



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:58 AM EDT

PDB ID : 9IS2 / pdb_00009is2
Title : Unheat-treated beta-conglycinin
Authors : Zhang, T.; Li, J.Y.
Deposited on : 2024-07-16
Resolution : 2.78 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

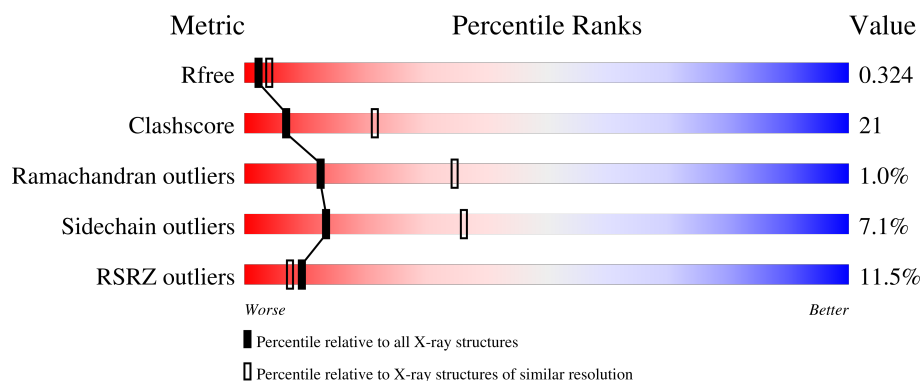
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	385	10% 51% 42% • •
1	B	385	15% 50% 41% • •
1	C	385	8% 51% 41% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9048 atoms, of which 0 are hydrogens and 0 are deuteriums.

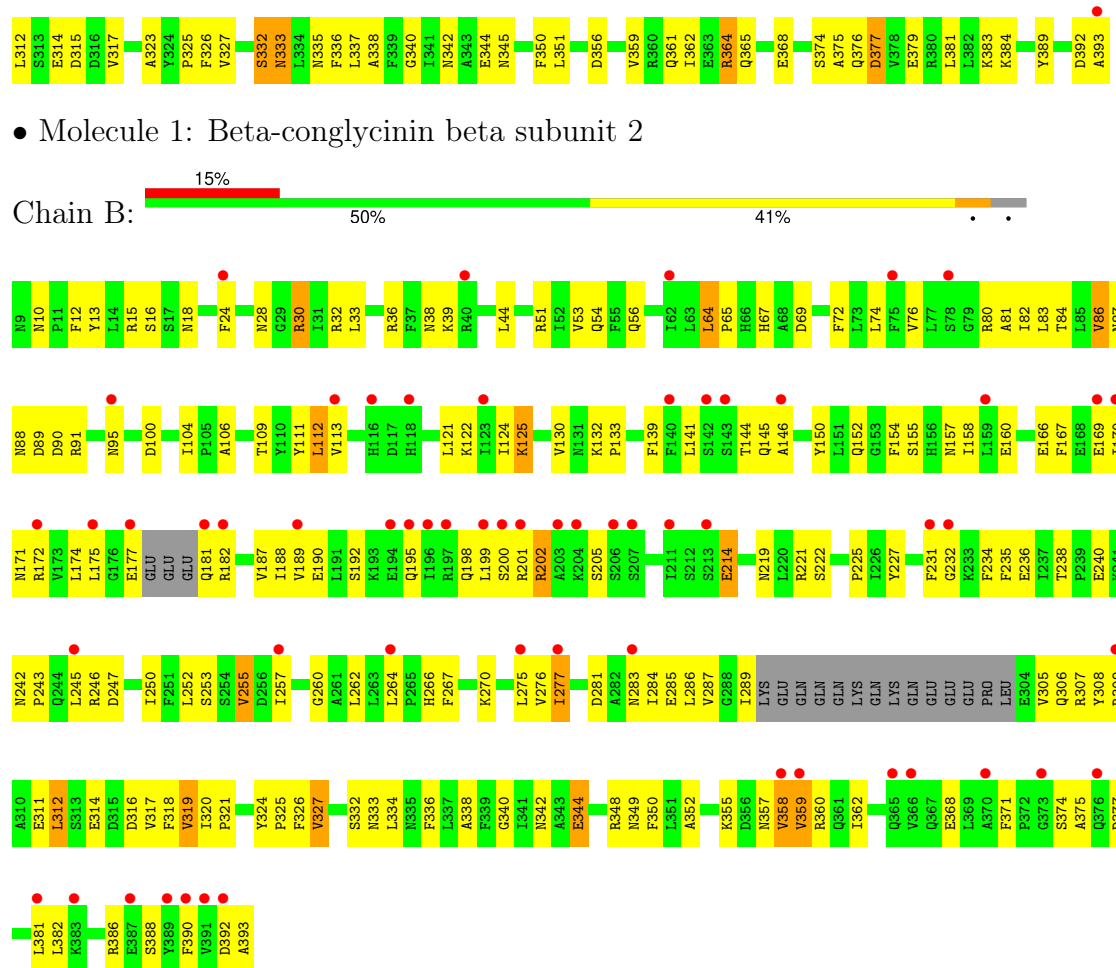
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-conglycinin beta subunit 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	C	368	Total	C	N	O	0	0	0
			2995	1890	537	568			
1	A	368	Total	C	N	O	0	0	0
			2995	1890	537	568			
1	B	368	Total	C	N	O	0	0	0
			2995	1890	537	568			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	28	Total	O	0	0
			28	28		
2	A	19	Total	O	0	0
			19	19		
2	B	16	Total	O	0	0
			16	16		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.02Å 63.10Å 121.85Å 90.00° 91.31° 90.00°	Depositor
Resolution (Å)	42.11 – 2.78 42.11 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.11-2.78) 99.3 (42.11-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.244 , 0.325 0.244 , 0.324	Depositor DCC
R_{free} test set	2007 reflections (5.83%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9048	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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

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	0.40	0/3053	0.67	0/4129
1	B	0.37	0/3053	0.59	0/4129
1	C	0.44	0/3053	0.67	0/4129
All	All	0.40	0/9159	0.65	0/12387

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

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	2995	0	2941	133	0
1	B	2995	0	2941	140	0
1	C	2995	0	2941	139	0
2	A	19	0	0	7	0
2	B	16	0	0	6	0
2	C	28	0	0	7	0
All	All	9048	0	8823	377	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 21.

All (377) 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:144:THR:HG22	1:B:146:ALA:H	1.17	1.06
1:B:246:ARG:NH2	2:B:401:HOH:O	1.89	1.05
1:A:304:GLU:N	2:A:401:HOH:O	1.97	0.95
1:C:23:LEU:HD11	1:C:33:LEU:HD12	1.45	0.95
1:C:46:ASN:ND2	1:B:130:VAL:O	2.01	0.93
1:C:144:THR:HG22	1:C:146:ALA:H	1.34	0.93
1:B:56:GLN:HE21	1:B:122:LYS:HD3	1.32	0.93
1:A:245:LEU:HD21	1:A:252:LEU:HD12	1.47	0.92
1:C:80:ARG:HH21	1:C:95:ASN:HD21	1.17	0.90
1:A:219:ASN:HB3	1:A:222:SER:HB3	1.55	0.88
1:A:142:SER:OG	1:A:147:GLN:NE2	2.08	0.85
1:B:195:GLN:NE2	2:B:402:HOH:O	2.13	0.81
1:C:181:GLN:N	2:C:402:HOH:O	2.14	0.80
1:B:33:LEU:HD11	1:B:51:ARG:HH21	1.47	0.79
1:C:364:ARG:HG2	1:C:375:ALA:HB1	1.64	0.78
1:A:248:LEU:HB3	1:A:250:ILE:HD12	1.66	0.78
1:C:181:GLN:N	2:C:404:HOH:O	2.17	0.77
1:A:255:VAL:CG1	1:A:336:PHE:CZ	2.68	0.76
1:C:363:GLU:HG3	1:B:91:ARG:NH1	2.00	0.75
1:C:34:LEU:O	1:C:51:ARG:NH1	2.19	0.75
1:A:220:LEU:HD12	1:A:237:ILE:HD13	1.67	0.75
1:B:306:GLN:NE2	1:B:307:ARG:O	2.20	0.75
1:C:359:VAL:HG22	1:B:141:LEU:HD21	1.70	0.74
1:C:239:PRO:HB3	1:C:246:ARG:HA	1.70	0.73
1:C:54:GLN:NE2	1:C:315:ASP:OD1	2.21	0.73
1:A:211:ILE:HD13	1:A:218:PHE:HB2	1.70	0.72
1:A:255:VAL:HG11	1:A:336:PHE:CZ	2.24	0.72
1:A:270:LYS:NZ	1:A:342:ASN:OD1	2.23	0.71
1:C:27:GLN:HG2	2:C:413:HOH:O	1.88	0.71
1:C:46:ASN:OD1	2:C:401:HOH:O	2.07	0.71
1:C:327:VAL:HG11	1:B:158:ILE:HG21	1.71	0.71
1:A:62:ILE:HG13	1:A:113:VAL:HG22	1.71	0.71
1:A:255:VAL:HG13	1:A:336:PHE:CE2	2.25	0.70
1:A:40:ARG:NH1	2:A:404:HOH:O	2.24	0.69
1:A:144:THR:HG22	1:A:146:ALA:H	1.57	0.69
1:B:198:GLN:NE2	2:B:404:HOH:O	2.25	0.69
1:C:102:GLN:HG2	1:C:103:ARG:H	1.58	0.68
1:C:207:SER:HB3	1:C:210:THR:HG23	1.75	0.68
1:A:74:LEU:HD23	1:A:104:ILE:HD11	1.75	0.68
1:A:71:ASP:OD1	2:A:402:HOH:O	2.12	0.68
1:A:233:LYS:O	1:A:255:VAL:HG23	1.93	0.67
1:C:192:SER:HB3	1:C:195:GLN:HE21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:PHE:HB2	1:B:104:ILE:HB	1.77	0.66
1:B:240:GLU:N	1:B:240:GLU:OE1	2.27	0.66
1:A:55:PHE:HE1	1:A:57:SER:HB3	1.59	0.66
1:B:155:SER:HB2	1:B:158:ILE:HD13	1.78	0.66
1:A:256:ASP:OD1	1:A:335:ASN:ND2	2.27	0.65
1:B:44:LEU:HD21	1:B:319:VAL:HG11	1.78	0.65
1:C:270:LYS:HB3	1:B:106:ALA:HB3	1.78	0.65
1:A:15:ARG:NH2	2:A:403:HOH:O	2.16	0.65
1:A:74:LEU:HD13	1:A:123:ILE:HD13	1.79	0.64
1:C:144:THR:CG2	1:C:146:ALA:H	2.09	0.64
1:B:181:GLN:N	1:B:181:GLN:OE1	2.31	0.64
1:B:257:ILE:HG12	1:B:390:PHE:HE2	1.61	0.64
1:A:253:SER:OG	1:A:338:ALA:HB3	1.98	0.64
1:A:270:LYS:HE3	1:A:344:GLU:O	1.98	0.63
1:B:24:PHE:CD2	1:B:187:VAL:HG22	2.33	0.63
1:B:82:ILE:HD12	1:B:113:VAL:HB	1.80	0.63
1:C:25:GLU:HB2	1:C:30:ARG:HB2	1.81	0.63
1:B:181:GLN:NE2	2:B:405:HOH:O	2.31	0.63
1:A:193:LYS:HE2	1:A:193:LYS:H	1.64	0.62
1:A:211:ILE:HG21	1:A:223:ARG:NH1	2.14	0.62
1:B:270:LYS:NZ	1:B:342:ASN:O	2.32	0.62
1:C:363:GLU:HG3	1:B:91:ARG:HH12	1.64	0.62
1:B:312:LEU:HD21	1:B:318:PHE:HB2	1.81	0.62
1:C:368:GLU:HG2	1:C:375:ALA:HB2	1.82	0.61
1:C:112:LEU:HD21	1:C:123:ILE:HD12	1.83	0.61
1:C:279:GLU:OE1	2:C:403:HOH:O	2.15	0.61
1:C:286:LEU:HD11	1:C:324:TYR:HB3	1.83	0.60
1:A:9:ASN:ND2	2:A:407:HOH:O	2.33	0.60
1:C:172:ARG:HD3	1:C:182:ARG:NH1	2.16	0.60
1:B:86:VAL:HG22	1:B:109:THR:HB	1.82	0.60
1:B:125:LYS:NZ	2:B:406:HOH:O	2.33	0.60
1:A:106:ALA:HB3	1:B:270:LYS:HB3	1.84	0.60
1:A:196:ILE:HA	1:A:199:LEU:HD12	1.84	0.60
1:B:16:SER:N	1:B:316:ASP:OD1	2.27	0.60
1:B:81:ALA:HB2	1:B:121:LEU:HD11	1.84	0.60
1:A:161:THR:HG21	1:B:393:ALA:HB2	1.84	0.59
1:B:236:GLU:CD	1:B:348:ARG:HH22	2.11	0.59
1:C:231:PHE:CE1	1:C:392:ASP:HB2	2.38	0.58
1:B:166:GLU:N	1:B:166:GLU:OE2	2.36	0.58
1:B:172:ARG:O	1:B:182:ARG:NH1	2.28	0.58
1:B:192:SER:H	1:B:195:GLN:HE21	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:VAL:O	1:A:46:ASN:ND2	2.37	0.58
1:B:287:VAL:HG23	1:B:325:PRO:HD2	1.86	0.58
1:B:214:GLU:HG3	1:B:243:PRO:HB2	1.86	0.57
1:C:75:PHE:CE2	1:C:337:LEU:HD13	2.40	0.57
1:C:277:ILE:HD13	1:C:336:PHE:HB3	1.86	0.57
1:A:223:ARG:HE	1:A:237:ILE:HD11	1.68	0.57
1:C:279:GLU:CG	1:C:335:ASN:HB3	2.34	0.57
1:C:360:ARG:HG3	1:C:382:LEU:HD13	1.86	0.57
1:B:28:ASN:HD21	1:B:190:GLU:HG3	1.69	0.57
1:B:33:LEU:CD1	1:B:51:ARG:HH21	2.16	0.57
1:A:374:SER:OG	1:A:377:ASP:HB2	2.05	0.57
1:A:55:PHE:CE1	1:A:57:SER:HB3	2.39	0.56
1:B:195:GLN:O	1:B:199:LEU:HD23	2.05	0.56
1:C:161:THR:HG21	1:A:393:ALA:HB2	1.88	0.56
1:A:208:ARG:NH1	1:A:211:ILE:HG13	2.21	0.56
1:B:56:GLN:HA	1:B:121:LEU:O	2.06	0.56
1:A:255:VAL:HG13	1:A:336:PHE:CZ	2.39	0.55
1:B:275:LEU:HD21	1:B:318:PHE:HB3	1.88	0.55
1:C:64:LEU:HD23	1:C:187:VAL:HA	1.87	0.55
1:B:276:VAL:HG22	1:B:317:VAL:HG22	1.88	0.55
1:C:264:LEU:HD12	1:C:389:TYR:C	2.31	0.55
1:C:383:LYS:HE3	1:C:386:ARG:NH1	2.21	0.55
1:C:226:ILE:HG22	1:C:227:TYR:CD2	2.42	0.55
1:C:10:ASN:HB3	1:C:13:TYR:HB3	1.89	0.55
1:C:265:PRO:HB3	1:B:154:PHE:CE2	2.42	0.55
1:A:55:PHE:HE2	1:A:63:LEU:HD22	1.72	0.55
1:C:152:GLN:HG2	1:C:175:LEU:HD22	1.89	0.54
1:C:279:GLU:HG2	1:C:335:ASN:HB3	1.89	0.54
1:A:231:PHE:CE1	1:A:392:ASP:HB2	2.43	0.54
1:C:286:LEU:HB3	1:C:308:TYR:HB2	1.88	0.54
1:C:381:LEU:HD12	1:B:169:GLU:HG2	1.88	0.54
1:C:277:ILE:HD12	1:C:334:LEU:HD11	1.89	0.54
1:C:287:VAL:HG22	1:C:325:PRO:HD2	1.88	0.54
1:C:236:GLU:HG3	1:C:253:SER:HB3	1.88	0.54
1:B:286:LEU:HD11	1:B:324:TYR:HB3	1.88	0.54
1:A:229:ASN:O	1:A:231:PHE:N	2.41	0.53
1:A:24:PHE:HZ	1:A:26:ASN:ND2	2.05	0.53
1:C:144:THR:HB	1:C:147:GLN:NE2	2.24	0.53
1:C:207:SER:OG	1:C:208:ARG:N	2.41	0.53
1:B:53:VAL:HB	1:B:125:LYS:HG3	1.90	0.53
1:C:246:ARG:CZ	1:C:246:ARG:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PHE:CE1	1:B:392:ASP:HB2	2.43	0.53
1:B:266:HIS:HB3	1:B:350:PHE:CD1	2.43	0.53
1:B:355:LYS:H	1:B:388:SER:HB3	1.74	0.53
1:C:35:GLN:HB2	1:C:39:LYS:HE3	1.89	0.53
1:A:192:SER:OG	1:A:195:GLN:NE2	2.28	0.53
1:C:281:ASP:HB2	1:C:332:SER:OG	2.08	0.53
1:A:214:GLU:HG2	1:A:243:PRO:HB2	1.89	0.53
1:C:358:VAL:HG12	1:B:87:ASN:O	2.09	0.53
1:B:56:GLN:NE2	1:B:122:LYS:HD3	2.13	0.53
1:C:169:GLU:OE1	1:A:384:LYS:NZ	2.31	0.53
1:C:153:GLY:O	1:A:307:ARG:HG3	2.09	0.52
1:C:381:LEU:HD11	1:B:170:ILE:HG22	1.91	0.52
1:B:30:ARG:HH11	1:B:56:GLN:HB2	1.75	0.52
1:A:153:GLY:HA3	1:B:287:VAL:CG1	2.39	0.52
1:A:38:ASN:OD1	1:A:48:ARG:NH1	2.43	0.52
1:A:80:ARG:O	1:A:121:LEU:HD13	2.11	0.51
1:A:277:ILE:HD11	1:A:312:LEU:HD13	1.92	0.51
1:C:24:PHE:HZ	1:C:186:GLY:HA3	1.75	0.51
1:C:380:ARG:O	1:C:384:LYS:HD3	2.10	0.51
1:A:28:ASN:HB3	1:A:61:THR:HG21	1.92	0.51
1:C:191:LEU:HD13	1:C:196:ILE:HG12	1.92	0.51
1:B:277:ILE:HG22	1:B:314:GLU:HA	1.92	0.51
1:C:236:GLU:OE2	1:C:348:ARG:NH2	2.25	0.51
1:A:116:HIS:CG	1:A:119:GLN:HB2	2.46	0.51
1:B:95:ASN:HB2	1:B:205:SER:HB2	1.93	0.51
1:B:281:ASP:O	1:B:334:LEU:HD13	2.11	0.51
1:C:226:ILE:HG22	1:C:227:TYR:CE2	2.46	0.51
1:B:201:ARG:O	1:B:202:ARG:HB2	2.10	0.51
1:C:144:THR:HG22	1:C:146:ALA:N	2.15	0.51
1:C:91:ARG:HD3	1:A:361:GLN:O	2.11	0.50
1:A:87:ASN:ND2	1:A:90:ASP:HB3	2.27	0.50
1:C:362:ILE:HG22	1:C:366:VAL:HB	1.94	0.50
1:A:207:SER:HB3	1:A:210:THR:HG23	1.93	0.50
1:B:76:VAL:HG22	1:B:100:ASP:O	2.12	0.50
1:A:265:PRO:HB2	1:A:351:LEU:HD12	1.94	0.50
1:B:90:ASP:OD1	1:B:91:ARG:N	2.38	0.50
1:B:225:PRO:HG3	1:B:235:PHE:CZ	2.47	0.50
1:A:64:LEU:HD22	1:A:187:VAL:O	2.11	0.50
1:B:30:ARG:CZ	1:B:32:ARG:HD2	2.42	0.50
1:C:13:TYR:OH	1:C:15:ARG:HG3	2.12	0.50
1:C:320:ILE:HG21	1:C:326:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD23	1:B:187:VAL:HA	1.94	0.49
1:C:305:VAL:HG21	1:B:150:TYR:HA	1.93	0.49
1:A:190:GLU:O	1:A:191:LEU:HD12	2.12	0.49
1:C:194:GLU:O	1:C:197:ARG:HB2	2.12	0.49
1:A:359:VAL:HA	1:A:362:ILE:HD12	1.94	0.49
1:B:253:SER:OG	1:B:338:ALA:HB3	2.12	0.49
1:C:383:LYS:HE3	1:C:386:ARG:HH11	1.77	0.49
1:B:15:ARG:HB3	1:B:18:ASN:OD1	2.13	0.49
1:B:10:ASN:HB3	1:B:13:TYR:HB3	1.94	0.49
1:A:148:GLN:HB2	1:B:305:VAL:HG23	1.95	0.49
1:A:238:THR:HG22	1:A:241:LYS:HG2	1.95	0.49
1:A:221:ARG:HD3	1:A:235:PHE:CE1	2.47	0.49
1:B:286:LEU:HB3	1:B:308:TYR:HB2	1.93	0.49
1:C:242:ASN:ND2	2:C:407:HOH:O	2.23	0.48
1:C:381:LEU:CD1	1:B:169:GLU:HG2	2.43	0.48
1:A:225:PRO:HG3	1:A:235:PHE:CZ	2.48	0.48
1:C:159:LEU:HB3	1:C:170:ILE:HD11	1.95	0.48
1:C:270:LYS:HE2	1:C:344:GLU:O	2.12	0.48
1:B:152:GLN:HE21	1:B:175:LEU:HB3	1.79	0.48
1:C:31:ILE:HG12	1:C:55:PHE:HD2	1.78	0.48
1:C:56:GLN:HA	1:C:121:LEU:O	2.14	0.48
1:B:36:ARG:HG2	1:B:38:ASN:OD1	2.14	0.48
1:B:231:PHE:CZ	1:B:392:ASP:HB2	2.49	0.48
1:C:150:TYR:HA	1:A:305:VAL:HG21	1.94	0.48
1:C:264:LEU:HD12	1:C:389:TYR:O	2.14	0.48
1:A:23:LEU:HD12	1:A:31:ILE:HG22	1.95	0.48
1:A:192:SER:HB2	1:A:195:GLN:HG3	1.95	0.48
1:B:219:ASN:OD1	1:B:221:ARG:HG3	2.14	0.48
1:A:13:TYR:OH	1:A:15:ARG:HG3	2.14	0.48
1:A:76:VAL:HG12	1:A:98:PRO:HA	1.96	0.48
1:A:141:LEU:HD21	1:B:359:VAL:HG13	1.96	0.48
1:A:231:PHE:CZ	1:A:392:ASP:HB2	2.49	0.48
1:B:270:LYS:NZ	1:B:344:GLU:O	2.43	0.48
1:C:323:ALA:HB3	1:B:69:ASP:HB3	1.96	0.48
1:C:192:SER:OG	1:C:195:GLN:HG3	2.13	0.47
1:C:36:ARG:H	1:C:39:LYS:HE3	1.79	0.47
1:A:13:TYR:CE1	1:A:312:LEU:HD23	2.49	0.47
1:A:34:LEU:O	1:A:51:ARG:NH1	2.47	0.47
1:A:185:GLU:OE1	1:A:185:GLU:N	2.44	0.47
1:A:38:ASN:ND2	2:A:409:HOH:O	2.47	0.47
1:C:73:LEU:HD12	1:C:102:GLN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HA	1:A:340:GLY:O	2.14	0.47
1:B:305:VAL:HG12	1:B:306:GLN:N	2.30	0.47
1:A:276:VAL:HG12	1:A:317:VAL:HG22	1.97	0.47
1:B:285:GLU:O	1:B:326:PHE:HA	2.15	0.47
1:B:53:VAL:HG11	1:B:125:LYS:HE2	1.97	0.47
1:B:158:ILE:HD12	1:B:158:ILE:H	1.79	0.47
1:B:285:GLU:HB2	1:B:327:VAL:HG12	1.96	0.47
1:B:286:LEU:CD1	1:B:320:ILE:HG23	2.44	0.47
1:C:263:LEU:O	1:C:327:VAL:HG23	2.15	0.46
1:A:153:GLY:O	1:B:307:ARG:HB2	2.16	0.46
1:A:229:ASN:C	1:A:231:PHE:H	2.21	0.46
1:C:153:GLY:HA3	1:A:287:VAL:CG1	2.46	0.46
1:C:83:LEU:CD1	1:C:112:LEU:HD13	2.46	0.46
1:A:184:GLN:HG3	1:A:185:GLU:OE1	2.15	0.46
1:B:266:HIS:O	1:B:325:PRO:HA	2.15	0.46
1:C:221:ARG:H	1:C:221:ARG:HG2	1.56	0.46
1:C:286:LEU:HD21	1:C:321:PRO:HD2	1.98	0.46
1:C:83:LEU:HD12	1:C:112:LEU:HD13	1.97	0.46
1:B:350:PHE:O	1:B:358:VAL:HG22	2.16	0.46
1:C:227:TYR:OH	1:C:348:ARG:HD2	2.15	0.46
1:C:227:TYR:HB3	1:C:389:TYR:CD1	2.50	0.46
1:A:350:PHE:HB2	1:A:356:ASP:O	2.15	0.46
1:A:74:LEU:CD2	1:A:104:ILE:HD11	2.42	0.46
1:B:10:ASN:OD1	1:B:318:PHE:HE2	1.99	0.46
1:C:84:THR:HA	1:C:92:ASP:O	2.16	0.46
1:C:374:SER:OG	1:C:375:ALA:N	2.48	0.46
1:C:219:ASN:HB3	1:C:222:SER:HB3	1.98	0.45
1:C:53:VAL:HG21	1:C:136:TYR:OH	2.16	0.45
1:C:156:HIS:O	1:C:160:GLU:HG3	2.15	0.45
1:B:167:PHE:CD1	1:B:170:ILE:HD11	2.50	0.45
1:C:103:ARG:NH1	1:C:247:ASP:OD1	2.49	0.45
1:A:111:TYR:CE1	1:B:362:ILE:HG23	2.51	0.45
1:B:139:PHE:HB3	1:B:150:TYR:CD2	2.51	0.45
1:C:62:ILE:HG23	1:C:189:VAL:HG13	1.99	0.45
1:A:307:ARG:NH1	1:A:309:ARG:HD3	2.32	0.45
1:C:250:ILE:HA	1:C:340:GLY:O	2.17	0.45
1:A:36:ARG:NH2	1:A:135:ARG:HD2	2.32	0.45
1:A:383:LYS:HA	1:A:383:LYS:HD2	1.81	0.45
1:B:171:ASN:OD1	1:B:177:GLU:HG3	2.15	0.45
1:B:192:SER:OG	1:B:195:GLN:HG3	2.16	0.45
1:B:284:ILE:O	1:B:309:ARG:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:HD21	1:A:177:GLU:HB2	1.82	0.45
1:B:368:GLU:CG	1:B:375:ALA:HB2	2.47	0.45
1:C:23:LEU:HD11	1:C:33:LEU:CD1	2.32	0.45
1:C:381:LEU:HD22	1:B:174:LEU:HG	1.97	0.45
1:B:255:VAL:HG13	1:B:336:PHE:CE1	2.52	0.45
1:A:52:ILE:HD11	1:A:274:ILE:HG21	1.99	0.45
1:A:227:TYR:HB3	1:A:389:TYR:CD2	2.52	0.45
1:A:236:GLU:HG3	1:A:253:SER:HB3	1.99	0.45
1:A:284:ILE:HG13	1:A:327:VAL:O	2.17	0.45
1:B:349:ASN:N	1:B:349:ASN:HD22	2.15	0.45
1:B:357:ASN:CG	1:B:360:ARG:HG3	2.42	0.45
1:C:85:LEU:HD22	1:C:104:ILE:HG23	1.99	0.44
1:C:112:LEU:HD21	1:C:123:ILE:CD1	2.47	0.44
1:A:202:ARG:O	1:A:202:ARG:NH1	2.42	0.44
1:C:69:ASP:HB3	1:A:323:ALA:HB3	1.99	0.44
1:C:75:PHE:HE1	1:C:220:LEU:HD13	1.81	0.44
1:C:82:ILE:HD13	1:C:200:SER:HA	1.98	0.44
1:A:272:ILE:H	1:A:272:ILE:HG13	1.63	0.44
1:C:34:LEU:HD23	1:C:52:ILE:HB	2.00	0.44
1:A:58:LYS:O	1:A:61:THR:OG1	2.34	0.44
1:B:321:PRO:HB2	1:B:324:TYR:CD1	2.52	0.44
1:C:374:SER:HB3	1:C:377:ASP:HB2	2.00	0.44
1:A:168:GLU:HB2	2:A:408:HOH:O	2.18	0.44
1:A:55:PHE:CE2	1:A:63:LEU:HD22	2.51	0.44
1:B:236:GLU:OE1	1:B:253:SER:HB3	2.17	0.44
1:C:259:GLU:HB2	1:C:333:ASN:H	1.82	0.44
1:C:332:SER:O	1:C:333:ASN:C	2.60	0.44
1:C:66:HIS:O	1:C:109:THR:HA	2.18	0.44
1:A:53:VAL:HB	1:A:125:LYS:HG2	2.00	0.44
1:A:74:LEU:HD23	1:A:104:ILE:CD1	2.47	0.44
1:A:153:GLY:HA3	1:B:287:VAL:HG12	1.99	0.44
1:C:184:GLN:NE2	1:C:189:VAL:HG21	2.32	0.44
1:A:152:GLN:HG3	1:A:175:LEU:HD13	1.98	0.44
1:B:132:LYS:HB2	1:B:132:LYS:HE3	1.67	0.44
1:B:374:SER:HB3	1:B:377:ASP:HB2	2.00	0.44
1:C:66:HIS:HB3	1:C:140:PHE:CD1	2.53	0.43
1:B:360:ARG:HG2	1:B:382:LEU:HB3	2.00	0.43
1:A:71:ASP:OD2	1:A:103:ARG:NE	2.45	0.43
1:B:160:GLU:OE2	2:B:403:HOH:O	2.21	0.43
1:A:38:ASN:ND2	1:A:38:ASN:H	2.16	0.43
1:A:208:ARG:HH12	1:A:211:ILE:HG13	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:HD22	1:B:189:VAL:HA	1.83	0.43
1:B:275:LEU:HD22	1:B:320:ILE:HD11	2.00	0.43
1:C:74:LEU:HD23	1:C:74:LEU:H	1.82	0.43
1:B:152:GLN:HG3	1:B:175:LEU:HD22	2.00	0.43
1:B:227:TYR:O	1:B:234:PHE:N	2.52	0.43
1:C:320:ILE:HD13	1:C:326:PHE:CZ	2.53	0.43
1:A:70:ALA:O	1:A:106:ALA:HA	2.18	0.43
1:A:87:ASN:OD1	1:A:87:ASN:N	2.50	0.43
1:B:225:PRO:HG3	1:B:235:PHE:CE1	2.53	0.43
1:B:245:LEU:HD22	1:B:250:ILE:O	2.19	0.43
1:B:289:ILE:HG22	1:B:289:ILE:O	2.18	0.43
1:C:36:ARG:HH21	1:C:135:ARG:HD3	1.84	0.43
1:C:383:LYS:HB3	2:C:411:HOH:O	2.19	0.43
1:B:83:LEU:HD13	1:B:112:LEU:HD13	2.01	0.43
1:B:152:GLN:HG3	1:B:175:LEU:HD13	2.01	0.43
1:B:381:LEU:O	1:B:381:LEU:HD12	2.18	0.43
1:A:55:PHE:CD1	1:A:55:PHE:C	2.96	0.43
1:A:62:ILE:HG22	1:A:189:VAL:HG13	2.01	0.43
1:A:67:HIS:CE1	1:B:267:PHE:CE2	3.07	0.43
1:B:84:THR:HB	1:B:111:TYR:CE2	2.53	0.43
1:B:267:PHE:CE1	1:B:349:ASN:HB2	2.54	0.43
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.48	0.42
1:C:356:ASP:HA	1:B:88:ASN:HB2	2.01	0.42
1:C:147:GLN:HE21	1:C:187:VAL:HG12	1.84	0.42
1:C:309:ARG:HG2	1:C:310:ALA:N	2.33	0.42
1:C:383:LYS:HD2	1:C:383:LYS:HA	1.64	0.42
1:B:28:ASN:ND2	1:B:190:GLU:HG3	2.34	0.42
1:B:167:PHE:HD1	1:B:170:ILE:HD11	1.85	0.42
1:A:118:HIS:O	1:A:118:HIS:ND1	2.51	0.42
1:B:260:GLY:O	1:B:393:ALA:HB3	2.19	0.42
1:A:75:PHE:CD2	1:A:337:LEU:HD13	2.54	0.42
1:A:238:THR:OG1	1:A:239:PRO:HD2	2.19	0.42
1:C:141:LEU:HD11	1:A:359:VAL:HG22	2.02	0.42
1:A:332:SER:O	1:A:333:ASN:C	2.63	0.42
1:B:250:ILE:HA	1:B:340:GLY:O	2.19	0.42
1:C:36:ARG:N	1:C:39:LYS:HE3	2.35	0.42
1:C:231:PHE:HB3	1:C:261:ALA:CB	2.50	0.42
1:B:275:LEU:HD23	1:B:318:PHE:O	2.20	0.42
1:A:236:GLU:O	1:A:237:ILE:HD12	2.20	0.42
1:B:65:PRO:HG3	1:B:111:TYR:CD1	2.55	0.42
1:C:287:VAL:CG2	1:C:325:PRO:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HD12	1:A:326:PHE:HB3	2.01	0.42
1:A:314:GLU:O	1:A:315:ASP:HB2	2.19	0.42
1:A:375:ALA:O	1:A:379:GLU:HB2	2.20	0.42
1:A:255:VAL:CG1	1:A:336:PHE:CE1	3.03	0.42
1:C:221:ARG:HA	1:C:235:PHE:CD2	2.55	0.42
1:B:283:ASN:OD1	1:B:311:GLU:HG3	2.20	0.42
1:A:181:GLN:NE2	1:A:182:ARG:HG3	2.34	0.41
1:A:185:GLU:H	1:A:185:GLU:CD	2.27	0.41
1:B:242:ASN:HB3	1:B:245:LEU:HD12	2.02	0.41
1:C:34:LEU:HD22	1:C:317:VAL:HG21	2.01	0.41
1:C:85:LEU:HD21	1:C:104:ILE:HG12	2.02	0.41
1:A:67:HIS:CD2	1:A:139:PHE:HB2	2.54	0.41
1:B:12:PHE:HB3	1:B:319:VAL:O	2.20	0.41
1:B:32:ARG:NH1	1:B:54:GLN:OE1	2.51	0.41
1:C:159:LEU:HB3	1:C:170:ILE:CD1	2.50	0.41
1:A:38:ASN:ND2	1:A:48:ARG:HA	2.35	0.41
1:A:194:GLU:O	1:A:197:ARG:HB2	2.20	0.41
1:C:189:VAL:HG22	1:C:190:GLU:O	2.20	0.41
1:A:267:PHE:HB3	1:A:325:PRO:HA	2.03	0.41
1:A:365:GLN:OE1	1:A:365:GLN:HA	2.20	0.41
1:C:367:GLN:HB3	1:C:378:VAL:HG11	2.02	0.41
1:C:283:ASN:OD1	1:C:311:GLU:HG2	2.20	0.41
1:B:33:LEU:HD23	1:B:53:VAL:HG22	2.01	0.41
1:C:169:GLU:O	1:C:173:VAL:HG23	2.21	0.41
1:C:263:LEU:HD13	1:C:390:PHE:CE1	2.55	0.41
1:C:362:ILE:H	1:C:362:ILE:HG13	1.56	0.41
1:A:74:LEU:CD1	1:A:123:ILE:HD13	2.48	0.41
1:B:332:SER:OG	1:B:333:ASN:N	2.53	0.41
1:C:361:GLN:NE2	1:B:89:ASP:C	2.79	0.41
1:A:238:THR:HG23	1:A:240:GLU:H	1.86	0.41
1:A:240:GLU:HB3	1:A:241:LYS:HD3	2.02	0.41
1:A:368:GLU:OE2	1:A:375:ALA:HB2	2.21	0.41
1:B:36:ARG:NH1	1:B:39:LYS:HG3	2.35	0.41
1:C:312:LEU:HD23	1:C:316:ASP:HB3	2.03	0.40
1:C:323:ALA:HB1	1:B:67:HIS:CE1	2.56	0.40
1:A:364:ARG:HE	1:A:364:ARG:HB3	1.43	0.40
1:B:38:ASN:OD1	1:B:38:ASN:N	2.54	0.40
1:B:221:ARG:HD2	1:B:222:SER:N	2.36	0.40
1:C:384:LYS:HA	1:C:384:LYS:HD2	1.81	0.40
1:A:208:ARG:O	1:A:208:ARG:NE	2.54	0.40
1:B:33:LEU:HD11	1:B:51:ARG:NH2	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.84	0.40
1:B:232:GLY:HA3	1:B:390:PHE:CD2	2.56	0.40
1:C:152:GLN:OE1	1:C:175:LEU:HD13	2.22	0.40
1:A:14:LEU:HB2	1:A:317:VAL:HB	2.03	0.40
1:A:68:ALA:HB1	1:A:136:TYR:HD2	1.86	0.40
1:A:344:GLU:O	1:A:345:ASN:HB2	2.20	0.40
1:B:264:LEU:HD13	1:B:352:ALA:O	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	362/385 (94%)	331 (91%)	27 (8%)	4 (1%)	11	32
1	B	362/385 (94%)	330 (91%)	30 (8%)	2 (1%)	21	47
1	C	362/385 (94%)	335 (92%)	22 (6%)	5 (1%)	9	26
All	All	1086/1155 (94%)	996 (92%)	79 (7%)	11 (1%)	12	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	ARG
1	B	202	ARG
1	A	230	ASN
1	C	314	GLU
1	C	333	ASN
1	A	332	SER
1	A	333	ASN
1	C	389	TYR
1	C	228	SER
1	A	221	ARG

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Mol	Chain	Res	Type
1	B	133	PRO

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	332/349 (95%)	310 (93%)	22 (7%)	15	40
1	B	332/349 (95%)	305 (92%)	27 (8%)	11	30
1	C	332/349 (95%)	310 (93%)	22 (7%)	15	40
All	All	996/1047 (95%)	925 (93%)	71 (7%)	13	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	SER
1	C	30	ARG
1	C	39	LYS
1	C	58	LYS
1	C	78	SER
1	C	86	VAL
1	C	120	ASN
1	C	125	LYS
1	C	132	LYS
1	C	141	LEU
1	C	143	SER
1	C	144	THR
1	C	149	SER
1	C	169	GLU
1	C	192	SER
1	C	206	SER
1	C	208	ARG
1	C	216	GLU
1	C	255	VAL
1	C	305	VAL
1	C	312	LEU

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Mol	Chain	Res	Type
1	C	374	SER
1	A	22	THR
1	A	54	GLN
1	A	64	LEU
1	A	71	ASP
1	A	73	LEU
1	A	87	ASN
1	A	108	THR
1	A	109	THR
1	A	158	ILE
1	A	172	ARG
1	A	184	GLN
1	A	192	SER
1	A	197	ARG
1	A	209	LYS
1	A	245	LEU
1	A	270	LYS
1	A	279	GLU
1	A	311	GLU
1	A	364	ARG
1	A	376	GLN
1	A	377	ASP
1	A	381	LEU
1	B	30	ARG
1	B	64	LEU
1	B	74	LEU
1	B	80	ARG
1	B	86	VAL
1	B	112	LEU
1	B	124	ILE
1	B	125	LYS
1	B	145	GLN
1	B	157	ASN
1	B	188	ILE
1	B	200	SER
1	B	214	GLU
1	B	238	THR
1	B	247	ASP
1	B	252	LEU
1	B	255	VAL
1	B	262	LEU
1	B	277	ILE

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Mol	Chain	Res	Type
1	B	312	LEU
1	B	319	VAL
1	B	327	VAL
1	B	344	GLU
1	B	358	VAL
1	B	359	VAL
1	B	371	PHE
1	B	386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
1	C	157	ASN
1	C	195	GLN
1	C	198	GLN
1	C	268	ASN
1	C	346	ASN
1	A	21	GLN
1	A	38	ASN
1	A	43	GLN
1	A	67	HIS
1	A	119	GLN
1	A	147	GLN
1	A	152	GLN
1	A	181	GLN
1	B	10	ASN
1	B	28	ASN
1	B	56	GLN
1	B	60	ASN
1	B	116	HIS
1	B	120	ASN
1	B	181	GLN
1	B	306	GLN
1	B	349	ASN
1	B	367	GLN

5.3.3 RNA ⓘ

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 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	368/385 (95%)	0.98	37 (10%) 12 10	12, 39, 71, 84	0
1	B	368/385 (95%)	1.27	59 (16%) 5 4	23, 49, 73, 87	0
1	C	368/385 (95%)	0.74	31 (8%) 17 13	11, 28, 58, 78	0
All	All	1104/1155 (95%)	0.99	127 (11%) 9 7	11, 39, 69, 87	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	ALA	5.3
1	B	200	SER	5.2
1	B	370	ALA	4.5
1	C	369	LEU	4.5
1	A	206	SER	4.4
1	B	203	ALA	4.2
1	A	205	SER	4.2
1	A	198	GLN	4.2
1	A	211	ILE	4.1
1	A	176	GLY	3.9
1	C	366	VAL	3.8
1	B	206	SER	3.8
1	C	194	GLU	3.7
1	C	195	GLN	3.7
1	B	194	GLU	3.7
1	A	204	LYS	3.6
1	B	211	ILE	3.6
1	B	257	ILE	3.6
1	A	199	LEU	3.5
1	A	212	SER	3.5
1	A	210	THR	3.4
1	B	116	HIS	3.4
1	B	390	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	200	SER	3.3
1	C	203	ALA	3.3
1	C	181	GLN	3.3
1	C	363	GLU	3.2
1	A	207	SER	3.2
1	B	204	LYS	3.2
1	A	177	GLU	3.1
1	B	201	ARG	3.1
1	C	177	GLU	3.1
1	A	213	SER	3.1
1	A	191	LEU	3.0
1	B	359	VAL	3.0
1	A	143	SER	3.0
1	B	232	GLY	3.0
1	A	167	PHE	2.9
1	A	172	ARG	2.9
1	B	62	ILE	2.9
1	A	166	GLU	2.9
1	B	207	SER	2.9
1	B	391	VAL	2.9
1	B	181	GLN	2.8
1	A	181	GLN	2.8
1	C	192	SER	2.8
1	A	195	GLN	2.8
1	C	304	GLU	2.8
1	B	196	ILE	2.7
1	B	140	PHE	2.7
1	C	309	ARG	2.7
1	B	376	GLN	2.7
1	B	199	LEU	2.7
1	A	305	VAL	2.7
1	A	393	ALA	2.7
1	A	175	LEU	2.7
1	A	168	GLU	2.7
1	B	40	ARG	2.6
1	C	379	GLU	2.6
1	C	378	VAL	2.6
1	A	184	GLN	2.5
1	B	170	ILE	2.5
1	B	264	LEU	2.5
1	B	169	GLU	2.5
1	C	393	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	309	ARG	2.5
1	A	169	GLU	2.5
1	B	389	TYR	2.5
1	A	208	ARG	2.4
1	B	182	ARG	2.4
1	C	191	LEU	2.4
1	A	192	SER	2.4
1	B	387	GLU	2.4
1	B	118	HIS	2.4
1	B	392	ASP	2.4
1	B	365	GLN	2.4
1	B	24	PHE	2.4
1	C	357	ASN	2.4
1	B	283	ASN	2.4
1	C	364	ARG	2.4
1	B	197	ARG	2.4
1	A	209	LYS	2.3
1	A	183	GLN	2.3
1	A	173	VAL	2.3
1	B	159	LEU	2.3
1	C	193	LYS	2.3
1	B	383	LYS	2.3
1	C	372	PRO	2.3
1	C	353	GLY	2.3
1	C	279	GLU	2.3
1	B	177	GLU	2.3
1	C	380	ARG	2.3
1	B	381	LEU	2.3
1	B	213	SER	2.3
1	A	118	HIS	2.2
1	A	201	ARG	2.2
1	C	359	VAL	2.2
1	B	366	VAL	2.2
1	C	362	ILE	2.2
1	A	163	PHE	2.2
1	B	95	ASN	2.2
1	B	275	LEU	2.2
1	C	375	ALA	2.2
1	C	9	ASN	2.2
1	C	382	LEU	2.2
1	B	373	GLY	2.2
1	B	231	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	277	ILE	2.2
1	B	358	VAL	2.2
1	B	172	ARG	2.1
1	A	9	ASN	2.1
1	B	245	LEU	2.1
1	C	247	ASP	2.1
1	B	113	VAL	2.1
1	B	143	SER	2.1
1	B	175	LEU	2.1
1	B	123	ILE	2.1
1	A	89	ASP	2.1
1	B	75	PHE	2.1
1	B	142	SER	2.1
1	B	195	GLN	2.1
1	B	78	SER	2.0
1	A	309	ARG	2.0
1	B	146	ALA	2.0
1	C	196	ILE	2.0
1	C	197	ARG	2.0
1	B	189	VAL	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.