Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 07:57 PM EDT

PDB ID	:	3DRU
Title	:	Crystal Structure of Gly117Phe Alpha1-Antitrypsin
Authors	:	Gooptu, B.; Nobeli, I.; Purkiss, A.; Phillips, R.L.; Mallya, M.; Lomas, D.A.; Barrett, T.E.
Deposited on	:	2008-07-11
Resolution	:	3.20 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 ⓘ symbol.

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

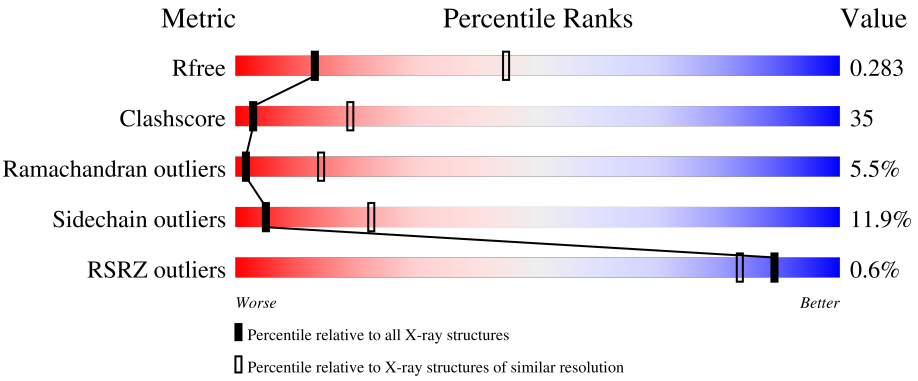
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	404	45% 37% 7% • 10%
1	B	404	40% 40% 8% • 10%
1	C	404	% 37% 40% 11% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8560 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 Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2861	1845	466	541	9			
1	B	362	Total	C	N	O	S	0	0	0
			2867	1849	467	542	9			
1	C	360	Total	C	N	O	S	0	0	0
			2832	1825	462	537	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP P01009
A	-8	ARG	-	expression tag	UNP P01009
A	-7	GLY	-	expression tag	UNP P01009
A	-6	SER	-	expression tag	UNP P01009
A	-5	HIS	-	expression tag	UNP P01009
A	-4	HIS	-	expression tag	UNP P01009
A	-3	HIS	-	expression tag	UNP P01009
A	-2	HIS	-	expression tag	UNP P01009
A	-1	HIS	-	expression tag	UNP P01009
A	0	HIS	-	expression tag	UNP P01009
A	1	THR	-	expression tag	UNP P01009
A	117	PHE	GLY	engineered mutation	UNP P01009
B	-9	MET	-	expression tag	UNP P01009
B	-8	ARG	-	expression tag	UNP P01009
B	-7	GLY	-	expression tag	UNP P01009
B	-6	SER	-	expression tag	UNP P01009
B	-5	HIS	-	expression tag	UNP P01009
B	-4	HIS	-	expression tag	UNP P01009
B	-3	HIS	-	expression tag	UNP P01009
B	-2	HIS	-	expression tag	UNP P01009
B	-1	HIS	-	expression tag	UNP P01009
B	0	HIS	-	expression tag	UNP P01009
B	1	THR	-	expression tag	UNP P01009

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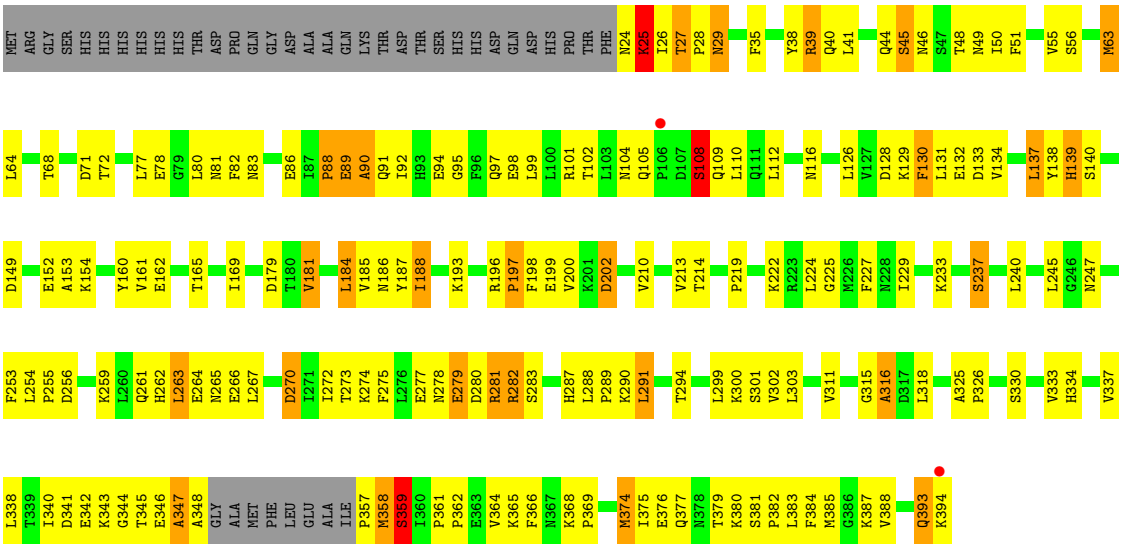
Chain	Residue	Modelled	Actual	Comment	Reference
B	117	PHE	GLY	engineered mutation	UNP P01009
C	-9	MET	-	expression tag	UNP P01009
C	-8	ARG	-	expression tag	UNP P01009
C	-7	GLY	-	expression tag	UNP P01009
C	-6	SER	-	expression tag	UNP P01009
C	-5	HIS	-	expression tag	UNP P01009
C	-4	HIS	-	expression tag	UNP P01009
C	-3	HIS	-	expression tag	UNP P01009
C	-2	HIS	-	expression tag	UNP P01009
C	-1	HIS	-	expression tag	UNP P01009
C	0	HIS	-	expression tag	UNP P01009
C	1	THR	-	expression tag	UNP P01009
C	117	PHE	GLY	engineered mutation	UNP P01009

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.

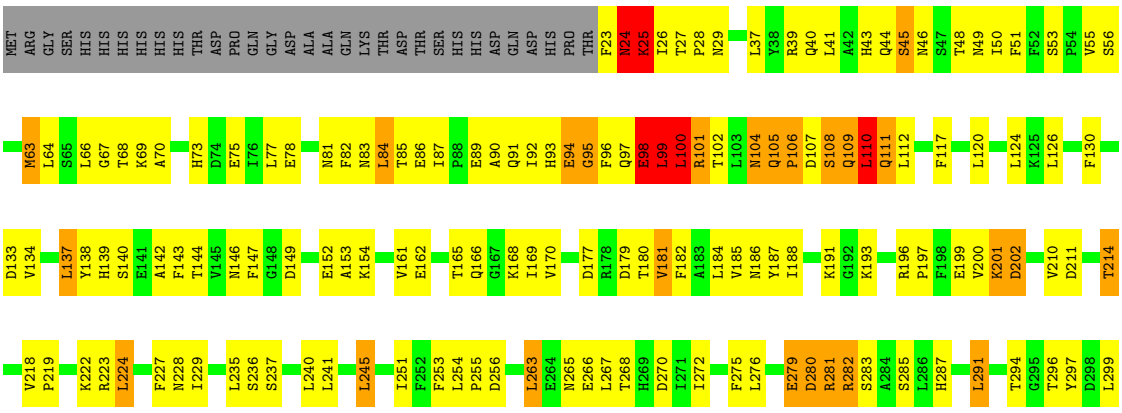
• Molecule 1: Alpha-1-antitrypsin

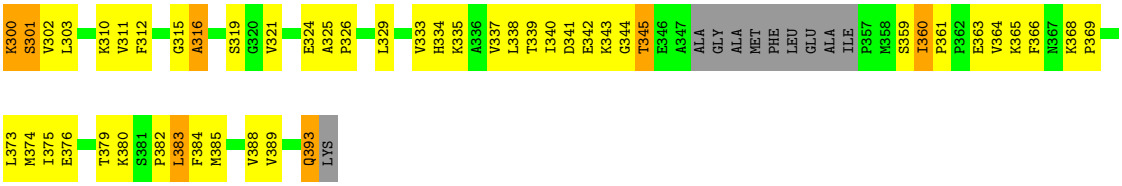
Chain A:



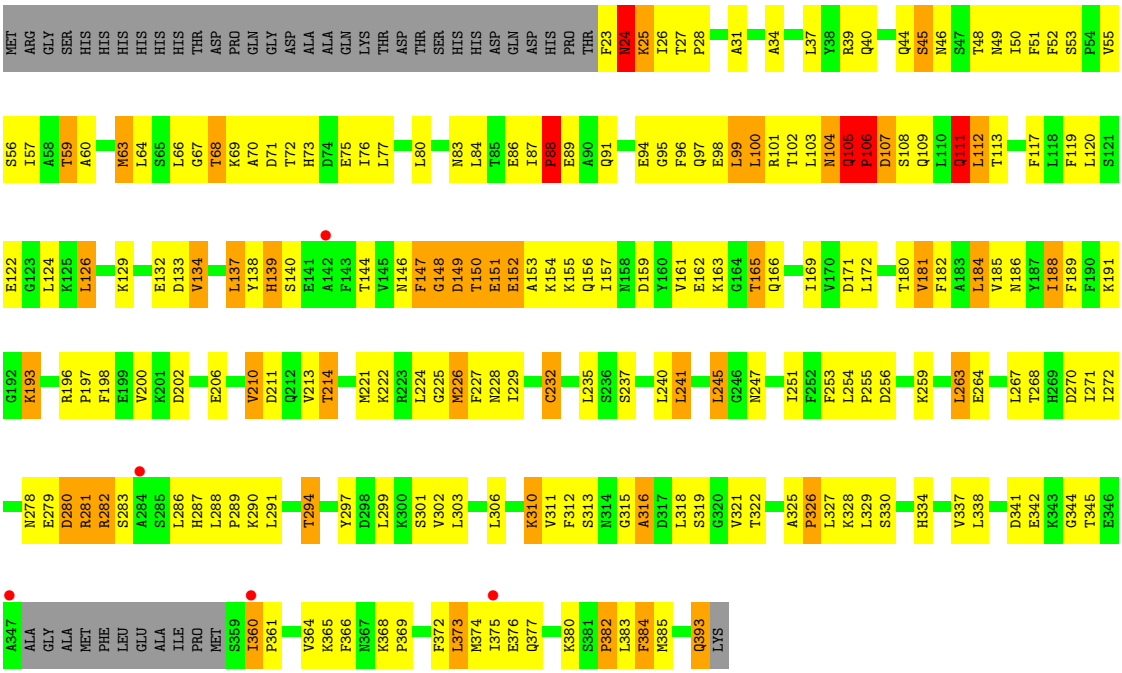
• Molecule 1: Alpha-1-antitrypsin

Chain B:





- Molecule 1: Alpha-1-antitrypsin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.84Å 149.30Å 77.29Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	55.00 – 3.20 77.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (55.00-3.20) 99.7 (77.09-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.290 0.238 , 0.283	Depositor DCC
R_{free} test set	1340 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	72.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8560	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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

5.1 Standard geometry

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	0.51	0/2920	0.73	0/3948
1	B	0.53	0/2926	0.79	4/3955 (0.1%)
1	C	0.46	0/2890	0.75	4/3911 (0.1%)
All	All	0.50	0/8736	0.76	8/11814 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	152	GLU	N-CA-C	-9.51	85.34	111.00
1	C	105	GLN	N-CA-C	-6.62	93.11	111.00
1	C	279	GLU	N-CA-C	-6.58	93.24	111.00
1	B	110	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	101	ARG	N-CA-C	-5.60	95.87	111.00
1	C	146	ASN	C-N-CA	5.54	135.55	121.70
1	B	99	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	224	LEU	CA-CB-CG	-5.08	103.61	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2861	0	2858	171	3
1	B	2867	0	2874	207	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2832	0	2814	219	0
All	All	8560	0	8546	595	3

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 35.

All (595) 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:100:LEU:HD12	1:C:100:LEU:H	1.13	1.12
1:A:348:ALA:HB2	1:C:98:GLU:HG3	1.16	1.10
1:B:294:THR:HG22	1:B:337:VAL:HG13	1.25	1.10
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.35	1.09
1:B:109:GLN:O	1:B:110:LEU:HB3	1.54	1.06
1:C:280:ASP:O	1:C:281:ARG:HG2	1.57	1.04
1:B:100:LEU:HD23	1:B:100:LEU:H	1.21	1.01
1:C:152:GLU:O	1:C:156:GLN:N	1.94	1.00
1:B:196:ARG:HH12	1:B:281:ARG:NH2	1.61	0.99
1:C:197:PRO:HB3	1:C:344:GLY:HA3	1.47	0.95
1:A:358:MET:O	1:A:358:MET:HG3	1.63	0.94
1:B:96:PHE:O	1:B:100:LEU:HD21	1.67	0.94
1:A:29:ASN:H	1:A:29:ASN:HD22	1.02	0.94
1:B:197:PRO:HB3	1:B:344:GLY:HA3	1.47	0.94
1:B:24:ASN:O	1:B:25:LYS:HB2	1.67	0.92
1:A:237:SER:HB3	1:A:255:PRO:HA	1.51	0.92
1:B:100:LEU:HD23	1:B:100:LEU:N	1.84	0.92
1:B:109:GLN:HG2	1:B:245:LEU:HD12	1.49	0.92
1:A:63:MET:HE1	1:A:64:LEU:HA	1.50	0.92
1:B:282:ARG:CB	1:B:282:ARG:HH11	1.84	0.91
1:B:254:LEU:HD11	1:B:368:LYS:HE2	1.52	0.89
1:B:294:THR:CG2	1:B:337:VAL:HG13	2.03	0.89
1:A:49:ASN:O	1:A:50:ILE:HD12	1.73	0.89
1:B:99:LEU:O	1:B:102:THR:N	2.07	0.88
1:A:49:ASN:H	1:A:393:GLN:HE22	1.21	0.87
1:B:25:LYS:NZ	1:B:25:LYS:HA	1.90	0.87
1:C:106:PRO:HG2	1:C:107:ASP:H	1.38	0.86
1:A:29:ASN:HD22	1:A:29:ASN:N	1.70	0.86
1:A:25:LYS:O	1:A:25:LYS:HD3	1.74	0.85
1:C:134:VAL:HG12	1:C:140:SER:HB2	1.59	0.84
1:B:282:ARG:HH11	1:B:282:ARG:HB3	1.42	0.84
1:B:99:LEU:O	1:B:101:ARG:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:NH1	1:B:281:ARG:HH22	1.74	0.83
1:A:358:MET:O	1:A:358:MET:CG	2.27	0.83
1:C:161:VAL:O	1:C:165:THR:HB	1.79	0.83
1:C:237:SER:HB3	1:C:255:PRO:HA	1.61	0.83
1:B:267:LEU:HD22	1:B:272:ILE:HD11	1.59	0.82
1:C:126:LEU:HD12	1:C:126:LEU:H	1.44	0.82
1:B:287:HIS:HB2	1:B:365:LYS:HA	1.62	0.82
1:C:100:LEU:HD12	1:C:100:LEU:N	1.94	0.81
1:A:294:THR:HG22	1:A:337:VAL:HG13	1.62	0.81
1:C:23:PHE:O	1:C:24:ASN:HB2	1.81	0.81
1:C:96:PHE:O	1:C:100:LEU:CD1	2.28	0.80
1:C:256:ASP:HB2	1:C:259:LYS:HG3	1.63	0.80
1:C:99:LEU:O	1:C:102:THR:HB	1.80	0.80
1:C:287:HIS:HB2	1:C:365:LYS:HA	1.63	0.79
1:A:197:PRO:HB3	1:A:344:GLY:HA3	1.63	0.78
1:C:282:ARG:HH11	1:C:282:ARG:HB3	1.46	0.78
1:A:287:HIS:HB2	1:A:365:LYS:HA	1.66	0.78
1:C:112:LEU:HD23	1:C:113:THR:N	1.99	0.78
1:A:375:ILE:HD12	1:A:380:LYS:O	1.83	0.78
1:B:254:LEU:HB2	1:B:366:PHE:CE2	2.19	0.77
1:C:96:PHE:O	1:C:100:LEU:HD11	1.84	0.77
1:B:106:PRO:HG2	1:B:107:ASP:H	1.51	0.76
1:B:100:LEU:H	1:B:100:LEU:CD2	1.97	0.76
1:A:29:ASN:N	1:A:29:ASN:ND2	2.31	0.76
1:C:280:ASP:O	1:C:281:ARG:CG	2.34	0.76
1:C:151:GLU:HA	1:C:154:LYS:HB3	1.67	0.75
1:B:25:LYS:HA	1:B:25:LYS:HZ3	1.49	0.75
1:C:98:GLU:O	1:C:99:LEU:CB	2.34	0.74
1:C:166:GLN:HA	1:C:166:GLN:HE21	1.52	0.74
1:B:91:GLN:O	1:B:94:GLU:HB3	1.86	0.74
1:C:55:VAL:HG23	1:C:382:PRO:O	1.88	0.73
1:B:99:LEU:HG	1:B:100:LEU:H	1.54	0.73
1:C:147:PHE:CE2	1:C:180:THR:HB	2.23	0.73
1:C:226:MET:HE2	1:C:226:MET:H	1.54	0.73
1:B:254:LEU:CD1	1:B:368:LYS:HE2	2.18	0.72
1:B:134:VAL:HG12	1:B:140:SER:HB2	1.70	0.72
1:B:96:PHE:O	1:B:100:LEU:CD2	2.38	0.72
1:B:196:ARG:NH1	1:B:281:ARG:NH2	2.31	0.72
1:C:222:LYS:HE2	1:C:287:HIS:CD2	2.24	0.72
1:A:83:ASN:HB3	1:A:86:GLU:HG2	1.72	0.72
1:A:27:THR:HG23	1:A:381:SER:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:PHE:HE2	1:C:181:VAL:N	1.89	0.71
1:A:97:GLN:HB3	1:A:101:ARG:HH21	1.55	0.71
1:A:49:ASN:N	1:A:393:GLN:HE22	1.88	0.70
1:C:198:PHE:HB2	1:C:342:GLU:HB3	1.73	0.70
1:B:237:SER:HB3	1:B:255:PRO:HA	1.73	0.70
1:C:120:LEU:HD22	1:C:126:LEU:HD23	1.71	0.70
1:B:360:ILE:HG22	1:B:360:ILE:O	1.91	0.70
1:C:210:VAL:HG13	1:C:214:THR:HB	1.72	0.70
1:A:29:ASN:H	1:A:29:ASN:ND2	1.80	0.70
1:A:56:SER:OG	1:A:186:ASN:ND2	2.22	0.69
1:B:55:VAL:HG23	1:B:382:PRO:O	1.93	0.69
1:C:282:ARG:HH11	1:C:282:ARG:CB	2.04	0.69
1:C:325:ALA:HB1	1:C:326:PRO:HD2	1.75	0.69
1:A:83:ASN:HD22	1:A:86:GLU:CG	2.06	0.69
1:B:109:GLN:CG	1:B:245:LEU:HD12	2.21	0.68
1:B:23:PHE:O	1:B:25:LYS:N	2.27	0.68
1:A:91:GLN:O	1:A:94:GLU:HB3	1.94	0.68
1:C:254:LEU:HB2	1:C:366:PHE:CE2	2.29	0.67
1:A:63:MET:CE	1:A:64:LEU:HA	2.24	0.67
1:A:364:VAL:HG12	1:A:364:VAL:O	1.95	0.67
1:C:37:LEU:HD13	1:C:306:LEU:HD11	1.77	0.67
1:C:122:GLU:HB2	1:C:144:THR:HB	1.77	0.67
1:C:383:LEU:C	1:C:384:PHE:HD2	1.99	0.67
1:A:108:SER:O	1:A:110:LEU:N	2.28	0.66
1:B:184:LEU:HD23	1:B:185:VAL:N	2.10	0.66
1:C:63:MET:HE1	1:C:64:LEU:HA	1.76	0.66
1:A:49:ASN:C	1:A:50:ILE:HD12	2.15	0.66
1:A:68:THR:HG22	1:A:318:LEU:HD23	1.78	0.66
1:B:83:ASN:HD22	1:B:86:GLU:HG2	1.61	0.66
1:C:299:LEU:HB3	1:C:303:LEU:CD1	2.26	0.66
1:C:156:GLN:O	1:C:159:ASP:HB2	1.96	0.66
1:B:197:PRO:HB3	1:B:344:GLY:CA	2.24	0.66
1:C:75:GLU:CD	1:C:310:LYS:HD2	2.16	0.66
1:A:89:GLU:C	1:A:91:GLN:H	1.99	0.65
1:C:318:LEU:HD12	1:C:327:LEU:HB3	1.79	0.65
1:A:346:GLU:O	1:A:347:ALA:HB2	1.97	0.65
1:C:112:LEU:HD23	1:C:112:LEU:C	2.17	0.65
1:B:44:GLN:O	1:B:45:SER:CB	2.45	0.64
1:B:315:GLY:O	1:B:316:ALA:C	2.34	0.64
1:C:104:ASN:CG	1:C:104:ASN:O	2.35	0.64
1:B:282:ARG:HB3	1:B:282:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:O	1:C:165:THR:HG22	1.97	0.64
1:A:83:ASN:HD22	1:A:86:GLU:HG2	1.62	0.64
1:C:153:ALA:O	1:C:157:ILE:N	2.31	0.64
1:B:137:LEU:H	1:B:137:LEU:HD23	1.62	0.64
1:C:129:LYS:O	1:C:132:GLU:HB3	1.98	0.64
1:A:358:MET:O	1:A:359:SER:HB2	1.98	0.64
1:B:184:LEU:HD23	1:B:184:LEU:C	2.18	0.64
1:B:179:ASP:O	1:B:181:VAL:HG13	1.99	0.63
1:B:199:GLU:O	1:B:202:ASP:HB2	1.97	0.63
1:B:291:LEU:HD23	1:B:340:ILE:HB	1.79	0.63
1:B:199:GLU:OE1	1:B:201:LYS:HG3	1.98	0.63
1:C:197:PRO:HB3	1:C:344:GLY:CA	2.25	0.63
1:C:83:ASN:ND2	1:C:86:GLU:HB2	2.14	0.63
1:A:299:LEU:HB3	1:A:303:LEU:CD1	2.29	0.63
1:C:88:PRO:HD2	1:C:91:GLN:HE21	1.63	0.63
1:C:287:HIS:CG	1:C:365:LYS:HG2	2.33	0.63
1:C:75:GLU:OE1	1:C:310:LYS:HD2	1.99	0.63
1:C:383:LEU:HB3	1:C:384:PHE:HD2	1.64	0.63
1:A:134:VAL:HG12	1:A:140:SER:HB2	1.81	0.62
1:B:44:GLN:O	1:B:45:SER:HB3	1.99	0.62
1:C:87:ILE:HG12	1:C:88:PRO:HD2	1.80	0.62
1:A:280:ASP:O	1:A:281:ARG:HG3	1.99	0.62
1:C:221:MET:SD	1:C:342:GLU:HG3	2.39	0.62
1:B:63:MET:HE1	1:B:64:LEU:HA	1.81	0.62
1:C:69:LYS:HE2	1:C:319:SER:OG	1.99	0.62
1:A:105:GLN:CB	1:A:108:SER:OG	2.48	0.62
1:A:25:LYS:O	1:A:25:LYS:CD	2.45	0.61
1:A:149:ASP:HB3	1:A:152:GLU:HB3	1.80	0.61
1:C:166:GLN:HA	1:C:166:GLN:NE2	2.14	0.61
1:B:92:ILE:HG22	1:B:96:PHE:CD2	2.36	0.61
1:C:294:THR:HG22	1:C:337:VAL:HG13	1.83	0.61
1:B:280:ASP:C	1:B:281:ARG:HG2	2.21	0.61
1:B:253:PHE:HB3	1:B:263:LEU:HD11	1.83	0.61
1:C:375:ILE:CG2	1:C:376:GLU:N	2.63	0.61
1:A:245:LEU:HD13	1:A:345:THR:CG2	2.31	0.61
1:B:50:ILE:HA	1:B:297:TYR:OH	1.99	0.61
1:B:104:ASN:O	1:B:105:GLN:O	2.18	0.60
1:B:130:PHE:O	1:B:134:VAL:HG23	2.01	0.60
1:C:288:LEU:HD12	1:C:289:PRO:HD2	1.83	0.60
1:B:44:GLN:O	1:B:44:GLN:HG3	2.02	0.60
1:B:229:ILE:HD11	1:B:364:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLU:OE1	1:C:98:GLU:HA	2.01	0.60
1:B:84:LEU:HD22	1:B:84:LEU:H	1.67	0.60
1:B:137:LEU:HD23	1:B:137:LEU:N	2.16	0.60
1:C:147:PHE:CE2	1:C:180:THR:C	2.75	0.60
1:C:256:ASP:HB2	1:C:259:LYS:CG	2.32	0.60
1:C:383:LEU:HB3	1:C:384:PHE:CD2	2.37	0.59
1:C:98:GLU:O	1:C:99:LEU:HB2	2.01	0.59
1:C:106:PRO:O	1:C:107:ASP:C	2.40	0.59
1:A:348:ALA:HB2	1:C:98:GLU:CG	2.11	0.59
1:C:299:LEU:HB3	1:C:303:LEU:HD12	1.84	0.59
1:A:196:ARG:HH22	1:A:281:ARG:NH2	2.00	0.59
1:A:374:MET:HB2	1:A:384:PHE:HB2	1.83	0.59
1:C:100:LEU:H	1:C:100:LEU:CD1	2.01	0.59
1:C:104:ASN:OD1	1:C:139:HIS:CE1	2.56	0.59
1:C:383:LEU:C	1:C:384:PHE:CD2	2.76	0.59
1:A:99:LEU:HD12	1:A:99:LEU:O	2.03	0.58
1:A:213:VAL:HG23	1:A:214:THR:N	2.18	0.58
1:B:210:VAL:HG13	1:B:214:THR:HB	1.85	0.58
1:A:222:LYS:HE2	1:A:287:HIS:CD2	2.38	0.58
1:B:165:THR:HG21	1:B:169:ILE:H	1.68	0.58
1:B:49:ASN:H	1:B:393:GLN:HE22	1.52	0.58
1:A:161:VAL:O	1:A:165:THR:HG22	2.04	0.58
1:B:25:LYS:HA	1:B:25:LYS:HZ2	1.66	0.58
1:B:99:LEU:HG	1:B:100:LEU:HD23	1.85	0.58
1:B:379:THR:O	1:B:380:LYS:HB2	2.03	0.58
1:C:147:PHE:CE2	1:C:181:VAL:N	2.72	0.58
1:B:325:ALA:HB1	1:B:326:PRO:CD	2.34	0.57
1:A:280:ASP:O	1:A:281:ARG:CG	2.52	0.57
1:B:27:THR:HB	1:B:28:PRO:HD3	1.86	0.57
1:A:282:ARG:HB3	1:A:282:ARG:HH11	1.69	0.57
1:B:210:VAL:HG23	1:B:389:VAL:O	2.04	0.57
1:C:237:SER:CB	1:C:255:PRO:HA	2.32	0.57
1:C:360:ILE:HD13	1:C:361:PRO:HD2	1.86	0.57
1:A:27:THR:N	1:A:28:PRO:CD	2.66	0.57
1:A:51:PHE:CZ	1:A:338:LEU:HB2	2.39	0.57
1:C:27:THR:HB	1:C:28:PRO:HD3	1.86	0.57
1:C:232:CYS:SG	1:C:235:LEU:HB2	2.44	0.57
1:C:373:LEU:HD23	1:C:373:LEU:O	2.04	0.57
1:B:228:ASN:HB3	1:B:241:LEU:HB3	1.87	0.57
1:C:228:ASN:HB3	1:C:241:LEU:HB3	1.86	0.57
1:A:184:LEU:HD23	1:A:185:VAL:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PHE:CE1	1:C:329:LEU:HD23	2.40	0.57
1:A:27:THR:HG23	1:A:381:SER:CA	2.33	0.57
1:C:51:PHE:CZ	1:C:384:PHE:HD1	2.23	0.57
1:A:77:LEU:O	1:A:82:PHE:HB2	2.05	0.57
1:C:98:GLU:O	1:C:99:LEU:HB3	2.04	0.57
1:C:211:ASP:HB3	1:C:214:THR:H	1.69	0.57
1:A:245:LEU:HD13	1:A:345:THR:HG22	1.87	0.56
1:B:82:PHE:CD2	1:B:92:ILE:HD13	2.39	0.56
1:B:287:HIS:CG	1:B:365:LYS:HG2	2.39	0.56
1:A:267:LEU:HD22	1:A:272:ILE:HD11	1.87	0.56
1:C:97:GLN:NE2	1:C:137:LEU:HD13	2.20	0.56
1:A:254:LEU:HB2	1:A:366:PHE:CE2	2.40	0.56
1:B:99:LEU:CG	1:B:100:LEU:H	2.16	0.56
1:C:60:ALA:HB2	1:C:186:ASN:ND2	2.21	0.56
1:C:134:VAL:CG1	1:C:140:SER:HB2	2.34	0.56
1:C:147:PHE:HD2	1:C:180:THR:O	1.88	0.56
1:A:63:MET:HE1	1:A:64:LEU:CA	2.32	0.56
1:A:229:ILE:HD11	1:A:364:VAL:HG21	1.87	0.56
1:C:99:LEU:O	1:C:102:THR:N	2.38	0.56
1:A:129:LYS:O	1:A:132:GLU:HB3	2.05	0.56
1:A:126:LEU:HD12	1:A:126:LEU:H	1.70	0.56
1:A:196:ARG:NH2	1:A:281:ARG:NH2	2.54	0.56
1:B:134:VAL:CG1	1:B:140:SER:HB2	2.35	0.56
1:B:126:LEU:H	1:B:126:LEU:HD12	1.71	0.56
1:C:166:GLN:HE21	1:C:166:GLN:CA	2.15	0.56
1:A:83:ASN:HB3	1:A:86:GLU:OE2	2.06	0.55
1:A:44:GLN:O	1:A:45:SER:HB3	2.06	0.55
1:B:63:MET:HE2	1:B:63:MET:O	2.07	0.55
1:B:112:LEU:HD11	1:B:383:LEU:HD21	1.88	0.55
1:B:300:LYS:HE3	1:B:312:PHE:HB3	1.88	0.55
1:C:104:ASN:OD1	1:C:139:HIS:HE1	1.89	0.55
1:C:188:ILE:HD11	1:C:384:PHE:CZ	2.42	0.55
1:C:322:THR:HG21	1:C:327:LEU:HD13	1.88	0.55
1:C:111:GLN:OE1	1:C:111:GLN:HA	2.05	0.55
1:B:99:LEU:HD12	1:B:100:LEU:N	2.22	0.55
1:C:311:VAL:HG23	1:C:318:LEU:HD21	1.89	0.55
1:B:68:THR:OG1	1:B:73:HIS:HB2	2.06	0.54
1:C:184:LEU:HD23	1:C:185:VAL:N	2.22	0.54
1:B:184:LEU:C	1:B:184:LEU:CD2	2.75	0.54
1:C:377:GLN:O	1:C:380:LYS:NZ	2.41	0.54
1:A:315:GLY:O	1:A:316:ALA:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:PHE:CE2	1:C:180:THR:CB	2.90	0.54
1:C:37:LEU:HD23	1:C:52:PHE:HE2	1.71	0.54
1:A:41:LEU:O	1:A:44:GLN:HG2	2.08	0.54
1:C:360:ILE:CD1	1:C:361:PRO:HD2	2.37	0.54
1:B:338:LEU:HD12	1:B:339:THR:H	1.72	0.54
1:C:106:PRO:CG	1:C:107:ASP:H	2.12	0.54
1:B:241:LEU:HD13	1:B:275:PHE:HE2	1.73	0.54
1:C:44:GLN:O	1:C:45:SER:HB3	2.08	0.54
1:A:229:ILE:HB	1:A:240:LEU:HD12	1.90	0.54
1:A:253:PHE:HB3	1:A:263:LEU:HD11	1.90	0.53
1:C:37:LEU:HD23	1:C:52:PHE:CE2	2.43	0.53
1:C:126:LEU:HD12	1:C:126:LEU:N	2.18	0.53
1:A:261:GLN:HE21	1:A:265:ASN:HD21	1.56	0.53
1:C:253:PHE:HB3	1:C:263:LEU:HD11	1.90	0.53
1:C:267:LEU:HD22	1:C:272:ILE:HD11	1.89	0.53
1:B:78:GLU:HG3	1:B:84:LEU:HD21	1.89	0.53
1:C:111:GLN:O	1:C:112:LEU:HB2	2.09	0.53
1:C:373:LEU:HD23	1:C:373:LEU:C	2.28	0.53
1:A:89:GLU:O	1:A:91:GLN:N	2.41	0.53
1:C:49:ASN:H	1:C:393:GLN:HE22	1.55	0.53
1:A:299:LEU:HB3	1:A:303:LEU:HD12	1.90	0.53
1:B:37:LEU:O	1:B:41:LEU:HG	2.09	0.53
1:B:312:PHE:CE1	1:B:329:LEU:HD23	2.43	0.53
1:C:23:PHE:O	1:C:24:ASN:CB	2.54	0.53
1:C:53:SER:HB3	1:C:56:SER:HB3	1.90	0.53
1:B:97:GLN:NE2	1:B:137:LEU:HB2	2.24	0.52
1:A:89:GLU:HG3	1:A:90:ALA:H	1.74	0.52
1:B:149:ASP:HB3	1:B:152:GLU:HB3	1.91	0.52
1:C:106:PRO:HG2	1:C:107:ASP:N	2.16	0.52
1:C:311:VAL:HG22	1:C:311:VAL:O	2.10	0.52
1:A:56:SER:HG	1:A:186:ASN:HD21	1.55	0.52
1:C:117:PHE:HB3	1:C:119:PHE:CE1	2.44	0.52
1:C:165:THR:O	1:C:166:GLN:HB2	2.09	0.52
1:A:165:THR:HG21	1:A:169:ILE:HB	1.91	0.52
1:A:196:ARG:HH12	1:A:281:ARG:HH21	1.57	0.52
1:B:25:LYS:O	1:B:25:LYS:HD3	2.09	0.52
1:B:369:PRO:HA	1:B:388:VAL:O	2.09	0.52
1:A:137:LEU:N	1:A:137:LEU:HD23	2.25	0.52
1:C:360:ILE:CG2	1:C:360:ILE:O	2.57	0.52
1:A:138:TYR:O	1:A:139:HIS:C	2.47	0.52
1:C:251:ILE:HG22	1:C:253:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:HIS:CD2	1:B:365:LYS:HG2	2.45	0.52
1:A:245:LEU:CD1	1:A:345:THR:HG22	2.40	0.52
1:B:92:ILE:HG22	1:B:96:PHE:HD2	1.75	0.52
1:C:165:THR:CG2	1:C:169:ILE:H	2.22	0.52
1:A:196:ARG:HH12	1:A:281:ARG:NH2	2.08	0.51
1:C:147:PHE:CD2	1:C:180:THR:O	2.63	0.51
1:C:39:ARG:NH2	1:C:264:GLU:O	2.43	0.51
1:C:51:PHE:CD1	1:C:372:PHE:HZ	2.27	0.51
1:A:92:ILE:O	1:A:95:GLY:N	2.43	0.51
1:B:99:LEU:CG	1:B:100:LEU:N	2.73	0.51
1:B:285:SER:HB2	1:B:363:GLU:HA	1.91	0.51
1:A:83:ASN:HB3	1:A:86:GLU:CG	2.38	0.51
1:A:279:GLU:C	1:A:279:GLU:OE1	2.48	0.51
1:A:227:PHE:O	1:A:281:ARG:HA	2.10	0.51
1:C:240:LEU:HG	1:C:241:LEU:N	2.26	0.51
1:A:133:ASP:O	1:A:137:LEU:HD23	2.11	0.51
1:C:59:THR:HG22	1:C:60:ALA:N	2.26	0.51
1:B:229:ILE:HB	1:B:240:LEU:HD12	1.93	0.51
1:C:225:GLY:O	1:C:283:SER:HA	2.11	0.51
1:A:55:VAL:HG23	1:A:382:PRO:O	2.11	0.51
1:B:191:LYS:HB2	1:B:339:THR:HB	1.92	0.51
1:B:267:LEU:HD22	1:B:272:ILE:CD1	2.34	0.51
1:C:120:LEU:HG	1:C:182:PHE:CD1	2.46	0.51
1:B:26:ILE:HA	1:B:29:ASN:HD22	1.76	0.51
1:B:81:ASN:HD22	1:B:81:ASN:N	2.08	0.50
1:B:120:LEU:O	1:B:144:THR:HA	2.11	0.50
1:B:253:PHE:CB	1:B:263:LEU:HD11	2.41	0.50
1:B:267:LEU:CD2	1:B:272:ILE:HD11	2.37	0.50
1:C:126:LEU:H	1:C:126:LEU:CD1	2.12	0.50
1:B:266:GLU:O	1:B:268:THR:HG23	2.12	0.50
1:A:40:GLN:HG2	1:A:302:VAL:HG13	1.92	0.50
1:B:177:ASP:HB3	1:B:180:THR:OG1	2.10	0.50
1:C:138:TYR:O	1:C:139:HIS:C	2.49	0.50
1:B:78:GLU:HG3	1:B:84:LEU:CD2	2.41	0.50
1:B:124:LEU:O	1:B:126:LEU:N	2.44	0.50
1:C:120:LEU:HG	1:C:182:PHE:CE1	2.47	0.50
1:C:224:LEU:HD12	1:C:225:GLY:H	1.76	0.50
1:A:273:THR:O	1:A:277:GLU:HG2	2.12	0.50
1:C:57:ILE:HD11	1:C:334:HIS:CD2	2.46	0.50
1:A:278:ASN:ND2	1:A:280:ASP:OD2	2.43	0.50
1:B:99:LEU:HG	1:B:100:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:THR:OG1	1:C:271:ILE:HG13	2.12	0.50
1:C:360:ILE:O	1:C:360:ILE:HG23	2.12	0.50
1:A:83:ASN:ND2	1:A:86:GLU:HG2	2.27	0.50
1:A:219:PRO:HG2	1:A:290:LYS:HB3	1.93	0.50
1:A:283:SER:OG	1:A:361:PRO:HB3	2.11	0.50
1:B:282:ARG:HH11	1:B:282:ARG:HB2	1.74	0.50
1:C:48:THR:HA	1:C:393:GLN:HE22	1.77	0.50
1:B:187:TYR:CD1	1:B:187:TYR:C	2.85	0.50
1:C:96:PHE:O	1:C:98:GLU:O	2.29	0.50
1:A:282:ARG:HH11	1:A:282:ARG:CG	2.25	0.49
1:B:112:LEU:HD23	1:B:112:LEU:C	2.32	0.49
1:B:299:LEU:O	1:B:300:LYS:C	2.51	0.49
1:C:193:LYS:O	1:C:245:LEU:HB2	2.12	0.49
1:A:78:GLU:O	1:A:81:ASN:N	2.44	0.49
1:B:89:GLU:HG2	1:B:90:ALA:N	2.27	0.49
1:C:102:THR:CG2	1:C:247:ASN:ND2	2.75	0.49
1:C:63:MET:CE	1:C:64:LEU:HA	2.41	0.49
1:A:98:GLU:OE1	1:A:98:GLU:HA	2.11	0.49
1:C:245:LEU:CD2	1:C:345:THR:HG22	2.42	0.49
1:A:196:ARG:NH1	1:A:281:ARG:NH2	2.60	0.49
1:B:296:THR:HG1	1:B:335:LYS:HZ3	1.59	0.49
1:B:196:ARG:HH12	1:B:281:ARG:HH21	1.55	0.49
1:C:104:ASN:C	1:C:105:GLN:O	2.50	0.49
1:C:224:LEU:HD12	1:C:225:GLY:N	2.26	0.49
1:C:290:LYS:O	1:C:290:LYS:HG2	2.13	0.49
1:B:84:LEU:HD22	1:B:84:LEU:N	2.26	0.49
1:A:130:PHE:O	1:A:131:LEU:C	2.50	0.49
1:A:287:HIS:CG	1:A:365:LYS:HG2	2.48	0.49
1:C:99:LEU:O	1:C:102:THR:CB	2.56	0.49
1:A:369:PRO:HA	1:A:388:VAL:O	2.13	0.48
1:C:88:PRO:HD2	1:C:91:GLN:NE2	2.28	0.48
1:A:325:ALA:HB1	1:A:326:PRO:CD	2.43	0.48
1:B:282:ARG:CB	1:B:282:ARG:NH1	2.65	0.48
1:C:76:ILE:O	1:C:80:LEU:HG	2.13	0.48
1:C:191:LYS:HE3	1:C:341:ASP:OD2	2.13	0.48
1:A:89:GLU:C	1:A:91:GLN:N	2.64	0.48
1:B:43:HIS:ND1	1:B:43:HIS:C	2.67	0.48
1:C:51:PHE:HD1	1:C:372:PHE:HZ	1.62	0.48
1:C:102:THR:HG22	1:C:247:ASN:ND2	2.27	0.48
1:A:25:LYS:C	1:A:25:LYS:HZ2	2.17	0.48
1:A:38:TYR:C	1:A:40:GLN:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:CG1	1:A:140:SER:HB2	2.44	0.48
1:B:91:GLN:O	1:B:94:GLU:N	2.46	0.48
1:B:227:PHE:HB2	1:B:229:ILE:HG22	1.95	0.48
1:B:49:ASN:N	1:B:393:GLN:HE22	2.11	0.48
1:B:373:LEU:C	1:B:373:LEU:HD23	2.34	0.48
1:C:213:VAL:HG23	1:C:214:THR:N	2.28	0.48
1:A:213:VAL:CG2	1:A:214:THR:N	2.76	0.48
1:B:51:PHE:CZ	1:B:338:LEU:HB2	2.49	0.48
1:B:63:MET:HB2	1:B:138:TYR:CG	2.49	0.48
1:B:360:ILE:O	1:B:360:ILE:CG2	2.62	0.48
1:B:237:SER:CB	1:B:255:PRO:HA	2.44	0.48
1:C:27:THR:HG23	1:C:380:LYS:O	2.14	0.48
1:A:188:ILE:HG23	1:A:188:ILE:O	2.13	0.48
1:B:53:SER:HB3	1:B:56:SER:HB3	1.95	0.48
1:B:299:LEU:HB3	1:B:303:LEU:HG	1.96	0.48
1:B:344:GLY:O	1:B:345:THR:C	2.52	0.48
1:C:256:ASP:O	1:C:259:LYS:HB2	2.14	0.48
1:C:374:MET:HG2	1:C:384:PHE:HB2	1.95	0.48
1:A:112:LEU:C	1:A:112:LEU:HD23	2.35	0.47
1:C:106:PRO:CG	1:C:107:ASP:N	2.74	0.47
1:C:315:GLY:O	1:C:316:ALA:C	2.53	0.47
1:A:38:TYR:OH	1:A:387:LYS:HE3	2.14	0.47
1:B:245:LEU:CD2	1:B:345:THR:HG22	2.44	0.47
1:C:147:PHE:CD2	1:C:180:THR:C	2.88	0.47
1:A:275:PHE:C	1:A:275:PHE:CD2	2.88	0.47
1:B:106:PRO:HG2	1:B:107:ASP:N	2.27	0.47
1:B:142:ALA:O	1:B:143:PHE:CD1	2.67	0.47
1:C:51:PHE:HZ	1:C:384:PHE:HD1	1.60	0.47
1:C:147:PHE:HE2	1:C:180:THR:C	2.16	0.47
1:A:89:GLU:HG3	1:A:90:ALA:N	2.29	0.47
1:B:51:PHE:CZ	1:B:384:PHE:CD1	3.02	0.47
1:B:94:GLU:O	1:B:96:PHE:N	2.48	0.47
1:B:240:LEU:O	1:B:251:ILE:HA	2.15	0.47
1:C:75:GLU:OE2	1:C:310:LYS:HD2	2.14	0.47
1:C:137:LEU:N	1:C:137:LEU:HD23	2.30	0.47
1:C:375:ILE:CG2	1:C:380:LYS:HA	2.44	0.47
1:A:341:ASP:OD2	1:A:343:LYS:HD3	2.14	0.47
1:B:211:ASP:HB3	1:B:214:THR:H	1.80	0.47
1:C:286:LEU:HD11	1:C:366:PHE:HE1	1.80	0.47
1:A:27:THR:HB	1:A:28:PRO:HD3	1.97	0.47
1:B:87:ILE:HG23	1:B:87:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD11	1:B:361:PRO:HG3	1.96	0.47
1:C:68:THR:OG1	1:C:73:HIS:HB2	2.15	0.47
1:C:152:GLU:O	1:C:155:LYS:N	2.48	0.47
1:C:227:PHE:C	1:C:229:ILE:H	2.17	0.47
1:A:253:PHE:CB	1:A:263:LEU:HD11	2.45	0.47
1:A:224:LEU:HD12	1:A:225:GLY:N	2.31	0.46
1:A:291:LEU:HD23	1:A:340:ILE:HB	1.97	0.46
1:A:368:LYS:O	1:A:369:PRO:C	2.54	0.46
1:B:66:LEU:CD2	1:B:93:HIS:CE1	2.98	0.46
1:C:56:SER:OG	1:C:186:ASN:OD1	2.34	0.46
1:C:384:PHE:CD2	1:C:384:PHE:N	2.82	0.46
1:B:186:ASN:O	1:B:334:HIS:HA	2.14	0.46
1:A:179:ASP:O	1:A:181:VAL:HG13	2.16	0.46
1:B:147:PHE:CE1	1:B:180:THR:CG2	2.99	0.46
1:C:48:THR:HA	1:C:393:GLN:NE2	2.30	0.46
1:C:222:LYS:HE2	1:C:287:HIS:NE2	2.30	0.46
1:C:84:LEU:O	1:C:87:ILE:O	2.33	0.46
1:C:213:VAL:CG2	1:C:214:THR:N	2.78	0.46
1:A:162:GLU:O	1:A:162:GLU:HG2	2.16	0.46
1:A:379:THR:O	1:A:380:LYS:HB2	2.16	0.46
1:B:97:GLN:NE2	1:B:137:LEU:CB	2.79	0.46
1:B:223:ARG:NH2	1:B:227:PHE:CE1	2.84	0.46
1:C:280:ASP:HB3	1:C:281:ARG:H	1.46	0.46
1:A:68:THR:HG22	1:A:318:LEU:CD2	2.44	0.46
1:B:69:LYS:HE2	1:B:319:SER:OG	2.15	0.46
1:C:325:ALA:HB1	1:C:326:PRO:CD	2.43	0.46
1:A:26:ILE:HG22	1:A:82:PHE:HE1	1.80	0.46
1:A:375:ILE:CG2	1:A:376:GLU:N	2.79	0.46
1:B:48:THR:HG22	1:B:49:ASN:N	2.31	0.46
1:B:75:GLU:CD	1:B:310:LYS:HD2	2.37	0.46
1:B:165:THR:CG2	1:B:169:ILE:H	2.28	0.45
1:B:383:LEU:HD22	1:B:384:PHE:CE2	2.51	0.45
1:C:95:GLY:O	1:C:98:GLU:HB2	2.16	0.45
1:C:99:LEU:O	1:C:103:LEU:N	2.44	0.45
1:C:282:ARG:HG3	1:C:283:SER:O	2.17	0.45
1:B:91:GLN:O	1:B:94:GLU:CB	2.60	0.45
1:B:110:LEU:O	1:B:110:LEU:HG	2.16	0.45
1:B:196:ARG:HA	1:B:197:PRO:HD2	1.83	0.45
1:C:25:LYS:HA	1:C:25:LYS:HD3	1.54	0.45
1:C:375:ILE:HG23	1:C:376:GLU:H	1.81	0.45
1:A:48:THR:HA	1:A:393:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HH11	1:A:282:ARG:CB	2.29	0.45
1:A:283:SER:O	1:A:362:PRO:HD2	2.16	0.45
1:B:341:ASP:OD2	1:B:343:LYS:HD3	2.17	0.45
1:B:106:PRO:CG	1:B:107:ASP:H	2.25	0.45
1:B:222:LYS:O	1:B:223:ARG:HB2	2.16	0.45
1:A:153:ALA:O	1:A:154:LYS:C	2.54	0.45
1:C:96:PHE:O	1:C:100:LEU:HD12	2.14	0.45
1:C:375:ILE:HG23	1:C:376:GLU:N	2.31	0.45
1:C:40:GLN:HG2	1:C:302:VAL:HG13	1.98	0.45
1:C:165:THR:HG21	1:C:169:ILE:H	1.80	0.45
1:A:39:ARG:NH2	1:A:264:GLU:O	2.47	0.45
1:C:87:ILE:CG1	1:C:88:PRO:HD2	2.46	0.45
1:C:280:ASP:O	1:C:281:ARG:CB	2.64	0.45
1:A:333:VAL:CG1	1:A:334:HIS:N	2.80	0.45
1:B:94:GLU:O	1:B:95:GLY:C	2.55	0.45
1:C:147:PHE:O	1:C:148:GLY:O	2.35	0.45
1:A:102:THR:HG22	1:A:247:ASN:ND2	2.32	0.44
1:A:129:LYS:HG2	1:A:133:ASP:OD2	2.16	0.44
1:A:299:LEU:O	1:A:300:LYS:C	2.56	0.44
1:A:346:GLU:O	1:A:347:ALA:CB	2.61	0.44
1:B:98:GLU:HA	1:B:98:GLU:OE1	2.16	0.44
1:B:120:LEU:HD22	1:B:126:LEU:HD23	1.99	0.44
1:B:165:THR:HG23	1:B:168:LYS:H	1.82	0.44
1:B:218:VAL:HB	1:B:219:PRO:HD2	1.99	0.44
1:C:50:ILE:HD13	1:C:50:ILE:HA	1.85	0.44
1:C:149:ASP:O	1:C:150:THR:O	2.35	0.44
1:B:299:LEU:O	1:B:301:SER:N	2.51	0.44
1:B:299:LEU:HB3	1:B:303:LEU:CD1	2.47	0.44
1:B:325:ALA:HB1	1:B:326:PRO:HD2	1.99	0.44
1:B:40:GLN:HG2	1:B:302:VAL:HG13	2.00	0.44
1:C:27:THR:CG2	1:C:380:LYS:O	2.65	0.44
1:C:71:ASP:O	1:C:72:THR:C	2.56	0.44
1:C:200:VAL:C	1:C:202:ASP:H	2.20	0.44
1:C:384:PHE:HD2	1:C:384:PHE:N	2.15	0.44
1:B:24:ASN:O	1:B:25:LYS:CB	2.50	0.44
1:C:51:PHE:CZ	1:C:338:LEU:HB2	2.53	0.44
1:C:193:LYS:HE3	1:C:193:LYS:H	1.83	0.44
1:C:326:PRO:O	1:C:326:PRO:HG2	2.17	0.44
1:A:198:PHE:O	1:A:342:GLU:HB3	2.17	0.44
1:A:280:ASP:O	1:A:281:ARG:CB	2.66	0.44
1:A:288:LEU:HD12	1:A:289:PRO:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:C	1:B:101:ARG:H	2.21	0.44
1:C:87:ILE:HG12	1:C:88:PRO:CD	2.48	0.44
1:B:66:LEU:HD21	1:B:93:HIS:CE1	2.53	0.44
1:C:77:LEU:HA	1:C:80:LEU:HD12	2.00	0.44
1:A:112:LEU:HD23	1:A:112:LEU:O	2.18	0.43
1:B:98:GLU:O	1:B:101:ARG:HB2	2.18	0.43
1:B:117:PHE:CD1	1:B:161:VAL:HG22	2.53	0.43
1:A:63:MET:C	1:A:63:MET:HE2	2.39	0.43
1:B:112:LEU:HD23	1:B:112:LEU:O	2.18	0.43
1:B:133:ASP:HB3	1:B:137:LEU:HD21	2.00	0.43
1:B:224:LEU:O	1:B:224:LEU:HG	2.16	0.43
1:B:342:GLU:O	1:B:343:LYS:C	2.56	0.43
1:C:226:MET:SD	1:C:226:MET:N	2.91	0.43
1:A:83:ASN:CB	1:A:86:GLU:OE2	2.66	0.43
1:B:39:ARG:HE	1:B:265:ASN:HA	1.83	0.43
1:B:120:LEU:HG	1:B:182:PHE:CD1	2.53	0.43
1:B:146:ASN:O	1:B:153:ALA:HB2	2.18	0.43
1:B:360:ILE:HD13	1:B:360:ILE:HA	1.76	0.43
1:A:137:LEU:HD23	1:A:137:LEU:H	1.83	0.43
1:B:98:GLU:OE1	1:B:101:ARG:NH1	2.52	0.43
1:B:48:THR:HG22	1:B:49:ASN:H	1.83	0.43
1:B:84:LEU:O	1:B:87:ILE:O	2.36	0.43
1:C:112:LEU:C	1:C:112:LEU:CD2	2.86	0.43
1:C:152:GLU:O	1:C:153:ALA:C	2.56	0.43
1:A:128:ASP:O	1:A:129:LYS:C	2.57	0.43
1:C:31:ALA:O	1:C:34:ALA:HB3	2.17	0.43
1:A:25:LYS:O	1:A:25:LYS:NZ	2.50	0.43
1:A:83:ASN:CB	1:A:86:GLU:HG2	2.46	0.43
1:A:187:TYR:CD1	1:A:187:TYR:C	2.92	0.43
1:A:270:ASP:O	1:A:274:LYS:HG3	2.18	0.43
1:B:245:LEU:HD23	1:B:345:THR:CG2	2.49	0.43
1:A:78:GLU:HA	1:A:82:PHE:O	2.19	0.43
1:B:77:LEU:HA	1:B:77:LEU:HD23	1.73	0.43
1:B:105:GLN:CB	1:B:108:SER:HB2	2.49	0.43
1:C:153:ALA:O	1:C:157:ILE:HB	2.19	0.43
1:C:163:LYS:C	1:C:165:THR:H	2.22	0.43
1:B:138:TYR:O	1:B:139:HIS:C	2.57	0.43
1:C:180:THR:HG23	1:C:330:SER:HB2	2.01	0.43
1:C:196:ARG:HA	1:C:197:PRO:HD2	1.87	0.43
1:A:256:ASP:O	1:A:259:LYS:HB2	2.19	0.42
1:B:162:GLU:HG3	1:B:170:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASP:HB2	1:A:259:LYS:HG3	2.01	0.42
1:C:67:GLY:O	1:C:321:VAL:HG23	2.18	0.42
1:A:116:ASN:HB2	1:A:140:SER:OG	2.19	0.42
1:A:229:ILE:CD1	1:A:364:VAL:HG21	2.48	0.42
1:A:393:GLN:HG2	1:A:394:LYS:N	2.34	0.42
1:B:333:VAL:CG1	1:B:334:HIS:N	2.81	0.42
1:C:368:LYS:HB2	1:C:369:PRO:HD2	2.02	0.42
1:C:375:ILE:HG22	1:C:376:GLU:N	2.34	0.42
1:A:71:ASP:O	1:A:72:THR:C	2.58	0.42
1:B:97:GLN:O	1:B:98:GLU:C	2.57	0.42
1:A:38:TYR:C	1:A:38:TYR:CD2	2.93	0.42
1:A:83:ASN:O	1:A:86:GLU:HG2	2.20	0.42
1:A:99:LEU:HD12	1:A:99:LEU:C	2.39	0.42
1:B:188:ILE:HD13	1:B:384:PHE:CE1	2.54	0.42
1:B:245:LEU:HD23	1:B:345:THR:HG22	2.01	0.42
1:B:24:ASN:HD22	1:B:24:ASN:HA	1.65	0.42
1:B:83:ASN:O	1:B:85:THR:N	2.53	0.42
1:B:235:LEU:O	1:B:236:SER:C	2.57	0.42
1:B:279:GLU:OE1	1:B:279:GLU:C	2.58	0.42
1:C:282:ARG:HB3	1:C:282:ARG:NH1	2.26	0.42
1:A:27:THR:CB	1:A:28:PRO:HD3	2.50	0.42
1:A:274:LYS:O	1:A:275:PHE:C	2.58	0.42
1:A:162:GLU:HA	1:A:165:THR:HG22	2.02	0.42
1:A:184:LEU:C	1:A:184:LEU:CD2	2.88	0.42
1:B:40:GLN:CG	1:B:302:VAL:HG13	2.49	0.42
1:B:235:LEU:HD22	1:B:263:LEU:HD23	2.01	0.42
1:C:383:LEU:HD23	1:C:383:LEU:HA	1.80	0.42
1:A:80:LEU:O	1:A:81:ASN:HB2	2.20	0.42
1:B:344:GLY:O	1:B:345:THR:O	2.37	0.42
1:C:200:VAL:C	1:C:202:ASP:N	2.73	0.42
1:B:92:ILE:CG2	1:B:96:PHE:CE2	3.03	0.41
1:B:112:LEU:HD11	1:B:383:LEU:CD2	2.50	0.41
1:C:26:ILE:HG13	1:C:27:THR:N	2.34	0.41
1:C:94:GLU:O	1:C:95:GLY:C	2.59	0.41
1:C:117:PHE:HB2	1:C:185:VAL:HB	2.01	0.41
1:A:196:ARG:NH2	1:A:281:ARG:HH22	2.16	0.41
1:C:133:ASP:O	1:C:134:VAL:C	2.59	0.41
1:A:198:PHE:N	1:A:198:PHE:CD2	2.89	0.41
1:B:147:PHE:CE1	1:B:180:THR:HG22	2.55	0.41
1:A:38:TYR:OH	1:A:264:GLU:OE2	2.28	0.41
1:A:49:ASN:C	1:A:50:ILE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:CG	1:A:282:ARG:NH1	2.81	0.41
1:B:48:THR:HA	1:B:393:GLN:NE2	2.36	0.41
1:B:375:ILE:CG2	1:B:376:GLU:N	2.82	0.41
1:B:153:ALA:O	1:B:154:LYS:C	2.58	0.41
1:A:200:VAL:C	1:A:202:ASP:N	2.73	0.41
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.81	0.41
1:C:63:MET:HE2	1:C:63:MET:O	2.19	0.41
1:C:169:ILE:HD11	1:C:189:PHE:CZ	2.56	0.41
1:A:35:PHE:O	1:A:39:ARG:HG2	2.20	0.41
1:A:44:GLN:O	1:A:45:SER:CB	2.69	0.41
1:A:63:MET:CE	1:A:64:LEU:CA	2.97	0.41
1:A:344:GLY:O	1:A:345:THR:C	2.59	0.41
1:B:282:ARG:HG3	1:B:283:SER:O	2.21	0.41
1:B:383:LEU:HD22	1:B:384:PHE:HE2	1.86	0.41
1:C:373:LEU:HD21	1:C:375:ILE:HG13	2.03	0.41
1:B:315:GLY:O	1:B:316:ALA:O	2.39	0.41
1:C:95:GLY:O	1:C:98:GLU:O	2.38	0.41
1:A:99:LEU:O	1:A:102:THR:HB	2.21	0.40
1:C:51:PHE:O	1:C:297:TYR:HE2	2.04	0.40
1:B:23:PHE:O	1:B:24:ASN:C	2.59	0.40
1:B:67:GLY:HA3	1:B:321:VAL:HG23	2.02	0.40
1:B:383:LEU:CD2	1:B:384:PHE:CE2	3.04	0.40
1:C:66:LEU:O	1:C:66:LEU:HD23	2.22	0.40
1:A:262:HIS:CE1	1:A:266:GLU:HG3	2.56	0.40
1:A:267:LEU:HD22	1:A:272:ILE:CD1	2.51	0.40
1:B:83:ASN:HD22	1:B:86:GLU:CG	2.33	0.40
1:C:229:ILE:HD11	1:C:364:VAL:HG21	2.04	0.40
1:B:368:LYS:O	1:B:369:PRO:C	2.60	0.40
1:C:245:LEU:HD23	1:C:345:THR:CG2	2.52	0.40
1:C:360:ILE:HA	1:C:361:PRO:HD2	1.99	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:MET:N	1:B:224:LEU:N[1_455]	1.73	0.47
1:A:357:PRO:N	1:B:223:ARG:O[1_455]	1.82	0.38
1:A:160:TYR:OH	1:A:233:LYS:NZ[1_655]	1.98	0.22

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	359/404 (89%)	284 (79%)	60 (17%)	15 (4%)	3	20
1	B	358/404 (89%)	277 (77%)	59 (16%)	22 (6%)	1	12
1	C	356/404 (88%)	277 (78%)	57 (16%)	22 (6%)	1	11
All	All	1073/1212 (88%)	838 (78%)	176 (16%)	59 (6%)	2	14

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	108	SER
1	A	109	GLN
1	A	281	ARG
1	A	316	ALA
1	A	347	ALA
1	A	359	SER
1	B	24	ASN
1	B	25	LYS
1	B	45	SER
1	B	84	LEU
1	B	99	LEU
1	B	100	LEU
1	B	105	GLN
1	B	110	LEU
1	B	111	GLN
1	B	345	THR
1	C	24	ASN
1	C	45	SER
1	C	70	ALA
1	C	99	LEU
1	C	106	PRO
1	C	150	THR
1	C	151	GLU

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Mol	Chain	Res	Type
1	C	280	ASP
1	C	281	ARG
1	C	316	ALA
1	A	25	LYS
1	A	90	ALA
1	A	130	PHE
1	A	188	ILE
1	B	200	VAL
1	B	300	LYS
1	B	316	ALA
1	C	109	GLN
1	C	139	HIS
1	C	148	GLY
1	A	181	VAL
1	B	94	GLU
1	B	95	GLY
1	B	256	ASP
1	B	324	GLU
1	C	172	LEU
1	A	139	HIS
1	B	70	ALA
1	C	112	LEU
1	C	134	VAL
1	C	326	PRO
1	C	382	PRO
1	A	88	PRO
1	A	377	GLN
1	B	98	GLU
1	B	106	PRO
1	B	360	ILE
1	C	111	GLN
1	C	188	ILE
1	B	181	VAL
1	C	88	PRO
1	C	181	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	316/358 (88%)	283 (90%)	33 (10%)	7 28
1	B	319/358 (89%)	286 (90%)	33 (10%)	7 29
1	C	312/358 (87%)	265 (85%)	47 (15%)	3 14
All	All	947/1074 (88%)	834 (88%)	113 (12%)	5 22

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	25	LYS
1	A	27	THR
1	A	29	ASN
1	A	39	ARG
1	A	46	ASN
1	A	63	MET
1	A	88	PRO
1	A	89	GLU
1	A	104	ASN
1	A	108	SER
1	A	137	LEU
1	A	184	LEU
1	A	193	LYS
1	A	197	PRO
1	A	199	GLU
1	A	202	ASP
1	A	210	VAL
1	A	237	SER
1	A	263	LEU
1	A	270	ASP
1	A	279	GLU
1	A	282	ARG
1	A	291	LEU
1	A	301	SER
1	A	311	VAL
1	A	330	SER
1	A	358	MET
1	A	359	SER
1	A	374	MET
1	A	383	LEU
1	A	385	MET

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Mol	Chain	Res	Type
1	A	393	GLN
1	B	24	ASN
1	B	25	LYS
1	B	46	ASN
1	B	63	MET
1	B	98	GLU
1	B	99	LEU
1	B	100	LEU
1	B	104	ASN
1	B	108	SER
1	B	109	GLN
1	B	110	LEU
1	B	111	GLN
1	B	137	LEU
1	B	166	GLN
1	B	193	LYS
1	B	201	LYS
1	B	202	ASP
1	B	214	THR
1	B	245	LEU
1	B	263	LEU
1	B	270	ASP
1	B	279	GLU
1	B	280	ASP
1	B	281	ARG
1	B	282	ARG
1	B	291	LEU
1	B	301	SER
1	B	311	VAL
1	B	359	SER
1	B	374	MET
1	B	383	LEU
1	B	385	MET
1	B	393	GLN
1	C	24	ASN
1	C	25	LYS
1	C	46	ASN
1	C	59	THR
1	C	63	MET
1	C	68	THR
1	C	88	PRO
1	C	89	GLU

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Mol	Chain	Res	Type
1	C	100	LEU
1	C	101	ARG
1	C	104	ASN
1	C	105	GLN
1	C	106	PRO
1	C	107	ASP
1	C	108	SER
1	C	111	GLN
1	C	124	LEU
1	C	126	LEU
1	C	137	LEU
1	C	147	PHE
1	C	149	ASP
1	C	165	THR
1	C	171	ASP
1	C	184	LEU
1	C	193	LYS
1	C	206	GLU
1	C	210	VAL
1	C	214	THR
1	C	226	MET
1	C	232	CYS
1	C	241	LEU
1	C	245	LEU
1	C	263	LEU
1	C	270	ASP
1	C	278	ASN
1	C	282	ARG
1	C	291	LEU
1	C	294	THR
1	C	301	SER
1	C	310	LYS
1	C	313	SER
1	C	328	LYS
1	C	360	ILE
1	C	373	LEU
1	C	384	PHE
1	C	385	MET
1	C	393	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	29	ASN
1	A	44	GLN
1	A	81	ASN
1	A	83	ASN
1	A	91	GLN
1	A	97	GLN
1	A	139	HIS
1	A	166	GLN
1	A	186	ASN
1	A	261	GLN
1	A	269	HIS
1	A	367	ASN
1	A	393	GLN
1	B	24	ASN
1	B	29	ASN
1	B	83	ASN
1	B	91	GLN
1	B	97	GLN
1	B	166	GLN
1	B	261	GLN
1	B	265	ASN
1	B	269	HIS
1	B	393	GLN
1	C	24	ASN
1	C	44	GLN
1	C	81	ASN
1	C	91	GLN
1	C	139	HIS
1	C	166	GLN
1	C	186	ASN
1	C	261	GLN
1	C	265	ASN
1	C	269	HIS
1	C	393	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)

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)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	363/404 (89%)	-0.21	2 (0%) 89 83	28, 57, 94, 109	0
1	B	362/404 (89%)	-0.22	0 100 100	27, 59, 92, 108	0
1	C	360/404 (89%)	-0.04	5 (1%) 75 63	53, 85, 117, 141	0
All	All	1085/1212 (89%)	-0.15	7 (0%) 89 83	27, 67, 105, 141	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	ALA	5.2
1	A	394	LYS	2.9
1	C	360	ILE	2.8
1	C	284	ALA	2.7
1	C	142	ALA	2.5
1	C	375	ILE	2.2
1	A	106	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.