Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:03 PM GMT

PDB ID	:	1DWF
Title	:	STUDY ON RADIATION DAMAGE ON A CRYOCOOLED CRYSTAL. PART 2: STRUCTURE AFTER IRRADIATION WITH 9.1*10E15 PHOTONS/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 (i) symbol.

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

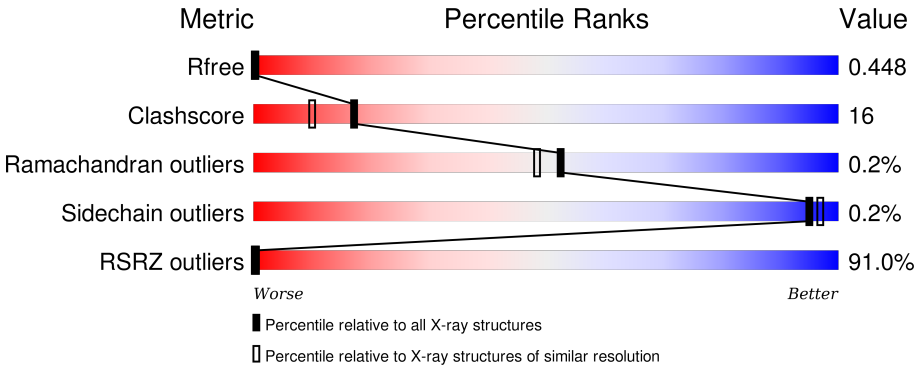
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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 <=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	91% 82% 16%

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	1506	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	M	1519	X	-	-	X
3	NAG	M	1505	-	-	-	X
5	BMA	M	1515	-	-	X	-
5	MAN	M	1518	X	-	X	-
7	SO4	M	1526	-	-	X	-
7	SO4	M	1527	-	-	X	-
7	SO4	M	1529	-	X	-	-
7	SO4	M	1532	-	X	X	X
8	GOL	M	1533	-	-	X	X
8	GOL	M	1534	-	-	-	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.

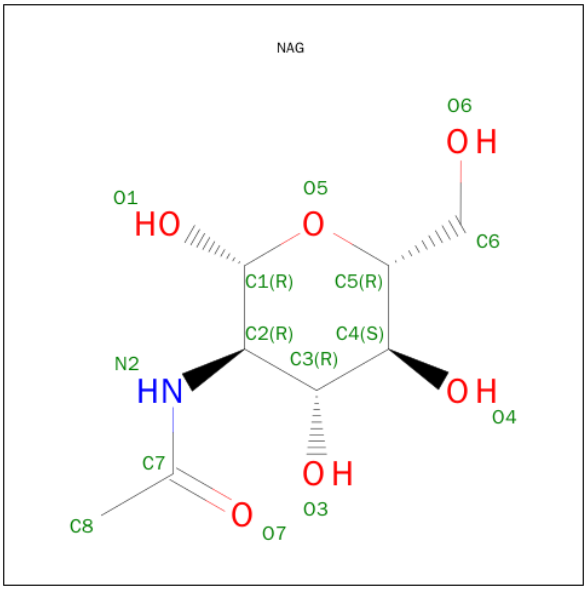
- Molecule 1 is a protein called MYROSINASE MA1.

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		

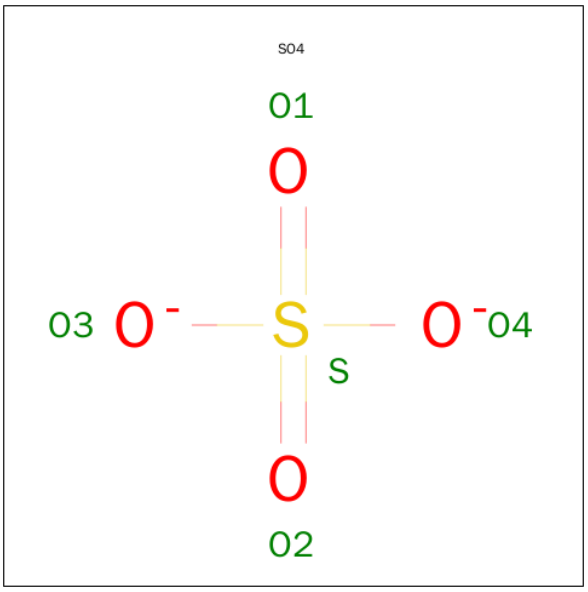
- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

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).

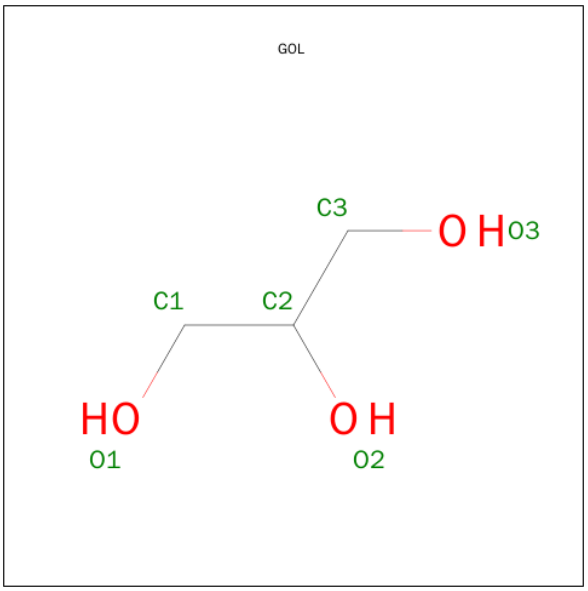
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Zn	0	0
			1	1		

- 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.

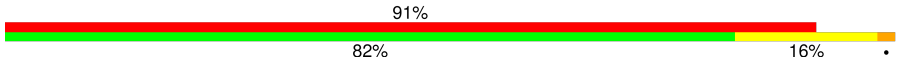
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	63	Total O 63 63	0	0
9	M	689	Total O 689 689	0	0
9	W	36	Total O 36 36	0	0

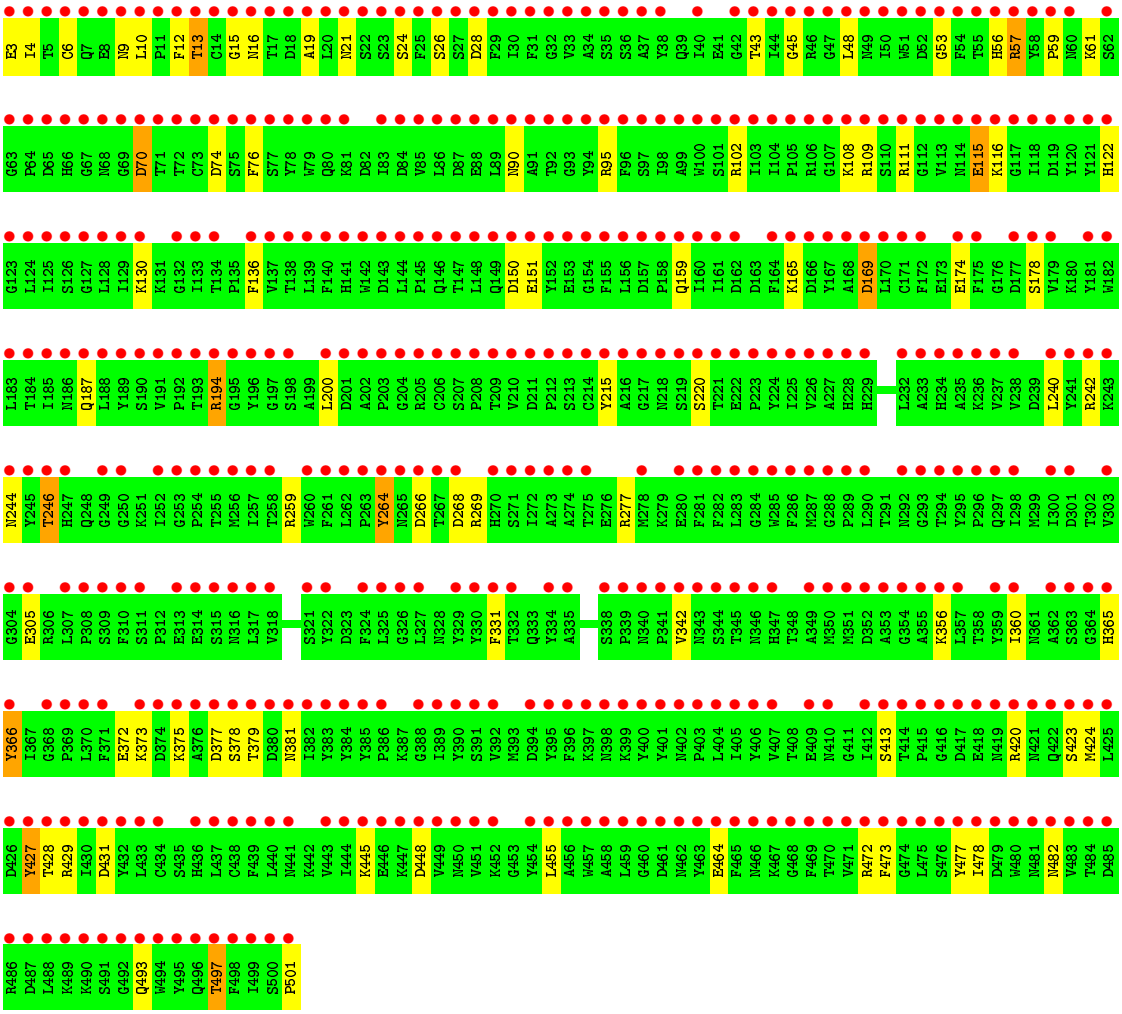
3 Residue-property plots (i)

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)	17.40 – 2.00 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (17.40-2.00) 98.7 (9.94-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	6.70 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.169 , 0.180 0.435 , 0.448	Depositor DCC
R_{free} test set	2440 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 58.2	EDS
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 50380 reflections	Xtriage
F_o,F_c correlation	0.66	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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	1.15	18/4291 (0.4%)	1.32	41/5835 (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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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	1518	MAN	C5

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	13	THR	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	3835	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	9	0
8	M	30	0	39	4	0
9	G	63	0	0	7	1
9	M	689	0	0	62	16
9	W	36	0	0	8	1
All	All	5220	0	4116	134	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 (134) 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:1506:NAG:C1	0.96	1.56
1:M:21:ASN:HD21	2:M:1502: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:1533:GOL:C1	9:W:2026: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:1504:NAG:O3	3:M:1504: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:1533:GOL:H11	9:W:2026: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:1533:GOL:C2	9:W:2026: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:1527:SO4:O2	7:M:1532:SO4:S	2.19	1.00
1:M:165:LYS:NZ	2:M:1506:NAG:H82	1.76	0.99
2:M:1519:NAG:H61	9:G:2056: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:1515:BMA:H61	5:M:1518:MAN:C6	2.03	0.89
5:M:1515:BMA:H61	5:M:1518: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:1506: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:1502:NAG:C2	1.88	0.83
1:M:151:GLU:OE1	9:M:2279:HOH:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1515:BMA:C6	5:M:1518: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:1532:SO4:O1	9:W:2024:HOH:O	2.00	0.78
1:M:70:ASP:HB3	9:M:2078:HOH:O	1.83	0.76
3:M:1522:NAG:H83	9:G:2062:HOH:O	1.86	0.76
5:M:1515:BMA:C6	5:M:1518: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:1503: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:W:2014:HOH:O	1.91	0.70
1:M:116:LYS:HG2	9:M:2225:HOH:O	1.92	0.70
3:M:1504:NAG:O3	9:G:2019: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:1527:SO4:S	7:M:1532: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:1526:SO4:O2	9:W:2006:HOH:O	2.14	0.66
5:M:1515:BMA:H61	5:M:1518: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:1526:SO4:O4	9:W:2006:HOH:O	2.16	0.63
1:M:200:LEU:HB3	9:M:2336:HOH:O	1.98	0.63
7:M:1527:SO4:O2	7:M:1532:SO4:O3	2.15	0.63
8:M:1533:GOL:O2	9:W:2026:HOH:O	2.01	0.61
7:M:1527:SO4:O1	7:M:1532: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:1527:SO4:S	7:M:1532: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
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:GLU:CD	9:M:2223:HOH:O	2.42	0.58
1:M:90:ASN:ND2	2:M:1503: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:1502: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:1532: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:1506:NAG:H82	1.67	0.55
5:M:1515:BMA:C6	9:G:2055:HOH:O	2.47	0.55
1:M:21:ASN:ND2	2:M:1502:NAG:C2	2.58	0.54
1:M:90:ASN:CG	2:M:1503: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:1506:NAG:C2	1.98	0.52
5:M:1518:MAN:C4	9:G:2053:HOH:O	2.58	0.52
3:M:1504:NAG:O3	3:M:1504: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:1502: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:1518:MAN:C5	9:G:2053:HOH:O	2.62	0.47
1:M:59:PRO:HB3	9:M:2100:HOH:O	2.14	0.47
5:M:1515:BMA:O6	5:M:1518: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:1506: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
1:M:244:ASN:ND2	2:M:1506:NAG:O5	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1519:NAG:C6	9:G:2056:HOH:O	2.41	0.41
1:M:244:ASN:ND2	2:M:1506: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:1524:ZN:ZN	6:M:1524: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:2085:HOH:O	9:G:2057:HOH:O[3_656]	2.12	0.08
9:W:2014:HOH:O	9:W:2014:HOH:O[4_576]	2.12	0.08

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	M	518/499 (104%)	504 (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	456/435 (105%)	455 (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 (i)

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	1504	1,3	14,14,15	5.95	7 (50%)	15,19,21	3.61	8 (53%)
3	NAG	M	1505	3	14,14,15	2.78	3 (21%)	15,19,21	3.87	7 (46%)
4	NAG	M	1507	1,4	14,14,15	0.55	0	15,19,21	1.98	4 (26%)
4	FUC	M	1508	4	10,10,11	1.57	2 (20%)	14,14,16	2.20	4 (28%)
4	NAG	M	1509	4	14,14,15	1.01	1 (7%)	15,19,21	1.33	2 (13%)
4	BMA	M	1510	4	11,11,12	1.87	2 (18%)	14,15,17	1.70	4 (28%)
4	XYP	M	1511	4	9,9,10	1.35	2 (22%)	12,12,14	2.70	4 (33%)
5	NAG	M	1512	1,5	14,14,15	1.89	3 (21%)	15,19,21	2.16	3 (20%)
5	FUC	M	1513	5	10,10,11	2.82	5 (50%)	14,14,16	1.90	2 (14%)
5	NAG	M	1514	5	14,14,15	1.43	3 (21%)	15,19,21	1.66	4 (26%)
5	BMA	M	1515	5	11,11,12	2.58	3 (27%)	14,15,17	4.51	8 (57%)
5	XYP	M	1516	5	9,9,10	1.93	3 (33%)	12,12,14	2.70	5 (41%)
5	MAN	M	1517	5	11,11,12	1.84	2 (18%)	14,15,17	2.80	8 (57%)
5	MAN	M	1518	5	11,11,12	2.95	6 (54%)	14,15,17	7.39	11 (78%)
3	NAG	M	1521	1,3	14,14,15	2.38	3 (21%)	15,19,21	2.45	3 (20%)
3	NAG	M	1522	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	1504	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	1505	3	-	0/6/23/26	0/1/1/1
4	NAG	M	1507	1,4	-	0/6/23/26	0/1/1/1
4	FUC	M	1508	4	-	0/0/17/20	0/1/1/1
4	NAG	M	1509	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	M	1510	4	-	0/2/19/22	0/1/1/1
4	XYP	M	1511	4	-	0/0/14/17	0/1/1/1
5	NAG	M	1512	1,5	-	0/6/23/26	0/1/1/1
5	FUC	M	1513	5	-	0/0/17/20	0/1/1/1
5	NAG	M	1514	5	-	0/6/23/26	0/1/1/1
5	BMA	M	1515	5	-	0/2/19/22	0/1/1/1
5	XYP	M	1516	5	-	0/0/14/17	0/1/1/1
5	MAN	M	1517	5	-	0/2/19/22	0/1/1/1
5	MAN	M	1518	5	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	M	1521	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	1522	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	1515	BMA	C2-C3	-7.12	1.42	1.52
3	M	1521	NAG	O7-C7	-6.36	1.08	1.23
3	M	1505	NAG	C6-C5	-5.84	1.31	1.51
5	M	1512	NAG	C1-C2	-5.26	1.45	1.52
3	M	1505	NAG	C4-C5	-4.54	1.43	1.53
3	M	1504	NAG	C7-N2	-4.31	1.17	1.34
4	M	1510	BMA	C2-C3	-4.28	1.46	1.52
5	M	1514	NAG	C3-C2	-3.08	1.45	1.52
5	M	1512	NAG	O5-C1	-2.45	1.39	1.43
5	M	1512	NAG	C2-N2	-2.37	1.42	1.46
5	M	1518	MAN	C6-C5	-2.23	1.44	1.51
3	M	1521	NAG	O5-C1	-2.21	1.40	1.43
5	M	1513	FUC	C4-C3	-2.02	1.47	1.52
4	M	1511	XYP	O3B-C3B	2.03	1.47	1.43
5	M	1515	BMA	O3-C3	2.05	1.47	1.43
3	M	1522	NAG	C8-C7	2.08	1.54	1.50
5	M	1518	MAN	O5-C1	2.10	1.47	1.43
4	M	1508	FUC	O2-C2	2.11	1.48	1.43
5	M	1514	NAG	C1-C2	2.17	1.55	1.52
3	M	1522	NAG	C4-C5	2.25	1.57	1.53
5	M	1514	NAG	O7-C7	2.30	1.28	1.23
4	M	1509	NAG	C1-C2	2.31	1.55	1.52
5	M	1513	FUC	C1-C2	2.36	1.57	1.52
4	M	1511	XYP	C4B-C3B	2.39	1.55	1.52
5	M	1516	XYP	O5B-C5B	2.55	1.47	1.42
5	M	1518	MAN	C1-C2	2.57	1.58	1.52
4	M	1510	BMA	O5-C5	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1504	NAG	O5-C5	2.70	1.49	1.43
3	M	1504	NAG	O4-C4	2.74	1.49	1.43
5	M	1516	XYP	O3B-C3B	2.83	1.49	1.43
4	M	1508	FUC	C2-C3	2.93	1.56	1.52
3	M	1522	NAG	C1-C2	3.03	1.56	1.52
3	M	1504	NAG	C4-C5	3.07	1.59	1.53
5	M	1518	MAN	O4-C4	3.10	1.50	1.43
5	M	1517	MAN	C4-C5	3.20	1.59	1.53
5	M	1516	XYP	C2B-C3B	3.29	1.57	1.52
5	M	1513	FUC	O4-C4	3.44	1.51	1.43
5	M	1515	BMA	C4-C5	3.44	1.60	1.53
3	M	1504	NAG	C3-C2	3.62	1.60	1.52
5	M	1518	MAN	C2-C3	3.68	1.57	1.52
5	M	1517	MAN	O5-C5	4.28	1.52	1.43
3	M	1521	NAG	C8-C7	4.65	1.59	1.50
5	M	1513	FUC	C2-C3	5.15	1.59	1.52
5	M	1513	FUC	C4-C5	5.16	1.63	1.52
3	M	1505	NAG	O5-C5	6.52	1.57	1.43
5	M	1518	MAN	O5-C5	7.21	1.59	1.43
3	M	1504	NAG	O7-C7	7.34	1.40	1.23
3	M	1504	NAG	O3-C3	19.50	1.89	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1518	MAN	C1-O5-C5	-17.00	90.67	112.25
5	M	1518	MAN	O5-C5-C6	-8.83	88.23	107.35
3	M	1505	NAG	C1-O5-C5	-8.27	101.75	112.25
3	M	1504	NAG	O3-C3-C2	-7.80	93.66	109.11
3	M	1504	NAG	C1-O5-C5	-6.76	103.67	112.25
5	M	1518	MAN	O4-C4-C3	-6.54	95.62	110.34
5	M	1515	BMA	O5-C5-C6	-6.47	93.34	107.35
5	M	1518	MAN	C2-C3-C4	-6.38	100.20	111.04
5	M	1515	BMA	O4-C4-C3	-6.11	96.58	110.34
5	M	1512	NAG	C1-O5-C5	-6.11	104.50	112.25
5	M	1513	FUC	C1-C2-C3	-5.77	102.72	109.54
4	M	1511	XYP	C5B-C4B-C3B	-5.69	102.81	109.54
3	M	1521	NAG	C8-C7-N2	-5.52	105.54	116.11
5	M	1515	BMA	C1-C2-C3	-5.40	103.16	109.54
4	M	1508	FUC	O3-C3-C2	-5.27	100.48	110.00
5	M	1515	BMA	O2-C2-C3	-4.92	100.22	110.12
3	M	1504	NAG	O4-C4-C5	-4.87	96.32	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1516	XYP	C5B-C4B-C3B	-4.83	103.83	109.54
5	M	1516	XYP	O5B-C1B-C2B	-4.80	101.33	110.31
4	M	1507	NAG	C1-O5-C5	-4.79	106.17	112.25
5	M	1518	MAN	O5-C1-C2	-4.53	103.51	110.86
5	M	1516	XYP	C4B-C3B-C2B	-4.43	106.86	111.24
4	M	1507	NAG	C2-N2-C7	-4.15	117.70	123.04
3	M	1504	NAG	C4-C3-C2	-4.10	104.86	111.23
4	M	1508	FUC	C1-C2-C3	-4.06	104.74	109.54
4	M	1511	XYP	O2B-C2B-C3B	-4.02	102.03	110.12
3	M	1522	NAG	C2-N2-C7	-4.01	117.89	123.04
4	M	1511	XYP	O3B-C3B-C2B	-3.92	102.91	110.00
5	M	1517	MAN	C3-C4-C5	-3.88	103.44	110.20
3	M	1504	NAG	O7-C7-C8	-3.85	114.99	122.06
5	M	1517	MAN	C2-C3-C4	-3.69	104.77	111.04
3	M	1505	NAG	C4-C3-C2	-3.63	105.59	111.23
3	M	1522	NAG	C1-O5-C5	-3.49	107.81	112.25
3	M	1521	NAG	C2-N2-C7	-3.48	118.56	123.04
3	M	1505	NAG	O6-C6-C5	-3.48	99.85	111.33
5	M	1517	MAN	O2-C2-C3	-3.46	103.16	110.12
5	M	1518	MAN	C3-C4-C5	-3.40	104.27	110.20
4	M	1508	FUC	O2-C2-C3	-3.33	103.43	110.12
4	M	1509	NAG	C2-N2-C7	-3.32	118.77	123.04
3	M	1504	NAG	O4-C4-C3	-3.30	102.91	110.34
3	M	1504	NAG	O3-C3-C4	-3.24	103.03	110.34
5	M	1517	MAN	O5-C5-C6	-3.20	100.42	107.35
3	M	1522	NAG	C3-C4-C5	-2.98	105.00	110.20
3	M	1522	NAG	O4-C4-C3	-2.96	103.67	110.34
3	M	1522	NAG	C6-C5-C4	-2.91	105.83	113.02
5	M	1515	BMA	C1-O5-C5	-2.86	108.62	112.25
5	M	1514	NAG	C2-N2-C7	-2.78	119.47	123.04
5	M	1512	NAG	O5-C5-C6	-2.76	101.37	107.35
5	M	1516	XYP	O4B-C4B-C3B	-2.69	104.70	110.12
4	M	1510	BMA	O5-C5-C6	-2.68	101.54	107.35
3	M	1505	NAG	O5-C5-C6	-2.68	101.54	107.35
5	M	1514	NAG	O4-C4-C3	-2.66	104.34	110.34
5	M	1518	MAN	O2-C2-C1	-2.62	103.96	109.21
3	M	1505	NAG	C3-C2-N2	-2.42	104.76	110.56
5	M	1517	MAN	C6-C5-C4	-2.35	107.22	113.02
5	M	1516	XYP	O2B-C2B-C3B	-2.34	105.41	110.12
4	M	1509	NAG	O4-C4-C3	-2.30	105.15	110.34
4	M	1508	FUC	O3-C3-C4	-2.26	105.25	110.34
5	M	1514	NAG	C1-O5-C5	-2.23	109.42	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1507	NAG	C8-C7-N2	-2.21	111.87	116.11
3	M	1522	NAG	C4-C3-C2	-2.12	107.94	111.23
5	M	1514	NAG	O6-C6-C5	-2.01	104.69	111.33
4	M	1507	NAG	C4-C3-C2	-2.01	108.11	111.23
5	M	1513	FUC	C6-C5-C4	-2.01	109.13	113.08
4	M	1510	BMA	C3-C4-C5	2.12	113.89	110.20
5	M	1512	NAG	C2-N2-C7	2.19	125.86	123.04
5	M	1517	MAN	C1-O5-C5	2.21	115.06	112.25
3	M	1504	NAG	C8-C7-N2	2.32	120.56	116.11
3	M	1522	NAG	O3-C3-C2	2.39	113.86	109.11
4	M	1510	BMA	O3-C3-C4	2.50	115.98	110.34
5	M	1517	MAN	O2-C2-C1	2.92	115.06	109.21
4	M	1510	BMA	C2-C3-C4	3.02	116.17	111.04
4	M	1511	XYP	C1B-C2B-C3B	3.59	113.78	109.54
5	M	1515	BMA	C3-C4-C5	3.72	116.67	110.20
3	M	1505	NAG	O3-C3-C4	4.26	119.92	110.34
5	M	1518	MAN	O6-C6-C5	4.44	126.02	111.33
5	M	1515	BMA	C6-C5-C4	5.69	127.05	113.02
5	M	1517	MAN	C1-C2-C3	5.72	116.31	109.54
5	M	1518	MAN	C1-C2-C3	5.91	116.53	109.54
3	M	1521	NAG	O7-C7-N2	6.01	134.11	121.86
5	M	1518	MAN	O4-C4-C5	8.20	130.98	109.24
3	M	1505	NAG	C3-C4-C5	9.24	126.30	110.20
5	M	1515	BMA	O4-C4-C5	9.40	134.15	109.24
5	M	1518	MAN	C6-C5-C4	12.21	143.14	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1518	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	1504	NAG	3	0
5	M	1515	BMA	7	0
5	M	1518	MAN	8	0
3	M	1522	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	$\#\|Z\| > 2$
2	NAG	M	1502	1	14,14,15	1.16	1 (7%)	15,19,21	1.98	2 (13%)
2	NAG	M	1503	1	14,14,15	1.59	2 (14%)	15,19,21	2.25	4 (26%)
2	NAG	M	1506	1	14,14,15	1.97	5 (35%)	15,19,21	7.88	11 (73%)
2	NAG	M	1519	1	14,14,15	1.33	2 (14%)	15,19,21	2.84	3 (20%)
2	NAG	M	1520	1	14,14,15	1.30	1 (7%)	15,19,21	1.90	6 (40%)
2	NAG	M	1523	1	14,14,15	1.22	1 (7%)	15,19,21	1.69	2 (13%)
7	SO4	M	1525	-	4,4,4	1.88	1 (25%)	6,6,6	1.04	0
7	SO4	M	1526	-	4,4,4	0.83	0	6,6,6	0.72	0
7	SO4	M	1527	7	4,4,4	2.13	1 (25%)	6,6,6	1.94	2 (33%)
7	SO4	M	1528	-	4,4,4	0.48	0	6,6,6	0.32	0
7	SO4	M	1529	-	4,4,4	2.85	1 (25%)	6,6,6	3.18	3 (50%)
7	SO4	M	1530	-	4,4,4	1.67	1 (25%)	6,6,6	1.32	1 (16%)
7	SO4	M	1531	-	4,4,4	1.13	0	6,6,6	0.47	0
7	SO4	M	1532	7	4,4,4	2.25	2 (50%)	6,6,6	3.61	3 (50%)
8	GOL	M	1533	-	5,5,5	0.67	0	5,5,5	1.16	1 (20%)
8	GOL	M	1534	-	5,5,5	1.26	1 (20%)	5,5,5	1.05	0
8	GOL	M	1535	-	5,5,5	0.91	0	5,5,5	1.13	0
8	GOL	M	1536	-	5,5,5	0.62	0	5,5,5	1.03	0
8	GOL	M	1537	-	5,5,5	0.80	0	5,5,5	1.17	1 (20%)

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
2	NAG	M	1502	1	-	0/6/23/26	0/1/1/1
2	NAG	M	1503	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	1506	1	-	0/6/23/26	0/1/1/1
2	NAG	M	1519	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	M	1520	1	-	0/6/23/26	0/1/1/1
2	NAG	M	1523	1	-	0/6/23/26	0/1/1/1
7	SO4	M	1525	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1526	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1527	7	-	0/0/0/0	0/0/0/0
7	SO4	M	1528	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1529	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1530	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1531	-	-	0/0/0/0	0/0/0/0
7	SO4	M	1532	7	-	0/0/0/0	0/0/0/0
8	GOL	M	1533	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1534	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1535	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1536	-	-	0/4/4/4	0/0/0/0
8	GOL	M	1537	-	-	0/4/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1520	NAG	O7-C7	-4.04	1.13	1.23
2	M	1506	NAG	O7-C7	-3.83	1.14	1.23
2	M	1523	NAG	O7-C7	-3.69	1.14	1.23
2	M	1506	NAG	C1-C2	-3.45	1.47	1.52
2	M	1503	NAG	O7-C7	-3.35	1.15	1.23
7	M	1525	SO4	O3-S	-3.28	1.35	1.47
2	M	1519	NAG	O7-C7	-3.28	1.15	1.23
2	M	1502	NAG	O7-C7	-2.74	1.16	1.23
2	M	1506	NAG	C2-N2	-2.54	1.41	1.46
2	M	1506	NAG	O5-C1	-2.09	1.40	1.43
7	M	1532	SO4	O2-S	2.08	1.54	1.47
2	M	1519	NAG	C2-N2	2.08	1.50	1.46
8	M	1534	GOL	O1-C1	2.13	1.51	1.42
7	M	1530	SO4	O2-S	2.15	1.54	1.47
2	M	1506	NAG	O4-C4	2.97	1.50	1.43
7	M	1532	SO4	O1-S	3.61	1.59	1.47
7	M	1527	SO4	O1-S	3.83	1.60	1.47
2	M	1503	NAG	O5-C5	3.85	1.51	1.43
7	M	1529	SO4	O2-S	5.52	1.66	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	1506	NAG	O7-C7-N2	-7.50	106.58	121.86
2	M	1506	NAG	C1-O5-C5	-7.16	103.16	112.25
7	M	1529	SO4	O2-S-O1	-6.97	87.42	109.50
7	M	1532	SO4	O2-S-O1	-6.78	88.00	109.50
2	M	1503	NAG	C1-O5-C5	-6.70	103.74	112.25
2	M	1502	NAG	C1-O5-C5	-6.58	103.90	112.25
2	M	1506	NAG	O7-C7-C8	-5.06	112.77	122.06
2	M	1523	NAG	C4-C3-C2	-4.47	104.28	111.23
2	M	1519	NAG	O3-C3-C2	-4.35	100.50	109.11
2	M	1523	NAG	O3-C3-C2	-3.78	101.62	109.11
2	M	1503	NAG	C4-C3-C2	-3.63	105.59	111.23
7	M	1527	SO4	O2-S-O1	-3.36	98.86	109.50
2	M	1506	NAG	O4-C4-C5	-3.19	100.79	109.24
2	M	1519	NAG	O4-C4-C5	-2.97	101.36	109.24
2	M	1520	NAG	O5-C5-C6	-2.82	101.24	107.35
2	M	1520	NAG	O3-C3-C2	-2.81	103.55	109.11
2	M	1506	NAG	O4-C4-C3	-2.64	104.40	110.34
2	M	1506	NAG	O5-C5-C6	-2.63	101.66	107.35
2	M	1506	NAG	C4-C3-C2	-2.47	107.39	111.23
8	M	1537	GOL	C3-C2-C1	-2.41	101.68	111.12
7	M	1530	SO4	O2-S-O1	-2.35	102.06	109.50
2	M	1502	NAG	C4-C3-C2	-2.15	107.88	111.23
2	M	1503	NAG	O5-C5-C6	-2.07	102.87	107.35
7	M	1529	SO4	O3-S-O2	-2.05	91.08	110.19
7	M	1532	SO4	O3-S-O1	-2.04	91.24	110.19
2	M	1503	NAG	O3-C3-C2	-2.01	105.13	109.11
7	M	1529	SO4	O4-S-O3	2.06	117.36	108.98
8	M	1533	GOL	O2-C2-C1	2.23	118.87	108.65
2	M	1520	NAG	O7-C7-C8	2.23	126.15	122.06
2	M	1520	NAG	C2-N2-C7	2.54	126.30	123.04
2	M	1520	NAG	C1-O5-C5	2.77	115.77	112.25
7	M	1527	SO4	O4-S-O3	3.25	122.18	108.98
2	M	1520	NAG	O4-C4-C3	3.32	117.82	110.34
2	M	1506	NAG	C3-C4-C5	3.98	117.13	110.20
2	M	1506	NAG	C3-C2-N2	4.16	120.53	110.56
7	M	1532	SO4	O4-S-O3	4.99	129.27	108.98
2	M	1519	NAG	C1-O5-C5	8.95	123.61	112.25
2	M	1506	NAG	C8-C7-N2	12.74	140.50	116.11
2	M	1506	NAG	C2-N2-C7	23.85	153.68	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	1519	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1502	NAG	5	0
2	M	1503	NAG	3	0
2	M	1506	NAG	8	0
2	M	1519	NAG	2	0
7	M	1526	SO4	2	0
7	M	1527	SO4	5	0
7	M	1532	SO4	7	0
8	M	1533	GOL	4	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, 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%)	3.33	454 (90%)	0	9, 13, 27, 54	3 (0%)

All (454) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	8.6
1	M	376	ALA	7.5
1	M	23	SER	7.5
1	M	378	SER	7.2
1	M	345	THR	7.0
1	M	469	PHE	6.7
1	M	417	ASP	6.5
1	M	380	ASP	6.4
1	M	419	ASN	6.4
1	M	420	ARG	6.3
1	M	375	LYS	6.1
1	M	17	THR	5.9
1	M	390	TYR	5.9
1	M	366[A]	TYR	5.9
1	M	206	CYS	5.8
1	M	481	ASN	5.8
1	M	339	PRO	5.8
1	M	360[A]	ILE	5.7
1	M	79	TRP	5.6
1	M	78	TYR	5.6
1	M	457	TRP	5.6
1	M	482	ASN	5.6
1	M	480	TRP	5.6
1	M	138	THR	5.5
1	M	374	ASP	5.4
1	M	83	ILE	5.4
1	M	471	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	M	497	THR	5.4
1	M	209	THR	5.3
1	M	4	ILE	5.3
1	M	18	ASP	5.3
1	M	10	LEU	5.3
1	M	197	GLY	5.2
1	M	144	LEU	5.1
1	M	283	LEU	5.1
1	M	196	TYR	5.1
1	M	449[A]	VAL	5.1
1	M	421	ASN	5.0
1	M	112	GLY	5.0
1	M	152	TYR	5.0
1	M	3	GLU	5.0
1	M	478	ILE	4.9
1	M	213[A]	SER	4.9
1	M	30[A]	ILE	4.9
1	M	444	ILE	4.9
1	M	12	PHE	4.9
1	M	458	ALA	4.9
1	M	167	TYR	4.8
1	M	362	ALA	4.8
1	M	55	THR	4.8
1	M	371	PHE	4.8
1	M	89	LEU	4.8
1	M	245	TYR	4.8
1	M	300	ILE	4.8
1	M	80	GLN	4.8
1	M	434	CYS	4.8
1	M	73	CYS	4.7
1	M	51	TRP	4.7
1	M	305[A]	GLU	4.7
1	M	142	TRP	4.7
1	M	25	PHE	4.7
1	M	50	ILE	4.7
1	M	36	SER	4.7
1	M	99	ALA	4.7
1	M	20[A]	LEU	4.7
1	M	219	SER	4.6
1	M	363[A]	SER	4.6
1	M	488	LEU	4.6
1	M	424	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	M	128	LEU	4.6
1	M	9	ASN	4.6
1	M	113	VAL	4.6
1	M	208	PRO	4.6
1	M	415	PRO	4.6
1	M	364	GLY	4.6
1	M	16	ASN	4.5
1	M	183	LEU	4.5
1	M	147	THR	4.5
1	M	210	VAL	4.5
1	M	465	PHE	4.5
1	M	71	THR	4.5
1	M	379	THR	4.5
1	M	377	ASP	4.5
1	M	97	SER	4.4
1	M	418	GLU	4.4
1	M	160	ILE	4.4
1	M	223	PRO	4.4
1	M	388	GLY	4.4
1	M	203	PRO	4.3
1	M	154	GLY	4.3
1	M	470	THR	4.3
1	M	13	THR	4.3
1	M	48	LEU	4.3
1	M	27	SER	4.3
1	M	140	PHE	4.3
1	M	330	TYR	4.3
1	M	433	LEU	4.3
1	M	349	ALA	4.3
1	M	215	TYR	4.2
1	M	257	ILE	4.2
1	M	344[A]	SER	4.2
1	M	94	TYR	4.2
1	M	43	THR	4.2
1	M	54	PHE	4.2
1	M	313	GLU	4.2
1	M	342[A]	VAL	4.2
1	M	317	LEU	4.2
1	M	459	LEU	4.2
1	M	396	PHE	4.2
1	M	404	LEU	4.2
1	M	359	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	129	ILE	4.1
1	M	191	VAL	4.1
1	M	298	ILE	4.1
1	M	485	ASP	4.1
1	M	45	GLY	4.1
1	M	334	TYR	4.1
1	M	400	TYR	4.1
1	M	281	PHE	4.1
1	M	338[A]	SER	4.1
1	M	59	PRO	4.1
1	M	430	ILE	4.1
1	M	499	ILE	4.1
1	M	484	THR	4.1
1	M	93	GLY	4.1
1	M	492	GLY	4.1
1	M	318	VAL	4.0
1	M	432	TYR	4.0
1	M	132	GLY	4.0
1	M	326	GLY	4.0
1	M	401	TYR	4.0
1	M	24	SER	4.0
1	M	101[A]	SER	4.0
1	M	370	LEU	4.0
1	M	474	GLY	4.0
1	M	500	SER	4.0
1	M	115	GLU	3.9
1	M	29	PHE	3.9
1	M	164	PHE	3.9
1	M	335	ALA	3.9
1	M	425	LEU	3.9
1	M	308	PRO	3.9
1	M	90	ASN	3.9
1	M	143	ASP	3.9
1	M	53	GLY	3.8
1	M	170	LEU	3.8
1	M	490	LYS	3.8
1	M	38	TYR	3.8
1	M	63	GLY	3.8
1	M	169[A]	ASP	3.8
1	M	310	PHE	3.8
1	M	365	HIS	3.8
1	M	479	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	139	LEU	3.7
1	M	88[A]	GLU	3.7
1	M	200	LEU	3.7
1	M	103	ILE	3.7
1	M	428	THR	3.7
1	M	249	GLY	3.7
1	M	357	LEU	3.7
1	M	414	THR	3.7
1	M	493	GLN	3.7
1	M	177	ASP	3.6
1	M	11	PRO	3.6
1	M	274	ALA	3.6
1	M	315	SER	3.6
1	M	395	TYR	3.6
1	M	52	ASP	3.6
1	M	60	ASN	3.6
1	M	148	LEU	3.6
1	M	264	TYR	3.6
1	M	260	TRP	3.6
1	M	285	TRP	3.6
1	M	324	PHE	3.6
1	M	409	GLU	3.6
1	M	498	PHE	3.6
1	M	211	ASP	3.6
1	M	106	ARG	3.6
1	M	350	MET	3.6
1	M	118[A]	ILE	3.5
1	M	204	GLY	3.5
1	M	157	ASP	3.5
1	M	275	THR	3.5
1	M	66	HIS	3.5
1	M	304	GLY	3.5
1	M	368	GLY	3.5
1	M	278	MET	3.5
1	M	192	PRO	3.5
1	M	443	VAL	3.5
1	M	240	LEU	3.5
1	M	5	THR	3.5
1	M	62[A]	SER	3.5
1	M	151	GLU	3.5
1	M	81	LYS	3.5
1	M	58	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	258	THR	3.4
1	M	69	GLY	3.4
1	M	77	SER	3.4
1	M	68	ASN	3.4
1	M	124	LEU	3.4
1	M	441	ASN	3.4
1	M	141	HIS	3.4
1	M	341	PRO	3.4
1	M	290	LEU	3.4
1	M	122	HIS	3.4
1	M	156	LEU	3.4
1	M	491	SER	3.4
1	M	121	TYR	3.4
1	M	85	VAL	3.3
1	M	104	ILE	3.3
1	M	149	GLN	3.3
1	M	382	ILE	3.3
1	M	120	TYR	3.3
1	M	49	ASN	3.3
1	M	84	ASP	3.3
1	M	271[A]	SER	3.3
1	M	311	SER	3.3
1	M	296	PRO	3.3
1	M	31	PHE	3.3
1	M	172	PHE	3.3
1	M	57	ARG	3.3
1	M	347	HIS	3.3
1	M	294	THR	3.3
1	M	26	SER	3.3
1	M	33	VAL	3.3
1	M	226	VAL	3.3
1	M	272	ILE	3.3
1	M	56	HIS	3.3
1	M	426	ASP	3.3
1	M	146	GLN	3.3
1	M	184	THR	3.3
1	M	75	SER	3.2
1	M	76	PHE	3.2
1	M	489	LYS	3.2
1	M	150	ASP	3.2
1	M	422	GLN	3.2
1	M	295	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	423	SER	3.2
1	M	28	ASP	3.2
1	M	42	GLY	3.2
1	M	353	ALA	3.2
1	M	381	ASN	3.2
1	M	220[A]	SER	3.2
1	M	47	GLY	3.2
1	M	329	TYR	3.2
1	M	406	TYR	3.2
1	M	237	VAL	3.2
1	M	126[A]	SER	3.2
1	M	448	ASP	3.2
1	M	403	PRO	3.2
1	M	214	CYS	3.2
1	M	224	TYR	3.2
1	M	162	ASP	3.1
1	M	22	SER	3.1
1	M	95	ARG	3.1
1	M	117	GLY	3.1
1	M	145	PRO	3.1
1	M	332	THR	3.1
1	M	384	TYR	3.1
1	M	452	LYS	3.1
1	M	494	TRP	3.1
1	M	451	VAL	3.1
1	M	171	CYS	3.1
1	M	286	PHE	3.1
1	M	487	ASP	3.1
1	M	373	LYS	3.1
1	M	217	GLY	3.1
1	M	327	LEU	3.0
1	M	72	THR	3.0
1	M	182	TRP	3.0
1	M	445	LYS	3.0
1	M	161	ILE	3.0
1	M	405	ILE	3.0
1	M	297	GLN	3.0
1	M	450	ASN	3.0
1	M	185	ILE	3.0
1	M	225	ILE	3.0
1	M	195	GLY	3.0
1	M	187	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	252	ILE	3.0
1	M	346	ASN	3.0
1	M	399	LYS	3.0
1	M	98	ILE	3.0
1	M	218	ASN	3.0
1	M	466	ASN	3.0
1	M	46	ARG	3.0
1	M	181	TYR	3.0
1	M	235	ALA	3.0
1	M	14	CYS	2.9
1	M	64	PRO	2.9
1	M	383	TYR	2.9
1	M	175	PHE	2.9
1	M	265	ASN	2.9
1	M	32	GLY	2.9
1	M	216	ALA	2.9
1	M	468	GLY	2.9
1	M	86	LEU	2.9
1	M	437	LEU	2.9
1	M	238	VAL	2.9
1	M	343	ASN	2.9
1	M	439	PHE	2.9
1	M	100	TRP	2.9
1	M	301	ASP	2.9
1	M	233	ALA	2.9
1	M	221	THR	2.9
1	M	108	LYS	2.9
1	M	6	CYS	2.9
1	M	91	ALA	2.9
1	M	386	PRO	2.9
1	M	455	LEU	2.9
1	M	303	VAL	2.9
1	M	37	ALA	2.9
1	M	114	ASN	2.9
1	M	463	TYR	2.9
1	M	134	THR	2.9
1	M	229	HIS	2.8
1	M	125	ILE	2.8
1	M	133	ILE	2.8
1	M	105	PRO	2.8
1	M	385	TYR	2.8
1	M	486	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	67	GLY	2.8
1	M	389	ILE	2.8
1	M	193	THR	2.8
1	M	123	GLY	2.8
1	M	322	TYR	2.8
1	M	287	MET	2.8
1	M	116	LYS	2.8
1	M	391	SER	2.8
1	M	427	TYR	2.8
1	M	309[A]	SER	2.8
1	M	188	LEU	2.8
1	M	501	PRO	2.8
1	M	356	LYS	2.8
1	M	70	ASP	2.8
1	M	107	GLY	2.8
1	M	316	ASN	2.8
1	M	496	GLN	2.8
1	M	246	THR	2.7
1	M	284	GLY	2.7
1	M	436	HIS	2.7
1	M	201	ASP	2.7
1	M	35	SER	2.7
1	M	186	ASN	2.7
1	M	467	LYS	2.7
1	M	130	LYS	2.7
1	M	293	GLY	2.7
1	M	179	VAL	2.7
1	M	266	ASP	2.7
1	M	456	ALA	2.7
1	M	153	GLU	2.7
1	M	96	PHE	2.7
1	M	198	SER	2.7
1	M	331	PHE	2.7
1	M	228	HIS	2.6
1	M	158	PRO	2.6
1	M	7	GLN	2.6
1	M	15	GLY	2.6
1	M	473	PHE	2.6
1	M	178	SER	2.6
1	M	413	SER	2.6
1	M	280	GLU	2.6
1	M	262	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	407	VAL	2.6
1	M	21	ASN	2.6
1	M	477	TYR	2.6
1	M	232	LEU	2.6
1	M	429	ARG	2.6
1	M	110	SER	2.6
1	M	168	ALA	2.6
1	M	136	PHE	2.6
1	M	119	ASP	2.6
1	M	207	SER	2.6
1	M	351	MET	2.6
1	M	464	GLU	2.6
1	M	392	VAL	2.6
1	M	241	TYR	2.5
1	M	253	GLY	2.5
1	M	92	THR	2.5
1	M	307	LEU	2.5
1	M	472	ARG	2.5
1	M	476	SER	2.5
1	M	398	ASN	2.5
1	M	454	TYR	2.5
1	M	261	PHE	2.5
1	M	34	ALA	2.5
1	M	227	ALA	2.5
1	M	250	GLY	2.5
1	M	40	ILE	2.5
1	M	461	ASP	2.5
1	M	462[A]	ASN	2.5
1	M	65	ASP	2.5
1	M	483	VAL	2.5
1	M	255	THR	2.5
1	M	205	ARG	2.5
1	M	410	ASN	2.5
1	M	242	ARG	2.5
1	M	194	ARG	2.4
1	M	137	VAL	2.4
1	M	431	ASP	2.4
1	M	314	GLU	2.4
1	M	263	PRO	2.4
1	M	247	HIS	2.4
1	M	352	ASP	2.4
1	M	438	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	159	GLN	2.3
1	M	127	GLY	2.3
1	M	416	GLY	2.3
1	M	74	ASP	2.3
1	M	475	LEU	2.3
1	M	202	ALA	2.3
1	M	44	ILE	2.3
1	M	19	ALA	2.3
1	M	325	LEU	2.3
1	M	102	ARG	2.3
1	M	495	TYR	2.3
1	M	165	LYS	2.3
1	M	166	ASP	2.3
1	M	236	LYS	2.3
1	M	292	ASN	2.3
1	M	412	ILE	2.2
1	M	447	LYS	2.2
1	M	189	TYR	2.2
1	M	267	THR	2.2
1	M	355	ALA	2.2
1	M	222	GLU	2.2
1	M	397	LYS	2.2
1	M	354	GLY	2.2
1	M	155	PHE	2.2
1	M	340	ASN	2.2
1	M	109	ARG	2.1
1	M	234	HIS	2.1
1	M	288	GLY	2.1
1	M	282	PHE	2.1
1	M	8	GLU	2.1
1	M	289	PRO	2.1
1	M	394	ASP	2.1
1	M	321	SER	2.1
1	M	440	LEU	2.1
1	M	369	PRO	2.1
1	M	270	HIS	2.1
1	M	268	ASP	2.1
1	M	174	GLU	2.1
1	M	254	PRO	2.1
1	M	244	ASN	2.1
1	M	273	ALA	2.1
1	M	460	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	111	ARG	2.0
1	M	256	MET	2.0
1	M	446	GLU	2.0
1	M	87	ASP	2.0
1	M	243	LYS	2.0
1	M	402	ASN	2.0
1	M	190	SER	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
3	NAG	M	1505	14/15	0.49	0.46	0.33	35,43,55,57	0
4	NAG	M	1507	14/15	0.64	0.34	0.18	13,20,25,25	0
3	NAG	M	1521	14/15	0.65	0.31	-0.11	7,14,19,21	0
3	NAG	M	1504	14/15	0.63	0.31	-0.23	17,21,30,35	0
5	NAG	M	1514	14/15	0.79	0.24	-	18,21,26,30	0
4	XYP	M	1511	9/10	0.54	0.34	-	39,46,50,52	0
4	FUC	M	1508	10/11	0.59	0.38	-	22,30,37,46	0
5	XYP	M	1516	9/10	0.48	0.42	-	30,36,41,61	0
3	NAG	M	1522	14/15	0.57	0.36	-	24,29,47,54	0
5	MAN	M	1518	11/12	0.54	0.56	-	31,41,52,53	0
5	NAG	M	1512	14/15	0.75	0.27	-	15,18,24,27	0
5	MAN	M	1517	11/12	0.42	0.47	-	23,37,49,54	0
5	FUC	M	1513	10/11	0.64	0.30	-	17,19,31,31	0
4	NAG	M	1509	14/15	0.71	0.30	-	19,25,31,36	0
4	BMA	M	1510	11/12	0.34	0.51	-	36,41,46,51	0
5	BMA	M	1515	11/12	0.53	0.27	-	23,28,33,45	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
7	SO4	M	1532	5/5	0.52	0.58	10.36	36,38,44,57	1
8	GOL	M	1533	6/6	0.47	0.52	9.74	34,40,42,49	6
2	NAG	M	1506	14/15	0.63	0.43	4.89	33,40,46,47	0
2	NAG	M	1519	14/15	0.57	0.64	4.79	41,48,60,66	0
8	GOL	M	1534	6/6	0.53	0.42	3.10	3,12,16,16	1
7	SO4	M	1525	5/5	0.81	0.38	1.19	24,27,30,35	5
2	NAG	M	1502	14/15	0.47	0.40	0.35	23,32,44,46	0
7	SO4	M	1527	5/5	0.77	0.27	-0.17	12,26,28,32	5
8	GOL	M	1537	6/6	0.65	0.28	-0.68	13,14,20,20	0
8	GOL	M	1535	6/6	0.74	0.23	-1.34	9,19,24,29	6
6	ZN	M	1524	1/1	0.84	0.19	-	34,34,34,34	0
2	NAG	M	1503	14/15	0.64	0.31	-	22,25,34,43	0
2	NAG	M	1523	14/15	0.35	0.66	-	32,38,51,54	0
7	SO4	M	1530	5/5	0.76	0.34	-	11,31,32,35	5
7	SO4	M	1531	5/5	0.74	0.33	-	31,33,36,37	5
7	SO4	M	1528	5/5	0.72	0.31	-	15,19,24,27	0
7	SO4	M	1529	5/5	0.78	0.49	-	24,28,32,33	5
2	NAG	M	1520	14/15	0.57	0.40	-	54,62,68,68	0
7	SO4	M	1526	5/5	0.60	0.53	-	23,26,33,34	5
8	GOL	M	1536	6/6	0.52	0.57	-	29,29,41,43	6

6.5 Other polymers

There are no such residues in this entry.