Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2023 – 05:37 PM EDT

PDB ID	:	1RF0
Title	:	Crystal Structure of Fragment D of gammaE132A Fibrinogen
Authors	:	Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on	:	2003-11-07
Resolution	:	2.81 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:

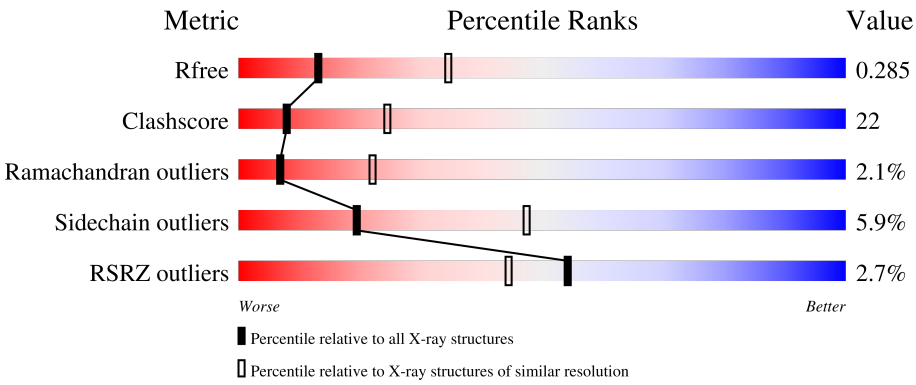
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.81 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))
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	66	2%, 62%, 32%, • •
1	D	66	2%, 44%, 38%, •, 15%
2	B	313	2%, 58%, 36%, • •
2	E	313	2%, 64%, 27%, • •
3	C	311	4%, 57%, 35%, • •

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Mol	Chain	Length	Quality of chain
3	F	311	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10772 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 Fibrinogen alpha/alpha-E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	64	523	322	99	99	3	0	0	0
1	D	56	458	280	87	88	3	0	0	0

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	306	2452	1528	432	470	22	0	0	0
2	E	300	2407	1503	425	457	22	0	0	0

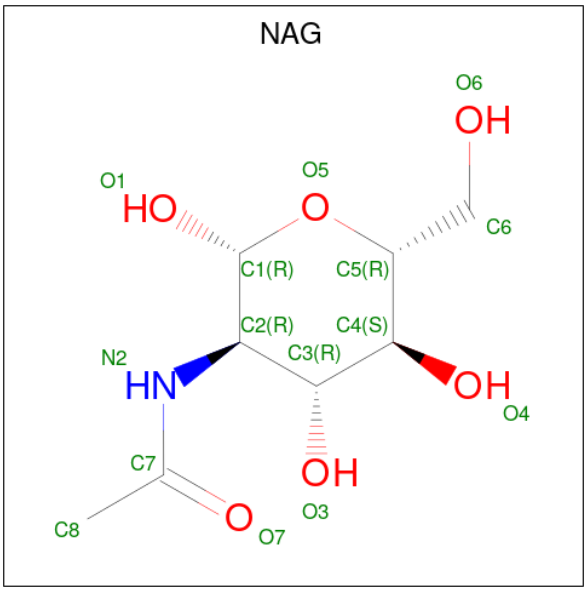
- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	298	2387	1515	402	459	11	0	0	0
3	F	299	2395	1521	403	460	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	ALA	GLU	engineered mutation	UNP P02679
F	132	ALA	GLU	engineered mutation	UNP P02679

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
4	E	1	14	8	1	5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	B	2	2	2	0	0
5	C	1	1	1	0	0
5	E	2	2	2	0	0
5	F	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	2	2	2	0	0
6	B	26	26	26	0	0
6	C	15	15	15	0	0

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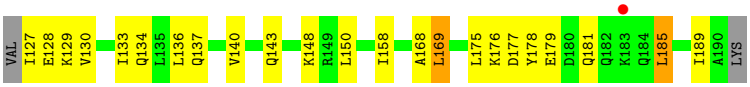
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	3	3	3	0	0
			Total	O		
6	E	50	50	50	0	0
			Total	O		
6	F	20	20	20	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: Fibrinogen alpha/alpha-E chain

Chain A:

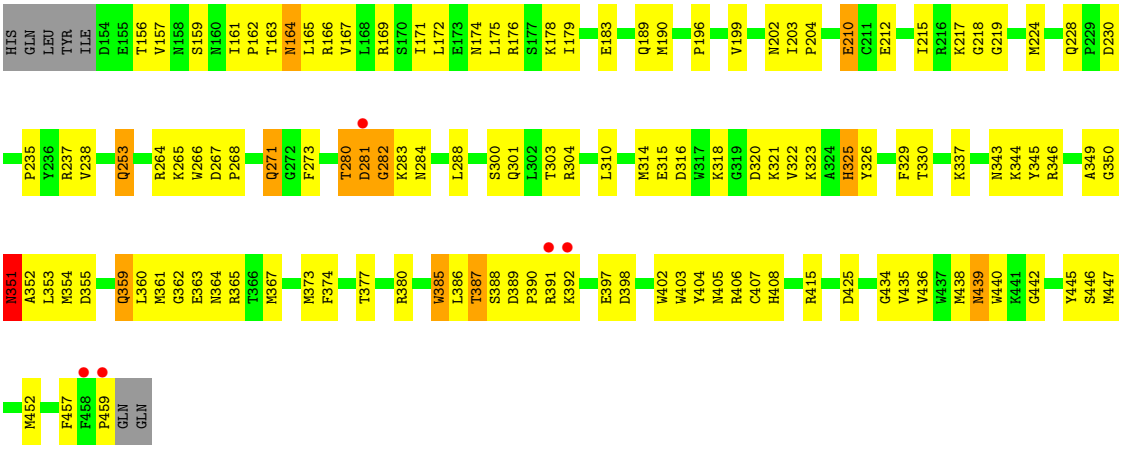


• Molecule 1: Fibrinogen alpha/alpha-E chain

Chain D:

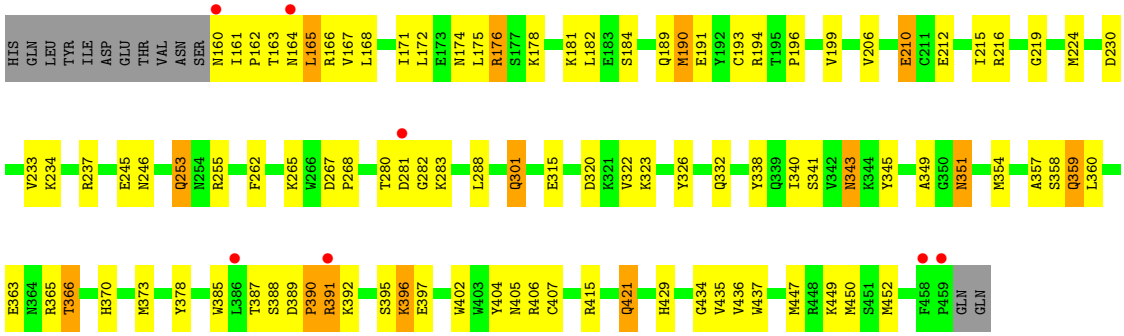
• Molecule 2: Fibrinogen beta chain

Chain B:



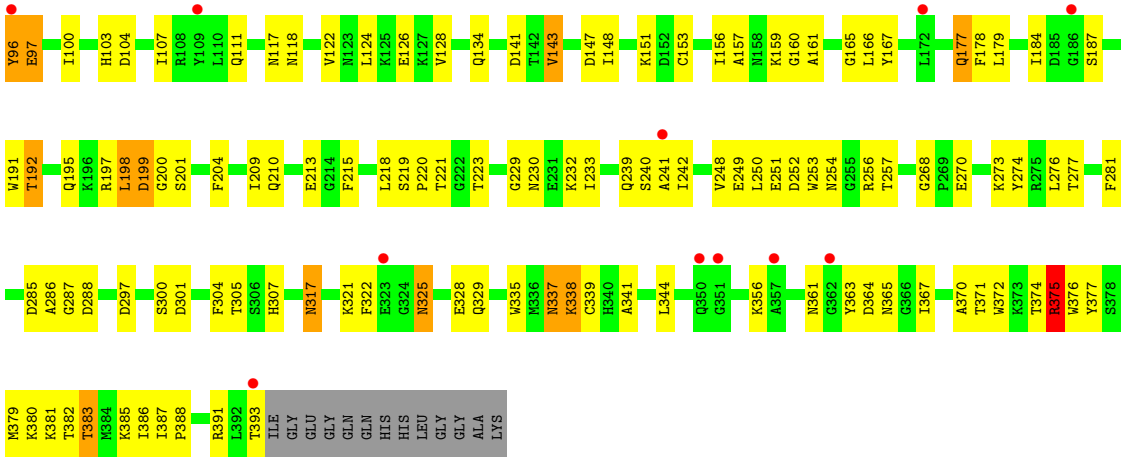
• Molecule 2: Fibrinogen beta chain

Chain E:



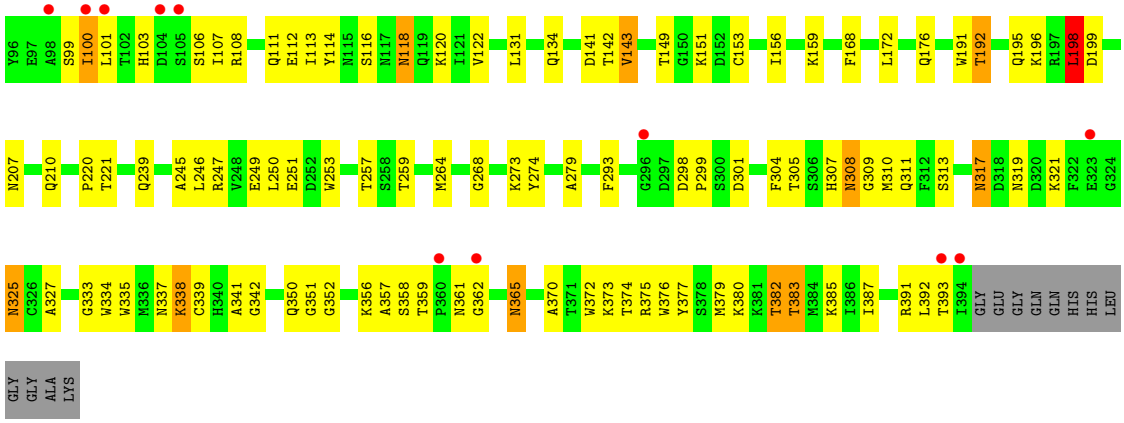
• Molecule 3: Fibrinogen gamma chain

Chain C:



• Molecule 3: Fibrinogen gamma chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.41Å 94.95Å 227.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.81 21.30 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.8 (17.97-2.81) 98.9 (21.30-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.84Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.286 0.233 , 0.285	Depositor DCC
R_{free} test set	2345 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10772	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: CA, NAG

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	0.30	0/524	0.53	0/699
1	D	0.32	0/458	0.56	0/610
2	B	0.37	0/2514	0.62	0/3397
2	E	0.40	0/2469	0.65	0/3335
3	C	0.37	0/2453	0.57	0/3319
3	F	0.38	0/2461	0.59	0/3330
All	All	0.37	0/10879	0.60	0/14690

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	523	0	547	32	0
1	D	458	0	477	39	0
2	B	2452	0	2312	116	0
2	E	2407	0	2275	106	0
3	C	2387	0	2234	105	0
3	F	2395	0	2245	96	0
4	B	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	14	0	13	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	B	26	0	0	1	0
6	C	15	0	0	3	0
6	D	3	0	0	0	0
6	E	50	0	0	2	0
6	F	20	0	0	0	0
All	All	10772	0	10116	447	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 22.

All (447) 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:A:168:ALA:HA	2:B:189:GLN:HE22	1.25	0.98
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.53	0.89
3:F:307:HIS:CE1	3:F:341:ALA:H	1.90	0.89
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.55	0.89
2:B:165:LEU:HD21	3:C:107:ILE:HD13	1.54	0.89
3:F:307:HIS:HE1	3:F:341:ALA:H	1.16	0.88
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.55	0.88
2:E:388:SER:O	2:E:390:PRO:HD3	1.73	0.88
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.56	0.85
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.57	0.85
2:B:439:ASN:H	2:B:439:ASN:HD22	1.23	0.84
3:C:325:ASN:ND2	3:C:328:GLU:H	1.78	0.81
2:B:388:SER:O	2:B:390:PRO:HD3	1.81	0.79
1:A:127:ILE:HG23	1:A:128:GLU:H	1.45	0.79
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.47	0.77
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.66	0.76
2:B:361:MET:HB2	4:B:500:NAG:H81	1.68	0.76
2:E:359:GLN:NE2	2:E:359:GLN:H	1.84	0.75
1:A:133:ILE:O	1:A:137:GLN:HG3	1.86	0.74
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.67	0.74
2:B:326:TYR:CE2	2:B:353:LEU:HD12	2.22	0.74
3:F:153:CYS:SG	3:F:192:THR:HB	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:LYS:N	3:C:339:CYS:HA	2.02	0.74
2:E:345:TYR:HB2	2:E:354:MET:CE	2.18	0.74
2:E:397:GLU:HB3	2:E:429:HIS:NE2	2.03	0.73
2:B:367:MET:HB2	2:B:406:ARG:HB2	1.72	0.72
2:B:408:HIS:O	2:B:438:MET:HE1	1.90	0.72
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.71	0.72
2:E:176:ARG:HB3	2:E:176:ARG:NH1	2.05	0.71
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.26	0.71
2:B:385:TRP:HE3	2:B:406:ARG:HG2	1.55	0.71
3:C:321:LYS:HB2	3:C:337:ASN:HD22	1.55	0.70
2:B:164:ASN:N	2:B:164:ASN:HD22	1.87	0.70
3:F:100:ILE:HG13	3:F:101:LEU:N	2.05	0.70
1:D:178:TYR:O	1:D:182:GLN:HG3	1.92	0.70
3:C:344:LEU:HB3	3:C:382:THR:HG21	1.74	0.70
3:F:321:LYS:O	3:F:338:LYS:HD3	1.93	0.69
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.75	0.69
3:C:344:LEU:HD13	3:C:382:THR:HG23	1.74	0.69
2:E:343:ASN:C	2:E:343:ASN:HD22	1.96	0.68
2:E:345:TYR:HB2	2:E:354:MET:HE3	1.74	0.68
2:E:406:ARG:HD3	6:E:92:HOH:O	1.93	0.68
3:F:338:LYS:N	3:F:339:CYS:HA	2.08	0.68
3:C:148:ILE:H	3:C:148:ILE:HD12	1.59	0.68
3:C:307:HIS:HE1	3:C:341:ALA:H	1.41	0.68
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.58	0.68
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.28	0.68
2:E:359:GLN:HE21	2:E:359:GLN:N	1.92	0.67
3:C:305:THR:HB	3:C:341:ALA:HB2	1.77	0.67
2:B:439:ASN:HD22	2:B:439:ASN:N	1.93	0.67
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.76	0.66
3:F:317:ASN:C	3:F:317:ASN:HD22	1.98	0.66
1:D:143:GLN:HE21	3:F:118:ASN:HD22	1.43	0.66
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.61	0.65
2:E:171:ILE:HD12	2:E:172:LEU:N	2.12	0.65
2:E:165:LEU:HD21	3:F:106:SER:HB2	1.78	0.65
2:B:163:THR:HA	2:B:166:ARG:HE	1.60	0.65
3:F:99:SER:O	3:F:101:LEU:N	2.30	0.65
3:F:307:HIS:CE1	3:F:342:GLY:H	2.13	0.65
3:C:200:GLY:HA2	6:C:421:HOH:O	1.96	0.64
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.98	0.64
1:A:127:ILE:HG12	1:A:128:GLU:N	2.11	0.64
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.62	0.64
3:F:103:HIS:O	3:F:107:ILE:HG12	1.97	0.64
3:C:322:PHE:HE2	3:C:329:GLN:HE22	1.46	0.64
2:E:176:ARG:HB3	2:E:176:ARG:HH11	1.63	0.63
1:A:140:VAL:HG12	2:B:172:LEU:HD21	1.80	0.63
3:C:192:THR:HG23	3:C:386:ILE:HG13	1.81	0.63
1:A:127:ILE:HG23	1:A:128:GLU:N	2.13	0.63
2:B:389:ASP:OD1	2:B:391:ARG:HB3	1.99	0.62
3:C:103:HIS:O	3:C:107:ILE:HG12	1.99	0.62
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.64	0.62
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.64	0.62
3:F:149:THR:HG22	3:F:168:PHE:O	2.00	0.62
2:E:172:LEU:HD22	3:F:113:ILE:HG13	1.82	0.61
3:F:356:LYS:O	3:F:362:GLY:HA2	1.99	0.61
2:B:169:ARG:HG2	2:B:169:ARG:HH11	1.66	0.61
2:B:176:ARG:HB2	3:C:117:ASN:HD21	1.66	0.61
1:D:134:GLN:O	1:D:138:LYS:HG3	1.99	0.61
2:B:351:ASN:ND2	2:B:354:MET:H	1.98	0.61
2:B:337:LYS:HE2	2:B:374:PHE:CG	2.35	0.61
3:C:248:VAL:HG13	3:C:344:LEU:HD11	1.82	0.61
3:C:281:PHE:HB2	3:C:288:ASP:OD2	2.00	0.61
3:C:321:LYS:HB2	3:C:337:ASN:ND2	2.15	0.61
2:B:165:LEU:HD21	3:C:107:ILE:CD1	2.31	0.60
2:B:280:THR:CG2	2:B:288:LEU:HG	2.32	0.60
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.16	0.60
3:C:252:ASP:OD2	3:C:256:ARG:HB2	2.01	0.60
1:D:169:LEU:H	2:E:189:GLN:HE22	1.50	0.60
2:E:391:ARG:O	2:E:391:ARG:HD3	2.00	0.60
2:B:389:ASP:OD1	2:B:392:LYS:HG3	2.01	0.60
2:B:351:ASN:HD22	2:B:351:ASN:C	2.03	0.60
1:A:178:TYR:CZ	2:B:178:LYS:HD3	2.37	0.60
1:D:171:ARG:HG3	1:D:171:ARG:HH11	1.66	0.60
3:C:251:GLU:HB2	3:C:257:THR:HG22	1.85	0.59
2:B:156:THR:O	2:B:159:SER:HB3	2.01	0.59
2:B:159:SER:C	2:B:162:PRO:HD2	2.22	0.59
2:B:343:ASN:OD1	2:B:344:LYS:HG3	2.03	0.59
2:E:199:VAL:O	3:F:142:THR:HG23	2.01	0.59
2:E:343:ASN:C	2:E:343:ASN:ND2	2.55	0.59
3:F:307:HIS:HE1	3:F:342:GLY:H	1.49	0.59
2:B:326:TYR:HE1	2:B:354:MET:HE2	1.68	0.59
2:B:439:ASN:H	2:B:439:ASN:ND2	1.97	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:LEU:O	2:E:172:LEU:HB2	2.02	0.59
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.02	0.59
3:C:118:ASN:O	3:C:122:VAL:HG23	2.03	0.59
3:C:307:HIS:HD2	3:C:335:TRP:O	1.86	0.59
2:B:323:LYS:NZ	2:B:325:HIS:HD2	2.00	0.58
3:F:251:GLU:CG	3:F:257:THR:HG22	2.31	0.58
2:B:217:LYS:HB3	3:C:213:GLU:HG3	1.85	0.58
3:F:250:LEU:HD12	3:F:379:MET:HG3	1.84	0.58
2:B:337:LYS:HE2	2:B:374:PHE:CD1	2.38	0.58
3:C:387:ILE:HG13	3:C:388:PRO:HD2	1.84	0.58
1:A:168:ALA:HA	2:B:189:GLN:NE2	2.08	0.58
1:D:140:VAL:HG23	1:D:141:ARG:N	2.19	0.58
2:E:165:LEU:HD21	3:F:106:SER:CB	2.33	0.58
1:A:185:LEU:O	1:A:189:ILE:HG13	2.04	0.57
1:D:169:LEU:H	2:E:189:GLN:NE2	2.01	0.57
2:B:224:MET:CE	2:B:237:ARG:HD3	2.35	0.57
2:B:385:TRP:NE1	2:B:392:LYS:HB3	2.20	0.57
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.05	0.57
2:E:233:VAL:HG22	2:E:234:LYS:H	1.70	0.57
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.85	0.57
3:F:359:THR:HG22	3:F:361:ASN:H	1.69	0.56
2:B:267:ASP:O	2:B:271:GLN:HG2	2.04	0.56
2:E:340:ILE:HG12	2:E:341:SER:N	2.19	0.56
3:F:107:ILE:O	3:F:111:GLN:HG2	2.05	0.56
2:B:385:TRP:HE1	2:B:392:LYS:HB3	1.70	0.56
3:C:160:GLY:O	3:C:161:ALA:C	2.42	0.56
3:C:276:LEU:HD12	3:C:277:THR:N	2.20	0.56
2:E:363:GLU:HA	2:E:366:THR:HG23	1.87	0.56
3:F:307:HIS:HE1	3:F:341:ALA:N	1.94	0.56
3:C:338:LYS:O	3:C:338:LYS:HG2	2.04	0.56
2:B:405:ASN:C	2:B:406:ARG:HG3	2.26	0.56
3:C:156:ILE:HG22	3:C:161:ALA:CB	2.36	0.56
3:C:270:GLU:HG3	3:C:274:TYR:CZ	2.40	0.56
3:F:357:ALA:O	3:F:359:THR:N	2.39	0.56
3:C:122:VAL:O	3:C:126:GLU:HG3	2.05	0.56
3:C:248:VAL:CG1	3:C:344:LEU:HD11	2.36	0.56
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.04	0.56
3:F:365:ASN:H	3:F:365:ASN:ND2	2.04	0.56
2:B:266:TRP:HA	2:B:377:THR:HG21	1.88	0.55
2:E:164:ASN:C	2:E:166:ARG:H	2.09	0.55
2:E:215:ILE:HA	2:E:219:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:THR:HA	2:B:166:ARG:NE	2.20	0.55
2:E:358:SER:HA	2:E:365:ARG:HH22	1.70	0.55
1:A:130:VAL:O	1:A:134:GLN:HG3	2.06	0.55
2:B:406:ARG:N	2:B:407:CYS:HA	2.20	0.55
2:B:439:ASN:N	2:B:439:ASN:ND2	2.53	0.55
2:E:358:SER:HA	2:E:365:ARG:NH2	2.22	0.55
3:F:264:MET:HB2	3:F:279:ALA:H	1.71	0.55
3:C:96:TYR:O	3:C:97:GLU:HB2	2.07	0.55
2:B:265:LYS:O	2:B:268:PRO:HD2	2.06	0.55
2:B:351:ASN:HD21	2:B:354:MET:H	1.55	0.55
2:B:389:ASP:CG	2:B:392:LYS:HG3	2.26	0.55
3:C:141:ASP:OD1	3:C:143:VAL:HG13	2.07	0.55
2:B:318:LYS:HD2	2:B:318:LYS:N	2.21	0.55
2:B:361:MET:HB2	4:B:500:NAG:C8	2.35	0.54
3:C:221:THR:O	3:C:223:THR:HG23	2.07	0.54
1:D:143:GLN:HE21	3:F:118:ASN:ND2	2.05	0.54
2:E:332:GLN:O	2:E:338:TYR:HA	2.08	0.54
3:C:325:ASN:C	3:C:325:ASN:HD22	2.10	0.54
2:E:265:LYS:O	2:E:268:PRO:HD2	2.08	0.54
2:E:326:TYR:HE1	2:E:354:MET:HE2	1.72	0.54
3:C:197:ARG:HB2	3:C:382:THR:HB	1.90	0.54
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.89	0.54
1:D:140:VAL:HG23	1:D:141:ARG:H	1.73	0.54
1:D:188:VAL:HB	2:E:164:ASN:OD1	2.08	0.54
2:E:233:VAL:HG22	2:E:234:LYS:N	2.22	0.54
3:C:248:VAL:HG12	3:C:250:LEU:CD1	2.38	0.54
2:E:397:GLU:HB3	2:E:429:HIS:CE1	2.43	0.54
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.89	0.54
2:E:359:GLN:H	2:E:359:GLN:HE21	1.48	0.54
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.89	0.53
3:F:374:THR:O	3:F:376:TRP:N	2.40	0.53
1:A:136:LEU:O	1:A:140:VAL:HG13	2.08	0.53
2:B:457:PHE:O	2:B:459:PRO:HD3	2.09	0.53
3:C:167:TYR:O	3:C:179:LEU:HD12	2.09	0.53
3:C:307:HIS:CE1	3:C:341:ALA:H	2.26	0.53
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.44	0.53
2:E:245:GLU:O	2:E:246:ASN:HB2	2.08	0.53
2:B:179:ILE:O	2:B:183:GLU:HG3	2.08	0.53
3:F:250:LEU:N	3:F:250:LEU:HD22	2.24	0.53
3:F:357:ALA:C	3:F:359:THR:H	2.12	0.53
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:O	1:D:140:VAL:HG22	2.08	0.52
1:A:177:ASP:O	1:A:181:GLN:HG3	2.10	0.52
1:D:175:LEU:HD22	1:D:175:LEU:H	1.75	0.52
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.92	0.52
2:B:434:GLY:O	2:B:436:VAL:N	2.43	0.52
2:B:253:GLN:HB3	2:B:452:MET:HB2	1.91	0.52
3:C:156:ILE:O	3:C:159:LYS:HB2	2.10	0.52
2:E:191:GLU:HA	2:E:194:ARG:HD2	1.91	0.52
1:A:178:TYR:OH	2:B:178:LYS:HD3	2.10	0.51
2:B:360:LEU:HD13	2:B:364:ASN:O	2.10	0.51
2:E:385:TRP:CE2	2:E:392:LYS:HD2	2.44	0.51
2:B:363:GLU:HG2	2:B:367:MET:CE	2.40	0.51
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.11	0.51
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.25	0.51
3:F:246:LEU:HD12	3:F:247:ARG:N	2.25	0.51
3:C:287:GLY:HA3	3:C:371:THR:OG1	2.11	0.51
3:F:196:LYS:HD2	3:F:383:THR:HB	1.92	0.51
1:D:133:ILE:HG12	3:F:107:ILE:HD12	1.93	0.51
2:E:160:ASN:HD22	2:E:163:THR:HB	1.76	0.51
2:E:172:LEU:HD22	3:F:113:ILE:CD1	2.40	0.51
2:E:359:GLN:NE2	2:E:359:GLN:N	2.52	0.51
2:E:392:LYS:O	2:E:392:LYS:HG3	2.10	0.51
2:B:164:ASN:N	2:B:164:ASN:ND2	2.57	0.50
2:B:434:GLY:O	2:B:436:VAL:HG23	2.11	0.50
3:F:374:THR:C	3:F:376:TRP:H	2.15	0.50
2:B:363:GLU:O	2:B:367:MET:HG2	2.11	0.50
2:E:406:ARG:N	2:E:407:CYS:HA	2.26	0.50
3:F:100:ILE:HG13	3:F:101:LEU:H	1.77	0.50
2:B:350:GLY:O	2:B:352:ALA:N	2.40	0.50
3:F:308:ASN:HD22	3:F:309:GLY:N	2.09	0.50
3:F:365:ASN:N	3:F:365:ASN:HD22	2.09	0.50
3:C:374:THR:C	3:C:376:TRP:H	2.14	0.50
3:F:273:LYS:HD2	3:F:319:ASN:OD1	2.12	0.50
2:E:391:ARG:HD3	2:E:396:LYS:NZ	2.27	0.50
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.94	0.49
2:B:325:HIS:HB2	2:B:346:ARG:O	2.12	0.49
3:C:153:CYS:SG	3:C:192:THR:HB	2.52	0.49
2:E:389:ASP:O	2:E:391:ARG:N	2.45	0.49
3:F:249:GLU:HG3	3:F:259:THR:HG22	1.93	0.49
3:F:268:GLY:O	3:F:274:TYR:HD1	1.95	0.49
3:F:304:PHE:HA	3:F:337:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ASN:O	2:E:178:LYS:HG2	2.12	0.49
2:B:228:GLN:HB2	2:B:235:PRO:HG3	1.93	0.49
3:C:361:ASN:HB2	3:C:363:TYR:CE1	2.48	0.49
3:C:364:ASP:OD2	3:C:375:ARG:NH1	2.45	0.49
3:F:108:ARG:O	3:F:112:GLU:HB2	2.12	0.49
3:F:304:PHE:C	3:F:337:ASN:ND2	2.65	0.49
3:F:172:LEU:CD2	3:F:239:GLN:HE21	2.25	0.49
2:B:385:TRP:CD1	2:B:392:LYS:HB3	2.47	0.49
3:C:166:LEU:HB3	3:C:179:LEU:HD11	1.93	0.49
3:C:107:ILE:O	3:C:111:GLN:HG3	2.13	0.49
3:F:307:HIS:HD2	3:F:335:TRP:O	1.95	0.49
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.12	0.49
1:A:169:LEU:H	2:B:189:GLN:NE2	2.11	0.49
3:C:253:TRP:CE3	3:C:380:LYS:HG3	2.48	0.49
1:A:127:ILE:CG2	1:A:129:LYS:HG2	2.42	0.49
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.13	0.49
3:C:165:GLY:O	3:C:167:TYR:HD1	1.96	0.49
1:D:133:ILE:HD11	3:F:107:ILE:HD11	1.95	0.49
2:B:300:SER:O	2:B:304:ARG:HG3	2.12	0.48
3:C:124:LEU:O	3:C:128:VAL:HG23	2.13	0.48
1:D:158:ILE:HG23	2:E:189:GLN:NE2	2.25	0.48
2:E:212:GLU:HG3	2:E:216:ARG:NH1	2.29	0.48
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.95	0.48
3:F:253:TRP:HA	3:F:380:LYS:HD2	1.95	0.48
2:B:386:LEU:O	2:B:387:THR:HB	2.13	0.48
2:B:385:TRP:CE3	2:B:406:ARG:HG2	2.44	0.48
1:A:127:ILE:CG2	1:A:128:GLU:H	2.15	0.48
3:C:166:LEU:HD21	3:C:219:SER:N	2.29	0.48
2:E:164:ASN:C	2:E:166:ARG:N	2.67	0.48
3:F:305:THR:HB	3:F:341:ALA:HB2	1.95	0.48
2:B:176:ARG:HB2	3:C:117:ASN:ND2	2.29	0.48
3:C:197:ARG:HD3	3:C:204:PHE:CZ	2.48	0.48
2:E:161:ILE:CB	2:E:162:PRO:HD3	2.31	0.48
2:E:434:GLY:O	2:E:436:VAL:HG23	2.14	0.48
2:B:316:ASP:OD2	2:B:320:ASP:HB2	2.14	0.47
2:B:373:MET:HE2	2:B:404:TYR:O	2.14	0.47
3:C:166:LEU:HD22	3:C:218:LEU:HB3	1.96	0.47
3:F:251:GLU:HG3	3:F:257:THR:CG2	2.35	0.47
3:C:100:ILE:O	3:C:100:ILE:HG22	2.14	0.47
2:B:175:LEU:O	2:B:179:ILE:HG13	2.15	0.47
2:B:352:ALA:HB2	2:B:439:ASN:ND2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:313:SER:OG	3:F:319:ASN:N	2.47	0.47
3:F:338:LYS:N	3:F:339:CYS:CA	2.78	0.47
2:E:281:ASP:O	2:E:283:LYS:N	2.47	0.47
3:F:325:ASN:HD22	3:F:325:ASN:C	2.18	0.47
3:C:304:PHE:HB3	3:C:338:LYS:O	2.14	0.47
2:E:167:VAL:HG23	2:E:168:LEU:N	2.30	0.47
2:E:255:ARG:HB2	2:E:450:MET:HB3	1.96	0.47
2:B:405:ASN:O	2:B:406:ARG:HG3	2.14	0.47
3:C:229:GLY:O	3:C:233:ILE:HG13	2.14	0.47
3:C:367:ILE:O	3:C:379:MET:HG2	2.15	0.47
3:C:393:THR:O	3:C:393:THR:HG22	2.15	0.47
3:F:118:ASN:O	3:F:122:VAL:HG23	2.14	0.47
2:B:397:GLU:HG2	2:B:398:ASP:N	2.30	0.47
3:C:177:GLN:HE21	3:C:177:GLN:HB2	1.53	0.47
3:F:365:ASN:H	3:F:365:ASN:HD22	1.60	0.47
3:C:230:ASN:HB3	3:C:274:TYR:CG	2.50	0.47
1:D:175:LEU:HD22	1:D:175:LEU:N	2.30	0.47
2:B:169:ARG:HG2	2:B:169:ARG:NH1	2.28	0.47
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.97	0.47
2:B:266:TRP:CE3	2:B:380:ARG:HG2	2.50	0.46
2:E:389:ASP:C	2:E:391:ARG:H	2.18	0.46
2:E:396:LYS:HG3	2:E:429:HIS:CD2	2.50	0.46
2:B:389:ASP:C	2:B:391:ARG:H	2.18	0.46
2:E:345:TYR:CB	2:E:354:MET:HE3	2.42	0.46
1:A:175:LEU:O	1:A:179:GLU:HG3	2.15	0.46
3:C:251:GLU:CB	3:C:257:THR:HG22	2.44	0.46
1:D:175:LEU:O	1:D:179:GLU:HG3	2.15	0.46
1:A:185:LEU:HD22	1:A:189:ILE:CG1	2.45	0.46
3:C:273:LYS:NZ	3:C:317:ASN:HD21	2.13	0.46
1:D:181:GLN:OE1	2:E:171:ILE:HA	2.15	0.46
1:A:127:ILE:HG12	1:A:128:GLU:H	1.80	0.46
2:B:237:ARG:HG3	6:B:62:HOH:O	2.14	0.46
3:C:209:ILE:HG13	6:C:409:HOH:O	2.15	0.46
1:D:135:LEU:HD13	1:D:139:ASN:OD1	2.16	0.46
2:E:322:VAL:HG23	2:E:349:ALA:HB2	1.98	0.46
2:E:436:VAL:HG13	6:E:51:HOH:O	2.14	0.46
2:B:363:GLU:HG2	2:B:367:MET:HE3	1.97	0.46
3:C:184:ILE:HD12	3:C:184:ILE:N	2.31	0.46
2:B:264:ARG:HD2	2:B:273:PHE:CD2	2.51	0.46
2:E:340:ILE:CG1	2:E:341:SER:N	2.78	0.46
2:E:171:ILE:HD12	2:E:171:ILE:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:LYS:HG2	2:E:182:LEU:N	2.30	0.46
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.98	0.46
2:B:345:TYR:HB2	2:B:354:MET:CE	2.45	0.46
2:B:440:TRP:HE3	2:B:447:MET:HE3	1.81	0.46
3:C:156:ILE:HG22	3:C:161:ALA:HB2	1.97	0.46
2:E:167:VAL:O	2:E:171:ILE:HG13	2.16	0.46
3:F:393:THR:HG22	3:F:393:THR:O	2.16	0.46
2:B:351:ASN:ND2	2:B:351:ASN:C	2.67	0.45
2:B:385:TRP:CZ3	2:B:406:ARG:HB3	2.50	0.45
3:F:143:VAL:HA	3:F:220:PRO:HG2	1.98	0.45
1:D:143:GLN:NE2	3:F:118:ASN:HD22	2.13	0.45
2:E:280:THR:HB	2:E:288:LEU:HG	1.99	0.45
1:A:175:LEU:O	1:A:178:TYR:HB2	2.16	0.45
3:C:387:ILE:HG13	3:C:388:PRO:CD	2.46	0.45
2:E:326:TYR:CE1	2:E:354:MET:HE2	2.51	0.45
3:F:249:GLU:HB3	3:F:383:THR:CG2	2.44	0.45
1:A:185:LEU:HD22	1:A:189:ILE:HG13	1.97	0.45
2:B:323:LYS:NZ	2:B:325:HIS:CD2	2.82	0.45
3:C:165:GLY:O	3:C:167:TYR:CD1	2.70	0.45
2:E:281:ASP:C	2:E:283:LYS:H	2.20	0.45
2:B:215:ILE:HA	2:B:219:GLY:O	2.16	0.45
2:B:315:GLU:OE1	2:B:321:LYS:HE2	2.17	0.45
1:D:165:CYS:HB3	2:E:193:CYS:HA	1.99	0.45
3:C:96:TYR:O	3:C:97:GLU:CB	2.64	0.45
3:C:177:GLN:H	3:C:177:GLN:HG3	1.44	0.45
1:D:136:LEU:HD21	3:F:111:GLN:HB3	1.97	0.45
2:E:436:VAL:HG12	2:E:437:TRP:N	2.31	0.45
3:F:374:THR:C	3:F:376:TRP:N	2.70	0.45
2:B:212:GLU:O	2:B:215:ILE:HG22	2.17	0.45
2:E:206:VAL:O	2:E:206:VAL:HG13	2.17	0.45
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.80	0.45
2:B:159:SER:CA	2:B:162:PRO:HD2	2.47	0.44
3:F:172:LEU:HD23	3:F:239:GLN:HE21	1.82	0.44
3:F:198:LEU:HD12	3:F:199:ASP:N	2.32	0.44
1:D:181:GLN:HG2	2:E:171:ILE:HG22	2.00	0.44
2:E:253:GLN:HB3	2:E:452:MET:HB2	1.99	0.44
3:C:337:ASN:HD22	3:C:337:ASN:C	2.20	0.44
1:D:186:GLU:C	1:D:188:VAL:H	2.21	0.44
2:E:351:ASN:ND2	2:E:354:MET:HB2	2.33	0.44
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.82	0.44
2:B:280:THR:O	2:B:281:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:LYS:HB2	2:B:374:PHE:CD1	2.52	0.44
3:C:157:ALA:C	3:C:159:LYS:H	2.21	0.44
2:E:172:LEU:HD22	3:F:113:ILE:CG1	2.45	0.44
2:E:224:MET:CE	2:E:237:ARG:HD3	2.47	0.44
3:F:293:PHE:CG	3:F:370:ALA:HB1	2.53	0.44
3:F:333:GLY:O	3:F:334:TRP:HB2	2.17	0.44
2:B:351:ASN:ND2	2:B:351:ASN:O	2.51	0.44
1:D:188:VAL:HG12	2:E:164:ASN:HD21	1.82	0.44
2:E:421:GLN:HE21	2:E:421:GLN:HB2	1.56	0.44
3:F:372:TRP:O	3:F:373:LYS:HD3	2.18	0.44
3:C:179:LEU:HD23	3:C:218:LEU:HD12	2.00	0.43
3:F:268:GLY:O	3:F:274:TYR:HA	2.17	0.43
3:F:373:LYS:HB3	3:F:377:TYR:HB3	2.00	0.43
3:C:300:SER:O	3:C:301:ASP:C	2.57	0.43
2:E:164:ASN:O	2:E:166:ARG:N	2.51	0.43
3:C:199:ASP:OD1	3:C:201:SER:N	2.50	0.43
1:D:171:ARG:HG3	1:D:171:ARG:NH1	2.33	0.43
2:E:255:ARG:HD3	2:E:262:PHE:CZ	2.53	0.43
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.36	0.43
3:F:172:LEU:HD22	3:F:172:LEU:H	1.84	0.43
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.53	0.43
3:C:270:GLU:HG3	3:C:274:TYR:CE2	2.54	0.43
2:B:280:THR:HG23	2:B:288:LEU:HG	1.99	0.43
3:C:297:ASP:OD1	3:C:375:ARG:NH2	2.51	0.43
3:C:338:LYS:N	3:C:339:CYS:CA	2.79	0.43
2:E:171:ILE:O	2:E:175:LEU:HG	2.19	0.43
3:C:156:ILE:CG2	3:C:161:ALA:HB2	2.49	0.43
1:D:175:LEU:H	1:D:175:LEU:CD2	2.31	0.43
3:F:305:THR:O	3:F:341:ALA:HB2	2.19	0.42
1:A:127:ILE:HG21	1:A:129:LYS:HG2	2.00	0.42
2:B:438:MET:O	2:B:442:GLY:HA2	2.20	0.42
2:E:373:MET:SD	2:E:405:ASN:ND2	2.93	0.42
3:F:311:GLN:O	3:F:335:TRP:HA	2.19	0.42
1:A:148:LYS:HD3	2:B:425:ASP:OD2	2.19	0.42
2:B:345:TYR:CG	2:B:346:ARG:N	2.86	0.42
3:C:240:SER:O	3:C:242:ILE:HG13	2.20	0.42
3:C:286:ALA:O	3:C:372:TRP:HB2	2.20	0.42
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.54	0.42
3:F:116:SER:O	3:F:120:LYS:HG3	2.19	0.42
2:E:163:THR:HG23	2:E:166:ARG:NH2	2.35	0.42
2:E:172:LEU:HD11	3:F:114:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:357:ALA:HB3	2:E:360:LEU:CD1	2.44	0.42
1:D:136:LEU:O	1:D:140:VAL:HG13	2.19	0.42
2:E:391:ARG:O	2:E:391:ARG:CD	2.68	0.42
3:F:245:ALA:HB1	3:F:392:LEU:HD11	2.00	0.42
2:B:310:LEU:HB2	2:B:329:PHE:CD2	2.54	0.42
2:E:160:ASN:ND2	2:E:163:THR:HB	2.34	0.42
3:C:356:LYS:HG3	3:C:376:TRP:CH2	2.55	0.42
1:A:143:GLN:HE22	3:C:117:ASN:HB2	1.85	0.42
1:A:185:LEU:HD22	1:A:189:ILE:CD1	2.49	0.42
2:E:415:ARG:O	2:E:434:GLY:HA2	2.19	0.42
3:F:246:LEU:HD12	3:F:247:ARG:H	1.84	0.42
2:B:355:ASP:O	2:B:365:ARG:HD3	2.19	0.41
1:D:150:LEU:O	1:D:154:ILE:HG13	2.19	0.41
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.45	0.41
2:B:157:VAL:C	2:B:159:SER:H	2.23	0.41
2:B:303:THR:HB	2:B:330:THR:HA	2.01	0.41
2:E:378:TYR:HA	2:E:395:SER:O	2.20	0.41
3:C:215:PHE:HA	6:C:410:HOH:O	2.20	0.41
3:C:219:SER:HA	3:C:220:PRO:HD3	1.89	0.41
2:E:190:MET:CE	3:F:131:LEU:HA	2.50	0.41
3:C:268:GLY:O	3:C:274:TYR:HA	2.20	0.41
3:C:387:ILE:CG1	3:C:388:PRO:HD2	2.48	0.41
3:C:304:PHE:CD1	3:C:338:LYS:HD3	2.55	0.41
1:D:175:LEU:O	1:D:178:TYR:HB2	2.21	0.41
1:A:136:LEU:HD21	3:C:111:GLN:HG2	2.01	0.41
2:B:282:GLY:O	2:B:283:LYS:HG2	2.20	0.41
2:B:322:VAL:HG23	2:B:349:ALA:HB2	2.02	0.41
2:B:359:GLN:O	2:B:360:LEU:HD23	2.20	0.41
2:E:395:SER:HB2	2:E:404:TYR:CE2	2.55	0.41
2:B:163:THR:O	2:B:167:VAL:HG23	2.21	0.41
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.93	0.41
2:B:314:MET:SD	2:B:447:MET:HE3	2.61	0.41
3:F:317:ASN:C	3:F:317:ASN:ND2	2.70	0.41
3:F:310:MET:HA	3:F:310:MET:CE	2.51	0.41
3:C:285:ASP:OD1	3:C:285:ASP:N	2.54	0.40
3:C:374:THR:O	3:C:376:TRP:N	2.53	0.40
1:D:188:VAL:HG12	2:E:164:ASN:ND2	2.36	0.40
2:E:301:GLN:NE2	2:E:301:GLN:C	2.74	0.40
2:E:351:ASN:C	2:E:351:ASN:HD22	2.23	0.40
2:E:436:VAL:CG1	2:E:437:TRP:N	2.84	0.40
3:F:298:ASP:HA	3:F:299:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLY:HA3	3:C:210:GLN:HG2	2.02	0.40
2:B:402:TRP:CG	2:B:403:TRP:N	2.89	0.40
3:C:148:ILE:HD12	3:C:148:ILE:N	2.32	0.40
3:F:149:THR:HA	3:F:156:ILE:HD11	2.03	0.40
3:F:373:LYS:HG3	3:F:377:TYR:HD2	1.86	0.40
2:B:171:ILE:O	2:B:174:ASN:HB3	2.21	0.40
2:B:415:ARG:O	2:B:434:GLY:HA2	2.21	0.40
1:D:141:ARG:O	1:D:145:VAL:HG23	2.22	0.40
1:A:176:LYS:O	1:A:179:GLU:N	2.55	0.40
2:E:212:GLU:O	2:E:215:ILE:HG22	2.21	0.40
2:E:281:ASP:C	2:E:283:LYS:N	2.75	0.40
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.86	0.40
2:E:163:THR:HG23	2:E:166:ARG:HH21	1.86	0.40
3:F:350:GLN:O	3:F:352:GLY:N	2.51	0.40
3:F:373:LYS:CG	3:F:377:TYR:HD2	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	62/66 (94%)	55 (89%)	7 (11%)	0	100	100
1	D	54/66 (82%)	48 (89%)	6 (11%)	0	100	100
2	B	304/313 (97%)	270 (89%)	27 (9%)	7 (2%)	6	20
2	E	298/313 (95%)	265 (89%)	28 (9%)	5 (2%)	9	27
3	C	296/311 (95%)	259 (88%)	27 (9%)	10 (3%)	3	12
3	F	297/311 (96%)	264 (89%)	27 (9%)	6 (2%)	7	23
All	All	1311/1380 (95%)	1161 (89%)	122 (9%)	28 (2%)	7	22

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	281	ASP
2	B	435	VAL
3	F	100	ILE
3	F	358	SER
2	B	282	GLY
2	B	351	ASN
3	C	198	LEU
3	C	241	ALA
3	C	254	ASN
3	C	338	LYS
3	C	375	ARG
3	F	375	ARG
3	C	199	ASP
3	C	370	ALA
2	E	387	THR
2	E	390	PRO
3	F	338	LYS
2	B	387	THR
3	C	97	GLU
3	C	187	SER
2	E	165	LEU
2	E	282	GLY
3	C	391	ARG
2	B	359	GLN
2	B	362	GLY
3	F	198	LEU
3	F	351	GLY
2	E	435	VAL

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	59/61 (97%)	57 (97%)	2 (3%)	37	69
1	D	52/61 (85%)	49 (94%)	3 (6%)	20	48
2	B	264/271 (97%)	249 (94%)	15 (6%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	258/271 (95%)	240 (93%)	18 (7%)	15	39
3	C	250/258 (97%)	236 (94%)	14 (6%)	21	49
3	F	251/258 (97%)	236 (94%)	15 (6%)	19	47
All	All	1134/1180 (96%)	1067 (94%)	67 (6%)	19	47

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	185	LEU
2	B	164	ASN
2	B	190	MET
2	B	196	PRO
2	B	210	GLU
2	B	230	ASP
2	B	238	VAL
2	B	253	GLN
2	B	271	GLN
2	B	280	THR
2	B	301	GLN
2	B	325	HIS
2	B	351	ASN
2	B	385	TRP
2	B	439	ASN
2	B	446	SER
3	C	96	TYR
3	C	104	ASP
3	C	134	GLN
3	C	143	VAL
3	C	147	ASP
3	C	177	GLN
3	C	192	THR
3	C	198	LEU
3	C	317	ASN
3	C	325	ASN
3	C	337	ASN
3	C	365	ASN
3	C	375	ARG
3	C	383	THR
1	D	135	LEU
1	D	176	LYS

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Mol	Chain	Res	Type
1	D	185	LEU
2	E	176	ARG
2	E	184	SER
2	E	190	MET
2	E	196	PRO
2	E	210	GLU
2	E	230	ASP
2	E	253	GLN
2	E	301	GLN
2	E	320	ASP
2	E	323	LYS
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	366	THR
2	E	391	ARG
2	E	396	LYS
2	E	421	GLN
2	E	447	MET
3	F	118	ASN
3	F	134	GLN
3	F	143	VAL
3	F	159	LYS
3	F	176	GLN
3	F	192	THR
3	F	198	LEU
3	F	221	THR
3	F	301	ASP
3	F	308	ASN
3	F	317	ASN
3	F	325	ASN
3	F	365	ASN
3	F	382	THR
3	F	383	THR

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	131	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN

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Mol	Chain	Res	Type
2	B	164	ASN
2	B	189	GLN
2	B	202	ASN
2	B	228	GLN
2	B	253	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	405	ASN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	117	ASN
3	C	119	GLN
3	C	136	GLN
3	C	144	GLN
3	C	163	GLN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	325	ASN
3	C	329	GLN
3	C	337	ASN
3	C	365	ASN
1	D	134	GLN
1	D	137	GLN
1	D	184	GLN
1	D	187	GLN
2	E	160	ASN
2	E	164	ASN
2	E	174	ASN
2	E	189	GLN
2	E	202	ASN
2	E	243	ASN
2	E	253	GLN
2	E	296	ASN
2	E	301	GLN

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Mol	Chain	Res	Type
2	E	325	HIS
2	E	339	GLN
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	421	GLN
2	E	439	ASN
3	F	118	ASN
3	F	134	GLN
3	F	136	GLN
3	F	176	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	308	ASN
3	F	317	ASN
3	F	325	ASN
3	F	337	ASN
3	F	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	NAG	B	500	2	14,14,15	0.56	0	17,19,21	0.76	1 (5%)
4	NAG	E	500	2	14,14,15	0.58	0	17,19,21	0.72	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	NAG	B	500	2	-	2/6/23/26	0/1/1/1
4	NAG	E	500	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	500	NAG	C2-N2-C7	-2.32	119.60	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	500	NAG	C8-C7-N2-C2
4	B	500	NAG	O7-C7-N2-C2
4	E	500	NAG	C8-C7-N2-C2
4	E	500	NAG	O7-C7-N2-C2
4	E	500	NAG	C4-C5-C6-O6
4	E	500	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	500	NAG	2	0

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	64/66 (96%)	-0.06	1 (1%)	72	65	20, 56, 85, 91	0
1	D	56/66 (84%)	0.15	1 (1%)	68	61	24, 52, 105, 113	0
2	B	306/313 (97%)	-0.32	5 (1%)	72	65	16, 33, 73, 94	0
2	E	300/313 (95%)	-0.40	7 (2%)	60	50	11, 25, 68, 114	0
3	C	298/311 (95%)	-0.09	11 (3%)	41	31	23, 43, 68, 89	0
3	F	299/311 (96%)	-0.11	11 (3%)	41	31	11, 34, 78, 101	0
All	All	1323/1380 (95%)	-0.21	36 (2%)	54	44	11, 35, 79, 114	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	393	THR	4.7
2	E	160	ASN	4.5
3	F	394	ILE	4.4
3	F	101	LEU	4.2
2	B	391	ARG	3.8
2	E	164	ASN	3.5
3	C	393	THR	3.3
2	E	391	ARG	3.3
3	F	296	GLY	3.1
3	C	96	TYR	2.8
3	F	360	PRO	2.7
2	B	281	ASP	2.7
1	A	183	LYS	2.6
2	B	459	PRO	2.6
3	C	351	GLY	2.6
3	C	357	ALA	2.6
3	C	323	GLU	2.5
3	F	100	ILE	2.5
3	C	350	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	362	GLY	2.4
3	F	98	ALA	2.4
3	C	362	GLY	2.3
2	E	386	LEU	2.3
2	E	458	PHE	2.3
2	B	458	PHE	2.3
3	F	105	SER	2.2
2	B	392	LYS	2.2
2	E	459	PRO	2.2
3	C	109	TYR	2.2
3	C	172	LEU	2.1
2	E	281	ASP	2.1
3	C	186	GLY	2.1
3	C	241	ALA	2.0
3	F	104	ASP	2.0
3	F	323	GLU	2.0
1	D	184	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	500	14/15	0.80	0.28	65,68,69,71	0
4	NAG	B	500	14/15	0.81	0.39	80,83,84,85	0
5	CA	C	407	1/1	0.87	0.05	50,50,50,50	0
5	CA	F	407	1/1	0.93	0.07	39,39,39,39	0
5	CA	E	502	1/1	0.96	0.08	37,37,37,37	0
5	CA	B	502	1/1	0.97	0.20	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	E	501	1/1	0.97	0.05	31,31,31,31	0
5	CA	B	501	1/1	0.99	0.06	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.