



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:53 AM UTC

PDB ID : 3UU2 / pdb_00003uu2
Title : Salmonella typhi osmoporin(OmpC):an Outer Membrane Protein
Authors : Prasanth, P.; Putcha, B.K.; Arockiasamy, A.; Krishnaswamy, S.
Deposited on : 2011-11-27
Resolution : 3.59 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

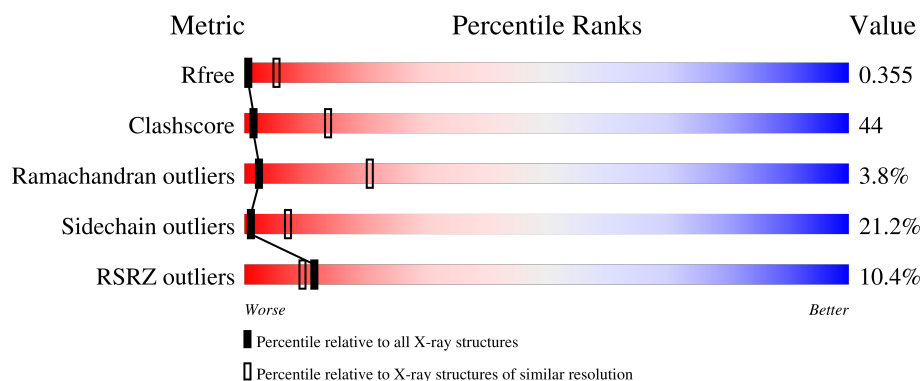
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	357	8% 29% 41% 13% 17%
1	B	357	10% 30% 43% 10% 17%
1	C	357	8% 31% 41% 11% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6988 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.

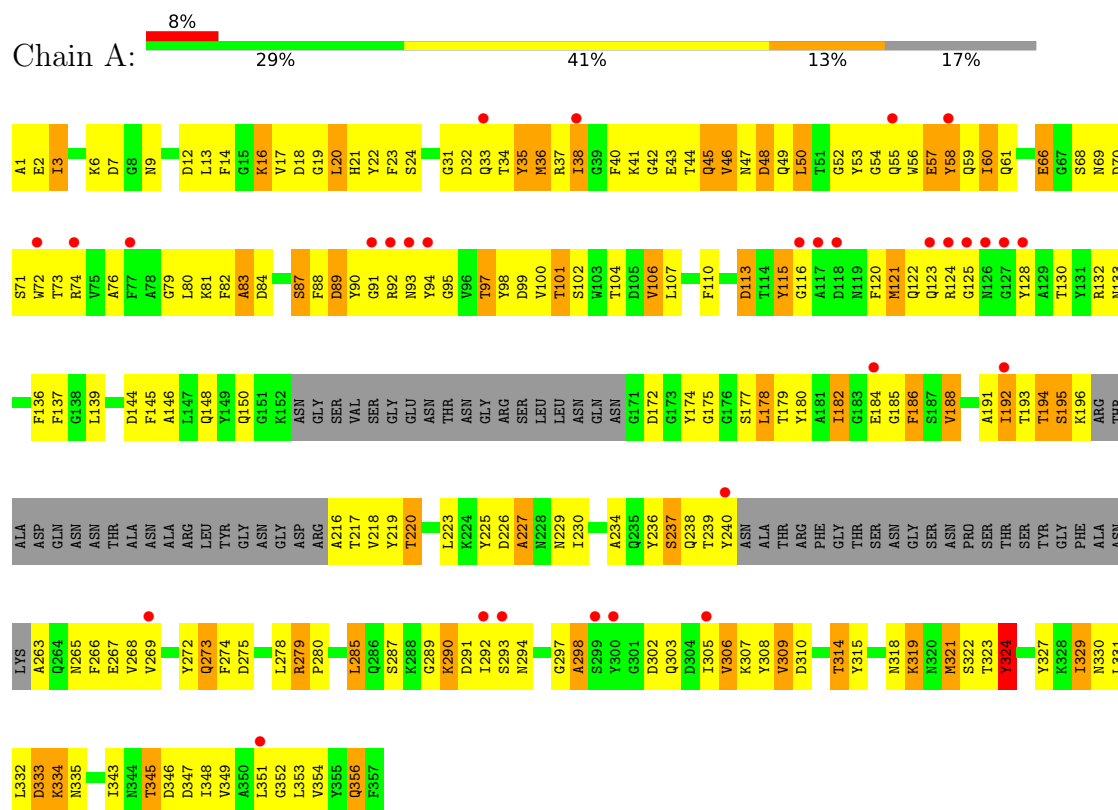
- Molecule 1 is a protein called Outer membrane protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2328	1476	374	475	3			
1	B	298	Total	C	N	O	S	0	0	0
			2333	1480	375	475	3			
1	C	298	Total	C	N	O	S	0	0	0
			2327	1476	373	475	3			

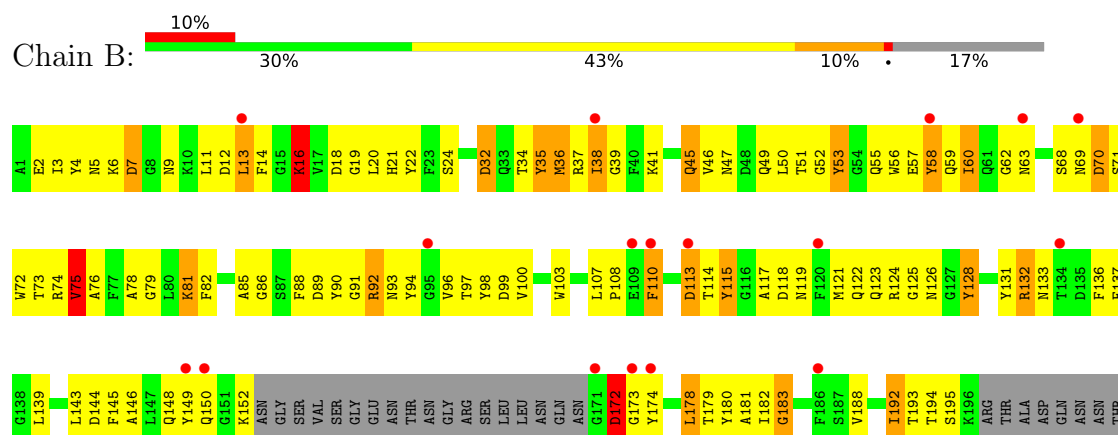
3 Residue-property plots

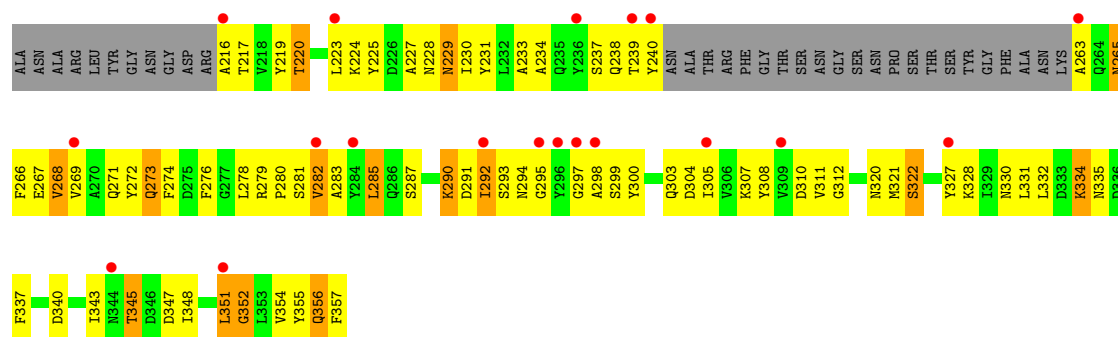
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Outer membrane protein C

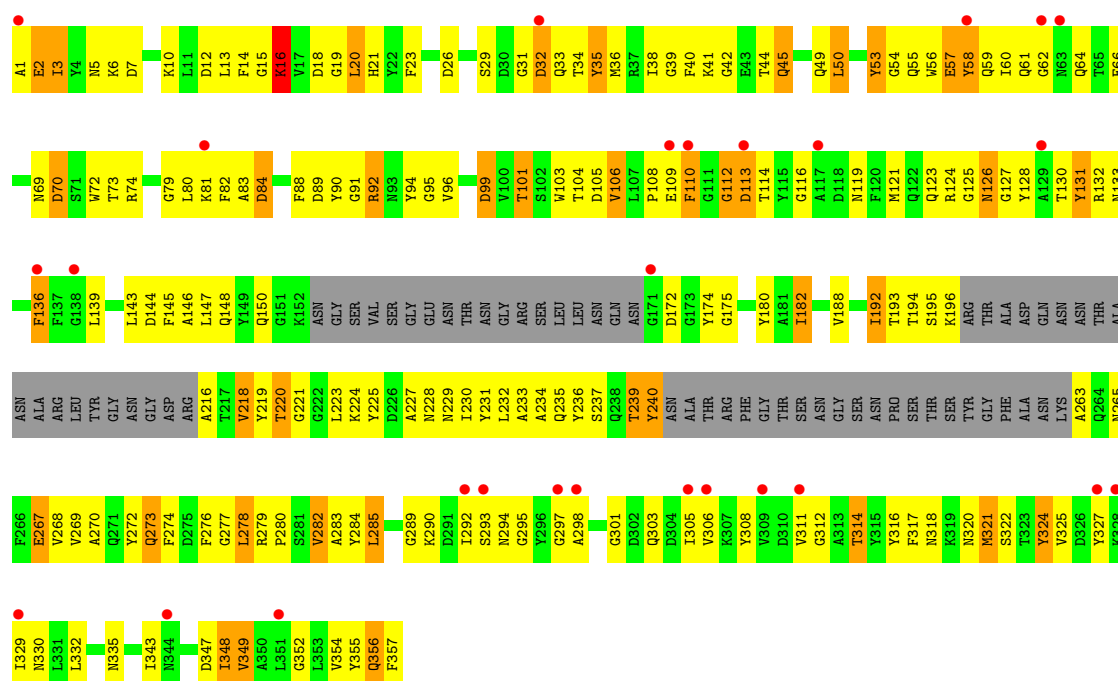


• Molecule 1: Outer membrane protein C





● Molecule 1: Outer membrane protein C



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.20Å 108.57Å 113.39Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	50.00 – 3.59 50.00 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.59) 98.8 (50.00-3.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.302 , 0.358 0.302 , 0.355	Depositor DCC
R_{free} test set	1383 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	108.5	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 158.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6988	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.82	1/2380 (0.0%)	1.02	5/3217 (0.2%)
1	B	0.77	1/2385 (0.0%)	1.00	9/3223 (0.3%)
1	C	0.72	1/2379 (0.0%)	0.92	0/3217
All	All	0.77	3/7144 (0.0%)	0.98	14/9657 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	LYS	CE-NZ	8.98	1.76	1.49
1	C	105	ASP	CB-CG	6.04	1.67	1.52
1	A	194	THR	CB-OG1	5.60	1.52	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	GLY	N-CA-C	8.56	122.21	110.56
1	B	352	GLY	N-CA-C	6.90	120.53	110.80
1	A	321	MET	N-CA-C	6.34	118.64	107.61
1	A	237	SER	N-CA-C	6.34	116.94	108.38
1	B	297	GLY	N-CA-C	5.95	117.39	111.21
1	A	275	ASP	N-CA-C	5.79	117.67	111.36
1	A	324	TYR	N-CA-C	5.78	118.64	108.75
1	B	75	VAL	N-CA-C	5.72	118.18	108.86
1	B	70	ASP	N-CA-C	5.58	117.77	107.73
1	B	46	VAL	N-CA-C	-5.50	107.08	111.81
1	B	268	VAL	N-CA-C	5.40	115.48	108.35
1	B	292	ILE	N-CA-C	5.28	116.33	108.46
1	B	183	GLY	N-CA-C	-5.10	106.93	112.08
1	A	17	VAL	N-CA-C	-5.02	100.52	107.80

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	2328	0	2118	228	0
1	B	2333	0	2133	219	0
1	C	2327	0	2115	174	0
All	All	6988	0	6366	582	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 44.

All (582) 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:B:334:LYS:CE	1:B:334:LYS:NZ	1.76	1.47
1:A:123:GLN:HG3	1:A:124:ARG:H	1.07	1.14
1:B:58:TYR:HB2	1:B:73:THR:HA	1.18	1.11
1:A:19:GLY:HA2	1:A:34:THR:HG22	1.16	1.05
1:C:236:TYR:HB2	1:C:265:ASN:O	1.57	1.04
1:B:22:TYR:HE1	1:B:110:PHE:CE1	1.76	1.03
1:B:263:ALA:HB2	1:B:290:LYS:HD2	1.42	1.02
1:B:22:TYR:CE1	1:B:110:PHE:HE1	1.78	1.01
1:B:123:GLN:HG2	1:B:124:ARG:H	1.27	0.99
1:A:22:TYR:HD2	1:A:33:GLN:OE1	1.41	0.99
1:A:334:LYS:HG3	1:A:345:THR:HG21	1.43	0.96
1:B:123:GLN:CG	1:B:124:ARG:H	1.78	0.96
1:A:324:TYR:HE2	1:A:352:GLY:HA3	1.31	0.96
1:A:123:GLN:CG	1:A:124:ARG:H	1.80	0.95
1:B:3:ILE:HD11	1:B:13:LEU:HD22	1.46	0.94
1:B:271:GLN:OE1	1:B:281:SER:HB3	1.66	0.94
1:C:322:SER:HB2	1:C:354:VAL:HG22	1.47	0.94
1:A:19:GLY:CA	1:A:34:THR:HG22	1.98	0.94
1:A:36:MET:HE2	1:A:60:ILE:CG2	1.99	0.93
1:C:18:ASP:HB3	1:C:35:TYR:HE1	1.30	0.93
1:A:234:ALA:HB2	1:A:268:VAL:HG23	1.49	0.92
1:A:19:GLY:HA2	1:A:34:THR:CG2	1.99	0.92
1:C:23:PHE:HB2	1:C:349:VAL:HG13	1.52	0.92
1:B:16:LYS:HD2	1:B:37:ARG:HD2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:HG3	1:A:124:ARG:N	1.81	0.90
1:A:36:MET:HE1	1:A:38:ILE:CD1	2.02	0.90
1:C:59:GLN:O	1:C:60:ILE:HG13	1.72	0.89
1:B:92:ARG:HD2	1:B:125:GLY:O	1.72	0.88
1:C:322:SER:HB2	1:C:354:VAL:CG2	2.04	0.88
1:A:18:ASP:HB3	1:A:35:TYR:HE1	1.38	0.88
1:B:303:GLN:HE22	1:B:335:ASN:HD21	1.21	0.87
1:C:18:ASP:HB3	1:C:35:TYR:CE1	2.08	0.87
1:A:16:LYS:HB2	1:A:16:LYS:NZ	1.89	0.87
1:B:57:GLU:OE2	1:B:74:ARG:NH2	2.06	0.87
1:C:53:TYR:OH	1:C:89:ASP:OD2	1.92	0.87
1:B:34:THR:HG21	1:C:91:GLY:HA2	1.56	0.86
1:A:267:GLU:HB3	1:A:285:LEU:HB3	1.58	0.85
1:A:303:GLN:HE22	1:A:335:ASN:HD21	1.23	0.85
1:C:277:GLY:O	1:C:278:LEU:HB2	1.78	0.83
1:A:22:TYR:HE1	1:A:110:PHE:HE1	1.23	0.83
1:B:36:MET:HE1	1:B:38:ILE:HG13	1.60	0.83
1:A:128:TYR:CE1	1:A:150:GLN:HG2	2.14	0.83
1:A:324:TYR:CE2	1:A:352:GLY:HA3	2.14	0.83
1:B:58:TYR:CB	1:B:73:THR:HA	2.05	0.82
1:A:309:VAL:HG13	1:A:329:ILE:HB	1.62	0.82
1:A:145:PHE:HB2	1:A:178:LEU:HD23	1.60	0.82
1:C:19:GLY:HA2	1:C:34:THR:HG22	1.62	0.81
1:A:36:MET:HE1	1:A:38:ILE:HG13	1.63	0.81
1:C:267:GLU:HB3	1:C:285:LEU:HB3	1.63	0.81
1:B:45:GLN:HA	1:B:51:THR:HG22	1.63	0.81
1:B:263:ALA:HB2	1:B:290:LYS:CD	2.11	0.81
1:A:216:ALA:HA	1:A:240:TYR:HB3	1.61	0.80
1:C:92:ARG:HH12	1:C:124:ARG:HB3	1.45	0.80
1:A:240:TYR:HD1	1:A:240:TYR:O	1.65	0.80
1:A:18:ASP:HB3	1:A:35:TYR:CE1	2.17	0.79
1:C:273:GLN:HG2	1:C:279:ARG:HD3	1.62	0.79
1:A:182:ILE:HD11	1:A:188:VAL:HB	1.65	0.79
1:C:132:ARG:HG3	1:C:146:ALA:HB2	1.65	0.78
1:B:303:GLN:HE22	1:B:335:ASN:ND2	1.81	0.78
1:A:229:ASN:HB2	1:A:272:TYR:CE1	2.19	0.78
1:C:19:GLY:CA	1:C:34:THR:HG22	2.13	0.78
1:B:303:GLN:NE2	1:B:335:ASN:HD21	1.81	0.78
1:A:20:LEU:O	1:A:20:LEU:HD23	1.84	0.77
1:A:47:ASN:O	1:A:49:GLN:N	2.17	0.77
1:B:97:THR:OG1	1:B:193:THR:HG21	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG11	1:C:317:PHE:HB3	1.66	0.76
1:A:132:ARG:HG3	1:A:146:ALA:HB2	1.67	0.76
1:B:117:ALA:O	1:B:118:ASP:HB2	1.85	0.76
1:B:121:MET:SD	1:B:150:GLN:OE1	2.45	0.75
1:C:239:THR:HG23	1:C:263:ALA:HB1	1.69	0.75
1:A:236:TYR:HB2	1:A:266:PHE:HA	1.67	0.75
1:B:19:GLY:O	1:B:352:GLY:HA3	1.87	0.74
1:A:36:MET:HE1	1:A:38:ILE:CG1	2.16	0.74
1:C:18:ASP:CG	1:C:354:VAL:HG12	2.12	0.74
1:A:36:MET:HE3	1:A:37:ARG:N	2.04	0.73
1:A:128:TYR:HE1	1:A:150:GLN:HG2	1.52	0.73
1:C:56:TRP:CZ2	1:C:58:TYR:HD2	2.06	0.73
1:B:263:ALA:CB	1:B:290:LYS:HD2	2.17	0.73
1:B:272:TYR:O	1:B:280:PRO:HD2	1.89	0.73
1:C:14:PHE:HE2	1:C:41:LYS:HG3	1.53	0.72
1:B:267:GLU:HB3	1:B:285:LEU:HB3	1.71	0.72
1:A:194:THR:HB	1:A:217:THR:HG22	1.72	0.72
1:B:107:LEU:HD23	1:B:310:ASP:OD1	1.88	0.72
1:A:218:VAL:HG22	1:A:219:TYR:O	1.90	0.71
1:A:36:MET:HE3	1:A:36:MET:C	2.16	0.71
1:A:91:GLY:HA2	1:C:34:THR:HG21	1.73	0.71
1:A:92:ARG:HD2	1:A:125:GLY:O	1.90	0.71
1:C:121:MET:HG3	1:C:128:TYR:HE1	1.55	0.71
1:B:57:GLU:CD	1:B:74:ARG:HH21	1.97	0.71
1:B:103:TRP:CD2	1:B:224:LYS:HD2	2.26	0.71
1:B:219:TYR:O	1:B:237:SER:CB	2.39	0.71
1:B:229:ASN:HB2	1:B:272:TYR:CE1	2.25	0.71
1:A:22:TYR:CE1	1:A:110:PHE:HE1	2.07	0.71
1:A:16:LYS:HZ1	1:A:18:ASP:HB2	1.57	0.70
1:A:50:LEU:HA	1:A:81:LYS:O	1.91	0.70
1:C:20:LEU:HD23	1:C:33:GLN:O	1.90	0.70
1:B:19:GLY:HA2	1:B:34:THR:HG22	1.72	0.70
1:B:123:GLN:CG	1:B:124:ARG:N	2.49	0.70
1:B:266:PHE:CZ	1:B:268:VAL:HB	2.26	0.70
1:B:3:ILE:CD1	1:B:13:LEU:HD22	2.21	0.70
1:A:22:TYR:CD2	1:A:33:GLN:OE1	2.34	0.70
1:B:56:TRP:HA	1:B:75:VAL:O	1.92	0.70
1:A:66:GLU:HG3	1:B:72:TRP:CD1	2.28	0.69
1:A:240:TYR:O	1:A:240:TYR:CD1	2.46	0.69
1:C:16:LYS:HB3	1:C:356:GLN:HB3	1.75	0.69
1:C:35:TYR:CD1	1:C:35:TYR:C	2.68	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HB2	1:A:16:LYS:HZ2	1.56	0.69
1:B:14:PHE:CE1	1:B:57:GLU:HB3	2.26	0.68
1:C:193:THR:OG1	1:C:218:VAL:HG13	1.93	0.68
1:A:79:GLY:HA3	1:A:89:ASP:HB3	1.73	0.68
1:C:56:TRP:HZ2	1:C:58:TYR:CD2	2.11	0.68
1:B:2:GLU:HA	1:B:12:ASP:HA	1.76	0.67
1:B:194:THR:HG22	1:B:217:THR:CG2	2.25	0.67
1:C:56:TRP:CZ2	1:C:58:TYR:CD2	2.83	0.67
1:B:273:GLN:NE2	1:B:279:ARG:HB2	2.09	0.67
1:A:194:THR:HA	1:A:217:THR:HA	1.76	0.67
1:B:145:PHE:HB3	1:B:178:LEU:HD13	1.75	0.67
1:C:88:PHE:HA	1:C:130:THR:O	1.95	0.67
1:A:121:MET:HE2	1:A:148:GLN:OE1	1.94	0.66
1:A:82:PHE:CD2	1:A:83:ALA:N	2.63	0.66
1:A:79:GLY:O	1:A:80:LEU:HD23	1.95	0.66
1:A:35:TYR:CD1	1:A:35:TYR:C	2.73	0.66
1:A:16:LYS:HB3	1:A:356:GLN:HA	1.76	0.66
1:C:121:MET:HA	1:C:128:TYR:OH	1.96	0.66
1:B:180:TYR:CE2	1:B:182:ILE:HA	2.31	0.66
1:C:50:LEU:HA	1:C:81:LYS:O	1.96	0.66
1:C:58:TYR:CB	1:C:73:THR:HA	2.26	0.65
1:B:216:ALA:HA	1:B:240:TYR:C	2.20	0.65
1:A:21:HIS:HB2	1:B:90:TYR:OH	1.96	0.65
1:A:36:MET:HE2	1:A:60:ILE:HG23	1.79	0.65
1:A:82:PHE:HD2	1:A:83:ALA:N	1.94	0.65
1:C:303:GLN:HE22	1:C:335:ASN:HD21	1.44	0.65
1:A:35:TYR:C	1:A:35:TYR:HD1	2.04	0.65
1:A:3:ILE:HD11	1:B:3:ILE:HG21	1.78	0.64
1:C:182:ILE:HD11	1:C:188:VAL:HB	1.80	0.64
1:C:308:TYR:HB2	1:C:329:ILE:O	1.97	0.64
1:A:18:ASP:CG	1:A:354:VAL:HG12	2.23	0.64
1:B:50:LEU:HA	1:B:81:LYS:O	1.97	0.64
1:B:92:ARG:HD3	1:B:126:ASN:OD1	1.97	0.64
1:B:355:TYR:CE2	1:C:42:GLY:HA3	2.33	0.64
1:A:145:PHE:CB	1:A:178:LEU:HD23	2.27	0.64
1:C:136:PHE:O	1:C:139:LEU:HD23	1.98	0.64
1:A:132:ARG:CG	1:A:146:ALA:HB2	2.28	0.64
1:A:95:GLY:HA3	1:A:121:MET:O	1.98	0.63
1:A:273:GLN:NE2	1:A:279:ARG:HB2	2.13	0.63
1:A:46:VAL:HG13	1:C:318:ASN:HD22	1.64	0.63
1:B:32:ASP:OD2	1:C:126:ASN:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:H	1:A:298:ALA:HB3	1.63	0.63
1:B:14:PHE:HE2	1:B:41:LYS:HG3	1.63	0.63
1:B:117:ALA:HB2	1:B:123:GLN:HE21	1.63	0.63
1:B:276:PHE:CE2	1:B:278:LEU:HB2	2.34	0.63
1:B:74:ARG:HG2	1:B:124:ARG:NH2	2.14	0.62
1:A:107:LEU:HD23	1:A:310:ASP:OD1	1.99	0.62
1:A:16:LYS:HB2	1:A:16:LYS:HZ3	1.61	0.62
1:A:59:GLN:NE2	1:A:72:TRP:CZ2	2.68	0.62
1:C:269:VAL:HG23	1:C:283:ALA:HB2	1.82	0.62
1:A:273:GLN:HE21	1:A:279:ARG:HD3	1.63	0.62
1:B:14:PHE:HE1	1:B:57:GLU:HB3	1.64	0.61
1:A:273:GLN:NE2	1:A:279:ARG:HD3	2.14	0.61
1:B:231:TYR:HB3	1:B:271:GLN:HB2	1.83	0.61
1:B:19:GLY:CA	1:B:34:THR:HG22	2.31	0.61
1:A:174:TYR:CD1	1:A:175:GLY:N	2.68	0.61
1:B:36:MET:HE1	1:B:38:ILE:CG1	2.28	0.61
1:C:1:ALA:N	1:C:357:PHE:OXT	2.33	0.61
1:A:306:VAL:HA	1:A:332:LEU:HD11	1.81	0.61
1:A:133:ASN:HB3	1:A:145:PHE:CE2	2.36	0.61
1:A:267:GLU:CB	1:A:285:LEU:HB3	2.28	0.61
1:A:36:MET:HE3	1:A:37:ARG:CA	2.30	0.60
1:C:58:TYR:HB2	1:C:73:THR:HA	1.83	0.60
1:A:52:GLY:HA3	1:C:321:MET:SD	2.41	0.60
1:B:82:PHE:HB3	1:B:85:ALA:HB3	1.82	0.60
1:C:16:LYS:NZ	1:C:18:ASP:HB2	2.16	0.60
1:A:16:LYS:HD2	1:A:37:ARG:HD2	1.84	0.60
1:B:16:LYS:HB3	1:B:356:GLN:HB3	1.84	0.60
1:B:121:MET:SD	1:B:193:THR:HB	2.41	0.60
1:B:334:LYS:NZ	1:B:334:LYS:CD	2.63	0.60
1:A:236:TYR:HB2	1:A:265:ASN:O	2.02	0.60
1:B:58:TYR:HD1	1:B:72:TRP:C	2.10	0.60
1:C:74:ARG:HG2	1:C:124:ARG:HH21	1.67	0.60
1:C:64:GLN:HG3	1:C:70:ASP:HB2	1.84	0.60
1:B:94:TYR:HE1	1:B:98:TYR:CE2	2.21	0.59
1:C:49:GLN:HB3	1:C:82:PHE:CE1	2.37	0.59
1:A:2:GLU:HA	1:A:12:ASP:HA	1.85	0.59
1:A:23:PHE:HB2	1:A:349:VAL:HG13	1.84	0.59
1:A:180:TYR:HB3	1:A:188:VAL:HG12	1.85	0.58
1:B:97:THR:HB	1:B:122:GLN:HA	1.85	0.58
1:B:273:GLN:HG2	1:B:279:ARG:HD3	1.85	0.58
1:A:278:LEU:HD23	1:A:280:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ASN:H	1:B:298:ALA:CB	2.17	0.58
1:B:3:ILE:HG22	1:B:3:ILE:O	2.03	0.58
1:A:123:GLN:CG	1:A:124:ARG:N	2.52	0.58
1:A:107:LEU:HD22	1:A:110:PHE:O	2.05	0.57
1:A:175:GLY:HA2	1:A:193:THR:HA	1.85	0.57
1:B:290:LYS:HG2	1:B:291:ASP:N	2.19	0.57
1:B:108:PRO:HD3	1:B:281:SER:OG	2.04	0.57
1:B:265:ASN:N	1:B:265:ASN:OD1	2.36	0.57
1:B:278:LEU:O	1:B:280:PRO:HD3	2.05	0.57
1:C:131:TYR:HD2	1:C:131:TYR:C	2.12	0.57
1:B:143:LEU:HD13	1:B:180:TYR:HD1	1.69	0.57
1:B:194:THR:HG22	1:B:217:THR:HG22	1.85	0.57
1:A:18:ASP:CB	1:A:35:TYR:HE1	2.16	0.57
1:B:145:PHE:HB3	1:B:178:LEU:CD1	2.35	0.57
1:C:324:TYR:HE2	1:C:352:GLY:HA3	1.70	0.57
1:A:58:TYR:HE1	1:A:71:SER:HB2	1.69	0.56
1:B:304:ASP:HB2	1:B:332:LEU:HD21	1.86	0.56
1:C:131:TYR:C	1:C:131:TYR:CD2	2.83	0.56
1:A:193:THR:OG1	1:A:218:VAL:HG12	2.04	0.56
1:B:6:LYS:HB3	1:B:7:ASP:OD1	2.06	0.56
1:C:45:GLN:O	1:C:45:GLN:HG3	2.04	0.56
1:A:226:ASP:O	1:A:227:ALA:HB2	2.05	0.56
1:A:266:PHE:CZ	1:A:268:VAL:HB	2.40	0.56
1:B:94:TYR:CD1	1:B:98:TYR:CD2	2.93	0.56
1:C:240:TYR:CD1	1:C:240:TYR:C	2.84	0.56
1:B:132:ARG:HG3	1:B:146:ALA:HB2	1.87	0.56
1:C:234:ALA:HB2	1:C:268:VAL:HG23	1.88	0.56
1:B:322:SER:HB2	1:B:354:VAL:HG22	1.88	0.56
1:A:324:TYR:CE2	1:A:352:GLY:CA	2.89	0.56
1:B:294:ASN:H	1:B:298:ALA:HB3	1.71	0.56
1:C:306:VAL:HA	1:C:332:LEU:HD11	1.87	0.56
1:A:353:LEU:HD23	1:B:78:ALA:O	2.06	0.56
1:A:16:LYS:HB3	1:A:356:GLN:CB	2.37	0.55
1:C:272:TYR:O	1:C:280:PRO:HD2	2.06	0.55
1:A:36:MET:HE2	1:A:60:ILE:HG22	1.87	0.55
1:B:276:PHE:HE2	1:B:278:LEU:HB2	1.69	0.55
1:C:14:PHE:CE2	1:C:41:LYS:HG3	2.38	0.55
1:C:230:ILE:CD1	1:C:272:TYR:HD1	2.20	0.55
1:C:219:TYR:O	1:C:237:SER:OG	2.23	0.55
1:A:16:LYS:NZ	1:A:18:ASP:HB2	2.21	0.55
1:A:46:VAL:HB	1:A:50:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:CD	1:A:319:LYS:H	2.19	0.55
1:B:148:GLN:HG2	1:B:149:TYR:N	2.21	0.55
1:C:227:ALA:O	1:C:229:ASN:N	2.40	0.55
1:A:263:ALA:N	1:A:289:GLY:HA2	2.21	0.55
1:B:114:THR:HB	1:B:265:ASN:HD22	1.71	0.55
1:B:36:MET:CE	1:B:38:ILE:HG13	2.35	0.54
1:C:36:MET:SD	1:C:36:MET:C	2.90	0.54
1:A:3:ILE:CD1	1:B:3:ILE:HG21	2.37	0.54
1:A:47:ASN:C	1:A:49:GLN:N	2.65	0.54
1:A:128:TYR:HE1	1:A:150:GLN:CG	2.19	0.54
1:A:321:MET:SD	1:B:52:GLY:HA3	2.48	0.54
1:B:285:LEU:HD11	1:B:308:TYR:CE1	2.43	0.54
1:A:334:LYS:HE2	1:A:345:THR:HG21	1.89	0.54
1:B:34:THR:O	1:B:62:GLY:N	2.41	0.54
1:C:293:SER:HA	1:C:298:ALA:O	2.08	0.54
1:A:47:ASN:C	1:A:49:GLN:H	2.14	0.54
1:B:266:PHE:HZ	1:B:268:VAL:HB	1.68	0.54
1:B:308:TYR:HA	1:B:331:LEU:HG	1.88	0.54
1:A:220:THR:HA	1:A:237:SER:HB2	1.90	0.54
1:A:278:LEU:CD2	1:A:280:PRO:HD3	2.38	0.54
1:C:126:ASN:N	1:C:126:ASN:HD22	2.06	0.54
1:A:16:LYS:HB3	1:A:356:GLN:CA	2.38	0.53
1:B:18:ASP:C	1:B:18:ASP:OD1	2.51	0.53
1:B:269:VAL:HG23	1:B:283:ALA:HB2	1.89	0.53
1:B:79:GLY:HA3	1:B:88:PHE:O	2.07	0.53
1:B:233:ALA:O	1:B:268:VAL:HG23	2.09	0.53
1:C:35:TYR:C	1:C:35:TYR:HD1	2.15	0.53
1:C:16:LYS:HZ1	1:C:354:VAL:HB	1.73	0.53
1:C:61:GLN:HG3	1:C:70:ASP:HB3	1.90	0.53
1:A:3:ILE:CG1	1:B:3:ILE:HG21	2.38	0.53
1:A:36:MET:HG2	1:B:56:TRP:CD1	2.43	0.53
1:B:58:TYR:HB2	1:B:73:THR:CA	2.13	0.53
1:C:92:ARG:HD2	1:C:125:GLY:O	2.08	0.53
1:A:16:LYS:HB3	1:A:356:GLN:HB3	1.90	0.53
1:B:357:PHE:HE1	1:C:40:PHE:CZ	2.26	0.53
1:C:174:TYR:CG	1:C:175:GLY:N	2.77	0.53
1:A:237:SER:OG	1:A:238:GLN:N	2.41	0.53
1:C:3:ILE:O	1:C:3:ILE:CG2	2.56	0.53
1:C:16:LYS:NZ	1:C:16:LYS:HB2	2.23	0.53
1:C:90:TYR:HA	1:C:128:TYR:O	2.09	0.53
1:B:311:VAL:HG12	1:B:327:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLY:HA2	1:C:56:TRP:CE3	2.44	0.53
1:C:311:VAL:HG12	1:C:327:TYR:HB3	1.91	0.53
1:B:96:VAL:HB	1:B:148:GLN:OE1	2.09	0.53
1:B:57:GLU:O	1:B:57:GLU:HG3	2.09	0.52
1:B:321:MET:HB2	1:C:44:THR:HG21	1.91	0.52
1:C:133:ASN:HB3	1:C:145:PHE:CE2	2.43	0.52
1:A:36:MET:HE1	1:A:38:ILE:HD11	1.86	0.52
1:A:334:LYS:HE2	1:A:345:THR:CG2	2.40	0.52
1:C:38:ILE:HG22	1:C:39:GLY:H	1.75	0.52
1:C:194:THR:O	1:C:196:LYS:NZ	2.25	0.52
1:C:324:TYR:HE2	1:C:352:GLY:CA	2.21	0.52
1:B:143:LEU:HD12	1:B:179:THR:O	2.08	0.52
1:B:36:MET:HE2	1:B:37:ARG:N	2.25	0.52
1:A:14:PHE:HE2	1:A:41:LYS:HG3	1.73	0.52
1:A:58:TYR:CE1	1:A:71:SER:HB2	2.44	0.52
1:A:97:THR:O	1:A:101:THR:OG1	2.24	0.52
1:A:24:SER:OG	1:A:348:ILE:HG22	2.09	0.52
1:B:14:PHE:HE1	1:B:57:GLU:CB	2.23	0.52
1:B:234:ALA:HB2	1:B:268:VAL:HG23	1.91	0.52
1:A:236:TYR:CB	1:A:266:PHE:HA	2.36	0.51
1:C:16:LYS:HA	1:C:355:TYR:O	2.10	0.51
1:C:18:ASP:OD2	1:C:354:VAL:HG12	2.10	0.51
1:B:94:TYR:CE1	1:B:98:TYR:CE2	2.98	0.51
1:A:54:GLY:HA3	1:C:355:TYR:CD2	2.46	0.51
1:B:18:ASP:CG	1:B:354:VAL:HG12	2.36	0.51
1:B:94:TYR:HD1	1:B:98:TYR:CD2	2.28	0.51
1:C:53:TYR:HD1	1:C:53:TYR:H	1.57	0.51
1:A:20:LEU:HD23	1:A:20:LEU:C	2.35	0.51
1:A:266:PHE:HZ	1:A:268:VAL:HB	1.75	0.51
1:A:293:SER:HA	1:A:298:ALA:O	2.10	0.51
1:B:62:GLY:O	1:C:126:ASN:OD1	2.28	0.51
1:C:83:ALA:O	1:C:84:ASP:HB2	2.10	0.51
1:C:223:LEU:O	1:C:233:ALA:HA	2.10	0.51
1:C:294:ASN:H	1:C:298:ALA:HB3	1.75	0.51
1:A:57:GLU:HG2	1:A:74:ARG:HB2	1.92	0.51
1:B:121:MET:HB3	1:B:150:GLN:NE2	2.26	0.51
1:C:103:TRP:CD2	1:C:224:LYS:HD2	2.45	0.51
1:A:22:TYR:CE1	1:A:110:PHE:CE1	2.95	0.51
1:A:185:GLY:HA3	1:A:226:ASP:O	2.11	0.51
1:C:42:GLY:N	1:C:54:GLY:O	2.44	0.51
1:B:282:VAL:HA	1:B:310:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE2	1:B:92:ARG:NH2	2.43	0.50
1:A:346:ASP:O	1:A:348:ILE:HG23	2.10	0.50
1:A:92:ARG:HH22	1:C:66:GLU:HB2	1.76	0.50
1:C:231:TYR:O	1:C:232:LEU:HD23	2.10	0.50
1:B:18:ASP:HB3	1:B:35:TYR:HE1	1.75	0.50
1:B:107:LEU:HD21	1:B:283:ALA:HB3	1.93	0.50
1:B:228:ASN:C	1:B:230:ILE:N	2.69	0.50
1:C:3:ILE:HD12	1:C:13:LEU:HB3	1.92	0.50
1:A:71:SER:O	1:A:72:TRP:HE3	1.95	0.50
1:B:292:ILE:HB	1:B:300:TYR:HB2	1.94	0.50
1:C:39:GLY:HA3	1:C:57:GLU:HB2	1.93	0.50
1:C:239:THR:OG1	1:C:240:TYR:N	2.44	0.50
1:A:18:ASP:HA	1:A:354:VAL:HA	1.94	0.50
1:A:240:TYR:CD1	1:A:240:TYR:C	2.90	0.50
1:B:22:TYR:CE1	1:B:110:PHE:CE1	2.68	0.50
1:B:103:TRP:CG	1:B:224:LYS:HD2	2.47	0.50
1:B:115:TYR:N	1:B:115:TYR:CD2	2.80	0.50
1:B:49:GLN:HB3	1:B:82:PHE:CE1	2.47	0.50
1:C:3:ILE:O	1:C:3:ILE:HG23	2.10	0.50
1:A:1:ALA:C	1:A:12:ASP:OD1	2.54	0.50
1:B:128:TYR:CD1	1:B:148:GLN:NE2	2.80	0.50
1:C:277:GLY:O	1:C:278:LEU:CB	2.53	0.50
1:A:182:ILE:HD12	1:A:186:PHE:HB3	1.94	0.49
1:B:228:ASN:C	1:B:230:ILE:H	2.19	0.49
1:A:20:LEU:H	1:A:34:THR:HG22	1.76	0.49
1:C:121:MET:HG3	1:C:128:TYR:CE1	2.41	0.49
1:C:294:ASN:N	1:C:297:GLY:O	2.45	0.49
1:B:3:ILE:HD11	1:B:13:LEU:CD2	2.32	0.49
1:B:36:MET:SD	1:C:56:TRP:NE1	2.85	0.49
1:B:278:LEU:O	1:B:280:PRO:CD	2.60	0.49
1:C:16:LYS:NZ	1:C:354:VAL:HB	2.27	0.49
1:C:59:GLN:C	1:C:60:ILE:HG13	2.37	0.49
1:C:104:THR:HG21	1:C:235:GLN:HB3	1.93	0.49
1:C:132:ARG:CG	1:C:146:ALA:HB2	2.41	0.49
1:A:98:TYR:O	1:A:102:SER:OG	2.21	0.49
1:A:333:ASP:OD1	1:A:333:ASP:N	2.45	0.49
1:B:225:TYR:OH	1:B:227:ALA:HB3	2.12	0.49
1:B:357:PHE:CE1	1:C:40:PHE:CZ	3.01	0.49
1:C:220:THR:HG22	1:C:235:GLN:HE21	1.78	0.49
1:A:266:PHE:CG	1:A:267:GLU:N	2.81	0.49
1:B:266:PHE:CG	1:B:267:GLU:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:HG2	1:B:149:TYR:H	1.77	0.49
1:C:192:ILE:N	1:C:192:ILE:HD13	2.28	0.49
1:C:292:ILE:HG22	1:C:293:SER:N	2.28	0.49
1:A:22:TYR:CD1	1:A:348:ILE:HD12	2.48	0.48
1:B:125:GLY:HA3	1:B:128:TYR:CZ	2.49	0.48
1:C:126:ASN:N	1:C:126:ASN:ND2	2.60	0.48
1:C:216:ALA:HA	1:C:240:TYR:HB3	1.96	0.48
1:A:66:GLU:OE1	1:B:124:ARG:NH2	2.45	0.48
1:C:180:TYR:CE2	1:C:182:ILE:HA	2.48	0.48
1:A:291:ASP:O	1:A:292:ILE:HG13	2.13	0.48
1:B:180:TYR:CD2	1:B:182:ILE:HA	2.48	0.48
1:A:21:HIS:C	1:A:21:HIS:CD2	2.92	0.48
1:A:192:ILE:HD13	1:A:192:ILE:H	1.78	0.48
1:B:53:TYR:HE2	1:B:81:LYS:NZ	2.12	0.48
1:B:334:LYS:HG2	1:B:345:THR:OG1	2.13	0.48
1:A:184:GLU:OE1	1:A:225:TYR:HE1	1.96	0.48
1:C:2:GLU:HA	1:C:12:ASP:HA	1.95	0.48
1:C:6:LYS:HE2	1:C:6:LYS:HB3	1.58	0.48
1:C:18:ASP:HA	1:C:354:VAL:HA	1.95	0.48
1:C:16:LYS:HB2	1:C:16:LYS:HZ3	1.78	0.47
1:C:110:PHE:CE1	1:C:348:ILE:HD11	2.49	0.47
1:B:14:PHE:CZ	1:B:57:GLU:HB3	2.48	0.47
1:C:61:GLN:CG	1:C:70:ASP:HB3	2.44	0.47
1:C:99:ASP:OD1	1:C:99:ASP:N	2.43	0.47
1:A:3:ILE:CG1	1:B:3:ILE:CG2	2.92	0.47
1:A:60:ILE:HD11	1:B:73:THR:OG1	2.15	0.47
1:B:53:TYR:CE2	1:B:81:LYS:NZ	2.82	0.47
1:B:237:SER:OG	1:B:238:GLN:N	2.47	0.47
1:C:74:ARG:HG2	1:C:124:ARG:NH2	2.29	0.47
1:C:240:TYR:C	1:C:240:TYR:HD1	2.21	0.47
1:A:121:MET:HB2	1:A:150:GLN:OE1	2.15	0.47
1:A:125:GLY:CA	1:A:128:TYR:HE2	2.28	0.47
1:B:355:TYR:CD2	1:C:54:GLY:HA3	2.50	0.47
1:C:103:TRP:CG	1:C:224:LYS:HD2	2.50	0.47
1:C:123:GLN:NE2	1:C:124:ARG:HD3	2.29	0.47
1:A:291:ASP:C	1:A:292:ILE:HG13	2.39	0.47
1:C:38:ILE:HG22	1:C:39:GLY:N	2.29	0.47
1:B:96:VAL:HG12	1:B:121:MET:HE2	1.96	0.47
1:B:192:ILE:C	1:B:193:THR:HG23	2.39	0.47
1:C:18:ASP:CB	1:C:35:TYR:HE1	2.13	0.47
1:C:89:ASP:OD1	1:C:130:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:HD13	1:C:180:TYR:HD1	1.80	0.47
1:A:128:TYR:CD1	1:A:150:GLN:HG2	2.50	0.47
1:A:90:TYR:HA	1:A:128:TYR:O	2.15	0.47
1:A:36:MET:CE	1:A:38:ILE:CD1	2.85	0.47
1:B:192:ILE:HD13	1:B:192:ILE:H	1.80	0.47
1:C:15:GLY:HA3	1:C:357:PHE:CZ	2.49	0.47
1:C:263:ALA:N	1:C:289:GLY:HA2	2.30	0.47
1:A:45:GLN:O	1:A:45:GLN:HG3	2.14	0.46
1:A:16:LYS:CE	1:A:18:ASP:HB2	2.45	0.46
1:C:32:ASP:OD1	1:C:34:THR:HG23	2.14	0.46
1:A:193:THR:OG1	1:A:218:VAL:CG1	2.63	0.46
1:B:354:VAL:HG23	1:B:354:VAL:O	2.15	0.46
1:A:3:ILE:HG12	1:B:3:ILE:HG21	1.98	0.46
1:A:47:ASN:O	1:A:48:ASP:C	2.58	0.46
1:A:18:ASP:OD1	1:A:18:ASP:C	2.58	0.46
1:A:22:TYR:HE1	1:A:110:PHE:CE1	2.15	0.46
1:A:59:GLN:NE2	1:A:61:GLN:OE1	2.49	0.46
1:B:172:ASP:O	1:B:195:SER:HB2	2.16	0.46
1:B:194:THR:HG22	1:B:217:THR:HB	1.97	0.46
1:C:96:VAL:HB	1:C:148:GLN:HB2	1.98	0.46
1:A:20:LEU:N	1:A:34:THR:HG22	2.31	0.46
1:B:267:GLU:CB	1:B:285:LEU:HB3	2.41	0.46
1:B:320:ASN:N	1:B:320:ASN:HD22	2.14	0.46
1:B:133:ASN:HB3	1:B:145:PHE:CE2	2.50	0.46
1:B:192:ILE:O	1:B:193:THR:CG2	2.64	0.46
1:A:184:GLU:OE1	1:A:225:TYR:CE1	2.69	0.46
1:C:16:LYS:HB3	1:C:356:GLN:CB	2.45	0.46
1:A:115:TYR:N	1:A:115:TYR:CD2	2.84	0.45
1:A:303:GLN:HE22	1:A:335:ASN:ND2	2.01	0.45
1:A:272:TYR:HD2	1:A:274:PHE:HD2	1.63	0.45
1:B:35:TYR:CE2	1:B:59:GLN:OE1	2.68	0.45
1:A:308:TYR:HA	1:A:331:LEU:HG	1.98	0.45
1:B:5:ASN:OD1	1:B:5:ASN:C	2.58	0.45
1:A:194:THR:CB	1:A:196:LYS:HZ1	2.28	0.45
1:B:47:ASN:HB3	1:B:49:GLN:H	1.80	0.45
1:B:355:TYR:CZ	1:C:42:GLY:HA3	2.51	0.45
1:C:55:GLN:HG2	1:C:56:TRP:H	1.82	0.45
1:A:3:ILE:HG12	1:B:3:ILE:CG2	2.47	0.45
1:A:88:PHE:HA	1:A:130:THR:O	2.17	0.45
1:B:45:GLN:O	1:B:45:GLN:HG3	2.17	0.45
1:B:181:ALA:C	1:B:183:GLY:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:MET:SD	1:C:150:GLN:HG3	2.55	0.45
1:B:128:TYR:HD2	1:B:128:TYR:N	2.14	0.45
1:B:263:ALA:HB2	1:B:290:LYS:CE	2.46	0.45
1:B:351:LEU:C	1:B:351:LEU:HD23	2.42	0.45
1:C:180:TYR:HE2	1:C:182:ILE:HA	1.81	0.45
1:A:80:LEU:O	1:A:87:SER:HB2	2.17	0.45
1:A:94:TYR:CD1	1:A:98:TYR:CD2	3.05	0.45
1:A:225:TYR:HE2	1:A:230:ILE:HB	1.81	0.45
1:B:35:TYR:C	1:B:35:TYR:CD1	2.95	0.45
1:C:58:TYR:HB3	1:C:73:THR:HA	1.97	0.45
1:A:236:TYR:HB2	1:A:266:PHE:CA	2.43	0.45
1:A:294:ASN:N	1:A:297:GLY:O	2.50	0.45
1:A:93:ASN:OD1	1:A:94:TYR:N	2.43	0.45
1:B:32:ASP:HB2	1:C:127:GLY:HA2	1.99	0.45
1:C:274:PHE:HD1	1:C:276:PHE:CE1	2.34	0.45
1:B:97:THR:HG23	1:B:220:THR:OG1	2.18	0.44
1:C:110:PHE:HE1	1:C:348:ILE:HD11	1.81	0.44
1:A:40:PHE:CD2	1:A:40:PHE:O	2.70	0.44
1:A:144:ASP:HB2	1:A:179:THR:OG1	2.17	0.44
1:B:14:PHE:CD1	1:B:14:PHE:C	2.95	0.44
1:B:59:GLN:O	1:B:60:ILE:HG13	2.16	0.44
1:B:290:LYS:HG2	1:B:291:ASP:H	1.79	0.44
1:C:92:ARG:NH1	1:C:124:ARG:HB3	2.22	0.44
1:A:46:VAL:HB	1:A:50:LEU:CD2	2.46	0.44
1:C:16:LYS:HZ1	1:C:354:VAL:CB	2.29	0.44
1:C:35:TYR:HD1	1:C:35:TYR:O	2.01	0.44
1:A:14:PHE:CE2	1:A:41:LYS:HG3	2.53	0.44
1:A:1:ALA:HB1	1:B:4:TYR:CD2	2.52	0.44
1:A:125:GLY:HA3	1:A:128:TYR:HE2	1.83	0.44
1:A:236:TYR:HB3	1:A:266:PHE:HD1	1.81	0.44
1:A:330:ASN:H	1:A:347:ASP:HB3	1.83	0.44
1:A:52:GLY:CA	1:C:321:MET:SD	3.06	0.44
1:A:121:MET:SD	1:A:193:THR:HB	2.57	0.44
1:B:39:GLY:HA3	1:B:57:GLU:HA	2.00	0.44
1:C:314:THR:HB	1:C:316:TYR:CE1	2.53	0.44
1:A:297:GLY:O	1:A:298:ALA:HB3	2.18	0.44
1:A:314:THR:HG22	1:A:324:TYR:HB3	2.00	0.44
1:B:59:GLN:HE21	1:B:72:TRP:HZ2	1.65	0.44
1:B:86:GLY:HA3	1:B:131:TYR:HE2	1.82	0.44
1:B:293:SER:HA	1:B:298:ALA:HB3	2.00	0.44
1:B:307:LYS:O	1:B:307:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:PHE:O	1:C:348:ILE:HB	2.18	0.43
1:A:42:GLY:HA3	1:C:355:TYR:CE2	2.53	0.43
1:A:60:ILE:HD13	1:B:56:TRP:HE1	1.83	0.43
1:A:92:ARG:HB2	1:C:62:GLY:O	2.18	0.43
1:B:11:LEU:O	1:B:11:LEU:HG	2.18	0.43
1:B:49:GLN:HB3	1:B:82:PHE:CZ	2.53	0.43
1:B:91:GLY:O	1:B:93:ASN:N	2.50	0.43
1:B:115:TYR:N	1:B:115:TYR:HD2	2.16	0.43
1:A:195:SER:CA	1:A:196:LYS:HE2	2.48	0.43
1:A:285:LEU:HD11	1:A:308:TYR:CZ	2.53	0.43
1:A:58:TYR:CD2	1:A:58:TYR:C	2.97	0.43
1:B:194:THR:HG22	1:B:217:THR:CB	2.48	0.43
1:B:128:TYR:N	1:B:128:TYR:CD2	2.86	0.43
1:C:95:GLY:HA3	1:C:121:MET:O	2.18	0.43
1:B:32:ASP:O	1:B:63:ASN:HB3	2.19	0.43
1:C:225:TYR:OH	1:C:227:ALA:HB3	2.19	0.43
1:A:36:MET:CE	1:A:38:ILE:HD11	2.48	0.43
1:A:116:GLY:O	1:A:123:GLN:HB3	2.19	0.43
1:A:226:ASP:O	1:A:227:ALA:CB	2.67	0.43
1:C:94:TYR:CZ	1:C:124:ARG:HD2	2.53	0.43
1:A:56:TRP:HD1	1:A:76:ALA:HB2	1.84	0.42
1:C:116:GLY:C	1:C:119:ASN:HB2	2.44	0.42
1:A:104:THR:HG21	1:A:267:GLU:HG3	2.01	0.42
1:A:307:LYS:HG3	1:A:331:LEU:HB2	2.00	0.42
1:B:14:PHE:CE2	1:B:41:LYS:HG3	2.49	0.42
1:B:21:HIS:HD2	1:B:22:TYR:O	2.01	0.42
1:B:98:TYR:O	1:B:99:ASP:C	2.60	0.42
1:C:330:ASN:H	1:C:347:ASP:HB3	1.83	0.42
1:A:36:MET:HE1	1:A:38:ILE:HD12	1.93	0.42
1:A:174:TYR:CG	1:A:175:GLY:N	2.88	0.42
1:B:96:VAL:N	1:B:148:GLN:OE1	2.52	0.42
1:C:108:PRO:HG2	1:C:312:GLY:HA3	2.00	0.42
1:B:305:ILE:O	1:B:343:ILE:HG21	2.19	0.42
1:B:321:MET:HE2	1:C:80:LEU:HD23	2.01	0.42
1:C:274:PHE:HB2	1:C:278:LEU:O	2.20	0.42
1:B:108:PRO:HG2	1:B:312:GLY:HA3	2.00	0.42
1:B:128:TYR:CE2	1:B:150:GLN:HG2	2.54	0.42
1:A:180:TYR:CE2	1:A:182:ILE:HA	2.54	0.42
1:B:181:ALA:C	1:B:183:GLY:N	2.77	0.42
1:C:92:ARG:HD3	1:C:126:ASN:CG	2.44	0.42
1:A:9:ASN:ND2	1:C:320:ASN:ND2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:O	1:A:237:SER:OG	2.35	0.42
1:B:24:SER:CB	1:B:348:ILE:HG22	2.50	0.42
1:B:94:TYR:CE1	1:B:98:TYR:CD2	3.08	0.42
1:B:123:GLN:HG3	1:B:124:ARG:N	2.33	0.42
1:C:58:TYR:HB2	1:C:72:TRP:C	2.45	0.42
1:A:234:ALA:HB2	1:A:268:VAL:CG2	2.36	0.42
1:B:180:TYR:HE2	1:B:182:ILE:HA	1.80	0.42
1:B:351:LEU:HD23	1:B:351:LEU:O	2.20	0.42
1:C:123:GLN:HE21	1:C:124:ARG:HD3	1.84	0.42
1:A:20:LEU:H	1:A:34:THR:CG2	2.33	0.41
1:A:35:TYR:HD1	1:A:35:TYR:O	2.03	0.41
1:A:55:GLN:O	1:A:76:ALA:HA	2.20	0.41
1:A:121:MET:HE3	1:A:150:GLN:CG	2.50	0.41
1:A:290:LYS:HA	1:A:302:ASP:OD2	2.20	0.41
1:B:229:ASN:O	1:B:272:TYR:HA	2.20	0.41
1:B:328:LYS:O	1:B:347:ASP:HB2	2.20	0.41
1:B:180:TYR:HB3	1:B:188:VAL:HG12	2.02	0.41
1:B:265:ASN:HB3	1:B:287:SER:HB3	2.02	0.41
1:C:21:HIS:CD2	1:C:31:GLY:O	2.73	0.41
1:C:348:ILE:HD12	1:C:349:VAL:N	2.35	0.41
1:A:31:GLY:C	1:A:33:GLN:HE22	2.28	0.41
1:A:16:LYS:HD2	1:A:37:ARG:CD	2.50	0.41
1:A:327:TYR:CD2	1:A:329:ILE:HD13	2.55	0.41
1:C:5:ASN:ND2	1:C:10:LYS:HG2	2.36	0.41
1:C:79:GLY:HA3	1:C:89:ASP:HB3	2.02	0.41
1:C:284:TYR:CG	1:C:285:LEU:N	2.88	0.41
1:A:84:ASP:O	1:A:137:PHE:HA	2.20	0.41
1:A:287:SER:OG	1:A:305:ILE:HB	2.20	0.41
1:B:45:GLN:HE21	1:B:45:GLN:HB2	1.60	0.41
1:B:58:TYR:CE1	1:B:71:SER:HB2	2.56	0.41
1:C:40:PHE:O	1:C:40:PHE:CD2	2.74	0.41
1:A:58:TYR:HB2	1:A:73:THR:HA	2.03	0.41
1:A:177:SER:HA	1:A:191:ALA:HA	2.02	0.41
1:A:182:ILE:H	1:A:182:ILE:HG13	1.54	0.41
1:B:53:TYR:HE1	1:B:89:ASP:HB3	1.85	0.41
1:B:148:GLN:CG	1:B:149:TYR:N	2.83	0.41
1:C:41:LYS:HA	1:C:55:GLN:HG3	2.02	0.41
1:C:59:GLN:CG	1:C:60:ILE:H	2.34	0.41
1:C:112:GLY:O	1:C:114:THR:N	2.51	0.41
1:A:353:LEU:HD21	1:B:79:GLY:HA2	2.03	0.41
1:A:40:PHE:CD2	1:A:40:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TYR:HB3	1:A:323:THR:HG22	2.03	0.41
1:B:18:ASP:HB3	1:B:35:TYR:CE1	2.55	0.41
1:B:53:TYR:HE1	1:B:79:GLY:HA3	1.86	0.41
1:B:55:GLN:O	1:B:76:ALA:HA	2.21	0.41
1:B:132:ARG:HE	1:B:132:ARG:HB2	1.75	0.41
1:B:303:GLN:HB2	1:B:337:PHE:CD1	2.55	0.41
1:C:26:ASP:HB3	1:C:29:SER:HB2	2.02	0.41
1:C:230:ILE:HD11	1:C:272:TYR:HD1	1.85	0.41
1:A:318:ASN:HB2	1:A:319:LYS:HD2	2.03	0.41
1:B:192:ILE:C	1:B:193:THR:CG2	2.94	0.41
1:B:274:PHE:HD1	1:B:276:PHE:CE1	2.40	0.41
1:B:219:TYR:O	1:B:237:SER:HB3	2.17	0.40
1:A:73:THR:HG21	1:A:76:ALA:HB2	2.03	0.40
1:A:94:TYR:CZ	1:A:124:ARG:HD2	2.56	0.40
1:A:97:THR:HB	1:A:122:GLN:HA	2.02	0.40
1:A:120:PHE:O	1:A:121:MET:HB3	2.21	0.40
1:C:231:TYR:O	1:C:270:ALA:HA	2.21	0.40
1:A:309:VAL:CG2	1:A:310:ASP:N	2.85	0.40
1:B:88:PHE:CD2	1:B:88:PHE:C	2.99	0.40
1:B:304:ASP:HB2	1:B:332:LEU:CD2	2.50	0.40
1:B:308:TYR:HB2	1:B:330:ASN:HA	2.03	0.40
1:C:221:GLY:O	1:C:235:GLN:HA	2.22	0.40
1:C:270:ALA:O	1:C:282:VAL:HG23	2.20	0.40
1:A:192:ILE:C	1:A:193:THR:CG2	2.95	0.40
1:C:56:TRP:O	1:C:57:GLU:HB3	2.21	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	290/357 (81%)	235 (81%)	44 (15%)	11 (4%)	2 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	290/357 (81%)	239 (82%)	42 (14%)	9 (3%)	3	25
1	C	290/357 (81%)	238 (82%)	39 (13%)	13 (4%)	2	17
All	All	870/1071 (81%)	712 (82%)	125 (14%)	33 (4%)	2	21

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	92	ARG
1	B	113	ASP
1	B	136	PHE
1	B	172	ASP
1	C	113	ASP
1	C	228	ASN
1	C	278	LEU
1	A	113	ASP
1	A	136	PHE
1	A	227	ALA
1	B	128	TYR
1	B	137	PHE
1	C	92	ARG
1	C	101	THR
1	C	301	GLY
1	C	305	ILE
1	A	121	MET
1	C	84	ASP
1	C	295	GLY
1	A	186	PHE
1	B	229	ASN
1	B	295	GLY
1	C	16	LYS
1	C	112	GLY
1	C	136	PHE
1	A	6	LYS
1	A	99	ASP
1	A	83	ALA
1	A	298	ALA
1	B	16	LYS
1	C	106	VAL
1	A	106	VAL

5.3.2 Protein sidechains ⓘ

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	233/282 (83%)	175 (75%)	58 (25%)	0	4
1	B	234/282 (83%)	189 (81%)	45 (19%)	1	9
1	C	232/282 (82%)	187 (81%)	45 (19%)	1	9
All	All	699/846 (83%)	551 (79%)	148 (21%)	1	7

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	7	ASP
1	A	13	LEU
1	A	16	LYS
1	A	20	LEU
1	A	32	ASP
1	A	35	TYR
1	A	36	MET
1	A	38	ILE
1	A	43	GLU
1	A	44	THR
1	A	45	GLN
1	A	46	VAL
1	A	50	LEU
1	A	53	TYR
1	A	57	GLU
1	A	58	TYR
1	A	60	ILE
1	A	66	GLU
1	A	68	SER
1	A	69	ASN
1	A	70	ASP
1	A	87	SER
1	A	89	ASP
1	A	97	THR
1	A	100	VAL

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Mol	Chain	Res	Type
1	A	101	THR
1	A	106	VAL
1	A	113	ASP
1	A	115	TYR
1	A	139	LEU
1	A	172	ASP
1	A	178	LEU
1	A	182	ILE
1	A	188	VAL
1	A	192	ILE
1	A	195	SER
1	A	220	THR
1	A	223	LEU
1	A	239	THR
1	A	269	VAL
1	A	273	GLN
1	A	279	ARG
1	A	285	LEU
1	A	290	LYS
1	A	306	VAL
1	A	309	VAL
1	A	314	THR
1	A	319	LYS
1	A	322	SER
1	A	324	TYR
1	A	329	ILE
1	A	333	ASP
1	A	334	LYS
1	A	343	ILE
1	A	345	THR
1	A	351	LEU
1	A	356	GLN
1	B	7	ASP
1	B	9	ASN
1	B	13	LEU
1	B	16	LYS
1	B	20	LEU
1	B	32	ASP
1	B	35	TYR
1	B	36	MET
1	B	38	ILE
1	B	45	GLN

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Mol	Chain	Res	Type
1	B	53	TYR
1	B	58	TYR
1	B	60	ILE
1	B	68	SER
1	B	69	ASN
1	B	70	ASP
1	B	75	VAL
1	B	81	LYS
1	B	100	VAL
1	B	110	PHE
1	B	113	ASP
1	B	115	TYR
1	B	119	ASN
1	B	132	ARG
1	B	139	LEU
1	B	144	ASP
1	B	152	LYS
1	B	172	ASP
1	B	174	TYR
1	B	178	LEU
1	B	192	ILE
1	B	220	THR
1	B	223	LEU
1	B	239	THR
1	B	265	ASN
1	B	273	GLN
1	B	282	VAL
1	B	285	LEU
1	B	290	LYS
1	B	299	SER
1	B	322	SER
1	B	340	ASP
1	B	345	THR
1	B	351	LEU
1	B	356	GLN
1	C	2	GLU
1	C	3	ILE
1	C	7	ASP
1	C	16	LYS
1	C	20	LEU
1	C	32	ASP
1	C	35	TYR

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Mol	Chain	Res	Type
1	C	45	GLN
1	C	50	LEU
1	C	53	TYR
1	C	57	GLU
1	C	58	TYR
1	C	69	ASN
1	C	70	ASP
1	C	99	ASP
1	C	101	THR
1	C	106	VAL
1	C	109	GLU
1	C	110	PHE
1	C	113	ASP
1	C	126	ASN
1	C	131	TYR
1	C	144	ASP
1	C	147	LEU
1	C	172	ASP
1	C	182	ILE
1	C	192	ILE
1	C	195	SER
1	C	218	VAL
1	C	220	THR
1	C	239	THR
1	C	240	TYR
1	C	267	GLU
1	C	273	GLN
1	C	282	VAL
1	C	285	LEU
1	C	290	LYS
1	C	314	THR
1	C	321	MET
1	C	324	TYR
1	C	325	VAL
1	C	343	ILE
1	C	348	ILE
1	C	349	VAL
1	C	356	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	ASN
1	A	45	GLN
1	A	59	GLN
1	A	69	ASN
1	A	119	ASN
1	A	273	GLN
1	A	335	ASN
1	B	9	ASN
1	B	45	GLN
1	B	61	GLN
1	B	63	ASN
1	B	64	GLN
1	B	119	ASN
1	B	123	GLN
1	B	318	ASN
1	B	320	ASN
1	B	335	ASN
1	B	356	GLN
1	C	5	ASN
1	C	9	ASN
1	C	21	HIS
1	C	45	GLN
1	C	55	GLN
1	C	59	GLN
1	C	61	GLN
1	C	63	ASN
1	C	123	GLN
1	C	235	GLN
1	C	303	GLN
1	C	320	ASN
1	C	335	ASN
1	C	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	298/357 (83%)	0.69	30 (10%)	12 10	109, 199, 280, 322	0
1	B	298/357 (83%)	0.60	36 (12%)	8 7	116, 235, 314, 335	0
1	C	298/357 (83%)	0.54	27 (9%)	15 11	136, 255, 343, 379	0
All	All	894/1071 (83%)	0.61	93 (10%)	11 9	109, 229, 322, 379	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	TYR	8.2
1	A	292	ILE	7.8
1	A	305	ILE	6.5
1	A	117	ALA	6.0
1	A	125	GLY	5.6
1	B	295	GLY	5.5
1	C	305	ILE	5.3
1	A	118	ASP	4.9
1	C	109	GLU	4.7
1	B	174	TYR	4.6
1	A	94	TYR	4.4
1	C	329	ILE	4.4
1	A	128	TYR	4.2
1	A	300	TYR	4.2
1	A	58	TYR	4.2
1	A	91	GLY	4.1
1	A	74	ARG	4.1
1	B	173	GLY	4.0
1	B	309	VAL	4.0
1	B	223	LEU	4.0
1	A	92	ARG	3.9
1	B	297	GLY	3.9
1	C	58	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	123	GLN	3.8
1	C	328	LYS	3.8
1	C	311	VAL	3.8
1	B	113	ASP	3.7
1	B	344	ASN	3.7
1	C	113	ASP	3.7
1	C	298	ALA	3.6
1	C	306	VAL	3.6
1	B	149	TYR	3.6
1	B	69	ASN	3.5
1	B	38	ILE	3.5
1	A	33	GLN	3.5
1	C	292	ILE	3.4
1	B	240	TYR	3.4
1	B	305	ILE	3.3
1	C	63	ASN	3.3
1	A	116	GLY	3.3
1	A	293	SER	3.2
1	A	351	LEU	3.2
1	A	124	ARG	3.1
1	B	63	ASN	3.1
1	A	184	GLU	3.0
1	A	299	SER	2.9
1	B	298	ALA	2.9
1	C	344	ASN	2.9
1	C	309	VAL	2.9
1	C	297	GLY	2.8
1	C	138	GLY	2.8
1	C	62	GLY	2.8
1	B	134	THR	2.8
1	A	127	GLY	2.8
1	B	239	THR	2.7
1	C	1	ALA	2.7
1	A	126	ASN	2.6
1	B	236	TYR	2.6
1	C	293	SER	2.5
1	B	171	GLY	2.5
1	C	136	PHE	2.5
1	B	95	GLY	2.5
1	C	32	ASP	2.5
1	B	292	ILE	2.5
1	A	269	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	263	ALA	2.5
1	A	240	TYR	2.5
1	B	110	PHE	2.4
1	B	186	PHE	2.4
1	B	351	LEU	2.4
1	C	171	GLY	2.4
1	B	282	VAL	2.4
1	A	93	ASN	2.4
1	B	13	LEU	2.4
1	B	58	TYR	2.4
1	B	327	TYR	2.3
1	C	110	PHE	2.3
1	B	109	GLU	2.3
1	B	284	TYR	2.2
1	C	351	LEU	2.2
1	C	117	ALA	2.1
1	B	150	GLN	2.1
1	A	38	ILE	2.1
1	A	77	PHE	2.1
1	C	129	ALA	2.1
1	B	120	PHE	2.1
1	A	72	TRP	2.1
1	C	81	LYS	2.1
1	A	55	GLN	2.1
1	A	192	ILE	2.0
1	B	269	VAL	2.0
1	C	327	TYR	2.0
1	B	216	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.