Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:03 PM GMT

PDB ID	:	1DWJ
Title	:	STUDY ON RADIATION DAMAGE ON A CRYOCOOLED CRYSTAL. REFINED PART 6: STRUCTURE AFTER A RADIATION DOSE OF 54*10E15 PHOTONS/MM2
Authors	:	Burmeister, W.P.
Deposited on	:	1999-12-05
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

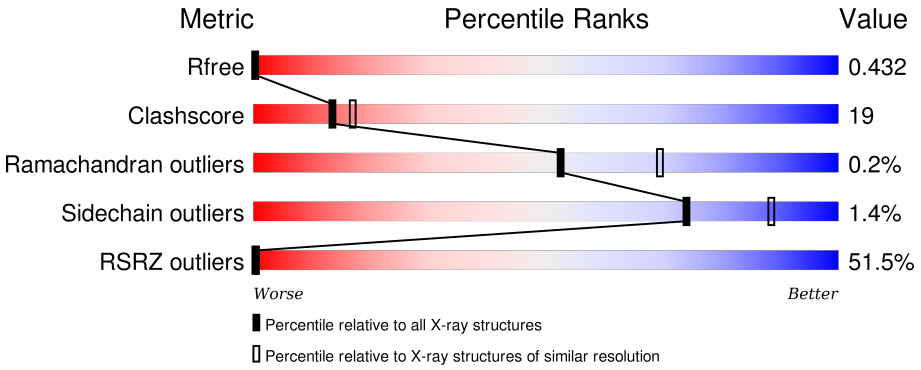
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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 <=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	M	499	52% 72% 27%

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
2	NAG	M	961	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	M	957	-	-	X	-
8	GOL	M	1010	-	-	-	X
8	GOL	M	1020	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5220 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.

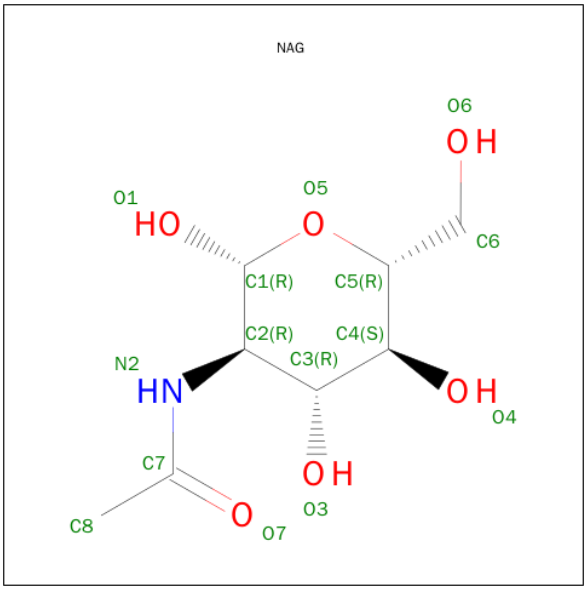
- Molecule 1 is a protein called MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4083	2619	660	788	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	497	THR	SER	SEE REMARK 999	UNP P29736

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	5	Total	C	N	O	0	0
			58	33	2	23		

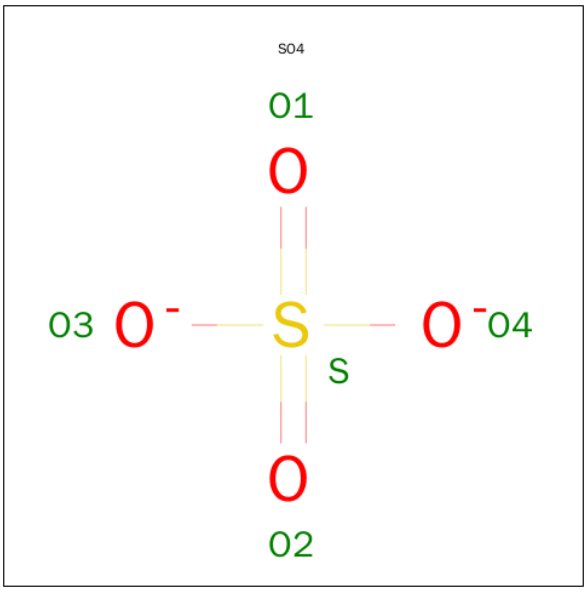
- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	7	Total	C	N	O	0	0
			80	45	2	33		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

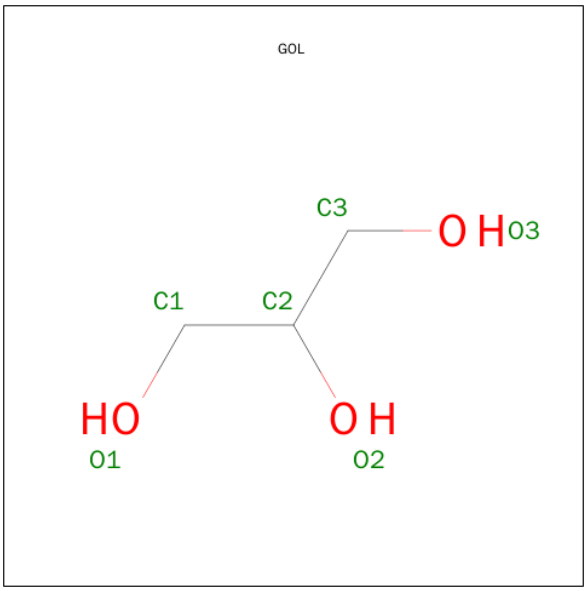
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Zn	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0
8	M	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

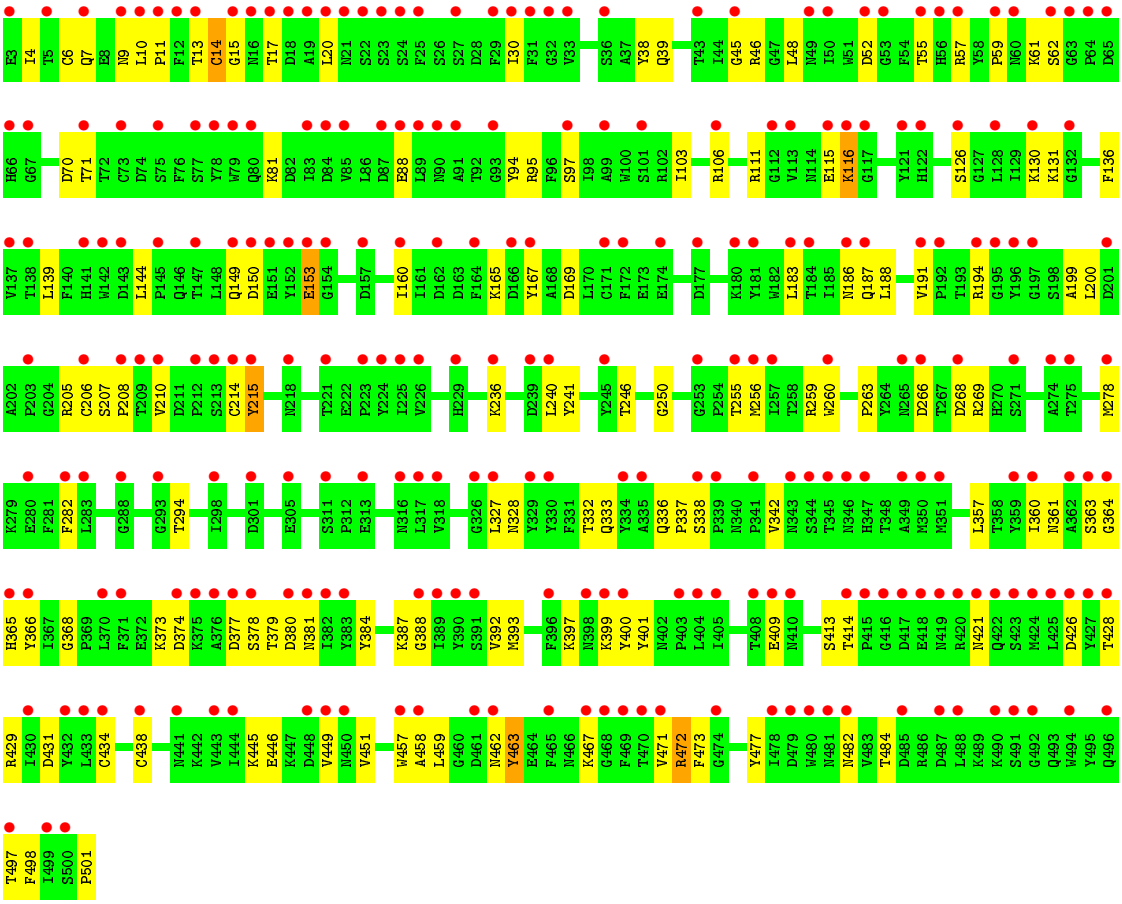
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	788	Total O 788 788	0	0

3 Residue-property plots (i)

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: MYROSINASE MA1

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.40) 95.1 (9.94-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.93 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.186 , 0.245 0.401 , 0.432	Depositor DCC
R_{free} test set	1356 reflections (2.81%)	DCC
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.3	EDS
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 50356 reflections	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: XYP, GOL, ZN, BMA, NAG, SO4, MAN, FUC

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	M	0.82	2/4291 (0.0%)	0.79	1/5835 (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	M	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	14	CYS	CB-SG	5.68	1.92	1.82
1	M	153	GLU	CG-CD	5.11	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	472	ARG	NE-CZ-NH1	5.32	122.96	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	215	TYR	Sidechain
1	M	401	TYR	Sidechain
1	M	446	GLU	Mainchain
1	M	463	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	M	482	ASN	Mainchain
1	M	94	TYR	Sidechain
1	M	97	SER	Mainchain

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	M	4083	0	3838	143	8
2	M	84	0	78	9	0
3	M	56	0	50	2	0
4	M	58	0	50	0	0
5	M	80	0	68	11	0
6	M	1	0	0	0	1
7	M	40	0	0	1	0
8	M	30	0	40	1	0
9	M	788	0	0	84	15
All	All	5220	0	4124	159	23

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 19.

All (159) 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)
5:M:957:MAN:O6	9:M:3053:HOH:O	1.55	1.22
1:M:15:GLY:HA3	9:M:2027:HOH:O	1.06	1.20
5:M:957:MAN:H61	9:M:3055:HOH:O	1.01	1.19
3:M:983:NAG:H83	9:M:3066:HOH:O	1.44	1.17
1:M:428:THR:HG23	9:M:2608:HOH:O	1.44	1.17
1:M:431:ASP:OD1	9:M:2612:HOH:O	1.63	1.13
1:M:215:TYR:O	9:M:2342:HOH:O	1.64	1.12
1:M:71:THR:HG23	9:M:2118:HOH:O	1.51	1.07
2:M:961:NAG:H61	9:M:3056:HOH:O	1.59	1.02
1:M:15:GLY:CA	9:M:2027:HOH:O	1.72	1.00
1:M:215:TYR:HB2	9:M:2093:HOH:O	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:379:THR:HG22	9:M:2542:HOH:O	0.80	0.97
1:M:246:THR:HG22	9:M:2360:HOH:O	1.66	0.95
2:M:961:NAG:C6	9:M:3056:HOH:O	2.14	0.95
1:M:6:CYS:HG	1:M:438:CYS:HG	0.90	0.89
1:M:379:THR:HG23	9:M:2537:HOH:O	1.74	0.87
1:M:20[B]:LEU:HG	1:M:498:PHE:HE2	1.44	0.82
1:M:70:ASP:OD2	9:M:2114:HOH:O	1.96	0.82
1:M:10:LEU:CD2	9:M:2020:HOH:O	2.27	0.81
5:M:954:BMA:H61	5:M:957:MAN:H5	1.63	0.81
5:M:957:MAN:C6	9:M:3053:HOH:O	2.18	0.80
1:M:150:ASP:OD2	9:M:2270:HOH:O	2.00	0.80
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE2	2.17	0.79
5:M:954:BMA:H61	5:M:957:MAN:C5	2.13	0.79
1:M:15:GLY:C	9:M:2027:HOH:O	2.03	0.78
1:M:14:CYS:HG	1:M:434:CYS:HG	0.81	0.78
1:M:278:MET:HE1	9:M:2323:HOH:O	1.84	0.77
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.67	0.76
1:M:130:LYS:HB3	9:M:2246:HOH:O	1.85	0.76
1:M:373:LYS:NZ	9:M:2528:HOH:O	2.15	0.75
1:M:10:LEU:HD23	9:M:2020:HOH:O	1.86	0.75
1:M:462[B]:ASN:OD1	9:M:2635:HOH:O	2.05	0.73
1:M:337:PRO:O	1:M:338[B]:SER:HB3	1.79	0.72
1:M:365:HIS:HE1	9:M:2519:HOH:O	1.75	0.69
1:M:215:TYR:CA	9:M:2342:HOH:O	2.40	0.69
1:M:20[B]:LEU:HG	1:M:498:PHE:CE2	2.28	0.67
1:M:59:PRO:HB3	9:M:2091:HOH:O	1.95	0.66
1:M:333:GLN:OE1	1:M:357:LEU:HD13	1.95	0.66
1:M:200:LEU:HB3	9:M:2328:HOH:O	1.96	0.65
1:M:240:LEU:HD13	2:M:931:NAG:H83	1.77	0.65
1:M:191:VAL:HG23	9:M:2326:HOH:O	1.98	0.64
1:M:428:THR:N	9:M:2608:HOH:O	2.20	0.64
5:M:954:BMA:C6	5:M:957:MAN:C5	2.76	0.64
1:M:126[B]:SER:OG	9:M:2236:HOH:O	2.15	0.63
1:M:208:PRO:HA	9:M:2335:HOH:O	1.97	0.63
1:M:81:LYS:HD2	9:M:2665:HOH:O	1.99	0.63
5:M:954:BMA:H61	9:M:3055:HOH:O	1.99	0.62
1:M:7:GLN:NE2	9:M:2009:HOH:O	2.32	0.62
5:M:957:MAN:C5	9:M:3053:HOH:O	2.45	0.62
1:M:205:ARG:O	1:M:206:CYS:HB3	1.98	0.62
5:M:954:BMA:C6	5:M:957:MAN:H5	2.30	0.62
1:M:484:THR:HB	9:M:2664:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:LEU:HD22	9:M:2020:HOH:O	1.95	0.60
1:M:111:ARG:C	9:M:2204:HOH:O	2.39	0.60
1:M:116:LYS:HE3	9:M:2074:HOH:O	2.01	0.60
1:M:194:ARG:NH2	9:M:2328:HOH:O	2.34	0.60
1:M:501:PRO:HB2	2:M:901:NAG:H82	1.83	0.60
1:M:165:LYS:HZ1	2:M:931:NAG:H82	1.66	0.60
1:M:414:THR:HG22	9:M:2609:HOH:O	2.02	0.59
1:M:497:THR:HG23	9:M:2682:HOH:O	2.03	0.59
1:M:7:GLN:NE2	1:M:13:THR:OG1	2.36	0.59
1:M:342[A]:VAL:HG13	9:M:2345:HOH:O	2.02	0.59
1:M:472:ARG:NE	9:M:2651:HOH:O	2.36	0.58
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.84	0.58
1:M:9:ASN:HB2	9:M:3080:HOH:O	2.03	0.58
1:M:39:GLN:HG2	1:M:463:TYR:O	2.03	0.58
1:M:445:LYS:HE2	9:M:2619:HOH:O	2.04	0.58
1:M:421:ASN:ND2	9:M:2600:HOH:O	2.37	0.58
1:M:378:SER:HB3	9:M:2528:HOH:O	2.03	0.57
5:M:952:FUC:H2	9:M:3040:HOH:O	2.03	0.57
1:M:165:LYS:NZ	2:M:931:NAG:H82	2.20	0.57
1:M:61:LYS:HE2	9:M:2337:HOH:O	2.04	0.57
1:M:88[B]:GLU:HG3	9:M:2147:HOH:O	2.05	0.56
2:M:961:NAG:H62	9:M:3056:HOH:O	1.92	0.55
1:M:360[B]:ILE:CG2	1:M:364:GLY:HA2	2.37	0.54
8:M:1024:GOL:H11	9:M:2291:HOH:O	2.07	0.54
1:M:259:ARG:HG3	1:M:282:PHE:CE2	2.43	0.53
1:M:215:TYR:HB2	9:M:2342:HOH:O	2.09	0.53
1:M:449[B]:VAL:HG23	1:M:451:VAL:HG23	1.90	0.53
1:M:130:LYS:HG2	9:M:2247:HOH:O	2.09	0.52
1:M:115:GLU:OE1	1:M:115:GLU:HA	2.09	0.52
1:M:188:LEU:HD12	1:M:256:MET:SD	2.49	0.52
1:M:55:THR:HG22	1:M:62[B]:SER:OG	2.10	0.52
1:M:360[B]:ILE:HG22	1:M:361:ASN:O	2.10	0.51
1:M:71:THR:CG2	9:M:2118:HOH:O	2.30	0.51
1:M:449[B]:VAL:CG2	1:M:451:VAL:HG23	2.40	0.51
1:M:38:TYR:HE1	1:M:52:ASP:OD1	1.93	0.51
5:M:957:MAN:O4	9:M:3053:HOH:O	1.90	0.51
1:M:428:THR:CB	9:M:2608:HOH:O	2.57	0.51
1:M:259:ARG:HG2	9:M:2466:HOH:O	2.11	0.51
1:M:477:TYR:HE1	9:M:2651:HOH:O	1.94	0.50
1:M:471:VAL:HG11	9:M:2587:HOH:O	2.11	0.50
1:M:207:SER:HB2	1:M:210:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:ARG:NH1	1:M:409:GLU:HG3	2.27	0.49
1:M:215:TYR:OH	9:M:2341:HOH:O	2.15	0.49
1:M:409:GLU:HG2	1:M:457:TRP:CE3	2.48	0.48
1:M:116:LYS:HA	1:M:116:LYS:HD2	1.61	0.47
1:M:365:HIS:CE1	3:M:981:NAG:H62	2.49	0.47
1:M:269:ARG:NH2	9:M:2397:HOH:O	2.44	0.47
1:M:259:ARG:HG3	1:M:282:PHE:CZ	2.50	0.47
1:M:387:LYS:HE3	9:M:2552:HOH:O	2.15	0.46
1:M:4:ILE:HG21	9:M:2618:HOH:O	2.16	0.46
1:M:103:ILE:HD11	1:M:167:TYR:HE1	1.80	0.46
1:M:336:GLN:HB2	1:M:337:PRO:HD2	1.98	0.46
1:M:194:ARG:HD2	7:M:1009:SO4:O1	2.16	0.45
1:M:241:TYR:OH	1:M:250:GLY:HA3	2.16	0.45
1:M:186:ASN:HA	1:M:255:THR:HB	1.99	0.45
1:M:327:LEU:HD12	1:M:393:MET:CE	2.46	0.45
1:M:363[B]:SER:HB3	9:M:2505:HOH:O	2.17	0.45
1:M:388:GLY:O	1:M:392:VAL:HG23	2.16	0.45
1:M:30[B]:ILE:CD1	9:M:2085:HOH:O	2.64	0.45
1:M:501:PRO:HB2	2:M:901:NAG:C8	2.47	0.45
1:M:374:ASP:HB3	1:M:377:ASP:O	2.17	0.44
1:M:360[B]:ILE:HG21	1:M:364:GLY:HA2	1.99	0.44
1:M:260:TRP:O	1:M:332:THR:HG23	2.16	0.44
1:M:95:ARG:HA	1:M:136:PHE:O	2.17	0.44
1:M:377:ASP:O	1:M:380:ASP:HB2	2.17	0.44
1:M:342[B]:VAL:HG11	9:M:2434:HOH:O	2.17	0.44
1:M:397:LYS:HD2	1:M:449[B]:VAL:HG12	2.00	0.44
1:M:467:LYS:HE3	9:M:2640:HOH:O	2.18	0.44
1:M:294:THR:HG22	9:M:2416:HOH:O	2.18	0.44
1:M:48:LEU:N	9:M:2081:HOH:O	2.27	0.43
1:M:149:GLN:O	1:M:153:GLU:HA	2.19	0.43
1:M:130:LYS:HE3	9:M:2235:HOH:O	2.17	0.43
1:M:328:ASN:CG	1:M:409:GLU:HB2	2.39	0.43
1:M:459:LEU:HD13	9:M:2166:HOH:O	2.18	0.43
1:M:215:TYR:HA	9:M:2342:HOH:O	2.15	0.43
1:M:426:ASP:OD2	1:M:429:ARG:NH1	2.48	0.43
1:M:39:GLN:O	1:M:462[A]:ASN:HB2	2.19	0.42
1:M:165:LYS:NZ	2:M:931:NAG:C8	2.80	0.42
1:M:381:ASN:ND2	9:M:2528:HOH:O	2.49	0.42
1:M:144:LEU:HD11	1:M:160:ILE:HD11	2.00	0.42
1:M:379:THR:CG2	9:M:2542:HOH:O	1.71	0.42
1:M:199:ALA:HB2	1:M:214:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:399:LYS:O	1:M:399:LYS:HG3	2.19	0.41
1:M:88[B]:GLU:CD	9:M:2154:HOH:O	2.58	0.41
1:M:457:TRP:HA	1:M:458:ALA:HA	1.90	0.41
1:M:363[A]:SER:HB2	9:M:2505:HOH:O	2.20	0.41
1:M:368:GLY:HA3	1:M:384:TYR:O	2.20	0.41
1:M:131:LYS:HA	1:M:131:LYS:HD3	1.82	0.41
1:M:337:PRO:O	1:M:338[B]:SER:CB	2.55	0.41
1:M:472:ARG:CZ	9:M:2651:HOH:O	2.67	0.41
1:M:214:CYS:HB2	9:M:2335:HOH:O	2.20	0.41
1:M:413:SER:HB3	1:M:473:PHE:CE1	2.55	0.41
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.41
1:M:139:LEU:HA	1:M:139:LEU:HD23	1.86	0.41
1:M:399:LYS:HG2	1:M:400:TYR:CE2	2.55	0.40
1:M:428:THR:CG2	9:M:2608:HOH:O	2.25	0.40
1:M:46:ARG:NE	9:M:2077:HOH:O	2.50	0.40

All (23) 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)
6:M:1001:ZN:ZN	6:M:1001:ZN:ZN[3_656]	1.10	1.10
9:M:2272:HOH:O	9:M:2272:HOH:O[3_656]	1.10	1.10
9:M:2010:HOH:O	9:M:2505:HOH:O[4_576]	1.43	0.77
9:M:2546:HOH:O	9:M:2546:HOH:O[4_576]	1.44	0.76
9:M:2017:HOH:O	9:M:2017:HOH:O[4_576]	1.63	0.57
9:M:2252:HOH:O	9:M:2252:HOH:O[4_576]	1.63	0.57
9:M:2408:HOH:O	9:M:3103:HOH:O[6_564]	1.63	0.57
1:M:373:LYS:CE	1:M:373:LYS:CE[4_576]	1.66	0.54
9:M:2241:HOH:O	9:M:2523:HOH:O[4_576]	1.67	0.53
9:M:2240:HOH:O	9:M:2240:HOH:O[4_576]	1.76	0.44
1:M:373:LYS:CD	1:M:373:LYS:NZ[4_576]	1.78	0.42
9:M:2108:HOH:O	9:M:2124:HOH:O[3_656]	1.83	0.37
1:M:45:GLY:N	1:M:57:ARG:O[3_656]	1.90	0.30
9:M:2173:HOH:O	9:M:2365:HOH:O[6_564]	1.92	0.28
9:M:2238:HOH:O	9:M:2613:HOH:O[4_576]	1.96	0.24
1:M:373:LYS:CG	1:M:373:LYS:NZ[4_576]	2.02	0.18
9:M:2058:HOH:O	9:M:2106:HOH:O[3_656]	2.02	0.18
1:M:106:ARG:CD	1:M:153:GLU:OE2[3_656]	2.07	0.13
9:M:2210:HOH:O	9:M:2339:HOH:O[3_656]	2.09	0.11
1:M:11:PRO:CG	9:M:2511:HOH:O[4_576]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:2017:HOH:O	9:M:2018:HOH:O[4_576]	2.12	0.08
1:M:106:ARG:NE	1:M:153:GLU:OE2[3_656]	2.17	0.03
1:M:373:LYS:CE	1:M:373:LYS:NZ[4_576]	2.18	0.02

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	M	518/499 (104%)	498 (96%)	19 (4%)	1 (0%)	52 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

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	M	456/435 (105%)	450 (99%)	6 (1%)	76 89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	116	LYS
1	M	183	LEU

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Mol	Chain	Res	Type
1	M	236	LYS
1	M	263	PRO
1	M	266	ASP
1	M	268	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules 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

16 carbohydrates 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	NAG	M	921	1,3	14,14,15	0.49	0	15,19,21	0.83	0
3	NAG	M	923	3	14,14,15	1.03	1 (7%)	15,19,21	0.84	1 (6%)
4	NAG	M	941	1,4	14,14,15	0.60	0	15,19,21	0.81	0
4	FUC	M	942	4	10,10,11	1.11	1 (10%)	14,14,16	1.00	2 (14%)
4	NAG	M	943	4	14,14,15	0.78	0	15,19,21	0.57	0
4	BMA	M	944	4	11,11,12	1.21	1 (9%)	14,15,17	0.75	0
4	XYP	M	945	4	9,9,10	0.90	0	12,12,14	1.49	1 (8%)
5	NAG	M	951	1,5	14,14,15	0.63	0	15,19,21	0.85	0
5	FUC	M	952	5	10,10,11	0.85	0	14,14,16	1.45	2 (14%)
5	NAG	M	953	5	14,14,15	0.72	0	15,19,21	1.04	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	M	954	5	11,11,12	1.08	1 (9%)	14,15,17	0.99	0
5	XYP	M	955	5	9,9,10	0.76	0	12,12,14	1.30	1 (8%)
5	MAN	M	956	5	11,11,12	0.82	0	14,15,17	0.60	0
5	MAN	M	957	5	11,11,12	1.04	1 (9%)	14,15,17	1.51	2 (14%)
3	NAG	M	981	1,3	14,14,15	0.55	0	15,19,21	0.61	0
3	NAG	M	983	3	14,14,15	0.79	0	15,19,21	0.78	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	NAG	M	921	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	923	3	-	0/6/23/26	0/1/1/1
4	NAG	M	941	1,4	-	0/6/23/26	0/1/1/1
4	FUC	M	942	4	-	0/0/17/20	0/1/1/1
4	NAG	M	943	4	-	0/6/23/26	0/1/1/1
4	BMA	M	944	4	-	0/2/19/22	0/1/1/1
4	XYP	M	945	4	-	0/0/14/17	0/1/1/1
5	NAG	M	951	1,5	-	0/6/23/26	0/1/1/1
5	FUC	M	952	5	-	0/0/17/20	0/1/1/1
5	NAG	M	953	5	-	0/6/23/26	0/1/1/1
5	BMA	M	954	5	-	0/2/19/22	0/1/1/1
5	XYP	M	955	5	-	0/0/14/17	0/1/1/1
5	MAN	M	956	5	-	0/2/19/22	0/1/1/1
5	MAN	M	957	5	-	0/2/19/22	0/1/1/1
3	NAG	M	981	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	983	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	954	BMA	C2-C3	-2.89	1.48	1.52
4	M	944	BMA	C4-C5	2.46	1.58	1.53
5	M	957	MAN	C2-C3	2.65	1.56	1.52
3	M	923	NAG	C1-C2	2.72	1.56	1.52
4	M	942	FUC	C2-C3	2.93	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	952	FUC	C1-C2-C3	-3.07	105.92	109.54
5	M	952	FUC	C2-C3-C4	-2.78	106.32	111.04
5	M	957	MAN	O5-C1-C2	-2.19	107.30	110.86
4	M	942	FUC	C1-C2-C3	-2.11	107.04	109.54
3	M	923	NAG	C2-N2-C7	2.07	125.69	123.04
4	M	942	FUC	C1-O5-C5	2.35	116.01	112.38
5	M	953	NAG	C3-C4-C5	2.77	115.03	110.20
5	M	955	XYP	C5B-C4B-C3B	3.90	114.16	109.54
5	M	957	MAN	C6-C5-C4	4.13	123.21	113.02
4	M	945	XYP	C1B-C2B-C3B	4.40	114.74	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	952	FUC	1	0
5	M	954	BMA	5	0
5	M	957	MAN	9	0
3	M	981	NAG	1	0
3	M	983	NAG	1	0

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
7	SO4	M	1002	-	4,4,4	0.92	0	6,6,6	0.11	0
7	SO4	M	1003	-	4,4,4	0.44	0	6,6,6	0.10	0
7	SO4	M	1004	-	4,4,4	0.51	0	6,6,6	0.33	0
7	SO4	M	1005	-	4,4,4	0.65	0	6,6,6	0.33	0
7	SO4	M	1006	-	4,4,4	0.84	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	M	1007	-	4,4,4	0.49	0	6,6,6	0.22	0
7	SO4	M	1008	-	4,4,4	0.79	0	6,6,6	0.15	0
7	SO4	M	1009	-	4,4,4	0.90	0	6,6,6	0.16	0
8	GOL	M	1010	-	5,5,5	0.09	0	5,5,5	0.57	0
8	GOL	M	1020	-	5,5,5	0.40	0	5,5,5	0.75	0
8	GOL	M	1021	-	5,5,5	0.29	0	5,5,5	0.30	0
8	GOL	M	1023	-	5,5,5	0.44	0	5,5,5	0.46	0
8	GOL	M	1024	-	5,5,5	0.54	0	5,5,5	0.37	0
2	NAG	M	901	1	14,14,15	0.62	0	15,19,21	0.87	0
2	NAG	M	911	1	14,14,15	0.77	0	15,19,21	0.62	0
2	NAG	M	931	1	14,14,15	0.67	0	15,19,21	1.20	1 (6%)
2	NAG	M	961	1	14,14,15	0.87	0	15,19,21	0.80	0
2	NAG	M	971	1	14,14,15	1.28	2 (14%)	15,19,21	0.59	0
2	NAG	M	991	1	14,14,15	0.80	0	15,19,21	0.91	1 (6%)

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
7	SO4	M	1002	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1003	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1004	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1005	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1006	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1007	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1008	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1009	-	-	0/0/0/0	0/0/0/0
8	GOL	M	1010	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1020	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1021	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1023	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1024	-	-	0/4/4/4	0/0/0/0
2	NAG	M	901	1	-	0/6/23/26	0/1/1/1
2	NAG	M	911	1	-	0/6/23/26	0/1/1/1
2	NAG	M	931	1	-	0/6/23/26	0/1/1/1
2	NAG	M	961	1	-	0/6/23/26	0/1/1/1
2	NAG	M	971	1	-	0/6/23/26	0/1/1/1
2	NAG	M	991	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	971	NAG	C4-C5	2.59	1.58	1.53
2	M	971	NAG	C1-C2	3.02	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	991	NAG	C4-C3-C2	-2.72	107.01	111.23
2	M	931	NAG	C2-N2-C7	3.66	127.74	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1009	SO4	1	0
8	M	1024	GOL	1	0
2	M	901	NAG	2	0
2	M	931	NAG	4	0
2	M	961	NAG	3	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

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^{th} 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	M	499/499 (100%)	2.17	257 (51%)	0 0	32, 36, 50, 77	37 (7%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	8.4
1	M	23	SER	6.6
1	M	18	ASP	5.8
1	M	345	THR	5.5
1	M	481	ASN	5.5
1	M	84	ASP	5.4
1	M	420	ARG	5.2
1	M	390	TYR	5.1
1	M	376	ALA	5.0
1	M	3	GLU	5.0
1	M	5	THR	5.0
1	M	482	ASN	5.0
1	M	374	ASP	4.9
1	M	213[A]	SER	4.8
1	M	375	LYS	4.8
1	M	380	ASP	4.6
1	M	13	THR	4.6
1	M	366[A]	TYR	4.4
1	M	335	ALA	4.4
1	M	377	ASP	4.4
1	M	90	ASN	4.3
1	M	17	THR	4.3
1	M	378	SER	4.3
1	M	418	GLU	4.2
1	M	305[A]	GLU	4.2
1	M	71	THR	4.2
1	M	206	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	313	GLU	4.0
1	M	43	THR	4.0
1	M	497	THR	4.0
1	M	480	TRP	4.0
1	M	27	SER	4.0
1	M	363[A]	SER	4.0
1	M	491	SER	3.9
1	M	55	THR	3.9
1	M	128	LEU	3.9
1	M	208	PRO	3.8
1	M	492	GLY	3.8
1	M	301	ASP	3.8
1	M	359	TYR	3.8
1	M	421	ASN	3.7
1	M	12	PHE	3.7
1	M	253	GLY	3.7
1	M	150	ASP	3.7
1	M	209	THR	3.7
1	M	19	ALA	3.7
1	M	151	GLU	3.6
1	M	469	PHE	3.6
1	M	214	CYS	3.6
1	M	485	ASP	3.6
1	M	10	LEU	3.6
1	M	164	PHE	3.6
1	M	330	TYR	3.6
1	M	341	PRO	3.5
1	M	77	SER	3.5
1	M	365	HIS	3.5
1	M	45	GLY	3.5
1	M	349	ALA	3.5
1	M	62[A]	SER	3.4
1	M	458	ALA	3.4
1	M	80	GLN	3.4
1	M	196	TYR	3.4
1	M	417	ASP	3.4
1	M	338[A]	SER	3.4
1	M	461	ASP	3.4
1	M	444	ILE	3.4
1	M	370	LEU	3.4
1	M	112	GLY	3.4
1	M	132	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	122	HIS	3.3
1	M	184	THR	3.3
1	M	143	ASP	3.3
1	M	257	ILE	3.3
1	M	53	GLY	3.2
1	M	449[A]	VAL	3.2
1	M	339	PRO	3.2
1	M	73	CYS	3.2
1	M	154	GLY	3.2
1	M	142	TRP	3.2
1	M	293	GLY	3.1
1	M	415	PRO	3.1
1	M	162	ASP	3.1
1	M	147	THR	3.1
1	M	166	ASP	3.1
1	M	400	TYR	3.1
1	M	59	PRO	3.1
1	M	334	TYR	3.1
1	M	152	TYR	3.1
1	M	223	PRO	3.1
1	M	434	CYS	3.1
1	M	419	ASN	3.1
1	M	424	MET	3.0
1	M	427	TYR	3.0
1	M	416	GLY	3.0
1	M	410	ASN	3.0
1	M	36	SER	3.0
1	M	16	ASN	3.0
1	M	245	TYR	3.0
1	M	448	ASP	3.0
1	M	474	GLY	3.0
1	M	116	LYS	3.0
1	M	89	LEU	3.0
1	M	404	LEU	3.0
1	M	97	SER	3.0
1	M	364	GLY	3.0
1	M	93	GLY	2.9
1	M	138	THR	2.9
1	M	399	LYS	2.9
1	M	79	TRP	2.9
1	M	167	TYR	2.9
1	M	11	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	271[A]	SER	2.9
1	M	283	LEU	2.9
1	M	274	ALA	2.9
1	M	422	GLN	2.9
1	M	85	VAL	2.9
1	M	471	VAL	2.9
1	M	255	THR	2.9
1	M	396	PHE	2.9
1	M	197	GLY	2.9
1	M	433	LEU	2.8
1	M	500	SER	2.8
1	M	177	ASP	2.8
1	M	210	VAL	2.8
1	M	344[A]	SER	2.8
1	M	191	VAL	2.8
1	M	268	ASP	2.8
1	M	494	TRP	2.7
1	M	441	ASN	2.7
1	M	24	SER	2.7
1	M	141	HIS	2.7
1	M	409	GLU	2.7
1	M	414	THR	2.7
1	M	57	ARG	2.7
1	M	275	THR	2.7
1	M	64	PRO	2.7
1	M	30[A]	ILE	2.7
1	M	33	VAL	2.7
1	M	121	TYR	2.7
1	M	499	ILE	2.7
1	M	75	SER	2.7
1	M	347	HIS	2.7
1	M	423	SER	2.7
1	M	215	TYR	2.7
1	M	432	TYR	2.7
1	M	346	ASN	2.7
1	M	183	LEU	2.7
1	M	25	PHE	2.7
1	M	298	ILE	2.6
1	M	488	LEU	2.6
1	M	101[A]	SER	2.6
1	M	326	GLY	2.6
1	M	113	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	350	MET	2.6
1	M	50	ILE	2.6
1	M	490	LYS	2.6
1	M	99	ALA	2.6
1	M	20[A]	LEU	2.5
1	M	426	ASP	2.5
1	M	67	GLY	2.5
1	M	360[A]	ILE	2.5
1	M	478	ILE	2.5
1	M	318	VAL	2.5
1	M	430	ILE	2.5
1	M	174	GLU	2.5
1	M	256	MET	2.5
1	M	126[A]	SER	2.5
1	M	443	VAL	2.5
1	M	398	ASN	2.5
1	M	389	ILE	2.5
1	M	130	LYS	2.5
1	M	171	CYS	2.4
1	M	388	GLY	2.4
1	M	52	ASP	2.4
1	M	7	GLN	2.4
1	M	468	GLY	2.4
1	M	425	LEU	2.4
1	M	382	ILE	2.4
1	M	381	ASN	2.4
1	M	172	PHE	2.4
1	M	153	GLU	2.4
1	M	496	GLN	2.4
1	M	181	TYR	2.3
1	M	66	HIS	2.3
1	M	192	PRO	2.3
1	M	221	THR	2.3
1	M	83	ILE	2.3
1	M	487	ASP	2.3
1	M	260	TRP	2.3
1	M	49	ASN	2.3
1	M	29	PHE	2.3
1	M	78	TYR	2.3
1	M	137	VAL	2.3
1	M	316	ASN	2.3
1	M	160	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	465	PHE	2.3
1	M	317	LEU	2.3
1	M	457	TRP	2.3
1	M	9	ASN	2.3
1	M	240	LEU	2.3
1	M	201	ASP	2.3
1	M	428	THR	2.3
1	M	149	GLN	2.2
1	M	218	ASN	2.2
1	M	229	HIS	2.2
1	M	470	THR	2.2
1	M	203	PRO	2.2
1	M	63	GLY	2.2
1	M	236	LYS	2.2
1	M	145	PRO	2.2
1	M	351	MET	2.2
1	M	450	ASN	2.2
1	M	88[A]	GLU	2.2
1	M	31	PHE	2.2
1	M	60	ASN	2.2
1	M	462[A]	ASN	2.2
1	M	479	ASP	2.2
1	M	239	ASP	2.2
1	M	65	ASP	2.2
1	M	224	TYR	2.1
1	M	311	SER	2.1
1	M	106	ARG	2.1
1	M	87	ASP	2.1
1	M	186	ASN	2.1
1	M	467	LYS	2.1
1	M	194	ARG	2.1
1	M	157	ASP	2.1
1	M	282	PHE	2.1
1	M	187	GLN	2.1
1	M	91	ALA	2.1
1	M	117	GLY	2.1
1	M	180	LYS	2.1
1	M	225	ILE	2.1
1	M	383	TYR	2.1
1	M	405	ILE	2.1
1	M	15	GLY	2.1
1	M	403	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	408	THR	2.1
1	M	362	ALA	2.1
1	M	391	SER	2.1
1	M	226	VAL	2.1
1	M	265	ASN	2.1
1	M	438	CYS	2.1
1	M	195	GLY	2.1
1	M	327	LEU	2.1
1	M	21	ASN	2.0
1	M	280	GLU	2.0
1	M	288	GLY	2.0
1	M	329	TYR	2.0
1	M	371	PHE	2.0
1	M	115	GLU	2.0
1	M	278	MET	2.0
1	M	56	HIS	2.0
1	M	22	SER	2.0
1	M	343	ASN	2.0
1	M	32	GLY	2.0
1	M	266	ASP	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)

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^{th} 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^2)	Q<0.9
4	NAG	M	941	14/15	0.69	0.31	-0.35	36,43,48,48	0
3	NAG	M	981	14/15	0.68	0.28	-0.58	30,38,42,44	0
3	NAG	M	921	14/15	0.78	0.20	-1.37	40,45,53,58	0
5	NAG	M	953	14/15	0.82	0.23	-	41,44,49,53	0
5	BMA	M	954	11/12	0.60	0.27	-	47,52,57,68	0
5	MAN	M	957	11/12	0.69	0.40	-	54,64,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	M	951	14/15	0.76	0.26	-	38,41,47,50	0
3	NAG	M	923	14/15	0.53	0.42	-	58,66,78,81	0
4	XYP	M	945	9/10	0.50	0.35	-	63,69,73,75	0
5	FUC	M	952	10/11	0.79	0.21	-	40,43,54,54	0
4	BMA	M	944	11/12	0.55	0.44	-	59,64,70,74	0
4	NAG	M	943	14/15	0.74	0.32	-	42,48,54,59	0
5	XYP	M	955	9/10	0.50	0.38	-	54,59,65,85	0
5	MAN	M	956	11/12	0.59	0.37	-	46,60,73,77	0
4	FUC	M	942	10/11	0.58	0.34	-	45,53,60,69	0
3	NAG	M	983	14/15	0.62	0.32	-	47,52,71,78	0

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, 95^{th} 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^2)	Q<0.9
8	GOL	M	1010	6/6	0.37	0.50	7.11	57,63,65,72	6
2	NAG	M	961	14/15	0.48	0.62	2.75	64,71,83,89	0
8	GOL	M	1020	6/6	0.48	0.43	2.49	27,35,39,39	1
7	SO4	M	1002	5/5	0.80	0.35	1.06	47,50,53,58	5
8	GOL	M	1021	6/6	0.59	0.31	0.72	32,42,47,52	6
2	NAG	M	901	14/15	0.51	0.29	-0.73	46,56,67,69	0
8	GOL	M	1024	6/6	0.78	0.28	-0.93	37,38,43,43	0
7	SO4	M	1004	5/5	0.84	0.42	-	35,49,51,56	5
7	SO4	M	1007	5/5	0.57	0.41	-	34,54,55,58	5
2	NAG	M	931	14/15	0.55	0.39	-	56,63,70,70	0
6	ZN	M	1001	1/1	0.91	0.21	-	33,33,33,33	0
2	NAG	M	991	14/15	0.44	0.49	-	56,61,74,77	0
7	SO4	M	1005	5/5	0.79	0.29	-	39,42,48,50	0
7	SO4	M	1003	5/5	0.64	0.51	-	46,49,57,57	5
8	GOL	M	1023	6/6	0.21	0.94	-	52,53,64,66	6
7	SO4	M	1009	5/5	0.36	0.58	-	59,61,67,80	1
7	SO4	M	1008	5/5	0.78	0.26	-	54,57,59,60	5
2	NAG	M	911	14/15	0.68	0.25	-	46,49,57,66	0
7	SO4	M	1006	5/5	0.90	0.40	-	47,52,55,56	5
2	NAG	M	971	14/15	0.55	0.39	-	77,85,91,91	0

6.5 Other polymers (i)

There are no such residues in this entry.