



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:25 PM GMT

PDB ID : 1UIK
Title : Crystal structure of soybean beta-conglycinin alpha prime homotrimer
Authors : Maruyama, Y.; Maruyama, N.; Mikami, B.; Utsumi, S.
Deposited on : 2003-07-16
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

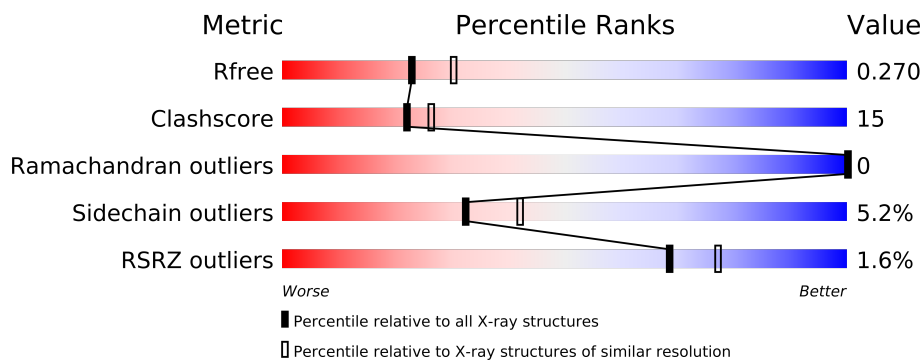
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	418	
1	B	418	
1	C	418	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9348 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called alpha prime subunit of beta-conglycinin.

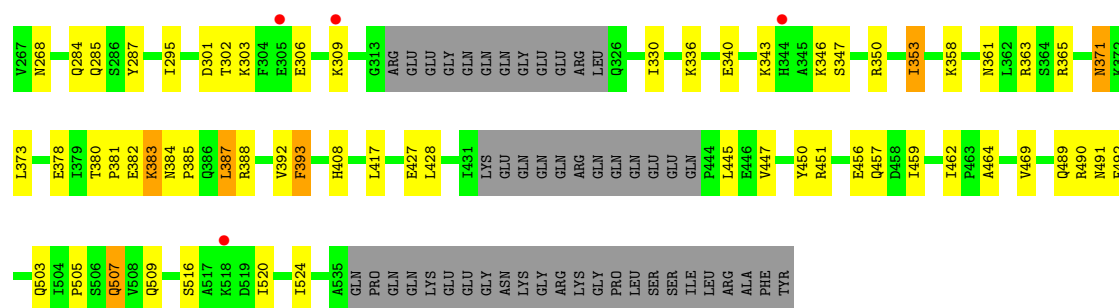
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2921	1857	504	558	2			
1	B	363	Total	C	N	O	S	0	1	0
			2919	1855	503	559	2			
1	C	364	Total	C	N	O	S	0	0	0
			2921	1857	504	558	2			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total	O	0	0
			188	188		
3	B	196	Total	O	0	0
			196	196		
3	C	200	Total	O	0	0
			200	200		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.96Å 164.96Å 110.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30 29.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 88.5 (29.99-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.269 0.223 , 0.270	Depositor DCC
R_{free} test set	3319 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	7 of 102805 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9348	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.62 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7719e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.36	0/2977	0.61	0/4026
1	B	0.38	0/2978	0.63	0/4027
1	C	0.36	0/2977	0.61	0/4026
All	All	0.37	0/8932	0.62	0/12079

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2921	0	2901	87	0
1	B	2919	0	2895	105	0
1	C	2921	0	2901	87	0
2	A	1	0	0	0	1
2	B	1	0	0	0	1
2	C	1	0	0	0	0
3	A	188	0	0	6	0
3	B	196	0	0	7	0
3	C	200	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9348	0	8697	261	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (261) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:507:GLN:HE21	1:A:507:GLN:H	1.02	0.99
1:A:507:GLN:NE2	1:A:507:GLN:H	1.66	0.94
1:B:507:GLN:HE21	1:B:507:GLN:H	1.05	0.93
1:C:193:ASN:HD21	1:C:259:ARG:HE	1.20	0.88
1:B:507:GLN:H	1:B:507:GLN:NE2	1.71	0.88
1:C:225:ASN:HD22	1:C:226:ASP:N	1.73	0.84
1:B:225:ASN:HD22	1:B:226:ASP:N	1.76	0.84
1:A:193:ASN:HD21	1:A:259:ARG:HE	1.28	0.81
1:C:507:GLN:HE21	1:C:507:GLN:H	1.31	0.77
1:A:507:GLN:HE21	1:A:507:GLN:N	1.82	0.76
1:A:381:PRO:HB3	1:A:388:ARG:HA	1.68	0.76
1:C:427:GLU:HG2	1:C:451:ARG:CD	2.16	0.76
1:C:158:GLN:HE21	1:C:159:THR:N	1.84	0.75
1:A:268:ASN:HD21	1:B:464:ALA:H	1.35	0.74
1:C:353:ILE:HD13	1:C:353:ILE:O	1.88	0.74
1:B:449:LYS:HB3	1:B:451:ARG:NH1	2.06	0.71
1:B:507:GLN:HE21	1:B:507:GLN:N	1.85	0.70
1:C:507:GLN:NE2	1:C:507:GLN:H	1.88	0.70
1:A:225:ASN:HD22	1:A:226:ASP:N	1.88	0.70
1:C:381:PRO:HB3	1:C:388:ARG:HA	1.74	0.68
1:C:158:GLN:HE21	1:C:158:GLN:C	1.97	0.68
1:B:350:ARG:HA	1:B:364:SER:OG	1.94	0.68
1:B:225:ASN:HD22	1:B:225:ASN:C	1.98	0.68
1:A:365:ARG:HH22	1:A:383:LYS:HE3	1.59	0.67
1:A:418:VAL:HG12	1:A:459:ILE:HD12	1.77	0.67
1:B:427:GLU:HG2	1:B:451:ARG:CD	2.25	0.67
1:B:225:ASN:HB3	1:C:491:ASN:HD22	1.61	0.66
1:B:336:LYS:HE3	1:B:340:GLU:OE2	1.96	0.66
1:A:371:ASN:HD22	1:A:371:ASN:C	1.98	0.66
1:B:169:ARG:HD3	1:B:191:GLU:OE1	1.96	0.66
1:A:491:ASN:HD22	1:C:225:ASN:HB3	1.61	0.65
1:C:382:GLU:HG2	1:C:383:LYS:HD2	1.79	0.64
1:B:268:ASN:HD21	1:C:464:ALA:H	1.45	0.64
1:A:336:LYS:O	1:A:340:GLU:HG3	1.99	0.63
1:C:445:LEU:HD22	3:C:1143:HOH:O	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:428:LEU:HB3	1:C:450:TYR:HB2	1.79	0.63
1:B:427:GLU:HG2	1:B:451:ARG:NE	2.13	0.62
1:A:371:ASN:ND2	1:A:373:LEU:H	1.97	0.62
1:A:153:ASN:C	1:A:153:ASN:HD22	2.02	0.61
1:B:364:SER:HB3	3:B:1178:HOH:O	1.99	0.61
1:C:193:ASN:ND2	1:C:259:ARG:HE	1.95	0.61
1:B:427:GLU:HG2	1:B:451:ARG:HD2	1.82	0.61
1:A:300:TYR:O	1:A:302:THR:HG23	2.01	0.61
1:B:227:ASP:HA	1:C:503:GLN:NE2	2.17	0.60
1:B:153:ASN:C	1:B:153:ASN:HD22	2.05	0.60
1:C:336:LYS:O	1:C:340:GLU:HG3	2.02	0.60
1:A:464:ALA:H	1:C:268:ASN:HD21	1.48	0.60
1:A:163:ASN:HD22	1:A:163:ASN:C	2.05	0.59
1:B:371:ASN:HD22	1:B:371:ASN:C	2.06	0.59
1:B:448:ARG:HD2	3:B:1090:HOH:O	2.02	0.59
1:C:427:GLU:HG2	1:C:451:ARG:HD3	1.85	0.59
1:B:429:VAL:CG1	1:B:467:PRO:HB2	2.33	0.59
1:B:350:ARG:O	1:B:353:ILE:HG23	2.03	0.59
1:C:213:ILE:HD13	1:C:260:MET:HG2	1.84	0.59
1:A:420:ASN:HB3	1:A:477:ASN:HD22	1.67	0.58
1:A:427:GLU:HG2	1:A:451:ARG:CD	2.33	0.58
1:B:427:GLU:HG2	1:B:451:ARG:HE	1.69	0.58
1:C:361:ASN:HD22	1:C:363:ARG:H	1.52	0.58
1:A:225:ASN:HB3	1:B:491:ASN:HD22	1.70	0.57
1:B:491:ASN:HB3	1:B:500:VAL:HG11	1.86	0.57
1:A:163:ASN:ND2	1:A:166:GLY:H	2.02	0.56
1:B:418:VAL:HG12	1:B:459:ILE:HD12	1.86	0.56
1:C:158:GLN:HE21	1:C:158:GLN:CA	2.17	0.56
1:C:163:ASN:C	1:C:163:ASN:HD22	2.08	0.56
1:C:427:GLU:HB2	1:C:469:VAL:HG12	1.86	0.56
1:B:491:ASN:HB3	1:B:500:VAL:CG1	2.35	0.56
1:C:371:ASN:HD22	1:C:371:ASN:C	2.07	0.56
1:C:365:ARG:HG3	1:C:365:ARG:HH11	1.68	0.56
1:B:259:ARG:HH11	1:B:420:ASN:HD22	1.54	0.55
1:A:404:LEU:HD11	1:A:469:VAL:HG13	1.87	0.55
1:C:211:ILE:O	1:C:238:ALA:HA	2.07	0.55
1:A:407:PRO:HG3	1:A:469:VAL:CG2	2.37	0.55
1:C:456:GLU:O	1:C:457:GLN:HB2	2.07	0.55
1:C:193:ASN:HD21	1:C:259:ARG:NE	2.00	0.55
1:A:191:GLU:OE2	1:A:457:GLN:NE2	2.40	0.55
1:A:361:ASN:HD22	1:A:363:ARG:H	1.55	0.54
1:C:225:ASN:HD22	1:C:225:ASN:C	2.10	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:353:ILE:HG12	3:C:1167:HOH:O	2.07	0.54
1:B:287:TYR:HA	1:C:447:VAL:HG11	1.90	0.54
1:A:448:ARG:NH2	1:A:449:LYS:O	2.40	0.54
1:A:456:GLU:O	1:A:457:GLN:HB2	2.07	0.54
1:B:336:LYS:O	1:B:340:GLU:HG3	2.08	0.54
1:A:220:LEU:HD13	1:A:239:LEU:HD23	1.90	0.54
1:B:234:GLN:HB2	3:B:1154:HOH:O	2.07	0.54
1:C:225:ASN:HD22	1:C:226:ASP:H	1.54	0.54
1:B:418:VAL:O	1:B:418:VAL:HG23	2.07	0.53
1:C:196:PRO:HD3	1:C:257:ASN:ND2	2.23	0.53
1:B:285:GLN:NE2	1:B:289:GLN:HE22	2.07	0.53
1:B:427:GLU:HB2	1:B:469:VAL:HG12	1.91	0.53
1:A:365:ARG:NH2	1:A:383:LYS:HE3	2.23	0.53
1:B:361:ASN:HD22	1:B:363:ARG:H	1.56	0.53
1:C:346:LYS:HD2	1:C:358:LYS:NZ	2.24	0.52
1:B:196:PRO:HB3	1:B:253:ASP:O	2.09	0.52
1:B:507:GLN:N	1:B:507:GLN:NE2	2.51	0.52
1:B:456:GLU:O	1:B:457:GLN:HB2	2.10	0.52
1:C:178:SER:OG	1:C:180:GLN:HB2	2.09	0.52
1:B:445:LEU:HD22	3:B:1149:HOH:O	2.08	0.52
1:B:225:ASN:HB3	1:C:491:ASN:ND2	2.25	0.52
1:C:353:ILE:HD12	1:C:383:LYS:HB3	1.91	0.52
1:B:353:ILE:HD12	1:B:383:LYS:NZ	2.25	0.52
1:A:285:GLN:NE2	1:A:289:GLN:NE2	2.58	0.52
1:A:152:PHE:HB2	1:A:459:ILE:HB	1.92	0.51
1:A:418:VAL:O	1:A:418:VAL:HG23	2.10	0.51
1:A:168:VAL:HG22	1:A:192:PHE:CD2	2.45	0.51
1:B:339:ARG:HH21	1:B:339:ARG:HG3	1.75	0.51
1:B:193:ASN:HD21	1:B:259:ARG:HE	1.59	0.51
1:A:378:GLU:CD	1:A:490:ARG:HH22	2.12	0.51
1:A:507:GLN:NE2	1:A:507:GLN:N	2.48	0.51
1:C:158:GLN:NE2	1:C:159:THR:N	2.57	0.51
1:C:350:ARG:HH21	1:C:350:ARG:HG2	1.75	0.51
1:A:384:ASN:OD1	1:A:386:GLN:HB2	2.11	0.51
1:C:371:ASN:ND2	1:C:373:LEU:H	2.08	0.51
1:A:445:LEU:HD22	3:A:1111:HOH:O	2.10	0.51
1:C:197:ASN:HD22	1:C:197:ASN:N	2.08	0.50
1:B:356[A]:GLU:HG2	3:B:1193:HOH:O	2.10	0.50
1:A:393:PHE:C	1:A:393:PHE:CD2	2.84	0.50
1:B:285:GLN:NE2	1:B:289:GLN:NE2	2.60	0.50
1:C:393:PHE:CD2	1:C:393:PHE:C	2.84	0.50
1:B:425:ASN:OD1	1:B:453:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:365:ARG:HD2	1:B:383:LYS:NZ	2.27	0.50
1:B:163:ASN:HD22	1:B:163:ASN:C	2.15	0.50
1:A:225:ASN:C	1:A:225:ASN:HD22	2.14	0.49
1:C:169:ARG:HG2	1:C:191:GLU:HB3	1.94	0.49
1:C:456:GLU:HG2	1:C:457:GLN:HG3	1.93	0.49
1:A:380:THR:HB	1:A:381:PRO:CD	2.43	0.49
1:B:213:ILE:HD13	1:B:260:MET:HG2	1.94	0.49
1:C:378:GLU:CD	1:C:490:ARG:HH22	2.14	0.49
1:C:153:ASN:HD22	1:C:153:ASN:C	2.14	0.49
1:A:516:SER:O	1:A:520:ILE:HG13	2.12	0.49
1:A:163:ASN:ND2	1:A:163:ASN:C	2.66	0.49
1:A:211:ILE:O	1:A:238:ALA:HA	2.12	0.49
1:A:336:LYS:HE2	1:A:340:GLU:OE2	2.12	0.49
1:A:446:GLU:HA	1:C:285:GLN:OE1	2.13	0.49
1:A:371:ASN:ND2	1:A:374:GLY:H	2.11	0.48
1:C:196:PRO:HD3	1:C:257:ASN:HD22	1.78	0.48
1:A:343:LYS:HB2	1:A:343:LYS:NZ	2.28	0.48
1:A:197:ASN:HD22	1:A:197:ASN:N	2.11	0.48
1:C:169:ARG:HD3	1:C:191:GLU:OE2	2.13	0.48
1:C:163:ASN:ND2	1:C:166:GLY:H	2.11	0.48
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.78	0.48
1:B:356[A]:GLU:HG3	1:B:357:ASP:N	2.28	0.48
1:B:197:ASN:HD22	1:B:197:ASN:N	2.11	0.48
1:A:214:LEU:HD22	1:A:479:PHE:CD2	2.49	0.48
1:C:330:ILE:HD12	1:C:330:ILE:N	2.29	0.48
1:B:381:PRO:HB3	1:B:388:ARG:HA	1.96	0.47
1:B:181:LEU:HD22	1:B:461:VAL:HG11	1.96	0.47
1:A:196:PRO:HB3	1:A:253:ASP:O	2.14	0.47
1:C:507:GLN:N	1:C:507:GLN:HE21	2.07	0.47
1:B:471:ASN:HD22	1:B:471:ASN:C	2.17	0.47
1:B:153:ASN:HD21	1:B:155:LYS:HB2	1.79	0.47
1:B:387:LEU:HG	1:B:392:VAL:O	2.15	0.47
1:B:228:ARG:HD3	1:C:505:PRO:HD3	1.97	0.47
1:B:193:ASN:HA	1:B:258:LEU:O	2.14	0.47
1:A:193:ASN:ND2	1:A:259:ARG:HE	2.06	0.47
1:A:228:ARG:HD3	1:B:503:GLN:O	2.14	0.47
1:B:219:ILE:HB	1:B:250:VAL:HB	1.97	0.47
1:C:427:GLU:HG2	1:C:451:ARG:NE	2.30	0.47
1:A:380:THR:HB	1:A:381:PRO:HD2	1.97	0.46
1:B:418:VAL:O	1:B:418:VAL:CG2	2.62	0.46
1:C:302:THR:HG22	1:C:303:LYS:N	2.30	0.46
1:C:365:ARG:HG3	1:C:365:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:520:ILE:O	1:B:524:ILE:HG12	2.14	0.46
1:B:152:PHE:HB2	1:B:459:ILE:HB	1.97	0.46
1:A:491:ASN:HB3	1:A:500:VAL:HG11	1.97	0.46
1:B:380:THR:HB	1:B:381:PRO:HD2	1.98	0.46
1:C:384:ASN:HA	1:C:385:PRO:HD3	1.76	0.46
1:A:383:LYS:HD3	3:A:1125:HOH:O	2.16	0.46
1:B:163:ASN:ND2	1:B:166:GLY:H	2.14	0.46
1:B:418:VAL:HG12	1:B:459:ILE:CD1	2.45	0.46
1:C:163:ASN:C	1:C:163:ASN:ND2	2.69	0.46
1:B:456:GLU:HG2	1:B:457:GLN:HG3	1.98	0.46
1:C:213:ILE:CD1	1:C:260:MET:HG2	2.46	0.45
1:A:413:ALA:H	1:A:488:ASN:ND2	2.14	0.45
1:B:423:GLU:HB3	3:B:1137:HOH:O	2.16	0.45
1:B:471:ASN:HD22	1:B:472:ALA:N	2.14	0.45
1:B:393:PHE:C	1:B:393:PHE:CD2	2.90	0.45
1:B:448:ARG:NH2	1:B:449:LYS:O	2.50	0.45
1:A:225:ASN:HB3	1:B:491:ASN:ND2	2.32	0.45
1:B:353:ILE:HD12	1:B:383:LYS:HZ1	1.81	0.45
1:C:371:ASN:ND2	1:C:371:ASN:C	2.70	0.45
1:B:217:THR:HG22	1:B:218:ALA:N	2.32	0.45
1:A:287:TYR:HA	1:B:447:VAL:HG11	1.99	0.45
1:C:214:LEU:HD11	1:C:261:ILE:HG13	1.98	0.44
1:A:387:LEU:HG	1:A:392:VAL:O	2.17	0.44
1:B:225:ASN:ND2	1:B:225:ASN:C	2.68	0.44
1:C:427:GLU:HB2	1:C:469:VAL:CG1	2.46	0.44
1:A:408:HIS:HB3	1:A:492:PHE:CD1	2.53	0.44
1:A:418:VAL:HG12	1:A:459:ILE:CD1	2.46	0.44
1:C:169:ARG:CG	1:C:191:GLU:HB3	2.47	0.44
1:B:365:ARG:HH21	1:B:365:ARG:HG2	1.82	0.44
1:A:382:GLU:HG2	1:A:383:LYS:HD2	1.98	0.44
1:A:427:GLU:OE2	1:C:295:ILE:HG13	2.18	0.44
1:B:365:ARG:NH2	1:B:365:ARG:HG2	2.33	0.43
1:B:169:ARG:HG2	1:B:191:GLU:HB3	2.01	0.43
1:B:339:ARG:HG3	1:B:339:ARG:NH2	2.34	0.43
1:A:306:GLU:HG3	3:A:1117:HOH:O	2.18	0.43
1:C:340:GLU:O	1:C:343:LYS:HE2	2.18	0.43
1:A:407:PRO:HG3	1:A:469:VAL:HG21	1.99	0.43
1:C:516:SER:O	1:C:520:ILE:HG13	2.18	0.43
1:C:186:ASP:O	1:C:266:PRO:HD2	2.18	0.43
1:B:371:ASN:ND2	1:B:374:GLY:H	2.16	0.43
1:C:361:ASN:ND2	1:C:363:ARG:H	2.14	0.43
1:B:259:ARG:HH11	1:B:420:ASN:ND2	2.15	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:ARG:HH11	1:A:420:ASN:HD22	1.66	0.43
1:A:384:ASN:HA	1:A:385:PRO:HD3	1.76	0.43
1:C:417:LEU:HD11	1:C:462:ILE:HD11	2.01	0.42
1:B:424:ALA:HB2	1:B:476:LEU:HD22	2.01	0.42
1:B:190:LEU:HB3	1:B:262:THR:HB	2.01	0.42
1:C:214:LEU:O	1:C:215:ASN:ND2	2.52	0.42
1:C:185:ARG:HB2	1:C:185:ARG:HH21	1.84	0.42
1:C:387:LEU:HG	1:C:392:VAL:O	2.19	0.42
1:A:448:ARG:HD2	3:A:1100:HOH:O	2.19	0.42
1:B:516:SER:O	1:B:520:ILE:HG13	2.20	0.42
1:C:417:LEU:O	1:C:459:ILE:HA	2.20	0.42
1:A:270:PRO:HG2	1:B:182:GLN:NE2	2.35	0.42
1:B:418:VAL:HG22	1:B:479:PHE:HB2	2.01	0.42
1:C:302:THR:CG2	1:C:306:GLU:HB3	2.50	0.42
1:C:148:ASN:HD22	1:C:148:ASN:C	2.22	0.42
1:B:500:VAL:HG23	1:B:501:ILE:N	2.33	0.42
1:C:380:THR:HB	1:C:381:PRO:CD	2.50	0.42
1:B:378:GLU:CD	1:B:490:ARG:HH12	2.23	0.42
1:B:418:VAL:HA	1:B:459:ILE:HD13	2.01	0.42
1:B:250:VAL:O	1:B:252:PRO:HD3	2.20	0.42
1:A:303:LYS:NZ	1:A:305:GLU:CD	2.72	0.42
1:A:219:ILE:HB	1:A:250:VAL:HB	2.02	0.41
1:A:226:ASP:O	1:A:227:ASP:HB3	2.21	0.41
1:C:520:ILE:O	1:C:524:ILE:HG12	2.20	0.41
1:B:353:ILE:HG22	3:B:1177:HOH:O	2.20	0.41
1:A:365:ARG:HH22	1:A:383:LYS:CE	2.29	0.41
1:C:505:PRO:O	1:C:509:GLN:HG3	2.20	0.41
1:C:309:LYS:HB2	1:C:309:LYS:HE3	1.89	0.41
1:A:185:ARG:HD2	3:A:1108:HOH:O	2.19	0.41
1:B:371:ASN:C	1:B:371:ASN:ND2	2.72	0.41
1:A:448:ARG:HH21	1:A:448:ARG:HG3	1.85	0.41
1:B:163:ASN:ND2	1:B:163:ASN:C	2.74	0.41
1:A:371:ASN:ND2	1:A:371:ASN:C	2.67	0.41
1:A:530:SER:O	1:A:531:TYR:HB2	2.20	0.41
1:C:347:SER:HB2	3:C:1071:HOH:O	2.19	0.41
1:A:259:ARG:HH11	1:A:420:ASN:ND2	2.19	0.41
1:B:451:ARG:CG	1:B:451:ARG:HH11	2.33	0.41
1:B:153:ASN:ND2	1:B:153:ASN:C	2.73	0.41
1:A:163:ASN:ND2	1:A:165:TYR:H	2.19	0.41
1:C:191:GLU:OE1	1:C:457:GLN:NE2	2.53	0.41
1:B:356[A]:GLU:HG3	1:B:357:ASP:OD1	2.20	0.41
1:B:384:ASN:HA	1:B:385:PRO:HD3	1.75	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:251:ASN:C	1:B:251:ASN:HD22	2.24	0.41
1:A:447:VAL:HG11	1:C:287:TYR:HA	2.03	0.41
1:C:408:HIS:HB3	1:C:492:PHE:CD1	2.56	0.41
1:A:268:ASN:ND2	1:B:414:ILE:HG12	2.36	0.41
1:B:240:ARG:H	1:B:386:GLN:NE2	2.19	0.40
1:B:471:ASN:C	1:B:471:ASN:ND2	2.75	0.40
1:C:219:ILE:HB	1:C:250:VAL:HB	2.02	0.40
1:A:418:VAL:O	1:A:418:VAL:CG2	2.68	0.40
1:A:214:LEU:HD22	1:A:479:PHE:CE2	2.56	0.40
1:B:380:THR:HB	1:B:381:PRO:CD	2.50	0.40
1:A:307:ILE:HG23	1:A:311:LEU:HD12	2.03	0.40
1:A:428:LEU:HB3	1:A:450:TYR:HB2	2.02	0.40
1:C:217:THR:HG22	1:C:218:ALA:N	2.37	0.40
1:A:153:ASN:ND2	1:A:153:ASN:C	2.72	0.40
1:B:148:ASN:HD22	1:B:148:ASN:C	2.24	0.40
1:A:350:ARG:HG3	3:A:1179:HOH:O	2.22	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	Distance(Å)	Clash(Å)
2:A:1001:MG:MG	2:B:1002:MG:MG[6_666]	0.06	2.14

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	358/418 (86%)	344 (96%)	14 (4%)	0	100	100
1	B	358/418 (86%)	346 (97%)	12 (3%)	0	100	100
1	C	358/418 (86%)	346 (97%)	12 (3%)	0	100	100
All	All	1074/1254 (86%)	1036 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	328/376 (87%)	315 (96%)	13 (4%)	42	56
1	B	328/376 (87%)	309 (94%)	19 (6%)	28	36
1	C	328/376 (87%)	309 (94%)	19 (6%)	28	36
All	All	984/1128 (87%)	933 (95%)	51 (5%)	32	42

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	153	ASN
1	A	158	GLN
1	A	163	ASN
1	A	197	ASN
1	A	225	ASN
1	A	240	ARG
1	A	251	ASN
1	A	284	GLN
1	A	371	ASN
1	A	387	LEU
1	A	393	PHE
1	A	507	GLN
1	B	148	ASN
1	B	153	ASN
1	B	158	GLN
1	B	163	ASN
1	B	169	ARG
1	B	185	ARG
1	B	197	ASN
1	B	200	LEU
1	B	225	ASN
1	B	240	ARG
1	B	251	ASN
1	B	284	GLN
1	B	341	LEU
1	B	371	ASN

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Mol	Chain	Res	Type
1	B	375	LYS
1	B	387	LEU
1	B	393	PHE
1	B	471	ASN
1	B	507	GLN
1	C	148	ASN
1	C	153	ASN
1	C	158	GLN
1	C	163	ASN
1	C	169	ARG
1	C	185	ARG
1	C	197	ASN
1	C	200	LEU
1	C	225	ASN
1	C	251	ASN
1	C	284	GLN
1	C	301	ASP
1	C	353	ILE
1	C	371	ASN
1	C	383	LYS
1	C	387	LEU
1	C	393	PHE
1	C	489	GLN
1	C	507	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	153	ASN
1	A	163	ASN
1	A	164	GLN
1	A	167	HIS
1	A	179	GLN
1	A	180	GLN
1	A	193	ASN
1	A	215	ASN
1	A	225	ASN
1	A	251	ASN
1	A	254	ASN
1	A	268	ASN
1	A	284	GLN

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Mol	Chain	Res	Type
1	A	289	GLN
1	A	294	ASN
1	A	326	GLN
1	A	337	GLN
1	A	361	ASN
1	A	371	ASN
1	A	386	GLN
1	A	400	ASN
1	A	420	ASN
1	A	477	ASN
1	A	484	ASN
1	A	487	ASN
1	A	488	ASN
1	A	491	ASN
1	A	503	GLN
1	A	507	GLN
1	A	522	ASN
1	B	148	ASN
1	B	153	ASN
1	B	163	ASN
1	B	172	GLN
1	B	179	GLN
1	B	182	GLN
1	B	193	ASN
1	B	225	ASN
1	B	251	ASN
1	B	254	ASN
1	B	257	ASN
1	B	268	ASN
1	B	289	GLN
1	B	294	ASN
1	B	326	GLN
1	B	361	ASN
1	B	371	ASN
1	B	386	GLN
1	B	400	ASN
1	B	420	ASN
1	B	471	ASN
1	B	477	ASN
1	B	484	ASN
1	B	487	ASN
1	B	488	ASN

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Mol	Chain	Res	Type
1	B	491	ASN
1	B	503	GLN
1	B	507	GLN
1	B	522	ASN
1	C	148	ASN
1	C	153	ASN
1	C	158	GLN
1	C	163	ASN
1	C	179	GLN
1	C	182	GLN
1	C	193	ASN
1	C	215	ASN
1	C	225	ASN
1	C	251	ASN
1	C	254	ASN
1	C	257	ASN
1	C	268	ASN
1	C	284	GLN
1	C	289	GLN
1	C	294	ASN
1	C	326	GLN
1	C	337	GLN
1	C	361	ASN
1	C	371	ASN
1	C	386	GLN
1	C	400	ASN
1	C	410	ASN
1	C	420	ASN
1	C	477	ASN
1	C	484	ASN
1	C	487	ASN
1	C	488	ASN
1	C	491	ASN
1	C	503	GLN
1	C	507	GLN
1	C	522	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	364/418 (87%)	-0.20	9 (2%) 54 65	20, 32, 47, 57	0
1	B	363/418 (86%)	-0.32	3 (0%) 83 90	18, 31, 46, 55	0
1	C	364/418 (87%)	-0.28	6 (1%) 68 77	17, 31, 46, 55	0
All	All	1091/1254 (87%)	-0.27	18 (1%) 68 77	17, 31, 47, 57	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	344	HIS	3.2
1	A	350	ARG	3.0
1	A	179	GLN	2.9
1	C	305	GLU	2.8
1	A	155	LYS	2.7
1	A	444	PRO	2.6
1	C	179	GLN	2.6
1	A	344	HIS	2.4
1	C	309	LYS	2.4
1	A	327	GLU	2.3
1	B	305	GLU	2.3
1	B	179	GLN	2.3
1	A	446	GLU	2.2
1	B	353	ILE	2.2
1	A	305	GLU	2.2
1	C	178	SER	2.1
1	A	178	SER	2.1
1	C	518	LYS	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	C	1003	1/1	0.11	0.68	34,34,34,34	1
2	MG	B	1002	1/1	0.04	-3.13	49,49,49,49	0
2	MG	A	1001	1/1	0.04	-3.19	47,47,47,47	0

6.5 Other polymers

There are no such residues in this entry.