



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:44 pm GMT

PDB ID : 1ABR  
Title : CRYSTAL STRUCTURE OF ABRIN-A  
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Deposited on : 1994-11-11  
Resolution : 2.14 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

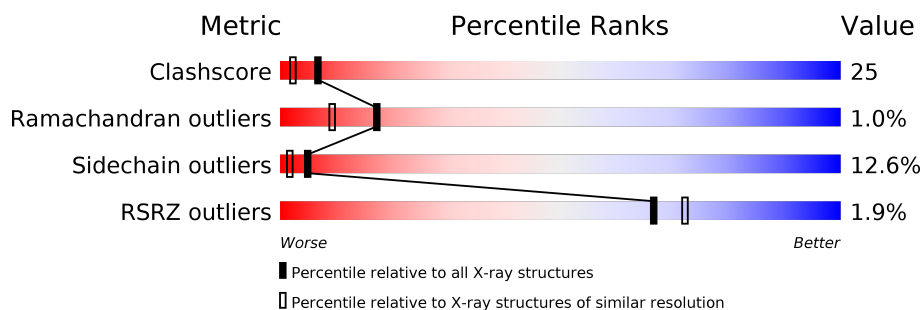
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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))
Clashscore	122126	2253 (2.16-2.12)
Ramachandran outliers	120053	2223 (2.16-2.12)
Sidechain outliers	120020	2222 (2.16-2.12)
RSRZ outliers	108989	2086 (2.16-2.12)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	251	<div> <div>2%</div> <div>53%</div> <div>38%</div> <div>10%</div> </div>
2	B	267	<div> <div>60%</div> <div>33%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDG	B	273(D)	-	-	X	-
3	NDG	B	274(D)	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	B	270(C)	X	-	-	-
5	MAN	B	276(D)	-	-	-	X
7	BGC	B	275(D)	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5798 atoms, of which 1387 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.

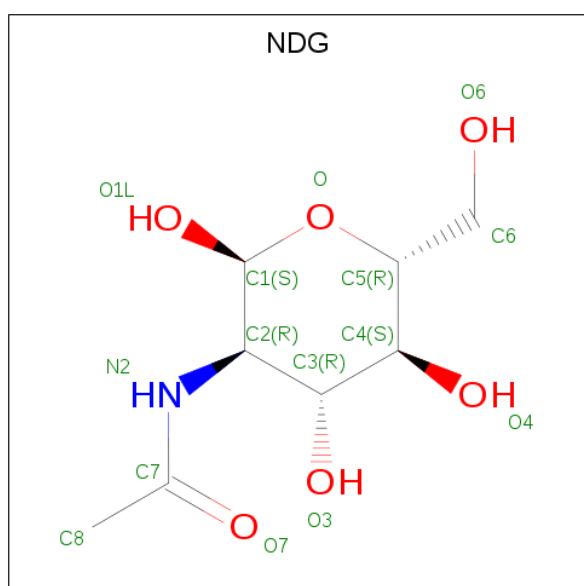
- Molecule 1 is a protein called ABRIN-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	H	N	O	S	0	0	0
			2441	1242	458	349	388	4			

- Molecule 2 is a protein called ABRIN-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	267	Total	C	H	N	O	S	0	0	0
			2603	1317	497	358	412	19			

- Molecule 3 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



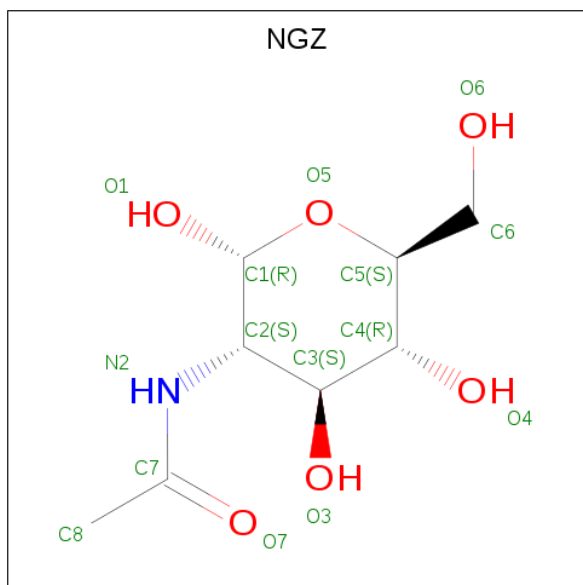
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O		0	0
			17	8	3	1	5			
3	B	1	Total	C	H	N	O		0	0
			17	8	3	1	5			

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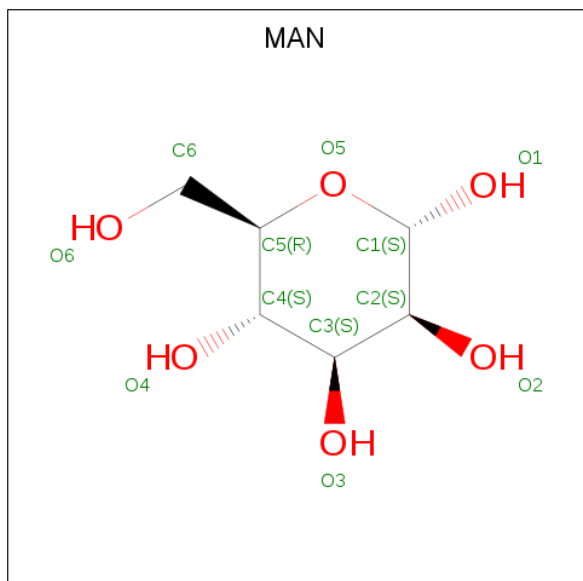
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	B	1	17	8	3	1	5	0	0

- Molecule 4 is 2-(ACETYLAMINO)-2-DEOXY-ALPHA-L-GLUCOPYRANOSE (three-letter code: NGZ) (formula:  $C_8H_{15}NO_6$ ).



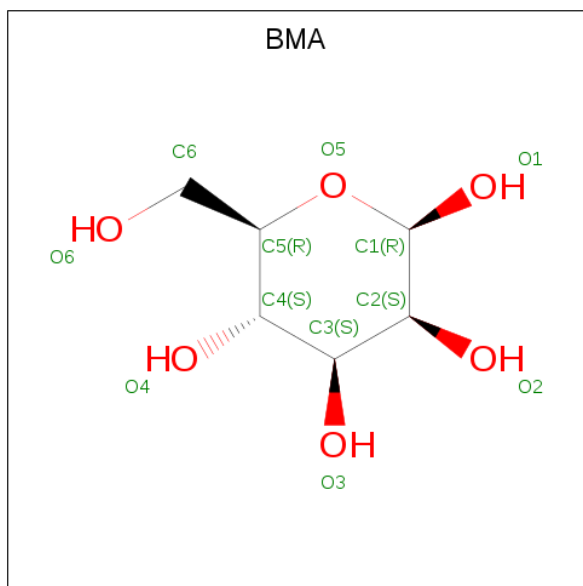
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	B	1	17	8	3	1	5	0	0

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



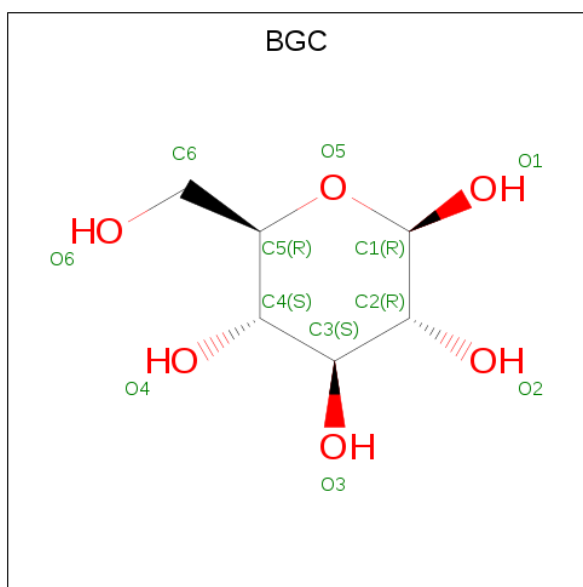
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			13	6	2	5		
5	B	1	Total	C	H	O	0	0
			15	6	4	5		
5	B	1	Total	C	H	O	0	0
			15	6	4	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			15	6	4	5		
6	B	1	Total	C	H	O	0	0
			15	6	4	5		

- Molecule 7 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			13	6	2	5		

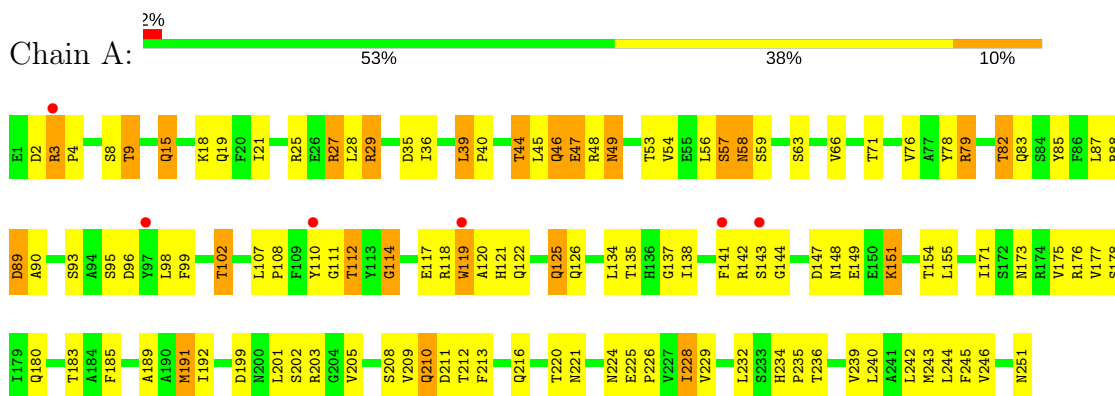
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	80	Total	H	O	0	0
			240	160	80		
8	B	120	Total	H	O	0	0
			360	240	120		

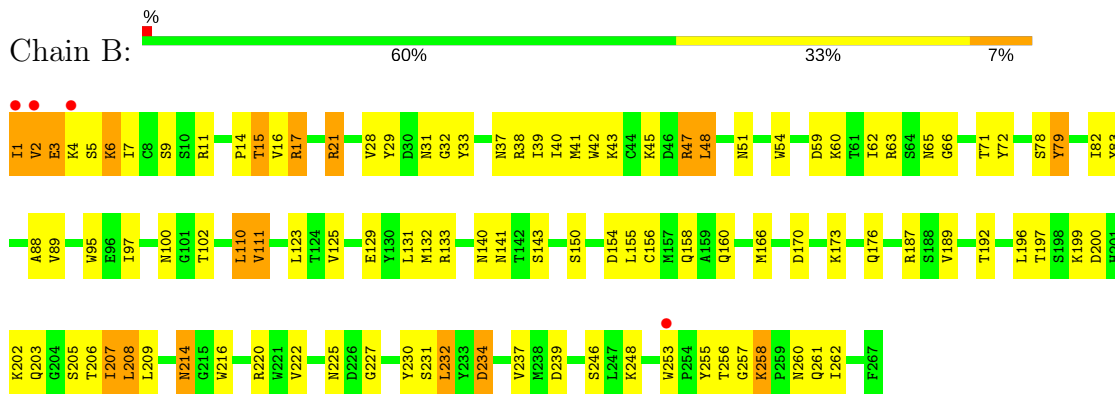
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ABRIN-A



#### • Molecule 2: ABRIN-A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.58Å 73.07Å 48.23Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.14 84.09 – 2.11	Depositor EDS
% Data completeness (in resolution range)	77.4 (10.00-2.14) 82.4 (84.09-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.10Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.189 , (Not available) 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 115.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, BMA, NGZ, NDG, MAN

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	0.59	0/2024	0.82	1/2755 (0.0%)
2	B	0.60	0/2153	0.85	2/2918 (0.1%)
All	All	0.60	0/4177	0.83	3/5673 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	234	ASP	N-CA-C	-5.94	94.96	111.00
2	B	17	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	114	GLY	N-CA-C	-5.13	100.28	113.10

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	1983	458	1932	120	0
2	B	2106	497	2025	92	2
3	B	42	9	36	20	0
4	B	14	3	12	0	0
5	B	33	10	28	2	0
6	B	22	8	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	11	2	8	0	0
8	A	80	160	0	4	0
8	B	120	240	0	5	2
All	All	4411	1387	4061	207	2

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 25.

All (207) 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)
2:B:48:LEU:HD23	3:B:274(D):NDG:H3	1.50	0.94
1:A:47:GLU:HG3	1:A:93:SER:HB2	1.49	0.91
1:A:147:ASP:HA	8:A:324:HOH:O	1.72	0.90
1:A:36:ILE:HB	8:A:329:HOH:O	1.77	0.84
1:A:243:MET:SD	8:A:329:HOH:O	2.35	0.84
1:A:216:GLN:HB3	1:A:228:ILE:HD13	1.60	0.83
2:B:41:MET:HG2	2:B:123:LEU:HD21	1.62	0.80
1:A:18:LYS:HD3	1:A:176:ARG:HD2	1.64	0.79
2:B:170:ASP:H	2:B:176:GLN:HE22	1.30	0.79
1:A:118:ARG:HD2	1:A:119:TRP:HZ3	1.51	0.74
1:A:151:LYS:NZ	1:A:151:LYS:HB2	2.03	0.73
2:B:100:ASN:ND2	3:B:268(C):NDG:C1	2.51	0.73
1:A:39:LEU:HD13	1:A:242:LEU:HD22	1.72	0.72
1:A:87:LEU:HB3	1:A:110:TYR:HD1	1.57	0.69
1:A:228:ILE:HD12	1:A:229:VAL:N	2.08	0.69
1:A:118:ARG:HB3	1:A:119:TRP:HE3	1.58	0.67
2:B:47:ARG:HB2	5:B:276(D):MAN:O3	1.96	0.66
1:A:78:TYR:OH	1:A:151:LYS:HE3	1.95	0.66
2:B:48:LEU:HD23	3:B:274(D):NDG:C3	2.25	0.66
1:A:118:ARG:HB3	1:A:119:TRP:CE3	2.32	0.65
1:A:245:PHE:HE2	2:B:6:LYS:HZ2	1.45	0.64
1:A:202:SER:HA	1:A:243:MET:HE2	1.80	0.64
1:A:28:LEU:O	1:A:40:PRO:HD3	1.97	0.64
1:A:216:GLN:HB3	1:A:228:ILE:CD1	2.27	0.63
1:A:220:THR:HG23	1:A:224:ASN:HA	1.81	0.63
1:A:15:GLN:HE21	1:A:15:GLN:HA	1.63	0.62
2:B:45:LYS:HB3	2:B:47:ARG:NH2	2.14	0.62
1:A:211:ASP:OD1	1:A:232:LEU:HB2	2.00	0.61
1:A:3:ARG:HH21	1:A:27:ARG:HH22	1.49	0.61
2:B:140:ASN:HD21	3:B:274(D):NDG:C1	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:HE	1:A:27:ARG:HH12	1.47	0.61
2:B:43:LYS:NZ	2:B:43:LYS:HB3	2.16	0.61
2:B:170:ASP:HB3	2:B:173:LYS:HD2	1.83	0.60
2:B:32:GLY:O	2:B:37:ASN:ND2	2.34	0.60
2:B:9:SER:OG	2:B:11:ARG:HG2	2.01	0.60
1:A:39:LEU:CD1	1:A:242:LEU:HD22	2.32	0.60
2:B:158:GLN:OE1	2:B:173:LYS:HD3	2.01	0.60
1:A:46:GLN:CG	1:A:48:ARG:HG2	2.32	0.60
1:A:199:ASP:O	1:A:203:ARG:HG3	2.01	0.59
1:A:118:ARG:HD2	1:A:119:TRP:CZ3	2.36	0.59
1:A:99:PHE:O	1:A:102:THR:HB	2.02	0.59
1:A:57:SER:HA	1:A:63:SER:HB3	1.83	0.59
2:B:15:THR:H	3:B:273(D):NDG:HA	1.50	0.59
2:B:2:VAL:HG22	2:B:3:GLU:H	1.67	0.59
2:B:231:SER:O	2:B:234:ASP:O	2.20	0.59
1:A:87:LEU:HD13	1:A:111:GLY:N	2.18	0.58
1:A:240:LEU:O	2:B:225:ASN:ND2	2.35	0.58
2:B:199:LYS:HE3	2:B:206:THR:H	1.66	0.58
1:A:88:ARG:HE	1:A:108:PRO:HA	1.67	0.58
1:A:216:GLN:HG3	3:B:273(D):NDG:H6C2	1.85	0.58
1:A:3:ARG:NH2	1:A:27:ARG:HH22	2.00	0.58
1:A:234:HIS:CE1	1:A:236:THR:HG23	2.39	0.57
1:A:171:ILE:O	1:A:175:VAL:HG23	2.04	0.57
1:A:208:SER:HA	1:A:212:THR:O	2.04	0.57
1:A:46:GLN:HG3	1:A:48:ARG:HG2	1.84	0.57
1:A:44:THR:HG23	2:B:1:ILE:N	2.20	0.57
1:A:235:PRO:CG	8:B:364:HOH:O	2.53	0.56
1:A:151:LYS:HZ3	1:A:151:LYS:HB2	1.69	0.56
2:B:48:LEU:CD2	3:B:274(D):NDG:H3	2.31	0.56
1:A:210:GLN:NE2	2:B:97:ILE:H	2.04	0.56
2:B:1:ILE:HD13	2:B:2:VAL:N	2.21	0.56
2:B:140:ASN:ND2	3:B:273(D):NDG:O4	2.39	0.56
1:A:236:THR:O	1:A:239:VAL:HG22	2.06	0.56
2:B:48:LEU:O	5:B:276(D):MAN:H2	2.05	0.55
1:A:58:ASN:HD21	1:A:135:THR:HA	1.71	0.55
1:A:245:PHE:HE2	2:B:6:LYS:NZ	2.05	0.55
1:A:220:THR:CG2	1:A:224:ASN:HA	2.37	0.54
2:B:17:ARG:NH2	2:B:45:LYS:O	2.41	0.54
2:B:100:ASN:ND2	3:B:268(C):NDG:O	2.35	0.54
1:A:44:THR:OG1	2:B:1:ILE:HA	2.08	0.54
1:A:44:THR:HG23	2:B:1:ILE:H2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:TYR:CD1	2:B:88:ALA:HB2	2.43	0.53
1:A:29:ARG:HD2	1:A:29:ARG:O	2.09	0.53
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.73	0.53
2:B:214:ASN:HB2	2:B:216:TRP:NE1	2.24	0.53
2:B:256:THR:OG1	2:B:258:LYS:HG3	2.06	0.53
2:B:33:TYR:OH	2:B:51:ASN:HA	2.09	0.53
2:B:232:LEU:HD12	3:B:268(C):NDG:O7	2.09	0.53
1:A:185:PHE:HE2	1:A:191:MET:HE1	1.73	0.53
1:A:79:ARG:NH1	1:A:79:ARG:HG3	2.23	0.53
2:B:16:VAL:HA	2:B:140:ASN:OD1	2.09	0.52
1:A:201:LEU:O	1:A:205:VAL:HG23	2.09	0.52
2:B:1:ILE:HD13	2:B:2:VAL:H	1.74	0.52
1:A:76:VAL:HB	1:A:90:ALA:HB1	1.92	0.52
1:A:176:ARG:CZ	1:A:176:ARG:HB3	2.39	0.51
2:B:199:LYS:HG3	2:B:200:ASP:N	2.25	0.51
1:A:110:TYR:HB3	1:A:112:THR:HG22	1.91	0.51
1:A:142:ARG:O	1:A:144:GLY:N	2.44	0.51
1:A:235:PRO:HG2	8:B:364:HOH:O	2.09	0.51
1:A:234:HIS:HE1	1:A:236:THR:HG23	1.76	0.50
1:A:114:GLY:O	1:A:118:ARG:HB2	2.12	0.50
2:B:140:ASN:ND2	3:B:274(D):NDG:C1	2.75	0.50
2:B:141:ASN:HD21	2:B:143:SER:HB2	1.77	0.50
1:A:141:PHE:CE1	1:A:151:LYS:HG3	2.46	0.50
3:B:274(D):NDG:O3	6:B:277(D):BMA:H5	2.12	0.50
2:B:42:TRP:CG	2:B:43:LYS:N	2.79	0.50
2:B:200:ASP:HB2	2:B:205:SER:OG	2.12	0.49
1:A:213:PHE:N	1:A:213:PHE:CD1	2.80	0.49
1:A:47:GLU:HG3	1:A:93:SER:CB	2.33	0.49
2:B:222:VAL:HG13	2:B:230:TYR:HB3	1.93	0.49
1:A:125:GLN:HG3	1:A:192:ILE:CD1	2.42	0.49
1:A:57:SER:HA	1:A:63:SER:CB	2.42	0.49
1:A:9:THR:HB	1:A:58:ASN:HD22	1.78	0.49
1:A:54:VAL:HB	1:A:66:VAL:HG22	1.92	0.49
1:A:209:VAL:HG23	1:A:210:GLN:H	1.77	0.49
1:A:202:SER:HA	1:A:243:MET:CE	2.41	0.49
1:A:178:SER:HB2	1:A:183:THR:O	2.13	0.48
2:B:21:ARG:HH21	2:B:133:ARG:HD2	1.78	0.48
2:B:129:GLU:HB2	2:B:131:LEU:HG	1.94	0.48
1:A:44:THR:HA	2:B:2:VAL:HG12	1.94	0.48
2:B:78:SER:O	2:B:125:VAL:HG22	2.12	0.48
2:B:197:THR:O	2:B:207:ILE:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:HB2	1:A:110:TYR:CG	2.49	0.48
2:B:15:THR:HA	2:B:54:TRP:O	2.14	0.48
1:A:120:ALA:C	1:A:122:GLN:H	2.18	0.47
2:B:63:ARG:HD3	2:B:66:GLY:O	2.15	0.47
2:B:45:LYS:HB3	2:B:47:ARG:HH21	1.79	0.47
3:B:268(C):NDG:H8C1	3:B:268(C):NDG:H2	1.57	0.47
1:A:180:GLN:HG2	8:B:372:HOH:O	2.15	0.47
1:A:87:LEU:HD13	1:A:111:GLY:CA	2.45	0.47
1:A:216:GLN:CG	3:B:273(D):NDG:H6C2	2.44	0.47
1:A:2:ASP:H	1:A:27:ARG:HH11	1.62	0.47
1:A:29:ARG:HD2	1:A:29:ARG:C	2.35	0.47
2:B:202:LYS:HG2	2:B:203:GLN:N	2.30	0.47
2:B:258:LYS:HB2	2:B:260:ASN:OD1	2.15	0.47
1:A:176:ARG:NH1	1:A:176:ARG:HB3	2.30	0.46
1:A:173:ASN:O	1:A:177:VAL:HG23	2.15	0.46
2:B:110:LEU:HB3	2:B:125:VAL:HB	1.97	0.46
2:B:2:VAL:HG22	2:B:3:GLU:N	2.29	0.46
2:B:72:TYR:CD1	2:B:79:TYR:HE1	2.34	0.46
1:A:117:GLU:O	1:A:120:ALA:O	2.34	0.46
1:A:122:GLN:HA	1:A:126:GLN:OE1	2.16	0.46
1:A:216:GLN:HG3	3:B:273(D):NDG:C6	2.46	0.46
2:B:29:TYR:HD1	2:B:40:ILE:HD13	1.80	0.46
1:A:56:LEU:O	1:A:138:ILE:HD13	2.16	0.46
1:A:3:ARG:N	1:A:4:PRO:CD	2.80	0.45
2:B:28:VAL:HG22	2:B:39:ILE:HD12	1.98	0.45
2:B:89:VAL:HG13	8:B:339:HOH:O	2.15	0.45
1:A:134:LEU:O	1:A:138:ILE:HG13	2.16	0.45
1:A:82:THR:O	1:A:83:GLN:HG2	2.17	0.45
2:B:62:ILE:CD1	2:B:95:TRP:HB2	2.47	0.45
2:B:239:ASP:OD1	2:B:253:TRP:CE3	2.70	0.45
3:B:273(D):NDG:H8C1	3:B:273(D):NDG:H2	1.80	0.45
1:A:141:PHE:HE1	1:A:151:LYS:HA	1.82	0.45
1:A:21:ILE:O	1:A:25:ARG:HG3	2.17	0.45
2:B:39:ILE:HD11	2:B:82:ILE:HB	1.99	0.45
1:A:54:VAL:HB	1:A:66:VAL:CG2	2.46	0.45
1:A:141:PHE:CE1	1:A:151:LYS:HA	2.53	0.44
1:A:3:ARG:N	1:A:4:PRO:HD2	2.32	0.44
1:A:76:VAL:HB	1:A:90:ALA:CB	2.48	0.44
2:B:62:ILE:HD12	2:B:95:TRP:CB	2.47	0.44
1:A:120:ALA:O	1:A:122:GLN:N	2.50	0.44
1:A:209:VAL:HG21	2:B:14:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:HB2	1:A:110:TYR:CD2	2.53	0.44
1:A:205:VAL:HB	1:A:243:MET:HE1	1.99	0.44
2:B:222:VAL:HG12	2:B:230:TYR:O	2.18	0.44
1:A:138:ILE:O	1:A:142:ARG:HB2	2.17	0.44
2:B:15:THR:O	3:B:273(D):NDG:H3	2.18	0.44
1:A:228:ILE:C	1:A:228:ILE:HD12	2.36	0.44
2:B:102:THR:CG2	2:B:111:VAL:HG21	2.48	0.44
2:B:37:ASN:HB3	2:B:82:ILE:HG22	1.99	0.43
2:B:187:ARG:HD3	2:B:192:THR:O	2.18	0.43
3:B:273(D):NDG:O3	3:B:274(D):NDG:C1	2.67	0.43
1:A:151:LYS:HZ2	1:A:151:LYS:HB2	1.81	0.43
1:A:189:ALA:HB1	1:A:220:THR:HG21	2.01	0.43
2:B:47:ARG:HG3	8:B:359:HOH:O	2.18	0.43
2:B:246:SER:O	2:B:248:LYS:HD2	2.19	0.43
1:A:225:GLU:HA	1:A:226:PRO:HD3	1.85	0.43
2:B:199:LYS:NZ	2:B:205:SER:HA	2.33	0.43
2:B:256:THR:H	2:B:261:GLN:HE22	1.67	0.43
1:A:221:ASN:OD1	1:A:225:GLU:HB2	2.17	0.43
2:B:255:TYR:CE1	2:B:257:GLY:HA2	2.54	0.43
1:A:63:SER:HA	1:A:138:ILE:CG2	2.49	0.43
2:B:47:ARG:HE	2:B:47:ARG:N	2.16	0.43
1:A:137:GLY:HA2	1:A:154:THR:HG21	2.01	0.42
2:B:155:LEU:CB	2:B:166:MET:HB3	2.50	0.42
1:A:15:GLN:O	1:A:19:GLN:HG3	2.20	0.42
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.90	0.42
2:B:14:PRO:HA	3:B:273(D):NDG:HA	1.83	0.42
1:A:85:TYR:HB3	1:A:107:LEU:HD21	2.01	0.42
2:B:21:ARG:NH2	2:B:133:ARG:HD2	2.35	0.42
1:A:3:ARG:N	1:A:3:ARG:HD2	2.35	0.42
2:B:100:ASN:HD21	3:B:268(C):NDG:C1	2.20	0.42
2:B:227:GLY:HA3	2:B:262:ILE:HG23	2.01	0.42
2:B:239:ASP:OD1	2:B:253:TRP:HE3	2.03	0.42
1:A:205:VAL:HB	1:A:243:MET:CE	2.50	0.41
2:B:150:SER:HA	2:B:156:CYS:HA	2.01	0.41
1:A:2:ASP:H	1:A:27:ARG:NH1	2.17	0.41
1:A:39:LEU:HD22	1:A:243:MET:O	2.19	0.41
2:B:2:VAL:O	2:B:4:LYS:N	2.53	0.41
2:B:28:VAL:HB	2:B:51:ASN:HB2	2.02	0.41
2:B:72:TYR:CD1	2:B:79:TYR:CE1	3.08	0.41
1:A:110:TYR:HB3	1:A:112:THR:CG2	2.50	0.41
2:B:237:VAL:HG22	2:B:253:TRP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:O	1:A:53:THR:O	2.39	0.41
1:A:87:LEU:HB3	1:A:110:TYR:CD1	2.47	0.41
2:B:59:ASP:O	2:B:60:LYS:HB2	2.21	0.41
2:B:132:MET:HA	2:B:220:ARG:HB2	2.03	0.40
2:B:208:LEU:HD22	2:B:209:LEU:O	2.20	0.40
2:B:208:LEU:HD22	2:B:209:LEU:N	2.36	0.40
2:B:47:ARG:HE	2:B:47:ARG:H	1.67	0.40
1:A:148:ASN:ND2	8:A:255:HOH:O	2.53	0.40
1:A:82:THR:C	1:A:83:GLN:HG2	2.41	0.40
1:A:3:ARG:HH22	1:A:49:ASN:HA	1.86	0.40
1:A:119:TRP:HE3	1:A:119:TRP:N	2.19	0.40
1:A:220:THR:HA	1:A:225:GLU:O	2.21	0.40
2:B:196:LEU:HD23	2:B:209:LEU:CD1	2.52	0.40

All (2) 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)
2:B:21:ARG:HH22	8:B:342:HOH:H2[2_656]	1.21	0.39
2:B:133:ARG:HH12	8:B:345:HOH:H2[2_656]	1.31	0.29

## 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	249/251 (99%)	224 (90%)	21 (8%)	4 (2%)	11	4
2	B	265/267 (99%)	245 (92%)	19 (7%)	1 (0%)	36	30
All	All	514/518 (99%)	469 (91%)	40 (8%)	5 (1%)	17	9

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	B	2	VAL
1	A	121	HIS
1	A	143	SER
1	A	47	GLU
1	A	3	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	219/219 (100%)	186 (85%)	33 (15%)	3	1
2	B	235/235 (100%)	211 (90%)	24 (10%)	8	4
All	All	454/454 (100%)	397 (87%)	57 (13%)	5	2

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	THR
1	A	15	GLN
1	A	27	ARG
1	A	29	ARG
1	A	35	ASP
1	A	39	LEU
1	A	44	THR
1	A	45	LEU
1	A	46	GLN
1	A	49	ASN
1	A	57	SER
1	A	58	ASN
1	A	59	SER
1	A	71	THR
1	A	79	ARG
1	A	82	THR
1	A	89	ASP
1	A	95	SER

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Mol	Chain	Res	Type
1	A	96	ASP
1	A	98	LEU
1	A	102	THR
1	A	112	THR
1	A	119	TRP
1	A	125	GLN
1	A	149	GLU
1	A	151	LYS
1	A	191	MET
1	A	210	GLN
1	A	228	ILE
1	A	244	LEU
1	A	246	VAL
1	A	251	ASN
2	B	1	ILE
2	B	3	GLU
2	B	5	SER
2	B	6	LYS
2	B	7	ILE
2	B	15	THR
2	B	21	ARG
2	B	31	ASN
2	B	38	ARG
2	B	47	ARG
2	B	48	LEU
2	B	65	ASN
2	B	71	THR
2	B	79	TYR
2	B	110	LEU
2	B	111	VAL
2	B	154	ASP
2	B	160	GLN
2	B	189	VAL
2	B	207	ILE
2	B	208	LEU
2	B	214	ASN
2	B	232	LEU
2	B	258	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	49	ASN
1	A	58	ASN
1	A	105	HIS
1	A	160	GLN
1	A	210	GLN
2	B	141	ASN
2	B	176	GLN
2	B	225	ASN
2	B	249	GLN
2	B	261	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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$
3	NDG	B	268(C)	4	14,14,15	0.62	0	17,19,21	1.30	2 (11%)
4	NGZ	B	269(C)	3,5	14,14,15	1.17	2 (14%)	17,19,21	0.81	0
5	MAN	B	270(C)	5,4,6	11,11,12	1.97	2 (18%)	15,15,17	1.90	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	B	271(C)	5	11,11,12	0.96	0	15,15,17	1.16	1 (6%)
6	BMA	B	272(C)	5	11,11,12	1.03	0	15,15,17	0.61	0
3	NDG	B	273(D)	3	14,14,15	0.84	1 (7%)	17,19,21	1.21	1 (5%)
3	NDG	B	274(D)	3,7	14,14,15	0.59	0	17,19,21	1.10	2 (11%)
7	BGC	B	275(D)	3,5,6	11,11,12	0.99	1 (9%)	15,15,17	0.76	0
5	MAN	B	276(D)	7	11,11,12	1.32	2 (18%)	15,15,17	0.86	1 (6%)
6	BMA	B	277(D)	7	11,11,12	0.74	0	15,15,17	0.64	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
3	NDG	B	268(C)	4	-	0/6/23/26	0/1/1/1
4	NGZ	B	269(C)	3,5	-	0/6/23/26	0/1/1/1
5	MAN	B	270(C)	5,4,6	2/2/4/5	0/2/19/22	0/1/1/1
5	MAN	B	271(C)	5	-	0/2/19/22	0/1/1/1
6	BMA	B	272(C)	5	-	0/2/19/22	0/1/1/1
3	NDG	B	273(D)	3	-	0/6/23/26	0/1/1/1
3	NDG	B	274(D)	3,7	4/4/6/7	0/6/23/26	1/1/1/1
7	BGC	B	275(D)	3,5,6	-	0/2/19/22	0/1/1/1
5	MAN	B	276(D)	7	-	0/2/19/22	1/1/1/1
6	BMA	B	277(D)	7	-	0/2/19/22	1/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	275(D)	BGC	C1-C2	2.10	1.57	1.52
4	B	269(C)	NGZ	C1-C2	2.38	1.55	1.52
3	B	273(D)	NDG	C3-C2	2.39	1.57	1.52
5	B	276(D)	MAN	C2-C3	2.54	1.56	1.52
5	B	276(D)	MAN	C1-C2	2.77	1.58	1.52
4	B	269(C)	NGZ	C4-C5	2.82	1.59	1.53
5	B	270(C)	MAN	C1-C2	3.22	1.59	1.52
5	B	270(C)	MAN	C2-C3	5.54	1.60	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	268(C)	NDG	C4-C3-C2	-3.40	106.04	111.02
3	B	268(C)	NDG	C1-O-C5	-2.58	108.63	112.19
3	B	273(D)	NDG	C6-C5-C4	-2.43	107.26	112.99
3	B	274(D)	NDG	C1-O-C5	-2.06	109.36	112.19
5	B	276(D)	MAN	O5-C5-C6	2.39	110.92	107.15
5	B	270(C)	MAN	O5-C5-C6	2.83	111.64	107.15
3	B	274(D)	NDG	O-C5-C6	3.14	112.12	107.15
5	B	271(C)	MAN	O5-C5-C6	3.46	112.62	107.15
5	B	270(C)	MAN	C1-C2-C3	6.03	117.28	109.66

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	270(C)	MAN	C2
5	B	270(C)	MAN	C1
3	B	274(D)	NDG	C5
3	B	274(D)	NDG	C3
3	B	274(D)	NDG	C1
3	B	274(D)	NDG	C4

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	274(D)	NDG	C1-C2-C3-C4-C5-O
5	B	276(D)	MAN	C1-C2-C3-C4-C5-O5
6	B	277(D)	BMA	C1-C2-C3-C4-C5-O5

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	268(C)	NDG	5	0
3	B	273(D)	NDG	9	0
3	B	274(D)	NDG	7	0
5	B	276(D)	MAN	2	0
6	B	277(D)	BMA	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	251/251 (100%)	0.05	6 (2%) 59 65	7, 26, 49, 79	0
2	B	267/267 (100%)	-0.11	4 (1%) 73 78	6, 21, 43, 69	0
All	All	518/518 (100%)	-0.03	10 (1%) 66 72	6, 22, 46, 79	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	TRP	6.5
2	B	4	LYS	4.1
2	B	2	VAL	4.0
1	A	97	TYR	3.9
1	A	3	ARG	3.7
1	A	110	TYR	2.9
2	B	1	ILE	2.7
1	A	143	SER	2.5
1	A	141	PHE	2.3
2	B	253	TRP	2.2

### 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	B	276(D)	11/12	0.31	0.63	20,83,86,87	0
6	BMA	B	272(C)	11/12	0.51	0.30	20,70,72,72	0
7	BGC	B	275(D)	11/12	0.53	0.51	20,67,75,80	0
5	MAN	B	270(C)	11/12	0.62	0.26	20,56,64,69	0
6	BMA	B	277(D)	11/12	0.67	0.37	20,77,79,82	0
5	MAN	B	271(C)	11/12	0.75	0.24	20,50,54,55	0
3	NDG	B	273(D)	14/15	0.81	0.23	20,33,46,46	0
3	NDG	B	274(D)	14/15	0.83	0.26	20,37,59,62	0
4	NGZ	B	269(C)	14/15	0.87	0.16	20,44,48,51	0
3	NDG	B	268(C)	14/15	0.91	0.13	17,27,33,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.