Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 12:47 AM EDT

PDB ID	:	1A2V
Title	:	COPPER AMINE OXIDASE FROM HANSENULA POLYMORPHA
Authors	:	Li, R.; Mathews, F.S.
Deposited on	:	1998-01-12
Resolution	:	2.40 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:

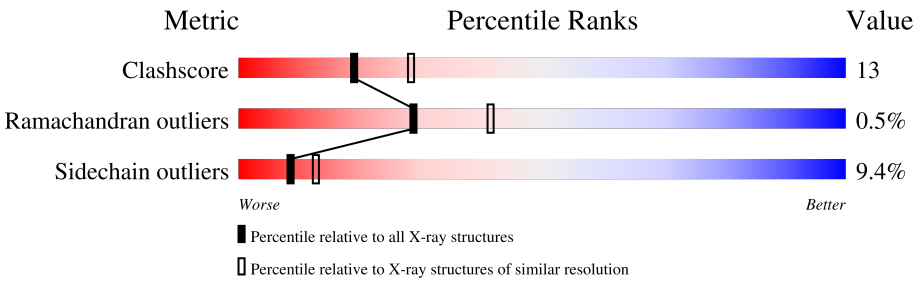
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	655	74% 22% •
1	B	655	73% 24% •
1	C	655	74% 22% •
1	D	655	69% 27% •
1	E	655	70% 26% •
1	F	655	73% 23% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 33726 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 METHYLAMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	655	5194	3305	892	974	23	0	0	0
1	B	655	5194	3305	892	974	23	0	0	0
1	C	655	5194	3305	892	974	23	0	0	0
1	D	655	5194	3305	892	974	23	0	0	0
1	E	655	5194	3305	892	974	23	0	0	0
1	F	655	5194	3305	892	974	23	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	TPQ	TYR	modified residue	UNP P12807
B	405	TPQ	TYR	modified residue	UNP P12807
C	405	TPQ	TYR	modified residue	UNP P12807
D	405	TPQ	TYR	modified residue	UNP P12807
E	405	TPQ	TYR	modified residue	UNP P12807
F	405	TPQ	TYR	modified residue	UNP P12807

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	D	1	1	1	0	0
			Total	Cu		
2	E	1	1	1	0	0
			Total	Cu		
2	F	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	499	499	499	0	0
			Total	O		
3	B	453	453	453	0	0
			Total	O		
3	C	474	474	474	0	0
			Total	O		
3	D	415	415	415	0	0
			Total	O		
3	E	335	335	335	0	0
			Total	O		
3	F	380	380	380	0	0

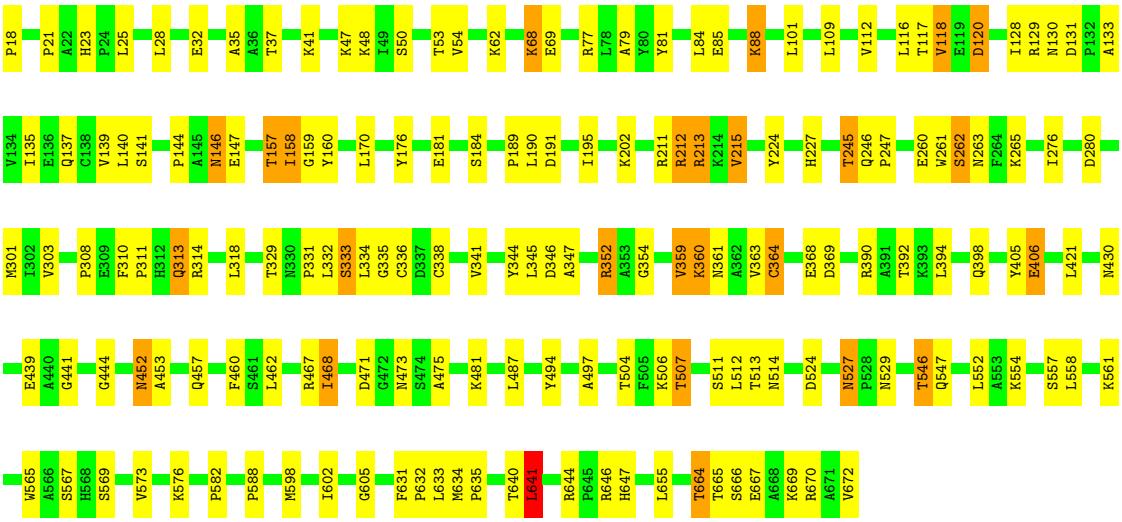
3 Residue-property plots (i)

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.

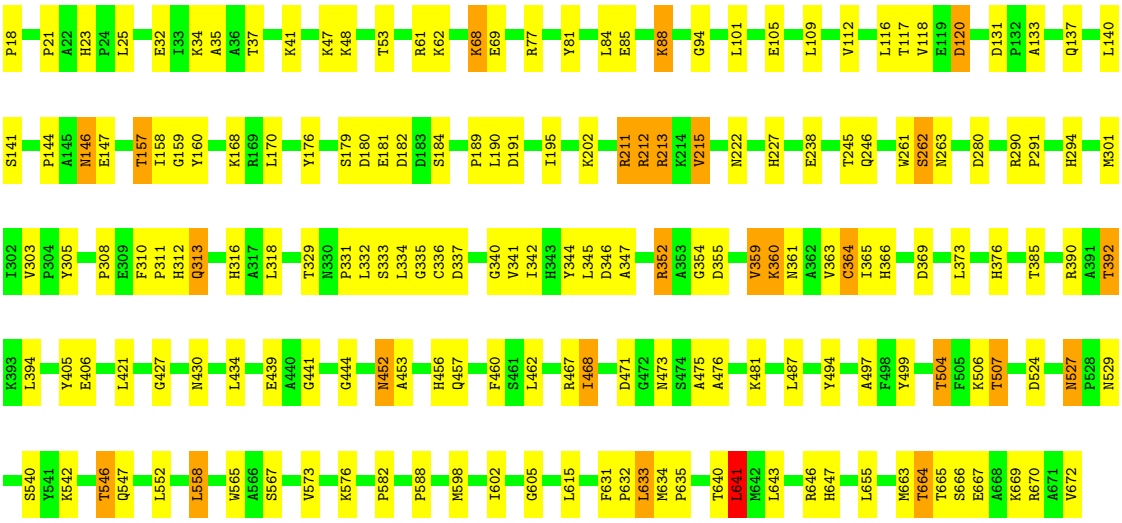
• Molecule 1: METHYLAMINE OXIDASE

Chain A: 74% 22% •



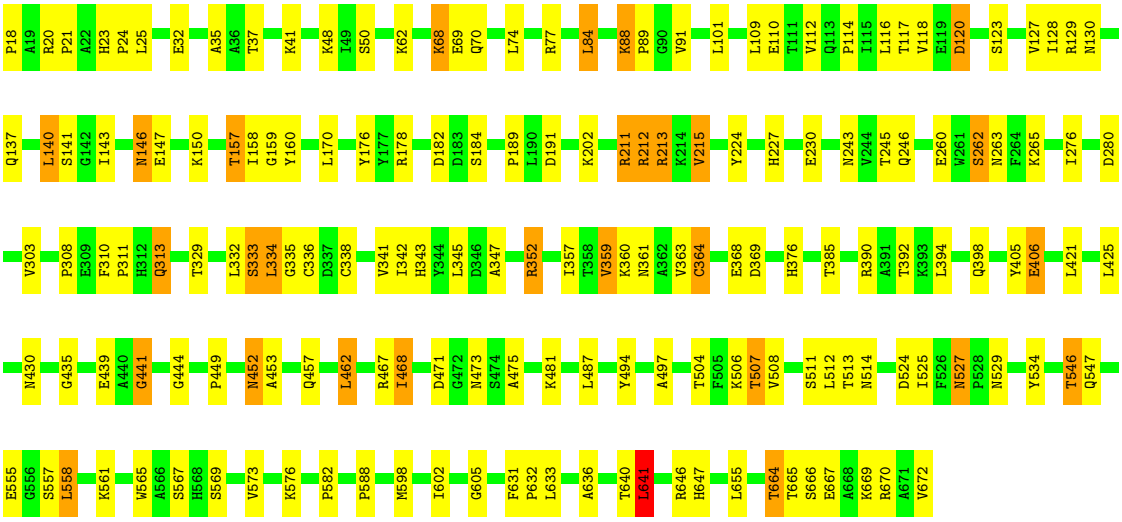
• Molecule 1: METHYLAMINE OXIDASE

Chain B: 73% 24% •



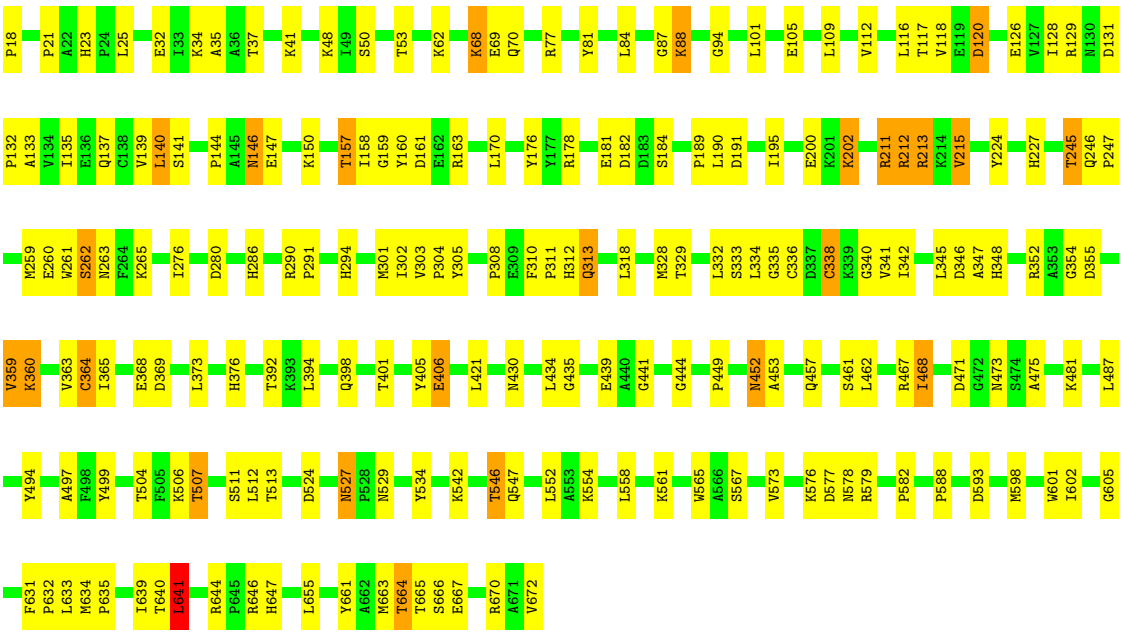
• Molecule 1: METHYLAMINE OXIDASE

Chain C: 74% 22% •



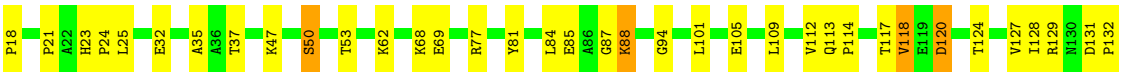
• Molecule 1: METHYLAMINE OXIDASE

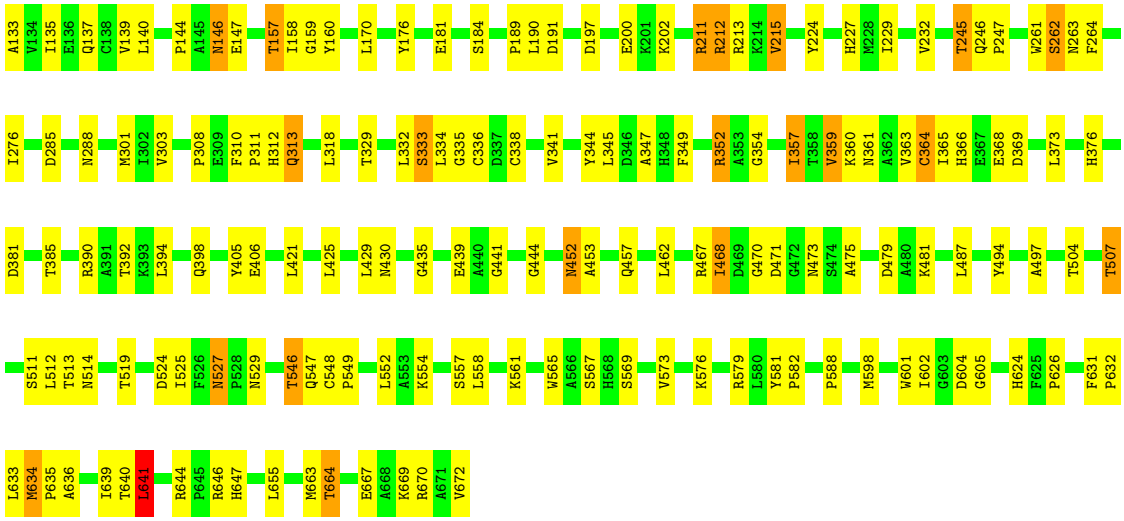
Chain D: 69% 27% •



• Molecule 1: METHYLAMINE OXIDASE

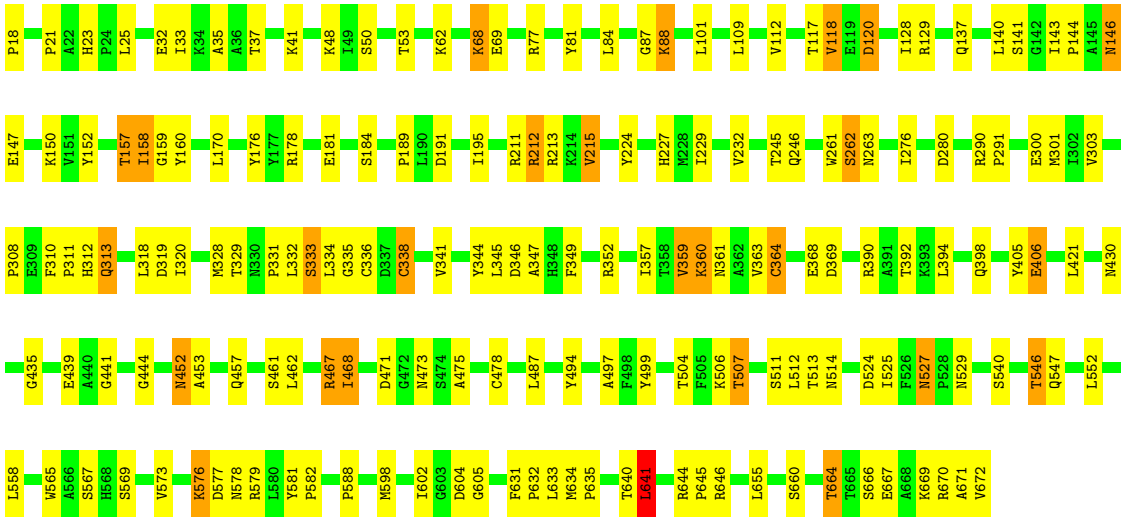
Chain E: 70% 26% •





- Molecule 1: METHYLAMINE OXIDASE

Chain F: 73% 23% •



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	138.77Å 148.22Å 234.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	83.6 (100.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.184 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33726	wwPDB-VP
Average B, all atoms (Å^2)	24.0	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: CU, TPQ

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	0.49	0/5329	0.74	2/7251 (0.0%)
1	B	0.53	1/5329 (0.0%)	0.77	2/7251 (0.0%)
1	C	0.53	0/5329	0.78	4/7251 (0.1%)
1	D	0.52	0/5329	0.77	2/7251 (0.0%)
1	E	0.50	0/5329	0.76	3/7251 (0.0%)
1	F	0.52	0/5329	0.77	3/7251 (0.0%)
All	All	0.52	1/31974 (0.0%)	0.76	16/43506 (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
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	CYS	CB-SG	-5.73	1.72	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	641	LEU	CA-CB-CG	7.25	131.96	115.30
1	A	641	LEU	CA-CB-CG	7.24	131.96	115.30
1	D	641	LEU	CA-CB-CG	7.03	131.47	115.30
1	E	641	LEU	CA-CB-CG	6.98	131.36	115.30
1	B	641	LEU	CA-CB-CG	6.80	130.95	115.30
1	F	641	LEU	CA-CB-CG	6.60	130.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	184	SER	N-CA-C	-5.71	95.60	111.00
1	F	184	SER	N-CA-C	-5.66	95.71	111.00
1	D	184	SER	N-CA-C	-5.66	95.72	111.00
1	A	184	SER	N-CA-C	-5.48	96.21	111.00
1	E	525	ILE	N-CA-C	-5.40	96.43	111.00
1	C	184	SER	N-CA-C	-5.34	96.57	111.00
1	C	525	ILE	N-CA-C	-5.26	96.80	111.00
1	E	184	SER	N-CA-C	-5.18	97.02	111.00
1	C	462	LEU	CA-CB-CG	5.11	127.05	115.30
1	F	525	ILE	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	305	TYR	Sidechain

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	5194	0	5033	129	0
1	B	5194	0	5033	141	0
1	C	5194	0	5033	129	0
1	D	5194	0	5033	150	0
1	E	5194	0	5033	150	0
1	F	5194	0	5033	140	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	499	0	0	7	0
3	B	453	0	0	6	0
3	C	474	0	0	5	0
3	D	415	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	335	0	0	5	0
3	F	380	0	0	7	0
All	All	33726	0	30198	791	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 13.

All (791) 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:C:546:THR:CG2	1:D:546:THR:HG21	1.57	1.32
1:A:546:THR:HG21	1:B:546:THR:CG2	1.64	1.27
1:E:546:THR:CG2	1:F:546:THR:HG21	1.64	1.26
1:A:546:THR:CG2	1:B:546:THR:HG21	1.67	1.24
1:C:546:THR:HG21	1:D:546:THR:CG2	1.69	1.22
1:E:546:THR:HG21	1:F:546:THR:CG2	1.81	1.09
1:D:664:THR:HG22	1:D:667:GLU:H	1.15	1.09
1:C:664:THR:HG22	1:C:667:GLU:H	1.17	1.07
1:A:664:THR:HG22	1:A:667:GLU:H	1.20	1.06
1:E:664:THR:HG22	1:E:667:GLU:H	1.20	1.05
1:E:439:GLU:HG3	1:E:441:GLY:H	1.22	1.00
1:F:664:THR:HG22	1:F:667:GLU:H	1.24	0.98
1:C:23:HIS:HD2	1:C:25:LEU:H	1.13	0.97
1:B:664:THR:HG22	1:B:667:GLU:H	1.30	0.96
1:A:494:TYR:CD1	1:B:313:GLN:HG2	2.02	0.95
1:C:130:ASN:HB3	3:C:716:HOH:O	1.68	0.93
1:D:23:HIS:HD2	1:D:25:LEU:H	1.14	0.93
1:E:311:PRO:HA	1:E:313:GLN:NE2	1.84	0.93
1:D:311:PRO:HA	1:D:313:GLN:NE2	1.83	0.93
1:A:23:HIS:HD2	1:A:25:LEU:H	1.16	0.92
1:E:311:PRO:HA	1:E:313:GLN:HE22	1.32	0.92
1:C:439:GLU:HG3	1:C:441:GLY:H	1.33	0.92
1:A:311:PRO:HA	1:A:313:GLN:NE2	1.85	0.91
1:A:130:ASN:HB3	3:A:1134:HOH:O	1.71	0.90
1:B:347:ALA:HB3	1:B:359:VAL:HG13	1.53	0.90
1:E:546:THR:HG21	1:F:546:THR:HG21	0.92	0.89
1:A:439:GLU:HG3	1:A:441:GLY:H	1.33	0.88
1:C:311:PRO:HA	1:C:313:GLN:NE2	1.89	0.88
1:B:311:PRO:HA	1:B:313:GLN:NE2	1.89	0.87
1:E:23:HIS:HD2	1:E:25:LEU:H	1.13	0.87
1:B:23:HIS:HD2	1:B:25:LEU:H	1.16	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLU:HG3	1:B:441:GLY:H	1.41	0.85
1:E:439:GLU:HG3	1:E:441:GLY:N	1.92	0.85
1:A:311:PRO:HA	1:A:313:GLN:HE22	1.42	0.84
1:F:439:GLU:HG3	1:F:441:GLY:H	1.41	0.84
1:F:23:HIS:HD2	1:F:25:LEU:H	1.26	0.83
1:D:439:GLU:HG3	1:D:441:GLY:H	1.44	0.83
1:F:311:PRO:HA	1:F:313:GLN:NE2	1.95	0.82
1:E:313:GLN:HG2	1:F:494:TYR:CD1	2.14	0.81
1:C:311:PRO:HA	1:C:313:GLN:HE22	1.46	0.81
1:D:468:ILE:H	1:D:473:ASN:HD21	1.24	0.80
1:D:527:ASN:HD22	1:D:529:ASN:H	1.29	0.80
1:A:313:GLN:HG2	1:B:494:TYR:CD1	2.17	0.79
1:C:347:ALA:HB3	1:C:359:VAL:HG13	1.65	0.78
1:C:494:TYR:CD1	1:D:313:GLN:HG2	2.18	0.78
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.12	0.78
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.13	0.78
1:E:347:ALA:HB3	1:E:359:VAL:HG13	1.65	0.78
1:F:527:ASN:HD22	1:F:529:ASN:H	1.33	0.76
1:C:468:ILE:H	1:C:473:ASN:HD21	1.32	0.76
1:C:313:GLN:HG2	1:D:494:TYR:CD1	2.20	0.76
1:D:311:PRO:HA	1:D:313:GLN:HE22	1.51	0.76
1:C:146:ASN:C	1:C:146:ASN:HD22	1.88	0.76
1:D:527:ASN:HD21	1:D:529:ASN:HB2	1.51	0.75
1:F:467:ARG:HD2	1:F:471:ASP:OD1	1.85	0.75
1:A:468:ILE:H	1:A:473:ASN:HD21	1.33	0.75
1:C:70:GLN:HG2	3:C:825:HOH:O	1.86	0.74
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.17	0.74
1:A:79:ALA:HB1	3:A:944:HOH:O	1.86	0.74
1:A:347:ALA:HB3	1:A:359:VAL:HG13	1.68	0.74
1:E:573:VAL:HG11	1:E:598:MET:HE1	1.68	0.74
1:F:468:ILE:H	1:F:473:ASN:HD21	1.35	0.74
1:B:157:THR:HG21	1:B:588:PRO:HB3	1.69	0.74
1:E:494:TYR:CD1	1:F:313:GLN:HG2	2.23	0.73
1:F:347:ALA:HB3	1:F:359:VAL:HG13	1.70	0.73
1:E:468:ILE:H	1:E:473:ASN:HD21	1.35	0.73
1:A:439:GLU:HG3	1:A:441:GLY:N	2.03	0.73
1:E:527:ASN:HD22	1:E:529:ASN:H	1.37	0.73
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.18	0.72
1:F:18:PRO:HG3	1:F:32:GLU:HA	1.70	0.72
1:B:527:ASN:HD22	1:B:529:ASN:H	1.37	0.72
1:B:137:GLN:OE1	1:B:212:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:PRO:HG3	1:E:32:GLU:HA	1.71	0.72
1:C:527:ASN:HD22	1:C:529:ASN:H	1.36	0.72
1:A:527:ASN:HD22	1:A:529:ASN:H	1.37	0.72
1:E:23:HIS:CD2	1:E:25:LEU:H	2.04	0.72
1:B:468:ILE:H	1:B:473:ASN:HD21	1.38	0.71
1:D:335:GLY:O	1:D:336:CYS:HB2	1.91	0.71
1:D:338:CYS:HG	1:D:364:CYS:CB	2.03	0.71
1:C:137:GLN:OE1	1:C:212:ARG:NH2	2.23	0.71
1:B:467:ARG:HD2	1:B:471:ASP:OD1	1.92	0.70
1:D:439:GLU:C	1:D:441:GLY:H	1.92	0.70
1:C:37:THR:O	1:C:41:LYS:HG3	1.92	0.69
1:D:467:ARG:HD2	1:D:471:ASP:OD1	1.92	0.69
1:C:565:TRP:CD1	1:C:582:PRO:HB2	2.28	0.69
1:C:439:GLU:HG3	1:C:441:GLY:N	2.05	0.69
1:A:146:ASN:C	1:A:146:ASN:HD22	1.95	0.69
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.22	0.69
1:C:406:GLU:OE2	1:D:376:HIS:ND1	2.20	0.69
1:E:338:CYS:CB	1:E:364:CYS:HG	2.05	0.69
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.23	0.69
1:D:146:ASN:C	1:D:146:ASN:HD22	1.94	0.69
1:D:507:THR:HG23	1:D:605:GLY:O	1.93	0.69
1:E:335:GLY:O	1:E:336:CYS:HB2	1.93	0.69
1:B:507:THR:HG23	1:B:605:GLY:O	1.93	0.69
1:D:68:LYS:HE2	1:D:280:ASP:OD2	1.92	0.69
1:E:439:GLU:C	1:E:441:GLY:H	1.96	0.68
1:E:507:THR:HG23	1:E:605:GLY:O	1.94	0.68
1:D:157:THR:HB	1:D:159:GLY:H	1.57	0.68
1:C:546:THR:HG21	1:D:546:THR:HG21	0.76	0.68
1:E:565:TRP:CD1	1:E:582:PRO:HB2	2.29	0.68
1:B:311:PRO:HA	1:B:313:GLN:HE22	1.56	0.68
1:B:146:ASN:HD22	1:B:146:ASN:C	1.96	0.68
1:C:335:GLY:O	1:C:336:CYS:HB2	1.92	0.68
1:B:168:LYS:HE2	3:B:944:HOH:O	1.93	0.68
1:F:146:ASN:C	1:F:146:ASN:HD22	1.96	0.68
1:F:338:CYS:HG	1:F:364:CYS:HG	0.76	0.68
1:B:507:THR:HG21	3:B:965:HOH:O	1.94	0.67
1:C:141:SER:O	1:C:215:VAL:HG23	1.93	0.67
1:C:146:ASN:HD22	1:C:147:GLU:N	1.92	0.67
1:E:137:GLN:OE1	1:E:212:ARG:NH2	2.27	0.67
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.42	0.67
1:C:546:THR:CG2	1:D:546:THR:CG2	2.48	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:546:THR:CG2	1:F:546:THR:CG2	2.55	0.67
1:A:467:ARG:HD2	1:A:471:ASP:OD1	1.93	0.67
1:B:439:GLU:HG3	1:B:441:GLY:N	2.10	0.67
1:A:18:PRO:HG3	1:A:32:GLU:HA	1.76	0.67
1:B:573:VAL:HG11	1:B:598:MET:HE1	1.75	0.67
1:E:467:ARG:HD2	1:E:471:ASP:OD1	1.95	0.67
1:A:335:GLY:O	1:A:336:CYS:HB2	1.94	0.67
1:A:137:GLN:OE1	1:A:212:ARG:NH2	2.28	0.67
1:B:345:LEU:HB2	1:B:363:VAL:HB	1.77	0.67
1:B:439:GLU:C	1:B:441:GLY:H	1.98	0.67
1:E:211:ARG:HD3	1:E:213:ARG:HD2	1.77	0.66
1:A:439:GLU:C	1:A:441:GLY:H	1.97	0.66
1:E:669:LYS:HE3	1:F:181:GLU:OE1	1.96	0.66
1:B:262:SER:O	1:B:263:ASN:HB2	1.96	0.66
1:C:157:THR:HB	1:C:159:GLY:H	1.60	0.66
1:C:439:GLU:C	1:C:441:GLY:H	2.00	0.65
1:F:137:GLN:OE1	1:F:212:ARG:NH2	2.29	0.65
1:C:507:THR:HG23	1:C:605:GLY:O	1.97	0.65
1:D:37:THR:O	1:D:41:LYS:HG3	1.96	0.65
1:E:308:PRO:HB3	1:F:497:ALA:HB2	1.79	0.65
1:F:338:CYS:CB	1:F:364:CYS:HG	2.06	0.65
1:F:439:GLU:HG3	1:F:441:GLY:N	2.10	0.65
1:F:507:THR:HG23	1:F:605:GLY:O	1.97	0.65
1:C:23:HIS:CD2	1:C:25:LEU:H	2.05	0.65
1:F:146:ASN:HD22	1:F:147:GLU:N	1.94	0.65
1:D:18:PRO:HG3	1:D:32:GLU:HA	1.79	0.65
1:A:507:THR:HG23	1:A:605:GLY:O	1.97	0.65
1:C:527:ASN:HD22	1:C:527:ASN:C	2.00	0.65
1:D:439:GLU:HG3	1:D:441:GLY:N	2.11	0.65
1:E:452:ASN:HD22	1:E:453:ALA:N	1.95	0.65
1:F:37:THR:O	1:F:41:LYS:HG3	1.97	0.65
1:E:18:PRO:HG2	1:E:32:GLU:HG2	1.79	0.64
1:E:211:ARG:CD	1:E:213:ARG:HD2	2.27	0.64
1:B:23:HIS:CD2	1:B:25:LEU:H	2.07	0.64
1:D:137:GLN:OE1	1:D:212:ARG:NH2	2.29	0.64
1:A:157:THR:HG21	1:A:588:PRO:HB3	1.79	0.64
1:E:144:PRO:HB2	1:E:146:ASN:ND2	2.13	0.64
1:A:146:ASN:HD22	1:A:147:GLU:N	1.96	0.64
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.78	0.64
1:E:457:GLN:HE22	1:E:552:LEU:H	1.46	0.64
1:C:527:ASN:ND2	1:C:529:ASN:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:THR:HG21	1:B:546:THR:HG21	0.76	0.63
1:A:669:LYS:HE3	1:B:181:GLU:OE1	1.98	0.63
1:F:160:TYR:CD2	1:F:558:LEU:HD21	2.33	0.63
1:A:262:SER:O	1:A:263:ASN:HB2	1.97	0.63
1:F:439:GLU:C	1:F:441:GLY:H	2.02	0.63
1:B:157:THR:CG2	1:B:588:PRO:HB3	2.29	0.63
1:F:18:PRO:HG2	1:F:32:GLU:HG2	1.81	0.63
1:D:468:ILE:N	1:D:473:ASN:HD21	1.96	0.62
1:C:669:LYS:HE3	1:D:181:GLU:OE1	1.99	0.62
1:D:573:VAL:HG11	1:D:598:MET:CE	2.28	0.62
1:F:527:ASN:ND2	1:F:529:ASN:H	1.97	0.62
1:D:157:THR:HG21	1:D:588:PRO:HB3	1.81	0.62
1:D:573:VAL:HG11	1:D:598:MET:HE1	1.80	0.62
1:D:262:SER:O	1:D:263:ASN:HB2	2.00	0.62
1:E:191:ASP:OD2	1:E:212:ARG:NH1	2.31	0.62
1:B:157:THR:HB	1:B:159:GLY:H	1.63	0.62
1:A:308:PRO:HB3	1:B:497:ALA:HB2	1.80	0.62
1:E:527:ASN:ND2	1:E:529:ASN:H	1.98	0.62
1:D:116:LEU:HD11	1:D:157:THR:HG23	1.82	0.61
1:D:527:ASN:ND2	1:D:529:ASN:H	1.97	0.61
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.47	0.61
1:D:664:THR:HG22	1:D:667:GLU:N	2.00	0.61
1:C:18:PRO:HG3	1:C:32:GLU:HA	1.82	0.61
1:B:146:ASN:HD22	1:B:147:GLU:N	1.98	0.61
1:A:160:TYR:CD2	1:A:558:LEU:HD21	2.35	0.61
1:F:335:GLY:O	1:F:336:CYS:HB2	2.01	0.61
1:F:452:ASN:HD22	1:F:453:ALA:N	1.98	0.61
1:F:141:SER:O	1:F:215:VAL:HG23	2.00	0.61
1:F:452:ASN:HD22	1:F:452:ASN:C	2.04	0.61
1:C:160:TYR:CD2	1:C:558:LEU:HD21	2.36	0.60
1:C:527:ASN:HD21	1:C:529:ASN:HB2	1.66	0.60
1:A:565:TRP:CD1	1:A:582:PRO:HB2	2.36	0.60
1:C:146:ASN:C	1:C:146:ASN:ND2	2.55	0.60
1:A:157:THR:HB	1:A:159:GLY:H	1.67	0.60
1:D:23:HIS:CD2	1:D:25:LEU:H	2.07	0.60
1:E:310:PHE:HA	1:E:313:GLN:HE21	1.66	0.60
1:E:547:GLN:NE2	1:E:640:THR:H	2.00	0.60
1:A:452:ASN:C	1:A:452:ASN:HD22	2.03	0.60
1:F:345:LEU:HB2	1:F:363:VAL:HB	1.84	0.60
1:A:452:ASN:HD22	1:A:453:ALA:N	2.00	0.60
1:C:276:ILE:HD11	1:C:398:GLN:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:ARG:HD2	1:C:471:ASP:OD1	2.01	0.60
1:B:18:PRO:HG3	1:B:32:GLU:HA	1.83	0.59
1:A:18:PRO:HG2	1:A:32:GLU:HG2	1.85	0.59
1:A:573:VAL:HG11	1:A:598:MET:HE1	1.83	0.59
1:D:565:TRP:CD1	1:D:582:PRO:HB2	2.37	0.59
1:E:146:ASN:HD22	1:E:147:GLU:N	2.01	0.59
1:B:35:ALA:HB1	1:B:101:LEU:HD21	1.83	0.59
1:E:157:THR:HB	1:E:159:GLY:H	1.68	0.59
1:E:527:ASN:ND2	1:E:529:ASN:HD22	1.99	0.59
1:A:527:ASN:ND2	1:A:529:ASN:H	2.01	0.59
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.38	0.59
1:E:262:SER:O	1:E:263:ASN:HB2	2.02	0.59
1:B:565:TRP:CD1	1:B:582:PRO:HB2	2.38	0.58
1:D:439:GLU:C	1:D:441:GLY:N	2.55	0.58
1:C:452:ASN:C	1:C:452:ASN:HD22	2.06	0.58
1:D:146:ASN:HD22	1:D:147:GLU:N	1.99	0.58
1:F:301:MET:HG3	1:F:320:ILE:HD12	1.84	0.58
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.39	0.58
1:F:68:LYS:HD2	3:F:873:HOH:O	2.02	0.58
1:C:157:THR:HG21	1:C:588:PRO:HB3	1.86	0.58
1:A:439:GLU:C	1:A:441:GLY:N	2.57	0.58
1:B:310:PHE:HA	1:B:313:GLN:HE21	1.69	0.58
1:C:468:ILE:N	1:C:473:ASN:HD21	2.02	0.57
1:D:146:ASN:C	1:D:146:ASN:ND2	2.57	0.57
1:A:468:ILE:N	1:A:473:ASN:HD21	2.01	0.57
1:C:439:GLU:C	1:C:441:GLY:N	2.58	0.57
1:E:47:LYS:HD2	1:E:85:GLU:OE2	2.04	0.57
1:E:276:ILE:HD11	1:E:398:GLN:HB3	1.87	0.57
1:A:68:LYS:HE2	1:A:280:ASP:OD2	2.04	0.57
1:A:23:HIS:CD2	1:A:25:LEU:H	2.09	0.57
1:E:547:GLN:HE22	1:E:639:ILE:HA	1.70	0.57
1:F:68:LYS:HE2	1:F:280:ASP:OD2	2.05	0.57
1:D:452:ASN:HD22	1:D:453:ALA:N	2.02	0.57
1:D:457:GLN:HE22	1:D:552:LEU:H	1.52	0.57
1:F:176:TYR:CE1	1:F:189:PRO:HB3	2.40	0.57
1:D:116:LEU:CD1	1:D:157:THR:HG23	2.35	0.57
1:C:117:THR:N	1:C:120:ASP:OD1	2.38	0.57
1:C:308:PRO:HB3	1:D:497:ALA:HB2	1.87	0.57
1:E:546:THR:HG23	1:F:546:THR:HG21	1.76	0.57
1:F:262:SER:O	1:F:263:ASN:HB2	2.04	0.57
1:C:573:VAL:HG11	1:C:598:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:ILE:N	1:F:473:ASN:HD21	2.03	0.56
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.70	0.56
1:E:573:VAL:CG1	1:E:598:MET:HE1	2.35	0.56
1:A:176:TYR:CE1	1:A:189:PRO:HB3	2.39	0.56
1:B:452:ASN:C	1:B:452:ASN:HD22	2.09	0.56
1:B:160:TYR:CD2	1:B:558:LEU:HD21	2.40	0.56
1:B:439:GLU:C	1:B:441:GLY:N	2.58	0.56
1:E:146:ASN:HD22	1:E:146:ASN:C	2.07	0.56
1:A:631:PHE:CG	1:A:632:PRO:HA	2.40	0.56
1:C:116:LEU:HD11	1:C:157:THR:HG23	1.87	0.56
1:E:598:MET:HE3	1:E:602:ILE:HG13	1.87	0.56
1:C:246:GLN:HB2	1:C:341:VAL:HG21	1.87	0.56
1:D:160:TYR:CD2	1:D:558:LEU:HD21	2.41	0.56
1:A:527:ASN:HD22	1:A:527:ASN:C	2.10	0.56
1:E:211:ARG:NE	1:E:213:ARG:HD2	2.20	0.56
1:E:439:GLU:HG3	1:E:441:GLY:CA	2.36	0.56
1:A:246:GLN:HB2	1:A:341:VAL:HG21	1.88	0.56
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.71	0.56
1:E:160:TYR:CD2	1:E:558:LEU:HD21	2.41	0.55
1:E:573:VAL:HG11	1:E:598:MET:CE	2.36	0.55
1:F:311:PRO:HA	1:F:313:GLN:HE22	1.70	0.55
1:A:546:THR:CG2	1:B:546:THR:CG2	2.50	0.55
1:B:344:TYR:CD1	1:B:361:ASN:HB3	2.41	0.55
1:D:70:GLN:HG2	3:D:980:HOH:O	2.06	0.55
1:F:261:TRP:CE3	1:F:262:SER:HB2	2.42	0.55
1:D:527:ASN:ND2	1:D:529:ASN:HB2	2.20	0.55
1:E:527:ASN:HD22	1:E:527:ASN:C	2.10	0.55
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.42	0.55
1:F:439:GLU:C	1:F:441:GLY:N	2.60	0.55
1:F:527:ASN:HD22	1:F:527:ASN:C	2.09	0.55
1:B:68:LYS:HE2	1:B:280:ASP:OD2	2.07	0.55
1:B:664:THR:CG2	1:B:667:GLU:H	2.09	0.55
1:D:261:TRP:CE3	1:D:262:SER:HB2	2.42	0.55
1:F:631:PHE:CG	1:F:632:PRO:HA	2.41	0.55
1:D:547:GLN:NE2	1:D:640:THR:H	2.05	0.55
1:E:37:THR:HG21	1:E:354:GLY:HA2	1.88	0.55
1:F:157:THR:HB	1:F:159:GLY:H	1.72	0.55
1:A:345:LEU:HB2	1:A:363:VAL:HB	1.87	0.54
1:A:146:ASN:C	1:A:146:ASN:ND2	2.60	0.54
1:A:117:THR:N	1:A:120:ASP:OD1	2.40	0.54
1:E:514:ASN:HA	1:E:569:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:TYR:CD1	1:F:361:ASN:HB3	2.43	0.54
1:A:35:ALA:HB1	1:A:101:LEU:HD21	1.89	0.54
1:C:35:ALA:HB1	1:C:101:LEU:HD21	1.88	0.54
1:A:157:THR:CG2	1:A:588:PRO:HB3	2.37	0.54
1:B:527:ASN:ND2	1:B:529:ASN:HD22	2.05	0.54
1:F:310:PHE:HA	1:F:313:GLN:HE21	1.72	0.54
1:B:47:LYS:HD2	1:B:85:GLU:OE2	2.07	0.54
1:B:631:PHE:CG	1:B:632:PRO:HA	2.43	0.54
1:D:294:HIS:HD2	3:D:847:HOH:O	1.89	0.54
1:C:655:LEU:HD11	1:D:632:PRO:HD2	1.89	0.54
1:E:452:ASN:HD22	1:E:452:ASN:C	2.08	0.54
1:A:547:GLN:NE2	1:A:640:THR:H	2.06	0.54
1:B:527:ASN:ND2	1:B:529:ASN:H	2.02	0.54
1:D:631:PHE:CG	1:D:632:PRO:HA	2.43	0.54
1:F:157:THR:HG21	1:F:588:PRO:HB3	1.90	0.54
1:F:506:LYS:HG2	3:F:975:HOH:O	2.08	0.54
1:B:346:ASP:OD1	1:B:360:LYS:HA	2.08	0.54
1:C:89:PRO:HG2	1:C:110:GLU:HB3	1.89	0.54
1:A:181:GLU:OE1	1:B:669:LYS:HE3	2.09	0.53
1:B:261:TRP:CE3	1:B:262:SER:HB2	2.43	0.53
1:C:557:SER:O	1:C:561:LYS:HG3	2.09	0.53
1:E:468:ILE:N	1:E:473:ASN:HD21	2.04	0.53
1:C:262:SER:O	1:C:263:ASN:HB2	2.08	0.53
1:B:452:ASN:HD22	1:B:453:ALA:N	2.06	0.53
1:D:135:ILE:O	1:D:139:VAL:HG23	2.08	0.53
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.73	0.53
1:B:573:VAL:CG1	1:B:598:MET:HE1	2.39	0.53
1:B:468:ILE:N	1:B:473:ASN:HD21	2.04	0.53
1:A:37:THR:O	1:A:41:LYS:HG3	2.09	0.53
1:B:392:THR:HG22	3:B:774:HOH:O	2.08	0.53
1:B:546:THR:HG23	1:B:546:THR:O	2.08	0.53
1:C:128:ILE:HG13	1:C:129:ARG:N	2.23	0.53
1:E:181:GLU:OE1	1:F:669:LYS:HE3	2.09	0.53
1:F:527:ASN:HD21	1:F:529:ASN:HB2	1.73	0.53
1:C:338:CYS:HG	1:C:364:CYS:CB	2.20	0.53
1:C:573:VAL:HG11	1:C:598:MET:CE	2.38	0.53
1:B:117:THR:N	1:B:120:ASP:OD1	2.41	0.53
1:C:664:THR:CG2	1:C:667:GLU:H	2.07	0.53
1:D:157:THR:CG2	1:D:588:PRO:HB3	2.38	0.53
1:E:144:PRO:HB2	1:E:146:ASN:HD21	1.74	0.53
1:E:303:VAL:HA	1:E:457:GLN:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:O	1:A:215:VAL:HG23	2.09	0.52
1:D:641:LEU:C	1:D:641:LEU:HD23	2.30	0.52
1:E:157:THR:HG21	1:E:588:PRO:HB3	1.91	0.52
1:B:180:ASP:OD2	1:B:182:ASP:HB2	2.09	0.52
1:C:452:ASN:HD22	1:C:453:ALA:N	2.07	0.52
1:F:565:TRP:CD1	1:F:582:PRO:HB2	2.43	0.52
1:A:276:ILE:HD11	1:A:398:GLN:HB3	1.91	0.52
1:B:211:ARG:HD3	1:B:213:ARG:HD2	1.92	0.52
1:C:68:LYS:HE2	1:C:280:ASP:OD2	2.09	0.52
1:F:191:ASP:OD2	1:F:212:ARG:NH1	2.42	0.52
1:B:146:ASN:C	1:B:146:ASN:ND2	2.61	0.52
1:D:598:MET:HE3	1:D:602:ILE:HG13	1.91	0.52
1:F:641:LEU:C	1:F:641:LEU:HD23	2.29	0.52
1:D:527:ASN:HD22	1:D:527:ASN:C	2.13	0.52
1:C:497:ALA:HB2	1:D:308:PRO:HB3	1.90	0.52
1:B:547:GLN:NE2	1:B:640:THR:H	2.08	0.52
1:D:452:ASN:HD22	1:D:452:ASN:C	2.12	0.52
1:F:346:ASP:OD1	1:F:360:LYS:HA	2.09	0.52
1:E:439:GLU:C	1:E:441:GLY:N	2.57	0.51
1:A:310:PHE:HA	1:A:313:GLN:HE21	1.75	0.51
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.76	0.51
1:F:211:ARG:NH2	1:F:435:GLY:HA3	2.25	0.51
1:C:18:PRO:HG2	1:C:32:GLU:HG2	1.93	0.51
1:F:246:GLN:HB2	1:F:341:VAL:HG21	1.92	0.51
1:C:116:LEU:CD1	1:C:157:THR:HG23	2.41	0.51
1:D:176:TYR:CE1	1:D:189:PRO:HB3	2.46	0.51
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.76	0.51
1:E:345:LEU:HB2	1:E:363:VAL:HB	1.92	0.51
1:F:664:THR:HG22	1:F:667:GLU:HG3	1.91	0.51
1:A:261:TRP:CE3	1:A:262:SER:HB2	2.45	0.51
1:B:527:ASN:HD21	1:B:529:ASN:HB2	1.76	0.51
1:B:335:GLY:O	1:B:336:CYS:HB2	2.10	0.51
1:F:35:ALA:HB1	1:F:101:LEU:HD21	1.93	0.51
1:A:573:VAL:HG11	1:A:598:MET:CE	2.40	0.50
1:B:21:PRO:HG3	1:B:77:ARG:NE	2.26	0.50
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.93	0.50
1:F:23:HIS:CD2	1:F:25:LEU:H	2.18	0.50
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.47	0.50
1:D:117:THR:N	1:D:120:ASP:OD1	2.43	0.50
1:F:468:ILE:H	1:F:473:ASN:ND2	2.08	0.50
1:D:246:GLN:HB2	1:D:341:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:OE2	1:A:467:ARG:NH2	2.44	0.50
1:E:117:THR:N	1:E:120:ASP:OD1	2.45	0.50
1:E:261:TRP:CE3	1:E:262:SER:HB2	2.47	0.50
1:F:444:GLY:HA3	1:F:452:ASN:HD21	1.75	0.50
1:A:457:GLN:HE22	1:A:552:LEU:H	1.57	0.50
1:B:246:GLN:HB2	1:B:341:VAL:HG21	1.92	0.50
1:A:191:ASP:OD2	1:A:212:ARG:NH1	2.43	0.50
1:A:527:ASN:HD21	1:A:529:ASN:HD22	1.59	0.50
1:B:190:LEU:HD21	1:B:215:VAL:HG13	1.94	0.50
1:C:157:THR:CG2	1:C:588:PRO:HB3	2.41	0.50
1:C:598:MET:HE2	1:C:602:ILE:HG13	1.93	0.50
1:E:246:GLN:HB2	1:E:341:VAL:HG21	1.94	0.50
1:C:632:PRO:HD2	1:D:655:LEU:HD11	1.93	0.50
1:D:191:ASP:OD2	1:D:212:ARG:NH1	2.44	0.50
1:D:311:PRO:HA	1:D:313:GLN:HE21	1.69	0.50
1:D:347:ALA:HB3	1:D:359:VAL:HG13	1.93	0.50
1:E:301:MET:O	1:E:318:LEU:HA	2.12	0.50
1:C:69:GLU:CD	1:C:467:ARG:HH22	2.15	0.49
1:D:18:PRO:HG2	1:D:32:GLU:HG2	1.94	0.49
1:D:35:ALA:HB1	1:D:101:LEU:HD21	1.95	0.49
1:D:189:PRO:HD2	3:D:782:HOH:O	2.11	0.49
1:D:211:ARG:NH2	1:D:435:GLY:HA3	2.27	0.49
1:E:157:THR:CG2	1:E:588:PRO:HB3	2.42	0.49
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.77	0.49
1:F:664:THR:CG2	1:F:667:GLU:H	2.11	0.49
1:F:670:ARG:C	1:F:672:VAL:H	2.14	0.49
1:E:118:VAL:HG13	3:E:928:HOH:O	2.11	0.49
1:A:670:ARG:C	1:A:672:VAL:H	2.15	0.49
1:C:345:LEU:HB2	1:C:363:VAL:HB	1.94	0.49
1:C:631:PHE:CG	1:C:632:PRO:HA	2.47	0.49
1:F:69:GLU:OE2	1:F:467:ARG:NH2	2.44	0.49
1:F:144:PRO:HB2	1:F:146:ASN:ND2	2.27	0.49
1:A:439:GLU:HG3	1:A:441:GLY:CA	2.42	0.49
1:B:352:ARG:NH1	1:B:352:ARG:HG3	2.27	0.49
1:D:126:GLU:HB2	3:D:1060:HOH:O	2.11	0.49
1:D:200:GLU:HB3	1:D:202:LYS:HE3	1.94	0.49
1:E:310:PHE:HA	1:E:313:GLN:NE2	2.26	0.49
1:B:439:GLU:HG3	1:B:441:GLY:CA	2.43	0.49
1:B:598:MET:HE3	1:B:602:ILE:HG13	1.94	0.49
1:C:141:SER:O	1:C:215:VAL:CG2	2.61	0.49
1:E:135:ILE:O	1:E:139:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:664:THR:CG2	1:F:667:GLU:HG3	2.42	0.49
1:D:211:ARG:HD3	1:D:213:ARG:HD2	1.95	0.49
1:F:146:ASN:C	1:F:146:ASN:ND2	2.59	0.49
1:F:641:LEU:C	1:F:641:LEU:CD2	2.81	0.49
1:B:573:VAL:HG11	1:B:598:MET:CE	2.42	0.49
1:D:468:ILE:H	1:D:473:ASN:ND2	2.01	0.49
1:F:452:ASN:C	1:F:452:ASN:ND2	2.66	0.49
1:A:646:ARG:O	1:A:647:HIS:HB2	2.13	0.49
1:C:670:ARG:C	1:C:672:VAL:H	2.16	0.49
1:E:131:ASP:OD2	1:E:133:ALA:HB3	2.13	0.49
1:B:303:VAL:HA	1:B:457:GLN:O	2.13	0.48
1:A:546:THR:HG23	1:A:546:THR:O	2.13	0.48
1:C:176:TYR:CE1	1:C:189:PRO:HB3	2.48	0.48
1:D:348:HIS:HD2	3:D:936:HOH:O	1.95	0.48
1:E:211:ARG:HE	1:E:213:ARG:HD2	1.78	0.48
1:A:118:VAL:HG13	3:A:828:HOH:O	2.12	0.48
1:D:311:PRO:CA	1:D:313:GLN:NE2	2.66	0.48
1:D:670:ARG:C	1:D:672:VAL:H	2.17	0.48
1:C:333:SER:HB2	1:C:361:ASN:OD1	2.12	0.48
1:E:632:PRO:HD2	1:F:655:LEU:HD11	1.95	0.48
1:B:34:LYS:NZ	1:B:355:ASP:OD1	2.45	0.48
1:C:385:THR:OG1	1:C:665:THR:HA	2.14	0.48
1:C:468:ILE:H	1:C:473:ASN:ND2	2.07	0.48
1:C:546:THR:HG23	1:C:546:THR:O	2.13	0.48
1:D:260:GLU:HG2	1:D:265:LYS:HG3	1.95	0.48
1:E:479:ASP:HB3	1:E:519:THR:HB	1.95	0.48
1:A:632:PRO:HD2	1:B:655:LEU:HD11	1.95	0.48
1:C:641:LEU:HD23	1:C:641:LEU:C	2.34	0.48
1:E:69:GLU:CD	1:E:467:ARG:HH22	2.17	0.48
1:E:128:ILE:HG13	1:E:129:ARG:N	2.29	0.48
1:B:476:ALA:CB	1:B:504:THR:HA	2.44	0.48
1:B:641:LEU:C	1:B:641:LEU:HD23	2.34	0.48
1:D:646:ARG:O	1:D:647:HIS:HB2	2.14	0.48
1:A:311:PRO:CA	1:A:313:GLN:NE2	2.67	0.48
1:B:37:THR:HG21	1:B:354:GLY:HA2	1.94	0.48
1:B:527:ASN:HD22	1:B:527:ASN:C	2.17	0.48
1:C:303:VAL:HA	1:C:457:GLN:O	2.14	0.48
1:C:547:GLN:NE2	1:C:640:THR:H	2.11	0.48
1:D:577:ASP:O	1:D:578:ASN:HB2	2.13	0.48
1:D:190:LEU:HD21	1:D:215:VAL:HG13	1.96	0.47
1:D:301:MET:O	1:D:318:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ASN:C	1:E:452:ASN:ND2	2.67	0.47
1:E:641:LEU:C	1:E:641:LEU:HD23	2.34	0.47
1:E:670:ARG:C	1:E:672:VAL:H	2.16	0.47
1:A:211:ARG:HD3	1:A:213:ARG:HD2	1.95	0.47
1:C:182:ASP:OD1	1:D:664:THR:HG23	2.14	0.47
1:C:334:LEU:HD13	1:D:661:TYR:CZ	2.48	0.47
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.49	0.47
1:E:579:ARG:HG2	1:E:601:TRP:CE2	2.50	0.47
1:B:61:ARG:HG3	1:B:294:HIS:CE1	2.49	0.47
1:B:141:SER:O	1:B:215:VAL:HG23	2.14	0.47
1:C:143:ILE:HG13	1:C:215:VAL:HG21	1.97	0.47
1:E:224:TYR:HB2	1:E:227:HIS:ND1	2.29	0.47
1:E:261:TRP:O	1:E:264:PHE:HB2	2.13	0.47
1:F:546:THR:O	1:F:546:THR:HG23	2.14	0.47
1:C:646:ARG:O	1:C:647:HIS:HB2	2.15	0.47
1:D:211:ARG:CD	1:D:213:ARG:HD2	2.45	0.47
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.49	0.47
1:E:69:GLU:OE2	1:E:467:ARG:NH2	2.45	0.47
1:E:311:PRO:CA	1:E:313:GLN:NE2	2.67	0.47
1:F:514:ASN:HA	1:F:569:SER:HB2	1.97	0.47
1:A:303:VAL:HA	1:A:457:GLN:O	2.15	0.47
1:B:598:MET:CE	1:B:602:ILE:HG13	2.44	0.47
1:C:69:GLU:OE2	1:C:467:ARG:NH2	2.47	0.47
1:C:475:ALA:HA	1:C:524:ASP:O	2.15	0.47
1:E:549:PRO:HB3	3:E:758:HOH:O	2.14	0.47
1:A:116:LEU:HD11	1:A:157:THR:HG23	1.95	0.47
1:B:191:ASP:OD1	1:B:212:ARG:NH1	2.48	0.47
1:B:331:PRO:HB3	1:B:360:LYS:O	2.15	0.47
1:D:69:GLU:OE2	1:D:467:ARG:NH2	2.44	0.47
1:E:190:LEU:HD21	1:E:215:VAL:HG13	1.97	0.47
1:E:467:ARG:HG3	1:E:470:GLY:O	2.14	0.47
1:E:631:PHE:CG	1:E:632:PRO:HA	2.50	0.47
1:A:664:THR:HG23	1:A:665:THR:N	2.30	0.47
1:D:224:TYR:HB2	1:D:227:HIS:ND1	2.29	0.47
1:B:670:ARG:C	1:B:672:VAL:H	2.18	0.47
1:D:634:MET:HA	1:D:635:PRO:HD3	1.74	0.47
1:A:468:ILE:H	1:A:473:ASN:ND2	2.06	0.47
1:B:468:ILE:H	1:B:473:ASN:ND2	2.09	0.47
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.49	0.47
1:B:664:THR:HG23	1:B:665:THR:N	2.30	0.46
1:F:150:LYS:HB3	1:F:178:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:CYS:SG	3:F:902:HOH:O	2.60	0.46
1:A:144:PRO:HB2	1:A:146:ASN:ND2	2.31	0.46
1:B:301:MET:O	1:B:318:LEU:HA	2.15	0.46
1:E:245:THR:OG1	1:E:247:PRO:HD3	2.15	0.46
1:C:664:THR:HG23	1:D:182:ASP:OD1	2.14	0.46
1:E:475:ALA:HA	1:E:524:ASP:O	2.16	0.46
1:F:439:GLU:HG3	1:F:441:GLY:CA	2.46	0.46
1:B:439:GLU:HG3	1:B:441:GLY:HA2	1.97	0.46
1:D:598:MET:CE	1:D:602:ILE:HG13	2.45	0.46
1:E:88:LYS:HZ3	1:E:88:LYS:HG2	1.69	0.46
1:F:670:ARG:C	1:F:672:VAL:N	2.68	0.46
1:B:664:THR:HG23	1:B:666:SER:H	1.81	0.46
1:A:224:TYR:HB2	1:A:227:HIS:ND1	2.30	0.46
1:A:655:LEU:HD11	1:B:632:PRO:HD2	1.98	0.46
1:B:340:GLY:O	1:B:342:ILE:HG12	2.16	0.46
1:B:457:GLN:HE22	1:B:552:LEU:H	1.64	0.46
1:E:53:THR:O	1:E:81:TYR:HA	2.15	0.46
1:E:349:PHE:HB2	1:E:357:ILE:HG13	1.96	0.46
1:F:158:ILE:HD12	1:F:195:ILE:HD12	1.98	0.46
1:F:573:VAL:HG11	1:F:598:MET:CE	2.46	0.46
1:A:69:GLU:CD	1:A:467:ARG:HH22	2.18	0.46
1:A:598:MET:HE3	1:A:602:ILE:HG13	1.98	0.46
1:B:53:THR:O	1:B:81:TYR:HA	2.16	0.46
1:C:664:THR:HG23	1:C:666:SER:H	1.80	0.46
1:C:664:THR:HG23	1:C:665:THR:N	2.30	0.46
1:D:53:THR:O	1:D:81:TYR:HA	2.15	0.46
1:D:140:LEU:HD13	3:D:977:HOH:O	2.15	0.46
1:E:23:HIS:CD2	1:E:24:PRO:HD2	2.51	0.46
1:E:191:ASP:OD1	1:E:212:ARG:NH1	2.49	0.46
1:E:581:TYR:HA	1:E:582:PRO:HD2	1.77	0.46
1:F:303:VAL:HA	1:F:457:GLN:O	2.15	0.46
1:A:452:ASN:C	1:A:452:ASN:ND2	2.67	0.46
1:A:664:THR:HG23	1:A:666:SER:H	1.81	0.46
1:C:452:ASN:C	1:C:452:ASN:ND2	2.68	0.46
1:E:333:SER:HB2	1:E:361:ASN:OD1	2.15	0.46
1:F:141:SER:O	1:F:215:VAL:CG2	2.64	0.46
1:F:576:LYS:HB2	1:F:579:ARG:HD2	1.97	0.46
1:A:135:ILE:O	1:A:139:VAL:HG23	2.16	0.46
1:A:557:SER:O	1:A:561:LYS:HG3	2.16	0.46
1:B:352:ARG:CG	1:B:352:ARG:HH11	2.29	0.46
1:C:160:TYR:HD2	1:C:558:LEU:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:GLY:O	1:C:336:CYS:CB	2.61	0.46
1:C:338:CYS:CB	1:C:364:CYS:HG	2.23	0.46
1:C:376:HIS:ND1	1:D:406:GLU:OE2	2.43	0.46
1:D:303:VAL:HA	1:D:457:GLN:O	2.16	0.46
1:F:468:ILE:HG21	1:F:540:SER:HA	1.97	0.46
1:F:598:MET:HE3	1:F:598:MET:O	2.16	0.46
1:C:352:ARG:NH1	1:C:352:ARG:HG3	2.31	0.45
1:D:345:LEU:HB2	1:D:363:VAL:HB	1.99	0.45
1:D:542:LYS:HB2	1:D:542:LYS:HE2	1.83	0.45
1:C:150:LYS:HB3	1:C:178:ARG:O	2.16	0.45
1:E:146:ASN:ND2	1:E:146:ASN:C	2.69	0.45
1:E:557:SER:O	1:E:561:LYS:HG3	2.16	0.45
1:F:33:ILE:O	1:F:37:THR:HG23	2.17	0.45
1:D:439:GLU:HG3	1:D:441:GLY:CA	2.46	0.45
1:F:21:PRO:HG3	1:F:77:ARG:NE	2.30	0.45
1:A:141:SER:O	1:A:215:VAL:CG2	2.64	0.45
1:A:641:LEU:C	1:A:641:LEU:HD23	2.37	0.45
1:B:37:THR:O	1:B:41:LYS:HG3	2.17	0.45
1:C:50:SER:HB3	3:C:770:HOH:O	2.16	0.45
1:C:211:ARG:HD3	1:C:213:ARG:HD2	1.98	0.45
1:D:37:THR:HG21	1:D:354:GLY:HA2	1.98	0.45
1:D:338:CYS:CB	1:D:364:CYS:SG	3.05	0.45
1:D:511:SER:O	1:D:513:THR:N	2.49	0.45
1:E:511:SER:O	1:E:513:THR:N	2.49	0.45
1:B:365:ILE:O	1:B:366:HIS:HB3	2.16	0.45
1:E:670:ARG:C	1:E:672:VAL:N	2.69	0.45
1:B:131:ASP:OD1	1:B:133:ALA:HB3	2.16	0.45
1:B:641:LEU:C	1:B:641:LEU:CD2	2.85	0.45
1:C:507:THR:HG21	3:C:759:HOH:O	2.15	0.45
1:C:598:MET:HE3	1:C:598:MET:O	2.17	0.45
1:F:499:TYR:CD1	1:F:499:TYR:N	2.84	0.45
1:F:117:THR:N	1:F:120:ASP:OD1	2.50	0.45
1:A:344:TYR:CD1	1:A:361:ASN:HB3	2.52	0.45
1:A:511:SER:O	1:A:513:THR:N	2.50	0.45
1:A:670:ARG:C	1:A:672:VAL:N	2.70	0.45
1:D:579:ARG:HG2	1:D:601:TRP:CE2	2.51	0.45
1:D:641:LEU:C	1:D:641:LEU:CD2	2.84	0.45
1:A:514:ASN:HA	1:A:569:SER:HB2	1.99	0.45
1:A:598:MET:CE	1:A:602:ILE:HG13	2.47	0.45
1:B:476:ALA:HB2	1:B:504:THR:HA	1.99	0.45
1:E:124:THR:HA	1:E:127:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:THR:CG2	1:F:588:PRO:HB3	2.46	0.45
1:A:21:PRO:HG3	1:A:77:ARG:NE	2.32	0.45
1:B:499:TYR:N	1:B:499:TYR:CD1	2.85	0.45
1:C:20:ARG:HG3	1:C:20:ARG:HH11	1.82	0.45
1:D:302:ILE:HG12	1:D:304:PRO:HD3	1.99	0.45
1:F:301:MET:O	1:F:318:LEU:HA	2.17	0.45
1:C:534:TYR:CE1	1:D:449:PRO:HD3	2.52	0.44
1:C:670:ARG:C	1:C:672:VAL:N	2.71	0.44
1:D:128:ILE:HG13	1:D:129:ARG:N	2.32	0.44
1:D:144:PRO:HB2	1:D:146:ASN:ND2	2.32	0.44
1:D:161:ASP:OD1	1:D:163:ARG:HB2	2.17	0.44
1:E:634:MET:HA	1:E:635:PRO:HD3	1.78	0.44
1:B:144:PRO:HB2	1:B:146:ASN:ND2	2.32	0.44
1:F:224:TYR:HB2	1:F:227:HIS:ND1	2.32	0.44
1:A:128:ILE:HG13	1:A:129:ARG:N	2.33	0.44
1:C:514:ASN:HA	1:C:569:SER:HB2	1.98	0.44
1:E:313:GLN:HG2	1:F:494:TYR:CE1	2.52	0.44
1:E:547:GLN:NE2	1:E:639:ILE:HA	2.33	0.44
1:B:385:THR:OG1	1:B:665:THR:HA	2.17	0.44
1:F:21:PRO:CD	1:F:77:ARG:HD3	2.47	0.44
1:F:290:ARG:HA	1:F:291:PRO:HD3	1.84	0.44
1:F:581:TYR:HB3	3:F:824:HOH:O	2.18	0.44
1:A:189:PRO:HD2	3:A:761:HOH:O	2.17	0.44
1:A:262:SER:O	1:A:263:ASN:CB	2.66	0.44
1:C:224:TYR:HB2	1:C:227:HIS:ND1	2.33	0.44
1:C:123:SER:O	1:C:127:VAL:HG13	2.17	0.44
1:D:670:ARG:C	1:D:672:VAL:N	2.71	0.44
1:A:439:GLU:O	1:A:441:GLY:N	2.51	0.44
1:B:634:MET:HA	1:B:635:PRO:HD3	1.75	0.44
1:B:664:THR:HG21	3:B:1053:HOH:O	2.17	0.44
1:D:157:THR:HG22	3:D:787:HOH:O	2.17	0.44
1:D:276:ILE:HD11	1:D:398:GLN:HB3	1.99	0.44
1:D:664:THR:HG23	1:D:665:THR:N	2.33	0.44
1:E:439:GLU:HG3	1:E:441:GLY:HA2	1.98	0.44
1:F:300:GLU:HG3	1:F:301:MET:N	2.33	0.44
1:D:601:TRP:N	1:D:601:TRP:CD1	2.85	0.44
1:A:88:LYS:HZ3	1:A:88:LYS:HG2	1.63	0.44
1:C:641:LEU:C	1:C:641:LEU:CD2	2.86	0.44
1:A:53:THR:O	1:A:81:TYR:HA	2.18	0.43
1:D:259:MET:CE	1:D:365:ILE:HG21	2.48	0.43
1:D:312:HIS:HD2	3:D:755:HOH:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLU:HG3	1:A:441:GLY:HA2	2.01	0.43
1:B:158:ILE:CD1	1:B:195:ILE:HD12	2.48	0.43
1:C:439:GLU:O	1:C:441:GLY:N	2.51	0.43
1:A:475:ALA:HA	1:A:524:ASP:O	2.18	0.43
1:B:262:SER:O	1:B:263:ASN:CB	2.65	0.43
1:B:646:ARG:O	1:B:647:HIS:HB2	2.17	0.43
1:D:310:PHE:HA	1:D:313:GLN:HE21	1.84	0.43
1:B:141:SER:O	1:B:215:VAL:CG2	2.67	0.43
1:D:94:GLY:HA3	1:D:105:GLU:O	2.18	0.43
1:E:23:HIS:HD2	1:E:25:LEU:N	1.97	0.43
1:F:229:ILE:O	1:F:232:VAL:O	2.36	0.43
1:F:333:SER:HB2	1:F:361:ASN:OD1	2.18	0.43
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.66	0.43
1:A:664:THR:HG21	3:A:1103:HOH:O	2.19	0.43
1:B:21:PRO:CD	1:B:77:ARG:HD3	2.48	0.43
1:D:340:GLY:O	1:D:342:ILE:HG12	2.19	0.43
1:D:439:GLU:O	1:D:441:GLY:N	2.51	0.43
1:E:373:LEU:HD12	1:E:373:LEU:HA	1.86	0.43
1:E:381:ASP:OD2	1:E:385:THR:OG1	2.33	0.43
1:E:664:THR:CG2	1:E:667:GLU:HG3	2.48	0.43
1:F:189:PRO:HD2	3:F:772:HOH:O	2.18	0.43
1:F:457:GLN:HE22	1:F:552:LEU:H	1.64	0.43
1:E:113:GLN:OE1	1:E:113:GLN:HA	2.18	0.43
1:E:646:ARG:O	1:E:647:HIS:HB2	2.19	0.43
1:B:116:LEU:HD11	1:B:157:THR:HG23	2.01	0.43
1:E:94:GLY:HA3	1:E:105:GLU:O	2.17	0.43
1:E:211:ARG:HD3	1:E:213:ARG:CD	2.47	0.43
1:B:452:ASN:C	1:B:452:ASN:ND2	2.71	0.43
1:B:670:ARG:C	1:B:672:VAL:N	2.72	0.43
1:C:91:VAL:HG11	1:C:114:PRO:HG3	2.00	0.43
1:C:439:GLU:HG3	1:C:441:GLY:CA	2.48	0.43
1:F:312:HIS:HE1	3:F:742:HOH:O	2.01	0.43
1:F:671:ALA:O	1:F:672:VAL:HB	2.19	0.43
1:A:211:ARG:CD	1:A:213:ARG:HD2	2.48	0.43
1:A:494:TYR:CE1	1:B:313:GLN:HG2	2.53	0.43
1:E:18:PRO:CG	1:E:32:GLU:HG2	2.47	0.43
1:A:352:ARG:NH1	1:A:352:ARG:HG3	2.33	0.43
1:B:434:LEU:HB2	1:B:452:ASN:HB2	2.01	0.43
1:C:191:ASP:OD1	1:C:212:ARG:NH1	2.52	0.43
1:C:511:SER:O	1:C:513:THR:N	2.51	0.43
1:D:461:SER:HB2	1:D:565:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:TYR:CD1	1:E:361:ASN:HB3	2.54	0.43
1:E:624:HIS:O	1:E:626:PRO:HD3	2.19	0.43
1:F:87:GLY:C	1:F:88:LYS:HZ2	2.22	0.43
1:F:311:PRO:HA	1:F:313:GLN:HE21	1.79	0.43
1:F:511:SER:O	1:F:513:THR:N	2.51	0.43
1:F:598:MET:HE3	1:F:598:MET:HA	2.01	0.43
1:A:190:LEU:HD21	1:A:215:VAL:HG13	2.00	0.42
1:F:143:ILE:HG13	1:F:215:VAL:HG21	2.01	0.42
1:A:333:SER:HB2	1:A:361:ASN:OD1	2.19	0.42
1:B:158:ILE:HD12	1:B:195:ILE:HD12	2.00	0.42
1:D:34:LYS:NZ	1:D:355:ASP:OD1	2.52	0.42
1:D:546:THR:HG23	1:D:546:THR:O	2.19	0.42
1:E:50:SER:HB3	3:E:961:HOH:O	2.18	0.42
1:E:548:CYS:HB3	3:E:774:HOH:O	2.20	0.42
1:A:28:LEU:CD1	3:A:944:HOH:O	2.66	0.42
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.86	0.42
1:D:150:LYS:HB3	1:D:178:ARG:O	2.20	0.42
1:F:439:GLU:HG3	1:F:441:GLY:HA2	2.01	0.42
1:A:641:LEU:C	1:A:641:LEU:CD2	2.88	0.42
1:C:342:ILE:HG22	1:C:343:HIS:N	2.34	0.42
1:E:335:GLY:O	1:E:336:CYS:CB	2.63	0.42
1:E:425:LEU:O	1:E:636:ALA:HA	2.20	0.42
1:F:69:GLU:CD	1:F:467:ARG:HH22	2.22	0.42
1:F:604:ASP:OD1	1:F:604:ASP:C	2.58	0.42
1:F:634:MET:HA	1:F:635:PRO:HD3	1.79	0.42
1:B:460:PHE:CD1	1:B:460:PHE:N	2.87	0.42
1:C:555:GLU:HG3	3:C:920:HOH:O	2.20	0.42
1:D:131:ASP:OD2	1:D:133:ALA:HB3	2.19	0.42
1:D:439:GLU:HG3	1:D:441:GLY:HA2	2.00	0.42
1:E:655:LEU:HD11	1:F:632:PRO:HD2	2.01	0.42
1:F:577:ASP:O	1:F:578:ASN:HB2	2.20	0.42
1:B:238:GLU:HG2	3:B:1092:HOH:O	2.19	0.42
1:D:475:ALA:HA	1:D:524:ASP:O	2.19	0.42
1:F:349:PHE:HB2	1:F:357:ILE:HG13	2.02	0.42
1:F:598:MET:CE	1:F:602:ILE:HG13	2.50	0.42
1:A:54:VAL:HG12	3:A:944:HOH:O	2.18	0.42
1:B:94:GLY:HA3	1:B:105:GLU:O	2.19	0.42
1:B:316:HIS:CE1	1:B:558:LEU:HD13	2.54	0.42
1:B:542:LYS:O	1:B:643:LEU:HA	2.20	0.42
1:C:598:MET:CE	1:C:602:ILE:HG13	2.50	0.42
1:D:346:ASP:OD1	1:D:360:LYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ALA:HB1	1:E:101:LEU:HD21	2.01	0.42
1:F:390:ARG:HG3	1:F:660:SER:OG	2.19	0.42
1:C:24:PRO:HG3	1:C:74:LEU:HD11	2.02	0.42
1:E:604:ASP:OD1	1:E:604:ASP:C	2.58	0.42
1:F:475:ALA:HA	1:F:524:ASP:O	2.20	0.42
1:C:507:THR:O	1:C:508:VAL:C	2.58	0.42
1:E:262:SER:O	1:E:263:ASN:CB	2.67	0.42
1:E:429:LEU:HD13	1:E:453:ALA:CB	2.50	0.42
1:F:331:PRO:HB3	1:F:360:LYS:O	2.19	0.42
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.34	0.42
1:D:131:ASP:HA	1:D:132:PRO:HD3	1.95	0.42
1:E:229:ILE:O	1:E:232:VAL:O	2.37	0.42
1:C:84:LEU:N	1:C:84:LEU:CD2	2.83	0.41
1:C:243:ASN:ND2	1:D:247:PRO:HG3	2.35	0.41
1:D:290:ARG:HA	1:D:291:PRO:HD3	1.87	0.41
1:E:285:ASP:N	1:E:288:ASN:O	2.51	0.41
1:E:312:HIS:HD2	3:E:779:HOH:O	2.03	0.41
1:E:376:HIS:ND1	1:F:406:GLU:OE2	2.37	0.41
1:B:212:ARG:HA	1:B:212:ARG:HD2	1.89	0.41
1:B:347:ALA:HB3	1:B:359:VAL:CG1	2.38	0.41
1:D:158:ILE:HD12	1:D:195:ILE:HG23	2.02	0.41
1:E:37:THR:HG21	1:E:354:GLY:CA	2.48	0.41
1:E:211:ARG:NH2	1:E:435:GLY:HA3	2.35	0.41
1:A:47:LYS:HD2	1:A:85:GLU:OE2	2.21	0.41
1:A:158:ILE:HD12	1:A:195:ILE:HD12	2.01	0.41
1:A:634:MET:HA	1:A:635:PRO:HD3	1.76	0.41
1:B:211:ARG:CD	1:B:213:ARG:HD2	2.50	0.41
1:F:319:ASP:HB3	1:F:328:MET:HE1	2.02	0.41
1:B:439:GLU:O	1:B:441:GLY:N	2.54	0.41
1:B:475:ALA:HA	1:B:524:ASP:O	2.21	0.41
1:D:328:MET:HB3	1:D:401:THR:O	2.21	0.41
1:F:160:TYR:HD2	1:F:558:LEU:HD21	1.84	0.41
1:A:158:ILE:HG13	1:A:314:ARG:HD2	2.02	0.41
1:A:338:CYS:CB	1:A:364:CYS:SG	3.09	0.41
1:C:449:PRO:HD3	1:D:534:TYR:CE1	2.55	0.41
1:D:245:THR:OG1	1:D:247:PRO:HD3	2.20	0.41
1:D:499:TYR:CD1	1:D:499:TYR:N	2.89	0.41
1:E:87:GLY:C	1:E:88:LYS:HZ2	2.24	0.41
1:E:365:ILE:O	1:E:366:HIS:HB3	2.20	0.41
1:E:457:GLN:NE2	1:E:552:LEU:H	2.15	0.41
1:A:18:PRO:HD3	1:A:35:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:THR:OG1	1:A:247:PRO:HD3	2.21	0.41
1:C:425:LEU:O	1:C:636:ALA:HA	2.20	0.41
1:D:191:ASP:OD1	1:D:212:ARG:NH1	2.54	0.41
1:D:664:THR:HG23	1:D:666:SER:H	1.85	0.41
1:F:53:THR:O	1:F:81:TYR:HA	2.21	0.41
1:B:305:TYR:CD2	1:B:456:HIS:HB3	2.56	0.41
1:B:427:GLY:O	1:B:633:LEU:HD23	2.21	0.41
1:C:35:ALA:HB1	1:C:101:LEU:CD2	2.50	0.41
1:D:561:LYS:NZ	1:D:593:ASP:OD1	2.53	0.41
1:F:118:VAL:HG13	3:F:821:HOH:O	2.21	0.41
1:A:460:PHE:CD1	1:A:460:PHE:N	2.88	0.41
1:B:69:GLU:CD	1:B:467:ARG:HH22	2.24	0.41
1:D:69:GLU:CD	1:D:467:ARG:HH22	2.23	0.41
1:D:286:HIS:CE1	3:D:908:HOH:O	2.74	0.41
1:E:191:ASP:CG	1:E:212:ARG:NH1	2.74	0.41
1:E:276:ILE:CD1	1:E:398:GLN:HB3	2.49	0.41
1:F:461:SER:HB2	1:F:565:TRP:CE3	2.55	0.41
1:F:664:THR:HG23	1:F:666:SER:H	1.84	0.41
1:A:301:MET:O	1:A:318:LEU:HA	2.20	0.41
1:B:190:LEU:CD2	1:B:215:VAL:HG13	2.50	0.41
1:B:352:ARG:HG3	1:B:352:ARG:HH11	1.84	0.41
1:C:88:LYS:HZ3	1:C:88:LYS:HG2	1.72	0.41
1:C:310:PHE:HA	1:C:313:GLN:HE21	1.86	0.41
1:D:87:GLY:C	1:D:88:LYS:HZ2	2.25	0.41
1:D:141:SER:O	1:D:215:VAL:CG2	2.69	0.41
1:D:547:GLN:HE22	1:D:639:ILE:HA	1.86	0.41
1:E:347:ALA:HB3	1:E:359:VAL:CG1	2.42	0.41
1:E:598:MET:CE	1:E:602:ILE:HG13	2.49	0.41
1:F:212:ARG:HA	1:F:212:ARG:HD2	1.88	0.41
1:F:666:SER:O	1:F:669:LYS:HB2	2.21	0.41
1:A:37:THR:HG21	1:A:354:GLY:HA2	2.03	0.41
1:A:131:ASP:OD2	1:A:133:ALA:HB3	2.22	0.41
1:B:37:THR:HG21	1:B:354:GLY:CA	2.51	0.41
1:B:88:LYS:HZ3	1:B:88:LYS:HG2	1.65	0.41
1:C:260:GLU:HG2	1:C:265:LYS:HG3	2.03	0.41
1:D:211:ARG:NE	1:D:213:ARG:HD2	2.35	0.41
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.90	0.41
1:E:114:PRO:O	1:E:588:PRO:HG2	2.20	0.41
1:E:197:ASP:CG	1:E:200:GLU:HB2	2.42	0.41
1:F:276:ILE:HD11	1:F:398:GLN:HB3	2.03	0.41
1:F:598:MET:HE2	1:F:602:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:LEU:HD23	1:B:615:LEU:HA	1.87	0.40
1:C:23:HIS:HD2	1:C:25:LEU:N	1.97	0.40
1:F:152:TYR:CD1	1:F:178:ARG:HG3	2.56	0.40
1:F:547:GLN:NE2	1:F:640:THR:H	2.19	0.40
1:A:346:ASP:OD1	1:A:360:LYS:HA	2.21	0.40
1:A:406:GLU:OE2	1:B:376:HIS:ND1	2.44	0.40
1:B:290:ARG:HA	1:B:291:PRO:HD3	1.88	0.40
1:D:434:LEU:HB2	1:D:452:ASN:HB2	2.03	0.40
1:E:131:ASP:HA	1:E:132:PRO:HD3	1.92	0.40
1:E:352:ARG:NH1	1:E:352:ARG:HG3	2.35	0.40
1:A:260:GLU:HG2	1:A:265:LYS:HG3	2.03	0.40
1:B:311:PRO:HA	1:B:313:GLN:HE21	1.78	0.40
1:B:312:HIS:HD2	3:B:792:HOH:O	2.05	0.40
1:C:224:TYR:O	1:C:227:HIS:HB2	2.21	0.40
1:D:527:ASN:HD22	1:D:529:ASN:N	2.08	0.40
1:A:331:PRO:HB3	1:A:360:LYS:O	2.21	0.40
1:C:140:LEU:HD12	1:C:140:LEU:HA	1.91	0.40
1:F:338:CYS:SG	1:F:364:CYS:CB	3.10	0.40
1:F:645:PRO:O	1:F:646:ARG:HD2	2.22	0.40
1:A:191:ASP:OD1	1:A:212:ARG:NH1	2.54	0.40
1:C:211:ARG:NH2	1:C:435:GLY:HA3	2.37	0.40
1:F:128:ILE:HG13	1:F:129:ARG:N	2.34	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	652/655 (100%)	616 (94%)	33 (5%)	3 (0%)	29	41
1	B	652/655 (100%)	616 (94%)	34 (5%)	2 (0%)	41	55
1	C	652/655 (100%)	616 (94%)	32 (5%)	4 (1%)	25	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	652/655 (100%)	617 (95%)	32 (5%)	3 (0%)	29	41
1	E	652/655 (100%)	619 (95%)	30 (5%)	3 (0%)	29	41
1	F	652/655 (100%)	613 (94%)	36 (6%)	3 (0%)	29	41
All	All	3912/3930 (100%)	3697 (94%)	197 (5%)	18 (0%)	29	41

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	512	LEU
1	E	468	ILE
1	E	512	LEU
1	A	512	LEU
1	D	333	SER
1	D	512	LEU
1	E	333	SER
1	F	512	LEU
1	A	333	SER
1	A	468	ILE
1	B	333	SER
1	B	468	ILE
1	C	333	SER
1	F	333	SER
1	C	468	ILE
1	F	468	ILE
1	D	468	ILE
1	C	441	GLY

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	565/565 (100%)	512 (91%)	53 (9%)	8	13
1	B	565/565 (100%)	511 (90%)	54 (10%)	8	12
1	C	565/565 (100%)	511 (90%)	54 (10%)	8	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	565/565 (100%)	511 (90%)	54 (10%)	8 12
1	E	565/565 (100%)	511 (90%)	54 (10%)	8 12
1	F	565/565 (100%)	515 (91%)	50 (9%)	10 15
All	All	3390/3390 (100%)	3071 (91%)	319 (9%)	8 13

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	50	SER
1	A	62	LYS
1	A	68	LYS
1	A	84	LEU
1	A	88	LYS
1	A	109	LEU
1	A	112	VAL
1	A	118	VAL
1	A	120	ASP
1	A	140	LEU
1	A	146	ASN
1	A	157	THR
1	A	158	ILE
1	A	170	LEU
1	A	202	LYS
1	A	212	ARG
1	A	213	ARG
1	A	215	VAL
1	A	245	THR
1	A	262	SER
1	A	313	GLN
1	A	329	THR
1	A	332	LEU
1	A	334	LEU
1	A	352	ARG
1	A	359	VAL
1	A	360	LYS
1	A	364	CYS
1	A	368	GLU
1	A	369	ASP
1	A	390	ARG
1	A	392	THR

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Mol	Chain	Res	Type
1	A	394	LEU
1	A	406	GLU
1	A	421	LEU
1	A	430	ASN
1	A	452	ASN
1	A	462	LEU
1	A	481	LYS
1	A	487	LEU
1	A	504	THR
1	A	506	LYS
1	A	507	THR
1	A	527	ASN
1	A	546	THR
1	A	554	LYS
1	A	567	SER
1	A	576	LYS
1	A	633	LEU
1	A	641	LEU
1	A	644	ARG
1	A	664	THR
1	B	48	LYS
1	B	62	LYS
1	B	68	LYS
1	B	84	LEU
1	B	88	LYS
1	B	109	LEU
1	B	112	VAL
1	B	118	VAL
1	B	120	ASP
1	B	140	LEU
1	B	146	ASN
1	B	157	THR
1	B	170	LEU
1	B	179	SER
1	B	202	LYS
1	B	211	ARG
1	B	212	ARG
1	B	213	ARG
1	B	215	VAL
1	B	245	THR
1	B	262	SER
1	B	313	GLN

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Mol	Chain	Res	Type
1	B	329	THR
1	B	332	LEU
1	B	334	LEU
1	B	337	ASP
1	B	352	ARG
1	B	359	VAL
1	B	360	LYS
1	B	364	CYS
1	B	369	ASP
1	B	390	ARG
1	B	392	THR
1	B	394	LEU
1	B	406	GLU
1	B	421	LEU
1	B	430	ASN
1	B	452	ASN
1	B	462	LEU
1	B	481	LYS
1	B	487	LEU
1	B	504	THR
1	B	506	LYS
1	B	507	THR
1	B	527	ASN
1	B	540	SER
1	B	546	THR
1	B	558	LEU
1	B	567	SER
1	B	576	LYS
1	B	633	LEU
1	B	641	LEU
1	B	663	MET
1	B	664	THR
1	C	48	LYS
1	C	62	LYS
1	C	68	LYS
1	C	84	LEU
1	C	88	LYS
1	C	109	LEU
1	C	112	VAL
1	C	118	VAL
1	C	120	ASP
1	C	140	LEU

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	157	THR
1	C	158	ILE
1	C	170	LEU
1	C	202	LYS
1	C	211	ARG
1	C	212	ARG
1	C	213	ARG
1	C	215	VAL
1	C	230	GLU
1	C	245	THR
1	C	262	SER
1	C	313	GLN
1	C	329	THR
1	C	332	LEU
1	C	334	LEU
1	C	352	ARG
1	C	357	ILE
1	C	359	VAL
1	C	360	LYS
1	C	364	CYS
1	C	368	GLU
1	C	369	ASP
1	C	390	ARG
1	C	392	THR
1	C	394	LEU
1	C	406	GLU
1	C	421	LEU
1	C	430	ASN
1	C	452	ASN
1	C	462	LEU
1	C	481	LYS
1	C	487	LEU
1	C	504	THR
1	C	506	LYS
1	C	507	THR
1	C	527	ASN
1	C	546	THR
1	C	558	LEU
1	C	567	SER
1	C	576	LYS
1	C	633	LEU

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Mol	Chain	Res	Type
1	C	641	LEU
1	C	664	THR
1	D	48	LYS
1	D	50	SER
1	D	62	LYS
1	D	68	LYS
1	D	84	LEU
1	D	88	LYS
1	D	109	LEU
1	D	112	VAL
1	D	118	VAL
1	D	120	ASP
1	D	140	LEU
1	D	146	ASN
1	D	157	THR
1	D	170	LEU
1	D	202	LYS
1	D	211	ARG
1	D	212	ARG
1	D	213	ARG
1	D	215	VAL
1	D	245	THR
1	D	262	SER
1	D	313	GLN
1	D	329	THR
1	D	332	LEU
1	D	334	LEU
1	D	338	CYS
1	D	352	ARG
1	D	359	VAL
1	D	360	LYS
1	D	364	CYS
1	D	368	GLU
1	D	369	ASP
1	D	392	THR
1	D	394	LEU
1	D	406	GLU
1	D	421	LEU
1	D	430	ASN
1	D	452	ASN
1	D	462	LEU
1	D	481	LYS

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Mol	Chain	Res	Type
1	D	487	LEU
1	D	504	THR
1	D	506	LYS
1	D	507	THR
1	D	527	ASN
1	D	546	THR
1	D	554	LYS
1	D	567	SER
1	D	576	LYS
1	D	633	LEU
1	D	641	LEU
1	D	644	ARG
1	D	663	MET
1	D	664	THR
1	E	50	SER
1	E	62	LYS
1	E	68	LYS
1	E	84	LEU
1	E	88	LYS
1	E	109	LEU
1	E	112	VAL
1	E	118	VAL
1	E	120	ASP
1	E	140	LEU
1	E	146	ASN
1	E	157	THR
1	E	158	ILE
1	E	170	LEU
1	E	202	LYS
1	E	211	ARG
1	E	212	ARG
1	E	215	VAL
1	E	245	THR
1	E	262	SER
1	E	313	GLN
1	E	329	THR
1	E	332	LEU
1	E	334	LEU
1	E	352	ARG
1	E	357	ILE
1	E	359	VAL
1	E	360	LYS

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Mol	Chain	Res	Type
1	E	364	CYS
1	E	368	GLU
1	E	369	ASP
1	E	390	ARG
1	E	392	THR
1	E	394	LEU
1	E	406	GLU
1	E	421	LEU
1	E	430	ASN
1	E	452	ASN
1	E	462	LEU
1	E	481	LYS
1	E	487	LEU
1	E	504	THR
1	E	507	THR
1	E	527	ASN
1	E	546	THR
1	E	554	LYS
1	E	567	SER
1	E	576	LYS
1	E	633	LEU
1	E	634	MET
1	E	641	LEU
1	E	644	ARG
1	E	663	MET
1	E	664	THR
1	F	48	LYS
1	F	50	SER
1	F	62	LYS
1	F	68	LYS
1	F	84	LEU
1	F	88	LYS
1	F	109	LEU
1	F	112	VAL
1	F	118	VAL
1	F	120	ASP
1	F	140	LEU
1	F	146	ASN
1	F	157	THR
1	F	158	ILE
1	F	170	LEU
1	F	212	ARG

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Mol	Chain	Res	Type
1	F	213	ARG
1	F	215	VAL
1	F	245	THR
1	F	262	SER
1	F	313	GLN
1	F	329	THR
1	F	332	LEU
1	F	334	LEU
1	F	338	CYS
1	F	352	ARG
1	F	359	VAL
1	F	360	LYS
1	F	364	CYS
1	F	368	GLU
1	F	369	ASP
1	F	392	THR
1	F	394	LEU
1	F	406	GLU
1	F	421	LEU
1	F	430	ASN
1	F	452	ASN
1	F	462	LEU
1	F	467	ARG
1	F	487	LEU
1	F	504	THR
1	F	507	THR
1	F	527	ASN
1	F	546	THR
1	F	567	SER
1	F	576	LYS
1	F	633	LEU
1	F	641	LEU
1	F	644	ARG
1	F	664	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	66	GLN
1	A	70	GLN
1	A	146	ASN

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Mol	Chain	Res	Type
1	A	288	ASN
1	A	294	HIS
1	A	312	HIS
1	A	313	GLN
1	A	330	ASN
1	A	382	ASN
1	A	450	ASN
1	A	452	ASN
1	A	457	GLN
1	A	473	ASN
1	A	527	ASN
1	A	547	GLN
1	B	23	HIS
1	B	66	GLN
1	B	70	GLN
1	B	146	ASN
1	B	246	GLN
1	B	288	ASN
1	B	294	HIS
1	B	312	HIS
1	B	313	GLN
1	B	330	ASN
1	B	343	HIS
1	B	450	ASN
1	B	452	ASN
1	B	457	GLN
1	B	473	ASN
1	B	527	ASN
1	B	547	GLN
1	C	23	HIS
1	C	66	GLN
1	C	70	GLN
1	C	146	ASN
1	C	243	ASN
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	313	GLN
1	C	330	ASN
1	C	382	ASN
1	C	450	ASN
1	C	452	ASN

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Mol	Chain	Res	Type
1	C	457	GLN
1	C	473	ASN
1	C	527	ASN
1	C	547	GLN
1	D	23	HIS
1	D	66	GLN
1	D	70	GLN
1	D	146	ASN
1	D	246	GLN
1	D	286	HIS
1	D	288	ASN
1	D	294	HIS
1	D	312	HIS
1	D	313	GLN
1	D	330	ASN
1	D	366	HIS
1	D	382	ASN
1	D	450	ASN
1	D	452	ASN
1	D	457	GLN
1	D	473	ASN
1	D	527	ASN
1	D	547	GLN
1	E	23	HIS
1	E	66	GLN
1	E	70	GLN
1	E	146	ASN
1	E	218	HIS
1	E	243	ASN
1	E	246	GLN
1	E	286	HIS
1	E	288	ASN
1	E	294	HIS
1	E	312	HIS
1	E	313	GLN
1	E	330	ASN
1	E	382	ASN
1	E	450	ASN
1	E	452	ASN
1	E	457	GLN
1	E	473	ASN
1	E	527	ASN

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Mol	Chain	Res	Type
1	E	547	GLN
1	F	23	HIS
1	F	66	GLN
1	F	70	GLN
1	F	146	ASN
1	F	243	ASN
1	F	246	GLN
1	F	288	ASN
1	F	294	HIS
1	F	312	HIS
1	F	313	GLN
1	F	330	ASN
1	F	382	ASN
1	F	450	ASN
1	F	452	ASN
1	F	457	GLN
1	F	473	ASN
1	F	527	ASN
1	F	547	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)

6 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	$\#\|Z\| > 2$
1	TPQ	B	405	1	13,14,15	2.50	5 (38%)	15,19,21	1.34	2 (13%)
1	TPQ	C	405	1	13,14,15	2.52	7 (53%)	15,19,21	1.40	2 (13%)
1	TPQ	A	405	1	13,14,15	2.47	6 (46%)	15,19,21	1.25	2 (13%)
1	TPQ	E	405	1	13,14,15	2.37	5 (38%)	15,19,21	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPQ	D	405	1	13,14,15	2.66	6 (46%)	15,19,21	1.32	2 (13%)
1	TPQ	F	405	1	13,14,15	2.58	4 (30%)	15,19,21	1.31	2 (13%)

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
1	TPQ	B	405	1	-	2/5/22/24	0/1/1/1
1	TPQ	C	405	1	-	3/5/22/24	0/1/1/1
1	TPQ	A	405	1	-	3/5/22/24	0/1/1/1
1	TPQ	E	405	1	-	3/5/22/24	0/1/1/1
1	TPQ	D	405	1	-	3/5/22/24	0/1/1/1
1	TPQ	F	405	1	-	4/5/22/24	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TPQ	C1-C2	-6.69	1.39	1.49
1	D	405	TPQ	C1-C2	-6.45	1.39	1.49
1	C	405	TPQ	C1-C2	-6.36	1.39	1.49
1	F	405	TPQ	C1-C2	-6.30	1.39	1.49
1	A	405	TPQ	C1-C2	-6.27	1.39	1.49
1	E	405	TPQ	C1-C2	-5.42	1.41	1.49
1	F	405	TPQ	O5-C5	3.79	1.34	1.24
1	D	405	TPQ	C3-C4	3.78	1.41	1.35
1	E	405	TPQ	C3-C4	3.65	1.41	1.35
1	A	405	TPQ	C3-C4	3.38	1.40	1.35
1	C	405	TPQ	C3-C4	3.33	1.40	1.35
1	F	405	TPQ	C3-C4	3.32	1.40	1.35
1	B	405	TPQ	C3-C4	3.14	1.40	1.35
1	D	405	TPQ	O5-C5	2.91	1.32	1.24
1	E	405	TPQ	C6-C1	2.84	1.42	1.34
1	C	405	TPQ	O5-C5	2.61	1.31	1.24
1	F	405	TPQ	C6-C1	2.57	1.41	1.34
1	D	405	TPQ	C6-C1	2.46	1.41	1.34
1	A	405	TPQ	C6-C1	2.45	1.41	1.34
1	A	405	TPQ	O5-C5	2.33	1.30	1.24
1	C	405	TPQ	C6-C1	2.30	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TPQ	C4-C5	-2.29	1.40	1.47
1	A	405	TPQ	C4-C5	-2.28	1.40	1.47
1	B	405	TPQ	O5-C5	2.28	1.30	1.24
1	B	405	TPQ	C6-C1	2.17	1.40	1.34
1	E	405	TPQ	O5-C5	2.17	1.30	1.24
1	C	405	TPQ	C4-C5	-2.14	1.41	1.47
1	E	405	TPQ	C4-C5	-2.14	1.41	1.47
1	A	405	TPQ	C3-C2	-2.11	1.39	1.44
1	C	405	TPQ	O4-C4	2.10	1.39	1.34
1	D	405	TPQ	C4-C5	-2.05	1.41	1.47
1	C	405	TPQ	C3-C2	-2.04	1.39	1.44
1	D	405	TPQ	O4-C4	2.02	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	405	TPQ	CB-CA-C	-3.60	104.71	111.47
1	B	405	TPQ	CB-CA-C	-3.43	105.05	111.47
1	D	405	TPQ	CB-CA-C	-3.18	105.50	111.47
1	A	405	TPQ	CB-CA-C	-2.99	105.86	111.47
1	F	405	TPQ	CB-CA-C	-2.85	106.12	111.47
1	E	405	TPQ	CB-CA-C	-2.44	106.90	111.47
1	F	405	TPQ	CA-CB-C1	2.37	118.04	113.51
1	B	405	TPQ	CA-CB-C1	2.22	117.76	113.51
1	A	405	TPQ	CA-CB-C1	2.20	117.72	113.51
1	C	405	TPQ	CA-CB-C1	2.16	117.64	113.51
1	D	405	TPQ	C6-C1-C2	2.04	120.20	118.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	405	TPQ	N-CA-CB-C1
1	A	405	TPQ	C-CA-CB-C1
1	B	405	TPQ	N-CA-CB-C1
1	B	405	TPQ	C-CA-CB-C1
1	C	405	TPQ	N-CA-CB-C1
1	C	405	TPQ	C-CA-CB-C1
1	D	405	TPQ	N-CA-CB-C1
1	D	405	TPQ	C-CA-CB-C1
1	E	405	TPQ	N-CA-CB-C1
1	E	405	TPQ	C-CA-CB-C1

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Mol	Chain	Res	Type	Atoms
1	F	405	TPQ	N-CA-CB-C1
1	F	405	TPQ	C-CA-CB-C1
1	F	405	TPQ	C2-C1-CB-CA
1	F	405	TPQ	C6-C1-CB-CA
1	A	405	TPQ	C2-C1-CB-CA
1	C	405	TPQ	C2-C1-CB-CA
1	D	405	TPQ	C2-C1-CB-CA
1	E	405	TPQ	C2-C1-CB-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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.