Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 06:46 AM EST

PDB ID	:	2NYL
Title	:	Crystal structure of Protein Phosphatase 2A (PP2A) holoenzyme with the catalytic subunit carboxyl terminus truncated
Authors	:	Xing, Y.; Xu, Y.; Chen, Y.; Chao, Y.; Lin, Z.; Shi, Y.
Deposited on	:	2006-11-20
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

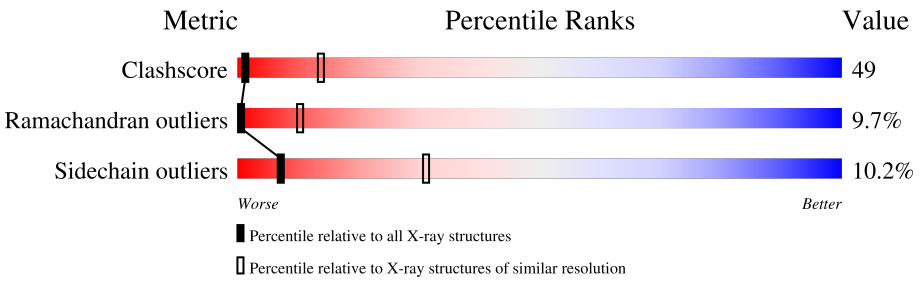
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	34% 54% 11% •
1	D	582	37% 49% 13% •
2	B	388	30% 56% 13% •
2	E	388	28% 55% 14% •
3	C	293	32% 58% 10%
3	F	293	38% 53% 9% •
4	G	7	43% 14% 43%
4	H	7	14% 71% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20212 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	582	4535	2881	764	863	14	13	0	0	0
1	D	582	4535	2881	764	863	14	13	0	0	0

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	388	3131	2043	513	561	3	11	0	0	0
2	E	388	3131	2043	513	561	3	11	0	0	0

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	293	2367	1497	405	450	15	0	0	0
3	F	293	2367	1497	405	450	15	0	0	0

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	7	71	49	10	12	0	0	0
4	H	7	71	49	10	12	0	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
5	C	2	2	2	0	0
5	F	2	2	2	0	0

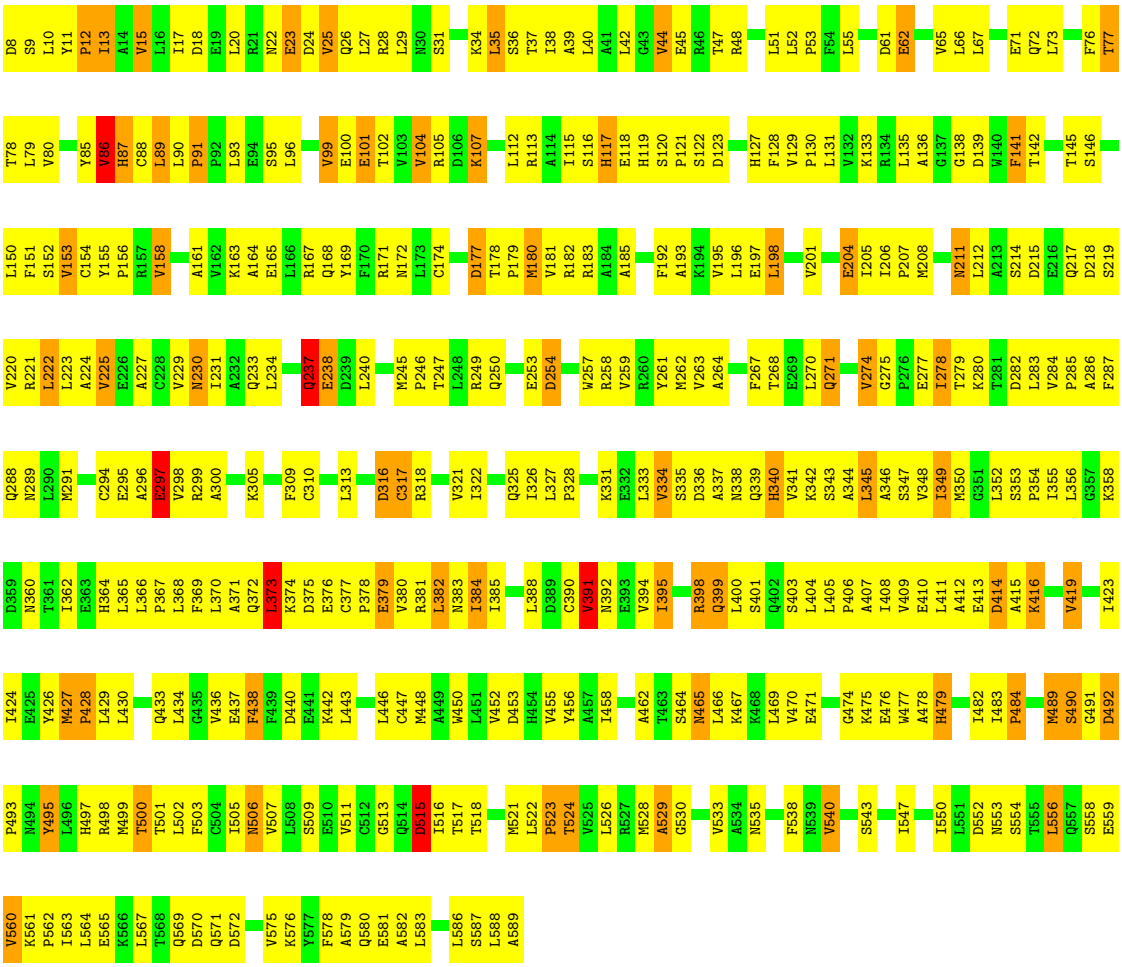
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

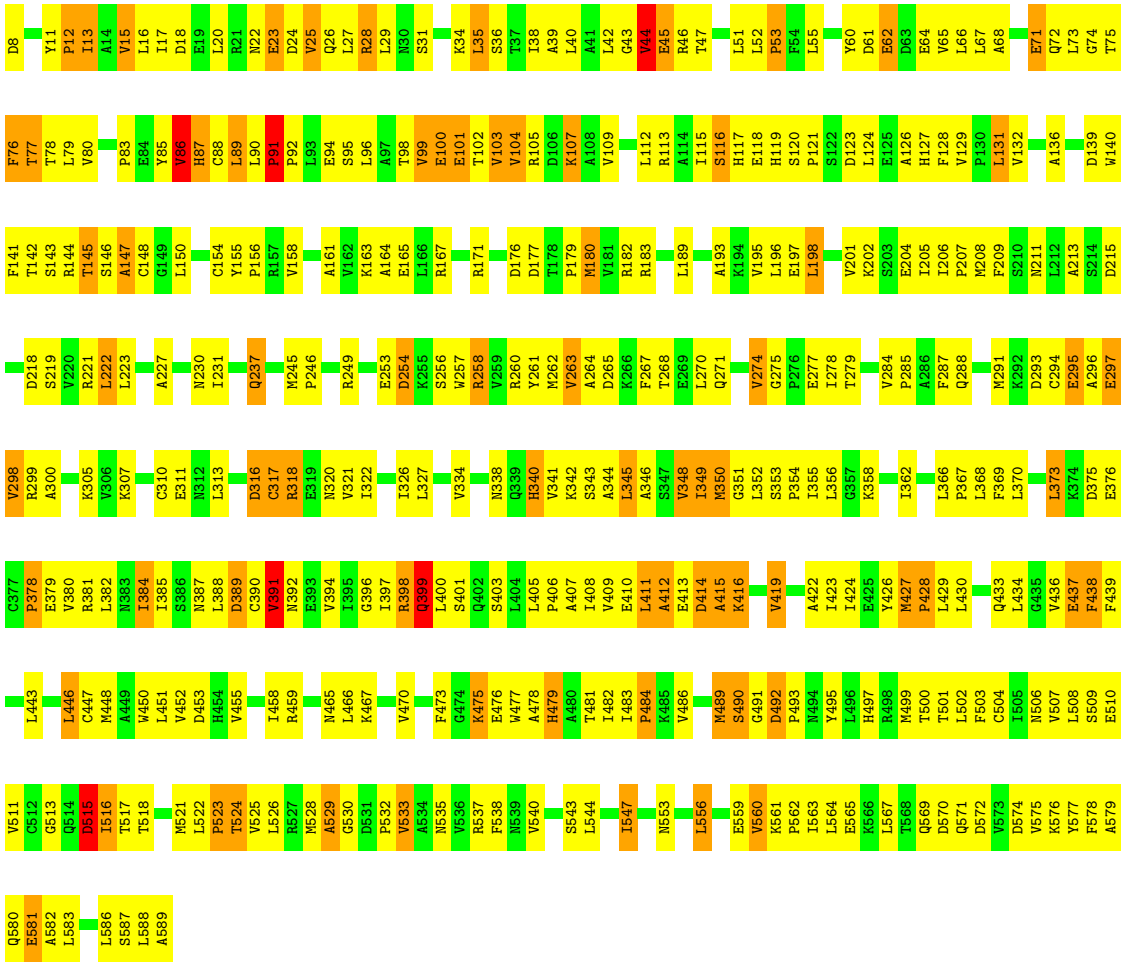
• Molecule 1: Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform

Chain A: 34% 54% 11%



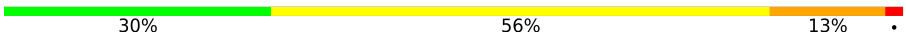
• Molecule 1: Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform

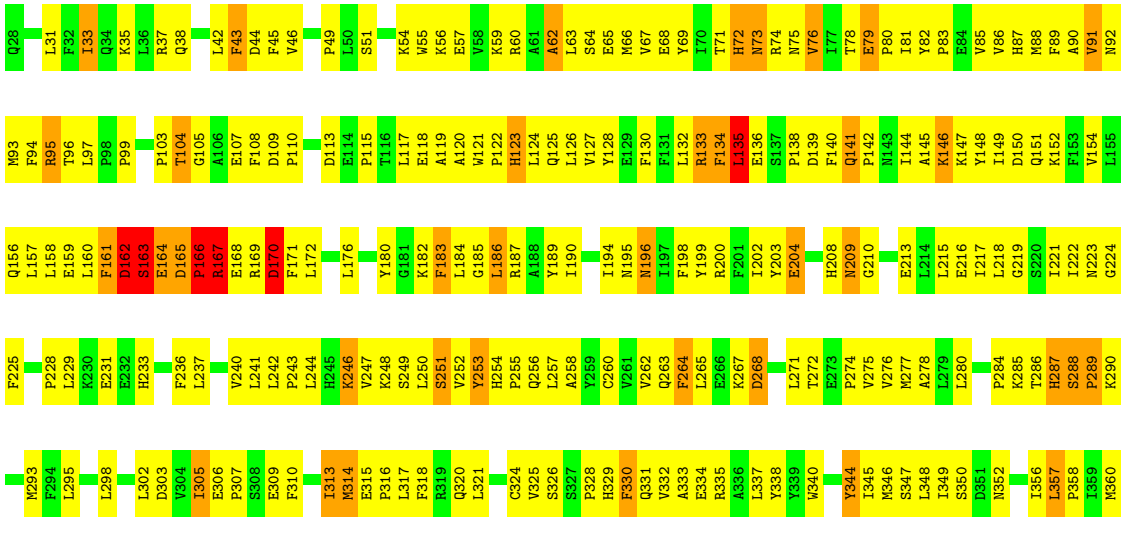
Chain D: 37% 49% 13%



• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

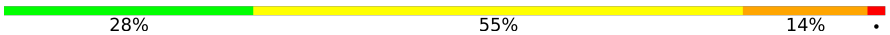
Chain B:

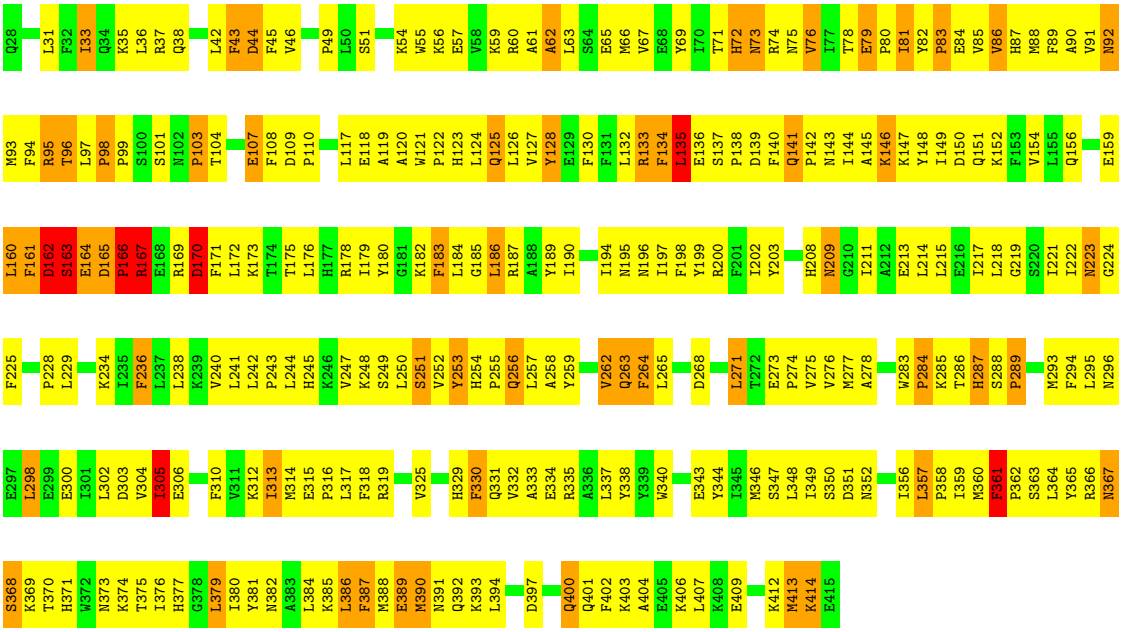




• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

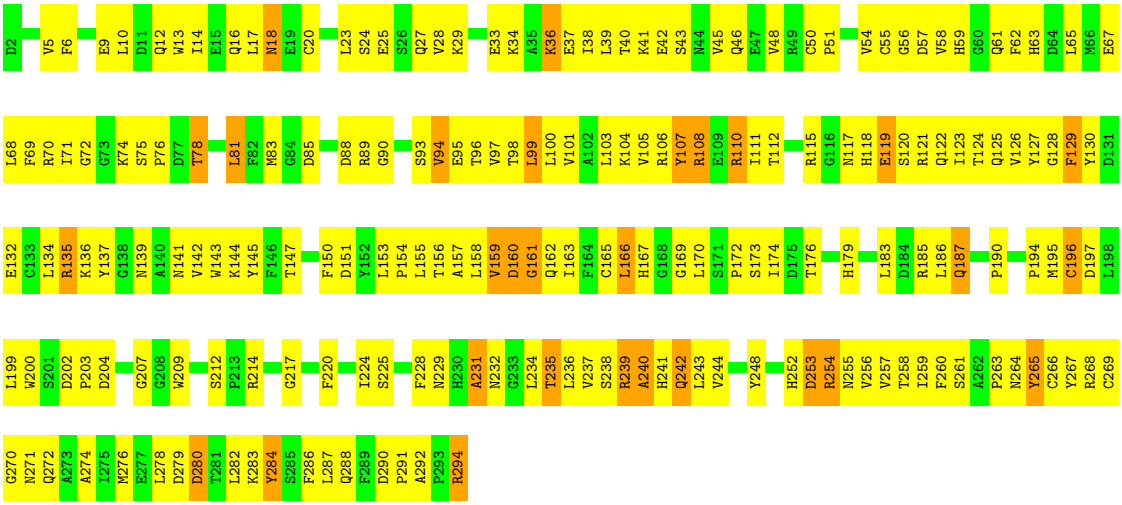
Chain E:





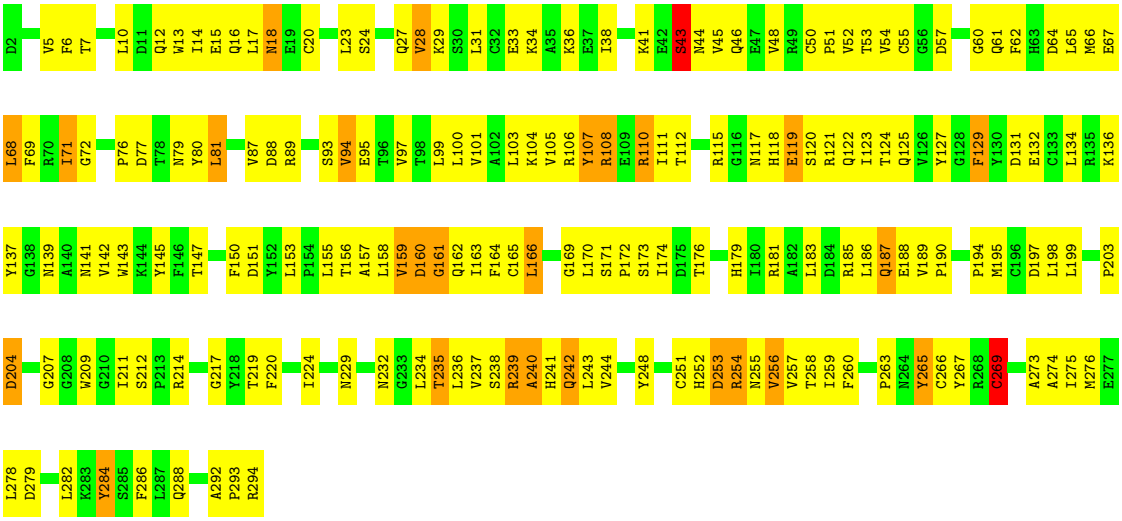
• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C:



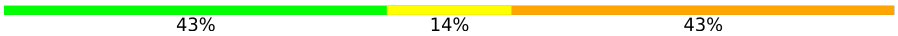
• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain F:



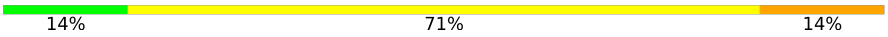
- Molecule 4: microcystin LR

Chain G:



- Molecule 4: microcystin LR

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.48Å 159.85Å 270.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.80	Depositor
% Data completeness (in resolution range)	99.6 (100.00-3.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20212	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, ACB, DAL, DAM, MN, FGA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.50	0/4596	0.72	0/6218
1	D	0.58	0/4596	0.75	0/6218
2	B	0.51	0/3202	0.74	3/4326 (0.1%)
2	E	0.53	0/3202	0.75	4/4326 (0.1%)
3	C	0.49	0/2424	0.73	0/3285
3	F	0.51	0/2424	0.74	1/3285 (0.0%)
4	G	0.36	0/17	0.80	0/19
4	H	0.38	0/17	0.89	0/19
All	All	0.53	0/20478	0.74	8/27696 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	3
4	H	0	3
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	162	ASP	N-CA-C	6.79	129.35	111.00
2	E	162	ASP	N-CA-C	6.71	129.12	111.00
2	E	163	SER	N-CA-C	6.21	127.77	111.00
2	B	163	SER	N-CA-C	5.95	127.06	111.00
2	E	219	GLY	N-CA-C	-5.95	98.24	113.10
2	E	49	PRO	N-CA-CB	5.48	109.88	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	49	PRO	N-CA-CB	5.41	109.79	103.30
3	F	269	CYS	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	4	ARG	Peptide
4	G	5	1ZN	Mainchain,Peptide
4	H	4	ARG	Peptide
4	H	5	1ZN	Mainchain,Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4637	449	0
1	D	4535	0	4637	431	0
2	B	3131	0	3050	330	0
2	E	3131	0	3050	359	0
3	C	2367	0	2268	221	0
3	F	2367	0	2268	215	0
4	G	71	0	61	1	0
4	H	71	0	61	3	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20212	0	20032	1982	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (1982) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ILE:H	1:D:278:ILE:HD12	1.10	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:325:VAL:HG13	2:E:337:LEU:HD11	1.29	1.11
1:D:350:MSE:HE1	1:D:391:VAL:HG13	1.24	1.10
2:B:277:MSE:HE1	2:B:316:PRO:HG3	1.35	1.08
2:E:340:TRP:HA	2:E:346:MSE:HE3	1.34	1.06
1:A:288:GLN:HA	1:A:291:MSE:HE3	1.34	1.06
2:E:146:LYS:HE3	2:E:147:LYS:HE3	1.35	1.05
1:A:278:ILE:H	1:A:278:ILE:HD12	1.18	1.02
1:D:500:THR:HA	1:D:503:PHE:HD1	1.25	1.01
3:C:13:TRP:HE1	3:C:27:GLN:NE2	1.58	1.00
1:D:416:LYS:O	1:D:419:VAL:HG23	1.61	1.00
1:A:535:ASN:HA	1:A:538:PHE:CE2	1.95	0.99
1:A:38:ILE:O	1:A:42:LEU:HB2	1.61	0.99
1:A:25:VAL:HG22	1:A:28:ARG:HH21	1.28	0.99
1:A:502:LEU:HD11	1:A:540:VAL:HG23	1.45	0.98
2:B:208:HIS:HD2	2:B:209:ASN:H	1.15	0.95
1:A:392:ASN:HB3	1:A:400:LEU:HD22	1.47	0.94
3:C:239:ARG:HH12	3:C:242:GLN:HG3	1.32	0.94
1:A:350:MSE:HE1	1:A:391:VAL:HG22	1.48	0.93
1:D:427:MSE:HA	1:D:427:MSE:HE3	1.47	0.93
1:A:427:MSE:HA	1:A:427:MSE:HE3	1.49	0.93
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.05	0.92
2:B:160:LEU:O	2:B:162:ASP:N	2.02	0.92
2:E:318:PHE:HD2	2:E:360:MSE:HE2	1.35	0.91
3:F:237:VAL:HB	3:F:256:VAL:HG23	1.49	0.91
1:A:526:LEU:HD22	1:A:563:ILE:HG21	1.51	0.91
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.53	0.91
1:D:338:ASN:HD22	1:D:341:VAL:HG23	1.36	0.91
3:F:159:VAL:HG23	3:F:163:ILE:HB	1.52	0.91
1:A:385:ILE:HD11	1:A:411:LEU:HG	1.52	0.90
1:D:392:ASN:HD21	1:D:433:GLN:HE22	1.18	0.90
1:D:448:MSE:HE2	1:D:448:MSE:HA	1.54	0.90
2:E:164:GLU:O	2:E:165:ASP:O	1.90	0.90
1:A:270:LEU:O	1:A:274:VAL:HG23	1.71	0.89
2:E:318:PHE:CD2	2:E:360:MSE:HE2	2.07	0.89
1:A:452:VAL:HG13	1:A:497:HIS:CD2	2.07	0.89
3:F:240:ALA:HA	3:F:258:THR:HG23	1.54	0.89
2:B:80:PRO:HG2	2:B:82:TYR:CE2	2.08	0.89
1:D:38:ILE:O	1:D:42:LEU:HB2	1.73	0.88
2:E:208:HIS:HD2	2:E:209:ASN:H	1.20	0.88
1:A:227:ALA:O	1:A:231:ILE:HG13	1.72	0.88
1:A:343:SER:CA	1:A:380:VAL:HG22	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:218:LEU:HD23	2:E:221:ILE:HD12	1.55	0.88
3:C:123:ILE:HG23	3:C:127:TYR:HD2	1.37	0.88
1:A:225:VAL:HG11	1:A:262:MSE:HB3	1.57	0.87
2:B:340:TRP:HA	2:B:346:MSE:HE3	1.55	0.87
1:D:180:MSE:HE3	1:D:180:MSE:H	1.40	0.87
2:E:128:TYR:HB3	2:E:171:PHE:CD2	2.08	0.87
1:D:278:ILE:H	1:D:278:ILE:CD1	1.88	0.87
1:D:409:VAL:HG13	1:D:446:LEU:HD21	1.56	0.87
2:B:251:SER:HA	2:B:293:MSE:HE1	1.55	0.86
1:A:362:ILE:HD13	1:A:399:GLN:HG3	1.56	0.86
3:F:239:ARG:HH12	3:F:242:GLN:HG3	1.39	0.86
1:A:300:ALA:HB2	1:A:341:VAL:HG22	1.56	0.86
2:B:318:PHE:HD2	2:B:360:MSE:HE2	1.41	0.86
1:D:77:THR:CG2	1:D:118:GLU:HG3	2.05	0.86
2:B:146:LYS:HE3	2:B:147:LYS:HE3	1.57	0.86
2:B:313:ILE:O	2:B:316:PRO:HD2	1.75	0.86
1:D:35:LEU:HD21	1:D:55:LEU:HD11	1.58	0.86
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.58	0.86
3:C:203:PRO:HD2	3:C:242:GLN:OE1	1.74	0.86
2:E:202:ILE:HD11	2:E:244:LEU:HG	1.58	0.85
1:A:25:VAL:HG22	1:A:28:ARG:NH2	1.91	0.85
1:A:405:LEU:O	1:A:409:VAL:HG23	1.76	0.85
2:E:277:MSE:HE1	2:E:316:PRO:HG3	1.57	0.85
1:A:477:TRP:CH2	1:A:482:ILE:HD11	2.11	0.84
2:B:329:HIS:CD2	2:B:331:GLN:HB2	2.12	0.84
1:D:392:ASN:ND2	1:D:433:GLN:HE22	1.73	0.84
2:B:318:PHE:CD2	2:B:360:MSE:HE2	2.12	0.84
2:B:388:MSE:HE2	2:B:392:GLN:HE22	1.41	0.84
1:A:352:LEU:HA	1:A:355:ILE:HD12	1.58	0.84
1:D:79:LEU:H	1:D:79:LEU:HD12	1.42	0.84
2:E:160:LEU:O	2:E:162:ASP:N	2.10	0.84
1:D:561:LYS:O	1:D:565:GLU:HG2	1.77	0.84
2:B:83:PRO:HB3	2:B:148:TYR:CD1	2.13	0.83
1:D:35:LEU:HD11	1:D:51:LEU:HD11	1.61	0.83
1:A:71:GLU:HG3	1:A:107:LYS:HE3	1.59	0.83
2:E:88:MSE:HE2	2:E:92:ASN:ND2	1.93	0.83
1:A:564:LEU:HD22	1:A:583:LEU:HD21	1.59	0.83
2:B:373:ASN:ND2	2:B:376:ILE:HG23	1.94	0.82
3:C:115:ARG:NH1	3:C:151:ASP:HA	1.93	0.82
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.95	0.82
1:D:310:CYS:HA	1:D:313:LEU:HD12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:HIS:HD2	2:B:209:ASN:N	1.78	0.82
1:D:407:ALA:O	1:D:411:LEU:HD22	1.79	0.81
2:E:251:SER:HA	2:E:293:MSE:HE1	1.61	0.81
3:F:123:ILE:HG23	3:F:127:TYR:HD2	1.44	0.81
2:B:78:THR:C	2:B:80:PRO:HD2	2.01	0.80
1:A:452:VAL:HG13	1:A:497:HIS:NE2	1.97	0.80
1:D:261:TYR:HA	1:D:298:VAL:HG22	1.62	0.80
1:D:405:LEU:O	1:D:409:VAL:HG23	1.82	0.80
1:D:390:CYS:O	1:D:392:ASN:N	2.15	0.80
3:F:239:ARG:HH12	3:F:242:GLN:CG	1.94	0.80
1:D:502:LEU:HD11	1:D:540:VAL:HG23	1.61	0.80
2:B:202:ILE:HD11	2:B:244:LEU:HG	1.60	0.80
3:C:159:VAL:HG23	3:C:163:ILE:HB	1.64	0.80
1:A:205:ILE:HA	1:A:208:MSE:HE3	1.62	0.79
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.47	0.79
1:A:347:SER:HB3	1:A:383:ASN:HD22	1.47	0.79
1:D:452:VAL:HG13	1:D:497:HIS:CD2	2.18	0.79
1:D:564:LEU:HD22	1:D:583:LEU:HD21	1.64	0.79
1:A:343:SER:HA	1:A:380:VAL:HG22	1.63	0.79
1:D:490:SER:HB2	1:D:528:MSE:HE3	1.64	0.79
3:C:237:VAL:HB	3:C:256:VAL:HG23	1.65	0.79
1:A:409:VAL:HG13	1:A:446:LEU:HD21	1.65	0.79
1:D:79:LEU:HD12	1:D:79:LEU:N	1.98	0.79
2:E:373:ASN:ND2	2:E:376:ILE:HG23	1.98	0.79
3:F:209:TRP:N	3:F:224:ILE:HD11	1.99	0.78
2:E:88:MSE:HE2	2:E:92:ASN:HD22	1.47	0.78
2:E:85:VAL:HG11	2:E:134:PHE:CD1	2.19	0.78
3:F:52:VAL:HG12	3:F:79:ASN:HB3	1.65	0.78
2:E:164:GLU:O	2:E:165:ASP:C	2.22	0.78
2:E:330:PHE:CE1	2:E:331:GLN:HG2	2.19	0.78
1:A:401:SER:HB3	1:A:434:LEU:HD21	1.66	0.77
1:D:427:MSE:HA	1:D:427:MSE:CE	2.15	0.77
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.67	0.77
1:A:564:LEU:O	1:A:564:LEU:HD23	1.83	0.77
3:C:209:TRP:N	3:C:224:ILE:HD11	1.99	0.77
2:E:59:LYS:HD3	2:E:123:HIS:NE2	2.00	0.77
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.64	0.77
1:A:482:ILE:C	1:A:484:PRO:HD2	2.05	0.77
1:D:427:MSE:HE1	1:D:430:LEU:HD12	1.64	0.77
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.66	0.77
1:A:495:TYR:O	1:A:499:MSE:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:GLU:HB3	2:B:168:GLU:HB2	1.67	0.77
3:C:214:ARG:HG2	3:C:214:ARG:HH11	1.50	0.77
1:A:500:THR:HA	1:A:503:PHE:HD1	1.48	0.77
2:B:128:TYR:HB3	2:B:171:PHE:CD2	2.20	0.77
1:A:416:LYS:O	1:A:419:VAL:HG23	1.85	0.77
2:B:164:GLU:O	2:B:165:ASP:O	2.02	0.77
1:A:278:ILE:H	1:A:278:ILE:CD1	1.93	0.77
2:E:223:ASN:HD22	2:E:263:GLN:HE21	1.33	0.77
1:D:25:VAL:HG22	1:D:28:ARG:NH2	1.99	0.77
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.15	0.76
2:B:190:ILE:O	2:B:194:ILE:HG13	1.83	0.76
3:F:203:PRO:HD2	3:F:242:GLN:OE1	1.85	0.76
1:A:561:LYS:O	1:A:565:GLU:HG2	1.86	0.76
2:B:208:HIS:CD2	2:B:209:ASN:H	2.02	0.76
2:B:80:PRO:HG2	2:B:82:TYR:HE2	1.50	0.76
2:E:78:THR:C	2:E:80:PRO:HD2	2.06	0.76
2:B:222:ILE:HD13	2:B:264:PHE:HD1	1.50	0.76
1:D:564:LEU:HD22	1:D:583:LEU:CD2	2.16	0.76
1:A:180:MSE:HE2	1:A:183:ARG:HH22	1.50	0.76
3:C:62:PHE:HD2	3:C:63:HIS:HD2	1.34	0.76
1:D:278:ILE:HD12	1:D:278:ILE:N	1.94	0.76
1:D:429:LEU:O	1:D:433:GLN:HG3	1.85	0.75
2:E:83:PRO:HB3	2:E:148:TYR:CD1	2.21	0.75
2:E:388:MSE:HE2	2:E:392:GLN:HE22	1.51	0.75
3:F:28:VAL:HG11	3:F:142:VAL:HG13	1.69	0.75
1:A:102:THR:HG22	1:A:105:ARG:NH2	2.00	0.75
2:E:85:VAL:HG11	2:E:134:PHE:HD1	1.52	0.75
1:A:237:GLN:NE2	1:A:278:ILE:HD11	2.02	0.75
1:D:500:THR:HA	1:D:503:PHE:CD1	2.17	0.75
2:B:165:ASP:O	2:B:167:ARG:N	2.20	0.74
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.52	0.74
2:E:325:VAL:CG1	2:E:337:LEU:HD11	2.14	0.74
2:B:242:LEU:HD13	2:B:278:ALA:CB	2.17	0.74
2:B:218:LEU:HD23	2:B:221:ILE:HD12	1.70	0.74
3:F:89:ARG:HD2	3:F:266:CYS:SG	2.28	0.74
3:F:104:LYS:N	3:F:111:ILE:HD11	2.01	0.74
2:E:134:PHE:CD2	2:E:135:LEU:N	2.56	0.74
2:B:118:GLU:HB3	2:B:164:GLU:CG	2.18	0.74
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.68	0.74
2:B:325:VAL:HG13	2:B:337:LEU:HD11	1.69	0.74
2:B:133:ARG:HA	2:B:136:GLU:OE2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:VAL:HG22	1:D:45:GLU:N	2.02	0.74
2:E:43:PHE:O	2:E:45:PHE:N	2.20	0.74
3:F:243:LEU:HD22	4:H:7:DAM:HM3	1.70	0.74
1:A:366:LEU:O	1:A:370:LEU:HD23	1.88	0.73
2:B:121:TRP:N	2:B:122:PRO:HD2	2.03	0.73
3:C:170:LEU:H	3:C:220:PHE:HE2	1.34	0.73
2:E:364:LEU:HB2	2:E:384:LEU:HD21	1.68	0.73
1:D:79:LEU:H	1:D:79:LEU:CD1	2.01	0.73
2:E:223:ASN:ND2	2:E:263:GLN:HE21	1.86	0.73
1:D:197:GLU:H	1:D:197:GLU:CD	1.89	0.73
1:D:401:SER:HB3	1:D:434:LEU:HD21	1.70	0.73
1:D:556:LEU:O	1:D:560:VAL:HB	1.88	0.73
2:E:391:ASN:ND2	2:E:394:LEU:HD12	2.03	0.73
1:A:564:LEU:HD22	1:A:583:LEU:CD2	2.18	0.73
1:A:556:LEU:O	1:A:560:VAL:HB	1.89	0.73
3:C:229:ASN:HA	3:C:234:LEU:HB2	1.71	0.73
2:E:80:PRO:HG2	2:E:82:TYR:CE2	2.24	0.73
1:A:278:ILE:HD12	1:A:278:ILE:N	2.00	0.73
2:E:208:HIS:HD2	2:E:209:ASN:N	1.87	0.73
2:E:242:LEU:HD13	2:E:278:ALA:CB	2.18	0.73
1:A:179:PRO:HB2	1:A:180:MSE:HE3	1.71	0.73
2:B:208:HIS:CD2	2:B:209:ASN:N	2.56	0.73
3:C:68:LEU:HD23	3:C:68:LEU:C	2.08	0.73
2:E:145:ALA:O	2:E:147:LYS:N	2.21	0.73
2:E:71:THR:HG21	2:E:133:ARG:HH11	1.53	0.72
3:F:214:ARG:HG2	3:F:214:ARG:HH11	1.54	0.72
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.24	0.72
1:D:495:TYR:HE2	1:D:535:ASN:HD22	1.36	0.72
2:E:371:HIS:CD2	2:E:376:ILE:HD11	2.25	0.72
3:F:143:TRP:CE2	3:F:147:THR:HG21	2.23	0.72
2:B:371:HIS:CD2	2:B:376:ILE:HD11	2.24	0.72
1:A:427:MSE:HA	1:A:427:MSE:CE	2.19	0.72
1:D:369:PHE:O	1:D:373:LEU:HB2	1.88	0.72
1:A:452:VAL:O	1:A:452:VAL:HG12	1.90	0.72
1:D:183:ARG:NH2	2:E:200:ARG:HD2	2.04	0.72
1:D:524:THR:O	1:D:528:MSE:HG3	1.90	0.72
2:E:208:HIS:CD2	2:E:209:ASN:H	2.07	0.72
1:D:109:VAL:HG13	1:D:150:LEU:HD21	1.71	0.72
2:E:313:ILE:HD12	2:E:313:ILE:N	2.05	0.72
2:B:118:GLU:HB3	2:B:164:GLU:HG2	1.72	0.71
2:E:313:ILE:HD12	2:E:313:ILE:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:TRP:N	2:E:122:PRO:HD2	2.05	0.71
2:E:190:ILE:O	2:E:194:ILE:HG13	1.90	0.71
1:D:104:VAL:HG12	1:D:105:ARG:N	2.05	0.71
2:E:391:ASN:OD1	2:E:394:LEU:HB2	1.91	0.71
2:E:406:LYS:O	2:E:406:LYS:HD3	1.89	0.71
1:A:362:ILE:CD1	1:A:399:GLN:HG3	2.21	0.71
2:B:313:ILE:H	2:B:313:ILE:HD12	1.55	0.71
3:C:220:PHE:HA	3:C:224:ILE:HD12	1.72	0.71
2:E:186:LEU:HB3	2:E:190:ILE:CD1	2.20	0.71
1:A:448:MSE:HA	1:A:448:MSE:HE2	1.72	0.71
1:A:261:TYR:HA	1:A:298:VAL:HG22	1.70	0.71
3:F:17:LEU:HD21	3:F:23:LEU:HG	1.72	0.70
2:B:240:VAL:O	2:B:243:PRO:HG2	1.91	0.70
3:F:197:ASP:OD1	3:F:217:GLY:HA2	1.89	0.70
1:A:35:LEU:HB3	1:A:72:GLN:HG2	1.71	0.70
2:E:208:HIS:CD2	2:E:209:ASN:N	2.60	0.70
2:E:151:GLN:HB3	2:E:189:TYR:CE2	2.25	0.70
2:E:165:ASP:O	2:E:167:ARG:N	2.25	0.70
2:E:376:ILE:HA	2:E:379:LEU:HB2	1.73	0.70
1:A:104:VAL:HG12	1:A:105:ARG:N	2.05	0.70
3:C:157:ALA:HB3	3:C:165:CYS:HB2	1.74	0.70
1:A:258:ARG:HH11	1:A:258:ARG:HG3	1.55	0.70
2:E:366:ARG:O	2:E:368:SER:N	2.24	0.70
1:A:407:ALA:O	1:A:411:LEU:HD22	1.92	0.69
1:D:66:LEU:HD22	1:D:96:LEU:HD23	1.75	0.69
2:E:167:ARG:CB	2:E:167:ARG:HH11	2.05	0.69
2:B:247:VAL:HG12	2:B:249:SER:H	1.57	0.69
3:C:89:ARG:HD2	3:C:266:CYS:SG	2.32	0.69
1:D:161:ALA:O	1:D:165:GLU:HG3	1.92	0.69
2:E:288:SER:HB2	2:E:289:PRO:HD3	1.74	0.69
3:F:160:ASP:O	3:F:162:GLN:N	2.25	0.69
1:A:35:LEU:HD11	1:A:51:LEU:HD11	1.73	0.69
1:D:115:ILE:HG13	1:D:115:ILE:O	1.92	0.69
2:E:166:PRO:O	2:E:167:ARG:C	2.30	0.69
3:F:137:TYR:CD2	3:F:142:VAL:HG21	2.28	0.69
2:B:310:PHE:O	2:B:314:MSE:HB2	1.93	0.69
1:D:452:VAL:O	1:D:452:VAL:HG12	1.92	0.69
1:A:193:ALA:HA	1:A:196:LEU:HD12	1.75	0.69
1:A:492:ASP:OD2	1:A:493:PRO:HD2	1.91	0.69
1:A:66:LEU:HD22	1:A:96:LEU:HD23	1.75	0.69
1:A:369:PHE:O	1:A:373:LEU:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:PHE:O	2:B:45:PHE:N	2.26	0.69
2:B:88:MSE:HE2	2:B:92:ASN:HD22	1.56	0.69
1:D:90:LEU:HB2	1:D:91:PRO:HD3	1.74	0.69
1:D:260:ARG:HH11	1:D:260:ARG:HG3	1.57	0.69
2:B:164:GLU:O	2:B:165:ASP:C	2.30	0.69
2:E:71:THR:HG21	2:E:133:ARG:NH1	2.08	0.69
3:F:13:TRP:HE1	3:F:27:GLN:NE2	1.90	0.69
2:E:169:ARG:HB3	2:E:213:GLU:HG2	1.75	0.69
3:F:165:CYS:SG	3:F:238:SER:HB3	2.33	0.69
1:A:286:ALA:O	1:A:289:ASN:HB2	1.94	0.68
2:B:305:ILE:HD13	2:B:306:GLU:H	1.56	0.68
3:C:194:PRO:HG2	3:C:195:MET:H	1.58	0.68
3:F:119:GLU:HG3	3:F:150:PHE:CD1	2.28	0.68
2:B:366:ARG:O	2:B:368:SER:N	2.27	0.68
1:D:288:GLN:HA	1:D:291:MSE:HE3	1.75	0.68
1:A:509:SER:OG	1:A:547:ILE:HG22	1.94	0.68
2:B:164:GLU:CB	2:B:168:GLU:HB2	2.23	0.68
1:D:428:PRO:HD3	1:D:465:ASN:ND2	2.08	0.68
1:A:428:PRO:HD3	1:A:465:ASN:ND2	2.08	0.68
2:B:132:LEU:C	2:B:134:PHE:H	1.97	0.68
1:D:499:MSE:HE1	3:F:77:ASP:O	1.94	0.68
1:D:20:LEU:HD23	1:D:31:SER:CB	2.24	0.68
3:F:139:ASN:CG	3:F:141:ASN:HD22	1.97	0.68
2:B:162:ASP:O	2:B:163:SER:HB2	1.94	0.68
2:E:176:LEU:HG	2:E:176:LEU:O	1.94	0.68
2:B:166:PRO:O	2:B:167:ARG:C	2.33	0.68
2:E:118:GLU:HB3	2:E:164:GLU:HG2	1.75	0.67
2:E:313:ILE:HG22	2:E:317:LEU:HB2	1.76	0.67
1:A:204:GLU:O	1:A:207:PRO:HD2	1.94	0.67
1:D:388:LEU:HD12	1:D:408:ILE:HD11	1.77	0.67
1:A:44:VAL:HG22	1:A:45:GLU:N	2.09	0.67
1:A:358:LYS:O	1:A:362:ILE:HG13	1.94	0.67
3:C:170:LEU:HB2	3:C:220:PHE:CD2	2.29	0.67
1:D:362:ILE:HD13	1:D:399:GLN:HG3	1.76	0.67
1:A:100:GLU:O	1:A:105:ARG:NH1	2.26	0.67
1:D:350:MSE:HE1	1:D:391:VAL:CG1	2.14	0.67
2:B:154:VAL:O	2:B:157:LEU:HB3	1.93	0.67
1:D:556:LEU:CD2	1:D:588:LEU:HD11	2.24	0.67
1:A:219:SER:HA	1:A:222:LEU:HD22	1.75	0.67
1:D:182:ARG:HH11	1:D:182:ARG:HG3	1.59	0.67
2:E:166:PRO:O	2:E:169:ARG:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:165:CYS:HA	3:F:238:SER:O	1.94	0.67
1:A:388:LEU:HD13	1:A:408:ILE:HD11	1.77	0.67
2:B:345:ILE:O	2:B:349:ILE:HG13	1.95	0.67
1:D:71:GLU:HG3	1:D:107:LYS:HE3	1.75	0.67
1:D:264:ALA:O	1:D:267:PHE:HB2	1.94	0.67
1:D:392:ASN:ND2	1:D:433:GLN:NE2	2.42	0.67
2:E:59:LYS:HA	2:E:62:ALA:HB3	1.77	0.67
2:B:286:THR:HG22	3:C:134:LEU:HB3	1.77	0.67
1:D:509:SER:HA	1:D:521:MSE:HE1	1.77	0.67
1:A:524:THR:O	1:A:528:MSE:HG3	1.95	0.67
2:B:313:ILE:HD12	2:B:313:ILE:N	2.09	0.67
2:E:93:MSE:HE2	2:E:128:TYR:OH	1.94	0.67
1:A:411:LEU:O	1:A:413:GLU:N	2.28	0.66
1:A:489:MSE:O	1:A:491:GLY:N	2.28	0.66
3:C:121:ARG:HH11	3:C:121:ARG:HG3	1.60	0.66
2:E:236:PHE:O	2:E:240:VAL:HB	1.95	0.66
3:C:94:VAL:HG23	3:C:132:GLU:OE2	1.95	0.66
1:D:180:MSE:H	1:D:180:MSE:CE	2.07	0.66
3:F:71:ILE:HG22	3:F:72:GLY:N	2.09	0.66
1:A:180:MSE:HE2	1:A:183:ARG:NH2	2.10	0.66
1:A:467:LYS:O	1:A:471:GLU:HG3	1.96	0.66
3:F:124:THR:HB	3:F:129:PHE:HB3	1.77	0.66
2:B:243:PRO:O	2:B:246:LYS:HB2	1.94	0.66
3:C:104:LYS:N	3:C:111:ILE:HD11	2.11	0.66
3:F:68:LEU:HD23	3:F:68:LEU:C	2.16	0.66
1:A:282:ASP:O	1:A:285:PRO:HD2	1.96	0.66
1:A:438:PHE:O	1:A:438:PHE:HD1	1.78	0.66
2:E:93:MSE:O	2:E:95:ARG:HG3	1.96	0.66
2:E:165:ASP:OD2	2:E:166:PRO:HD2	1.96	0.66
1:A:364:HIS:O	1:A:367:PRO:HD2	1.96	0.66
2:B:134:PHE:CD2	2:B:135:LEU:N	2.64	0.66
1:D:388:LEU:CD1	1:D:408:ILE:HD11	2.26	0.66
1:D:427:MSE:CE	1:D:430:LEU:HD12	2.26	0.66
2:E:381:TYR:CE2	2:E:385:LYS:HD2	2.30	0.66
1:D:35:LEU:HG	1:D:35:LEU:O	1.96	0.65
2:B:194:ILE:HG21	2:B:218:LEU:HD11	1.79	0.65
3:C:54:VAL:HG22	3:C:81:LEU:HD22	1.78	0.65
1:D:52:LEU:HB2	1:D:53:PRO:HD3	1.76	0.65
3:F:229:ASN:HA	3:F:234:LEU:HB2	1.78	0.65
1:A:24:ASP:O	1:A:26:GLN:N	2.29	0.65
1:A:427:MSE:HE1	1:A:430:LEU:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.77	0.65
2:E:340:TRP:CH2	2:E:360:MSE:HE3	2.30	0.65
2:E:344:TYR:O	2:E:347:SER:HB3	1.97	0.65
1:A:411:LEU:HD22	1:A:411:LEU:H	1.62	0.65
1:D:100:GLU:O	1:D:105:ARG:NH1	2.29	0.65
2:B:85:VAL:HG13	2:B:130:PHE:CE2	2.32	0.65
1:D:78:THR:HB	1:D:79:LEU:HD12	1.77	0.65
1:D:490:SER:CB	1:D:528:MSE:HE3	2.26	0.65
2:E:356:ILE:C	2:E:358:PRO:HD2	2.17	0.65
3:F:240:ALA:HB2	3:F:259:ILE:H	1.62	0.65
2:B:167:ARG:CB	2:B:167:ARG:HH11	2.10	0.65
2:B:200:ARG:HA	2:B:204:GLU:HG3	1.78	0.65
3:C:42:GLU:HB3	3:C:46:GLN:OE1	1.97	0.65
3:F:141:ASN:HB3	3:F:145:TYR:CE1	2.32	0.65
1:A:22:ASN:ND2	1:A:24:ASP:HB3	2.12	0.65
2:E:97:LEU:H	2:E:97:LEU:HD12	1.62	0.65
2:E:329:HIS:CD2	2:E:331:GLN:HB2	2.31	0.65
3:F:157:ALA:HB3	3:F:165:CYS:HB2	1.79	0.65
3:F:174:ILE:HD11	3:F:194:PRO:HB2	1.79	0.65
2:B:218:LEU:O	2:B:222:ILE:HG13	1.97	0.65
2:B:367:ASN:O	2:B:369:LYS:N	2.23	0.65
1:D:408:ILE:HD13	1:D:426:TYR:HE2	1.61	0.65
3:F:143:TRP:O	3:F:147:THR:HG23	1.96	0.65
1:A:388:LEU:CD1	1:A:408:ILE:HD11	2.26	0.65
2:B:157:LEU:O	2:B:160:LEU:HB2	1.96	0.65
2:E:128:TYR:HB3	2:E:171:PHE:HD2	1.58	0.65
3:F:159:VAL:CG2	3:F:163:ILE:HB	2.25	0.65
1:A:427:MSE:HB3	1:A:428:PRO:CD	2.27	0.64
2:B:288:SER:HB2	2:B:289:PRO:HD3	1.78	0.64
1:A:325:GLN:O	1:A:328:PRO:HD2	1.96	0.64
1:A:345:LEU:HD23	1:A:346:ALA:N	2.12	0.64
2:B:330:PHE:CE2	3:C:122:GLN:HG3	2.31	0.64
1:D:470:VAL:HG11	1:D:511:VAL:HG23	1.79	0.64
2:E:42:LEU:O	2:E:59:LYS:HE3	1.97	0.64
3:C:76:PRO:HB3	3:C:107:TYR:CD1	2.32	0.64
3:C:119:GLU:HG3	3:C:150:PHE:CD1	2.32	0.64
1:D:131:LEU:HD23	1:D:131:LEU:C	2.18	0.64
3:F:97:VAL:O	3:F:101:VAL:HG23	1.98	0.64
2:B:59:LYS:HD3	2:B:123:HIS:NE2	2.13	0.64
1:A:211:ASN:HD22	1:A:211:ASN:N	1.95	0.64
1:D:517:THR:HA	1:D:521:MSE:HE2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG13	1:A:45:GLU:H	1.62	0.64
2:B:391:ASN:ND2	2:B:394:LEU:HD12	2.12	0.64
2:E:240:VAL:O	2:E:243:PRO:HG2	1.98	0.64
1:D:113:ARG:O	1:D:116:SER:HB3	1.98	0.64
1:D:535:ASN:HA	1:D:538:PHE:HE2	1.61	0.64
3:F:115:ARG:HH12	3:F:151:ASP:HA	1.63	0.64
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.63	0.64
2:B:85:VAL:HG11	2:B:134:PHE:CD1	2.33	0.64
3:C:71:ILE:HG22	3:C:72:GLY:N	2.13	0.64
3:C:155:LEU:HD21	3:C:185:ARG:HB2	1.80	0.64
3:C:274:ALA:HB2	3:C:288:GLN:HA	1.80	0.64
1:D:556:LEU:HD22	1:D:588:LEU:HD11	1.80	0.64
2:E:149:ILE:HG22	2:E:149:ILE:O	1.96	0.64
1:A:158:VAL:HG23	1:A:163:LYS:HG3	1.80	0.63
2:E:375:THR:HG22	2:E:379:LEU:HD12	1.80	0.63
3:F:170:LEU:H	3:F:220:PHE:HE2	1.44	0.63
1:A:528:MSE:C	1:A:530:GLY:H	2.01	0.63
3:C:137:TYR:CD2	3:C:142:VAL:HG21	2.33	0.63
1:A:113:ARG:O	1:A:116:SER:HB3	1.98	0.63
1:A:346:ALA:HB2	1:A:380:VAL:HG13	1.80	0.63
1:A:427:MSE:CE	1:A:430:LEU:HD12	2.28	0.63
2:B:88:MSE:HE2	2:B:92:ASN:ND2	2.13	0.63
2:E:186:LEU:HB3	2:E:190:ILE:HD12	1.80	0.63
1:D:35:LEU:HD21	1:D:55:LEU:CD1	2.27	0.63
2:E:364:LEU:CB	2:E:384:LEU:HD21	2.29	0.63
2:B:166:PRO:O	2:B:169:ARG:N	2.32	0.63
3:C:158:LEU:CD2	3:C:161:GLY:HA2	2.28	0.63
1:D:35:LEU:HB3	1:D:72:GLN:HG2	1.81	0.63
3:F:194:PRO:HG2	3:F:195:MET:H	1.62	0.63
3:C:203:PRO:HA	3:C:220:PHE:CE1	2.34	0.63
1:A:556:LEU:CD2	1:A:588:LEU:HD11	2.29	0.62
2:B:151:GLN:HB3	2:B:189:TYR:CE2	2.34	0.62
2:E:73:ASN:C	2:E:75:ASN:H	2.01	0.62
2:E:329:HIS:CE1	3:F:125:GLN:HB3	2.34	0.62
2:B:244:LEU:HD22	2:B:253:TYR:CE1	2.34	0.62
2:B:364:LEU:HB2	2:B:384:LEU:HD21	1.81	0.62
3:C:159:VAL:CG2	3:C:163:ILE:HB	2.28	0.62
2:E:330:PHE:O	2:E:334:GLU:HB2	1.99	0.62
2:B:236:PHE:O	2:B:240:VAL:HB	1.99	0.62
3:C:239:ARG:NH1	3:C:242:GLN:HG3	2.11	0.62
3:C:276:MET:CE	3:C:278:LEU:HD21	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLN:NE2	1:D:278:ILE:HD11	2.15	0.62
1:D:528:MSE:C	1:D:530:GLY:H	2.01	0.62
2:E:389:GLU:O	2:E:390:MSE:HB2	1.99	0.62
1:A:349:ILE:HG23	1:A:350:MSE:N	2.13	0.62
2:B:169:ARG:O	2:B:172:LEU:N	2.33	0.62
1:D:300:ALA:HB2	1:D:341:VAL:HG22	1.80	0.62
2:E:209:ASN:N	2:E:209:ASN:ND2	2.47	0.62
2:E:313:ILE:CG2	2:E:317:LEU:HB2	2.28	0.62
3:F:115:ARG:NH1	3:F:151:ASP:HA	2.14	0.62
1:A:495:TYR:CD2	1:A:533:VAL:HG11	2.34	0.62
1:D:11:TYR:N	1:D:12:PRO:HD2	2.15	0.62
2:E:144:ILE:O	2:E:144:ILE:HG22	2.00	0.62
3:F:158:LEU:HD12	3:F:163:ILE:O	2.00	0.62
1:A:497:HIS:O	1:A:500:THR:HB	1.99	0.62
1:A:25:VAL:CG2	1:A:28:ARG:HH21	2.09	0.62
1:D:20:LEU:HD23	1:D:31:SER:HB2	1.80	0.62
2:E:133:ARG:HG2	2:E:136:GLU:OE2	2.00	0.62
2:E:170:ASP:O	2:E:173:LYS:HB3	2.00	0.62
1:A:382:LEU:HD12	1:A:419:VAL:HG22	1.81	0.62
2:B:233:HIS:O	2:B:236:PHE:HB3	2.00	0.62
2:E:110:PRO:HG3	2:E:249:SER:HB2	1.81	0.62
3:F:209:TRP:H	3:F:224:ILE:HD11	1.65	0.62
3:C:13:TRP:HE1	3:C:27:GLN:HE21	1.45	0.62
3:C:55:CYS:SG	3:C:68:LEU:HD11	2.39	0.62
3:F:62:PHE:O	3:F:65:LEU:HB3	1.99	0.62
1:A:502:LEU:HD22	1:A:543:SER:OG	1.99	0.61
1:D:455:VAL:HG23	3:F:71:ILE:HG13	1.82	0.61
2:E:180:TYR:CE1	2:E:187:ARG:HA	2.35	0.61
2:E:391:ASN:CG	2:E:394:LEU:HD12	2.21	0.61
3:F:183:LEU:HD21	3:F:194:PRO:HG3	1.82	0.61
3:F:236:LEU:HD11	3:F:257:VAL:HG12	1.81	0.61
3:C:25:GLU:CD	3:C:139:ASN:HD21	2.03	0.61
1:D:561:LYS:HB3	1:D:562:PRO:HD3	1.81	0.61
2:E:180:TYR:HE1	2:E:187:ARG:HA	1.65	0.61
2:E:80:PRO:HG2	2:E:82:TYR:CD2	2.36	0.61
1:A:245:MSE:O	1:A:249:ARG:HG3	1.99	0.61
2:B:118:GLU:H	2:B:164:GLU:HG2	1.65	0.61
2:B:329:HIS:CE1	3:C:125:GLN:HB3	2.35	0.61
3:C:13:TRP:NE1	3:C:27:GLN:NE2	2.39	0.61
1:D:34:LYS:O	1:D:36:SER:N	2.33	0.61
1:D:398:ARG:HB3	1:D:398:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:SER:HB3	1:D:434:LEU:CD2	2.31	0.61
1:D:427:MSE:O	1:D:429:LEU:N	2.34	0.61
1:A:482:ILE:C	1:A:484:PRO:CD	2.68	0.61
1:D:258:ARG:HG3	1:D:258:ARG:HH11	1.66	0.61
3:F:155:LEU:HD21	3:F:185:ARG:HB2	1.83	0.61
2:B:222:ILE:HD13	2:B:264:PHE:CD1	2.35	0.61
1:D:538:PHE:HB3	1:D:575:VAL:HA	1.83	0.61
2:E:72:HIS:O	2:E:74:ARG:N	2.34	0.61
1:D:66:LEU:HD22	1:D:96:LEU:CD2	2.31	0.61
1:A:77:THR:HG21	1:A:118:GLU:HG3	1.83	0.61
3:C:33:GLU:O	3:C:36:LYS:HB2	2.01	0.61
2:E:373:ASN:O	2:E:375:THR:N	2.32	0.61
3:F:103:LEU:HB3	3:F:111:ILE:HD13	1.82	0.61
1:A:35:LEU:HD21	1:A:55:LEU:HD11	1.81	0.61
1:A:39:ALA:HB1	1:A:47:THR:HG21	1.83	0.61
1:A:66:LEU:HB3	1:A:104:VAL:HG21	1.83	0.61
1:A:180:MSE:CE	1:A:183:ARG:HH22	2.13	0.61
1:A:346:ALA:CB	1:A:380:VAL:HG13	2.31	0.61
1:A:438:PHE:HE1	1:A:442:LYS:HB2	1.66	0.61
1:D:385:ILE:HD11	1:D:411:LEU:HG	1.83	0.61
1:A:171:ARG:HG3	1:A:208:MSE:SE	2.50	0.60
2:B:97:LEU:H	2:B:97:LEU:HD12	1.66	0.60
2:B:321:LEU:HB3	2:B:360:MSE:HE1	1.83	0.60
2:E:361:PHE:O	2:E:363:SER:N	2.34	0.60
1:A:258:ARG:HG3	1:A:258:ARG:NH1	2.15	0.60
2:B:364:LEU:CB	2:B:384:LEU:HD21	2.32	0.60
3:C:97:VAL:HG13	3:C:98:THR:N	2.16	0.60
1:D:526:LEU:HD22	1:D:563:ILE:HG21	1.83	0.60
2:E:132:LEU:C	2:E:134:PHE:H	2.05	0.60
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.36	0.60
1:A:477:TRP:CH2	1:A:482:ILE:CD1	2.83	0.60
1:D:427:MSE:HE2	1:D:430:LEU:HB2	1.84	0.60
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.31	0.60
2:E:325:VAL:HG22	2:E:337:LEU:HD12	1.84	0.60
1:A:79:LEU:HD12	1:A:79:LEU:N	2.17	0.60
1:D:205:ILE:HA	1:D:208:MSE:HE3	1.83	0.60
2:E:54:LYS:O	2:E:56:LYS:N	2.29	0.60
2:E:313:ILE:O	2:E:316:PRO:HD2	2.01	0.60
2:E:375:THR:CG2	2:E:379:LEU:HD12	2.32	0.60
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.82	0.60
2:B:376:ILE:HA	2:B:379:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:LEU:O	1:D:413:GLU:N	2.34	0.60
1:D:436:VAL:HG13	1:D:437:GLU:H	1.65	0.60
3:F:166:LEU:O	3:F:239:ARG:HA	2.02	0.60
1:A:388:LEU:HA	1:A:391:VAL:CG2	2.31	0.60
2:B:217:ILE:O	2:B:221:ILE:HG13	2.02	0.60
2:B:248:LYS:HD3	2:B:290:LYS:HZ2	1.66	0.60
1:D:564:LEU:O	1:D:564:LEU:HD23	2.02	0.60
2:E:329:HIS:HB3	2:E:332:VAL:HG23	1.83	0.60
1:A:180:MSE:HE3	1:A:180:MSE:H	1.67	0.60
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.83	0.60
2:B:373:ASN:HD22	2:B:376:ILE:HG23	1.67	0.60
2:B:412:LYS:O	2:B:414:LYS:N	2.34	0.60
2:E:141:GLN:HB3	2:E:142:PRO:HD2	1.84	0.60
3:F:214:ARG:HG2	3:F:214:ARG:NH1	2.15	0.60
3:F:220:PHE:HA	3:F:224:ILE:HD12	1.84	0.60
1:A:509:SER:HA	1:A:521:MSE:HE1	1.83	0.60
1:D:85:TYR:O	1:D:87:HIS:N	2.35	0.60
1:D:140:TRP:HH2	2:E:199:TYR:HH	1.49	0.60
2:E:79:GLU:N	2:E:80:PRO:CD	2.64	0.60
2:E:165:ASP:CG	2:E:166:PRO:HD2	2.22	0.60
2:B:357:LEU:N	2:B:358:PRO:HD2	2.17	0.60
2:B:361:PHE:O	2:B:363:SER:N	2.35	0.60
3:C:14:ILE:O	3:C:18:ASN:HB2	2.01	0.60
1:D:24:ASP:O	1:D:26:GLN:N	2.35	0.60
1:D:25:VAL:CG2	1:D:28:ARG:HH21	2.14	0.60
1:D:268:THR:HG23	1:D:305:LYS:HD2	1.84	0.60
2:B:222:ILE:HG21	2:B:264:PHE:CD1	2.37	0.59
1:A:579:ALA:O	1:A:582:ALA:HB3	2.02	0.59
3:C:141:ASN:HB3	3:C:145:TYR:CE1	2.38	0.59
1:D:270:LEU:O	1:D:274:VAL:HG23	2.02	0.59
1:D:448:MSE:HA	1:D:448:MSE:CE	2.31	0.59
2:E:325:VAL:HG22	2:E:337:LEU:CD1	2.32	0.59
1:A:154:CYS:O	1:A:158:VAL:HG13	2.02	0.59
2:B:60:ARG:C	2:B:60:ARG:HD3	2.22	0.59
1:D:179:PRO:HB2	1:D:180:MSE:HE3	1.83	0.59
2:E:253:TYR:H	2:E:253:TYR:HD2	1.48	0.59
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.83	0.59
1:A:470:VAL:HG22	1:A:478:ALA:HB2	1.84	0.59
1:D:261:TYR:CA	1:D:298:VAL:HG22	2.33	0.59
2:E:134:PHE:HD2	2:E:135:LEU:N	1.99	0.59
2:B:93:MSE:O	2:B:95:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:PRO:HA	2:B:113:ASP:OD2	2.03	0.59
2:B:251:SER:HA	2:B:293:MSE:CE	2.31	0.59
3:C:166:LEU:O	3:C:239:ARG:HA	2.03	0.59
1:D:25:VAL:CG2	1:D:28:ARG:NH2	2.66	0.59
1:D:274:VAL:HG12	1:D:278:ILE:HB	1.85	0.59
1:D:455:VAL:HG23	3:F:71:ILE:HA	1.85	0.59
1:D:528:MSE:O	1:D:530:GLY:N	2.36	0.59
2:E:169:ARG:O	2:E:172:LEU:N	2.36	0.59
3:F:240:ALA:CB	3:F:259:ILE:H	2.16	0.59
3:C:160:ASP:O	3:C:162:GLN:N	2.36	0.59
3:C:214:ARG:HG2	3:C:214:ARG:NH1	2.18	0.59
2:E:276:VAL:HG11	2:E:313:ILE:HG21	1.85	0.59
3:C:57:ASP:O	3:C:261:SER:HB2	2.03	0.58
2:E:79:GLU:N	2:E:80:PRO:HD2	2.17	0.58
1:A:438:PHE:HD1	1:A:438:PHE:C	2.07	0.58
3:C:284:TYR:N	3:C:284:TYR:CD2	2.68	0.58
1:D:22:ASN:ND2	1:D:24:ASP:HB3	2.17	0.58
2:E:83:PRO:C	2:E:85:VAL:H	2.07	0.58
2:E:183:PHE:N	2:E:183:PHE:CD1	2.71	0.58
1:A:247:THR:O	1:A:250:GLN:HB3	2.03	0.58
1:A:270:LEU:C	1:A:274:VAL:HG23	2.24	0.58
1:D:350:MSE:HE2	1:D:369:PHE:CE1	2.38	0.58
2:E:186:LEU:O	2:E:190:ILE:HD12	2.02	0.58
2:B:176:LEU:HD11	2:B:190:ILE:HG12	1.86	0.58
3:C:261:SER:O	3:C:263:PRO:HD3	2.03	0.58
1:D:570:ASP:OD2	1:D:571:GLN:N	2.36	0.58
1:D:588:LEU:O	1:D:589:ALA:HB2	2.03	0.58
3:F:29:LYS:HD2	3:F:145:TYR:CE2	2.38	0.58
1:A:572:ASP:OD2	3:C:110:ARG:NH2	2.36	0.58
2:B:164:GLU:HB3	2:B:168:GLU:CB	2.34	0.58
2:B:253:TYR:H	2:B:253:TYR:HD2	1.52	0.58
2:B:313:ILE:O	2:B:315:GLU:N	2.36	0.58
2:E:60:ARG:C	2:E:60:ARG:HD3	2.23	0.58
2:E:83:PRO:C	2:E:85:VAL:N	2.57	0.58
1:A:79:LEU:HD12	1:A:79:LEU:H	1.68	0.58
2:B:183:PHE:N	2:B:183:PHE:CD1	2.71	0.58
3:C:45:VAL:HG22	3:C:156:THR:OG1	2.04	0.58
1:D:109:VAL:O	1:D:113:ARG:HG3	2.02	0.58
2:E:71:THR:O	2:E:73:ASN:N	2.34	0.58
3:F:147:THR:HA	3:F:150:PHE:CD2	2.38	0.58
2:B:128:TYR:O	2:B:132:LEU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:LEU:HB3	3:C:111:ILE:HD13	1.85	0.58
1:A:464:SER:O	1:A:466:LEU:N	2.37	0.58
1:A:588:LEU:O	1:A:589:ALA:HB2	2.04	0.58
1:D:227:ALA:O	1:D:231:ILE:HG13	2.04	0.58
3:F:46:GLN:O	3:F:157:ALA:HA	2.02	0.58
2:E:169:ARG:O	2:E:170:ASP:C	2.42	0.58
2:E:373:ASN:C	2:E:375:THR:H	2.06	0.58
3:F:170:LEU:HB2	3:F:220:PHE:CD2	2.39	0.58
1:A:34:LYS:O	1:A:36:SER:N	2.37	0.58
1:A:77:THR:CG2	1:A:118:GLU:HG3	2.33	0.58
2:B:65:GLU:C	2:B:67:VAL:H	2.06	0.58
2:B:242:LEU:N	2:B:243:PRO:HD2	2.19	0.58
1:D:219:SER:HA	1:D:222:LEU:HD22	1.86	0.58
2:E:333:ALA:O	2:E:337:LEU:HD13	2.04	0.57
3:C:117:ASN:ND2	3:C:241:HIS:HE1	2.01	0.57
2:E:119:ALA:O	2:E:120:ALA:HB3	2.04	0.57
2:E:134:PHE:HD2	2:E:134:PHE:C	2.07	0.57
2:E:316:PRO:HG2	2:E:317:LEU:H	1.69	0.57
2:E:330:PHE:CE2	3:F:122:GLN:HG3	2.38	0.57
2:E:337:LEU:HD21	2:E:380:ILE:HG13	1.84	0.57
1:A:20:LEU:HD23	1:A:31:SER:CB	2.34	0.57
1:D:60:TYR:CD2	1:D:65:VAL:HG11	2.39	0.57
1:D:262:MSE:O	1:D:264:ALA:N	2.38	0.57
2:E:244:LEU:HD22	2:E:253:TYR:HE1	1.69	0.57
1:A:163:LYS:O	1:A:167:ARG:HG3	2.04	0.57
1:A:509:SER:CA	1:A:521:MSE:HE1	2.34	0.57
3:C:115:ARG:HG3	3:C:119:GLU:HB2	1.84	0.57
1:D:509:SER:CA	1:D:521:MSE:HE1	2.35	0.57
1:D:533:VAL:HG12	1:D:535:ASN:HB2	1.86	0.57
2:E:209:ASN:H	2:E:209:ASN:HD22	1.50	0.57
1:A:129:VAL:HB	1:A:130:PRO:HD3	1.85	0.57
1:A:483:ILE:N	1:A:484:PRO:CD	2.68	0.57
1:A:529:ALA:HB2	1:A:540:VAL:HG11	1.85	0.57
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.86	0.57
3:C:197:ASP:OD1	3:C:217:GLY:HA2	2.05	0.57
1:A:427:MSE:HE2	1:A:430:LEU:HB2	1.85	0.57
2:B:289:PRO:O	2:B:293:MSE:HG3	2.04	0.57
1:D:72:GLN:O	1:D:74:GLY:N	2.37	0.57
3:F:106:ARG:O	3:F:108:ARG:N	2.36	0.57
1:A:22:ASN:O	1:A:23:GLU:CB	2.52	0.57
3:C:143:TRP:O	3:C:147:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:ALA:HA	3:C:258:THR:HG23	1.87	0.57
3:C:244:VAL:HG23	3:C:244:VAL:O	2.05	0.57
1:D:261:TYR:C	1:D:261:TYR:CD2	2.77	0.57
1:D:297:GLU:O	1:D:298:VAL:C	2.42	0.57
1:D:479:HIS:ND1	1:D:479:HIS:O	2.34	0.57
1:A:88:CYS:O	1:A:91:PRO:HD2	2.05	0.57
1:D:438:PHE:CD1	1:D:438:PHE:C	2.77	0.57
2:E:406:LYS:HD3	2:E:406:LYS:C	2.25	0.57
3:F:117:ASN:ND2	3:F:241:HIS:HE1	2.03	0.57
1:A:217:GLN:O	1:A:220:VAL:HB	2.05	0.57
2:B:384:LEU:O	2:B:387:PHE:N	2.35	0.57
3:C:29:LYS:HD2	3:C:145:TYR:CE2	2.40	0.57
3:C:160:ASP:C	3:C:162:GLN:H	2.08	0.57
2:E:118:GLU:HB3	2:E:164:GLU:CG	2.35	0.57
2:E:218:LEU:O	2:E:222:ILE:HG13	2.03	0.57
2:E:315:GLU:HB3	2:E:319:ARG:NH2	2.20	0.57
2:B:80:PRO:HG2	2:B:82:TYR:CD2	2.39	0.57
1:D:179:PRO:HG3	1:D:182:ARG:HH22	1.70	0.57
2:E:340:TRP:HH2	2:E:360:MSE:HE3	1.69	0.57
3:F:176:THR:HA	3:F:232:ASN:OD1	2.05	0.57
1:A:390:CYS:O	1:A:392:ASN:N	2.37	0.56
2:B:79:GLU:N	2:B:80:PRO:CD	2.67	0.56
2:B:340:TRP:HH2	2:B:360:MSE:HE3	1.70	0.56
3:C:5:VAL:O	3:C:5:VAL:HG12	2.04	0.56
3:C:62:PHE:O	3:C:65:LEU:HB3	2.05	0.56
2:E:134:PHE:CD2	2:E:134:PHE:C	2.78	0.56
1:A:343:SER:N	1:A:380:VAL:HG22	2.19	0.56
1:A:535:ASN:HA	1:A:538:PHE:HE2	1.61	0.56
2:B:302:LEU:HD11	2:B:317:LEU:HD21	1.87	0.56
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.20	0.56
1:D:409:VAL:O	1:D:409:VAL:HG12	2.04	0.56
2:E:124:LEU:O	2:E:126:LEU:N	2.38	0.56
2:E:305:ILE:HD13	2:E:306:GLU:H	1.69	0.56
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.87	0.56
1:A:336:ASP:OD1	1:A:337:ALA:N	2.38	0.56
1:A:352:LEU:HD23	1:A:355:ILE:HD12	1.88	0.56
2:B:118:GLU:HB3	2:B:164:GLU:HG3	1.86	0.56
2:B:340:TRP:CH2	2:B:360:MSE:HE3	2.40	0.56
3:C:100:LEU:HA	3:C:103:LEU:HD12	1.86	0.56
1:D:115:ILE:O	1:D:119:HIS:CD2	2.58	0.56
1:D:427:MSE:HB3	1:D:428:PRO:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:VAL:CG1	1:D:535:ASN:HB2	2.35	0.56
2:E:162:ASP:O	2:E:163:SER:HB2	2.05	0.56
2:E:262:VAL:O	2:E:265:LEU:N	2.38	0.56
3:F:266:CYS:SG	4:H:2:LEU:HD12	2.45	0.56
1:A:201:VAL:O	1:A:205:ILE:HB	2.05	0.56
1:A:342:LYS:O	1:A:346:ALA:HB2	2.05	0.56
1:A:395:ILE:HD11	1:A:400:LEU:CA	2.35	0.56
1:A:489:MSE:C	1:A:491:GLY:H	2.09	0.56
3:F:265:TYR:HB3	3:F:269:CYS:HB2	1.86	0.56
1:A:438:PHE:C	1:A:438:PHE:CD1	2.77	0.56
3:C:276:MET:HB2	3:C:286:PHE:CE1	2.40	0.56
2:E:255:PRO:HG2	2:E:256:GLN:CD	2.25	0.56
3:F:101:VAL:O	3:F:105:VAL:HG23	2.05	0.56
3:F:240:ALA:HB1	3:F:259:ILE:O	2.05	0.56
1:A:24:ASP:O	1:A:25:VAL:C	2.42	0.56
1:A:237:GLN:O	1:A:238:GLU:C	2.43	0.56
3:F:284:TYR:N	3:F:284:TYR:CD2	2.72	0.56
2:B:121:TRP:CZ2	2:B:167:ARG:HB3	2.40	0.56
1:D:206:ILE:HB	1:D:207:PRO:HD3	1.88	0.56
2:B:35:LYS:C	2:B:37:ARG:H	2.08	0.56
2:B:180:TYR:CE1	2:B:187:ARG:HA	2.41	0.56
1:D:438:PHE:C	1:D:438:PHE:HD1	2.09	0.56
2:E:164:GLU:OE2	2:E:164:GLU:C	2.43	0.56
3:F:45:VAL:HA	3:F:156:THR:OG1	2.06	0.56
1:A:409:VAL:O	1:A:409:VAL:HG12	2.06	0.56
1:D:145:THR:HG22	1:D:146:SER:N	2.21	0.56
2:E:254:HIS:N	2:E:255:PRO:HD2	2.21	0.56
3:F:53:THR:HG21	3:F:275:ILE:HD12	1.87	0.56
1:A:526:LEU:CD2	1:A:563:ILE:HG21	2.32	0.56
3:C:253:ASP:O	3:C:255:ASN:N	2.39	0.56
1:D:491:GLY:O	1:D:492:ASP:C	2.44	0.56
2:E:412:LYS:O	2:E:414:LYS:N	2.39	0.56
3:F:176:THR:HG23	3:F:179:HIS:HD2	1.69	0.56
1:A:261:TYR:CA	1:A:298:VAL:HG22	2.36	0.55
1:A:350:MSE:HE3	1:A:391:VAL:HG13	1.88	0.55
2:B:119:ALA:O	2:B:120:ALA:HB3	2.05	0.55
3:C:240:ALA:HB1	3:C:259:ILE:O	2.05	0.55
2:E:218:LEU:CD2	2:E:221:ILE:HD12	2.32	0.55
3:C:139:ASN:CG	3:C:141:ASN:HD22	2.08	0.55
1:D:436:VAL:HG13	1:D:437:GLU:N	2.20	0.55
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PHE:O	1:A:582:ALA:HB2	2.06	0.55
2:E:373:ASN:ND2	2:E:376:ILE:H	2.05	0.55
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.87	0.55
3:C:115:ARG:HH12	3:C:151:ASP:HA	1.67	0.55
1:D:424:ILE:HG12	1:D:450:TRP:CE3	2.41	0.55
3:F:76:PRO:HB3	3:F:107:TYR:CD1	2.41	0.55
2:B:333:ALA:O	2:B:337:LEU:HD13	2.06	0.55
1:D:66:LEU:HB3	1:D:104:VAL:HG21	1.88	0.55
3:F:162:GLN:HB3	3:F:235:THR:CG2	2.36	0.55
2:B:134:PHE:O	2:B:136:GLU:N	2.39	0.55
1:D:412:ALA:O	1:D:413:GLU:HG3	2.07	0.55
1:A:556:LEU:HD22	1:A:588:LEU:HD11	1.89	0.55
2:B:310:PHE:CD1	2:B:348:LEU:HD13	2.42	0.55
1:D:12:PRO:O	1:D:15:VAL:HG12	2.07	0.55
1:D:154:CYS:O	1:D:158:VAL:HG13	2.07	0.55
2:E:357:LEU:N	2:E:358:PRO:HD2	2.22	0.55
3:F:244:VAL:O	3:F:244:VAL:HG23	2.07	0.55
1:A:29:LEU:HA	1:A:65:VAL:HG22	1.89	0.55
1:A:360:ASN:O	1:A:364:HIS:N	2.38	0.55
1:D:559:GLU:O	1:D:563:ILE:HG22	2.07	0.55
1:A:182:ARG:HH11	1:A:182:ARG:HG3	1.70	0.55
1:A:517:THR:HA	1:A:521:MSE:HE2	1.88	0.55
2:B:31:LEU:C	2:B:33:ILE:H	2.10	0.55
1:D:470:VAL:HG22	1:D:478:ALA:HB2	1.88	0.55
2:B:330:PHE:O	2:B:334:GLU:HB2	2.06	0.54
2:B:406:LYS:O	2:B:406:LYS:HD3	2.06	0.54
3:C:101:VAL:O	3:C:105:VAL:HG23	2.07	0.54
1:D:260:ARG:HG3	1:D:260:ARG:NH1	2.22	0.54
2:E:83:PRO:O	2:E:85:VAL:N	2.40	0.54
3:F:265:TYR:CD2	3:F:266:CYS:N	2.74	0.54
1:A:197:GLU:H	1:A:197:GLU:CD	2.09	0.54
2:B:158:LEU:O	2:B:161:PHE:HD1	1.90	0.54
2:B:356:ILE:C	2:B:358:PRO:HD2	2.28	0.54
2:B:409:GLU:O	2:B:413:MSE:HB2	2.08	0.54
3:C:253:ASP:O	3:C:254:ARG:C	2.45	0.54
2:E:189:TYR:O	2:E:190:ILE:C	2.45	0.54
2:E:255:PRO:HG2	2:E:256:GLN:NE2	2.22	0.54
3:F:28:VAL:O	3:F:31:LEU:N	2.41	0.54
3:F:203:PRO:HA	3:F:220:PHE:CE1	2.42	0.54
1:A:438:PHE:CE1	1:A:442:LYS:HB2	2.42	0.54
2:B:73:ASN:C	2:B:75:ASN:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:LEU:HD13	3:C:106:ARG:HB2	1.90	0.54
3:C:65:LEU:O	3:C:68:LEU:HB3	2.08	0.54
3:C:170:LEU:HD12	3:C:220:PHE:CD2	2.43	0.54
3:C:248:TYR:CE2	3:C:286:PHE:CD2	2.95	0.54
2:E:244:LEU:HD22	2:E:253:TYR:CE1	2.42	0.54
2:E:350:SER:O	2:E:352:ASN:N	2.39	0.54
1:A:367:PRO:O	1:A:370:LEU:HB2	2.07	0.54
1:D:477:TRP:CH2	1:D:482:ILE:HD11	2.42	0.54
3:F:76:PRO:HG3	3:F:107:TYR:CE1	2.43	0.54
3:F:160:ASP:C	3:F:162:GLN:H	2.11	0.54
2:B:310:PHE:CG	2:B:348:LEU:HD13	2.42	0.54
1:D:91:PRO:HB2	1:D:92:PRO:HD3	1.89	0.54
1:A:366:LEU:N	1:A:367:PRO:CD	2.70	0.54
1:A:381:ARG:HH12	1:A:414:ASP:CG	2.11	0.54
2:B:43:PHE:C	2:B:45:PHE:H	2.09	0.54
2:B:250:LEU:HA	2:B:253:TYR:CE2	2.42	0.54
1:D:24:ASP:O	1:D:25:VAL:C	2.46	0.54
1:D:131:LEU:HD23	1:D:132:VAL:N	2.23	0.54
1:D:381:ARG:O	1:D:385:ILE:HG12	2.07	0.54
2:E:152:LYS:O	2:E:156:GLN:HG3	2.08	0.54
2:B:158:LEU:O	2:B:159:GLU:C	2.44	0.54
1:D:452:VAL:HG13	1:D:497:HIS:HD2	1.72	0.54
2:B:373:ASN:C	2:B:375:THR:H	2.11	0.54
3:C:97:VAL:O	3:C:101:VAL:HG23	2.08	0.54
1:D:317:CYS:O	1:D:320:ASN:N	2.38	0.54
2:E:316:PRO:HG2	2:E:317:LEU:N	2.23	0.54
2:E:332:VAL:O	2:E:335:ARG:N	2.40	0.54
1:D:262:MSE:O	1:D:263:VAL:C	2.47	0.54
1:D:348:VAL:O	1:D:350:MSE:N	2.41	0.54
2:E:381:TYR:HE2	2:E:385:LYS:HD2	1.71	0.54
2:B:380:ILE:HG22	2:B:381:TYR:N	2.22	0.54
1:D:144:ARG:HH21	1:D:176:ASP:CG	2.12	0.54
1:D:158:VAL:HG23	1:D:163:LYS:HG3	1.90	0.54
1:D:375:ASP:OD2	1:D:376:GLU:N	2.41	0.54
1:D:408:ILE:CD1	1:D:426:TYR:HE2	2.20	0.54
2:E:138:PRO:O	2:E:140:PHE:CD1	2.61	0.54
2:E:211:ILE:HG21	2:E:253:TYR:CD1	2.43	0.54
3:F:190:PRO:HD3	3:F:195:MET:CE	2.38	0.54
1:A:36:SER:C	1:A:38:ILE:H	2.11	0.53
2:B:79:GLU:N	2:B:80:PRO:HD2	2.22	0.53
2:B:121:TRP:H	2:B:122:PRO:HD2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:PHE:HD2	3:C:63:HIS:CD2	2.23	0.53
2:E:165:ASP:O	2:E:166:PRO:C	2.45	0.53
1:A:570:ASP:OD2	1:A:571:GLN:N	2.41	0.53
1:D:211:ASN:HD22	1:D:211:ASN:N	2.04	0.53
1:A:423:ILE:O	1:A:426:TYR:N	2.36	0.53
2:B:141:GLN:HB3	2:B:142:PRO:HD2	1.91	0.53
2:B:165:ASP:O	2:B:166:PRO:C	2.46	0.53
1:D:47:THR:HG23	1:D:51:LEU:HD23	1.90	0.53
2:B:89:PHE:CE2	2:B:93:MSE:HG3	2.44	0.53
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.29	0.53
1:D:171:ARG:HG3	1:D:208:MSE:SE	2.58	0.53
3:F:10:LEU:HD23	3:F:13:TRP:CE3	2.43	0.53
1:A:178:THR:HB	1:A:180:MSE:HG2	1.89	0.53
1:A:326:ILE:N	1:A:326:ILE:HD12	2.24	0.53
1:A:479:HIS:O	1:A:479:HIS:ND1	2.39	0.53
2:B:389:GLU:O	2:B:390:MSE:HB2	2.09	0.53
1:D:79:LEU:N	1:D:79:LEU:CD1	2.65	0.53
3:F:189:VAL:HA	3:F:195:MET:HE2	1.90	0.53
1:A:429:LEU:O	1:A:433:GLN:HG3	2.09	0.53
1:A:455:VAL:HG23	3:C:71:ILE:HA	1.90	0.53
2:B:149:ILE:O	2:B:149:ILE:HG22	2.08	0.53
1:D:284:VAL:HB	1:D:285:PRO:HD3	1.90	0.53
1:D:310:CYS:HB3	1:D:322:ILE:HD11	1.90	0.53
1:A:88:CYS:C	1:A:90:LEU:H	2.11	0.53
1:A:116:SER:HB2	1:A:128:PHE:CE1	2.44	0.53
1:A:352:LEU:HA	1:A:355:ILE:CD1	2.36	0.53
2:B:124:LEU:O	2:B:126:LEU:N	2.42	0.53
3:C:36:LYS:O	3:C:39:LEU:N	2.40	0.53
1:D:489:MSE:O	1:D:491:GLY:N	2.41	0.53
2:E:197:ILE:HD13	2:E:208:HIS:HE1	1.74	0.53
3:F:185:ARG:O	3:F:187:GLN:N	2.37	0.53
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.39	0.53
2:B:393:LYS:HG2	2:B:397:ASP:OD2	2.08	0.53
1:D:104:VAL:CG1	1:D:105:ARG:N	2.72	0.53
1:D:405:LEU:HB3	1:D:406:PRO:HD3	1.91	0.53
1:D:528:MSE:C	1:D:530:GLY:N	2.61	0.53
1:D:586:LEU:O	1:D:587:SER:HB2	2.09	0.53
1:A:390:CYS:SG	1:A:391:VAL:N	2.82	0.53
1:A:491:GLY:O	1:A:492:ASP:C	2.47	0.53
2:B:54:LYS:O	2:B:56:LYS:N	2.33	0.53
2:B:208:HIS:CD2	2:B:210:GLY:H	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:CYS:O	1:D:391:VAL:C	2.47	0.53
2:E:234:LYS:O	2:E:238:LEU:HD23	2.08	0.53
2:E:247:VAL:HG12	2:E:249:SER:H	1.73	0.53
1:A:470:VAL:HG11	1:A:511:VAL:HG23	1.89	0.53
2:B:380:ILE:O	2:B:381:TYR:C	2.48	0.53
3:C:83:MET:HE3	3:C:240:ALA:HB3	1.90	0.53
3:C:185:ARG:O	3:C:187:GLN:N	2.40	0.53
1:D:198:LEU:CD1	1:D:202:LYS:HE3	2.39	0.53
2:E:91:VAL:O	2:E:91:VAL:HG12	2.08	0.53
2:E:211:ILE:CG2	2:E:253:TYR:CD1	2.92	0.53
2:E:365:TYR:O	2:E:366:ARG:C	2.47	0.53
3:F:253:ASP:O	3:F:254:ARG:C	2.46	0.53
1:A:489:MSE:C	1:A:491:GLY:N	2.61	0.52
2:B:42:LEU:CB	2:B:63:LEU:HD21	2.39	0.52
2:B:108:PHE:HB3	3:C:268:ARG:NH2	2.24	0.52
2:E:42:LEU:CB	2:E:63:LEU:HD21	2.39	0.52
1:A:105:ARG:HD2	1:A:146:SER:OG	2.09	0.52
1:A:350:MSE:HE1	1:A:391:VAL:CG2	2.33	0.52
1:A:405:LEU:N	1:A:406:PRO:CD	2.71	0.52
2:E:87:HIS:O	2:E:91:VAL:HG23	2.09	0.52
3:F:162:GLN:OE1	3:F:235:THR:HG21	2.09	0.52
1:A:325:GLN:C	1:A:328:PRO:HD2	2.29	0.52
2:B:180:TYR:HE1	2:B:187:ARG:HA	1.73	0.52
2:B:254:HIS:O	2:B:257:LEU:HB3	2.10	0.52
1:D:448:MSE:HE1	1:D:466:LEU:HD21	1.92	0.52
2:E:43:PHE:C	2:E:45:PHE:H	2.12	0.52
1:A:29:LEU:HD12	1:A:65:VAL:HG22	1.90	0.52
1:A:35:LEU:HD21	1:A:55:LEU:CD1	2.40	0.52
1:A:77:THR:HG23	1:A:86:VAL:HG21	1.90	0.52
2:B:285:LYS:O	2:B:286:THR:HG23	2.09	0.52
1:A:77:THR:O	1:A:80:VAL:HG12	2.09	0.52
1:A:130:PRO:O	1:A:133:LYS:HB2	2.10	0.52
1:A:358:LYS:HA	1:A:394:VAL:HG12	1.92	0.52
2:B:85:VAL:HG11	2:B:134:PHE:HD1	1.74	0.52
1:D:119:HIS:CD2	1:D:119:HIS:H	2.27	0.52
1:D:155:TYR:N	1:D:156:PRO:CD	2.72	0.52
2:E:304:VAL:O	2:E:304:VAL:HG12	2.09	0.52
1:A:408:ILE:HD13	1:A:426:TYR:HE2	1.74	0.52
2:B:71:THR:HG21	2:B:133:ARG:HH11	1.74	0.52
3:C:128:GLY:O	3:C:129:PHE:C	2.46	0.52
1:D:506:ASN:HD21	1:D:543:SER:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:VAL:HG12	1:D:561:LYS:N	2.25	0.52
2:E:42:LEU:O	2:E:43:PHE:O	2.27	0.52
2:E:262:VAL:HG12	2:E:263:GLN:N	2.23	0.52
1:A:506:ASN:HD21	1:A:543:SER:CB	2.23	0.52
3:C:17:LEU:HD21	3:C:23:LEU:HG	1.91	0.52
3:C:170:LEU:HD12	3:C:220:PHE:CG	2.45	0.52
3:C:252:HIS:O	3:C:253:ASP:O	2.28	0.52
3:C:252:HIS:O	3:C:255:ASN:HB2	2.10	0.52
1:D:345:LEU:HD23	1:D:346:ALA:N	2.25	0.52
2:E:73:ASN:C	2:E:75:ASN:N	2.63	0.52
2:E:250:LEU:O	2:E:252:VAL:N	2.43	0.52
3:F:137:TYR:CG	3:F:142:VAL:HG21	2.44	0.52
3:C:166:LEU:O	3:C:166:LEU:HD23	2.10	0.52
1:D:105:ARG:HD2	1:D:146:SER:OG	2.10	0.52
1:D:358:LYS:O	1:D:362:ILE:HG13	2.10	0.52
1:A:12:PRO:O	1:A:15:VAL:HG12	2.10	0.52
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.90	0.52
1:A:500:THR:HA	1:A:503:PHE:CD1	2.36	0.52
2:B:88:MSE:HE1	2:B:127:VAL:HG22	1.92	0.52
2:B:254:HIS:CD2	2:B:293:MSE:HE2	2.44	0.52
3:C:166:LEU:CD2	3:C:239:ARG:HB3	2.40	0.52
1:D:141:PHE:CD1	1:D:142:THR:N	2.78	0.52
1:D:277:GLU:C	1:D:279:THR:N	2.60	0.52
2:E:250:LEU:C	2:E:252:VAL:H	2.11	0.52
2:E:286:THR:HG22	3:F:134:LEU:HB3	1.91	0.52
2:E:310:PHE:O	2:E:314:MSE:HB2	2.09	0.52
2:B:134:PHE:C	2:B:136:GLU:H	2.13	0.52
3:C:209:TRP:H	3:C:224:ILE:HD11	1.73	0.52
1:D:20:LEU:HD21	1:D:31:SER:O	2.09	0.52
1:D:164:ALA:HA	1:D:167:ARG:NH1	2.25	0.52
1:D:349:ILE:HG23	1:D:350:MSE:N	2.25	0.52
2:E:256:GLN:CD	2:E:256:GLN:H	2.13	0.52
3:F:166:LEU:HD12	3:F:198:LEU:HD22	1.92	0.52
1:A:89:LEU:N	1:A:89:LEU:CD1	2.72	0.51
1:A:586:LEU:O	1:A:587:SER:HB2	2.10	0.51
3:C:166:LEU:HD21	3:C:239:ARG:HB3	1.91	0.51
1:D:438:PHE:HD1	1:D:438:PHE:O	1.94	0.51
2:E:35:LYS:C	2:E:37:ARG:H	2.11	0.51
3:F:189:VAL:HA	3:F:195:MET:CE	2.40	0.51
1:A:29:LEU:HD12	1:A:65:VAL:CG2	2.40	0.51
1:A:90:LEU:CB	1:A:91:PRO:HD3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ILE:HA	1:A:450:TRP:CZ3	2.45	0.51
1:D:128:PHE:O	1:D:129:VAL:C	2.47	0.51
1:D:366:LEU:HB3	1:D:367:PRO:HD3	1.90	0.51
2:E:249:SER:O	2:E:252:VAL:HG23	2.10	0.51
2:E:373:ASN:HD21	2:E:376:ILE:HG23	1.75	0.51
3:F:13:TRP:NE1	3:F:27:GLN:NE2	2.57	0.51
3:F:121:ARG:HH11	3:F:121:ARG:HG3	1.75	0.51
1:A:17:ILE:HG12	1:A:38:ILE:HG23	1.92	0.51
2:B:72:HIS:O	2:B:74:ARG:N	2.44	0.51
2:B:87:HIS:O	2:B:91:VAL:HG23	2.11	0.51
2:B:189:TYR:O	2:B:190:ILE:C	2.48	0.51
2:B:363:SER:HA	2:B:366:ARG:HB2	1.92	0.51
2:B:373:ASN:ND2	2:B:376:ILE:H	2.09	0.51
3:C:118:HIS:ND1	3:C:123:ILE:HG21	2.24	0.51
1:D:155:TYR:CE2	1:D:196:LEU:HD23	2.45	0.51
1:D:410:GLU:O	1:D:411:LEU:C	2.47	0.51
2:E:134:PHE:CE2	2:E:135:LEU:HD22	2.45	0.51
2:E:136:GLU:OE1	2:E:178:ARG:NH1	2.40	0.51
2:B:121:TRP:N	2:B:122:PRO:CD	2.73	0.51
2:B:262:VAL:O	2:B:265:LEU:N	2.43	0.51
3:C:81:LEU:HD23	3:C:81:LEU:O	2.10	0.51
1:D:155:TYR:N	1:D:156:PRO:HD3	2.25	0.51
2:E:65:GLU:C	2:E:67:VAL:H	2.13	0.51
2:E:242:LEU:N	2:E:243:PRO:HD2	2.25	0.51
3:F:6:PHE:HE2	3:F:34:LYS:HG3	1.75	0.51
1:A:11:TYR:N	1:A:12:PRO:HD2	2.26	0.51
1:A:174:CYS:SG	1:A:185:ALA:HB1	2.50	0.51
1:A:215:ASP:O	1:A:221:ARG:NH1	2.42	0.51
2:B:145:ALA:O	2:B:147:LYS:N	2.44	0.51
2:B:346:MSE:CE	2:B:349:ILE:HD12	2.41	0.51
3:C:68:LEU:C	3:C:68:LEU:CD2	2.79	0.51
3:C:121:ARG:HG3	3:C:121:ARG:NH1	2.25	0.51
1:D:91:PRO:HB2	1:D:92:PRO:CD	2.41	0.51
2:E:271:LEU:O	2:E:274:PRO:HG2	2.10	0.51
1:A:515:ASP:O	1:A:518:THR:N	2.43	0.51
2:E:88:MSE:HE1	2:E:127:VAL:HG22	1.93	0.51
2:E:202:ILE:HD11	2:E:244:LEU:CG	2.36	0.51
1:D:414:ASP:OD2	1:D:415:ALA:N	2.44	0.51
1:D:419:VAL:O	1:D:422:ALA:HB3	2.10	0.51
2:E:167:ARG:HH11	2:E:167:ARG:CG	2.23	0.51
2:E:180:TYR:HE2	2:E:221:ILE:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:SER:O	1:A:562:PRO:HG2	2.10	0.51
2:B:134:PHE:CD2	2:B:134:PHE:C	2.83	0.51
2:B:257:LEU:O	2:B:258:ALA:C	2.49	0.51
3:F:95:GLU:OE1	3:F:95:GLU:N	2.38	0.51
3:C:142:VAL:HA	3:C:145:TYR:HD1	1.76	0.51
1:D:155:TYR:CZ	1:D:163:LYS:HB3	2.46	0.51
1:D:343:SER:HA	1:D:380:VAL:HG22	1.92	0.51
2:B:267:LYS:O	2:B:268:ASP:HB2	2.11	0.51
2:E:194:ILE:HG21	2:E:218:LEU:HD11	1.92	0.51
3:F:155:LEU:HD11	3:F:195:MET:HG3	1.93	0.51
1:A:104:VAL:CG1	1:A:105:ARG:N	2.73	0.50
1:A:161:ALA:O	1:A:164:ALA:HB3	2.11	0.50
1:A:168:GLN:NE2	1:A:171:ARG:HH12	2.09	0.50
3:C:162:GLN:OE1	3:C:235:THR:HG21	2.11	0.50
3:C:239:ARG:O	3:C:240:ALA:HB2	2.11	0.50
1:D:155:TYR:CE1	1:D:163:LYS:HB3	2.46	0.50
1:D:205:ILE:HD13	1:D:208:MSE:HE3	1.93	0.50
1:D:439:PHE:CD1	1:D:443:LEU:HB3	2.47	0.50
2:E:79:GLU:O	2:E:80:PRO:C	2.50	0.50
3:F:33:GLU:O	3:F:36:LYS:HB2	2.11	0.50
3:F:141:ASN:O	3:F:145:TYR:CD1	2.64	0.50
3:F:194:PRO:HG2	3:F:195:MET:N	2.26	0.50
3:F:274:ALA:HB2	3:F:288:GLN:HA	1.94	0.50
2:B:94:PHE:N	2:B:94:PHE:CD2	2.79	0.50
3:C:34:LYS:O	3:C:38:ILE:HG13	2.11	0.50
1:D:52:LEU:HD11	1:D:89:LEU:HD12	1.93	0.50
1:D:245:MSE:O	1:D:249:ARG:HG3	2.10	0.50
1:D:338:ASN:ND2	1:D:341:VAL:HG23	2.17	0.50
1:D:502:LEU:HD21	1:D:540:VAL:HG22	1.93	0.50
1:D:518:THR:HG22	1:D:518:THR:O	2.10	0.50
1:D:538:PHE:CB	1:D:575:VAL:HA	2.41	0.50
2:E:183:PHE:C	2:E:185:GLY:N	2.63	0.50
2:E:310:PHE:CG	2:E:348:LEU:HD13	2.45	0.50
1:A:453:ASP:OD2	1:A:458:ILE:HG21	2.11	0.50
2:E:257:LEU:O	2:E:258:ALA:C	2.50	0.50
2:E:287:HIS:CE1	2:E:289:PRO:HB2	2.46	0.50
3:F:181:ARG:HH11	3:F:181:ARG:HG3	1.76	0.50
1:A:257:TRP:CH2	2:B:99:PRO:HB3	2.46	0.50
1:A:282:ASP:C	1:A:285:PRO:HD2	2.32	0.50
3:C:51:PRO:HB3	3:C:279:ASP:C	2.31	0.50
3:C:81:LEU:HA	3:C:112:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:ALA:HB2	1:D:540:VAL:HG11	1.93	0.50
2:E:380:ILE:O	2:E:381:TYR:C	2.46	0.50
1:A:502:LEU:HA	1:A:505:ILE:HD12	1.94	0.50
1:A:560:VAL:HG12	1:A:561:LYS:N	2.26	0.50
1:D:427:MSE:O	1:D:428:PRO:C	2.49	0.50
1:D:581:GLU:HG3	1:D:581:GLU:O	2.11	0.50
2:E:332:VAL:O	2:E:333:ALA:C	2.48	0.50
3:F:34:LYS:O	3:F:38:ILE:HG13	2.12	0.50
3:F:243:LEU:HD12	3:F:260:PHE:CE2	2.47	0.50
1:A:230:ASN:O	1:A:234:LEU:HG	2.11	0.50
2:B:144:ILE:HG22	2:B:144:ILE:O	2.11	0.50
3:C:74:LYS:O	3:C:78:THR:HG22	2.12	0.50
3:C:143:TRP:CE2	3:C:147:THR:HG21	2.45	0.50
1:D:489:MSE:HB3	1:D:501:THR:OG1	2.11	0.50
2:E:121:TRP:CZ2	2:E:167:ARG:HB3	2.46	0.50
1:A:372:GLN:O	1:A:374:LYS:N	2.45	0.50
1:A:456:TYR:CD1	1:A:456:TYR:C	2.84	0.50
2:B:134:PHE:C	2:B:134:PHE:HD2	2.15	0.50
3:C:225:SER:OG	3:C:252:HIS:ND1	2.33	0.50
1:D:44:VAL:CG2	1:D:45:GLU:N	2.74	0.50
1:D:180:MSE:HE2	1:D:183:ARG:NH2	2.27	0.50
1:D:397:ILE:O	1:D:397:ILE:HG13	2.11	0.50
2:E:397:ASP:O	2:E:400:GLN:HB3	2.11	0.50
2:E:400:GLN:O	2:E:401:GLN:C	2.49	0.50
1:A:377:CYS:SG	1:A:380:VAL:HG23	2.51	0.50
3:C:106:ARG:HG3	3:C:107:TYR:N	2.26	0.50
3:C:190:PRO:O	3:C:196:CYS:HB2	2.11	0.50
1:D:112:LEU:HD13	1:D:150:LEU:HD11	1.92	0.50
1:D:256:SER:OG	2:E:96:THR:HG21	2.11	0.50
2:E:88:MSE:HE1	2:E:127:VAL:HG13	1.94	0.50
3:F:100:LEU:HA	3:F:103:LEU:HD12	1.94	0.50
3:F:141:ASN:HB3	3:F:145:TYR:HE1	1.73	0.50
1:A:127:HIS:C	1:A:130:PRO:HD2	2.32	0.50
3:C:190:PRO:HD3	3:C:195:MET:HE1	1.93	0.50
1:D:423:ILE:O	1:D:426:TYR:N	2.42	0.50
2:E:218:LEU:HD13	2:E:236:PHE:HZ	1.76	0.50
3:F:276:MET:CE	3:F:278:LEU:HD21	2.42	0.50
1:D:20:LEU:HD23	1:D:31:SER:HB3	1.92	0.49
1:D:426:TYR:CG	1:D:426:TYR:O	2.65	0.49
2:E:35:LYS:O	2:E:38:GLN:N	2.44	0.49
1:D:16:LEU:HD23	1:D:16:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ILE:HG21	1:D:356:LEU:HD21	1.93	0.49
1:D:412:ALA:O	1:D:413:GLU:CG	2.60	0.49
2:E:89:PHE:CE2	2:E:93:MSE:HG3	2.47	0.49
2:E:223:ASN:HD22	2:E:263:GLN:NE2	2.05	0.49
2:E:250:LEU:HA	2:E:253:TYR:CE2	2.47	0.49
3:F:183:LEU:HD21	3:F:194:PRO:CG	2.41	0.49
1:A:583:LEU:HD22	1:A:588:LEU:HB2	1.93	0.49
2:B:195:ASN:O	2:B:198:PHE:N	2.45	0.49
3:C:243:LEU:HD12	3:C:260:PHE:CD2	2.47	0.49
1:D:570:ASP:OD1	1:D:575:VAL:HG11	2.12	0.49
2:E:164:GLU:C	2:E:165:ASP:O	2.50	0.49
2:E:253:TYR:CD2	2:E:253:TYR:N	2.79	0.49
3:F:190:PRO:HD3	3:F:195:MET:HE2	1.94	0.49
3:F:239:ARG:C	3:F:239:ARG:HD3	2.32	0.49
1:A:85:TYR:O	1:A:87:HIS:N	2.45	0.49
1:A:155:TYR:OH	1:A:167:ARG:HD3	2.11	0.49
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.94	0.49
2:B:65:GLU:C	2:B:67:VAL:N	2.64	0.49
3:C:162:GLN:HB3	3:C:235:THR:CG2	2.42	0.49
2:E:65:GLU:O	2:E:67:VAL:N	2.44	0.49
2:E:97:LEU:HD22	2:E:162:ASP:CB	2.42	0.49
2:E:121:TRP:C	2:E:123:HIS:H	2.16	0.49
2:E:183:PHE:O	2:E:185:GLY:N	2.46	0.49
3:F:276:MET:HB2	3:F:286:PHE:CE1	2.47	0.49
1:A:77:THR:HG23	1:A:86:VAL:CG2	2.43	0.49
1:A:129:VAL:CB	1:A:130:PRO:HD3	2.42	0.49
1:A:411:LEU:C	1:A:413:GLU:N	2.66	0.49
1:A:580:GLN:C	1:A:582:ALA:H	2.16	0.49
2:B:248:LYS:NZ	2:B:290:LYS:HZ2	2.10	0.49
1:D:120:SER:O	1:D:121:PRO:C	2.49	0.49
1:D:245:MSE:O	1:D:246:PRO:C	2.48	0.49
1:D:342:LYS:O	1:D:346:ALA:HB2	2.12	0.49
1:D:489:MSE:C	1:D:491:GLY:H	2.16	0.49
2:E:121:TRP:C	2:E:123:HIS:N	2.66	0.49
3:F:158:LEU:HA	3:F:163:ILE:O	2.12	0.49
3:F:251:CYS:SG	3:F:256:VAL:HG12	2.53	0.49
1:A:141:PHE:CD1	1:A:142:THR:N	2.80	0.49
1:A:364:HIS:C	1:A:367:PRO:HD2	2.31	0.49
1:A:399:GLN:NE2	1:A:403:SER:OG	2.46	0.49
1:A:559:GLU:O	1:A:563:ILE:HG22	2.13	0.49
2:B:67:VAL:C	2:B:69:TYR:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:MSE:SE	2:B:127:VAL:HG13	2.62	0.49
3:C:104:LYS:CA	3:C:111:ILE:HD11	2.41	0.49
1:D:426:TYR:O	1:D:426:TYR:CD1	2.64	0.49
1:D:517:THR:HG23	1:D:521:MSE:HE3	1.95	0.49
2:E:175:THR:O	2:E:179:ILE:HG13	2.13	0.49
1:A:112:LEU:HD13	1:A:150:LEU:HD11	1.94	0.49
1:A:270:LEU:O	1:A:271:GLN:C	2.51	0.49
1:A:552:ASP:OD1	1:A:554:SER:HB3	2.12	0.49
2:B:64:SER:O	2:B:68:GLU:HG3	2.13	0.49
3:C:209:TRP:CD2	3:C:224:ILE:HD13	2.48	0.49
1:D:179:PRO:HG3	1:D:182:ARG:NH2	2.27	0.49
1:D:410:GLU:O	1:D:412:ALA:N	2.46	0.49
2:E:262:VAL:O	2:E:263:GLN:C	2.51	0.49
3:F:118:HIS:ND1	3:F:123:ILE:HG21	2.27	0.49
1:A:24:ASP:O	1:A:24:ASP:OD2	2.30	0.49
1:A:204:GLU:C	1:A:207:PRO:HD2	2.32	0.49
1:D:297:GLU:O	1:D:299:ARG:N	2.46	0.49
1:D:481:THR:O	1:D:481:THR:HG22	2.13	0.49
1:D:588:LEU:O	1:D:589:ALA:CB	2.60	0.49
2:E:167:ARG:HH11	2:E:167:ARG:HB3	1.78	0.49
3:F:153:LEU:O	3:F:185:ARG:HD2	2.12	0.49
3:F:166:LEU:CD2	3:F:239:ARG:HB3	2.42	0.49
1:A:29:LEU:HD12	1:A:65:VAL:HA	1.94	0.49
1:A:178:THR:OG1	1:A:181:VAL:HG23	2.12	0.49
1:A:283:LEU:O	1:A:287:PHE:N	2.42	0.49
1:A:305:LYS:O	1:A:309:PHE:HB2	2.12	0.49
2:B:118:GLU:H	2:B:164:GLU:CG	2.25	0.49
2:B:329:HIS:NE2	2:B:331:GLN:HB2	2.26	0.49
2:B:371:HIS:NE2	2:B:376:ILE:HD11	2.27	0.49
3:C:24:SER:OG	3:C:27:GLN:HG3	2.13	0.49
2:E:118:GLU:H	2:E:164:GLU:HG2	1.76	0.49
2:E:141:GLN:HB2	2:E:144:ILE:HG13	1.93	0.49
2:E:367:ASN:O	2:E:369:LYS:N	2.32	0.49
3:F:57:ASP:HB2	3:F:260:PHE:CE1	2.48	0.49
1:A:88:CYS:O	1:A:90:LEU:N	2.46	0.49
1:A:89:LEU:CD1	1:A:89:LEU:H	2.25	0.49
2:B:330:PHE:CE1	2:B:331:GLN:HG2	2.48	0.49
2:E:86:VAL:O	2:E:87:HIS:C	2.51	0.49
3:F:45:VAL:HG22	3:F:156:THR:OG1	2.12	0.49
3:F:181:ARG:HG3	3:F:181:ARG:NH1	2.27	0.49
3:F:244:VAL:O	3:F:244:VAL:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TYR:HE1	1:A:167:ARG:HG2	1.78	0.48
1:A:347:SER:HB3	1:A:383:ASN:ND2	2.24	0.48
1:D:183:ARG:CZ	2:E:200:ARG:HD2	2.43	0.48
1:D:405:LEU:C	1:D:405:LEU:HD13	2.33	0.48
2:E:121:TRP:N	2:E:122:PRO:CD	2.75	0.48
1:A:66:LEU:HD22	1:A:96:LEU:CD2	2.42	0.48
1:A:179:PRO:HD2	2:B:196:ASN:ND2	2.27	0.48
2:B:63:LEU:O	2:B:67:VAL:HG23	2.13	0.48
2:B:132:LEU:C	2:B:134:PHE:N	2.66	0.48
2:B:337:LEU:HD21	2:B:380:ILE:HG13	1.94	0.48
3:C:46:GLN:O	3:C:157:ALA:HA	2.13	0.48
3:C:119:GLU:HG2	3:C:153:LEU:HD12	1.95	0.48
1:D:86:VAL:C	1:D:88:CYS:H	2.17	0.48
1:D:489:MSE:C	1:D:491:GLY:N	2.67	0.48
1:D:574:ASP:OD2	3:F:110:ARG:NE	2.46	0.48
2:E:388:MSE:O	2:E:390:MSE:N	2.46	0.48
3:F:55:CYS:SG	3:F:68:LEU:HD11	2.53	0.48
3:F:237:VAL:CB	3:F:256:VAL:HG23	2.32	0.48
1:A:24:ASP:O	1:A:27:LEU:N	2.39	0.48
1:A:277:GLU:O	1:A:279:THR:N	2.47	0.48
3:C:58:VAL:O	3:C:61:GLN:HG3	2.14	0.48
3:C:115:ARG:HB2	3:C:153:LEU:HB2	1.95	0.48
3:C:239:ARG:HH12	3:C:242:GLN:CG	2.16	0.48
1:D:67:LEU:HA	1:D:104:VAL:HG22	1.94	0.48
2:E:217:ILE:O	2:E:221:ILE:HG13	2.13	0.48
2:B:68:GLU:HB3	2:B:72:HIS:HD2	1.79	0.48
2:B:250:LEU:C	2:B:252:VAL:H	2.16	0.48
3:C:176:THR:HA	3:C:232:ASN:OD1	2.13	0.48
1:D:260:ARG:NE	1:D:293:ASP:OD2	2.42	0.48
1:D:399:GLN:NE2	1:D:403:SER:OG	2.45	0.48
3:F:123:ILE:HG23	3:F:127:TYR:CD2	2.35	0.48
1:A:89:LEU:N	1:A:89:LEU:HD12	2.27	0.48
1:A:277:GLU:C	1:A:279:THR:N	2.67	0.48
1:D:94:GLU:HB2	1:D:131:LEU:CD1	2.44	0.48
1:D:353:SER:N	1:D:354:PRO:HD2	2.29	0.48
1:D:389:ASP:OD2	1:D:389:ASP:N	2.46	0.48
2:E:80:PRO:HG2	2:E:82:TYR:HE2	1.73	0.48
2:E:195:ASN:O	2:E:198:PHE:N	2.46	0.48
2:E:373:ASN:HD22	2:E:376:ILE:HG23	1.75	0.48
3:F:253:ASP:O	3:F:255:ASN:N	2.45	0.48
1:A:39:ALA:HB1	1:A:47:THR:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASN:ND2	1:A:543:SER:HA	2.29	0.48
2:B:344:TYR:O	2:B:347:SER:HB3	2.12	0.48
3:C:158:LEU:HD21	3:C:161:GLY:HA2	1.96	0.48
1:D:12:PRO:O	1:D:13:ILE:C	2.52	0.48
2:E:259:TYR:O	2:E:263:GLN:HB2	2.12	0.48
1:A:25:VAL:HG13	1:A:62:GLU:HG2	1.95	0.48
1:A:502:LEU:O	1:A:506:ASN:OD1	2.32	0.48
3:C:202:ASP:HA	3:C:239:ARG:NH2	2.29	0.48
3:C:237:VAL:CB	3:C:256:VAL:HG23	2.41	0.48
3:C:276:MET:HE3	3:C:278:LEU:HD21	1.95	0.48
1:D:75:THR:C	1:D:77:THR:H	2.17	0.48
1:D:398:ARG:O	1:D:399:GLN:C	2.52	0.48
2:E:245:HIS:CE1	2:E:257:LEU:HD21	2.49	0.48
2:B:313:ILE:C	2:B:316:PRO:HD2	2.33	0.48
3:C:236:LEU:HD11	3:C:257:VAL:HG12	1.95	0.48
1:D:77:THR:O	1:D:80:VAL:HG12	2.13	0.48
2:E:236:PHE:CD2	2:E:236:PHE:C	2.86	0.48
2:E:287:HIS:O	2:E:288:SER:C	2.52	0.48
2:E:296:ASN:O	2:E:300:GLU:HG3	2.13	0.48
2:B:325:VAL:HG22	2:B:337:LEU:HD12	1.96	0.48
2:B:325:VAL:HG22	2:B:337:LEU:CD1	2.44	0.48
2:B:391:ASN:CG	2:B:394:LEU:HD12	2.34	0.48
1:D:198:LEU:HD12	1:D:202:LYS:HE3	1.96	0.48
2:E:121:TRP:O	2:E:123:HIS:N	2.47	0.48
3:F:68:LEU:C	3:F:68:LEU:CD2	2.81	0.48
3:F:142:VAL:HA	3:F:145:TYR:HD1	1.77	0.48
3:F:251:CYS:SG	3:F:256:VAL:CG1	3.02	0.48
1:A:52:LEU:HD11	1:A:89:LEU:HD12	1.95	0.48
2:B:42:LEU:O	2:B:59:LYS:HE3	2.14	0.48
2:B:315:GLU:HB2	2:B:316:PRO:HD3	1.96	0.48
2:B:407:LEU:HD23	2:B:407:LEU:C	2.34	0.48
3:C:176:THR:HG23	3:C:179:HIS:HD2	1.78	0.48
3:C:239:ARG:HD3	3:C:240:ALA:N	2.29	0.48
1:D:22:ASN:O	1:D:23:GLU:CB	2.61	0.48
1:D:482:ILE:O	1:D:486:VAL:HG23	2.14	0.48
2:E:356:ILE:O	2:E:359:ILE:N	2.46	0.48
3:F:120:SER:O	3:F:124:THR:HG23	2.13	0.48
1:A:179:PRO:CB	1:A:183:ARG:NH1	2.76	0.47
1:A:375:ASP:OD2	1:A:376:GLU:N	2.47	0.47
1:A:455:VAL:HG13	1:A:458:ILE:HB	1.95	0.47
2:B:400:GLN:O	2:B:401:GLN:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLY:O	1:D:44:VAL:C	2.52	0.47
1:D:102:THR:O	1:D:103:VAL:C	2.52	0.47
1:D:245:MSE:HA	1:D:245:MSE:HE3	1.96	0.47
2:E:255:PRO:HG2	2:E:256:GLN:H	1.79	0.47
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.94	0.47
1:A:218:ASP:C	1:A:220:VAL:H	2.16	0.47
1:A:327:LEU:O	1:A:331:LYS:HG3	2.13	0.47
2:B:365:TYR:O	2:B:366:ARG:C	2.52	0.47
2:E:183:PHE:C	2:E:185:GLY:H	2.15	0.47
3:F:28:VAL:HG21	3:F:142:VAL:HG13	1.95	0.47
1:A:102:THR:HG22	1:A:105:ARG:HH22	1.77	0.47
1:A:466:LEU:O	1:A:469:LEU:N	2.43	0.47
1:A:509:SER:O	1:A:550:ILE:HD13	2.14	0.47
1:A:533:VAL:HG12	1:A:535:ASN:HB2	1.95	0.47
3:C:122:GLN:O	3:C:126:VAL:HG23	2.15	0.47
3:C:166:LEU:HD11	3:C:169:GLY:C	2.34	0.47
3:C:276:MET:HE2	3:C:278:LEU:HD21	1.95	0.47
1:D:398:ARG:O	1:D:400:LEU:N	2.47	0.47
2:E:215:LEU:HD13	2:E:257:LEU:HA	1.97	0.47
2:E:288:SER:HB2	2:E:289:PRO:CD	2.43	0.47
3:F:17:LEU:O	3:F:20:CYS:N	2.36	0.47
1:A:382:LEU:HD12	1:A:419:VAL:HG13	1.97	0.47
2:B:132:LEU:O	2:B:134:PHE:N	2.47	0.47
1:D:40:LEU:C	1:D:42:LEU:N	2.67	0.47
2:E:97:LEU:HB3	2:E:98:PRO:HD2	1.97	0.47
2:E:151:GLN:O	2:E:154:VAL:N	2.47	0.47
2:E:241:LEU:HA	2:E:241:LEU:HD23	1.66	0.47
2:E:409:GLU:O	2:E:413:MSE:HB2	2.13	0.47
3:F:119:GLU:HG3	3:F:150:PHE:CE1	2.49	0.47
1:A:115:ILE:O	1:A:119:HIS:CD2	2.67	0.47
1:A:141:PHE:CD1	1:A:141:PHE:C	2.87	0.47
1:A:377:CYS:SG	1:A:379:GLU:HB2	2.55	0.47
2:B:186:LEU:O	2:B:190:ILE:HD12	2.14	0.47
2:B:242:LEU:HD13	2:B:278:ALA:HB2	1.94	0.47
2:E:285:LYS:HE3	2:E:285:LYS:HB2	1.74	0.47
1:A:100:GLU:O	1:A:101:GLU:C	2.53	0.47
1:A:499:MSE:O	1:A:501:THR:N	2.47	0.47
1:D:317:CYS:O	1:D:318:ARG:C	2.53	0.47
1:A:76:PHE:HB2	1:A:89:LEU:HD21	1.95	0.47
1:A:96:LEU:HA	1:A:99:VAL:HG23	1.96	0.47
2:B:59:LYS:HA	2:B:62:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:THR:OG1	2:B:105:GLY:N	2.46	0.47
2:B:118:GLU:CB	2:B:164:GLU:HG2	2.43	0.47
2:B:158:LEU:HD23	2:B:161:PHE:CE1	2.50	0.47
2:B:335:ARG:HH11	2:B:335:ARG:HG3	1.78	0.47
3:C:45:VAL:HA	3:C:156:THR:OG1	2.14	0.47
3:C:106:ARG:O	3:C:108:ARG:N	2.36	0.47
3:C:117:ASN:HB2	3:C:200:TRP:CZ2	2.49	0.47
3:C:119:GLU:HG3	3:C:150:PHE:CG	2.49	0.47
3:C:294:ARG:HG2	3:C:294:ARG:HH11	1.80	0.47
1:D:67:LEU:HD12	1:D:67:LEU:O	2.15	0.47
1:D:94:GLU:HB2	1:D:131:LEU:HD12	1.96	0.47
1:D:193:ALA:HB2	1:D:205:ILE:HG13	1.97	0.47
1:D:385:ILE:HD12	1:D:423:ILE:HD11	1.96	0.47
2:E:72:HIS:C	2:E:74:ARG:H	2.17	0.47
2:E:117:LEU:HD23	2:E:164:GLU:OE1	2.15	0.47
1:A:177:ASP:OD1	1:A:177:ASP:N	2.48	0.47
1:A:288:GLN:CA	1:A:291:MSE:HE3	2.25	0.47
1:A:349:ILE:HG23	1:A:350:MSE:H	1.80	0.47
2:B:169:ARG:O	2:B:170:ASP:C	2.53	0.47
3:C:10:LEU:HD23	3:C:13:TRP:CE3	2.50	0.47
1:D:307:LYS:HD2	1:D:351:GLY:HA3	1.97	0.47
3:F:248:TYR:CE2	3:F:286:PHE:CD2	3.03	0.47
1:A:76:PHE:CB	1:A:89:LEU:HD21	2.45	0.47
1:A:225:VAL:HG11	1:A:262:MSE:CB	2.37	0.47
1:A:349:ILE:CG2	1:A:350:MSE:N	2.78	0.47
2:B:35:LYS:C	2:B:37:ARG:N	2.68	0.47
2:B:169:ARG:HB3	2:B:213:GLU:HG2	1.97	0.47
2:B:250:LEU:O	2:B:252:VAL:N	2.48	0.47
2:B:324:CYS:O	2:B:325:VAL:C	2.53	0.47
3:C:94:VAL:O	3:C:97:VAL:HG12	2.15	0.47
3:C:220:PHE:CA	3:C:224:ILE:HD12	2.44	0.47
1:D:17:ILE:HG12	1:D:38:ILE:HG23	1.95	0.47
1:D:119:HIS:CD2	1:D:119:HIS:N	2.83	0.47
1:D:348:VAL:O	1:D:349:ILE:C	2.53	0.47
1:D:411:LEU:C	1:D:413:GLU:N	2.67	0.47
1:D:492:ASP:OD2	1:D:493:PRO:HD2	2.15	0.47
2:E:315:GLU:O	2:E:319:ARG:HB2	2.14	0.47
3:F:244:VAL:HG21	3:F:248:TYR:N	2.30	0.47
1:A:119:HIS:CD2	1:A:119:HIS:H	2.33	0.47
1:A:452:VAL:HG13	1:A:497:HIS:HE2	1.75	0.47
2:B:305:ILE:HD13	2:B:306:GLU:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:MSE:HE2	2:B:392:GLN:NE2	2.19	0.47
1:D:352:LEU:HD23	1:D:355:ILE:HD12	1.96	0.47
1:D:522:LEU:N	1:D:523:PRO:CD	2.77	0.47
2:E:251:SER:HA	2:E:293:MSE:CE	2.41	0.47
3:F:87:VAL:O	3:F:88:ASP:HB2	2.14	0.47
3:F:88:ASP:O	3:F:89:ARG:HB2	2.15	0.47
3:F:171:SER:HB2	3:F:197:ASP:HB3	1.96	0.47
1:A:340:HIS:O	1:A:344:ALA:HB2	2.15	0.46
1:A:353:SER:N	1:A:354:PRO:HD2	2.30	0.46
1:A:399:GLN:CA	1:A:399:GLN:HE21	2.27	0.46
2:B:222:ILE:O	2:B:224:GLY:N	2.47	0.46
1:D:350:MSE:CE	1:D:391:VAL:HG13	2.18	0.46
1:D:535:ASN:HA	1:D:538:PHE:CD2	2.49	0.46
2:E:313:ILE:HG22	2:E:314:MSE:N	2.30	0.46
3:F:5:VAL:O	3:F:5:VAL:HG12	2.14	0.46
3:F:103:LEU:C	3:F:111:ILE:HD11	2.34	0.46
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.61	0.46
2:B:335:ARG:HG3	2:B:335:ARG:NH1	2.30	0.46
1:D:61:ASP:N	1:D:62:GLU:OE2	2.47	0.46
1:D:215:ASP:O	1:D:221:ARG:NH1	2.49	0.46
1:D:495:TYR:O	1:D:499:MSE:HG3	2.14	0.46
2:E:61:ALA:O	2:E:63:LEU:N	2.48	0.46
2:B:186:LEU:HB3	2:B:190:ILE:CD1	2.45	0.46
2:B:329:HIS:HD2	2:B:332:VAL:HG23	1.80	0.46
3:C:97:VAL:HG13	3:C:98:THR:H	1.79	0.46
1:D:182:ARG:HG3	1:D:182:ARG:NH1	2.29	0.46
3:F:106:ARG:HG3	3:F:107:TYR:N	2.30	0.46
1:A:80:VAL:HG22	1:A:80:VAL:O	2.16	0.46
2:B:83:PRO:HD3	2:B:148:TYR:CE1	2.50	0.46
3:C:59:HIS:HE1	3:C:118:HIS:CD2	2.34	0.46
3:C:174:ILE:HD11	3:C:194:PRO:HB2	1.98	0.46
1:D:349:ILE:HD11	1:D:368:LEU:HD12	1.97	0.46
1:D:384:ILE:CG2	1:D:385:ILE:N	2.78	0.46
1:D:388:LEU:HA	1:D:391:VAL:HG22	1.97	0.46
2:E:45:PHE:CB	2:E:59:LYS:HD2	2.46	0.46
2:E:97:LEU:HD22	2:E:162:ASP:HB3	1.97	0.46
2:E:145:ALA:O	2:E:146:LYS:C	2.54	0.46
3:F:236:LEU:HD11	3:F:257:VAL:CG1	2.45	0.46
3:F:265:TYR:HD2	3:F:266:CYS:H	1.63	0.46
1:A:22:ASN:O	1:A:23:GLU:HB2	2.16	0.46
1:A:79:LEU:H	1:A:79:LEU:CD1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB3	1:A:183:ARG:NH1	2.31	0.46
1:A:182:ARG:HG3	1:A:182:ARG:NH1	2.31	0.46
1:A:222:LEU:HD23	1:A:223:LEU:N	2.30	0.46
1:A:476:GLU:CD	1:A:476:GLU:H	2.18	0.46
2:B:63:LEU:C	2:B:65:GLU:N	2.68	0.46
2:B:215:LEU:HD13	2:B:257:LEU:HA	1.97	0.46
3:C:50:CYS:HB2	3:C:51:PRO:CA	2.43	0.46
1:D:388:LEU:HA	1:D:391:VAL:CG2	2.46	0.46
1:D:482:ILE:C	1:D:484:PRO:HD2	2.35	0.46
1:D:495:TYR:CD2	1:D:533:VAL:HG11	2.50	0.46
2:E:65:GLU:C	2:E:67:VAL:N	2.67	0.46
2:E:133:ARG:HA	2:E:136:GLU:OE2	2.15	0.46
3:F:76:PRO:HB3	3:F:107:TYR:CG	2.51	0.46
3:F:171:SER:HB2	3:F:197:ASP:CB	2.45	0.46
1:A:316:ASP:O	1:A:317:CYS:HB3	2.15	0.46
1:A:470:VAL:HG11	1:A:511:VAL:CG2	2.45	0.46
1:D:338:ASN:HD21	1:D:340:HIS:HB2	1.81	0.46
1:D:579:ALA:O	1:D:582:ALA:HB3	2.16	0.46
1:D:580:GLN:C	1:D:582:ALA:H	2.19	0.46
3:F:43:SER:HG	3:F:45:VAL:C	2.19	0.46
3:F:158:LEU:CD2	3:F:161:GLY:HA2	2.45	0.46
1:A:141:PHE:HE2	2:B:199:TYR:CD2	2.34	0.46
1:A:211:ASN:N	1:A:211:ASN:ND2	2.62	0.46
1:A:229:VAL:O	1:A:233:GLN:HG3	2.16	0.46
1:A:339:GLN:HE21	1:A:377:CYS:HB2	1.79	0.46
1:A:522:LEU:N	1:A:523:PRO:CD	2.79	0.46
2:B:121:TRP:O	2:B:123:HIS:N	2.48	0.46
2:B:186:LEU:HB3	2:B:190:ILE:HD12	1.97	0.46
3:C:36:LYS:O	3:C:37:GLU:C	2.53	0.46
3:C:141:ASN:O	3:C:145:TYR:CD1	2.68	0.46
3:C:258:THR:C	3:C:259:ILE:HG13	2.35	0.46
3:C:272:GLN:OE1	3:C:288:GLN:NE2	2.48	0.46
1:D:253:GLU:O	1:D:254:ASP:C	2.54	0.46
1:D:504:CYS:HB3	1:D:508:LEU:HD23	1.96	0.46
3:F:162:GLN:HB3	3:F:235:THR:HG21	1.98	0.46
1:A:388:LEU:C	1:A:390:CYS:N	2.67	0.46
1:A:399:GLN:HE21	1:A:399:GLN:C	2.19	0.46
1:A:564:LEU:O	1:A:564:LEU:CD2	2.60	0.46
1:D:277:GLU:C	1:D:279:THR:H	2.19	0.46
2:E:107:GLU:H	2:E:107:GLU:HG2	1.55	0.46
2:B:313:ILE:CG2	2:B:317:LEU:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:ASN:HD21	1:D:543:SER:CB	2.29	0.46
2:E:35:LYS:O	2:E:37:ARG:N	2.48	0.46
2:E:137:SER:O	2:E:140:PHE:HD1	1.99	0.46
3:F:12:GLN:HE22	3:F:16:GLN:HB2	1.81	0.46
1:A:67:LEU:HD11	1:A:107:LYS:HG3	1.97	0.46
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.80	0.46
2:B:313:ILE:HG22	2:B:314:MSE:N	2.31	0.46
2:B:313:ILE:HG22	2:B:317:LEU:HB2	1.98	0.46
3:C:12:GLN:O	3:C:12:GLN:NE2	2.49	0.46
3:C:183:LEU:HD21	3:C:194:PRO:HG3	1.97	0.46
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.97	0.46
1:D:126:ALA:C	1:D:127:HIS:HD2	2.19	0.46
1:D:179:PRO:O	1:D:180:MSE:C	2.53	0.46
1:D:326:ILE:HG22	1:D:327:LEU:N	2.31	0.46
1:D:378:PRO:O	1:D:379:GLU:C	2.54	0.46
2:E:330:PHE:CD1	2:E:331:GLN:N	2.84	0.46
2:B:237:LEU:HD12	2:B:241:LEU:HD12	1.98	0.45
2:B:305:ILE:HD12	2:B:310:PHE:N	2.31	0.45
3:C:76:PRO:HB3	3:C:107:TYR:CG	2.51	0.45
1:D:455:VAL:O	1:D:455:VAL:HG13	2.16	0.45
1:D:525:VAL:HG11	1:D:544:LEU:CD2	2.46	0.45
3:F:118:HIS:C	3:F:120:SER:H	2.20	0.45
3:F:166:LEU:HD23	3:F:239:ARG:HB3	1.97	0.45
1:A:528:MSE:C	1:A:530:GLY:N	2.65	0.45
2:B:257:LEU:O	2:B:260:CYS:N	2.49	0.45
2:B:407:LEU:HD23	2:B:407:LEU:O	2.16	0.45
3:C:67:GLU:HA	3:C:70:ARG:NH1	2.31	0.45
1:D:146:SER:O	1:D:147:ALA:C	2.54	0.45
1:D:401:SER:HA	1:D:405:LEU:HB2	1.98	0.45
1:D:405:LEU:HD13	1:D:409:VAL:CG2	2.46	0.45
2:E:242:LEU:HD13	2:E:278:ALA:HB2	1.96	0.45
3:F:103:LEU:CB	3:F:111:ILE:HD13	2.46	0.45
3:F:115:ARG:HG3	3:F:119:GLU:HB2	1.98	0.45
1:A:77:THR:HA	1:A:86:VAL:HG23	1.97	0.45
1:A:395:ILE:HD11	1:A:400:LEU:HA	1.97	0.45
1:A:528:MSE:O	1:A:530:GLY:N	2.49	0.45
2:B:97:LEU:HD22	2:B:162:ASP:CB	2.47	0.45
2:B:184:LEU:HA	2:B:187:ARG:HG3	1.97	0.45
3:C:119:GLU:HB3	3:C:150:PHE:HB3	1.98	0.45
1:D:348:VAL:CG2	1:D:349:ILE:N	2.78	0.45
1:D:370:LEU:HD13	1:D:370:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:TYR:CZ	2:E:75:ASN:ND2	2.85	0.45
2:E:103:PRO:HG3	2:E:108:PHE:CD2	2.51	0.45
1:A:390:CYS:O	1:A:391:VAL:C	2.54	0.45
1:A:400:LEU:HD12	1:A:404:LEU:HD23	1.98	0.45
1:A:408:ILE:HA	1:A:411:LEU:HD23	1.98	0.45
2:B:67:VAL:C	2:B:69:TYR:N	2.70	0.45
2:B:164:GLU:HB2	2:B:168:GLU:HB2	1.99	0.45
2:B:167:ARG:O	2:B:168:GLU:C	2.54	0.45
2:B:183:PHE:HB2	2:B:186:LEU:HD22	1.97	0.45
2:B:265:LEU:HD21	2:B:272:THR:HA	1.98	0.45
3:C:165:CYS:HA	3:C:238:SER:O	2.16	0.45
3:C:265:TYR:HB3	3:C:269:CYS:HB2	1.98	0.45
1:D:42:LEU:HD23	1:D:47:THR:HA	1.99	0.45
1:D:410:GLU:C	1:D:412:ALA:N	2.69	0.45
1:D:495:TYR:CD2	1:D:499:MSE:HE2	2.51	0.45
2:E:273:GLU:OE1	2:E:312:LYS:HD3	2.16	0.45
2:E:294:PHE:O	2:E:295:LEU:C	2.53	0.45
1:A:490:SER:HB2	1:A:528:MSE:HE3	1.99	0.45
1:A:552:ASP:O	1:A:554:SER:N	2.50	0.45
2:B:65:GLU:O	2:B:67:VAL:N	2.49	0.45
2:B:124:LEU:C	2:B:126:LEU:N	2.70	0.45
2:B:298:LEU:HA	2:B:298:LEU:HD12	1.45	0.45
3:C:294:ARG:HG2	3:C:294:ARG:NH1	2.32	0.45
1:D:295:GLU:O	1:D:296:ALA:C	2.54	0.45
1:D:327:LEU:O	1:D:327:LEU:HG	2.16	0.45
2:E:126:LEU:C	2:E:128:TYR:N	2.70	0.45
3:F:95:GLU:OE1	3:F:136:LYS:NZ	2.49	0.45
3:F:176:THR:HG23	3:F:179:HIS:CD2	2.49	0.45
3:F:252:HIS:O	3:F:253:ASP:O	2.34	0.45
1:A:12:PRO:O	1:A:13:ILE:C	2.55	0.45
1:A:52:LEU:HD12	1:A:88:CYS:HB3	1.98	0.45
1:A:88:CYS:C	1:A:90:LEU:N	2.70	0.45
1:A:179:PRO:CB	1:A:183:ARG:HH12	2.29	0.45
1:A:343:SER:CB	1:A:380:VAL:HG22	2.46	0.45
1:A:365:LEU:C	1:A:367:PRO:HD2	2.37	0.45
2:B:242:LEU:HD11	2:B:275:VAL:HA	1.99	0.45
3:C:120:SER:O	3:C:124:THR:HG23	2.15	0.45
1:D:560:VAL:O	1:D:561:LYS:C	2.55	0.45
2:E:118:GLU:HG3	2:E:119:ALA:O	2.16	0.45
3:F:24:SER:OG	3:F:27:GLN:HG3	2.17	0.45
1:A:237:GLN:CD	1:A:278:ILE:HD11	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:N	1:A:328:PRO:CD	2.78	0.45
1:A:400:LEU:HD12	1:A:404:LEU:CD2	2.45	0.45
2:B:182:LYS:HB2	2:B:183:PHE:CD1	2.52	0.45
3:C:137:TYR:CG	3:C:142:VAL:HG21	2.51	0.45
1:D:22:ASN:HD21	1:D:24:ASP:HB3	1.82	0.45
1:D:35:LEU:O	1:D:76:PHE:HZ	1.99	0.45
1:D:262:MSE:O	1:D:265:ASP:N	2.49	0.45
2:E:402:PHE:O	2:E:403:LYS:C	2.55	0.45
3:F:12:GLN:O	3:F:15:GLU:HB3	2.16	0.45
3:F:194:PRO:CG	3:F:195:MET:H	2.30	0.45
1:A:384:ILE:HG22	1:A:385:ILE:N	2.31	0.45
1:A:581:GLU:O	1:A:581:GLU:HG3	2.17	0.45
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.51	0.45
3:C:203:PRO:HB3	3:C:220:PHE:HE1	1.82	0.45
1:D:38:ILE:HD12	1:D:38:ILE:N	2.32	0.45
1:D:257:TRP:CZ2	2:E:99:PRO:HD3	2.52	0.45
1:D:405:LEU:HD13	1:D:409:VAL:HG23	1.99	0.45
2:E:44:ASP:O	2:E:45:PHE:C	2.55	0.45
2:E:85:VAL:HG11	2:E:134:PHE:CE1	2.52	0.45
2:E:121:TRP:CE2	2:E:167:ARG:NH1	2.85	0.45
3:F:14:ILE:O	3:F:18:ASN:HB2	2.17	0.45
3:F:134:LEU:HD12	3:F:134:LEU:N	2.32	0.45
2:B:152:LYS:O	2:B:156:GLN:HG3	2.17	0.45
2:B:237:LEU:HA	2:B:241:LEU:HB2	1.98	0.45
1:D:120:SER:O	1:D:123:ASP:N	2.50	0.45
1:D:211:ASN:N	1:D:211:ASN:ND2	2.65	0.45
1:D:287:PHE:CD2	1:D:291:MSE:HE2	2.52	0.45
1:D:451:LEU:HD12	1:D:451:LEU:HA	1.64	0.45
1:D:525:VAL:CG1	1:D:544:LEU:HD21	2.47	0.45
2:E:162:ASP:O	2:E:163:SER:CB	2.62	0.45
2:E:182:LYS:HB2	2:E:183:PHE:CE1	2.51	0.45
1:A:197:GLU:O	1:A:198:LEU:C	2.55	0.45
1:A:333:LEU:O	1:A:335:SER:N	2.49	0.45
1:A:369:PHE:CD2	1:A:369:PHE:N	2.83	0.45
2:B:71:THR:HG21	2:B:133:ARG:NH1	2.31	0.45
3:C:93:SER:O	3:C:94:VAL:C	2.55	0.45
3:C:121:ARG:HG2	3:C:147:THR:HB	1.98	0.45
3:C:203:PRO:CA	3:C:220:PHE:CE1	2.99	0.45
1:D:34:LYS:C	1:D:36:SER:H	2.20	0.45
1:D:90:LEU:HB2	1:D:91:PRO:CD	2.45	0.45
2:E:250:LEU:C	2:E:252:VAL:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:GLN:NE2	3:F:64:ASP:OD2	2.50	0.45
1:A:44:VAL:CG2	1:A:45:GLU:N	2.79	0.44
1:A:221:ARG:O	1:A:224:ALA:HB3	2.17	0.44
1:A:297:GLU:O	1:A:298:VAL:C	2.56	0.44
1:A:384:ILE:CG2	1:A:385:ILE:N	2.80	0.44
1:A:515:ASP:O	1:A:517:THR:N	2.50	0.44
2:B:314:MSE:O	2:B:315:GLU:C	2.56	0.44
3:C:166:LEU:HD11	3:C:169:GLY:CA	2.47	0.44
1:D:146:SER:O	1:D:148:CYS:N	2.49	0.44
1:D:205:ILE:HG22	1:D:206:ILE:N	2.32	0.44
1:D:307:LYS:O	1:D:311:GLU:HG3	2.17	0.44
2:E:43:PHE:HA	2:E:88:MSE:HG2	1.98	0.44
2:E:93:MSE:HE2	2:E:128:TYR:CZ	2.52	0.44
2:E:350:SER:C	2:E:352:ASN:N	2.71	0.44
1:A:115:ILE:O	1:A:115:ILE:HG13	2.14	0.44
1:A:229:VAL:HG22	1:A:270:LEU:CD2	2.46	0.44
1:A:588:LEU:O	1:A:589:ALA:CB	2.64	0.44
2:B:71:THR:O	2:B:73:ASN:N	2.42	0.44
2:B:209:ASN:N	2:B:209:ASN:ND2	2.65	0.44
2:B:244:LEU:HD22	2:B:253:TYR:HE1	1.78	0.44
3:C:43:SER:OG	3:C:45:VAL:C	2.56	0.44
3:C:118:HIS:C	3:C:120:SER:H	2.20	0.44
1:D:44:VAL:HG13	1:D:45:GLU:H	1.82	0.44
1:D:499:MSE:O	1:D:502:LEU:N	2.50	0.44
2:E:31:LEU:C	2:E:33:ILE:H	2.19	0.44
3:F:119:GLU:HG2	3:F:153:LEU:HD12	1.99	0.44
3:F:293:PRO:O	3:F:293:PRO:HG2	2.17	0.44
1:A:11:TYR:O	1:A:12:PRO:C	2.55	0.44
1:A:271:GLN:HA	1:A:283:LEU:CD1	2.48	0.44
1:A:288:GLN:O	1:A:291:MSE:N	2.50	0.44
1:A:560:VAL:O	1:A:563:ILE:HG22	2.17	0.44
2:B:121:TRP:C	2:B:123:HIS:N	2.69	0.44
2:B:250:LEU:C	2:B:252:VAL:N	2.71	0.44
2:B:315:GLU:HB2	2:B:316:PRO:CD	2.47	0.44
3:C:118:HIS:CE1	3:C:123:ILE:HG21	2.51	0.44
3:C:144:LYS:O	3:C:145:TYR:C	2.56	0.44
1:D:218:ASP:HB3	1:D:221:ARG:NH2	2.33	0.44
1:D:439:PHE:CE1	1:D:443:LEU:HB3	2.52	0.44
2:E:289:PRO:O	2:E:293:MSE:HG3	2.17	0.44
2:E:344:TYR:HE1	2:E:348:LEU:HD11	1.83	0.44
3:F:12:GLN:NE2	3:F:16:GLN:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:VAL:HG22	1:A:440:ASP:OD2	2.17	0.44
3:C:185:ARG:HG2	3:C:185:ARG:HH11	1.83	0.44
2:E:182:LYS:HB2	2:E:183:PHE:CD1	2.52	0.44
3:F:156:THR:HG22	3:F:166:LEU:HB3	1.98	0.44
2:B:93:MSE:HA	2:B:93:MSE:HE3	1.99	0.44
2:B:121:TRP:HB3	2:B:122:PRO:CD	2.48	0.44
2:B:242:LEU:HA	2:B:242:LEU:HD23	1.62	0.44
2:B:248:LYS:CD	2:B:290:LYS:HZ2	2.29	0.44
3:C:123:ILE:HG23	3:C:127:TYR:CD2	2.29	0.44
1:D:39:ALA:HB3	1:D:79:LEU:HD23	1.99	0.44
1:D:123:ASP:O	1:D:124:LEU:C	2.54	0.44
1:D:206:ILE:O	1:D:209:PHE:HB3	2.17	0.44
1:D:497:HIS:O	1:D:500:THR:HB	2.18	0.44
3:F:115:ARG:HB2	3:F:153:LEU:HB2	1.98	0.44
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.33	0.44
2:B:365:TYR:HD2	2:B:402:PHE:HE2	1.66	0.44
2:B:397:ASP:O	2:B:400:GLN:HB3	2.18	0.44
1:D:100:GLU:O	1:D:101:GLU:C	2.55	0.44
1:D:587:SER:O	1:D:588:LEU:HD23	2.18	0.44
2:E:247:VAL:HG12	2:E:248:LYS:N	2.33	0.44
3:F:7:THR:O	3:F:7:THR:HG22	2.18	0.44
3:F:87:VAL:HG23	3:F:88:ASP:OD2	2.17	0.44
3:F:199:LEU:N	3:F:199:LEU:CD1	2.80	0.44
3:F:239:ARG:HD3	3:F:240:ALA:N	2.33	0.44
1:A:61:ASP:N	1:A:62:GLU:OE2	2.50	0.44
1:A:450:TRP:HB3	1:A:462:ALA:HB2	2.00	0.44
1:A:498:ARG:NH2	3:C:280:ASP:OD1	2.44	0.44
1:A:506:ASN:HD21	1:A:543:SER:HA	1.82	0.44
2:B:302:LEU:HA	2:B:305:ILE:HB	1.99	0.44
1:D:80:VAL:HG21	1:D:88:CYS:HB2	1.99	0.44
2:E:121:TRP:H	2:E:122:PRO:HD2	1.82	0.44
2:E:143:ASN:C	2:E:145:ALA:H	2.18	0.44
2:E:236:PHE:CE2	2:E:241:LEU:HG	2.52	0.44
1:A:277:GLU:O	1:A:280:LYS:N	2.51	0.44
2:B:85:VAL:HG13	2:B:130:PHE:CZ	2.52	0.44
2:B:97:LEU:HD22	2:B:162:ASP:HB3	1.98	0.44
2:B:117:LEU:HA	2:B:164:GLU:OE1	2.18	0.44
3:C:12:GLN:NE2	3:C:16:GLN:HB2	2.33	0.44
1:D:36:SER:C	1:D:38:ILE:H	2.22	0.44
1:D:213:ALA:O	1:D:221:ARG:HG2	2.17	0.44
1:D:265:ASP:O	1:D:305:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LEU:N	1:D:406:PRO:CD	2.81	0.44
1:D:509:SER:OG	1:D:547:ILE:HG22	2.17	0.44
1:D:567:LEU:C	1:D:569:GLN:N	2.70	0.44
2:E:35:LYS:C	2:E:37:ARG:N	2.71	0.44
2:E:94:PHE:CD2	2:E:94:PHE:N	2.84	0.44
2:E:186:LEU:O	2:E:190:ILE:CD1	2.65	0.44
2:E:382:ASN:OD1	2:E:386:LEU:CD1	2.66	0.44
1:A:261:TYR:C	1:A:261:TYR:CD2	2.91	0.44
2:B:73:ASN:C	2:B:75:ASN:N	2.71	0.44
2:B:236:PHE:C	2:B:236:PHE:CD2	2.91	0.44
2:B:302:LEU:HA	2:B:302:LEU:HD23	1.85	0.44
3:C:190:PRO:HD3	3:C:195:MET:CE	2.48	0.44
1:D:221:ARG:NE	1:D:254:ASP:OD2	2.51	0.44
1:D:381:ARG:HH12	1:D:414:ASP:CG	2.21	0.44
1:D:448:MSE:CE	1:D:466:LEU:HD21	2.47	0.44
2:E:124:LEU:O	2:E:125:GLN:C	2.55	0.44
2:E:313:ILE:N	2:E:313:ILE:CD1	2.77	0.44
1:A:24:ASP:OD2	1:A:24:ASP:C	2.56	0.43
2:B:326:SER:OG	2:B:363:SER:HB3	2.18	0.43
2:B:373:ASN:O	2:B:375:THR:N	2.47	0.43
3:C:51:PRO:HB3	3:C:279:ASP:O	2.18	0.43
3:C:68:LEU:O	3:C:71:ILE:HB	2.18	0.43
1:A:169:TYR:HA	1:A:172:ASN:HD22	1.83	0.43
1:A:277:GLU:C	1:A:279:THR:H	2.21	0.43
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.96	0.43
1:A:502:LEU:HD21	1:A:540:VAL:HG22	2.00	0.43
1:D:438:PHE:CD1	1:D:438:PHE:O	2.71	0.43
2:E:67:VAL:C	2:E:69:TYR:N	2.71	0.43
2:E:85:VAL:HG13	2:E:130:PHE:CE2	2.53	0.43
3:F:81:LEU:HD23	3:F:81:LEU:O	2.18	0.43
3:F:118:HIS:ND1	3:F:123:ILE:CG2	2.80	0.43
1:A:120:SER:O	1:A:121:PRO:C	2.56	0.43
2:B:287:HIS:O	2:B:288:SER:C	2.56	0.43
3:C:125:GLN:HA	3:C:130:TYR:HB2	1.99	0.43
1:D:475:LYS:HB2	1:D:516:ILE:CD1	2.47	0.43
1:D:483:ILE:N	1:D:484:PRO:CD	2.81	0.43
2:E:245:HIS:HD1	2:E:245:HIS:H	1.66	0.43
2:E:283:TRP:HA	2:E:284:PRO:HD3	1.76	0.43
3:F:43:SER:OG	3:F:44:ASN:N	2.50	0.43
3:F:48:VAL:O	3:F:159:VAL:HA	2.18	0.43
1:A:250:GLN:NE2	1:A:250:GLN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LEU:HD11	2:B:317:LEU:HA	2.01	0.43
1:D:11:TYR:O	1:D:12:PRO:C	2.56	0.43
1:D:40:LEU:C	1:D:42:LEU:H	2.22	0.43
1:D:500:THR:O	1:D:503:PHE:HB2	2.18	0.43
1:A:27:LEU:O	1:A:28:ARG:C	2.56	0.43
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.83	0.43
1:A:322:ILE:CD1	1:A:355:ILE:HG21	2.49	0.43
1:A:570:ASP:OD1	1:A:575:VAL:HG11	2.17	0.43
2:B:79:GLU:O	2:B:80:PRO:C	2.55	0.43
2:B:89:PHE:CZ	2:B:93:MSE:HG3	2.54	0.43
2:B:138:PRO:O	2:B:140:PHE:CD1	2.72	0.43
2:B:202:ILE:HD11	2:B:244:LEU:CG	2.41	0.43
3:C:76:PRO:HG3	3:C:107:TYR:CE1	2.53	0.43
3:C:117:ASN:H	3:C:167:HIS:CD2	2.36	0.43
3:C:187:GLN:HE21	3:C:187:GLN:HB2	1.66	0.43
1:D:189:LEU:HD11	1:D:205:ILE:HD12	1.99	0.43
2:E:43:PHE:C	2:E:45:PHE:N	2.70	0.43
2:E:78:THR:O	2:E:78:THR:HG22	2.17	0.43
2:E:222:ILE:HD13	2:E:264:PHE:HD1	1.83	0.43
2:E:242:LEU:HD11	2:E:275:VAL:HA	2.00	0.43
2:E:387:PHE:HD1	2:E:387:PHE:HA	1.68	0.43
3:F:51:PRO:HB3	3:F:279:ASP:C	2.38	0.43
3:F:123:ILE:N	3:F:123:ILE:HD12	2.34	0.43
1:A:180:MSE:CE	1:A:180:MSE:H	2.29	0.43
1:A:206:ILE:HB	1:A:207:PRO:HD3	2.00	0.43
2:B:254:HIS:N	2:B:255:PRO:HD2	2.33	0.43
2:B:271:LEU:O	2:B:274:PRO:HD2	2.19	0.43
1:D:40:LEU:O	1:D:42:LEU:N	2.51	0.43
1:D:270:LEU:O	1:D:271:GLN:C	2.56	0.43
1:D:408:ILE:HD13	1:D:426:TYR:CE2	2.48	0.43
1:D:506:ASN:ND2	1:D:543:SER:HA	2.34	0.43
2:E:313:ILE:HG22	2:E:317:LEU:CB	2.46	0.43
1:A:78:THR:HB	1:A:79:LEU:HD12	2.00	0.43
1:A:136:ALA:C	1:A:138:GLY:H	2.22	0.43
1:A:155:TYR:CE1	1:A:167:ARG:HG2	2.54	0.43
1:A:253:GLU:O	1:A:254:ASP:C	2.56	0.43
1:A:535:ASN:HA	1:A:538:PHE:CD2	2.50	0.43
2:B:176:LEU:HG	2:B:176:LEU:O	2.19	0.43
2:B:332:VAL:O	2:B:335:ARG:N	2.52	0.43
1:D:141:PHE:CD1	1:D:141:PHE:C	2.92	0.43
1:D:142:THR:OG1	1:D:143:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:316:PRO:CG	2:E:317:LEU:N	2.82	0.43
2:E:361:PHE:C	2:E:363:SER:H	2.22	0.43
3:F:65:LEU:O	3:F:66:MET:C	2.56	0.43
1:A:24:ASP:OD2	1:A:26:GLN:HB3	2.19	0.43
2:B:88:MSE:HE1	2:B:127:VAL:HG13	2.00	0.43
3:C:24:SER:O	3:C:27:GLN:HB2	2.18	0.43
3:C:48:VAL:O	3:C:159:VAL:HA	2.18	0.43
3:C:274:ALA:CB	3:C:288:GLN:HA	2.46	0.43
1:D:578:PHE:O	1:D:582:ALA:HB2	2.18	0.43
2:E:63:LEU:C	2:E:65:GLU:N	2.72	0.43
2:E:256:GLN:CD	2:E:256:GLN:N	2.72	0.43
2:E:335:ARG:HG3	2:E:335:ARG:O	2.18	0.43
3:F:131:ASP:O	3:F:132:GLU:C	2.57	0.43
1:A:9:SER:OG	1:A:10:LEU:N	2.51	0.43
1:A:179:PRO:HB2	1:A:183:ARG:HH12	1.84	0.43
2:B:254:HIS:CD2	2:B:293:MSE:HB3	2.54	0.43
2:B:361:PHE:N	2:B:362:PRO:HD2	2.33	0.43
3:C:162:GLN:HB3	3:C:235:THR:HG21	2.00	0.43
1:D:145:THR:CG2	1:D:146:SER:N	2.78	0.43
1:D:353:SER:HB3	1:D:394:VAL:HG21	2.01	0.43
1:D:515:ASP:O	1:D:516:ILE:C	2.57	0.43
1:D:522:LEU:O	1:D:522:LEU:HD12	2.19	0.43
3:F:17:LEU:CD1	3:F:99:LEU:HA	2.48	0.43
1:A:499:MSE:O	1:A:500:THR:C	2.58	0.43
2:B:35:LYS:O	2:B:38:GLN:N	2.52	0.43
1:D:565:GLU:C	1:D:567:LEU:H	2.22	0.43
2:E:222:ILE:O	2:E:224:GLY:N	2.52	0.43
2:E:242:LEU:HA	2:E:242:LEU:HD23	1.75	0.43
2:E:302:LEU:HD11	2:E:317:LEU:HD21	1.99	0.43
1:A:11:TYR:HD2	1:A:11:TYR:HA	1.69	0.42
1:A:317:CYS:O	1:A:321:VAL:HG13	2.19	0.42
1:D:506:ASN:HD21	1:D:543:SER:CA	2.32	0.42
2:E:393:LYS:HG2	2:E:397:ASP:OD2	2.18	0.42
1:A:506:ASN:HD21	1:A:543:SER:CA	2.32	0.42
2:B:145:ALA:O	2:B:146:LYS:C	2.58	0.42
2:B:402:PHE:O	2:B:403:LYS:C	2.56	0.42
3:C:17:LEU:O	3:C:20:CYS:N	2.42	0.42
3:C:279:ASP:OD1	3:C:283:LYS:N	2.51	0.42
1:D:179:PRO:O	1:D:182:ARG:N	2.52	0.42
1:D:350:MSE:HG3	1:D:387:ASN:HB3	2.01	0.42
1:D:507:VAL:HA	1:D:510:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:SER:CB	1:D:547:ILE:HG22	2.50	0.42
2:E:67:VAL:C	2:E:69:TYR:H	2.22	0.42
2:E:124:LEU:C	2:E:126:LEU:N	2.72	0.42
1:A:38:ILE:HD12	1:A:38:ILE:N	2.34	0.42
1:A:131:LEU:HD23	1:A:131:LEU:C	2.39	0.42
1:A:438:PHE:O	1:A:438:PHE:CD1	2.66	0.42
1:A:517:THR:HG23	1:A:521:MSE:HE3	2.00	0.42
1:A:538:PHE:HB3	1:A:575:VAL:HA	2.01	0.42
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.82	0.42
3:C:85:ASP:OD1	3:C:117:ASN:OD1	2.37	0.42
1:D:90:LEU:HD23	1:D:90:LEU:HA	1.76	0.42
1:D:260:ARG:NH1	1:D:260:ARG:CG	2.82	0.42
1:D:275:GLY:HA3	1:D:278:ILE:HD13	2.01	0.42
2:E:76:VAL:O	2:E:76:VAL:HG12	2.19	0.42
2:E:314:MSE:O	2:E:315:GLU:C	2.58	0.42
3:F:28:VAL:O	3:F:29:LYS:C	2.57	0.42
3:F:68:LEU:O	3:F:71:ILE:N	2.47	0.42
3:F:240:ALA:HA	3:F:258:THR:CG2	2.38	0.42
1:A:333:LEU:O	1:A:334:VAL:C	2.57	0.42
1:A:388:LEU:HA	1:A:391:VAL:HG22	2.01	0.42
1:A:482:ILE:O	1:A:484:PRO:N	2.53	0.42
2:B:63:LEU:O	2:B:65:GLU:N	2.53	0.42
2:B:97:LEU:HD12	2:B:97:LEU:N	2.32	0.42
2:B:133:ARG:HA	2:B:136:GLU:CD	2.40	0.42
1:D:85:TYR:O	1:D:86:VAL:C	2.57	0.42
1:D:141:PHE:HA	1:D:144:ARG:HD3	2.01	0.42
1:D:205:ILE:HA	1:D:205:ILE:HD13	1.79	0.42
1:D:222:LEU:HG	1:D:223:LEU:HD23	2.00	0.42
1:D:537:ARG:HG3	1:D:537:ARG:HH11	1.84	0.42
2:E:176:LEU:O	2:E:176:LEU:CG	2.64	0.42
2:E:202:ILE:HG22	2:E:203:TYR:CD2	2.55	0.42
1:A:326:ILE:N	1:A:326:ILE:CD1	2.82	0.42
2:B:85:VAL:O	2:B:88:MSE:HB3	2.19	0.42
2:B:183:PHE:C	2:B:185:GLY:H	2.22	0.42
2:B:254:HIS:CG	2:B:293:MSE:HE2	2.55	0.42
2:B:306:GLU:O	2:B:309:GLU:N	2.47	0.42
3:C:97:VAL:CG1	3:C:98:THR:N	2.83	0.42
3:C:124:THR:HB	3:C:129:PHE:HB3	2.00	0.42
3:C:125:GLN:HA	3:C:130:TYR:CB	2.50	0.42
3:C:155:LEU:CD1	3:C:195:MET:HG3	2.50	0.42
1:D:65:VAL:O	1:D:68:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:166:LEU:O	3:F:166:LEU:HD23	2.20	0.42
3:F:187:GLN:HE21	3:F:187:GLN:HB2	1.68	0.42
3:F:204:ASP:HB2	3:F:219:THR:HB	2.01	0.42
3:F:263:PRO:N	3:F:273:ALA:HB2	2.35	0.42
1:A:560:VAL:O	1:A:561:LYS:C	2.56	0.42
2:B:287:HIS:O	2:B:287:HIS:ND1	2.53	0.42
2:B:329:HIS:CD2	2:B:332:VAL:HG23	2.55	0.42
2:B:337:LEU:HD12	2:B:337:LEU:N	2.34	0.42
2:B:392:GLN:O	2:B:393:LYS:C	2.58	0.42
3:C:274:ALA:HB1	3:C:287:LEU:O	2.20	0.42
1:D:180:MSE:HE2	1:D:183:ARG:HH22	1.84	0.42
2:E:69:TYR:O	2:E:74:ARG:HB2	2.19	0.42
2:E:222:ILE:HD13	2:E:264:PHE:CD1	2.54	0.42
2:E:288:SER:O	2:E:289:PRO:C	2.57	0.42
2:E:313:ILE:H	2:E:313:ILE:CD1	2.27	0.42
1:A:22:ASN:HD22	1:A:24:ASP:HB3	1.80	0.42
1:A:40:LEU:C	1:A:42:LEU:N	2.73	0.42
1:A:161:ALA:O	1:A:165:GLU:HG3	2.18	0.42
1:A:275:GLY:HA3	1:A:278:ILE:HD13	2.00	0.42
1:A:500:THR:O	1:A:503:PHE:HB2	2.19	0.42
1:A:552:ASP:OD1	1:A:552:ASP:O	2.38	0.42
2:B:71:THR:CG2	2:B:133:ARG:HH11	2.32	0.42
2:B:83:PRO:C	2:B:85:VAL:H	2.22	0.42
2:B:164:GLU:CB	2:B:168:GLU:CB	2.95	0.42
2:B:268:ASP:C	2:B:268:ASP:OD1	2.58	0.42
2:B:325:VAL:HG11	2:B:364:LEU:CD2	2.50	0.42
3:C:135:ARG:HG2	3:C:135:ARG:HH11	1.83	0.42
3:C:156:THR:HG22	3:C:166:LEU:HB3	2.02	0.42
1:D:587:SER:C	1:D:588:LEU:HD23	2.40	0.42
2:E:61:ALA:C	2:E:63:LEU:N	2.72	0.42
2:E:119:ALA:O	2:E:120:ALA:CB	2.68	0.42
2:E:134:PHE:HE2	2:E:135:LEU:HD22	1.84	0.42
2:E:373:ASN:C	2:E:375:THR:N	2.71	0.42
3:F:131:ASP:O	3:F:134:LEU:N	2.53	0.42
4:G:6:FGA:HG3	4:G:7:DAM:HM1	1.79	0.42
1:A:85:TYR:O	1:A:86:VAL:C	2.58	0.42
1:A:178:THR:OG1	1:A:181:VAL:CG2	2.67	0.42
1:A:362:ILE:HD13	1:A:399:GLN:CG	2.39	0.42
1:A:368:LEU:O	1:A:371:ALA:HB3	2.19	0.42
2:B:157:LEU:HD11	2:B:172:LEU:HD23	2.02	0.42
3:C:61:GLN:HA	3:C:267:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PHE:O	1:D:80:VAL:HG12	2.19	0.42
1:D:572:ASP:OD2	3:F:110:ARG:NH2	2.52	0.42
2:E:132:LEU:O	2:E:134:PHE:N	2.52	0.42
3:F:17:LEU:HD12	3:F:99:LEU:HA	2.01	0.42
3:F:66:MET:O	3:F:69:PHE:HB2	2.19	0.42
1:A:343:SER:OG	1:A:379:GLU:HB3	2.19	0.42
2:B:276:VAL:HG11	2:B:313:ILE:HG21	2.02	0.42
2:B:295:LEU:HA	2:B:295:LEU:HD23	1.79	0.42
3:C:39:LEU:O	3:C:40:THR:C	2.58	0.42
3:C:71:ILE:CG2	3:C:72:GLY:N	2.83	0.42
1:D:197:GLU:O	1:D:201:VAL:HG23	2.19	0.42
2:E:72:HIS:C	2:E:74:ARG:N	2.71	0.42
3:F:164:PHE:HB2	3:F:234:LEU:HD13	2.01	0.42
3:F:185:ARG:HG2	3:F:185:ARG:HH11	1.85	0.42
1:A:20:LEU:HD23	1:A:31:SER:HB3	2.01	0.42
1:A:245:MSE:O	1:A:246:PRO:C	2.56	0.42
1:A:368:LEU:O	1:A:371:ALA:N	2.53	0.42
1:D:180:MSE:HE3	1:D:180:MSE:N	2.21	0.42
1:D:277:GLU:O	1:D:279:THR:N	2.53	0.42
1:D:567:LEU:C	1:D:569:GLN:H	2.22	0.42
2:E:134:PHE:O	2:E:136:GLU:N	2.53	0.42
3:F:54:VAL:HG21	3:F:276:MET:CE	2.50	0.42
1:A:257:TRP:CZ2	2:B:99:PRO:HD3	2.55	0.41
2:B:76:VAL:O	2:B:76:VAL:HG12	2.20	0.41
2:B:202:ILE:HG22	2:B:203:TYR:CG	2.55	0.41
1:D:44:VAL:O	1:D:46:ARG:N	2.53	0.41
1:D:105:ARG:O	1:D:109:VAL:HG23	2.20	0.41
1:D:334:VAL:O	1:D:334:VAL:HG12	2.20	0.41
2:E:368:SER:O	2:E:377:HIS:ND1	2.52	0.41
3:F:54:VAL:HB	3:F:276:MET:HB3	2.02	0.41
3:F:104:LYS:CA	3:F:111:ILE:HD11	2.50	0.41
4:H:2:LEU:H	4:H:7:DAM:C	2.33	0.41
1:A:40:LEU:C	1:A:42:LEU:H	2.23	0.41
1:A:90:LEU:HB2	1:A:91:PRO:CD	2.43	0.41
1:A:127:HIS:O	1:A:130:PRO:HD2	2.20	0.41
2:B:241:LEU:HD22	2:B:257:LEU:CD1	2.50	0.41
3:C:94:VAL:HB	3:C:95:GLU:OE1	2.20	0.41
3:C:134:LEU:O	3:C:136:LYS:N	2.54	0.41
3:C:203:PRO:HA	3:C:220:PHE:CD1	2.55	0.41
3:C:228:PHE:O	3:C:231:ALA:HB3	2.20	0.41
1:D:128:PHE:O	1:D:131:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:HG3	1:D:258:ARG:NH1	2.32	0.41
1:D:373:LEU:HD11	1:D:385:ILE:HD13	2.02	0.41
2:E:258:ALA:O	2:E:259:TYR:C	2.59	0.41
2:E:361:PHE:C	2:E:363:SER:N	2.73	0.41
2:E:375:THR:HG22	2:E:376:ILE:N	2.35	0.41
3:F:93:SER:O	3:F:94:VAL:C	2.58	0.41
3:F:107:TYR:HB3	3:F:110:ARG:HG3	2.02	0.41
1:A:151:PHE:O	1:A:153:VAL:N	2.54	0.41
1:A:295:GLU:O	1:A:296:ALA:C	2.58	0.41
2:B:69:TYR:CZ	2:B:75:ASN:ND2	2.87	0.41
3:C:59:HIS:CE1	3:C:85:ASP:HB3	2.55	0.41
1:D:343:SER:O	1:D:346:ALA:HB3	2.20	0.41
2:E:305:ILE:CG2	2:E:348:LEU:HD11	2.50	0.41
3:F:203:PRO:HB3	3:F:220:PHE:HE1	1.85	0.41
2:B:78:THR:O	2:B:78:THR:HG22	2.21	0.41
2:B:183:PHE:C	2:B:185:GLY:N	2.74	0.41
2:B:183:PHE:CB	2:B:186:LEU:HD22	2.51	0.41
2:B:350:SER:C	2:B:352:ASN:N	2.73	0.41
2:B:406:LYS:HD3	2:B:406:LYS:C	2.40	0.41
3:C:6:PHE:O	3:C:9:GLU:N	2.53	0.41
3:C:286:PHE:O	3:C:287:LEU:HD23	2.20	0.41
1:D:219:SER:HA	1:D:222:LEU:CD2	2.50	0.41
1:D:245:MSE:HE3	1:D:245:MSE:CA	2.50	0.41
2:E:132:LEU:C	2:E:134:PHE:N	2.71	0.41
2:E:184:LEU:HA	2:E:187:ARG:HG3	2.01	0.41
2:E:295:LEU:HA	2:E:295:LEU:HD23	1.77	0.41
3:F:99:LEU:O	3:F:100:LEU:C	2.57	0.41
3:F:172:PRO:C	3:F:174:ILE:H	2.23	0.41
3:F:211:ILE:HD12	3:F:212:SER:H	1.85	0.41
1:A:73:LEU:HB2	1:A:93:LEU:HD21	2.03	0.41
1:A:119:HIS:CD2	1:A:119:HIS:N	2.89	0.41
1:A:377:CYS:O	1:A:378:PRO:C	2.59	0.41
1:A:455:VAL:HG13	1:A:455:VAL:O	2.20	0.41
1:A:509:SER:N	1:A:521:MSE:HE1	2.36	0.41
2:B:357:LEU:HD12	2:B:361:PHE:CE1	2.56	0.41
1:D:378:PRO:O	1:D:381:ARG:N	2.53	0.41
1:D:515:ASP:O	1:D:518:THR:N	2.52	0.41
1:D:522:LEU:O	1:D:526:LEU:HG	2.20	0.41
2:E:121:TRP:CD1	2:E:167:ARG:NH1	2.89	0.41
3:F:76:PRO:HD3	3:F:107:TYR:CZ	2.55	0.41
3:F:121:ARG:N	3:F:188:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:169:GLY:HA3	3:F:220:PHE:HE2	1.85	0.41
3:F:276:MET:HE3	3:F:278:LEU:HD21	2.02	0.41
1:A:90:LEU:CB	1:A:91:PRO:CD	2.97	0.41
1:A:196:LEU:CD1	1:A:205:ILE:HD11	2.51	0.41
1:A:411:LEU:C	1:A:413:GLU:H	2.23	0.41
1:A:423:ILE:HD13	1:A:423:ILE:HA	1.81	0.41
2:B:83:PRO:C	2:B:85:VAL:N	2.74	0.41
2:B:316:PRO:HG2	2:B:317:LEU:N	2.36	0.41
2:B:365:TYR:CD2	2:B:402:PHE:HE2	2.37	0.41
2:B:387:PHE:HD1	2:B:387:PHE:HA	1.76	0.41
3:C:96:THR:O	3:C:99:LEU:HB3	2.20	0.41
3:C:100:LEU:HA	3:C:100:LEU:HD23	1.87	0.41
3:C:170:LEU:HB2	3:C:220:PHE:HD2	1.80	0.41
1:D:285:PRO:HA	1:D:288:GLN:OE1	2.20	0.41
1:D:475:LYS:HB2	1:D:516:ILE:HD11	2.01	0.41
1:D:482:ILE:C	1:D:484:PRO:CD	2.89	0.41
1:D:503:PHE:O	1:D:504:CYS:C	2.59	0.41
1:D:521:MSE:C	1:D:523:PRO:CD	2.89	0.41
2:E:145:ALA:O	2:E:148:TYR:N	2.31	0.41
2:E:313:ILE:C	2:E:316:PRO:HD2	2.40	0.41
1:A:205:ILE:HD13	1:A:208:MSE:HE3	2.03	0.41
1:A:426:TYR:CD1	1:A:426:TYR:O	2.73	0.41
2:B:124:LEU:O	2:B:127:VAL:N	2.54	0.41
2:B:134:PHE:CE2	2:B:135:LEU:HD22	2.56	0.41
2:B:285:LYS:HB2	2:B:285:LYS:HE3	1.87	0.41
3:C:118:HIS:ND1	3:C:123:ILE:CG2	2.83	0.41
1:D:52:LEU:CB	1:D:53:PRO:HD3	2.48	0.41
1:D:90:LEU:CB	1:D:91:PRO:HD3	2.47	0.41
1:D:398:ARG:HH11	1:D:398:ARG:CB	2.32	0.41
1:D:427:MSE:CE	1:D:430:LEU:HB2	2.50	0.41
1:D:563:ILE:O	1:D:563:ILE:HG12	2.20	0.41
2:E:184:LEU:HD23	2:E:187:ARG:CZ	2.51	0.41
2:E:346:MSE:CE	2:E:349:ILE:HD12	2.51	0.41
3:F:194:PRO:CG	3:F:195:MET:N	2.84	0.41
1:A:155:TYR:CE2	1:A:163:LYS:HD3	2.56	0.41
1:A:174:CYS:O	1:A:212:LEU:HD21	2.21	0.41
1:A:237:GLN:O	1:A:240:LEU:HB2	2.20	0.41
1:A:259:VAL:O	1:A:262:MSE:HB2	2.20	0.41
1:A:264:ALA:O	1:A:267:PHE:HB2	2.21	0.41
1:A:274:VAL:HG12	1:A:278:ILE:HB	2.02	0.41
1:A:400:LEU:CD1	1:A:404:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:VAL:O	2:B:87:HIS:C	2.58	0.41
2:B:271:LEU:O	2:B:274:PRO:HG2	2.21	0.41
3:C:68:LEU:HD23	3:C:69:PHE:N	2.35	0.41
3:C:153:LEU:HA	3:C:154:PRO:HD2	1.90	0.41
3:C:154:PRO:HA	3:C:185:ARG:NE	2.35	0.41
1:D:316:ASP:O	1:D:317:CYS:HB3	2.21	0.41
2:E:180:TYR:CE2	2:E:221:ILE:HG23	2.54	0.41
2:E:248:LYS:C	2:E:250:LEU:H	2.23	0.41
2:E:407:LEU:HD23	2:E:407:LEU:C	2.40	0.41
1:A:34:LYS:C	1:A:36:SER:H	2.24	0.41
1:A:424:ILE:HG12	1:A:450:TRP:CD2	2.55	0.41
2:B:68:GLU:HG3	2:B:68:GLU:H	1.72	0.41
2:B:109:ASP:HA	2:B:110:PRO:HD2	1.87	0.41
2:B:134:PHE:C	2:B:136:GLU:N	2.74	0.41
2:B:150:ASP:O	2:B:151:GLN:C	2.59	0.41
2:B:320:GLN:O	2:B:321:LEU:C	2.58	0.41
3:C:43:SER:OG	3:C:45:VAL:O	2.35	0.41
3:C:163:ILE:HG23	3:C:236:LEU:O	2.20	0.41
3:C:199:LEU:HD12	3:C:199:LEU:N	2.36	0.41
3:C:264:ASN:O	3:C:265:TYR:O	2.39	0.41
1:D:136:ALA:O	1:D:144:ARG:HG2	2.20	0.41
1:D:176:ASP:OD1	1:D:177:ASP:N	2.54	0.41
1:D:189:LEU:HD11	1:D:205:ILE:CD1	2.51	0.41
1:D:436:VAL:HB	1:D:473:PHE:CE1	2.55	0.41
1:D:564:LEU:O	1:D:564:LEU:CD2	2.67	0.41
2:E:75:ASN:OD1	2:E:78:THR:OG1	2.38	0.41
2:E:80:PRO:O	2:E:81:ILE:C	2.59	0.41
2:E:97:LEU:HD12	2:E:97:LEU:N	2.31	0.41
2:E:150:ASP:O	2:E:151:GLN:C	2.58	0.41
2:E:316:PRO:CG	2:E:317:LEU:H	2.32	0.41
2:E:401:GLN:O	2:E:404:ALA:HB3	2.21	0.41
3:F:204:ASP:N	3:F:220:PHE:O	2.51	0.41
3:F:244:VAL:HG21	3:F:248:TYR:CA	2.51	0.41
1:A:192:PHE:O	1:A:195:VAL:HG22	2.21	0.41
1:D:98:THR:O	1:D:99:VAL:C	2.58	0.41
1:D:270:LEU:C	1:D:274:VAL:HG23	2.41	0.41
2:E:63:LEU:O	2:E:67:VAL:HG23	2.21	0.41
2:E:159:GLU:O	2:E:161:PHE:N	2.53	0.41
1:A:67:LEU:HA	1:A:104:VAL:HG22	2.02	0.40
1:A:79:LEU:N	1:A:79:LEU:CD1	2.84	0.40
1:A:398:ARG:O	1:A:399:GLN:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:PHE:C	2:B:45:PHE:N	2.72	0.40
2:B:158:LEU:O	2:B:161:PHE:CD1	2.74	0.40
2:B:202:ILE:HG22	2:B:203:TYR:CD1	2.57	0.40
2:B:216:GLU:O	2:B:219:GLY:N	2.49	0.40
1:D:366:LEU:N	1:D:367:PRO:CD	2.83	0.40
1:D:384:ILE:HG22	1:D:385:ILE:N	2.36	0.40
1:D:455:VAL:HG13	1:D:458:ILE:HB	2.02	0.40
1:A:86:VAL:C	1:A:88:CYS:H	2.24	0.40
1:A:131:LEU:HD23	1:A:135:LEU:HD12	2.03	0.40
1:A:218:ASP:C	1:A:220:VAL:N	2.74	0.40
1:A:262:MSE:O	1:A:263:VAL:C	2.59	0.40
1:A:353:SER:HB3	1:A:394:VAL:HG21	2.03	0.40
1:A:379:GLU:O	1:A:383:ASN:HB2	2.21	0.40
2:B:72:HIS:C	2:B:74:ARG:H	2.24	0.40
2:B:372:TRP:O	2:B:374:LYS:N	2.54	0.40
3:C:56:GLY:N	3:C:261:SER:OG	2.49	0.40
1:D:94:GLU:O	1:D:94:GLU:HG2	2.21	0.40
2:E:97:LEU:HD22	2:E:162:ASP:HB2	2.03	0.40
2:E:332:VAL:O	2:E:334:GLU:N	2.54	0.40
2:E:337:LEU:HD12	2:E:337:LEU:N	2.36	0.40
3:F:43:SER:OG	3:F:45:VAL:C	2.60	0.40
3:F:266:CYS:O	3:F:267:TYR:HB2	2.21	0.40
1:A:120:SER:O	1:A:123:ASP:N	2.54	0.40
1:A:410:GLU:O	1:A:411:LEU:C	2.59	0.40
1:D:124:LEU:O	1:D:126:ALA:N	2.54	0.40
2:E:283:TRP:HZ3	2:E:298:LEU:CD2	2.34	0.40
3:F:50:CYS:HB2	3:F:51:PRO:CA	2.43	0.40
3:F:81:LEU:HA	3:F:112:THR:O	2.21	0.40
1:A:353:SER:HB2	1:A:354:PRO:CD	2.52	0.40
1:A:395:ILE:HD11	1:A:400:LEU:HB2	2.04	0.40
1:A:427:MSE:N	1:A:428:PRO:HD2	2.36	0.40
1:A:587:SER:C	1:A:588:LEU:HD23	2.41	0.40
3:C:155:LEU:HD11	3:C:195:MET:HG3	2.03	0.40
3:C:212:SER:OG	3:C:214:ARG:HB2	2.22	0.40
1:D:25:VAL:O	1:D:26:GLN:C	2.60	0.40
1:D:29:LEU:HD13	1:D:64:GLU:HG2	2.03	0.40
1:D:453:ASP:O	1:D:459:ARG:HD3	2.21	0.40
2:E:67:VAL:O	2:E:69:TYR:N	2.53	0.40
2:E:109:ASP:OD1	2:E:110:PRO:HD2	2.21	0.40
2:E:117:LEU:HA	2:E:164:GLU:OE1	2.21	0.40
3:F:121:ARG:HG3	3:F:121:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:162:GLN:O	3:F:235:THR:HG22	2.21	0.40
1:A:274:VAL:HG21	1:A:283:LEU:HD11	2.02	0.40
1:A:567:LEU:C	1:A:569:GLN:N	2.74	0.40
1:A:572:ASP:CG	3:C:110:ARG:HH21	2.25	0.40
2:B:306:GLU:O	2:B:307:PRO:C	2.59	0.40
1:D:23:GLU:HG2	1:D:23:GLU:O	2.20	0.40
1:D:76:PHE:N	1:D:76:PHE:CD1	2.90	0.40
2:E:85:VAL:HB	2:E:134:PHE:HE1	1.86	0.40
2:E:121:TRP:HB3	2:E:122:PRO:CD	2.51	0.40
2:E:161:PHE:CD2	2:E:214:LEU:HG	2.56	0.40
2:E:208:HIS:HB3	2:E:211:ILE:HD13	2.03	0.40
3:F:51:PRO:O	3:F:52:VAL:HG13	2.22	0.40
3:F:209:TRP:CD2	3:F:224:ILE:HD13	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	580/582 (100%)	411 (71%)	124 (21%)	45 (8%)	1 15
1	D	580/582 (100%)	411 (71%)	119 (20%)	50 (9%)	1 12
2	B	386/388 (100%)	234 (61%)	97 (25%)	55 (14%)	0 4
2	E	386/388 (100%)	234 (61%)	95 (25%)	57 (15%)	0 4
3	C	291/293 (99%)	203 (70%)	69 (24%)	19 (6%)	1 19
3	F	291/293 (99%)	210 (72%)	63 (22%)	18 (6%)	1 20
4	G	1/7 (14%)	1 (100%)	0	0	100 100
4	H	1/7 (14%)	1 (100%)	0	0	100 100
All	All	2516/2540 (99%)	1705 (68%)	567 (22%)	244 (10%)	0 10

All (244) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	LEU
1	A	44	VAL
1	A	317	CYS
1	A	391	VAL
1	A	412	ALA
1	A	560	VAL
2	B	33	ILE
2	B	43	PHE
2	B	44	ASP
2	B	46	VAL
2	B	55	TRP
2	B	57	GLU
2	B	73	ASN
2	B	81	ILE
2	B	103	PRO
2	B	104	THR
2	B	146	LYS
2	B	161	PHE
2	B	165	ASP
2	B	166	PRO
2	B	167	ARG
2	B	229	LEU
2	B	268	ASP
2	B	367	ASN
2	B	368	SER
2	B	390	MSE
2	B	413	MSE
3	C	94	VAL
3	C	254	ARG
3	C	265	TYR
1	D	25	VAL
1	D	35	LEU
1	D	44	VAL
1	D	73	LEU
1	D	391	VAL
1	D	415	ALA
1	D	515	ASP
2	E	33	ILE
2	E	43	PHE
2	E	44	ASP
2	E	46	VAL

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Mol	Chain	Res	Type
2	E	55	TRP
2	E	57	GLU
2	E	72	HIS
2	E	73	ASN
2	E	146	LYS
2	E	161	PHE
2	E	165	ASP
2	E	166	PRO
2	E	167	ARG
2	E	229	LEU
2	E	367	ASN
2	E	368	SER
2	E	390	MSE
2	E	413	MSE
3	F	94	VAL
3	F	254	ARG
3	F	265	TYR
1	A	23	GLU
1	A	86	VAL
1	A	89	LEU
1	A	238	GLU
1	A	254	ASP
1	A	274	VAL
1	A	318	ARG
1	A	349	ILE
1	A	373	LEU
1	A	415	ALA
1	A	465	ASN
1	A	474	GLY
1	A	490	SER
1	A	500	THR
1	A	513	GLY
1	A	515	ASP
1	A	553	ASN
2	B	72	HIS
2	B	76	VAL
2	B	125	GLN
2	B	135	LEU
2	B	223	ASN
2	B	287	HIS
2	B	314	MSE
2	B	374	LYS

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Mol	Chain	Res	Type
2	B	389	GLU
3	C	41	LYS
3	C	135	ARG
3	C	161	GLY
3	C	207	GLY
3	C	240	ALA
3	C	253	ASP
3	C	270	GLY
1	D	76	PHE
1	D	86	VAL
1	D	147	ALA
1	D	254	ASP
1	D	263	VAL
1	D	274	VAL
1	D	297	GLU
1	D	317	CYS
1	D	349	ILE
1	D	412	ALA
1	D	513	GLY
1	D	529	ALA
1	D	560	VAL
1	D	576	LYS
2	E	51	SER
2	E	76	VAL
2	E	81	ILE
2	E	104	THR
2	E	125	GLN
2	E	160	LEU
2	E	223	ASN
2	E	251	SER
2	E	313	ILE
2	E	351	ASP
2	E	374	LYS
2	E	389	GLU
2	E	414	LYS
3	F	108	ARG
3	F	129	PHE
3	F	161	GLY
3	F	207	GLY
3	F	240	ALA
3	F	269	CYS
1	A	37	THR

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Mol	Chain	Res	Type
1	A	152	SER
1	A	484	PRO
1	A	529	ALA
2	B	51	SER
2	B	90	ALA
2	B	163	SER
2	B	170	ASP
2	B	204	GLU
2	B	251	SER
2	B	284	PRO
2	B	362	PRO
3	C	108	ARG
3	C	231	ALA
1	D	23	GLU
1	D	318	ARG
1	D	344	ALA
1	D	399	GLN
1	D	416	LYS
1	D	428	PRO
1	D	490	SER
1	D	553	ASN
2	E	36	LEU
2	E	62	ALA
2	E	90	ALA
2	E	135	LEU
2	E	287	HIS
2	E	361	PHE
2	E	400	GLN
3	F	41	LYS
3	F	60	GLY
3	F	107	TYR
3	F	173	SER
3	F	186	LEU
3	F	253	ASP
1	A	99	VAL
1	A	117	HIS
1	A	297	GLU
1	A	334	VAL
2	B	62	ALA
2	B	66	MSE
2	B	133	ARG
2	B	196	ASN

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Mol	Chain	Res	Type
2	B	313	ILE
2	B	361	PHE
2	B	400	GLN
2	B	414	LYS
3	C	36	LYS
3	C	129	PHE
3	C	186	LEU
3	C	282	LEU
1	D	12	PRO
1	D	100	GLU
1	D	103	VAL
1	D	298	VAL
1	D	533	VAL
1	D	577	TYR
2	E	66	MSE
2	E	84	GLU
2	E	103	PRO
2	E	170	ASP
2	E	268	ASP
2	E	271	LEU
2	E	362	PRO
1	A	12	PRO
1	A	87	HIS
1	A	237	GLN
1	A	271	GLN
1	A	416	LYS
1	A	428	PRO
1	A	506	ASN
2	B	141	GLN
2	B	330	PHE
3	C	107	TYR
1	D	28	ARG
1	D	45	GLU
1	D	87	HIS
1	D	117	HIS
1	D	516	ILE
1	D	547	ILE
1	D	581	GLU
2	E	86	VAL
2	E	133	ARG
2	E	163	SER
2	E	196	ASN

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Mol	Chain	Res	Type
2	E	330	PHE
3	F	43	SER
3	F	282	LEU
1	A	516	ILE
1	A	523	PRO
1	A	576	LYS
2	B	79	GLU
2	B	303	ASP
2	B	328	PRO
3	C	88	ASP
1	D	396	GLY
1	D	492	ASP
1	D	532	PRO
2	E	343	GLU
2	B	228	PRO
1	D	91	PRO
2	E	141	GLN
2	E	305	ILE
3	F	28	VAL
1	A	13	ILE
1	A	158	VAL
1	A	492	ASP
2	B	91	VAL
1	D	484	PRO
2	E	284	PRO
2	B	115	PRO
2	B	288	SER
1	D	13	ILE
1	D	99	VAL
2	E	79	GLU
2	E	228	PRO
2	E	262	VAL
3	C	90	GLY
1	D	523	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/496 (103%)	450 (88%)	59 (12%)	5	27
1	D	509/496 (103%)	450 (88%)	59 (12%)	5	27
2	B	331/351 (94%)	299 (90%)	32 (10%)	8	33
2	E	331/351 (94%)	295 (89%)	36 (11%)	6	29
3	C	259/259 (100%)	239 (92%)	20 (8%)	13	43
3	F	259/259 (100%)	241 (93%)	18 (7%)	15	46
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2202/2216 (99%)	1978 (90%)	224 (10%)	7	31

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	15	VAL
1	A	18	ASP
1	A	48	ARG
1	A	62	GLU
1	A	77	THR
1	A	86	VAL
1	A	91	PRO
1	A	95	SER
1	A	101	GLU
1	A	104	VAL
1	A	107	LYS
1	A	117	HIS
1	A	122	SER
1	A	139	ASP
1	A	141	PHE
1	A	145	THR
1	A	153	VAL
1	A	177	ASP
1	A	180	MSE
1	A	198	LEU
1	A	204	GLU
1	A	211	ASN
1	A	214	SER
1	A	222	LEU
1	A	225	VAL
1	A	230	ASN

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Mol	Chain	Res	Type
1	A	237	GLN
1	A	268	THR
1	A	278	ILE
1	A	294	CYS
1	A	297	GLU
1	A	316	ASP
1	A	340	HIS
1	A	345	LEU
1	A	348	VAL
1	A	373	LEU
1	A	379	GLU
1	A	382	LEU
1	A	384	ILE
1	A	391	VAL
1	A	395	ILE
1	A	398	ARG
1	A	399	GLN
1	A	414	ASP
1	A	419	VAL
1	A	427	MSE
1	A	437	GLU
1	A	438	PHE
1	A	443	LEU
1	A	447	CYS
1	A	475	LYS
1	A	479	HIS
1	A	489	MSE
1	A	495	TYR
1	A	515	ASP
1	A	524	THR
1	A	540	VAL
1	A	556	LEU
2	B	95	ARG
2	B	96	THR
2	B	107	GLU
2	B	123	HIS
2	B	134	PHE
2	B	135	LEU
2	B	139	ASP
2	B	162	ASP
2	B	164	GLU
2	B	166	PRO

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Mol	Chain	Res	Type
2	B	167	ARG
2	B	170	ASP
2	B	183	PHE
2	B	186	LEU
2	B	209	ASN
2	B	225	PHE
2	B	231	GLU
2	B	246	LYS
2	B	253	TYR
2	B	256	GLN
2	B	263	GLN
2	B	264	PHE
2	B	289	PRO
2	B	305	ILE
2	B	338	TYR
2	B	344	TYR
2	B	357	LEU
2	B	361	PHE
2	B	375	THR
2	B	380	ILE
2	B	386	LEU
2	B	387	PHE
3	C	18	ASN
3	C	75	SER
3	C	78	THR
3	C	81	LEU
3	C	99	LEU
3	C	110	ARG
3	C	119	GLU
3	C	159	VAL
3	C	160	ASP
3	C	166	LEU
3	C	173	SER
3	C	187	GLN
3	C	196	CYS
3	C	204	ASP
3	C	235	THR
3	C	239	ARG
3	C	242	GLN
3	C	280	ASP
3	C	284	TYR
3	C	294	ARG

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Mol	Chain	Res	Type
1	D	8	ASP
1	D	15	VAL
1	D	18	ASP
1	D	44	VAL
1	D	53	PRO
1	D	62	GLU
1	D	71	GLU
1	D	77	THR
1	D	83	PRO
1	D	86	VAL
1	D	89	LEU
1	D	91	PRO
1	D	95	SER
1	D	101	GLU
1	D	104	VAL
1	D	107	LYS
1	D	116	SER
1	D	131	LEU
1	D	139	ASP
1	D	145	THR
1	D	180	MSE
1	D	195	VAL
1	D	198	LEU
1	D	204	GLU
1	D	222	LEU
1	D	230	ASN
1	D	237	GLN
1	D	258	ARG
1	D	294	CYS
1	D	295	GLU
1	D	316	ASP
1	D	321	VAL
1	D	340	HIS
1	D	345	LEU
1	D	348	VAL
1	D	350	MSE
1	D	373	LEU
1	D	378	PRO
1	D	382	LEU
1	D	384	ILE
1	D	389	ASP
1	D	391	VAL

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Mol	Chain	Res	Type
1	D	398	ARG
1	D	399	GLN
1	D	411	LEU
1	D	414	ASP
1	D	419	VAL
1	D	427	MSE
1	D	437	GLU
1	D	438	PHE
1	D	446	LEU
1	D	447	CYS
1	D	475	LYS
1	D	476	GLU
1	D	479	HIS
1	D	489	MSE
1	D	515	ASP
1	D	524	THR
1	D	556	LEU
2	E	83	PRO
2	E	92	ASN
2	E	95	ARG
2	E	96	THR
2	E	98	PRO
2	E	101	SER
2	E	107	GLU
2	E	128	TYR
2	E	134	PHE
2	E	135	LEU
2	E	139	ASP
2	E	162	ASP
2	E	164	GLU
2	E	166	PRO
2	E	167	ARG
2	E	170	ASP
2	E	183	PHE
2	E	186	LEU
2	E	209	ASN
2	E	225	PHE
2	E	236	PHE
2	E	253	TYR
2	E	256	GLN
2	E	263	GLN
2	E	264	PHE

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Mol	Chain	Res	Type
2	E	289	PRO
2	E	298	LEU
2	E	303	ASP
2	E	305	ILE
2	E	338	TYR
2	E	357	LEU
2	E	361	PHE
2	E	370	THR
2	E	379	LEU
2	E	386	LEU
2	E	387	PHE
3	F	18	ASN
3	F	43	SER
3	F	68	LEU
3	F	71	ILE
3	F	81	LEU
3	F	110	ARG
3	F	119	GLU
3	F	159	VAL
3	F	160	ASP
3	F	166	LEU
3	F	187	GLN
3	F	204	ASP
3	F	235	THR
3	F	239	ARG
3	F	242	GLN
3	F	256	VAL
3	F	284	TYR
3	F	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	26	GLN
1	A	119	HIS
1	A	168	GLN
1	A	172	ASN
1	A	200	ASN
1	A	211	ASN
1	A	230	ASN
1	A	271	GLN

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Mol	Chain	Res	Type
1	A	338	ASN
1	A	339	GLN
1	A	383	ASN
1	A	399	GLN
1	A	465	ASN
1	A	506	ASN
1	A	580	GLN
2	B	72	HIS
2	B	92	ASN
2	B	177	HIS
2	B	196	ASN
2	B	208	HIS
2	B	209	ASN
2	B	254	HIS
2	B	329	HIS
2	B	373	ASN
2	B	392	GLN
3	C	12	GLN
3	C	27	GLN
3	C	44	ASN
3	C	63	HIS
3	C	141	ASN
3	C	179	HIS
3	C	187	GLN
3	C	288	GLN
1	D	22	ASN
1	D	119	HIS
1	D	127	HIS
1	D	200	ASN
1	D	211	ASN
1	D	230	ASN
1	D	271	GLN
1	D	338	ASN
1	D	392	ASN
1	D	399	GLN
1	D	465	ASN
1	D	506	ASN
1	D	539	ASN
1	D	580	GLN
2	E	72	HIS
2	E	92	ASN
2	E	177	HIS

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Mol	Chain	Res	Type
2	E	208	HIS
2	E	209	ASN
2	E	223	ASN
2	E	254	HIS
2	E	329	HIS
2	E	373	ASN
2	E	392	GLN
3	F	12	GLN
3	F	27	GLN
3	F	44	ASN
3	F	63	HIS
3	F	141	ASN
3	F	179	HIS
3	F	187	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	1ZN	H	5	4	23,23,24	0.99	0	24,29,31	0.83	0
4	FGA	H	6	4	7,8,9	2.45	2 (28%)	7,9,11	1.74	2 (28%)
4	FGA	G	6	4	7,8,9	2.33	2 (28%)	7,9,11	1.93	2 (28%)
4	1ZN	G	5	4	23,23,24	1.19	1 (4%)	24,29,31	0.92	1 (4%)
4	ACB	H	3	-	7,8,9	1.74	2 (28%)	8,10,12	0.73	0
4	DAM	G	7	4,3	4,5,6	1.92	1 (25%)	3,5,7	3.89	3 (100%)
4	DAM	H	7	4,3	4,5,6	1.96	1 (25%)	3,5,7	4.23	3 (100%)
4	ACB	G	3	-	7,8,9	1.34	0	8,10,12	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1ZN	H	5	4	-	3/22/25/27	0/1/1/1
4	FGA	H	6	4	-	2/7/8/9	-
4	FGA	G	6	4	-	3/7/8/9	-
4	1ZN	G	5	4	-	3/22/25/27	0/1/1/1
4	ACB	H	3	-	-	1/9/10/12	-
4	DAM	G	7	4,3	-	0/0/4/6	-
4	DAM	H	7	4,3	-	0/0/4/6	-
4	ACB	G	3	-	-	1/9/10/12	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	FGA	O-C	5.27	1.38	1.22
4	G	6	FGA	O-C	5.15	1.37	1.22
4	G	7	DAM	C-CA	3.47	1.50	1.45
4	H	7	DAM	C-CA	3.45	1.50	1.45
4	H	3	ACB	CB-CG	2.86	1.55	1.50
4	H	6	FGA	OXT-C	-2.82	1.21	1.30
4	G	6	FGA	OXT-C	-2.33	1.22	1.30
4	H	3	ACB	CB-CA	2.30	1.57	1.55
4	G	5	1ZN	C18-C	2.09	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	7	DAM	O-C-CA	-4.96	118.85	125.22
4	H	7	DAM	CM-N-CA	-4.89	116.01	123.45
4	G	7	DAM	CM-N-CA	-4.83	116.11	123.45
4	G	7	DAM	O-C-CA	-4.19	119.85	125.22
4	G	6	FGA	O-C-CA	-3.44	110.01	122.14
4	G	6	FGA	OXT-C-CA	3.43	125.07	113.38
4	H	6	FGA	OXT-C-CA	3.10	123.93	113.38
4	H	6	FGA	O-C-CA	-3.02	111.48	122.14
4	H	7	DAM	CB-CA-N	-2.29	120.35	125.91
4	G	5	1ZN	CA-C16-C15	-2.17	120.26	123.59
4	G	7	DAM	CB-CA-N	-2.13	120.75	125.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	ACB	CA-CB-CG-OD1
4	G	5	1ZN	C12-C13-C15-C16
4	G	5	1ZN	C14-C13-C15-C16
4	H	5	1ZN	C12-C13-C15-C16
4	H	5	1ZN	C14-C13-C15-C16
4	G	6	FGA	O-C-CA-N
4	H	6	FGA	O-C-CA-N
4	H	6	FGA	OXT-C-CA-N
4	G	6	FGA	OXT-C-CA-N
4	G	6	FGA	CA-CB-CG-CD
4	H	3	ACB	CA-CB-CG-OD1
4	G	5	1ZN	C10-C2-C3-C4
4	H	5	1ZN	C10-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	6	FGA	1	0
4	G	7	DAM	1	0
4	H	7	DAM	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.