



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:05 PM UTC

PDB ID : 9IS1 / pdb_00009is1
Title : Pasteurization-treated beta-conglycinin
Authors : Zhang, T.; Li, J.Y.
Deposited on : 2024-07-16
Resolution : 2.01 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

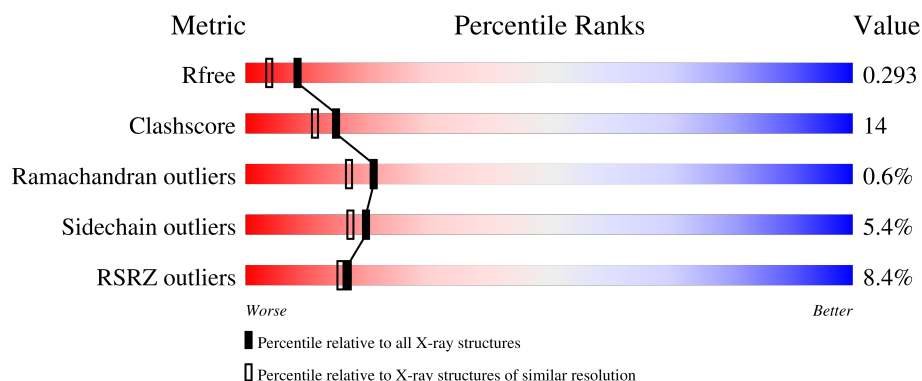
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 66% 26% • •
1	B	385	7% 71% 23% • •
1	C	385	8% 66% 28% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9461 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			

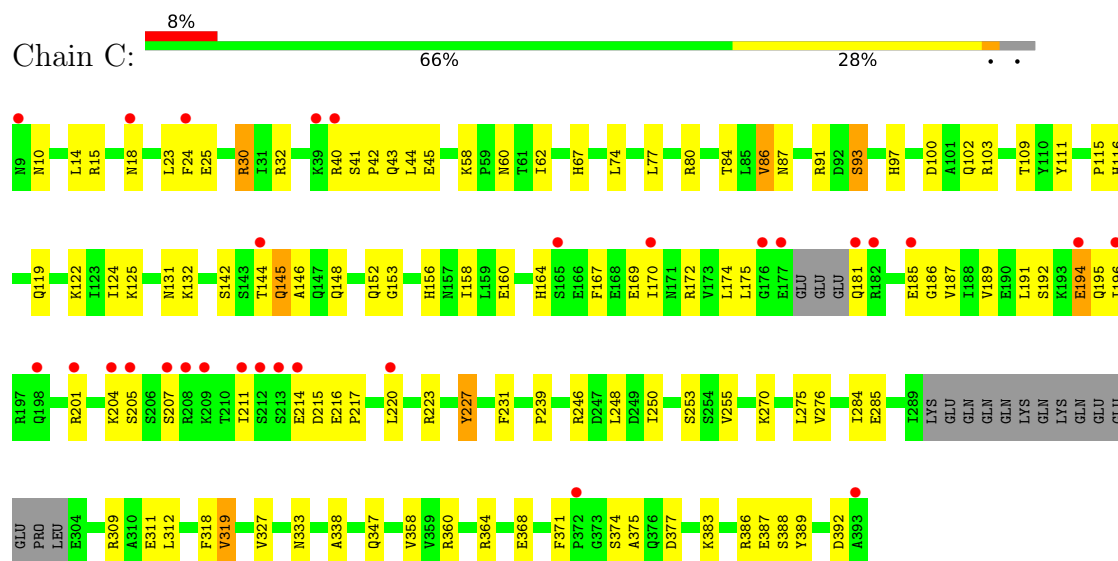
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	163	Total	O	0	0
			163	163		
2	A	171	Total	O	0	0
			171	171		
2	B	142	Total	O	0	0
			142	142		

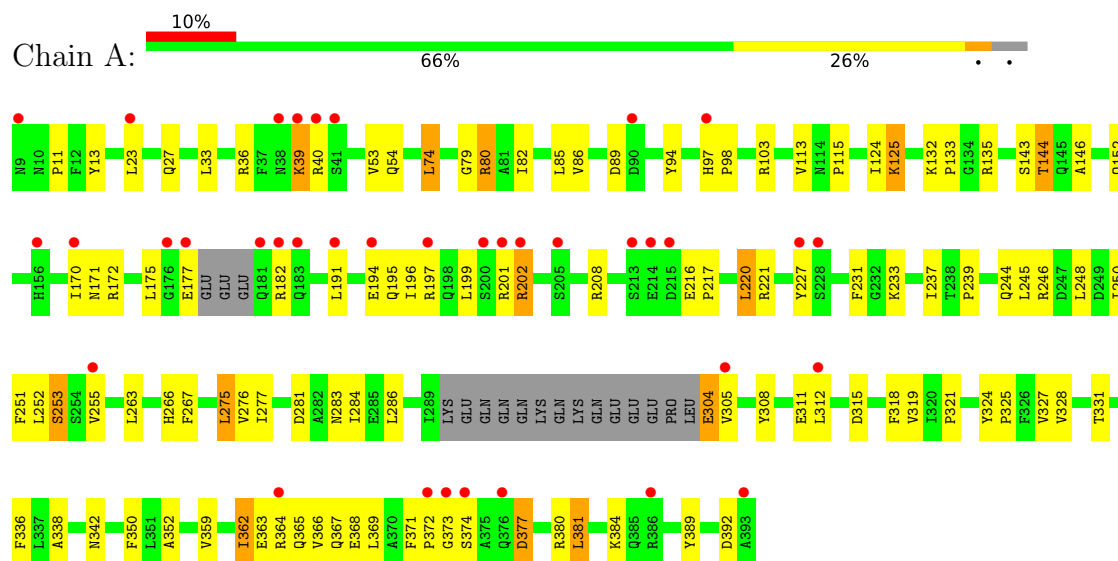
3 Residue-property plots

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.

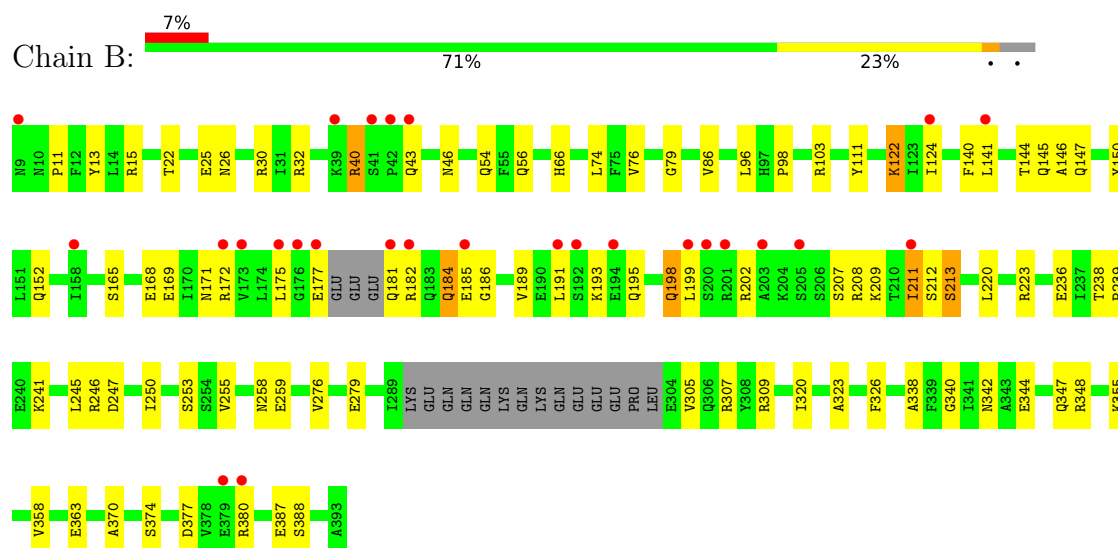
• Molecule 1: Beta-conglycinin beta subunit 2



• Molecule 1: Beta-conglycinin beta subunit 2



• Molecule 1: Beta-conglycinin beta subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.11Å 83.46Å 86.92Å 90.00° 118.36° 90.00°	Depositor
Resolution (Å)	37.45 – 2.01 37.45 – 2.01	Depositor EDS
% Data completeness (in resolution range)	89.5 (37.45-2.01) 90.9 (37.45-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.244 , 0.294 0.244 , 0.293	Depositor DCC
R_{free} test set	1921 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.022 for h,-k,-h-l 0.017 for -h-l,-k,l 0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9461	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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	0.39	0/3053	0.63	1/4129 (0.0%)
1	B	0.35	0/3053	0.58	1/4129 (0.0%)
1	C	0.41	0/3053	0.64	0/4129
All	All	0.38	0/9159	0.62	2/12387 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CA-CB-CG	6.43	138.80	116.30
1	A	74	LEU	CA-CB-CG	5.23	134.59	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2995	0	2941	91	1
1	B	2995	0	2941	79	0
1	C	2995	0	2941	92	1
2	A	171	0	0	18	0
2	B	142	0	0	13	0
2	C	163	0	0	25	0
All	All	9461	0	8823	245	1

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 14.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:NH2	2:A:401:HOH:O	1.85	1.09
1:A:36:ARG:HE	1:A:39:LYS:HG3	1.31	0.94
1:C:181:GLN:N	2:C:402:HOH:O	1.99	0.94
1:B:207:SER:OG	1:B:209:LYS:HD3	1.71	0.91
1:C:214:GLU:OE1	2:C:401:HOH:O	1.89	0.89
1:A:371:PHE:O	2:A:403:HOH:O	1.95	0.85
1:B:144:THR:HG22	1:B:146:ALA:H	1.41	0.84
1:C:44:LEU:HD11	1:C:319:VAL:HG11	1.59	0.84
1:B:259:GLU:OE1	2:B:401:HOH:O	1.97	0.82
1:B:202:ARG:NH1	2:B:407:HOH:O	2.11	0.81
1:A:53:VAL:HB	1:A:125:LYS:HG3	1.63	0.80
1:A:172:ARG:HG3	1:A:182:ARG:HH12	1.48	0.78
1:C:215:ASP:O	2:C:403:HOH:O	2.03	0.76
1:A:132:LYS:HE3	1:A:135:ARG:HD3	1.69	0.75
1:A:36:ARG:HE	1:A:39:LYS:CG	2.01	0.74
1:B:181:GLN:OE1	2:B:402:HOH:O	2.05	0.73
1:A:143:SER:O	2:A:404:HOH:O	2.07	0.73
1:A:27:GLN:CD	1:A:27:GLN:H	1.99	0.70
1:A:143:SER:OG	2:A:405:HOH:O	2.09	0.70
1:B:13:TYR:O	2:B:404:HOH:O	2.09	0.69
1:A:384:LYS:NZ	1:B:169:GLU:OE2	2.25	0.69
1:A:82:ILE:HG12	1:A:115:PRO:HG3	1.73	0.69
1:A:369:LEU:HD21	1:B:195:GLN:HE22	1.57	0.69
1:C:62:ILE:HB	1:C:191:LEU:HD11	1.75	0.69
1:A:36:ARG:NE	1:A:39:LYS:HG3	2.05	0.68
1:A:239:PRO:HB3	1:A:246:ARG:HA	1.75	0.68
1:B:344:GLU:OE1	2:B:406:HOH:O	2.11	0.68
1:C:231:PHE:CE2	1:C:392:ASP:HB2	2.29	0.68
1:B:213:SER:HB2	2:B:445:HOH:O	1.94	0.68
1:C:87:ASN:ND2	2:C:406:HOH:O	2.18	0.67
1:C:144:THR:HG22	1:C:146:ALA:H	1.60	0.66
1:C:383:LYS:CG	2:C:425:HOH:O	2.43	0.66
1:A:23:LEU:HD11	1:A:33:LEU:HB2	1.78	0.65
1:C:360:ARG:NH2	1:C:383:LYS:HG2	2.13	0.64
1:B:171:ASN:HD21	1:B:177:GLU:HG3	1.61	0.64
1:A:89:ASP:OD2	2:A:407:HOH:O	2.15	0.64
1:B:239:PRO:HB3	1:B:246:ARG:HA	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TYR:OH	1:B:363:GLU:HG2	1.98	0.63
1:C:45:GLU:OE2	2:C:404:HOH:O	2.16	0.63
1:A:284:ILE:CD1	1:A:312:LEU:HD11	2.30	0.62
1:B:144:THR:HB	1:B:147:GLN:NE2	2.15	0.62
1:A:208:ARG:HD3	1:A:208:ARG:H	1.65	0.62
1:C:148:GLN:HB2	1:B:305:VAL:HG23	1.81	0.62
1:B:236:GLU:OE2	1:B:348:ARG:NH2	2.33	0.61
1:A:275:LEU:HD21	1:A:318:PHE:HB3	1.82	0.61
1:A:172:ARG:HG3	1:A:182:ARG:NH1	2.14	0.61
1:B:347:GLN:OE1	2:B:408:HOH:O	2.16	0.60
1:C:41:SER:C	1:C:43:GLN:H	2.10	0.60
1:A:248:LEU:HB3	1:A:250:ILE:HD12	1.84	0.59
1:C:204:LYS:HD3	1:C:205:SER:N	2.17	0.59
1:A:342:ASN:ND2	2:A:418:HOH:O	2.35	0.59
1:B:198:GLN:OE1	2:B:409:HOH:O	2.17	0.59
1:C:74:LEU:HD23	1:C:102:GLN:O	2.03	0.58
1:C:204:LYS:HD3	1:C:205:SER:H	1.69	0.58
1:B:171:ASN:HD21	1:B:177:GLU:H	1.51	0.58
1:C:124:ILE:HD13	1:C:276:VAL:HG11	1.84	0.58
1:A:208:ARG:H	1:A:208:ARG:CD	2.17	0.58
1:C:152:GLN:HG3	1:C:175:LEU:HD22	1.85	0.58
1:A:144:THR:HG22	1:A:146:ALA:H	1.67	0.58
1:B:172:ARG:O	1:B:182:ARG:NH1	2.37	0.57
1:C:386:ARG:HG3	1:C:386:ARG:HH11	1.67	0.57
1:B:25:GLU:HG3	1:B:30:ARG:HB3	1.86	0.57
1:A:195:GLN:NE2	2:A:421:HOH:O	2.38	0.57
1:A:263:LEU:O	1:A:327:VAL:HG23	2.05	0.57
1:B:212:SER:O	1:B:212:SER:OG	2.23	0.57
1:C:25:GLU:HB2	1:C:30:ARG:HB2	1.87	0.56
1:C:201:ARG:NH2	2:C:415:HOH:O	2.27	0.56
1:A:132:LYS:HD2	1:A:133:PRO:HD2	1.88	0.56
1:A:311:GLU:OE1	2:A:408:HOH:O	2.17	0.56
1:B:355:LYS:NZ	2:B:416:HOH:O	2.36	0.56
1:C:84:THR:HG1	1:C:93:SER:HG	1.53	0.55
1:B:195:GLN:O	1:B:199:LEU:HG	2.06	0.55
1:C:170:ILE:HG13	1:C:174:LEU:HD12	1.88	0.55
1:C:383:LYS:HG2	2:C:425:HOH:O	2.06	0.55
1:A:40:ARG:NH2	2:A:422:HOH:O	2.38	0.55
1:C:86:VAL:HG22	1:C:109:THR:HB	1.87	0.55
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.72	0.55
1:C:181:GLN:NE2	2:C:427:HOH:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:CD1	1:A:276:VAL:HG11	2.37	0.55
1:C:145:GLN:HB2	1:C:185:GLU:HA	1.89	0.54
1:A:23:LEU:HD11	1:A:33:LEU:CB	2.36	0.54
1:C:371:PHE:O	2:C:407:HOH:O	2.18	0.54
1:A:13:TYR:CE1	1:A:312:LEU:HD23	2.42	0.54
1:A:80:ARG:HD2	1:A:97:HIS:HE1	1.71	0.54
1:C:24:PHE:CD2	1:C:187:VAL:HG22	2.42	0.54
1:A:286:LEU:HB3	1:A:308:TYR:HB2	1.90	0.54
1:B:66:HIS:HB3	1:B:140:PHE:CD1	2.43	0.54
1:A:191:LEU:O	2:A:409:HOH:O	2.18	0.54
1:C:43:GLN:O	2:C:408:HOH:O	2.19	0.53
1:C:14:LEU:CD2	1:C:40:ARG:HD3	2.39	0.53
1:C:364:ARG:HD2	2:C:410:HOH:O	2.08	0.53
1:A:377:ASP:OD1	1:A:380:ARG:NH2	2.40	0.53
1:C:181:GLN:HB2	2:C:537:HOH:O	2.08	0.53
1:A:331:THR:OG1	2:A:402:HOH:O	1.87	0.53
1:A:359:VAL:HG22	1:B:141:LEU:HD21	1.91	0.53
1:A:266:HIS:HB3	1:A:350:PHE:CD1	2.44	0.53
1:A:244:GLN:NE2	2:A:426:HOH:O	2.41	0.52
1:A:36:ARG:NE	1:A:39:LYS:HE3	2.24	0.52
1:B:245:LEU:HB3	1:B:250:ILE:O	2.09	0.52
1:C:43:GLN:C	2:C:411:HOH:O	2.53	0.52
1:A:304:GLU:N	2:A:427:HOH:O	2.43	0.52
1:A:305:VAL:HG21	1:B:150:TYR:HA	1.92	0.52
1:B:253:SER:OG	1:B:338:ALA:HB3	2.09	0.51
1:A:144:THR:CG2	1:A:146:ALA:H	2.23	0.51
1:B:250:ILE:HA	1:B:340:GLY:O	2.10	0.51
1:C:156:HIS:O	1:C:160:GLU:HG3	2.10	0.51
1:B:32:ARG:HH21	1:B:54:GLN:HE22	1.57	0.51
1:A:366:VAL:HG21	1:B:111:TYR:CE2	2.46	0.50
1:C:84:THR:OG1	1:C:93:SER:OG	2.22	0.50
1:C:215:ASP:HA	2:C:403:HOH:O	2.11	0.50
1:C:14:LEU:HD21	1:C:40:ARG:HD3	1.93	0.50
1:A:374:SER:HB3	1:A:377:ASP:HB2	1.93	0.50
1:C:62:ILE:CB	1:C:191:LEU:HD11	2.42	0.50
1:B:193:LYS:HB2	2:B:462:HOH:O	2.11	0.50
1:A:103:ARG:HB3	1:A:244:GLN:HE21	1.76	0.49
1:B:11:PRO:O	1:B:40:ARG:HD3	2.11	0.49
1:C:211:ILE:HD11	1:C:223:ARG:HD2	1.95	0.49
1:C:311:GLU:N	2:C:433:HOH:O	2.45	0.49
1:B:387:GLU:HG3	1:B:388:SER:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:CD2	1:A:318:PHE:HB3	2.41	0.49
1:B:22:THR:HA	1:B:32:ARG:HG2	1.94	0.49
1:C:169:GLU:OE2	1:B:380:ARG:NH1	2.46	0.49
1:C:285:GLU:HB2	1:C:327:VAL:HG12	1.95	0.49
1:C:248:LEU:HB3	1:C:250:ILE:HD12	1.95	0.48
1:A:82:ILE:HB	1:A:113:VAL:HB	1.95	0.48
1:C:124:ILE:CD1	1:C:276:VAL:HG11	2.43	0.48
1:C:142:SER:HB3	1:B:370:ALA:HB1	1.94	0.48
1:A:364:ARG:NH2	2:A:431:HOH:O	2.47	0.48
1:A:191:LEU:HD23	1:A:196:ILE:HG13	1.95	0.48
1:B:307:ARG:HG2	1:B:309:ARG:HH21	1.77	0.48
1:C:41:SER:C	1:C:43:GLN:N	2.71	0.48
1:B:40:ARG:HG3	1:B:40:ARG:HH11	1.79	0.48
1:B:171:ASN:ND2	1:B:177:GLU:H	2.12	0.48
1:C:194:GLU:OE1	2:C:409:HOH:O	2.20	0.48
1:A:284:ILE:HD12	1:A:312:LEU:HD11	1.95	0.48
1:C:91:ARG:NE	1:B:363:GLU:OE1	2.47	0.48
1:A:54:GLN:HE22	1:A:315:ASP:CG	2.22	0.47
1:A:220:LEU:HD22	1:A:237:ILE:HG22	1.94	0.47
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.28	0.47
1:C:77:LEU:HD11	1:C:124:ILE:HD12	1.96	0.47
1:A:283:ASN:OD1	1:A:311:GLU:HG2	2.14	0.47
1:B:145:GLN:HB2	1:B:185:GLU:HA	1.95	0.47
1:C:172:ARG:NH2	2:C:422:HOH:O	2.35	0.47
1:A:194:GLU:O	1:A:197:ARG:HB2	2.14	0.47
1:C:24:PHE:HZ	1:C:186:GLY:HA3	1.78	0.47
1:C:60:ASN:HA	1:C:196:ILE:HD11	1.96	0.47
1:C:386:ARG:HB2	2:C:412:HOH:O	2.15	0.47
1:A:171:ASN:HD21	1:A:177:GLU:HB2	1.80	0.47
1:B:79:GLY:O	1:B:98:PRO:HD3	2.14	0.47
1:A:36:ARG:CZ	1:A:39:LYS:HE3	2.44	0.47
1:A:275:LEU:HD23	1:A:318:PHE:O	2.15	0.47
1:B:208:ARG:NH2	2:B:420:HOH:O	2.47	0.47
1:C:164:HIS:O	1:C:164:HIS:CD2	2.68	0.47
1:B:374:SER:OG	1:B:377:ASP:OD2	2.32	0.47
1:C:164:HIS:O	1:C:164:HIS:CG	2.68	0.46
1:A:80:ARG:HG3	1:A:97:HIS:ND1	2.30	0.46
1:B:152:GLN:HG2	1:B:175:LEU:HD13	1.95	0.46
1:A:11:PRO:O	1:A:40:ARG:HD3	2.15	0.46
1:B:124:ILE:CD1	1:B:276:VAL:HG11	2.44	0.46
1:B:342:ASN:HB2	2:B:534:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HD11	1:A:312:LEU:HD13	1.97	0.46
1:A:284:ILE:HG12	1:A:328:VAL:HG22	1.98	0.46
1:C:216:GLU:HB3	1:C:217:PRO:HD2	1.97	0.46
1:C:239:PRO:HB3	1:C:246:ARG:HA	1.97	0.46
1:A:372:PRO:HB3	1:B:182:ARG:C	2.41	0.46
1:C:62:ILE:CG2	1:C:191:LEU:HD11	2.46	0.46
1:C:309:ARG:NH2	1:C:311:GLU:OE2	2.47	0.46
1:A:27:GLN:CD	1:A:27:GLN:N	2.72	0.46
1:A:40:ARG:NH2	2:A:417:HOH:O	2.35	0.46
1:B:241:LYS:HE2	1:B:241:LYS:HB2	1.61	0.46
1:B:13:TYR:OH	1:B:15:ARG:HG3	2.16	0.46
1:A:237:ILE:HG23	1:A:245:LEU:HD11	1.98	0.45
1:C:144:THR:O	1:C:146:ALA:N	2.49	0.45
1:C:364:ARG:HG2	1:C:375:ALA:HB1	1.97	0.45
1:A:352:ALA:HA	2:A:406:HOH:O	2.16	0.45
1:C:80:ARG:HD2	1:C:116:HIS:HD2	1.82	0.45
1:B:184:GLN:HG2	1:B:189:VAL:CG1	2.46	0.45
1:A:362:ILE:HG22	1:A:367:GLN:HG3	1.99	0.45
1:B:103:ARG:HH12	1:B:247:ASP:HB3	1.82	0.44
1:B:258:ASN:HB3	2:B:423:HOH:O	2.17	0.44
1:C:41:SER:O	1:C:43:GLN:N	2.49	0.44
1:C:284:ILE:HD13	1:C:318:PHE:CD1	2.53	0.44
1:B:387:GLU:HG3	1:B:388:SER:N	2.32	0.44
1:C:191:LEU:N	1:C:191:LEU:HD12	2.33	0.44
1:C:32:ARG:HD2	2:C:405:HOH:O	2.17	0.44
1:B:32:ARG:HH21	1:B:54:GLN:NE2	2.14	0.44
1:C:169:GLU:HA	2:C:422:HOH:O	2.17	0.44
1:C:347:GLN:HG3	2:C:523:HOH:O	2.17	0.44
1:A:36:ARG:NE	1:A:39:LYS:CE	2.81	0.43
1:A:79:GLY:O	1:A:98:PRO:HD3	2.18	0.43
1:A:124:ILE:HD11	1:A:276:VAL:HG11	1.99	0.43
1:A:152:GLN:HG3	1:A:175:LEU:HD22	2.00	0.43
1:B:171:ASN:HD22	1:B:175:LEU:HB2	1.83	0.43
1:B:184:GLN:HG2	1:B:189:VAL:HG11	1.99	0.43
1:B:320:ILE:HG21	1:B:326:PHE:CD1	2.54	0.43
1:C:153:GLY:O	1:B:307:ARG:HG2	2.19	0.43
1:A:231:PHE:CE1	1:A:392:ASP:HB2	2.53	0.43
1:C:360:ARG:HH22	1:C:383:LYS:HG2	1.82	0.43
1:B:76:VAL:HG21	1:B:96:LEU:HB3	2.01	0.43
1:B:141:LEU:HD13	1:B:150:TYR:CZ	2.54	0.43
1:A:94:TYR:CD1	1:A:217:PRO:HD3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.84	0.43
1:B:144:THR:HG21	1:B:186:GLY:C	2.44	0.43
1:A:251:PHE:CD1	1:A:251:PHE:C	2.97	0.43
1:B:56:GLN:HG3	1:B:122:LYS:HG3	2.00	0.43
1:A:377:ASP:OD2	2:A:410:HOH:O	2.21	0.42
1:B:26:ASN:HD22	1:B:186:GLY:HA3	1.84	0.42
1:C:115:PRO:HA	1:C:196:ILE:HD13	2.01	0.42
1:A:275:LEU:HD12	1:A:336:PHE:CD1	2.54	0.42
1:C:111:TYR:HH	1:B:363:GLU:HG2	1.83	0.42
1:A:381:LEU:HD23	1:B:169:GLU:OE2	2.20	0.42
1:B:152:GLN:CG	1:B:175:LEU:HD22	2.50	0.42
1:C:270:LYS:NZ	2:C:416:HOH:O	2.27	0.42
1:C:368:GLU:O	2:C:407:HOH:O	2.22	0.42
1:A:364:ARG:HG2	1:A:365:GLN:N	2.34	0.42
1:C:67:HIS:CD2	1:B:323:ALA:HB1	2.55	0.42
1:C:333:ASN:ND2	2:C:434:HOH:O	2.45	0.42
1:A:245:LEU:HB3	1:A:250:ILE:O	2.19	0.42
1:B:211:ILE:HD13	1:B:211:ILE:HA	1.77	0.42
1:C:102:GLN:HG3	1:C:103:ARG:N	2.34	0.42
1:C:80:ARG:HH11	1:C:116:HIS:CD2	2.38	0.41
1:C:167:PHE:HA	1:C:170:ILE:CG2	2.50	0.41
1:C:192:SER:OG	1:C:195:GLN:HG3	2.19	0.41
1:C:253:SER:OG	1:C:338:ALA:HB3	2.20	0.41
1:C:387:GLU:HG3	1:C:388:SER:H	1.86	0.41
1:C:312:LEU:HD21	1:C:318:PHE:HB2	2.01	0.41
1:A:253:SER:OG	1:A:338:ALA:HB3	2.20	0.41
1:B:238:THR:HB	1:B:239:PRO:HD2	2.03	0.41
1:C:227:TYR:HB3	1:C:389:TYR:CD2	2.56	0.41
1:A:267:PHE:HB3	1:A:325:PRO:HA	2.03	0.41
1:A:373:GLY:HA2	2:A:410:HOH:O	2.19	0.41
1:B:168:GLU:O	1:B:172:ARG:HB2	2.21	0.41
1:B:171:ASN:ND2	1:B:175:LEU:HB2	2.36	0.41
1:C:97:HIS:O	1:C:100:ASP:HB2	2.20	0.41
1:C:58:LYS:HA	1:C:58:LYS:HD3	1.87	0.41
1:C:131:ASN:O	1:B:46:ASN:HB2	2.21	0.41
1:A:202:ARG:HA	1:A:202:ARG:NE	2.36	0.41
1:A:220:LEU:HD21	1:A:252:LEU:HB2	2.03	0.41
1:A:321:PRO:HB2	1:A:324:TYR:CD1	2.55	0.41
1:B:165:SER:OG	1:B:169:GLU:OE1	2.32	0.41
1:C:15:ARG:HD2	1:C:18:ASN:OD1	2.21	0.40
1:C:91:ARG:CZ	1:B:363:GLU:OE1	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:H	1:A:221:ARG:HG2	1.67	0.40
1:A:227:TYR:HB3	1:A:389:TYR:CD2	2.56	0.40
1:C:144:THR:C	1:C:146:ALA:H	2.30	0.40

All (1) 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:C:386:ARG:O	1:A:39:LYS:NZ[2_545]	2.17	0.03

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%)	348 (96%)	12 (3%)	2 (1%)	21	17
1	B	362/385 (94%)	351 (97%)	10 (3%)	1 (0%)	36	35
1	C	362/385 (94%)	349 (96%)	10 (3%)	3 (1%)	16	11
All	All	1086/1155 (94%)	1048 (96%)	32 (3%)	6 (1%)	21	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	GLN
1	A	202	ARG
1	A	220	LEU
1	C	10	ASN
1	C	42	PRO
1	B	40	ARG

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	12
1	B	332/349 (95%)	320 (96%)	12 (4%)	31	31
1	C	332/349 (95%)	312 (94%)	20 (6%)	17	14
All	All	996/1047 (95%)	942 (95%)	54 (5%)	20	17

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	30	ARG
1	C	86	VAL
1	C	93	SER
1	C	119	GLN
1	C	122	LYS
1	C	125	LYS
1	C	132	LYS
1	C	158	ILE
1	C	189	VAL
1	C	194	GLU
1	C	207	SER
1	C	220	LEU
1	C	227	TYR
1	C	255	VAL
1	C	275	LEU
1	C	319	VAL
1	C	358	VAL
1	C	374	SER
1	C	377	ASP
1	A	39	LYS
1	A	74	LEU
1	A	80	ARG
1	A	85	LEU
1	A	86	VAL
1	A	125	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	THR
1	A	170	ILE
1	A	201	ARG
1	A	216	GLU
1	A	233	LYS
1	A	253	SER
1	A	255	VAL
1	A	275	LEU
1	A	281	ASP
1	A	304	GLU
1	A	319	VAL
1	A	362	ILE
1	A	363	GLU
1	A	368	GLU
1	A	377	ASP
1	A	381	LEU
1	B	43	GLN
1	B	74	LEU
1	B	86	VAL
1	B	122	LYS
1	B	184	GLN
1	B	191	LEU
1	B	198	GLN
1	B	211	ILE
1	B	213	SER
1	B	255	VAL
1	B	279	GLU
1	B	358	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	21	GLN
1	C	28	ASN
1	C	164	HIS
1	C	244	GLN
1	C	333	ASN
1	C	365	GLN
1	A	87	ASN
1	A	97	HIS
1	A	145	GLN
1	A	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	306	GLN
1	A	342	ASN
1	A	345	ASN
1	B	21	GLN
1	B	54	GLN
1	B	145	GLN
1	B	147	GLN
1	B	156	HIS
1	B	164	HIS
1	B	171	ASN
1	B	183	GLN
1	B	195	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 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%)	0.72	37 (10%)	12 11	17, 29, 50, 69	0
1	B	368/385 (95%)	0.78	27 (7%)	21 19	17, 33, 51, 70	0
1	C	368/385 (95%)	0.66	29 (7%)	18 17	17, 28, 50, 63	0
All	All	1104/1155 (95%)	0.72	93 (8%)	17 15	17, 30, 50, 70	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ARG	5.2
1	C	181	GLN	5.0
1	C	212	SER	4.4
1	C	177	GLU	4.3
1	C	9	ASN	4.3
1	A	39	LYS	4.2
1	B	182	ARG	4.1
1	A	393	ALA	4.0
1	A	202	ARG	3.7
1	B	181	GLN	3.5
1	A	214	GLU	3.4
1	C	207	SER	3.2
1	A	40	ARG	3.2
1	B	177	GLU	3.1
1	A	227	TYR	3.1
1	B	172	ARG	2.9
1	A	213	SER	2.9
1	A	305	VAL	2.9
1	B	176	GLY	2.9
1	A	386	ARG	2.8
1	C	170	ILE	2.8
1	B	191	LEU	2.8
1	A	182	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	41	SER	2.7
1	A	177	GLU	2.7
1	B	203	ALA	2.7
1	A	181	GLN	2.7
1	C	194	GLU	2.7
1	B	194	GLU	2.7
1	C	214	GLU	2.6
1	B	124	ILE	2.6
1	B	380	ARG	2.6
1	A	183	GLN	2.6
1	A	376	GLN	2.6
1	C	196	ILE	2.6
1	B	39	LYS	2.6
1	B	205	SER	2.5
1	C	220	LEU	2.5
1	C	24	PHE	2.5
1	A	228	SER	2.5
1	A	215	ASP	2.5
1	C	213	SER	2.5
1	C	40	ARG	2.5
1	C	176	GLY	2.5
1	A	38	ASN	2.5
1	C	144	THR	2.4
1	B	141	LEU	2.4
1	A	373	GLY	2.4
1	B	173	VAL	2.4
1	A	41	SER	2.4
1	A	200	SER	2.4
1	C	372	PRO	2.4
1	B	175	LEU	2.4
1	C	182	ARG	2.4
1	A	374	SER	2.4
1	C	185	GLU	2.3
1	A	170	ILE	2.3
1	A	191	LEU	2.3
1	C	39	LYS	2.3
1	C	165	SER	2.3
1	A	205	SER	2.3
1	B	42	PRO	2.3
1	B	43	GLN	2.3
1	C	201	ARG	2.3
1	A	194	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	364	ARG	2.3
1	C	198	GLN	2.2
1	C	204	LYS	2.2
1	B	158	ILE	2.2
1	B	200	SER	2.2
1	C	209	LYS	2.2
1	A	197	ARG	2.1
1	B	211	ILE	2.1
1	A	312	LEU	2.1
1	B	199	LEU	2.1
1	B	379	GLU	2.1
1	A	255	VAL	2.1
1	C	205	SER	2.1
1	C	393	ALA	2.1
1	B	192	SER	2.1
1	C	18	ASN	2.0
1	A	9	ASN	2.0
1	B	9	ASN	2.0
1	A	90	ASP	2.0
1	C	208	ARG	2.0
1	B	201	ARG	2.0
1	C	211	ILE	2.0
1	B	185	GLU	2.0
1	A	23	LEU	2.0
1	A	97	HIS	2.0
1	A	156	HIS	2.0
1	A	372	PRO	2.0
1	A	176	GLY	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 ⓘ

There are no such residues in this entry.