



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:48 am GMT

PDB ID : 3BGA  
Title : Crystal structure of beta-galactosidase from Bacteroides thetaiotaomicron VPI-5482  
Authors : Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-11-26  
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

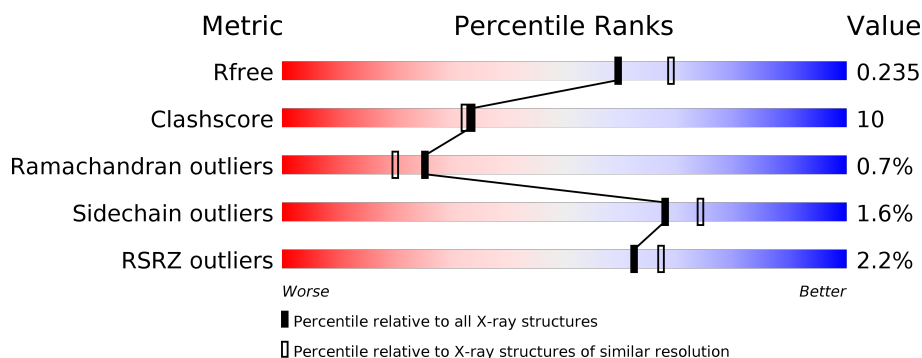
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	1010	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	1010	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17243 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-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1003	Total	C	N	O	S	Se	0	0	0
			8064	5124	1390	1516	14	20			
1	B	1000	Total	C	N	O	S	Se	0	0	0
			8034	5109	1379	1512	14	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	-	EXPRESSION TAG	UNP Q8A799
A	22	SER	-	EXPRESSION TAG	UNP Q8A799
A	23	LEU	-	EXPRESSION TAG	UNP Q8A799
A	1023	GLU	-	EXPRESSION TAG	UNP Q8A799
A	1024	GLY	-	EXPRESSION TAG	UNP Q8A799
A	1025	HIS	-	EXPRESSION TAG	UNP Q8A799
A	1026	HIS	-	EXPRESSION TAG	UNP Q8A799
A	1027	HIS	-	EXPRESSION TAG	UNP Q8A799
A	1028	HIS	-	EXPRESSION TAG	UNP Q8A799
A	1029	HIS	-	EXPRESSION TAG	UNP Q8A799
A	1030	HIS	-	EXPRESSION TAG	UNP Q8A799
B	21	MSE	-	EXPRESSION TAG	UNP Q8A799
B	22	SER	-	EXPRESSION TAG	UNP Q8A799
B	23	LEU	-	EXPRESSION TAG	UNP Q8A799
B	1023	GLU	-	EXPRESSION TAG	UNP Q8A799
B	1024	GLY	-	EXPRESSION TAG	UNP Q8A799
B	1025	HIS	-	EXPRESSION TAG	UNP Q8A799
B	1026	HIS	-	EXPRESSION TAG	UNP Q8A799
B	1027	HIS	-	EXPRESSION TAG	UNP Q8A799
B	1028	HIS	-	EXPRESSION TAG	UNP Q8A799
B	1029	HIS	-	EXPRESSION TAG	UNP Q8A799
B	1030	HIS	-	EXPRESSION TAG	UNP Q8A799

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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0
3	A	2	Total Na 2 2	0	0

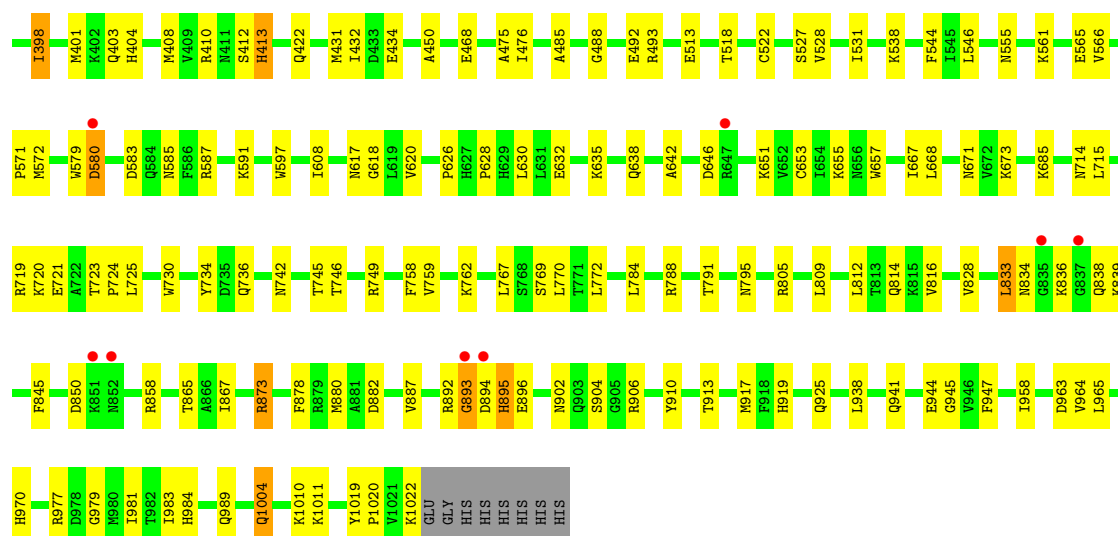
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	563	Total O 563 563	0	0
5	B	574	Total O 574 574	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.33Å 138.86Å 102.82Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	49.76 – 2.10 49.76 – 2.09	Depositor EDS
% Data completeness (in resolution range)	84.7 (49.76-2.10) 84.0 (49.76-2.09)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.200 , 0.234 0.200 , 0.235	Depositor DCC
$R_{free}$ test set	5795 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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

### 5.1 Standard geometry

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

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	0/8256	0.65	1/11168 (0.0%)
1	B	0.35	0/8222	0.64	5/11122 (0.0%)
All	All	0.36	0/16478	0.65	6/22290 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	893	GLY	N-CA-C	7.27	131.28	113.10
1	B	893	GLY	N-CA-C	5.46	126.75	113.10
1	B	81	LYS	N-CA-C	-5.29	96.72	111.00
1	B	173	ILE	CA-C-N	-5.27	105.60	117.20
1	B	173	ILE	C-N-CA	5.00	134.21	121.70
1	B	174	SER	N-CA-CB	5.00	118.01	110.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8064	0	7787	159	0
1	B	8034	0	7782	148	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	563	0	0	8	0
5	B	574	0	0	14	0
All	All	17243	0	15569	307	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (307) 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:173:ILE:HG13	1:A:174:SER:N	1.77	1.00
1:B:431:MSE:HE3	1:B:476:ILE:CG1	1.93	0.97
1:B:723:THR:HG22	1:B:725:LEU:H	1.25	0.95
1:A:714:ASN:HD21	1:A:736:GLN:HE21	1.12	0.94
1:B:431:MSE:HE3	1:B:476:ILE:HG13	1.49	0.93
1:B:1004:GLN:H	1:B:1004:GLN:NE2	1.65	0.93
1:B:1004:GLN:H	1:B:1004:GLN:HE21	0.96	0.91
1:A:1004:GLN:H	1:A:1004:GLN:HE21	1.15	0.89
1:A:723:THR:HG23	1:A:725:LEU:H	1.43	0.84
1:B:431:MSE:CE	1:B:476:ILE:HG13	2.06	0.84
1:B:356:ARG:HB2	1:B:368:ASN:HD21	1.41	0.83
1:B:1004:GLN:HE21	1:B:1004:GLN:N	1.75	0.83
1:B:836:LYS:HB2	1:B:838:GLN:HE21	1.45	0.82
1:B:431:MSE:HE2	1:B:475:ALA:HB3	1.59	0.82
1:A:1004:GLN:H	1:A:1004:GLN:NE2	1.80	0.80
1:B:60:GLY:H	1:B:422:GLN:HE22	1.29	0.80
1:B:788:ARG:HH11	1:B:989:GLN:HE21	1.30	0.80
1:B:579:TRP:HE1	1:B:617:ASN:HD22	1.30	0.79
1:B:60:GLY:H	1:B:422:GLN:NE2	1.80	0.78
1:A:723:THR:HG21	5:A:1542:HOH:O	1.82	0.78
1:B:723:THR:HG21	5:B:1545:HOH:O	1.83	0.77
1:A:356:ARG:HB2	1:A:368:ASN:HD21	1.49	0.76
1:B:431:MSE:HE3	1:B:476:ILE:HG12	1.66	0.76
1:A:579:TRP:HE1	1:A:617:ASN:HD22	1.30	0.76
1:B:964:VAL:HG23	5:B:1572:HOH:O	1.85	0.75
1:A:947:PHE:HB3	1:A:1019:TYR:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HD2	1:A:401:MSE:HE1	1.68	0.74
1:A:834:ASN:HD21	1:A:838:GLN:HB2	1.54	0.72
1:A:640:ILE:HD12	1:A:663:LEU:HD21	1.71	0.72
1:A:483:ASN:ND2	1:A:484:GLU:HG2	2.06	0.71
1:A:788:ARG:HH11	1:A:989:GLN:HE21	1.38	0.71
1:B:296:LEU:HG	1:B:318:ILE:HD11	1.73	0.70
1:A:357:THR:H	1:A:368:ASN:ND2	1.90	0.70
1:A:118:ILE:HG12	1:A:608:ILE:HD11	1.72	0.69
1:A:173:ILE:HG13	1:A:174:SER:H	1.52	0.69
1:B:379:ARG:HD2	1:B:401:MSE:HE1	1.73	0.69
1:A:878:PHE:CE1	1:A:880:MSE:HE2	2.27	0.69
1:A:670:TRP:HE1	1:A:685:LYS:HZ3	1.41	0.69
1:A:965:LEU:HD21	1:A:976:GLU:H	1.57	0.69
1:B:880:MSE:CE	1:B:938:LEU:HD23	2.23	0.68
1:A:528:VAL:HG13	1:A:566:VAL:HG21	1.76	0.68
1:B:357:THR:H	1:B:368:ASN:ND2	1.92	0.67
1:A:357:THR:H	1:A:368:ASN:HD22	1.42	0.67
1:A:579:TRP:CZ2	1:A:580:ASP:OD1	2.48	0.67
1:A:878:PHE:HE1	1:A:880:MSE:HE2	1.59	0.66
1:B:356:ARG:CB	1:B:368:ASN:HD21	2.07	0.65
1:A:478:ILE:HD13	1:A:506:PRO:HD2	1.77	0.65
1:A:1004:GLN:N	1:A:1004:GLN:HE21	1.93	0.65
1:A:914:VAL:HA	1:A:917:MSE:HE2	1.78	0.64
1:B:178:VAL:HG13	1:B:185:LEU:HB2	1.79	0.64
1:A:378:ASN:OD1	1:A:410:ARG:HD3	1.98	0.64
1:A:723:THR:HG22	1:A:726:VAL:H	1.63	0.64
1:B:893:GLY:HA3	1:B:910:TYR:CE2	2.33	0.64
1:B:385:LEU:HB2	5:B:1256:HOH:O	1.98	0.64
1:A:832:ILE:HG22	1:A:840:VAL:HB	1.80	0.63
1:A:527:SER:O	1:A:531:ILE:HG12	1.99	0.63
1:A:287:LEU:O	1:A:295:VAL:HG22	1.99	0.63
1:A:723:THR:CG2	1:A:726:VAL:H	2.12	0.63
1:B:1011:LYS:HG2	5:B:1459:HOH:O	2.00	0.62
1:A:444:TYR:OH	1:A:484:GLU:HB2	2.00	0.62
1:B:828:VAL:HG13	1:B:845:PHE:HB2	1.81	0.62
1:A:623:VAL:HG23	1:A:625:GLU:HG3	1.81	0.61
1:A:173:ILE:CG1	1:A:174:SER:N	2.56	0.61
1:B:71:LEU:HD11	1:B:240:LEU:HD13	1.83	0.61
1:B:357:THR:H	1:B:368:ASN:HD22	1.46	0.61
1:A:180:VAL:HG23	1:A:185:LEU:HD11	1.81	0.61
1:B:555:ASN:H	1:B:925:GLN:NE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HA	1:B:422:GLN:HE21	1.67	0.60
1:A:71:LEU:HD11	1:A:240:LEU:HD13	1.84	0.59
1:B:834:ASN:HD21	1:B:838:GLN:HB2	1.67	0.59
1:A:714:ASN:ND2	1:A:736:GLN:HE21	1.92	0.59
1:A:670:TRP:HE1	1:A:685:LYS:NZ	1.99	0.59
1:B:176:TYR:CD1	1:B:212:LEU:HD12	2.37	0.59
1:B:719:ARG:HD3	1:B:721:GLU:O	2.02	0.59
1:A:873:ARG:HD3	1:A:986:ASP:OD1	2.03	0.59
1:B:180:VAL:HG23	1:B:185:LEU:HD11	1.85	0.59
1:B:561:LYS:O	1:B:565:GLU:HG3	2.02	0.59
1:B:894:ASP:O	1:B:895:HIS:HB3	2.03	0.59
1:A:296:LEU:HG	1:A:318:ILE:HD11	1.84	0.59
1:A:153:THR:HG22	5:A:1458:HOH:O	2.03	0.59
1:B:667:ILE:HD11	1:B:720:LYS:HE3	1.83	0.58
1:B:378:ASN:OD1	1:B:410:ARG:HD3	2.03	0.58
1:A:356:ARG:CB	1:A:368:ASN:HD21	2.16	0.58
1:B:173:ILE:CG1	1:B:174:SER:N	2.67	0.58
1:B:887:VAL:HG22	1:B:938:LEU:HD13	1.86	0.58
1:A:684:THR:C	1:A:685:LYS:HD2	2.24	0.58
1:A:759:VAL:HB	1:A:769:SER:HB3	1.86	0.57
1:B:580:ASP:O	1:B:618:GLY:HA2	2.03	0.57
1:B:784:LEU:H	1:B:814:GLN:NE2	2.03	0.57
1:B:880:MSE:HE3	1:B:938:LEU:HD23	1.87	0.57
1:B:118:ILE:HG12	1:B:608:ILE:HD11	1.86	0.57
1:B:364:ARG:HD3	1:B:571:PRO:O	2.04	0.57
1:B:723:THR:HG23	1:B:724:PRO:HD2	1.87	0.57
1:B:153:THR:HG23	1:B:207:GLU:HG3	1.86	0.56
1:A:784:LEU:HD23	1:A:832:ILE:HG12	1.85	0.56
1:B:173:ILE:HG13	1:B:174:SER:N	2.20	0.56
1:B:723:THR:HG22	1:B:725:LEU:N	2.08	0.56
1:B:538:LYS:HE2	5:B:1539:HOH:O	2.05	0.56
1:B:635:LYS:O	1:B:638:GLN:HG2	2.05	0.56
1:A:561:LYS:O	1:A:565:GLU:HG3	2.05	0.56
1:A:635:LYS:O	1:A:638:GLN:HG2	2.06	0.56
1:A:784:LEU:H	1:A:814:GLN:NE2	2.04	0.56
1:A:378:ASN:HB3	1:A:412:SER:OG	2.07	0.55
1:B:356:ARG:CA	1:B:368:ASN:HD21	2.20	0.55
1:B:528:VAL:HG13	1:B:566:VAL:HG21	1.88	0.55
1:B:527:SER:O	1:B:531:ILE:HG12	2.06	0.55
1:A:850:ASP:OD2	1:A:852:ASN:HB2	2.05	0.55
1:B:880:MSE:HE1	1:B:938:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:ASN:HD21	1:B:736:GLN:HE21	1.53	0.54
1:A:555:ASN:H	1:A:925:GLN:NE2	2.05	0.54
1:A:839:LYS:HD2	1:A:842:MSE:HE2	1.90	0.54
1:A:906:ARG:HD3	5:A:1566:HOH:O	2.07	0.54
1:B:1010:LYS:HB2	5:B:1114:HOH:O	2.07	0.54
1:B:173:ILE:HG13	1:B:174:SER:H	1.72	0.54
1:B:244:PRO:HG2	1:B:246:GLN:O	2.08	0.54
1:B:591:LYS:HG3	5:B:1178:HOH:O	2.08	0.54
1:A:938:LEU:HD21	1:A:981:ILE:CD1	2.38	0.53
1:A:828:VAL:CG1	1:A:845:PHE:HB2	2.39	0.53
1:A:626:PRO:HB3	1:A:630:LEU:HD23	1.90	0.53
1:A:742:ASN:O	1:A:745:THR:HG22	2.09	0.53
1:B:947:PHE:HB3	1:B:1019:TYR:HB2	1.90	0.53
1:A:160:TRP:HA	1:A:163:ARG:HD3	1.90	0.53
1:A:784:LEU:H	1:A:814:GLN:HE22	1.56	0.53
1:B:266:ILE:HD12	1:B:317:LYS:HE2	1.89	0.53
1:A:226:GLN:HG2	1:A:413:HIS:HB2	1.91	0.53
1:A:621:ASN:ND2	1:A:625:GLU:HB2	2.24	0.53
1:B:878:PHE:CE1	1:B:880:MSE:HE2	2.45	0.52
1:A:413:HIS:HA	1:A:434:GLU:OE1	2.09	0.52
1:A:795:ASN:ND2	1:A:805:ARG:HH22	2.06	0.52
1:B:809:LEU:HA	1:B:812:LEU:HD21	1.91	0.52
1:B:226:GLN:HG2	1:B:413:HIS:HB2	1.91	0.52
1:A:762:LYS:O	1:A:816:VAL:HG21	2.09	0.52
1:B:759:VAL:HB	1:B:769:SER:HB3	1.92	0.51
1:A:706:ASN:HB2	1:A:742:ASN:HD22	1.75	0.51
1:A:887:VAL:HG21	1:A:917:MSE:CE	2.40	0.51
1:B:300:ILE:HG12	1:B:313:PHE:CE1	2.45	0.51
1:A:646:ASP:OD2	1:A:648:LYS:HG2	2.10	0.51
1:A:531:ILE:HD13	1:A:544:PHE:CE1	2.45	0.51
1:A:914:VAL:HA	1:A:917:MSE:CE	2.40	0.51
1:A:869:LYS:HA	5:A:1431:HOH:O	2.10	0.51
1:B:379:ARG:HD2	1:B:401:MSE:CE	2.41	0.51
1:A:49:PRO:HG3	1:A:242:SER:O	2.11	0.50
1:A:938:LEU:HD21	1:A:981:ILE:HD12	1.92	0.50
1:A:153:THR:OG1	1:A:207:GLU:HG3	2.11	0.50
1:B:488:GLY:O	1:B:492:GLU:HG3	2.11	0.50
1:A:632:GLU:HA	1:A:904:SER:HB3	1.92	0.50
1:B:254:SER:HB3	1:B:268:ASN:HB2	1.92	0.50
1:B:493:ARG:HG3	1:B:493:ARG:HH11	1.76	0.50
1:B:363:GLY:HA3	1:B:572:MSE:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLN:HG2	1:A:726:VAL:HG22	1.93	0.50
1:A:834:ASN:ND2	1:A:838:GLN:HB2	2.25	0.50
1:B:318:ILE:HD13	5:B:1574:HOH:O	2.12	0.50
1:B:655:LYS:HE2	1:B:657:TRP:CZ2	2.47	0.50
1:B:583:ASP:HB3	1:B:585:ASN:ND2	2.27	0.50
1:A:958:ILE:HG23	1:A:983:ILE:HD13	1.93	0.49
1:A:340:ASP:OD2	1:A:344:LYS:HB3	2.12	0.49
1:A:887:VAL:HG22	1:A:938:LEU:HD13	1.94	0.49
1:B:173:ILE:HG23	1:B:232:SER:HA	1.93	0.49
1:B:160:TRP:HA	1:B:163:ARG:HD3	1.95	0.49
1:A:477:VAL:HG23	1:A:478:ILE:HG12	1.94	0.49
1:A:727:ASP:HB2	5:A:1362:HOH:O	2.12	0.49
1:B:356:ARG:HB2	1:B:368:ASN:ND2	2.19	0.49
1:B:398:ILE:HD13	1:B:398:ILE:O	2.12	0.49
1:A:356:ARG:CA	1:A:368:ASN:HD21	2.25	0.49
1:A:817:VAL:HG12	1:A:829:ARG:O	2.13	0.49
1:A:639:ASN:O	1:A:640:ILE:HD13	2.13	0.49
1:A:69:MSE:HE2	1:A:240:LEU:HD22	1.95	0.48
1:B:23:LEU:HD13	1:B:27:LEU:HD13	1.94	0.48
1:B:431:MSE:HE2	1:B:475:ALA:CB	2.36	0.48
1:B:408:MSE:SE	1:B:432:ILE:HG13	2.63	0.48
1:A:282:SER:HB3	1:A:301:ASN:HD22	1.78	0.48
1:A:871:MSE:HG3	1:A:1009:VAL:HG22	1.95	0.48
1:B:795:ASN:ND2	1:B:805:ARG:HH22	2.11	0.48
1:B:893:GLY:HA3	1:B:910:TYR:CD2	2.48	0.48
1:B:110:GLU:HA	1:B:114:TYR:O	2.14	0.48
1:B:958:ILE:HG23	1:B:983:ILE:HD13	1.96	0.48
1:B:668:LEU:HD11	1:B:715:LEU:HD22	1.96	0.48
1:B:628:PRO:HD3	1:B:919:HIS:CE1	2.49	0.48
1:A:40:LYS:HG2	1:A:197:TRP:CE2	2.49	0.47
1:A:933:VAL:HG21	1:A:956:PHE:HD2	1.79	0.47
1:B:646:ASP:HB3	1:B:651:LYS:HB3	1.94	0.47
1:A:133:PHE:CG	1:A:141:PRO:HG3	2.48	0.47
1:A:579:TRP:CE2	1:A:580:ASP:OD1	2.68	0.47
1:B:894:ASP:O	1:B:894:ASP:CG	2.50	0.47
1:B:43:PRO:HB2	1:B:468:GLU:HG3	1.96	0.47
1:B:49:PRO:HG3	1:B:242:SER:O	2.13	0.47
1:A:509:TYR:CZ	1:A:511:ARG:HB2	2.50	0.47
1:B:71:LEU:CD1	1:B:240:LEU:HD13	2.44	0.47
1:A:828:VAL:HG13	1:A:845:PHE:HB2	1.96	0.47
1:A:818:SER:HB3	1:A:829:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:LEU:HD22	1:B:833:LEU:N	2.29	0.47
1:A:977:ARG:HH11	1:A:977:ARG:HG3	1.80	0.47
1:B:667:ILE:HD11	1:B:720:LYS:HG2	1.96	0.47
1:B:74:LYS:NZ	1:B:104:ASN:HD21	2.11	0.47
1:B:788:ARG:NH1	1:B:989:GLN:HE21	2.06	0.47
1:B:671:ASN:OD1	1:B:673:LYS:HG3	2.15	0.47
1:A:948:MSE:HG2	1:A:1018:LEU:HD22	1.96	0.47
1:B:746:THR:HB	1:B:749:ARG:HD2	1.96	0.47
1:A:887:VAL:HG21	1:A:917:MSE:HE1	1.97	0.47
1:B:882:ASP:OD2	1:B:979:GLY:HA2	2.15	0.47
1:A:180:VAL:CG2	1:A:185:LEU:HD11	2.46	0.46
1:A:244:PRO:HG2	1:A:246:GLN:O	2.14	0.46
1:A:619:LEU:HB3	1:A:630:LEU:HD13	1.96	0.46
1:B:620:VAL:HG12	1:B:626:PRO:HA	1.98	0.46
1:A:880:MSE:HE3	1:A:983:ILE:HG13	1.96	0.46
1:B:965:LEU:HD12	5:B:1135:HOH:O	2.16	0.46
1:A:257:LEU:HA	1:A:264:GLU:O	2.16	0.46
1:B:385:LEU:HD12	5:B:1256:HOH:O	2.14	0.46
1:B:834:ASN:ND2	1:B:838:GLN:HB2	2.28	0.46
1:A:820:LYS:NZ	1:A:820:LYS:HB3	2.31	0.46
1:A:655:LYS:HE2	1:A:657:TRP:CZ2	2.51	0.45
1:B:795:ASN:HD21	1:B:805:ARG:HH12	1.64	0.45
1:B:938:LEU:HD21	1:B:981:ILE:CD1	2.46	0.45
1:B:892:ARG:HD2	1:B:902:ASN:HB2	1.97	0.45
1:B:311:ILE:HD12	1:B:311:ILE:N	2.31	0.45
1:A:511:ARG:NE	1:A:511:ARG:HA	2.31	0.45
1:A:766:ALA:HB1	1:A:782:ILE:O	2.17	0.45
1:A:109:TRP:CE2	1:A:232:SER:HB2	2.52	0.45
1:B:40:LYS:HG2	1:B:197:TRP:CE2	2.52	0.45
1:B:385:LEU:HD22	5:B:1275:HOH:O	2.17	0.45
1:B:742:ASN:O	1:B:745:THR:HG22	2.17	0.44
1:B:944:GLU:HG2	1:B:1022:LYS:HG3	1.99	0.44
1:A:124:TYR:CE2	1:A:222:TYR:HA	2.53	0.44
1:A:921:TYR:O	1:A:972:ILE:HD11	2.17	0.44
1:A:882:ASP:OD2	1:A:979:GLY:HA2	2.17	0.44
1:B:858:ARG:HH11	1:B:858:ARG:HG2	1.81	0.44
1:A:82:ASN:OD1	1:A:82:ASN:C	2.55	0.44
1:B:116:THR:HG21	1:B:608:ILE:HD12	2.00	0.44
1:A:705:PRO:HG2	1:A:708:VAL:HG22	1.99	0.44
1:A:261:LYS:O	1:A:263:LYS:HG2	2.16	0.44
1:B:388:THR:HB	5:B:1256:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:VAL:HG21	1:A:956:PHE:CD2	2.52	0.43
1:B:493:ARG:HG3	1:B:493:ARG:NH1	2.33	0.43
1:B:791:THR:HA	1:B:925:GLN:HB2	2.00	0.43
1:B:977:ARG:HH11	1:B:977:ARG:HG3	1.82	0.43
1:A:300:ILE:HG12	1:A:313:PHE:CE1	2.53	0.43
1:A:273:VAL:O	1:A:308:SER:HA	2.18	0.43
1:A:509:TYR:CE2	1:A:511:ARG:HB2	2.54	0.43
1:A:71:LEU:CD1	1:A:240:LEU:HD13	2.49	0.43
1:A:477:VAL:O	1:A:478:ILE:HD13	2.19	0.43
1:A:178:VAL:HG23	1:A:212:LEU:CD2	2.49	0.43
1:B:137:PRO:HG3	1:B:222:TYR:CE2	2.54	0.43
1:B:413:HIS:N	1:B:413:HIS:ND1	2.66	0.43
1:B:839:LYS:O	1:B:867:ILE:HD12	2.19	0.43
1:A:254:SER:HB3	1:A:268:ASN:HB2	2.01	0.42
1:A:551:HIS:CG	1:A:997:CYS:HB3	2.55	0.42
1:A:880:MSE:CE	1:A:983:ILE:HG13	2.49	0.42
1:B:642:ALA:HA	1:B:653:CYS:O	2.19	0.42
1:A:399:ARG:O	1:A:403:GLN:HG3	2.19	0.42
1:B:356:ARG:HA	1:B:368:ASN:HD21	1.84	0.42
1:B:90:PHE:HA	1:B:95:TYR:CG	2.54	0.42
1:B:984:HIS:HD2	5:B:1071:HOH:O	2.02	0.42
1:A:432:ILE:HG12	1:A:478:ILE:HB	2.01	0.42
1:A:719:ARG:HG2	5:A:1494:HOH:O	2.18	0.42
1:A:668:LEU:HB2	1:A:717:TRP:CZ3	2.54	0.42
1:B:772:LEU:HD13	1:B:1020:PRO:HB2	2.00	0.42
1:B:788:ARG:HA	1:B:873:ARG:HH21	1.85	0.42
1:A:110:GLU:HA	1:A:114:TYR:O	2.20	0.42
1:A:178:VAL:HG13	1:A:185:LEU:HB2	2.01	0.42
1:A:890:LEU:HD22	5:A:1374:HOH:O	2.19	0.42
1:B:587:ARG:HB2	1:B:597:TRP:CZ3	2.55	0.42
1:A:151:ARG:HG3	1:A:211:ALA:HB2	2.02	0.42
1:A:513:GLU:HA	5:A:1057:HOH:O	2.18	0.42
1:A:640:ILE:HD12	1:A:663:LEU:CD2	2.44	0.42
1:B:404:HIS:CD2	1:B:630:LEU:HG	2.55	0.42
1:B:685:LYS:HB2	1:B:685:LYS:NZ	2.35	0.42
1:B:723:THR:HG23	1:B:724:PRO:CD	2.48	0.42
1:A:141:PRO:O	1:A:145:ASN:HB2	2.19	0.42
1:A:768:SER:HA	1:A:781:PRO:HB3	2.02	0.42
1:A:823:LYS:HD3	1:A:823:LYS:O	2.20	0.42
1:A:484:GLU:HA	1:A:511:ARG:CG	2.50	0.42
1:A:893:GLY:N	1:A:906:ARG:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ALA:HB2	1:B:485:ALA:O	2.20	0.42
1:A:255:ALA:HB1	1:A:355:PHE:CD1	2.55	0.41
1:B:938:LEU:O	1:B:945:GLY:HA3	2.20	0.41
1:B:632:GLU:HA	1:B:904:SER:HB3	2.02	0.41
1:B:880:MSE:CE	1:B:983:ILE:HG13	2.50	0.41
1:A:360:ILE:CD1	1:A:506:PRO:HB3	2.51	0.41
1:A:431:MSE:HB2	1:A:476:ILE:HA	2.03	0.41
1:A:839:LYS:HD2	1:A:842:MSE:CE	2.50	0.41
1:A:831:GLU:HG2	1:A:842:MSE:SE	2.71	0.41
1:A:791:THR:HA	1:A:925:GLN:HB2	2.01	0.41
1:B:304:SER:HB2	5:B:1312:HOH:O	2.19	0.41
1:A:408:MSE:SE	1:A:432:ILE:HG13	2.70	0.41
1:A:285:TYR:CD1	1:A:285:TYR:C	2.94	0.41
1:B:784:LEU:H	1:B:814:GLN:HE22	1.65	0.41
1:A:782:ILE:HA	1:A:878:PHE:HB3	2.02	0.41
1:B:628:PRO:HB3	1:B:896:GLU:HB3	2.03	0.41
1:B:762:LYS:O	1:B:816:VAL:HG21	2.21	0.41
1:A:620:VAL:HG12	1:A:626:PRO:HA	2.02	0.41
1:B:403:GLN:HB3	1:B:730:TRP:CZ2	2.56	0.41
1:B:878:PHE:HE1	1:B:880:MSE:HE2	1.86	0.41
1:B:723:THR:CG2	1:B:724:PRO:N	2.83	0.41
1:A:74:LYS:NZ	1:A:104:ASN:HD21	2.19	0.41
1:A:965:LEU:O	1:A:965:LEU:HD12	2.21	0.41
1:B:758:PHE:HA	1:B:769:SER:O	2.21	0.41
1:A:807:ALA:HB3	1:A:809:LEU:HG	2.03	0.40
1:A:884:TYR:HB3	1:A:938:LEU:HG	2.03	0.40
1:B:413:HIS:HA	1:B:434:GLU:OE1	2.20	0.40
1:A:691:PRO:O	1:A:692:HIS:HB2	2.21	0.40
1:A:880:MSE:CE	1:A:938:LEU:HD23	2.52	0.40
1:A:178:VAL:HG23	1:A:212:LEU:HD22	2.02	0.40
1:A:977:ARG:HG3	1:A:977:ARG:NH1	2.36	0.40
1:B:913:THR:O	1:B:917:MSE:HG3	2.21	0.40
1:A:580:ASP:O	1:A:618:GLY:HA2	2.20	0.40
1:B:635:LYS:HE3	1:B:734:TYR:O	2.22	0.40
1:B:963:ASP:OD2	1:B:984:HIS:HE1	2.04	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1001/1010 (99%)	954 (95%)	41 (4%)	6 (1%)	28	24
1	B	998/1010 (99%)	948 (95%)	43 (4%)	7 (1%)	25	20
All	All	1999/2020 (99%)	1902 (95%)	84 (4%)	13 (1%)	25	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	SER
1	B	412	SER
1	A	893	GLY
1	B	513	GLU
1	B	895	HIS
1	B	174	SER
1	A	82	ASN
1	A	174	SER
1	A	484	GLU
1	A	580	ASP
1	B	82	ASN
1	B	865	THR
1	B	518	THR

### 5.3.2 Protein sidechains [i](#)

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	854/840 (102%)	844 (99%)	10 (1%)	75	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	852/840 (101%)	834 (98%)	18 (2%)	59	64
All	All	1706/1680 (102%)	1678 (98%)	28 (2%)	68	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	A	356	ARG
1	A	471	LYS
1	A	522	CYS
1	A	544	PHE
1	A	546	LEU
1	A	580	ASP
1	A	755	GLU
1	A	820	LYS
1	A	1004	GLN
1	B	174	SER
1	B	232	SER
1	B	356	ARG
1	B	398	ILE
1	B	413	HIS
1	B	522	CYS
1	B	544	PHE
1	B	546	LEU
1	B	580	ASP
1	B	767	LEU
1	B	770	LEU
1	B	833	LEU
1	B	850	ASP
1	B	873	ARG
1	B	906	ARG
1	B	941	GLN
1	B	970	HIS
1	B	1004	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	85	ASN
1	A	104	ASN

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Mol	Chain	Res	Type
1	A	297	GLN
1	A	301	ASN
1	A	330	ASN
1	A	368	ASN
1	A	380	HIS
1	A	490	ASN
1	A	585	ASN
1	A	639	ASN
1	A	649	ASN
1	A	714	ASN
1	A	744	ASN
1	A	795	ASN
1	A	814	GLN
1	A	838	GLN
1	A	862	GLN
1	A	925	GLN
1	A	929	ASN
1	A	941	GLN
1	A	970	HIS
1	A	989	GLN
1	A	1004	GLN
1	B	85	ASN
1	B	104	ASN
1	B	297	GLN
1	B	301	ASN
1	B	328	HIS
1	B	330	ASN
1	B	368	ASN
1	B	380	HIS
1	B	422	GLN
1	B	481	GLN
1	B	490	ASN
1	B	508	GLN
1	B	569	ASN
1	B	585	ASN
1	B	639	ASN
1	B	649	ASN
1	B	714	ASN
1	B	795	ASN
1	B	814	GLN
1	B	838	GLN
1	B	925	GLN

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Mol	Chain	Res	Type
1	B	929	ASN
1	B	984	HIS
1	B	989	GLN
1	B	1004	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](#)

Of 8 ligands modelled in this entry, 8 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.

No monomer is involved in short contacts.

### 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, 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	983/1010 (97%)	0.06	26 (2%) 56 62	10, 24, 43, 55	0
1	B	980/1010 (97%)	-0.10	18 (1%) 69 73	11, 23, 39, 58	0
All	All	1963/2020 (97%)	-0.02	44 (2%) 62 67	10, 23, 41, 58	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	ARG	7.1
1	B	304	SER	5.3
1	B	306	GLY	4.4
1	B	303	LYS	4.3
1	A	819	LEU	3.7
1	A	817	VAL	3.5
1	A	205	GLU	3.3
1	A	703	LYS	3.3
1	B	302	ILE	3.2
1	A	697	VAL	3.1
1	A	893	GLY	2.9
1	A	751	GLN	2.9
1	A	174	SER	2.9
1	A	580	ASP	2.8
1	B	580	ASP	2.8
1	A	670	TRP	2.7
1	A	823	LYS	2.6
1	B	278	ALA	2.6
1	A	158	ALA	2.5
1	B	893	GLY	2.5
1	B	837	GLY	2.5
1	B	894	ASP	2.5
1	B	280	ALA	2.5
1	A	699	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	174	SER	2.4
1	B	647	ARG	2.3
1	A	851	LYS	2.3
1	A	645	SER	2.3
1	A	816	VAL	2.3
1	A	522	CYS	2.2
1	B	852	ASN	2.2
1	A	828	VAL	2.1
1	A	822	GLU	2.1
1	B	57	GLY	2.1
1	A	824	THR	2.1
1	A	305	ARG	2.1
1	B	835	GLY	2.1
1	A	291	SER	2.0
1	B	851	LYS	2.0
1	A	700	GLY	2.0
1	A	850	ASP	2.0
1	A	681	ALA	2.0
1	B	205	GLU	2.0
1	A	683	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 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	1	1/1	0.98	0.10	-0.47	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	B	5	1/1	0.99	0.08	-1.05	18,18,18,18	0
3	NA	B	3	1/1	0.95	0.09	-1.06	18,18,18,18	0
3	NA	A	4	1/1	0.98	0.07	-1.72	15,15,15,15	0
3	NA	A	6	1/1	0.98	0.06	-1.88	21,21,21,21	0
2	MG	B	2	1/1	0.98	0.06	-2.84	20,20,20,20	0
4	CL	A	7	1/1	0.99	0.07	-2.90	12,12,12,12	0
4	CL	B	8	1/1	0.99	0.04	-3.87	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.