



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:53 AM GMT

PDB ID : 1NWG
Title : BETA-1,4-GALACTOSYLTRANSFERASECOMPLEX WITH ALPHA-LACTALBUMIN AND N-BUTANOYL-GLUCOAMINE
Authors : Ramakrishnan, B.; Shah, P.S.; Qasba, P.K.
Deposited on : 2003-02-06
Resolution : 2.32 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>

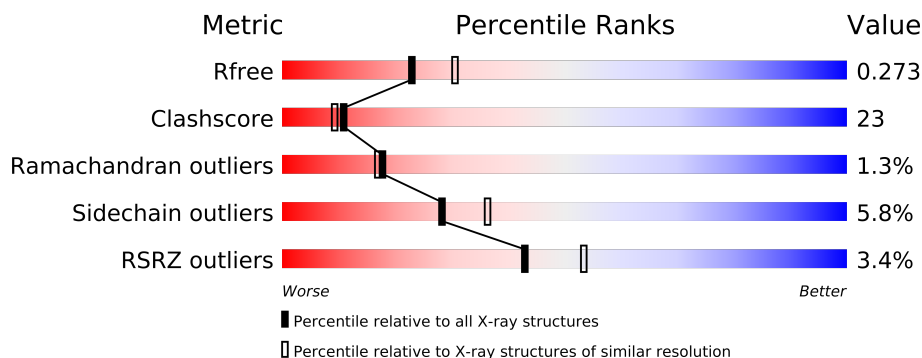
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.32 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	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (2.34-2.30)

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	123	
1	C	123	
2	B	286	
2	D	286	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7260 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-lactalbumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			
1	C	123	Total	C	N	O	S	0	0	0
			980	620	156	195	9			

- Molecule 2 is a protein called beta-1,4-galactosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	0	0	0
			2218	1424	382	398	14			
2	D	272	Total	C	N	O	S	0	0	0
			2218	1424	382	398	14			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
D	117	ALA	-	SEE REMARK 999	UNP P08037
D	118	SER	-	SEE REMARK 999	UNP P08037
D	119	MET	-	SEE REMARK 999	UNP P08037

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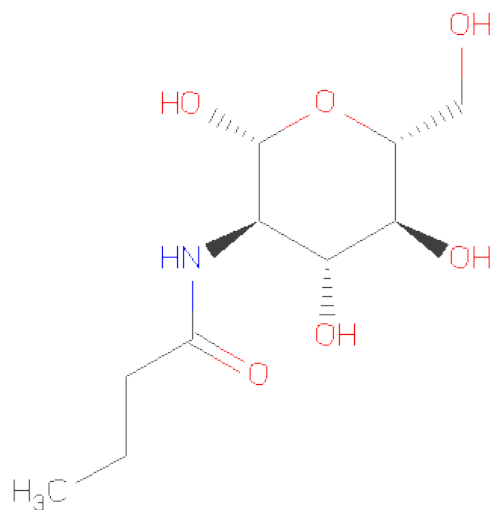
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Chain	Residue	Modelled	Actual	Comment	Reference
D	120	THR	-	SEE REMARK 999	UNP P08037
D	121	GLY	-	SEE REMARK 999	UNP P08037
D	122	GLY	-	SEE REMARK 999	UNP P08037
D	123	GLN	-	SEE REMARK 999	UNP P08037
D	124	GLN	-	SEE REMARK 999	UNP P08037
D	125	MET	-	SEE REMARK 999	UNP P08037
D	126	GLY	-	SEE REMARK 999	UNP P08037
D	127	ARG	-	SEE REMARK 999	UNP P08037
D	128	GLY	-	SEE REMARK 999	UNP P08037
D	129	SER	-	SEE REMARK 999	UNP P08037

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is N-BUTANOYL-2-AMINO-2-DEOXY-GLUCOPYRANOSIDE (three-letter code: BGN) (formula: C₁₀H₁₉NO₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 17 10 1 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			17	10	1	6		

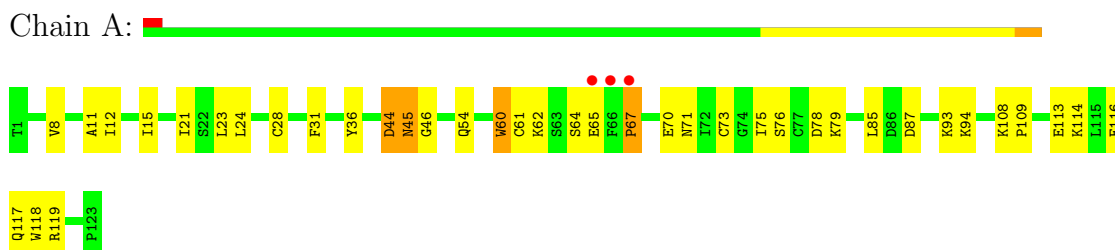
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	0
			179	179		
5	B	274	Total	O	0	0
			274	274		
5	C	167	Total	O	0	0
			167	167		
5	D	208	Total	O	0	0
			208	208		

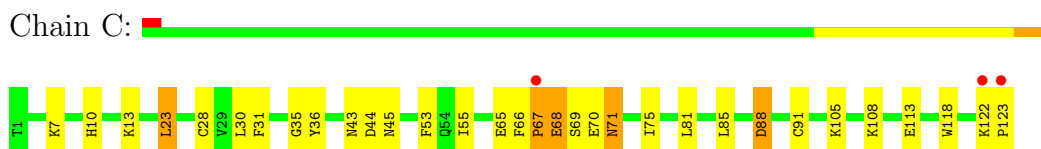
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

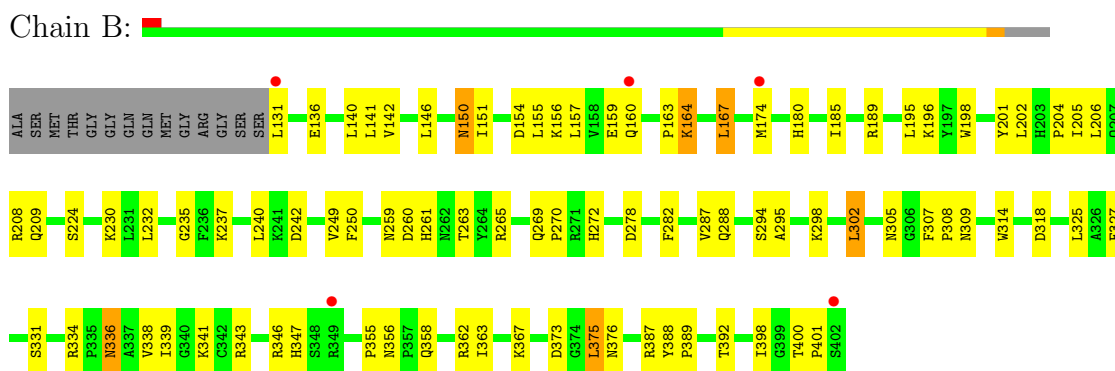
- Molecule 1: Alpha-lactalbumin



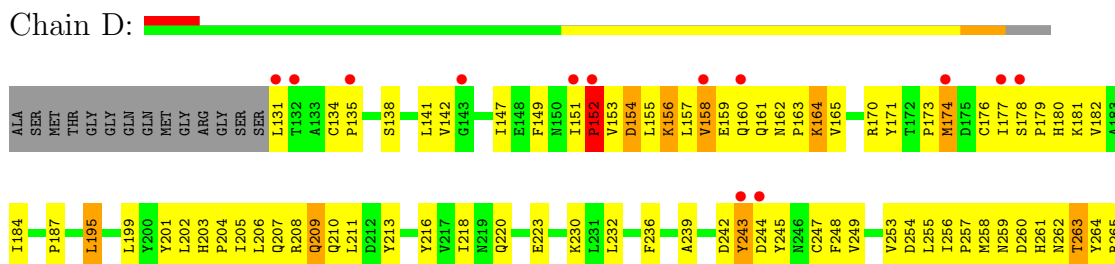
- Molecule 1: Alpha-lactalbumin

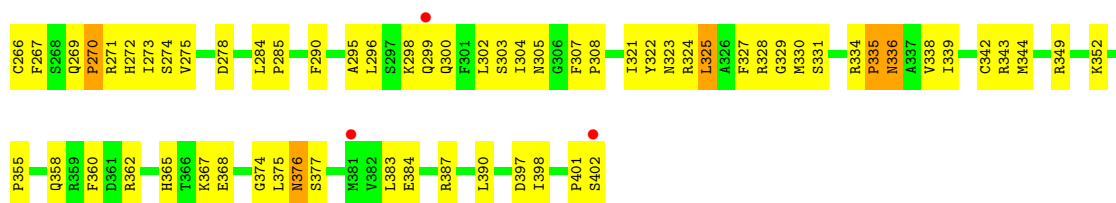


- Molecule 2: beta-1,4-galactosyltransferase



- Molecule 2: beta-1,4-galactosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.20Å 97.11Å 99.70Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	19.72 – 2.32 19.71 – 2.32	Depositor EDS
% Data completeness (in resolution range)	87.8 (19.72-2.32) 87.8 (19.71-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.33Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.277 0.205 , 0.273	Depositor DCC
R_{free} test set	4107 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40644 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7260	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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: CA, BGN

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	0.52	0/1001	0.75	1/1350 (0.1%)
1	C	0.58	0/1001	0.79	0/1350
2	B	0.51	0/2278	0.74	0/3085
2	D	0.48	0/2278	0.73	1/3085 (0.0%)
All	All	0.51	0/6558	0.75	2/8870 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	335	PRO	N-CA-C	-5.75	97.16	112.10
1	A	60	TRP	N-CA-C	5.43	125.67	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	PHE	Sidechain

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	980	0	936	27	0
1	C	980	0	936	31	0
2	B	2218	0	2185	67	0
2	D	2218	0	2185	165	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	17	0	19	2	0
4	D	17	0	19	0	0
5	A	179	0	0	6	0
5	B	274	0	0	4	0
5	C	167	0	0	15	0
5	D	208	0	0	15	0
All	All	7260	0	6280	288	0

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 23.

All (288) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:10:HIS:HA	1:C:13:LYS:HE2	1.48	0.93
2:B:150:ASN:HD22	2:B:151:ILE:H	1.08	0.91
2:D:243:TYR:HD1	2:D:244:ASP:H	1.16	0.90
2:B:155:LEU:O	2:B:159:GLU:HG3	1.73	0.89
2:D:275:VAL:HG21	2:D:335:PRO:HD2	1.53	0.89
2:D:336:ASN:H	2:D:339:ILE:HD11	1.38	0.88
2:D:327:PHE:CE2	2:D:367:LYS:HB2	2.08	0.88
2:D:335:PRO:HB2	2:D:339:ILE:HG13	1.55	0.88
2:B:150:ASN:HD22	2:B:151:ILE:N	1.74	0.85
2:D:160:GLN:O	2:D:163:PRO:HD3	1.78	0.84
2:D:154:ASP:OD1	2:D:156:LYS:HB2	1.79	0.83
2:D:263:THR:HG21	2:D:265:ARG:HD3	1.61	0.81
2:D:323:ASN:O	2:D:327:PHE:HD1	1.64	0.81
1:C:69:SER:HA	5:C:1426:HOH:O	1.79	0.81
2:D:170:ARG:HB3	2:D:170:ARG:NH1	1.96	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:336:ASN:HD22	2:D:338:VAL:H	1.31	0.79
2:D:265:ARG:HA	5:D:997:HOH:O	1.82	0.78
1:C:69:SER:HB2	5:C:903:HOH:O	1.83	0.78
2:B:305:ASN:HD21	2:B:376:ASN:H	1.29	0.78
2:D:209:GLN:HE21	2:D:263:THR:HA	1.48	0.78
1:C:71:ASN:HD21	1:C:75:ILE:H	1.31	0.78
1:A:62:LYS:HE3	1:A:67:PRO:O	1.84	0.77
2:B:150:ASN:ND2	2:B:151:ILE:H	1.82	0.77
2:B:155:LEU:HD11	2:B:196:LYS:HG2	1.65	0.76
2:D:159:GLU:HG2	2:D:390:LEU:HG	1.66	0.75
1:C:68:GLU:HG2	5:C:1725:HOH:O	1.87	0.74
2:D:205:ILE:HG22	2:D:209:GLN:OE1	1.86	0.74
2:D:138:SER:HB3	2:D:141:LEU:HD13	1.69	0.74
2:B:363:ILE:HD13	4:B:403:BGN:H92	1.70	0.72
2:D:272:HIS:HB3	2:D:334:ARG:HG2	1.72	0.70
2:D:131:LEU:HD22	2:D:177:ILE:HD11	1.74	0.70
2:D:164:LYS:HB3	2:D:207:GLN:HE22	1.56	0.69
2:B:272:HIS:HB3	2:B:334:ARG:HG2	1.75	0.69
1:C:7:LYS:HE3	5:C:1689:HOH:O	1.92	0.68
2:D:230:LYS:HD3	2:D:398:ILE:HB	1.74	0.68
2:D:322:TYR:HA	2:D:325:LEU:HD11	1.75	0.68
2:B:327:PHE:CZ	2:B:367:LYS:HB2	2.28	0.68
1:C:31:PHE:HA	5:C:1597:HOH:O	1.94	0.67
2:D:170:ARG:HB3	2:D:170:ARG:HH11	1.60	0.66
2:B:230:LYS:HD3	2:B:398:ILE:HB	1.77	0.66
2:B:150:ASN:ND2	2:B:151:ILE:N	2.41	0.66
2:D:336:ASN:ND2	2:D:338:VAL:H	1.93	0.65
2:D:243:TYR:HD1	2:D:244:ASP:N	1.93	0.65
1:C:66:PHE:HD1	5:C:1725:HOH:O	1.79	0.65
1:C:10:HIS:O	1:C:13:LYS:HG2	1.95	0.65
2:D:263:THR:CG2	2:D:265:ARG:HD3	2.27	0.65
2:D:349:ARG:HD3	5:D:1195:HOH:O	1.96	0.65
2:B:249:VAL:HG22	2:B:295:ALA:HB2	1.79	0.64
2:D:208:ARG:C	2:D:210:GLN:H	2.01	0.64
2:B:150:ASN:ND2	2:B:150:ASN:H	1.96	0.64
2:D:259:ASN:OD1	2:D:261:HIS:HB2	1.98	0.63
2:D:164:LYS:HG2	2:D:171:TYR:CE1	2.34	0.63
2:D:349:ARG:HG2	2:D:349:ARG:HH11	1.64	0.63
2:D:323:ASN:O	2:D:327:PHE:CD1	2.51	0.62
2:D:154:ASP:O	2:D:158:VAL:HG23	1.98	0.62
2:D:321:ILE:O	2:D:325:LEU:HD13	2.00	0.61
2:B:327:PHE:CD2	2:B:367:LYS:HD3	2.35	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:174:MET:CE	2:D:174:MET:H	2.12	0.61
2:D:271:ARG:HB2	5:D:990:HOH:O	2.00	0.61
2:D:274:SER:HA	2:D:342:CYS:SG	2.41	0.61
1:A:71:ASN:HD21	1:A:75:ILE:H	1.48	0.61
2:D:258:MET:HG3	2:D:342:CYS:HA	1.82	0.61
2:D:170:ARG:CB	2:D:170:ARG:HH11	2.14	0.60
2:B:363:ILE:CD1	4:B:403:BGN:H92	2.32	0.60
2:D:184:ILE:HG13	2:D:249:VAL:HB	1.83	0.60
2:D:203:HIS:HB2	2:D:204:PRO:HD3	1.82	0.60
2:D:164:LYS:HG2	2:D:171:TYR:HE1	1.66	0.60
2:B:205:ILE:O	2:B:209:GLN:HG3	2.02	0.60
1:A:78:ASP:HB2	5:A:1082:HOH:O	2.01	0.60
2:D:358:GLN:O	2:D:362:ARG:HG3	2.02	0.60
2:D:272:HIS:CD2	2:D:290:PHE:HA	2.36	0.59
2:B:343:ARG:HH11	2:B:343:ARG:HG2	1.67	0.59
2:D:275:VAL:HG13	2:D:284:LEU:HD13	1.85	0.59
2:D:304:ILE:HB	2:D:324:ARG:HB3	1.84	0.59
2:D:325:LEU:HD13	2:D:325:LEU:H	1.68	0.59
2:D:257:PRO:HD3	2:D:264:TYR:OH	2.01	0.58
2:D:174:MET:H	2:D:174:MET:HE2	1.69	0.58
1:A:12:ILE:O	1:A:15:ILE:HG22	2.02	0.58
2:D:157:LEU:O	2:D:160:GLN:NE2	2.37	0.58
2:D:176:CYS:SG	2:D:210:GLN:OE1	2.62	0.57
2:D:171:TYR:CD2	2:D:207:GLN:HG2	2.38	0.57
2:D:220:GLN:CD	2:D:398:ILE:HD11	2.24	0.57
2:B:278:ASP:HB3	2:B:282:PHE:CE2	2.40	0.57
2:D:295:ALA:C	2:D:296:LEU:HD12	2.25	0.57
2:D:247:CYS:SG	5:D:997:HOH:O	2.58	0.57
2:B:154:ASP:CG	2:B:157:LEU:HD23	2.26	0.56
2:B:180:HIS:CE1	2:B:265:ARG:HD3	2.41	0.56
2:B:150:ASN:HD22	2:B:150:ASN:N	2.04	0.56
2:B:338:VAL:O	2:B:341:LYS:HG3	2.05	0.56
2:D:216:TYR:CE2	2:D:239:ALA:HA	2.41	0.56
2:D:155:LEU:O	2:D:159:GLU:HG3	2.06	0.56
2:B:307:PHE:HB3	2:B:308:PRO:HD2	1.88	0.56
2:D:223:GLU:O	2:D:352:LYS:HE2	2.05	0.56
2:D:182:VAL:HG12	2:D:184:ILE:HD12	1.87	0.56
1:C:69:SER:CB	5:C:903:HOH:O	2.47	0.55
2:D:401:PRO:O	2:D:402:SER:HB3	2.06	0.55
2:D:142:VAL:HG12	5:D:907:HOH:O	2.05	0.55
2:D:275:VAL:CG2	2:D:335:PRO:HD2	2.32	0.55
2:D:208:ARG:O	2:D:210:GLN:N	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:159:GLU:HA	2:D:390:LEU:HD21	1.89	0.55
1:C:122:LYS:HG3	5:C:1603:HOH:O	2.08	0.54
2:D:179:PRO:HG2	2:D:180:HIS:CE1	2.43	0.54
2:D:278:ASP:OD1	2:D:343:ARG:HA	2.09	0.53
2:D:201:TYR:O	2:D:205:ILE:HG13	2.07	0.53
2:D:262:ASN:HB3	5:D:1600:HOH:O	2.09	0.53
2:D:322:TYR:O	2:D:325:LEU:HD22	2.08	0.53
1:A:8:VAL:HG21	1:A:36:TYR:CD1	2.43	0.53
2:D:267:PHE:HB2	5:D:990:HOH:O	2.07	0.53
2:D:179:PRO:HD2	5:D:1358:HOH:O	2.09	0.53
2:B:202:LEU:O	2:B:206:LEU:HG	2.08	0.53
2:B:201:TYR:O	2:B:204:PRO:HD2	2.09	0.53
2:D:298:LYS:O	2:D:302:LEU:HB2	2.10	0.52
1:C:105:LYS:HE3	2:D:360:PHE:CD1	2.45	0.52
2:B:237:LYS:HE2	2:B:375:LEU:HD21	1.90	0.52
2:D:269:GLN:HB3	2:D:331:SER:O	2.09	0.52
2:D:131:LEU:CD2	2:D:177:ILE:HD11	2.40	0.52
2:D:336:ASN:ND2	2:D:339:ILE:HG12	2.25	0.52
2:D:149:PHE:CE2	2:D:256:ILE:HG13	2.45	0.52
1:A:64:SER:O	1:A:67:PRO:HD3	2.10	0.52
2:D:328:ARG:O	2:D:330:MET:N	2.43	0.52
2:B:336:ASN:ND2	2:B:339:ILE:H	2.08	0.52
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.26	0.51
1:A:75:ILE:HD11	1:A:79:LYS:HB3	1.91	0.51
2:D:305:ASN:HD21	2:D:376:ASN:H	1.59	0.51
2:B:230:LYS:NZ	2:B:398:ILE:O	2.39	0.51
1:C:55:ILE:HD13	1:C:91:CYS:SG	2.50	0.51
2:D:152:PRO:HD2	5:D:1118:HOH:O	2.11	0.51
1:C:68:GLU:HG3	5:C:1078:HOH:O	2.10	0.51
2:D:170:ARG:HH21	2:D:243:TYR:HD2	1.58	0.50
2:B:288:GLN:N	2:B:288:GLN:OE1	2.42	0.50
1:C:10:HIS:HB2	5:C:1043:HOH:O	2.12	0.50
2:D:349:ARG:NH1	2:D:349:ARG:HG2	2.26	0.50
2:B:270:PRO:HG2	2:B:325:LEU:HD22	1.93	0.50
2:D:263:THR:HB	2:D:265:ARG:HG2	1.92	0.50
2:D:171:TYR:CD1	2:D:207:GLN:NE2	2.78	0.50
2:D:149:PHE:HE2	2:D:256:ILE:HG13	1.76	0.50
2:D:202:LEU:O	2:D:206:LEU:HG	2.11	0.50
2:B:347:HIS:HE1	5:B:1411:HOH:O	1.94	0.50
2:D:253:VAL:HG22	2:D:253:VAL:O	2.12	0.50
1:A:24:LEU:HG	5:A:1621:HOH:O	2.11	0.50
1:A:44:ASP:O	1:A:45:ASN:HB3	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:307:PHE:HB3	2:D:308:PRO:HD2	1.93	0.49
1:A:21:ILE:HD13	1:A:21:ILE:N	2.27	0.49
2:D:349:ARG:NH1	5:D:1270:HOH:O	2.45	0.49
2:D:218:ILE:HD13	2:D:218:ILE:N	2.28	0.49
2:D:327:PHE:CD2	2:D:367:LYS:HD3	2.47	0.49
2:B:198:TRP:CZ2	2:B:202:LEU:HG	2.47	0.49
1:C:105:LYS:HE2	5:C:1294:HOH:O	2.12	0.49
2:B:259:ASN:OD1	2:B:261:HIS:HB2	2.13	0.49
2:D:383:LEU:HD11	2:D:397:ASP:HB2	1.94	0.49
2:D:254:ASP:O	2:D:344:MET:HA	2.13	0.49
2:D:266:CYS:C	2:D:267:PHE:CD1	2.86	0.48
2:D:295:ALA:O	2:D:296:LEU:HD12	2.12	0.48
2:B:140:LEU:HB2	2:B:208:ARG:HG2	1.94	0.48
2:D:180:HIS:CB	2:D:211:LEU:HD22	2.43	0.48
2:B:298:LYS:HG2	2:B:302:LEU:HD22	1.94	0.48
2:B:150:ASN:N	2:B:150:ASN:ND2	2.57	0.48
1:C:13:LYS:HD3	1:C:23:LEU:HD11	1.95	0.48
2:D:134:CYS:HB3	2:D:135:PRO:HD2	1.94	0.48
2:D:181:LYS:O	2:D:245:TYR:HB3	2.14	0.48
1:A:70:GLU:N	1:A:70:GLU:OE2	2.47	0.48
2:D:327:PHE:HD2	2:D:367:LYS:HD3	1.79	0.48
1:A:114:LYS:HE2	5:B:1633:HOH:O	2.13	0.48
2:B:358:GLN:OE1	2:B:362:ARG:NH1	2.47	0.48
2:D:160:GLN:NE2	2:D:161:GLN:HG3	2.29	0.48
1:C:44:ASP:HA	5:C:1614:HOH:O	2.12	0.47
2:D:159:GLU:HG2	2:D:390:LEU:CG	2.38	0.47
2:B:338:VAL:HG23	1:C:81:LEU:HD13	1.95	0.47
2:D:138:SER:CB	2:D:210:GLN:HE21	2.28	0.47
2:D:307:PHE:O	2:D:374:GLY:HA2	2.14	0.47
2:B:327:PHE:CE2	2:B:367:LYS:HD3	2.49	0.47
2:D:170:ARG:CA	2:D:170:ARG:HH11	2.28	0.47
2:B:174:MET:HE3	5:B:1441:HOH:O	2.15	0.46
2:B:388:TYR:HB3	2:B:389:PRO:HD2	1.96	0.46
2:B:309:ASN:HB2	2:B:373:ASP:OD1	2.15	0.46
2:D:173:PRO:HG2	2:D:178:SER:HB2	1.97	0.46
2:D:375:LEU:C	2:D:377:SER:H	2.18	0.46
2:D:195:LEU:HD22	2:D:199:LEU:CD1	2.46	0.46
2:D:147:ILE:HB	2:D:343:ARG:HD2	1.98	0.46
2:B:167:LEU:HD22	2:B:387:ARG:HB3	1.98	0.46
2:B:146:LEU:HD12	5:B:1443:HOH:O	2.15	0.46
2:D:205:ILE:HG23	2:D:260:ASP:HB3	1.98	0.46
2:D:171:TYR:OH	2:D:173:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:160:GLN:O	2:B:163:PRO:HD3	2.15	0.46
2:D:328:ARG:O	2:D:330:MET:HE3	2.16	0.46
2:D:262:ASN:ND2	2:D:273:ILE:HG23	2.31	0.45
2:B:198:TRP:O	2:B:202:LEU:HB2	2.16	0.45
2:B:224:SER:OG	2:B:400:THR:HG22	2.17	0.45
2:B:185:ILE:HG21	2:B:235:GLY:HA3	1.99	0.45
2:B:336:ASN:HD22	2:B:336:ASN:C	2.19	0.45
1:C:108:LYS:HB3	1:C:108:LYS:HE2	1.87	0.45
2:B:343:ARG:HG2	2:B:343:ARG:NH1	2.30	0.45
2:D:352:LYS:HE3	2:D:352:LYS:HA	1.98	0.45
2:B:140:LEU:O	2:B:208:ARG:HD3	2.16	0.45
2:B:167:LEU:HA	2:B:389:PRO:HA	1.99	0.45
2:B:318:ASP:OD1	2:B:318:ASP:N	2.46	0.45
2:D:270:PRO:HD3	2:D:300:GLN:NE2	2.32	0.45
1:A:75:ILE:HD12	1:A:87:ASP:HB2	1.99	0.45
2:D:358:GLN:OE1	2:D:362:ARG:NH1	2.50	0.44
2:D:157:LEU:O	2:D:161:GLN:HG3	2.16	0.44
2:D:138:SER:HB3	2:D:141:LEU:CD1	2.42	0.44
2:D:259:ASN:C	2:D:261:HIS:H	2.20	0.44
1:C:122:LYS:HA	1:C:123:PRO:HD3	1.53	0.44
1:A:114:LYS:O	1:A:117:GLN:HG2	2.17	0.44
2:B:269:GLN:HB3	2:B:331:SER:O	2.17	0.44
1:C:43:ASN:HB3	5:C:1103:HOH:O	2.18	0.44
2:D:236:PHE:HE1	2:D:248:PHE:CE2	2.36	0.44
2:D:180:HIS:HB2	2:D:211:LEU:HD22	2.00	0.44
2:D:207:GLN:O	2:D:210:GLN:N	2.50	0.44
1:C:31:PHE:HB2	1:C:36:TYR:CZ	2.53	0.44
2:D:335:PRO:HB2	2:D:339:ILE:CG1	2.37	0.43
2:D:255:LEU:CD2	2:D:344:MET:HB2	2.48	0.43
1:C:88:ASP:OD2	1:C:88:ASP:N	2.50	0.43
2:D:202:LEU:HB3	2:D:206:LEU:HD11	2.01	0.43
2:D:157:LEU:O	2:D:158:VAL:C	2.56	0.43
2:D:269:GLN:O	2:D:270:PRO:C	2.54	0.43
1:A:28:CYS:HB2	1:A:118:TRP:CD1	2.53	0.43
1:C:70:GLU:O	1:C:71:ASN:C	2.55	0.43
1:C:68:GLU:N	5:C:1725:HOH:O	2.52	0.43
2:D:375:LEU:O	2:D:377:SER:N	2.52	0.43
1:A:46:GLY:HA2	5:A:1221:HOH:O	2.18	0.43
2:B:150:ASN:HD22	2:B:150:ASN:H	1.60	0.43
2:B:232:LEU:HD22	2:B:250:PHE:HD2	1.82	0.43
2:D:187:PRO:HD3	2:D:232:LEU:CD2	2.48	0.43
2:D:242:ASP:OD2	2:D:387:ARG:NH1	2.41	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:299:GLN:OE1	2:D:299:GLN:HA	2.19	0.43
1:C:35:GLY:HA2	5:C:1597:HOH:O	2.18	0.43
2:D:208:ARG:C	2:D:210:GLN:N	2.68	0.43
2:D:162:ASN:O	2:D:165:VAL:HB	2.19	0.43
2:D:209:GLN:NE2	2:D:263:THR:HA	2.26	0.43
2:D:258:MET:HE1	2:D:343:ARG:CZ	2.49	0.43
2:D:285:PRO:HA	5:D:1311:HOH:O	2.19	0.43
1:C:28:CYS:HB2	1:C:118:TRP:CD1	2.53	0.43
2:B:249:VAL:HA	2:B:294:SER:O	2.19	0.42
2:B:356:ASN:OD1	2:B:356:ASN:C	2.58	0.42
2:D:151:ILE:HG22	2:D:151:ILE:O	2.18	0.42
2:D:182:VAL:HG12	2:D:184:ILE:CD1	2.48	0.42
2:D:271:ARG:HD3	5:D:990:HOH:O	2.18	0.42
1:A:116:GLU:OE1	1:A:119:ARG:NH2	2.52	0.42
2:D:182:VAL:O	2:D:213:TYR:HA	2.20	0.42
2:D:156:LYS:O	2:D:157:LEU:C	2.57	0.42
2:D:275:VAL:HG21	2:D:334:ARG:HB3	2.01	0.42
2:D:184:ILE:HD12	2:D:184:ILE:N	2.35	0.42
1:A:108:LYS:HB3	1:A:109:PRO:HD3	2.01	0.42
1:C:31:PHE:C	1:C:31:PHE:CD2	2.93	0.42
2:B:156:LYS:HD3	2:B:156:LYS:HA	1.90	0.42
2:D:182:VAL:HG22	2:D:247:CYS:HB3	2.01	0.42
2:D:207:GLN:O	2:D:208:ARG:C	2.57	0.42
2:D:202:LEU:HD13	2:D:202:LEU:HA	1.85	0.42
1:A:93:LYS:HD2	5:A:1433:HOH:O	2.18	0.42
1:A:61:CYS:HA	1:A:71:ASN:ND2	2.35	0.42
2:B:142:VAL:HG22	2:B:260:ASP:OD1	2.20	0.42
2:D:209:GLN:HB3	5:D:1430:HOH:O	2.20	0.41
2:B:164:LYS:HD2	2:B:174:MET:CE	2.50	0.41
2:D:195:LEU:HD22	2:D:199:LEU:HD11	2.00	0.41
2:D:384:GLU:HG2	5:D:916:HOH:O	2.19	0.41
2:B:387:ARG:HD3	2:B:392:THR:HG23	2.01	0.41
1:A:60:TRP:O	1:A:73:CYS:HB2	2.20	0.41
2:D:275:VAL:HG22	2:D:334:ARG:HD3	2.02	0.41
2:D:153:VAL:HG12	2:D:154:ASP:N	2.35	0.41
2:D:336:ASN:HD22	2:D:336:ASN:C	2.24	0.41
2:D:154:ASP:OD1	2:D:157:LEU:HD22	2.21	0.41
2:D:216:TYR:CD1	2:D:216:TYR:N	2.87	0.41
2:D:202:LEU:N	2:D:202:LEU:HD22	2.35	0.41
2:D:365:HIS:O	2:D:368:GLU:HG2	2.20	0.41
2:D:157:LEU:O	2:D:159:GLU:N	2.53	0.41
2:D:181:LYS:HB3	2:D:245:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:30:LEU:HD21	1:C:53:PHE:CD1	2.56	0.41
2:D:401:PRO:O	2:D:402:SER:CB	2.69	0.41
2:B:298:LYS:O	2:B:302:LEU:HB2	2.20	0.41
2:D:334:ARG:HB3	2:D:335:PRO:HD2	2.02	0.41
2:D:153:VAL:HA	5:D:1552:HOH:O	2.21	0.41
1:A:45:ASN:O	1:A:45:ASN:ND2	2.54	0.41
2:B:327:PHE:CE1	2:B:367:LYS:HB2	2.54	0.41
1:A:11:ALA:HB2	5:A:1286:HOH:O	2.20	0.41
1:C:75:ILE:HG23	1:C:75:ILE:O	2.20	0.40
1:A:94:LYS:HE3	5:A:1171:HOH:O	2.21	0.40
2:D:170:ARG:NH1	2:D:213:TYR:O	2.54	0.40
2:D:135:PRO:CG	2:D:210:GLN:HE22	2.34	0.40
2:D:202:LEU:O	2:D:206:LEU:CG	2.69	0.40
2:B:314:TRP:HB3	2:B:355:PRO:HA	2.01	0.40
2:D:243:TYR:CD1	2:D:244:ASP:N	2.78	0.40
2:D:322:TYR:HA	2:D:325:LEU:CD1	2.46	0.40
2:D:203:HIS:CB	2:D:204:PRO:HD3	2.48	0.40
2:B:154:ASP:O	2:B:157:LEU:HB2	2.22	0.40
2:B:198:TRP:CE2	2:B:202:LEU:HG	2.56	0.40
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.90	0.40
1:A:76:SER:O	1:A:79:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

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	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	27	30
1	C	121/123 (98%)	113 (93%)	6 (5%)	2 (2%)	14	11
2	B	270/286 (94%)	256 (95%)	13 (5%)	1 (0%)	43	52
2	D	270/286 (94%)	234 (87%)	30 (11%)	6 (2%)	10	7
All	All	782/818 (96%)	715 (91%)	57 (7%)	10 (1%)	18	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	156	LYS
1	C	67	PRO
2	D	209	GLN
2	D	329	GLY
2	D	376	ASN
1	A	67	PRO
1	C	68	GLU
2	D	152	PRO
2	B	401	PRO
2	D	158	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	109/109 (100%)	104 (95%)	5 (5%)	37	48	
1	C	109/109 (100%)	101 (93%)	8 (7%)	20	24	
2	B	245/254 (96%)	229 (94%)	16 (6%)	24	30	
2	D	245/254 (96%)	233 (95%)	12 (5%)	35	46	
All	All	708/726 (98%)	667 (94%)	41 (6%)	28	36	

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	45	ASN
1	A	65	GLU
1	A	85	LEU
1	A	113	GLU
2	B	131	LEU
2	B	136	GLU
2	B	141	LEU
2	B	150	ASN
2	B	164	LYS
2	B	167	LEU

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Mol	Chain	Res	Type
2	B	189	ARG
2	B	195	LEU
2	B	240	LEU
2	B	242	ASP
2	B	263	THR
2	B	287	VAL
2	B	302	LEU
2	B	336	ASN
2	B	346	ARG
2	B	375	LEU
1	C	23	LEU
1	C	45	ASN
1	C	65	GLU
1	C	67	PRO
1	C	71	ASN
1	C	85	LEU
1	C	88	ASP
1	C	113	GLU
2	D	152	PRO
2	D	154	ASP
2	D	164	LYS
2	D	174	MET
2	D	195	LEU
2	D	243	TYR
2	D	263	THR
2	D	270	PRO
2	D	303	SER
2	D	325	LEU
2	D	336	ASN
2	D	355	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	45	ASN
1	A	54	GLN
1	A	71	ASN
2	B	150	ASN
2	B	160	GLN
2	B	161	GLN
2	B	180	HIS

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Mol	Chain	Res	Type
2	B	207	GLN
2	B	210	GLN
2	B	219	ASN
2	B	305	ASN
2	B	336	ASN
1	C	32	HIS
1	C	45	ASN
1	C	71	ASN
2	D	150	ASN
2	D	160	GLN
2	D	161	GLN
2	D	162	ASN
2	D	180	HIS
2	D	209	GLN
2	D	210	GLN
2	D	305	ASN
2	D	310	ASN
2	D	336	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BGN	B	403	-	17,17,17	0.64	0	23,23,23	0.90	1 (4%)
4	BGN	D	527	-	17,17,17	1.13	3 (17%)	23,23,23	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGN	B	403	-	-	0/9/29/29	0/1/1/1
4	BGN	D	527	-	-	0/9/29/29	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	527	BGN	C2-N2	2.42	1.50	1.45
4	D	527	BGN	C4-C5	2.35	1.58	1.53
4	D	527	BGN	O5-C1	-2.32	1.38	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	BGN	C9-C8-C7	-2.58	107.76	113.41

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	123/123 (100%)	-0.31	3 (2%) 56 67	12, 31, 55, 79	0
1	C	123/123 (100%)	-0.35	3 (2%) 56 67	18, 29, 56, 84	0
2	B	272/286 (95%)	-0.20	5 (1%) 65 75	17, 36, 64, 74	0
2	D	272/286 (95%)	0.35	16 (5%) 22 31	19, 48, 78, 85	0
All	All	790/818 (96%)	-0.05	27 (3%) 43 53	12, 37, 68, 85	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	131	LEU	6.6
2	D	402	SER	5.8
1	C	123	PRO	4.9
2	D	132	THR	4.0
2	B	131	LEU	3.9
2	B	402	SER	3.8
1	A	66	PHE	3.6
2	D	177	ILE	3.4
1	C	67	PRO	3.0
2	D	174	MET	2.9
2	B	349	ARG	2.9
2	D	243	TYR	2.9
2	B	174	MET	2.8
2	D	135	PRO	2.6
2	D	143	GLY	2.5
2	D	299	GLN	2.5
2	D	151	ILE	2.4
2	B	160	GLN	2.4
1	A	67	PRO	2.4
2	D	158	VAL	2.3
1	A	65	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	122	LYS	2.3
2	D	152	PRO	2.3
2	D	244	ASP	2.1
2	D	160	GLN	2.0
2	D	381	MET	2.0
2	D	178	SER	2.0

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
4	BGN	D	527	17/17	0.11	0.21	19,22,24,28	0
4	BGN	B	403	17/17	0.09	0.09	20,24,29,30	0
3	CA	A	124	1/1	0.10	0.02	27,27,27,27	0
3	CA	C	526	1/1	0.05	-2.52	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.