



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DWG
Title : STUDY ON RADIATION DAMAGE ON A CRYOCOOLED CRYSTAL:
PART 3 STRUCTURE AFTER IRRADIATION WITH 18.2*10E15 PHO-
TONS/MM2.
Authors : Burmeister, W.P.
Deposited on : 1999-12-05
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

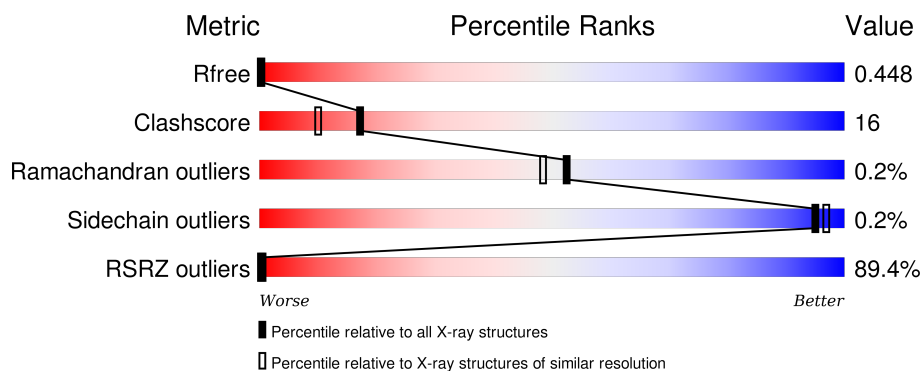
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	M	499	

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	931	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	M	961	X	-	-	X
3	NAG	M	923	-	-	-	X
5	BMA	M	954	-	-	X	-
5	MAN	M	957	X	-	X	-
7	SO4	M	1003	-	-	X	-
7	SO4	M	1004	-	-	X	-
7	SO4	M	1006	-	X	-	-
7	SO4	M	1009	-	X	X	X
8	GOL	M	1010	-	-	X	X
8	GOL	M	1020	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5217 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
			Total	C	N	O	S			
1	M	499	4080	2616	660	788	16	0	20	0

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
			Total	C	N	O		
2	M	1	14	8	1	5	0	0
2	M	1	14	8	1	5	0	0

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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: O₄S).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

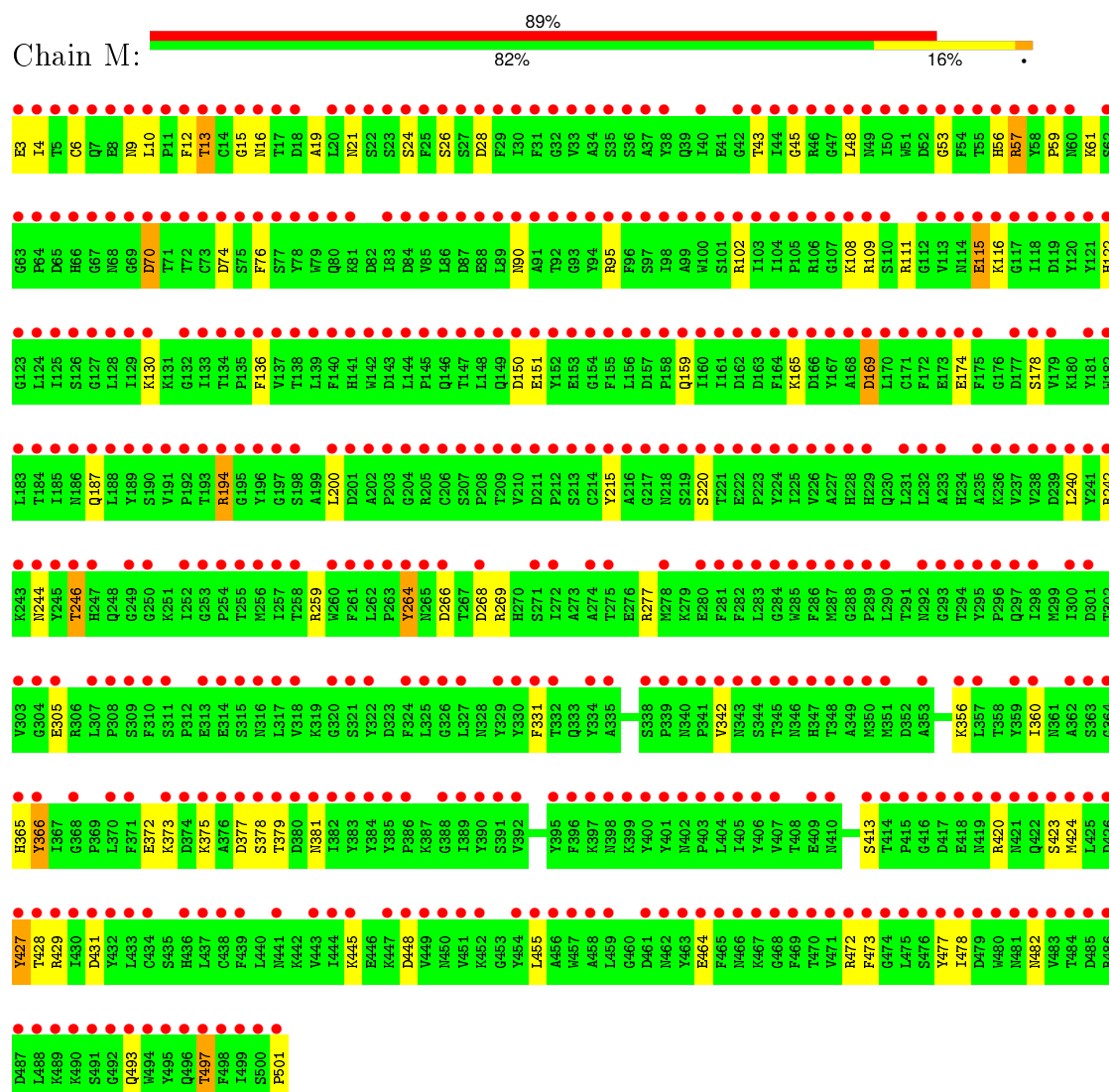
- Molecule 9 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



4 Data and refinement statistics

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 – 2.00 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.00) 98.4 (9.94-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.184 , 0.193 0.434 , 0.448	Depositor DCC
R_{free} test set	2401 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 53.8	EDS
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 50364 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	5217	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.15	18/4283 (0.4%)	1.32	41/5824 (0.7%)

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	1
5	M	1	0
All	All	1	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	264	TYR	CE1-CZ	-21.78	1.10	1.38
1	M	264	TYR	CZ-OH	20.20	1.72	1.37
1	M	16	ASN	CG-ND2	12.66	1.64	1.32
1	M	356	LYS	CE-NZ	-11.08	1.21	1.49
1	M	423	SER	CB-OG	9.83	1.55	1.42
1	M	13	THR	C-O	-9.72	1.04	1.23
1	M	6	CYS	CB-SG	-9.15	1.66	1.82
1	M	178	SER	CB-OG	8.91	1.53	1.42
1	M	501	PRO	CA-C	7.25	1.67	1.52
1	M	24	SER	CB-OG	7.00	1.51	1.42
1	M	115	GLU	CD-OE2	6.86	1.33	1.25
1	M	26	SER	CB-OG	5.51	1.49	1.42
1	M	413	SER	CB-OG	-5.36	1.35	1.42
1	M	246	THR	CB-CG2	-5.35	1.34	1.52
1	M	61	LYS	CD-CE	-5.18	1.38	1.51
1	M	501	PRO	N-CD	5.17	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	242	ARG	NE-CZ	5.11	1.39	1.33
1	M	464	GLU	CG-CD	-5.06	1.44	1.51

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	448	ASP	CB-CG-OD2	-18.65	101.51	118.30
1	M	115	GLU	OE1-CD-OE2	-15.25	105.00	123.30
1	M	264	TYR	CZ-CE2-CD2	-12.25	108.77	119.80
1	M	264	TYR	CE1-CZ-CE2	11.60	138.36	119.80
1	M	109	ARG	NE-CZ-NH1	-11.36	114.62	120.30
1	M	269	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	M	372	GLU	OE1-CD-OE2	-10.19	111.07	123.30
1	M	169[A]	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	M	169[B]	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	M	194	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	M	242	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	M	268	ASP	CB-CG-OD1	8.74	126.17	118.30
1	M	269	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	M	266	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	M	74	ASP	CB-CG-OD1	7.91	125.42	118.30
1	M	427	TYR	CG-CD1-CE1	-7.74	115.11	121.30
1	M	448	ASP	OD1-CG-OD2	7.70	137.92	123.30
1	M	264	TYR	OH-CZ-CE2	-7.51	99.82	120.10
1	M	264	TYR	CD1-CE1-CZ	-6.94	113.55	119.80
1	M	372	GLU	CG-CD-OE2	6.55	131.39	118.30
1	M	109	ARG	NH1-CZ-NH2	6.45	126.50	119.40
1	M	246	THR	OG1-CB-CG2	-6.39	95.31	110.00
1	M	482	ASN	CB-CG-OD1	6.24	134.09	121.60
1	M	76	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	M	482	ASN	CA-CB-CG	-6.03	100.13	113.40
1	M	194	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	M	70	ASP	CB-CG-OD1	5.82	123.54	118.30
1	M	377	ASP	O-C-N	-5.62	113.70	122.70
1	M	497	THR	OG1-CB-CG2	-5.55	97.24	110.00
1	M	102	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	M	420	ARG	CD-NE-CZ	5.51	131.31	123.60
1	M	429	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	M	420	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	M	277	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	M	427	TYR	CZ-CE2-CD2	-5.34	114.99	119.80
1	M	19	ALA	CB-CA-C	-5.24	102.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	366[A]	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	366[B]	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	M	57	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	M	473	PHE	CB-CG-CD2	5.14	124.40	120.80
1	M	478	ILE	CB-CG1-CD1	5.08	128.13	113.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	957	MAN	C5

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	13	THR	Mainchain

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	M	4080	0	3828	104	4
2	M	84	0	77	18	0
3	M	56	0	49	4	0
4	M	58	0	50	0	0
5	M	80	0	66	9	0
6	M	1	0	0	0	1
7	M	40	0	0	10	0
8	M	30	0	39	4	0
9	M	788	0	0	77	17
All	All	5217	0	4109	135	21

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 16.

All (135) 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:M:244:ASN:HD21	2:M:931:NAG:C1	0.96	1.56
1:M:21:ASN:HD21	2:M:901:NAG:C1	0.90	1.52
1:M:264:TYR:OH	1:M:264:TYR:CZ	1.72	1.42
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.57	1.37
8:M:1010:GOL:C1	9:M:4026:HOH:O	1.71	1.34
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	2.14	1.30
1:M:15:GLY:HA3	9:M:2032:HOH:O	1.25	1.28
1:M:427:TYR:HE2	9:M:2614:HOH:O	1.19	1.25
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.33	1.24
1:M:428:THR:HG23	9:M:2617:HOH:O	1.27	1.24
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE2	2.22	1.23
3:M:921:NAG:O3	3:M:921:NAG:C3	1.89	1.19
1:M:477:TYR:HE1	9:M:2659:HOH:O	1.21	1.18
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE2	1.78	1.17
1:M:431:ASP:OD1	9:M:2620:HOH:O	1.66	1.10
1:M:477:TYR:CE1	9:M:2659:HOH:O	1.94	1.08
8:M:1010:GOL:H11	9:M:4026:HOH:O	1.27	1.08
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE2	2.33	1.07
1:M:215:TYR:O	9:M:2355:HOH:O	1.69	1.07
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD2	1.92	1.05
8:M:1010:GOL:C2	9:M:4026:HOH:O	1.91	1.04
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.03	1.03
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE2	1.91	1.02
1:M:427:TYR:CE2	9:M:2614:HOH:O	1.95	1.01
7:M:1004:SO4:O2	7:M:1009:SO4:S	2.19	1.00
1:M:165:LYS:NZ	2:M:931:NAG:H82	1.76	0.99
2:M:961:NAG:H61	9:M:3056:HOH:O	1.62	0.98
1:M:259:ARG:HG2	9:M:2483:HOH:O	1.64	0.96
1:M:472:ARG:CZ	9:M:2659:HOH:O	2.12	0.95
1:M:246:THR:HG22	9:M:2377:HOH:O	1.66	0.94
1:M:150:ASP:OD2	9:M:2277:HOH:O	1.88	0.91
1:M:379:THR:HG23	9:M:2548:HOH:O	1.71	0.90
1:M:53:GLY:O	9:M:2097:HOH:O	1.90	0.89
5:M:954:BMA:H61	5:M:957:MAN:C6	2.03	0.89
7:M:1004:SO4:O2	7:M:1009:SO4:O2	1.91	0.88
5:M:954:BMA:H61	5:M:957:MAN:H61	1.55	0.88
1:M:130:LYS:HB3	9:M:2253:HOH:O	1.72	0.88
1:M:215:TYR:HB2	9:M:2102:HOH:O	1.72	0.86
1:M:165:LYS:HZ1	2:M:931:NAG:H82	1.34	0.86
1:M:130:LYS:HG3	9:M:2243:HOH:O	1.76	0.84
1:M:15:GLY:CA	9:M:2032:HOH:O	1.93	0.84
1:M:21:ASN:HD21	2:M:901:NAG:C2	1.88	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:151:GLU:OE1	9:M:2279:HOH:O	1.97	0.82
5:M:954:BMA:C6	5:M:957:MAN:H61	2.11	0.81
1:M:381:ASN:ND2	9:M:2554:HOH:O	2.14	0.79
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD2	2.61	0.78
7:M:1009:SO4:O1	9:M:4024:HOH:O	2.00	0.78
1:M:70:ASP:HB3	9:M:2078:HOH:O	1.83	0.76
3:M:983:NAG:H83	9:M:3062:HOH:O	1.86	0.76
5:M:954:BMA:C6	5:M:957:MAN:C6	2.65	0.74
1:M:373:LYS:NZ	9:M:2554:HOH:O	2.21	0.74
1:M:130:LYS:HB3	9:M:2091:HOH:O	1.87	0.74
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	2.22	0.74
1:M:90:ASN:ND2	2:M:911:NAG:C2	2.53	0.72
1:M:264:TYR:OH	1:M:264:TYR:CE2	2.42	0.71
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE2	2.24	0.71
1:M:9:ASN:HB2	9:M:4014:HOH:O	1.91	0.70
1:M:116:LYS:HG2	9:M:2225:HOH:O	1.92	0.70
3:M:921:NAG:O3	9:M:3019:HOH:O	2.10	0.70
1:M:472:ARG:NE	9:M:2659:HOH:O	2.20	0.70
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.67	0.69
1:M:493:GLN:NE2	9:M:2681:HOH:O	2.24	0.69
7:M:1004:SO4:S	7:M:1009:SO4:O3	2.51	0.68
1:M:70:ASP:OD2	9:M:2125:HOH:O	2.11	0.68
1:M:45:GLY:HA2	9:M:2085:HOH:O	1.93	0.68
7:M:1003:SO4:O2	9:M:4006:HOH:O	2.14	0.66
5:M:954:BMA:H61	5:M:957:MAN:H62	1.76	0.66
1:M:115:GLU:HG3	9:M:2223:HOH:O	1.95	0.66
1:M:111:ARG:O	9:M:2213:HOH:O	2.14	0.66
1:M:169[B]:ASP:HB2	1:M:240:LEU:HD21	1.78	0.65
1:M:472:ARG:NH2	9:M:2659:HOH:O	2.26	0.65
1:M:220[A]:SER:OG	9:M:2359:HOH:O	2.15	0.64
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.80	0.64
7:M:1003:SO4:O4	9:M:4006:HOH:O	2.16	0.63
1:M:200:LEU:HB3	9:M:2336:HOH:O	1.98	0.63
7:M:1004:SO4:O2	7:M:1009:SO4:O3	2.15	0.63
8:M:1010:GOL:O2	9:M:4026:HOH:O	2.01	0.61
7:M:1004:SO4:O1	7:M:1009:SO4:O3	2.20	0.60
1:M:365:HIS:HE1	9:M:2532:HOH:O	1.83	0.60
1:M:342[A]:VAL:HG13	9:M:2359:HOH:O	2.02	0.60
7:M:1004:SO4:S	7:M:1009:SO4:S	3.00	0.59
1:M:45:GLY:HA2	9:M:2086:HOH:O	2.03	0.58
1:M:159:GLN:NE2	9:M:2288:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.33	0.58
1:M:115:GLU:CD	9:M:2223:HOH:O	2.42	0.58
1:M:90:ASN:ND2	2:M:911:NAG:O5	2.36	0.58
1:M:115:GLU:OE2	9:M:2223:HOH:O	2.17	0.57
1:M:21:ASN:CG	2:M:901:NAG:C1	2.67	0.56
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.40	0.56
1:M:424:MET:HE3	9:M:2681:HOH:O	2.05	0.56
1:M:194:ARG:NH1	7:M:1009:SO4:O4	2.40	0.55
1:M:331:PHE:CD1	9:M:2483:HOH:O	2.53	0.55
1:M:165:LYS:HZ2	2:M:931:NAG:H82	1.67	0.55
5:M:954:BMA:C6	9:M:3055:HOH:O	2.47	0.55
1:M:21:ASN:ND2	2:M:901:NAG:C2	2.58	0.54
1:M:90:ASN:CG	2:M:911:NAG:C1	2.68	0.52
1:M:4:ILE:HD11	1:M:445:LYS:CD	2.39	0.52
1:M:244:ASN:HD21	2:M:931:NAG:C2	1.98	0.52
5:M:957:MAN:C4	9:M:3053:HOH:O	2.58	0.52
3:M:921:NAG:O3	3:M:921:NAG:C2	2.56	0.51
1:M:472:ARG:HG2	9:M:2658:HOH:O	2.11	0.51
1:M:21:ASN:ND2	2:M:901:NAG:O5	2.40	0.51
1:M:130:LYS:CB	9:M:2253:HOH:O	2.43	0.51
1:M:28:ASP:HA	9:M:2053:HOH:O	2.10	0.51
1:M:115:GLU:CG	9:M:2223:HOH:O	2.56	0.50
1:M:360[A]:ILE:HG23	9:M:2518:HOH:O	2.10	0.50
1:M:10:LEU:HD23	9:M:2023:HOH:O	2.12	0.49
1:M:108:LYS:HD2	9:M:2298:HOH:O	2.12	0.49
1:M:15:GLY:C	9:M:2032:HOH:O	2.34	0.48
1:M:70:ASP:CB	9:M:2078:HOH:O	2.51	0.48
1:M:360[A]:ILE:CG2	9:M:2518:HOH:O	2.61	0.48
1:M:95:ARG:HA	1:M:136:PHE:O	2.14	0.47
5:M:957:MAN:C5	9:M:3053:HOH:O	2.62	0.47
1:M:59:PRO:HB3	9:M:2100:HOH:O	2.14	0.47
5:M:954:BMA:O6	5:M:957:MAN:C6	2.49	0.46
1:M:12:PHE:HD2	9:M:2023:HOH:O	2.00	0.45
1:M:165:LYS:CE	2:M:931:NAG:H82	2.46	0.45
1:M:373:LYS:NZ	1:M:378:SER:OG	2.46	0.44
1:M:45:GLY:CA	9:M:2085:HOH:O	2.57	0.44
1:M:122:HIS:HE1	1:M:174:GLU:O	1.99	0.44
1:M:95:ARG:HB2	1:M:455:LEU:HD13	2.00	0.43
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:OH	2.05	0.43
1:M:497:THR:HG23	9:M:2689:HOH:O	2.19	0.42
1:M:59:PRO:HG3	9:M:2117:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:244:ASN:ND2	2:M:931:NAG:O5	2.42	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.42
1:M:12:PHE:N	9:M:2023:HOH:O	2.26	0.42
2:M:961:NAG:C6	9:M:3056:HOH:O	2.41	0.41
1:M:244:ASN:ND2	2:M:931:NAG:C2	2.68	0.41
1:M:48:LEU:N	9:M:2090:HOH:O	2.35	0.40
1:M:111:ARG:C	9:M:2213:HOH:O	2.58	0.40

All (21) 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:2279:HOH:O	9:M:2279:HOH:O[3_656]	1.10	1.10
9:M:2009:HOH:O	9:M:2520:HOH:O[4_576]	1.36	0.84
9:M:2248:HOH:O	9:M:2534:HOH:O[4_576]	1.37	0.83
9:M:2247:HOH:O	9:M:2247:HOH:O[4_576]	1.42	0.78
9:M:2555:HOH:O	9:M:2555:HOH:O[4_576]	1.44	0.76
9:M:2018:HOH:O	9:M:2018:HOH:O[4_576]	1.63	0.57
9:M:2258:HOH:O	9:M:2258:HOH:O[4_576]	1.63	0.57
9:M:2385:HOH:O	9:M:2426:HOH:O[6_565]	1.71	0.49
9:M:2116:HOH:O	9:M:2132:HOH:O[3_656]	1.76	0.44
9:M:2245:HOH:O	9:M:2621:HOH:O[4_576]	1.90	0.30
1:M:45:GLY:N	1:M:57:ARG:O[3_656]	1.95	0.25
9:M:2523:HOH:O	9:M:2622:HOH:O[4_576]	2.01	0.19
1:M:375:LYS:O	1:M:375:LYS:CD[4_576]	2.04	0.16
9:M:2388:HOH:O	9:M:2441:HOH:O[6_565]	2.06	0.14
1:M:379:THR:CG2	9:M:2603:HOH:O[4_576]	2.07	0.13
9:M:2018:HOH:O	9:M:2019:HOH:O[4_576]	2.08	0.12
1:M:43:THR:OG1	1:M:56:HIS:O[3_656]	2.10	0.10
9:M:2047:HOH:O	9:M:2127:HOH:O[3_656]	2.10	0.10
9:M:3057:HOH:O	9:M:2085:HOH:O[3_656]	2.12	0.08
9:M:4014:HOH:O	9:M:4014:HOH:O[4_576]	2.12	0.08

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	517/499 (104%)	503 (97%)	13 (2%)	1 (0%)	52 48

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	455/435 (105%)	454 (100%)	1 (0%)	95 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	244	ASN
1	M	365	HIS

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	5.95	7 (50%)	15,19,21	3.61	8 (53%)
3	NAG	M	923	3	14,14,15	2.78	3 (21%)	15,19,21	3.87	7 (46%)
4	NAG	M	941	1,4	14,14,15	0.55	0	15,19,21	1.98	4 (26%)
4	FUC	M	942	4	10,10,11	1.57	2 (20%)	14,14,16	2.20	4 (28%)
4	NAG	M	943	4	14,14,15	1.01	1 (7%)	15,19,21	1.33	2 (13%)
4	BMA	M	944	4	11,11,12	1.87	2 (18%)	14,15,17	1.70	4 (28%)
4	XYP	M	945	4	9,9,10	1.35	2 (22%)	12,12,14	2.70	4 (33%)
5	NAG	M	951	1,5	14,14,15	1.89	3 (21%)	15,19,21	2.16	3 (20%)
5	FUC	M	952	5	10,10,11	2.82	5 (50%)	14,14,16	1.90	2 (14%)
5	NAG	M	953	5	14,14,15	1.43	3 (21%)	15,19,21	1.66	4 (26%)
5	BMA	M	954	5	11,11,12	2.58	3 (27%)	14,15,17	4.51	8 (57%)
5	XYP	M	955	5	9,9,10	1.93	3 (33%)	12,12,14	2.70	5 (41%)
5	MAN	M	956	5	11,11,12	1.84	2 (18%)	14,15,17	2.80	8 (57%)
5	MAN	M	957	5	11,11,12	2.95	6 (54%)	14,15,17	7.39	11 (78%)
3	NAG	M	981	1,3	14,14,15	2.38	3 (21%)	15,19,21	2.45	3 (20%)
3	NAG	M	983	3	14,14,15	1.40	3 (21%)	15,19,21	2.22	7 (46%)

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	1/1/4/5	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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	954	BMA	C2-C3	-7.12	1.42	1.52
3	M	981	NAG	O7-C7	-6.36	1.08	1.23
3	M	923	NAG	C6-C5	-5.84	1.31	1.51
5	M	951	NAG	C1-C2	-5.26	1.45	1.52
3	M	923	NAG	C4-C5	-4.54	1.43	1.53
3	M	921	NAG	C7-N2	-4.31	1.17	1.34
4	M	944	BMA	C2-C3	-4.28	1.46	1.52
5	M	953	NAG	C3-C2	-3.08	1.45	1.52
5	M	951	NAG	O5-C1	-2.45	1.39	1.43
5	M	951	NAG	C2-N2	-2.37	1.42	1.46
5	M	957	MAN	C6-C5	-2.23	1.44	1.51
3	M	981	NAG	O5-C1	-2.21	1.40	1.43
5	M	952	FUC	C4-C3	-2.02	1.47	1.52
4	M	945	XYP	O3B-C3B	2.03	1.47	1.43
5	M	954	BMA	O3-C3	2.05	1.47	1.43
3	M	983	NAG	C8-C7	2.08	1.54	1.50
5	M	957	MAN	O5-C1	2.10	1.47	1.43
4	M	942	FUC	O2-C2	2.11	1.48	1.43
5	M	953	NAG	C1-C2	2.17	1.55	1.52
3	M	983	NAG	C4-C5	2.25	1.57	1.53
5	M	953	NAG	O7-C7	2.30	1.28	1.23
4	M	943	NAG	C1-C2	2.31	1.55	1.52
5	M	952	FUC	C1-C2	2.36	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	945	XYP	C4B-C3B	2.39	1.55	1.52
5	M	955	XYP	O5B-C5B	2.55	1.47	1.42
5	M	957	MAN	C1-C2	2.57	1.58	1.52
4	M	944	BMA	O5-C5	2.58	1.49	1.43
3	M	921	NAG	O5-C5	2.70	1.49	1.43
3	M	921	NAG	O4-C4	2.74	1.49	1.43
5	M	955	XYP	O3B-C3B	2.83	1.49	1.43
4	M	942	FUC	C2-C3	2.93	1.56	1.52
3	M	983	NAG	C1-C2	3.03	1.56	1.52
3	M	921	NAG	C4-C5	3.07	1.59	1.53
5	M	957	MAN	O4-C4	3.10	1.50	1.43
5	M	956	MAN	C4-C5	3.20	1.59	1.53
5	M	955	XYP	C2B-C3B	3.29	1.57	1.52
5	M	952	FUC	O4-C4	3.44	1.51	1.43
5	M	954	BMA	C4-C5	3.44	1.60	1.53
3	M	921	NAG	C3-C2	3.62	1.60	1.52
5	M	957	MAN	C2-C3	3.68	1.57	1.52
5	M	956	MAN	O5-C5	4.28	1.52	1.43
3	M	981	NAG	C8-C7	4.65	1.59	1.50
5	M	952	FUC	C2-C3	5.15	1.59	1.52
5	M	952	FUC	C4-C5	5.16	1.63	1.52
3	M	923	NAG	O5-C5	6.52	1.57	1.43
5	M	957	MAN	O5-C5	7.21	1.59	1.43
3	M	921	NAG	O7-C7	7.34	1.40	1.23
3	M	921	NAG	O3-C3	19.50	1.89	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	957	MAN	C1-O5-C5	-17.00	90.67	112.25
5	M	957	MAN	O5-C5-C6	-8.83	88.23	107.35
3	M	923	NAG	C1-O5-C5	-8.27	101.75	112.25
3	M	921	NAG	O3-C3-C2	-7.80	93.66	109.11
3	M	921	NAG	C1-O5-C5	-6.76	103.67	112.25
5	M	957	MAN	O4-C4-C3	-6.54	95.62	110.34
5	M	954	BMA	O5-C5-C6	-6.47	93.34	107.35
5	M	957	MAN	C2-C3-C4	-6.38	100.20	111.04
5	M	954	BMA	O4-C4-C3	-6.11	96.58	110.34
5	M	951	NAG	C1-O5-C5	-6.11	104.50	112.25
5	M	952	FUC	C1-C2-C3	-5.77	102.72	109.54
4	M	945	XYP	C5B-C4B-C3B	-5.69	102.81	109.54
3	M	981	NAG	C8-C7-N2	-5.52	105.54	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	954	BMA	C1-C2-C3	-5.40	103.16	109.54
4	M	942	FUC	O3-C3-C2	-5.27	100.48	110.00
5	M	954	BMA	O2-C2-C3	-4.92	100.22	110.12
3	M	921	NAG	O4-C4-C5	-4.87	96.32	109.24
5	M	955	XYP	C5B-C4B-C3B	-4.83	103.83	109.54
5	M	955	XYP	O5B-C1B-C2B	-4.80	101.33	110.31
4	M	941	NAG	C1-O5-C5	-4.79	106.17	112.25
5	M	957	MAN	O5-C1-C2	-4.53	103.51	110.86
5	M	955	XYP	C4B-C3B-C2B	-4.43	106.86	111.24
4	M	941	NAG	C2-N2-C7	-4.15	117.70	123.04
3	M	921	NAG	C4-C3-C2	-4.10	104.86	111.23
4	M	942	FUC	C1-C2-C3	-4.06	104.74	109.54
4	M	945	XYP	O2B-C2B-C3B	-4.02	102.03	110.12
3	M	983	NAG	C2-N2-C7	-4.01	117.89	123.04
4	M	945	XYP	O3B-C3B-C2B	-3.92	102.91	110.00
5	M	956	MAN	C3-C4-C5	-3.88	103.44	110.20
3	M	921	NAG	O7-C7-C8	-3.85	114.99	122.06
5	M	956	MAN	C2-C3-C4	-3.69	104.77	111.04
3	M	923	NAG	C4-C3-C2	-3.63	105.59	111.23
3	M	983	NAG	C1-O5-C5	-3.49	107.81	112.25
3	M	981	NAG	C2-N2-C7	-3.48	118.56	123.04
3	M	923	NAG	O6-C6-C5	-3.48	99.85	111.33
5	M	956	MAN	O2-C2-C3	-3.46	103.16	110.12
5	M	957	MAN	C3-C4-C5	-3.40	104.27	110.20
4	M	942	FUC	O2-C2-C3	-3.33	103.43	110.12
4	M	943	NAG	C2-N2-C7	-3.32	118.77	123.04
3	M	921	NAG	O4-C4-C3	-3.30	102.91	110.34
3	M	921	NAG	O3-C3-C4	-3.24	103.03	110.34
5	M	956	MAN	O5-C5-C6	-3.20	100.42	107.35
3	M	983	NAG	C3-C4-C5	-2.98	105.00	110.20
3	M	983	NAG	O4-C4-C3	-2.96	103.67	110.34
3	M	983	NAG	C6-C5-C4	-2.91	105.83	113.02
5	M	954	BMA	C1-O5-C5	-2.86	108.62	112.25
5	M	953	NAG	C2-N2-C7	-2.78	119.47	123.04
5	M	951	NAG	O5-C5-C6	-2.76	101.37	107.35
5	M	955	XYP	O4B-C4B-C3B	-2.69	104.70	110.12
4	M	944	BMA	O5-C5-C6	-2.68	101.54	107.35
3	M	923	NAG	O5-C5-C6	-2.68	101.54	107.35
5	M	953	NAG	O4-C4-C3	-2.66	104.34	110.34
5	M	957	MAN	O2-C2-C1	-2.62	103.96	109.21
3	M	923	NAG	C3-C2-N2	-2.42	104.76	110.56
5	M	956	MAN	C6-C5-C4	-2.35	107.22	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	955	XYP	O2B-C2B-C3B	-2.34	105.41	110.12
4	M	943	NAG	O4-C4-C3	-2.30	105.15	110.34
4	M	942	FUC	O3-C3-C4	-2.26	105.25	110.34
5	M	953	NAG	C1-O5-C5	-2.23	109.42	112.25
4	M	941	NAG	C8-C7-N2	-2.21	111.87	116.11
3	M	983	NAG	C4-C3-C2	-2.12	107.94	111.23
5	M	953	NAG	O6-C6-C5	-2.01	104.69	111.33
4	M	941	NAG	C4-C3-C2	-2.01	108.11	111.23
5	M	952	FUC	C6-C5-C4	-2.01	109.13	113.08
4	M	944	BMA	C3-C4-C5	2.12	113.89	110.20
5	M	951	NAG	C2-N2-C7	2.19	125.86	123.04
5	M	956	MAN	C1-O5-C5	2.21	115.06	112.25
3	M	921	NAG	C8-C7-N2	2.32	120.56	116.11
3	M	983	NAG	O3-C3-C2	2.39	113.86	109.11
4	M	944	BMA	O3-C3-C4	2.50	115.98	110.34
5	M	956	MAN	O2-C2-C1	2.92	115.06	109.21
4	M	944	BMA	C2-C3-C4	3.02	116.17	111.04
4	M	945	XYP	C1B-C2B-C3B	3.59	113.78	109.54
5	M	954	BMA	C3-C4-C5	3.72	116.67	110.20
3	M	923	NAG	O3-C3-C4	4.26	119.92	110.34
5	M	957	MAN	O6-C6-C5	4.44	126.02	111.33
5	M	954	BMA	C6-C5-C4	5.69	127.05	113.02
5	M	956	MAN	C1-C2-C3	5.72	116.31	109.54
5	M	957	MAN	C1-C2-C3	5.91	116.53	109.54
3	M	981	NAG	O7-C7-N2	6.01	134.11	121.86
5	M	957	MAN	O4-C4-C5	8.20	130.98	109.24
3	M	923	NAG	C3-C4-C5	9.24	126.30	110.20
5	M	954	BMA	O4-C4-C5	9.40	134.15	109.24
5	M	957	MAN	C6-C5-C4	12.21	143.14	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	957	MAN	C5

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	921	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	954	BMA	7	0
5	M	957	MAN	8	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	1.88	1 (25%)	6,6,6	1.04	0
7	SO4	M	1003	-	4,4,4	0.83	0	6,6,6	0.72	0
7	SO4	M	1004	-	4,4,4	2.13	1 (25%)	6,6,6	1.94	2 (33%)
7	SO4	M	1005	-	4,4,4	0.48	0	6,6,6	0.32	0
7	SO4	M	1006	-	4,4,4	2.85	1 (25%)	6,6,6	3.18	3 (50%)
7	SO4	M	1007	-	4,4,4	1.67	1 (25%)	6,6,6	1.32	1 (16%)
7	SO4	M	1008	-	4,4,4	1.13	0	6,6,6	0.47	0
7	SO4	M	1009	-	4,4,4	2.25	2 (50%)	6,6,6	3.61	3 (50%)
8	GOL	M	1010	-	5,5,5	0.67	0	5,5,5	1.16	1 (20%)
8	GOL	M	1020	-	5,5,5	1.26	1 (20%)	5,5,5	1.05	0
8	GOL	M	1021	-	5,5,5	0.91	0	5,5,5	1.13	0
8	GOL	M	1023	-	5,5,5	0.62	0	5,5,5	1.03	0
8	GOL	M	1024	-	5,5,5	0.80	0	5,5,5	1.17	1 (20%)
2	NAG	M	901	1	14,14,15	1.16	1 (7%)	15,19,21	1.98	2 (13%)
2	NAG	M	911	1	14,14,15	1.59	2 (14%)	15,19,21	2.25	4 (26%)
2	NAG	M	931	1	14,14,15	1.97	5 (35%)	15,19,21	7.88	11 (73%)
2	NAG	M	961	1	14,14,15	1.33	2 (14%)	15,19,21	2.84	3 (20%)
2	NAG	M	971	1	14,14,15	1.30	1 (7%)	15,19,21	1.90	6 (40%)
2	NAG	M	991	1	14,14,15	1.22	1 (7%)	15,19,21	1.69	2 (13%)

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	1/1/5/7	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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	971	NAG	O7-C7	-4.04	1.13	1.23
2	M	931	NAG	O7-C7	-3.83	1.14	1.23
2	M	991	NAG	O7-C7	-3.69	1.14	1.23
2	M	931	NAG	C1-C2	-3.45	1.47	1.52
2	M	911	NAG	O7-C7	-3.35	1.15	1.23
7	M	1002	SO4	O3-S	-3.28	1.35	1.47
2	M	961	NAG	O7-C7	-3.28	1.15	1.23
2	M	901	NAG	O7-C7	-2.74	1.16	1.23
2	M	931	NAG	C2-N2	-2.54	1.41	1.46
2	M	931	NAG	O5-C1	-2.09	1.40	1.43
7	M	1009	SO4	O2-S	2.08	1.54	1.47
2	M	961	NAG	C2-N2	2.08	1.50	1.46
8	M	1020	GOL	O1-C1	2.13	1.51	1.42
7	M	1007	SO4	O2-S	2.15	1.54	1.47
2	M	931	NAG	O4-C4	2.97	1.50	1.43
7	M	1009	SO4	O1-S	3.61	1.59	1.47
7	M	1004	SO4	O1-S	3.83	1.60	1.47
2	M	911	NAG	O5-C5	3.85	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1006	SO4	O2-S	5.52	1.66	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	O7-C7-N2	-7.50	106.58	121.86
2	M	931	NAG	C1-O5-C5	-7.16	103.16	112.25
7	M	1006	SO4	O2-S-O1	-6.97	87.42	109.50
7	M	1009	SO4	O2-S-O1	-6.78	88.00	109.50
2	M	911	NAG	C1-O5-C5	-6.70	103.74	112.25
2	M	901	NAG	C1-O5-C5	-6.58	103.90	112.25
2	M	931	NAG	O7-C7-C8	-5.06	112.77	122.06
2	M	991	NAG	C4-C3-C2	-4.47	104.28	111.23
2	M	961	NAG	O3-C3-C2	-4.35	100.50	109.11
2	M	991	NAG	O3-C3-C2	-3.78	101.62	109.11
2	M	911	NAG	C4-C3-C2	-3.63	105.59	111.23
7	M	1004	SO4	O2-S-O1	-3.36	98.86	109.50
2	M	931	NAG	O4-C4-C5	-3.19	100.79	109.24
2	M	961	NAG	O4-C4-C5	-2.97	101.36	109.24
2	M	971	NAG	O5-C5-C6	-2.82	101.24	107.35
2	M	971	NAG	O3-C3-C2	-2.81	103.55	109.11
2	M	931	NAG	O4-C4-C3	-2.64	104.40	110.34
2	M	931	NAG	O5-C5-C6	-2.63	101.66	107.35
2	M	931	NAG	C4-C3-C2	-2.47	107.39	111.23
8	M	1024	GOL	C3-C2-C1	-2.41	101.68	111.12
7	M	1007	SO4	O2-S-O1	-2.35	102.06	109.50
2	M	901	NAG	C4-C3-C2	-2.15	107.88	111.23
2	M	911	NAG	O5-C5-C6	-2.07	102.87	107.35
7	M	1006	SO4	O3-S-O2	-2.05	91.08	110.19
7	M	1009	SO4	O3-S-O1	-2.04	91.24	110.19
2	M	911	NAG	O3-C3-C2	-2.01	105.13	109.11
7	M	1006	SO4	O4-S-O3	2.06	117.36	108.98
8	M	1010	GOL	O2-C2-C1	2.23	118.87	108.65
2	M	971	NAG	O7-C7-C8	2.23	126.15	122.06
2	M	971	NAG	C2-N2-C7	2.54	126.30	123.04
2	M	971	NAG	C1-O5-C5	2.77	115.77	112.25
7	M	1004	SO4	O4-S-O3	3.25	122.18	108.98
2	M	971	NAG	O4-C4-C3	3.32	117.82	110.34
2	M	931	NAG	C3-C4-C5	3.98	117.13	110.20
2	M	931	NAG	C3-C2-N2	4.16	120.53	110.56
7	M	1009	SO4	O4-S-O3	4.99	129.27	108.98
2	M	961	NAG	C1-O5-C5	8.95	123.61	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	C8-C7-N2	12.74	140.50	116.11
2	M	931	NAG	C2-N2-C7	23.85	153.68	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	961	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1003	SO4	2	0
7	M	1004	SO4	6	0
7	M	1009	SO4	8	0
8	M	1010	GOL	4	0
2	M	901	NAG	5	0
2	M	911	NAG	3	0
2	M	931	NAG	8	0
2	M	961	NAG	2	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M	499/499 (100%)	3.32	446 (89%) 0 0	12, 16, 30, 57	11 (2%)

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	8.9
1	M	376	ALA	7.8
1	M	23	SER	7.7
1	M	378	SER	7.4
1	M	345	THR	6.7
1	M	417	ASP	6.5
1	M	469	PHE	6.4
1	M	419	ASN	6.2
1	M	206	CYS	6.1
1	M	375	LYS	6.1
1	M	380	ASP	6.1
1	M	420	ARG	6.0
1	M	390	TYR	5.9
1	M	366[A]	TYR	5.9
1	M	482	ASN	5.8
1	M	12	PHE	5.8
1	M	10	LEU	5.7
1	M	360[A]	ILE	5.6
1	M	480	TRP	5.6
1	M	209	THR	5.6
1	M	18	ASP	5.6
1	M	374	ASP	5.6
1	M	457	TRP	5.6
1	M	481	ASN	5.5
1	M	17	THR	5.5
1	M	497	THR	5.4
1	M	20	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	M	79	TRP	5.3
1	M	339	PRO	5.3
1	M	152	TYR	5.2
1	M	138	THR	5.2
1	M	78	TYR	5.2
1	M	471	VAL	5.2
1	M	99	ALA	5.1
1	M	3	GLU	5.1
1	M	55	THR	5.1
1	M	144	LEU	5.1
1	M	362	ALA	5.0
1	M	283	LEU	5.0
1	M	30[A]	ILE	5.0
1	M	142	TRP	5.0
1	M	196	TYR	5.0
1	M	4	ILE	5.0
1	M	434	CYS	4.9
1	M	245	TYR	4.9
1	M	478	ILE	4.9
1	M	203	PRO	4.9
1	M	25	PHE	4.8
1	M	377	ASP	4.8
1	M	183	LEU	4.8
1	M	300	ILE	4.8
1	M	449[A]	VAL	4.8
1	M	89	LEU	4.8
1	M	167	TYR	4.8
1	M	305[A]	GLU	4.8
1	M	363[A]	SER	4.8
1	M	313	GLU	4.7
1	M	364	GLY	4.7
1	M	444	ILE	4.7
1	M	421	ASN	4.7
1	M	73	CYS	4.7
1	M	83	ILE	4.7
1	M	9	ASN	4.7
1	M	458	ALA	4.7
1	M	154	GLY	4.7
1	M	197	GLY	4.7
1	M	191	VAL	4.7
1	M	257	ILE	4.7
1	M	223	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	M	112	GLY	4.6
1	M	213[A]	SER	4.6
1	M	349	ALA	4.6
1	M	219	SER	4.6
1	M	404	LEU	4.6
1	M	140	PHE	4.6
1	M	371	PHE	4.6
1	M	71	THR	4.6
1	M	330	TYR	4.6
1	M	50	ILE	4.5
1	M	326	GLY	4.5
1	M	401	TYR	4.5
1	M	16	ASN	4.5
1	M	160	ILE	4.5
1	M	424	MET	4.5
1	M	492	GLY	4.5
1	M	36	SER	4.5
1	M	418	GLU	4.4
1	M	359	TYR	4.4
1	M	51	TRP	4.4
1	M	430	ILE	4.4
1	M	433	LEU	4.4
1	M	80	GLN	4.4
1	M	432	TYR	4.4
1	M	335	ALA	4.4
1	M	210	VAL	4.4
1	M	488	LEU	4.3
1	M	143	ASP	4.3
1	M	113	VAL	4.3
1	M	474	GLY	4.3
1	M	147	THR	4.3
1	M	132	GLY	4.3
1	M	342[A]	VAL	4.3
1	M	388	GLY	4.3
1	M	317	LEU	4.3
1	M	97	SER	4.3
1	M	465	PHE	4.2
1	M	396	PHE	4.2
1	M	208	PRO	4.2
1	M	128	LEU	4.2
1	M	13	THR	4.2
1	M	425	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	93	GLY	4.2
1	M	365	HIS	4.2
1	M	45	GLY	4.1
1	M	400	TYR	4.1
1	M	318	VAL	4.1
1	M	101[A]	SER	4.0
1	M	298	ILE	4.0
1	M	43	THR	4.0
1	M	52	ASP	4.0
1	M	490	LYS	4.0
1	M	500	SER	4.0
1	M	54	PHE	4.0
1	M	48	LEU	4.0
1	M	77	SER	4.0
1	M	334	TYR	4.0
1	M	415	PRO	4.0
1	M	485	ASP	3.9
1	M	164	PHE	3.9
1	M	115	GLU	3.9
1	M	370	LEU	3.9
1	M	459	LEU	3.9
1	M	129	ILE	3.9
1	M	59	PRO	3.9
1	M	341	PRO	3.9
1	M	310	PHE	3.9
1	M	274	ALA	3.9
1	M	63	GLY	3.9
1	M	5	THR	3.8
1	M	170	LEU	3.8
1	M	150	ASP	3.8
1	M	24	SER	3.8
1	M	94	TYR	3.8
1	M	470	THR	3.8
1	M	204	GLY	3.8
1	M	338[A]	SER	3.8
1	M	379	THR	3.8
1	M	139	LEU	3.8
1	M	357	LEU	3.8
1	M	215	TYR	3.8
1	M	90	ASN	3.7
1	M	344[A]	SER	3.7
1	M	350	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	11	PRO	3.7
1	M	53	GLY	3.7
1	M	200	LEU	3.7
1	M	29	PHE	3.7
1	M	157	ASP	3.7
1	M	226	VAL	3.7
1	M	260	TRP	3.7
1	M	308	PRO	3.7
1	M	240	LEU	3.7
1	M	281	PHE	3.6
1	M	141	HIS	3.6
1	M	182	TRP	3.6
1	M	324	PHE	3.6
1	M	177	ASP	3.6
1	M	272	ILE	3.6
1	M	151	GLU	3.6
1	M	443	VAL	3.6
1	M	103	ILE	3.6
1	M	499	ILE	3.6
1	M	428	THR	3.6
1	M	347	HIS	3.6
1	M	285	TRP	3.6
1	M	409	GLU	3.6
1	M	171	CYS	3.6
1	M	224	TYR	3.5
1	M	406	TYR	3.5
1	M	423	SER	3.5
1	M	118[A]	ILE	3.5
1	M	487	ASP	3.5
1	M	184	THR	3.5
1	M	148	LEU	3.5
1	M	290	LEU	3.5
1	M	38	TYR	3.5
1	M	395	TYR	3.5
1	M	26	SER	3.5
1	M	27	SER	3.5
1	M	264	TYR	3.5
1	M	66	HIS	3.5
1	M	124	LEU	3.5
1	M	146	GLN	3.5
1	M	403	PRO	3.4
1	M	211	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	304	GLY	3.4
1	M	162	ASP	3.4
1	M	169[A]	ASP	3.4
1	M	448	ASP	3.4
1	M	498	PHE	3.4
1	M	353	ALA	3.4
1	M	6	CYS	3.4
1	M	493	GLN	3.4
1	M	49	ASN	3.4
1	M	68	ASN	3.4
1	M	441	ASN	3.4
1	M	120	TYR	3.4
1	M	126[A]	SER	3.4
1	M	88[A]	GLU	3.4
1	M	33	VAL	3.4
1	M	301	ASP	3.4
1	M	479	ASP	3.4
1	M	56	HIS	3.4
1	M	106	ARG	3.4
1	M	7	GLN	3.4
1	M	491	SER	3.4
1	M	253	GLY	3.4
1	M	57	ARG	3.3
1	M	81	LYS	3.3
1	M	368	GLY	3.3
1	M	185	ILE	3.3
1	M	329	TYR	3.3
1	M	343	ASN	3.3
1	M	426	ASP	3.3
1	M	149	GLN	3.3
1	M	258	THR	3.3
1	M	275	THR	3.3
1	M	294	THR	3.3
1	M	221	THR	3.3
1	M	220[A]	SER	3.3
1	M	311	SER	3.3
1	M	192	PRO	3.3
1	M	42	GLY	3.3
1	M	455	LEU	3.3
1	M	161	ILE	3.3
1	M	76	PHE	3.3
1	M	85	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	172	PHE	3.3
1	M	145	PRO	3.3
1	M	452	LYS	3.2
1	M	60	ASN	3.2
1	M	121	TYR	3.2
1	M	484	THR	3.2
1	M	494	TRP	3.2
1	M	450	ASN	3.2
1	M	217	GLY	3.2
1	M	249	GLY	3.2
1	M	225	ILE	3.2
1	M	31	PHE	3.2
1	M	69	GLY	3.2
1	M	195	GLY	3.2
1	M	468	GLY	3.2
1	M	22	SER	3.2
1	M	75	SER	3.1
1	M	104	ILE	3.1
1	M	14	CYS	3.1
1	M	295	TYR	3.1
1	M	62[A]	SER	3.1
1	M	315	SER	3.1
1	M	296	PRO	3.1
1	M	28	ASP	3.1
1	M	98	ILE	3.1
1	M	265	ASN	3.1
1	M	271[A]	SER	3.1
1	M	322	TYR	3.1
1	M	214	CYS	3.1
1	M	47	GLY	3.1
1	M	303	VAL	3.1
1	M	156	LEU	3.1
1	M	186	ASN	3.1
1	M	255	THR	3.1
1	M	414	THR	3.1
1	M	84	ASP	3.1
1	M	399	LYS	3.1
1	M	286	PHE	3.1
1	M	381	ASN	3.1
1	M	187	GLN	3.1
1	M	95	ARG	3.1
1	M	37	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	278	MET	3.0
1	M	383	TYR	3.0
1	M	91	ALA	3.0
1	M	233	ALA	3.0
1	M	122	HIS	3.0
1	M	58	TYR	3.0
1	M	229	HIS	3.0
1	M	280	GLU	3.0
1	M	327	LEU	3.0
1	M	405	ILE	3.0
1	M	293	GLY	3.0
1	M	489	LYS	3.0
1	M	501	PRO	3.0
1	M	175	PHE	3.0
1	M	133	ILE	3.0
1	M	218	ASN	3.0
1	M	439	PHE	3.0
1	M	46	ARG	2.9
1	M	386	PRO	2.9
1	M	467	LYS	2.9
1	M	384	TYR	2.9
1	M	117	GLY	2.9
1	M	105	PRO	2.9
1	M	114	ASN	2.9
1	M	407	VAL	2.9
1	M	67	GLY	2.9
1	M	373	LYS	2.9
1	M	252	ILE	2.9
1	M	466	ASN	2.9
1	M	266	ASP	2.9
1	M	477	TYR	2.9
1	M	382	ILE	2.9
1	M	297	GLN	2.9
1	M	32	GLY	2.9
1	M	389	ILE	2.9
1	M	237	VAL	2.9
1	M	436	HIS	2.8
1	M	235	ALA	2.8
1	M	238	VAL	2.8
1	M	96	PHE	2.8
1	M	158	PRO	2.8
1	M	486	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	456	ALA	2.8
1	M	179	VAL	2.8
1	M	181	TYR	2.8
1	M	153	GLU	2.8
1	M	86	LEU	2.8
1	M	125	ILE	2.8
1	M	422	GLN	2.8
1	M	463	TYR	2.8
1	M	116	LYS	2.8
1	M	316	ASN	2.7
1	M	332	THR	2.7
1	M	472	ARG	2.7
1	M	130	LYS	2.7
1	M	356	LYS	2.7
1	M	427	TYR	2.7
1	M	246	THR	2.7
1	M	262	LEU	2.7
1	M	241	TYR	2.7
1	M	193	THR	2.7
1	M	227	ALA	2.7
1	M	451	VAL	2.7
1	M	437	LEU	2.7
1	M	201	ASP	2.7
1	M	21	ASN	2.7
1	M	287	MET	2.7
1	M	309[A]	SER	2.7
1	M	40	ILE	2.6
1	M	228	HIS	2.6
1	M	72	THR	2.6
1	M	65	ASP	2.6
1	M	100	TRP	2.6
1	M	398	ASN	2.6
1	M	496	GLN	2.6
1	M	194	ARG	2.6
1	M	207	SER	2.6
1	M	70	ASP	2.6
1	M	108	LYS	2.6
1	M	445	LYS	2.6
1	M	166	ASP	2.6
1	M	127	GLY	2.6
1	M	454	TYR	2.6
1	M	198	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	391	SER	2.6
1	M	64	PRO	2.6
1	M	107	GLY	2.6
1	M	232	LEU	2.6
1	M	168	ALA	2.6
1	M	202	ALA	2.6
1	M	216	ALA	2.6
1	M	346	ASN	2.6
1	M	188	LEU	2.5
1	M	137	VAL	2.5
1	M	392	VAL	2.5
1	M	178	SER	2.5
1	M	464	GLU	2.5
1	M	385	TYR	2.5
1	M	92	THR	2.5
1	M	473	PHE	2.5
1	M	325	LEU	2.5
1	M	410	ASN	2.5
1	M	247	HIS	2.5
1	M	331	PHE	2.5
1	M	307	LEU	2.5
1	M	205	ARG	2.5
1	M	462[A]	ASN	2.5
1	M	159	GLN	2.5
1	M	263	PRO	2.5
1	M	461	ASP	2.5
1	M	495	TYR	2.4
1	M	134	THR	2.4
1	M	8	GLU	2.4
1	M	476	SER	2.4
1	M	123	GLY	2.4
1	M	250	GLY	2.4
1	M	268	ASP	2.4
1	M	256	MET	2.4
1	M	431	ASP	2.4
1	M	35	SER	2.4
1	M	110	SER	2.4
1	M	321	SER	2.4
1	M	34	ALA	2.3
1	M	254	PRO	2.3
1	M	119	ASP	2.3
1	M	429	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	314	GLU	2.3
1	M	15	GLY	2.3
1	M	413	SER	2.3
1	M	174	GLU	2.3
1	M	190	SER	2.3
1	M	284	GLY	2.3
1	M	136	PHE	2.3
1	M	397	LYS	2.3
1	M	483	VAL	2.3
1	M	351	MET	2.3
1	M	109	ARG	2.3
1	M	475	LEU	2.3
1	M	438	CYS	2.3
1	M	416	GLY	2.2
1	M	261	PHE	2.2
1	M	236	LYS	2.2
1	M	447	LYS	2.2
1	M	102	ARG	2.2
1	M	44	ILE	2.2
1	M	155	PHE	2.2
1	M	87	ASP	2.2
1	M	222	GLU	2.2
1	M	282	PHE	2.2
1	M	292	ASN	2.1
1	M	239	ASP	2.1
1	M	231	LEU	2.1
1	M	244	ASN	2.1
1	M	189	TYR	2.1
1	M	74	ASP	2.1
1	M	289	PRO	2.1
1	M	320	GLY	2.1
1	M	340	ASN	2.1
1	M	242	ARG	2.1
1	M	288	GLY	2.1
1	M	163	ASP	2.1
1	M	402	ASN	2.0
1	M	348	THR	2.0
1	M	165	LYS	2.0
1	M	173	GLU	2.0
1	M	135	PRO	2.0
1	M	243	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	M	923	14/15	0.48	0.45	0.23	38,46,58,60	0
4	NAG	M	941	14/15	0.63	0.34	0.16	15,23,27,28	0
3	NAG	M	921	14/15	0.64	0.30	-0.34	20,24,33,38	0
3	NAG	M	981	14/15	0.66	0.30	-0.38	10,17,22,24	0
4	BMA	M	944	11/12	0.36	0.52	-	39,44,49,53	0
5	FUC	M	952	10/11	0.68	0.28	-	19,22,34,34	0
5	XYP	M	955	9/10	0.49	0.42	-	33,39,44,64	0
3	NAG	M	983	14/15	0.60	0.36	-	27,32,50,57	0
5	MAN	M	957	11/12	0.56	0.55	-	34,44,55,56	0
4	NAG	M	943	14/15	0.72	0.28	-	22,28,34,39	0
5	NAG	M	953	14/15	0.79	0.23	-	21,24,29,33	0
5	MAN	M	956	11/12	0.46	0.46	-	26,40,52,57	0
4	FUC	M	942	10/11	0.57	0.37	-	25,33,40,48	0
5	NAG	M	951	14/15	0.74	0.27	-	18,21,27,29	0
4	XYP	M	945	9/10	0.54	0.33	-	42,48,53,54	0
5	BMA	M	954	11/12	0.58	0.25	-	26,31,36,48	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	GOL	M	1010	6/6	0.47	0.54	9.42	36,43,45,52	6
7	SO4	M	1009	5/5	0.52	0.58	9.10	39,40,47,60	1
2	NAG	M	931	14/15	0.64	0.41	5.27	36,43,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	M	961	14/15	0.57	0.64	5.04	44,51,63,69	0
8	GOL	M	1020	6/6	0.52	0.42	2.29	6,15,19,19	1
7	SO4	M	1002	5/5	0.82	0.34	0.66	27,30,33,38	5
2	NAG	M	901	14/15	0.49	0.39	0.17	26,35,47,49	0
7	SO4	M	1004	5/5	0.80	0.26	-0.41	15,28,31,35	5
8	GOL	M	1024	6/6	0.66	0.30	-0.44	16,17,23,23	0
8	GOL	M	1021	6/6	0.73	0.23	-1.10	12,22,27,32	6
7	SO4	M	1006	5/5	0.79	0.50	-	26,31,35,36	5
2	NAG	M	971	14/15	0.52	0.38	-	57,65,70,71	0
2	NAG	M	991	14/15	0.37	0.65	-	35,41,54,57	0
7	SO4	M	1007	5/5	0.77	0.35	-	14,34,35,38	5
7	SO4	M	1008	5/5	0.80	0.30	-	34,36,39,39	5
7	SO4	M	1005	5/5	0.73	0.31	-	18,22,27,29	0
7	SO4	M	1003	5/5	0.63	0.52	-	26,29,36,37	5
2	NAG	M	911	14/15	0.65	0.29	-	25,28,37,46	0
8	GOL	M	1023	6/6	0.47	0.61	-	31,32,43,46	6
6	ZN	M	1001	1/1	0.85	0.18	-	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.