



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2017 – 05:58 PM EDT

PDB ID : 1DWF
Title : Study on radiation damage on a cryocooled crystal. Part 2: Structure after irradiation with 9.1×10^{15} 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

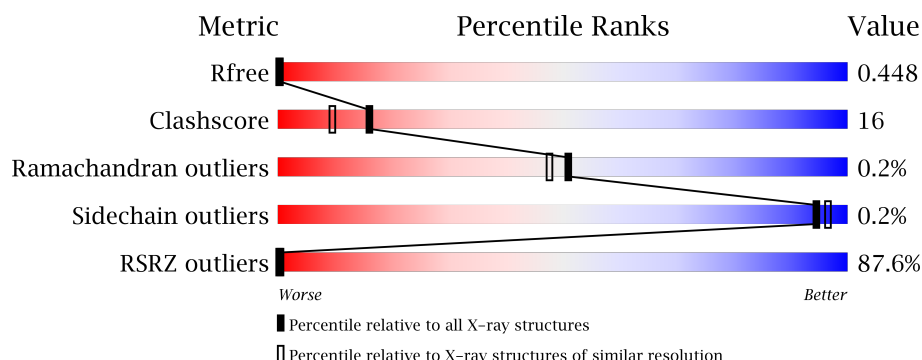
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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	<div> <div>88%</div> <div>82%16%.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	M	1505	-	-	-	X
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
4	BMA	M	1515	-	-	X	-
6	MAN	M	1518	X	-	X	-
8	SO4	M	1526	-	-	X	-
8	SO4	M	1527	-	-	X	-
8	SO4	M	1529	-	X	-	-
8	SO4	M	1532	-	X	X	X
9	GOL	M	1533	-	-	X	X
9	GOL	M	1534	-	-	-	X

2 Entry composition [i](#)

There are 10 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.

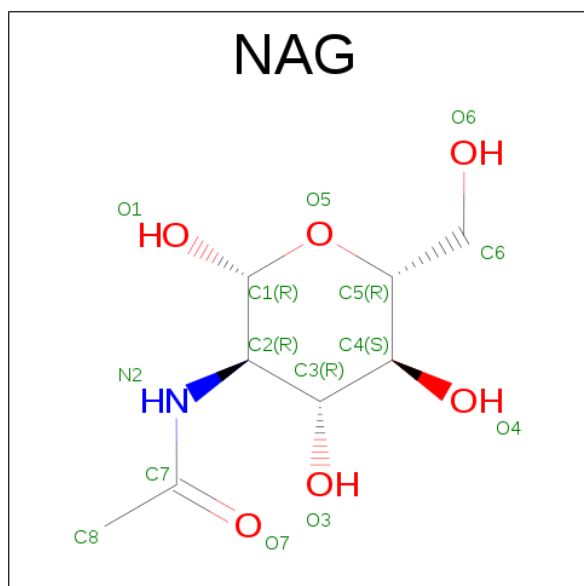
- Molecule 1 is a protein called MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	499	4083	2619	660	788	16	0	21	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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



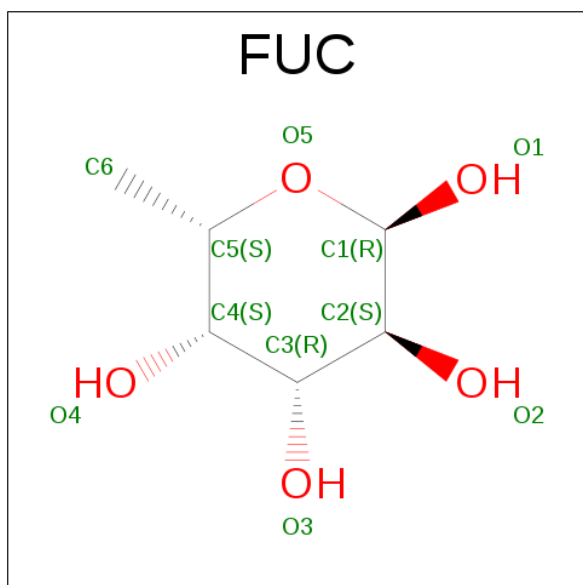
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	M	1	14	8	1	5	0	0
2	M	1	14	8	1	5	0	0
2	M	1	14	8	1	5	0	0

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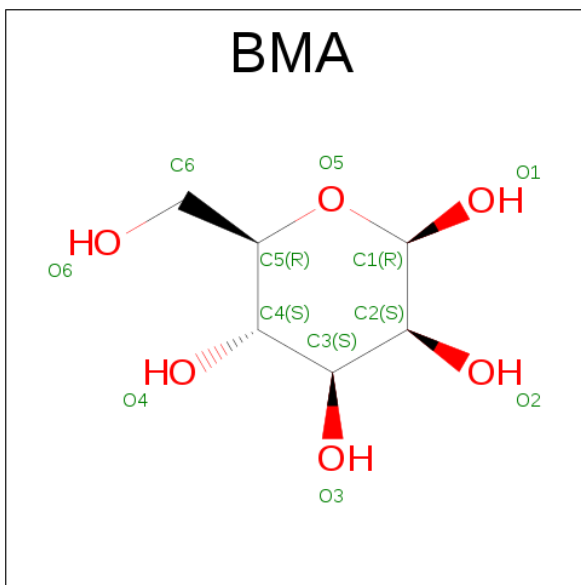
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1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

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



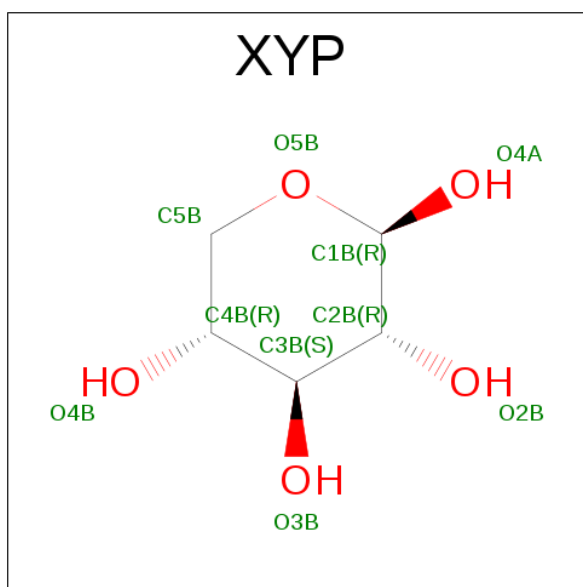
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			10	6	4		
3	M	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



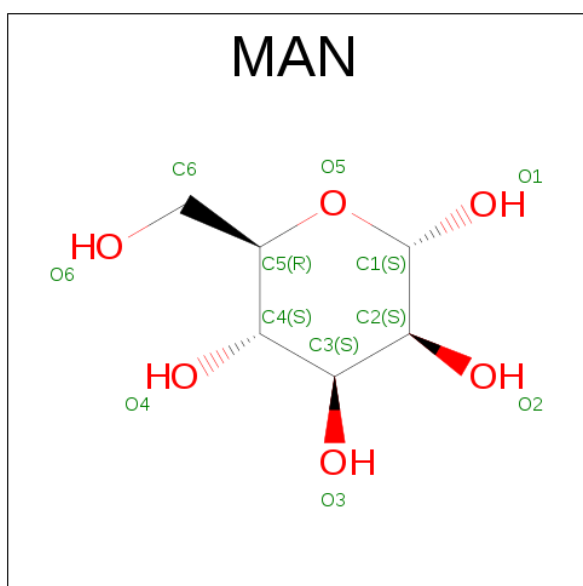
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			11	6	5		
4	M	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is BETA-D-XYLOPYRANOSE (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	C	O	0	0
			9	5	4		
5	M	1	Total	C	O	0	0
			9	5	4		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

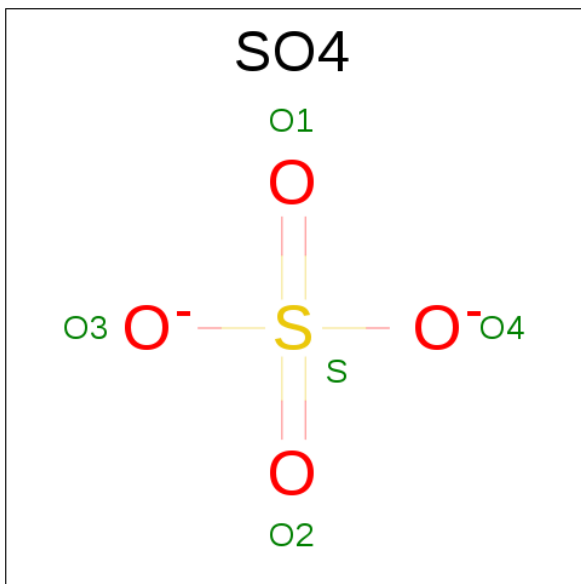


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			11	6	5		
6	M	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

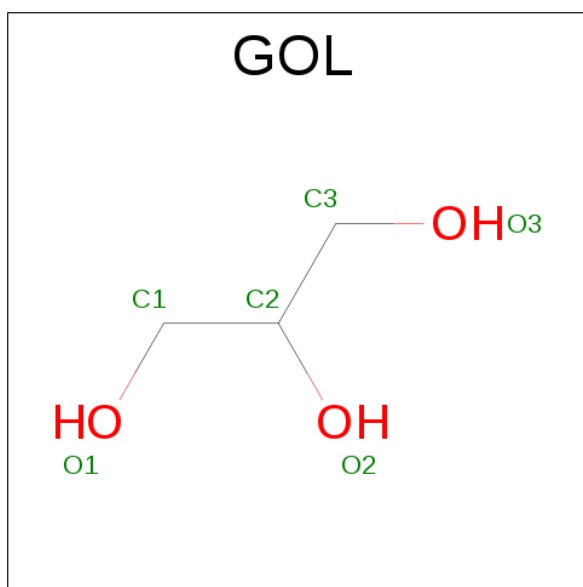
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Zn	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

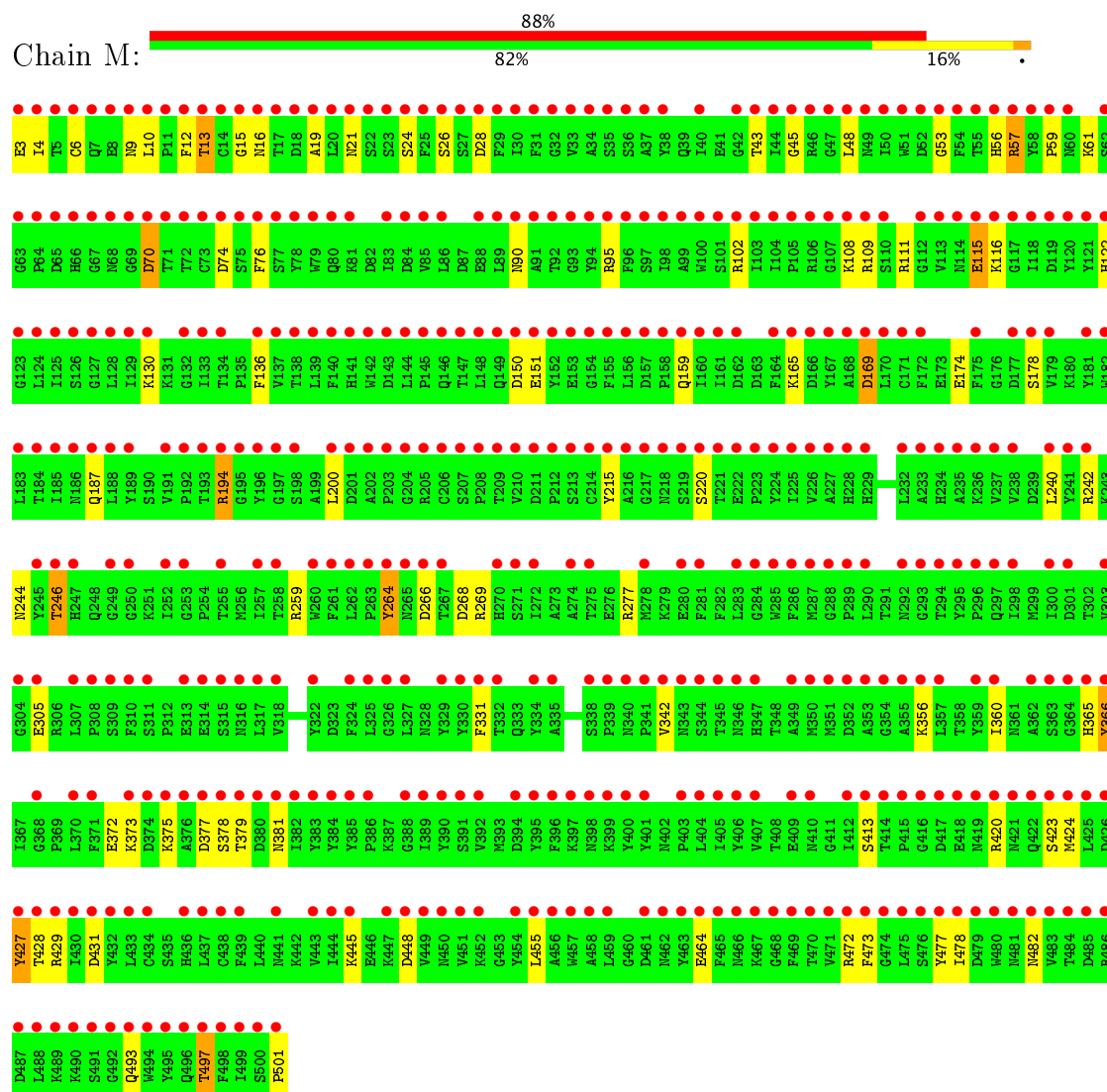
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	134.30 Å 136.40 Å 80.30 Å 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
$\langle I/\sigma(I) \rangle$ ¹	6.70 (at 1.99 Å)	Xtriage
Refinement program	X-PLOR	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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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
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
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

There are no chirality outliers.

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	4083	0	3835	104	4
2	M	196	0	172	22	0
3	M	20	0	20	0	0
4	M	22	0	15	7	0
5	M	18	0	16	0	0
6	M	22	0	19	8	0
7	M	1	0	0	0	1
8	M	40	0	0	9	0
9	M	30	0	39	4	0
10	M	788	0	0	77	17
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
9:M:1533:GOL:C1	10:M:3026: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	10:M:2032:HOH:O	1.25	1.28
1:M:427:TYR:HE2	10: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	10:M:2617:HOH:O	1.27	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE2	2.22	1.23
2:M:1504:NAG:O3	2:M:1504:NAG:C3	1.89	1.19
1:M:477:TYR:HE1	10: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	10:M:2620:HOH:O	1.66	1.10
1:M:477:TYR:CE1	10:M:2659:HOH:O	1.94	1.08
9:M:1533:GOL:H11	10:M:3026: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	10:M:2355:HOH:O	1.69	1.07
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD2	1.92	1.05
9:M:1533:GOL:C2	10:M:3026: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	10:M:2614:HOH:O	1.95	1.01
8:M:1527:SO4:O2	8: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	10:M:1056:HOH:O	1.62	0.98
1:M:259:ARG:HG2	10:M:2483:HOH:O	1.64	0.96
1:M:472:ARG:CZ	10:M:2659:HOH:O	2.12	0.95
1:M:246:THR:HG22	10:M:2377:HOH:O	1.66	0.94
1:M:150:ASP:OD2	10:M:2277:HOH:O	1.88	0.91
1:M:379:THR:HG23	10:M:2548:HOH:O	1.71	0.90
1:M:53:GLY:O	10:M:2097:HOH:O	1.90	0.89
4:M:1515:BMA:H61	6:M:1518:MAN:C6	2.03	0.89
1:M:130:LYS:HB3	10:M:2253:HOH:O	1.72	0.88
4:M:1515:BMA:H61	6:M:1518:MAN:H61	1.55	0.88
1:M:215:TYR:HB2	10: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	10:M:2243:HOH:O	1.76	0.84
1:M:15:GLY:CA	10: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	10:M:2279:HOH:O	1.97	0.82
4:M:1515:BMA:C6	6:M:1518:MAN:H61	2.11	0.81
1:M:381:ASN:ND2	10:M:2554:HOH:O	2.14	0.79
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD2	2.61	0.78
8:M:1532:SO4:O1	10:M:3024:HOH:O	2.00	0.78
1:M:70:ASP:HB3	10:M:2078:HOH:O	1.83	0.76
2:M:1522:NAG:H83	10:M:1062:HOH:O	1.86	0.76
4:M:1515:BMA:C6	6:M:1518:MAN:C6	2.65	0.74
1:M:373:LYS:NZ	10:M:2554:HOH:O	2.21	0.74
1:M:130:LYS:HB3	10:M:2091:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:LYS:HG2	10:M:2225:HOH:O	1.92	0.70
1:M:9:ASN:HB2	10:M:3014:HOH:O	1.91	0.70
2:M:1504:NAG:O3	10:M:1019:HOH:O	2.10	0.70
1:M:472:ARG:NE	10: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	10:M:2681:HOH:O	2.24	0.69
8:M:1527:SO4:S	8:M:1532:SO4:O3	2.51	0.68
1:M:45:GLY:HA2	10:M:2085:HOH:O	1.93	0.68
1:M:70:ASP:OD2	10:M:2125:HOH:O	2.11	0.68
8:M:1526:SO4:O2	10:M:3006:HOH:O	2.14	0.66
1:M:115:GLU:HG3	10:M:2223:HOH:O	1.95	0.66
4:M:1515:BMA:H61	6:M:1518:MAN:H62	1.76	0.66
1:M:111:ARG:O	10: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	10:M:2659:HOH:O	2.26	0.65
1:M:220[A]:SER:OG	10:M:2359:HOH:O	2.15	0.64
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.80	0.64
8:M:1526:SO4:O4	10:M:3006:HOH:O	2.16	0.63
1:M:200:LEU:HB3	10:M:2336:HOH:O	1.98	0.63
8:M:1527:SO4:O2	8:M:1532:SO4:O3	2.15	0.63
9:M:1533:GOL:O2	10:M:3026:HOH:O	2.01	0.61
8:M:1527:SO4:O1	8:M:1532:SO4:O3	2.20	0.60
1:M:365:HIS:HE1	10:M:2532:HOH:O	1.83	0.60
1:M:342[A]:VAL:HG13	10:M:2359:HOH:O	2.02	0.60
8:M:1527:SO4:S	8:M:1532:SO4:S	3.00	0.59
1:M:45:GLY:HA2	10:M:2086:HOH:O	2.03	0.58
1:M:159:GLN:NE2	10:M:2288:HOH:O	2.36	0.58
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CZ	2.33	0.58
1:M:115:GLU:CD	10: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	10: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	10:M:2681:HOH:O	2.05	0.56
1:M:194:ARG:NH1	8:M:1532:SO4:O4	2.40	0.55
1:M:331:PHE:CD1	10:M:2483:HOH:O	2.53	0.55
1:M:165:LYS:HZ2	2:M:1506:NAG:H82	1.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1515:BMA:C6	10:M:1055: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
6:M:1518:MAN:C4	10:M:1053:HOH:O	2.58	0.52
2:M:1504:NAG:O3	2:M:1504:NAG:C2	2.56	0.51
1:M:472:ARG:HG2	10: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	10:M:2253:HOH:O	2.43	0.51
1:M:28:ASP:HA	10:M:2053:HOH:O	2.10	0.51
1:M:115:GLU:CG	10:M:2223:HOH:O	2.56	0.50
1:M:360[A]:ILE:HG23	10:M:2518:HOH:O	2.10	0.50
1:M:10:LEU:HD23	10:M:2023:HOH:O	2.12	0.49
1:M:108:LYS:HD2	10:M:2298:HOH:O	2.12	0.49
1:M:15:GLY:C	10:M:2032:HOH:O	2.34	0.48
1:M:70:ASP:CB	10:M:2078:HOH:O	2.51	0.48
1:M:360[A]:ILE:CG2	10:M:2518:HOH:O	2.61	0.48
1:M:95:ARG:HA	1:M:136:PHE:O	2.14	0.47
6:M:1518:MAN:C5	10:M:1053:HOH:O	2.62	0.47
1:M:59:PRO:HB3	10:M:2100:HOH:O	2.14	0.47
4:M:1515:BMA:O6	6:M:1518:MAN:C6	2.49	0.46
1:M:12:PHE:HD2	10: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	10: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	10:M:2689:HOH:O	2.19	0.42
1:M:59:PRO:HG3	10:M:2117:HOH:O	2.19	0.42
1:M:244:ASN:ND2	2:M:1506:NAG:O5	2.42	0.42
1:M:12:PHE:N	10:M:2023:HOH:O	2.26	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.49	0.42
2:M:1519:NAG:C6	10:M:1056: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	10:M:2090:HOH:O	2.35	0.40
1:M:111:ARG:C	10: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)
7:M:1524:ZN:ZN	7:M:1524:ZN:ZN[3_656]	1.10	1.10
10:M:2279:HOH:O	10:M:2279:HOH:O[3_656]	1.10	1.10
10:M:2009:HOH:O	10:M:2520:HOH:O[4_576]	1.36	0.84
10:M:2248:HOH:O	10:M:2534:HOH:O[4_576]	1.37	0.83
10:M:2247:HOH:O	10:M:2247:HOH:O[4_576]	1.42	0.78
10:M:2555:HOH:O	10:M:2555:HOH:O[4_576]	1.44	0.76
10:M:2018:HOH:O	10:M:2018:HOH:O[4_576]	1.63	0.57
10:M:2258:HOH:O	10:M:2258:HOH:O[4_576]	1.63	0.57
10:M:2385:HOH:O	10:M:2426:HOH:O[6_565]	1.71	0.49
10:M:2116:HOH:O	10:M:2132:HOH:O[3_656]	1.76	0.44
10:M:2245:HOH:O	10: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
10:M:2523:HOH:O	10: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
10:M:2388:HOH:O	10:M:2441:HOH:O[6_565]	2.06	0.14
1:M:379:THR:CG2	10:M:2603:HOH:O[4_576]	2.07	0.13
10:M:2018:HOH:O	10: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
10:M:2047:HOH:O	10:M:2127:HOH:O[3_656]	2.10	0.10
10:M:1057:HOH:O	10:M:2085:HOH:O[3_656]	2.12	0.08
10:M:3014:HOH:O	10:M:3014: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	518/499 (104%)	504 (97%)	13 (2%)	1 (0%)	51 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	456/435 (105%)	455 (100%)	1 (0%)	94	96

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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 1 is monoatomic - leaving 35 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	1.18	1 (7%)	15,19,21	1.97	3 (20%)
2	NAG	M	1503	1	14,14,15	1.63	2 (14%)	15,19,21	2.08	2 (13%)
2	NAG	M	1504	1,2	14,14,15	6.16	7 (50%)	15,19,21	3.51	8 (53%)
2	NAG	M	1505	2	14,14,15	2.86	3 (21%)	15,19,21	3.90	7 (46%)
2	NAG	M	1506	1	14,14,15	1.98	5 (35%)	15,19,21	8.50	11 (73%)
2	NAG	M	1507	1,3,2	14,14,15	0.56	0	15,19,21	2.03	5 (33%)
3	FUC	M	1508	2	9,10,11	1.65	2 (22%)	13,14,16	2.26	4 (30%)
2	NAG	M	1509	2,4	14,14,15	1.03	1 (7%)	15,19,21	1.38	3 (20%)
4	BMA	M	1510	2,5	11,11,12	1.92	2 (18%)	13,15,17	1.61	4 (30%)
5	XYP	M	1511	4	9,9,10	1.37	2 (22%)	10,12,14	2.80	4 (40%)
2	NAG	M	1512	1,3,2	14,14,15	1.91	3 (21%)	15,19,21	2.52	2 (13%)
3	FUC	M	1513	2	9,10,11	3.07	5 (55%)	13,14,16	1.93	2 (15%)
2	NAG	M	1514	2,4	14,14,15	1.47	3 (21%)	15,19,21	1.71	3 (20%)
4	BMA	M	1515	2,5,6	11,11,12	2.64	3 (27%)	13,15,17	4.43	7 (53%)
5	XYP	M	1516	4	9,9,10	1.95	3 (33%)	10,12,14	2.32	4 (40%)
6	MAN	M	1517	4	11,11,12	1.90	2 (18%)	13,15,17	2.69	7 (53%)
6	MAN	M	1518	4	11,11,12	3.06	7 (63%)	13,15,17	7.12	10 (76%)
2	NAG	M	1519	1	14,14,15	1.34	2 (14%)	15,19,21	2.91	4 (26%)
2	NAG	M	1520	1	14,14,15	1.30	1 (7%)	15,19,21	2.49	6 (40%)
2	NAG	M	1521	1,2	14,14,15	2.34	4 (28%)	15,19,21	2.51	3 (20%)
2	NAG	M	1522	2	14,14,15	1.42	2 (14%)	15,19,21	2.67	9 (60%)
2	NAG	M	1523	1	14,14,15	1.22	1 (7%)	15,19,21	1.99	4 (26%)
8	SO4	M	1525	-	4,4,4	0.82	0	6,6,6	1.34	1 (16%)
8	SO4	M	1526	-	4,4,4	0.57	0	6,6,6	0.50	0
8	SO4	M	1527	8	4,4,4	1.44	1 (25%)	6,6,6	1.46	1 (16%)
8	SO4	M	1528	-	4,4,4	0.20	0	6,6,6	0.35	0
8	SO4	M	1529	-	4,4,4	1.97	1 (25%)	6,6,6	2.43	3 (50%)
8	SO4	M	1530	-	4,4,4	1.14	0	6,6,6	1.34	1 (16%)
8	SO4	M	1531	-	4,4,4	0.83	0	6,6,6	0.34	0
8	SO4	M	1532	8	4,4,4	1.55	1 (25%)	6,6,6	2.88	5 (83%)
9	GOL	M	1533	-	5,5,5	0.69	0	5,5,5	1.11	1 (20%)
9	GOL	M	1534	-	5,5,5	1.29	1 (20%)	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	M	1535	-	5,5,5	0.93	0	5,5,5	1.07	0
9	GOL	M	1536	-	5,5,5	0.64	0	5,5,5	1.05	0
9	GOL	M	1537	-	5,5,5	0.82	0	5,5,5	1.20	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
2	NAG	M	1504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	1505	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1506	1	-	0/6/23/26	0/1/1/1
2	NAG	M	1507	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	M	1508	2	-	0/0/17/20	0/1/1/1
2	NAG	M	1509	2,4	-	0/6/23/26	0/1/1/1
4	BMA	M	1510	2,5	-	0/2/19/22	0/1/1/1
5	XYP	M	1511	4	-	0/0/14/17	0/1/1/1
2	NAG	M	1512	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	M	1513	2	-	0/0/17/20	0/1/1/1
2	NAG	M	1514	2,4	-	0/6/23/26	0/1/1/1
4	BMA	M	1515	2,5,6	-	0/2/19/22	0/1/1/1
5	XYP	M	1516	4	-	0/0/14/17	0/1/1/1
6	MAN	M	1517	4	-	0/2/19/22	0/1/1/1
6	MAN	M	1518	4	1/1/4/5	0/2/19/22	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	1521	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	1522	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1523	1	-	0/6/23/26	0/1/1/1
8	SO4	M	1525	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1526	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1527	8	-	0/0/0/0	0/0/0/0
8	SO4	M	1528	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1529	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1530	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1531	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1532	8	-	0/0/0/0	0/0/0/0
9	GOL	M	1533	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1534	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	M	1535	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1536	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1537	-	-	0/4/4/4	0/0/0/0

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1515	BMA	C2-C3	-7.27	1.42	1.52
2	M	1521	NAG	O7-C7	-6.30	1.08	1.23
2	M	1505	NAG	C6-C5	-6.06	1.31	1.51
2	M	1512	NAG	C1-C2	-5.26	1.45	1.52
2	M	1505	NAG	C4-C5	-4.53	1.43	1.53
2	M	1504	NAG	C7-N2	-4.50	1.17	1.34
4	M	1510	BMA	C2-C3	-4.37	1.46	1.52
2	M	1520	NAG	O7-C7	-4.01	1.13	1.23
2	M	1506	NAG	O7-C7	-3.81	1.14	1.23
2	M	1523	NAG	O7-C7	-3.67	1.14	1.23
2	M	1506	NAG	C1-C2	-3.44	1.47	1.52
2	M	1503	NAG	O7-C7	-3.33	1.15	1.23
2	M	1514	NAG	C3-C2	-3.31	1.45	1.52
2	M	1519	NAG	O7-C7	-3.26	1.15	1.23
2	M	1502	NAG	O7-C7	-2.73	1.16	1.23
2	M	1506	NAG	C2-N2	-2.56	1.41	1.46
2	M	1512	NAG	O5-C1	-2.50	1.39	1.43
2	M	1512	NAG	C2-N2	-2.38	1.42	1.46
6	M	1518	MAN	C6-C5	-2.31	1.44	1.51
2	M	1521	NAG	O5-C1	-2.26	1.40	1.43
2	M	1506	NAG	O5-C1	-2.13	1.40	1.43
3	M	1513	FUC	C4-C3	-2.07	1.47	1.52
2	M	1521	NAG	O4-C4	2.03	1.47	1.43
6	M	1518	MAN	C4-C3	2.06	1.57	1.52
2	M	1519	NAG	C2-N2	2.09	1.50	1.46
5	M	1511	XYP	O3B-C3B	2.12	1.47	1.43
4	M	1515	BMA	O3-C3	2.14	1.47	1.43
6	M	1518	MAN	O5-C1	2.15	1.47	1.43
3	M	1508	FUC	O2-C2	2.16	1.48	1.43
9	M	1534	GOL	O1-C1	2.17	1.51	1.42
2	M	1514	NAG	C1-C2	2.19	1.55	1.52
2	M	1514	NAG	O7-C7	2.25	1.28	1.23
2	M	1522	NAG	C4-C5	2.26	1.57	1.53
2	M	1509	NAG	C1-C2	2.33	1.55	1.52
3	M	1513	FUC	C1-C2	2.38	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1511	XYP	C4B-C3B	2.42	1.55	1.52
5	M	1516	XYP	O5B-C5B	2.50	1.47	1.42
8	M	1532	SO4	O1-S	2.57	1.59	1.45
6	M	1518	MAN	C1-C2	2.60	1.58	1.52
8	M	1527	SO4	O1-S	2.70	1.60	1.45
4	M	1510	BMA	O5-C5	2.70	1.49	1.43
2	M	1504	NAG	O5-C5	2.82	1.49	1.43
2	M	1504	NAG	O4-C4	2.86	1.49	1.43
5	M	1516	XYP	O3B-C3B	2.95	1.49	1.43
3	M	1508	FUC	C2-C3	2.97	1.56	1.52
2	M	1522	NAG	C1-C2	3.05	1.56	1.52
2	M	1504	NAG	C4-C5	3.09	1.59	1.53
2	M	1506	NAG	O4-C4	3.10	1.50	1.43
6	M	1517	MAN	C4-C5	3.22	1.59	1.53
6	M	1518	MAN	O4-C4	3.23	1.50	1.43
5	M	1516	XYP	C2B-C3B	3.34	1.57	1.52
4	M	1515	BMA	C4-C5	3.46	1.60	1.53
3	M	1513	FUC	O4-C4	3.58	1.51	1.43
6	M	1518	MAN	C2-C3	3.73	1.57	1.52
8	M	1529	SO4	O2-S	3.75	1.66	1.45
2	M	1504	NAG	C3-C2	3.80	1.60	1.52
2	M	1503	NAG	O5-C5	4.03	1.51	1.43
2	M	1521	NAG	C8-C7	4.31	1.59	1.50
6	M	1517	MAN	O5-C5	4.47	1.52	1.43
3	M	1513	FUC	C2-C3	5.23	1.59	1.52
3	M	1513	FUC	C4-C5	5.42	1.63	1.53
2	M	1505	NAG	O5-C5	6.82	1.57	1.43
2	M	1504	NAG	O7-C7	7.23	1.40	1.23
6	M	1518	MAN	O5-C5	7.54	1.59	1.43
2	M	1504	NAG	O3-C3	20.29	1.89	1.43

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1518	MAN	C1-O5-C5	-15.59	90.67	112.17
2	M	1506	NAG	O7-C7-N2	-7.97	106.58	121.92
2	M	1505	NAG	C1-O5-C5	-7.55	101.75	112.17
2	M	1504	NAG	O3-C3-C2	-7.34	93.66	109.39
2	M	1520	NAG	O5-C1-C2	-6.84	101.95	111.47
6	M	1518	MAN	O4-C4-C3	-6.77	95.62	110.36
2	M	1506	NAG	C1-O5-C5	-6.53	103.16	112.17
4	M	1515	BMA	O4-C4-C3	-6.33	96.58	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1504	NAG	C1-O5-C5	-6.17	103.67	112.17
6	M	1518	MAN	C2-C3-C4	-6.12	100.20	110.88
2	M	1503	NAG	C1-O5-C5	-6.11	103.74	112.17
2	M	1502	NAG	C1-O5-C5	-5.99	103.90	112.17
2	M	1521	NAG	C8-C7-N2	-5.85	105.54	116.11
2	M	1512	NAG	C1-O5-C5	-5.56	104.50	112.17
3	M	1513	FUC	C1-C2-C3	-5.47	102.72	109.65
5	M	1511	XYP	C5B-C4B-C3B	-5.40	102.81	109.65
3	M	1508	FUC	O3-C3-C2	-5.24	100.48	110.02
2	M	1504	NAG	O4-C4-C5	-5.14	96.32	109.28
4	M	1515	BMA	C1-C2-C3	-5.12	103.16	109.65
2	M	1506	NAG	O7-C7-C8	-5.10	112.77	122.06
4	M	1515	BMA	O2-C2-C3	-5.07	100.22	110.17
2	M	1522	NAG	O5-C1-C2	-4.85	104.72	111.47
6	M	1518	MAN	O5-C1-C2	-4.65	103.51	110.79
2	M	1523	NAG	C4-C3-C2	-4.60	104.28	111.02
5	M	1516	XYP	C5B-C4B-C3B	-4.59	103.83	109.65
2	M	1519	NAG	C1-C2-N2	-4.41	102.95	110.49
2	M	1507	NAG	C1-O5-C5	-4.35	106.17	112.17
2	M	1522	NAG	C1-C2-N2	-4.21	103.29	110.49
2	M	1504	NAG	C4-C3-C2	-4.20	104.86	111.02
5	M	1511	XYP	O2B-C2B-C3B	-4.15	102.03	110.17
2	M	1519	NAG	O3-C3-C2	-4.15	100.50	109.39
5	M	1511	XYP	O3B-C3B-C2B	-3.91	102.91	110.02
2	M	1504	NAG	O7-C7-C8	-3.88	114.99	122.06
3	M	1508	FUC	C1-C2-C3	-3.87	104.74	109.65
6	M	1517	MAN	C3-C4-C5	-3.85	103.44	110.22
2	M	1503	NAG	C4-C3-C2	-3.71	105.59	111.02
2	M	1505	NAG	C4-C3-C2	-3.70	105.59	111.02
2	M	1523	NAG	O3-C3-C2	-3.62	101.62	109.39
2	M	1507	NAG	C2-N2-C7	-3.59	117.70	122.94
6	M	1517	MAN	O2-C2-C3	-3.57	103.16	110.17
6	M	1517	MAN	C2-C3-C4	-3.50	104.77	110.88
2	M	1522	NAG	C2-N2-C7	-3.47	117.89	122.94
5	M	1516	XYP	C4B-C3B-C2B	-3.44	106.86	110.86
3	M	1508	FUC	O2-C2-C3	-3.44	103.43	110.17
2	M	1504	NAG	O4-C4-C3	-3.42	102.91	110.36
2	M	1505	NAG	O6-C6-C5	-3.42	99.85	111.34
6	M	1518	MAN	C3-C4-C5	-3.38	104.27	110.22
2	M	1506	NAG	O4-C4-C5	-3.37	100.79	109.28
2	M	1504	NAG	O3-C3-C4	-3.37	103.03	110.36
8	M	1529	SO4	O3-S-O2	-3.30	91.08	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1532	SO4	O3-S-O1	-3.27	91.24	109.26
8	M	1529	SO4	O2-S-O1	-3.18	87.42	109.64
2	M	1522	NAG	C1-O5-C5	-3.16	107.81	112.17
2	M	1519	NAG	O4-C4-C5	-3.14	101.36	109.28
8	M	1532	SO4	O2-S-O1	-3.10	88.00	109.64
2	M	1522	NAG	O4-C4-C3	-3.07	103.67	110.36
2	M	1522	NAG	C6-C5-C4	-3.07	105.83	113.00
2	M	1521	NAG	C2-N2-C7	-3.00	118.56	122.94
2	M	1522	NAG	C3-C4-C5	-2.96	105.00	110.22
2	M	1509	NAG	C2-N2-C7	-2.86	118.77	122.94
2	M	1514	NAG	O5-C1-C2	-2.80	107.58	111.47
5	M	1516	XYP	O4B-C4B-C3B	-2.79	104.70	110.17
2	M	1514	NAG	O4-C4-C3	-2.76	104.34	110.36
2	M	1506	NAG	O4-C4-C3	-2.74	104.40	110.36
2	M	1520	NAG	O3-C3-C2	-2.73	103.55	109.39
2	M	1507	NAG	O5-C1-C2	-2.63	107.82	111.47
2	M	1523	NAG	C1-C2-N2	-2.62	106.02	110.49
4	M	1515	BMA	C1-O5-C5	-2.57	108.62	112.17
6	M	1518	MAN	O2-C2-C1	-2.56	103.96	109.18
2	M	1506	NAG	C4-C3-C2	-2.48	107.39	111.02
9	M	1537	GOL	C3-C2-C1	-2.48	101.68	111.52
6	M	1517	MAN	C6-C5-C4	-2.47	107.22	113.00
2	M	1507	NAG	C1-C2-N2	-2.45	106.30	110.49
5	M	1516	XYP	O2B-C2B-C3B	-2.43	105.41	110.17
2	M	1509	NAG	O4-C4-C3	-2.39	105.15	110.36
2	M	1514	NAG	C2-N2-C7	-2.38	119.47	122.94
3	M	1508	FUC	O3-C3-C4	-2.35	105.25	110.36
2	M	1507	NAG	C8-C7-N2	-2.35	111.87	116.11
8	M	1532	SO4	O4-S-O1	-2.28	96.69	109.26
2	M	1509	NAG	O5-C1-C2	-2.22	108.38	111.47
3	M	1513	FUC	C6-C5-C4	-2.22	109.13	113.07
2	M	1502	NAG	C4-C3-C2	-2.14	107.88	111.02
2	M	1522	NAG	C4-C3-C2	-2.10	107.94	111.02
2	M	1505	NAG	C8-C7-N2	-2.04	112.43	116.11
4	M	1510	BMA	O4-C4-C5	2.00	114.33	109.28
8	M	1532	SO4	O3-S-O2	2.02	120.41	109.26
2	M	1522	NAG	O3-C3-C2	2.09	113.86	109.39
4	M	1510	BMA	C3-C4-C5	2.09	113.89	110.22
6	M	1517	MAN	C1-O5-C5	2.10	115.06	112.17
9	M	1533	GOL	O2-C2-C1	2.12	118.87	108.84
2	M	1520	NAG	O7-C7-C8	2.25	126.15	122.06
8	M	1530	SO4	O4-S-O1	2.28	121.83	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1506	NAG	C1-C2-N2	2.28	114.39	110.49
8	M	1525	SO4	O3-S-O2	2.29	121.88	109.26
2	M	1520	NAG	C2-N2-C7	2.30	126.30	122.94
8	M	1529	SO4	O4-S-O1	2.41	122.53	109.26
2	M	1504	NAG	C8-C7-N2	2.46	120.56	116.11
4	M	1510	BMA	O3-C3-C4	2.58	115.98	110.36
2	M	1520	NAG	C1-O5-C5	2.61	115.77	112.17
2	M	1502	NAG	O5-C1-C2	2.85	115.44	111.47
6	M	1517	MAN	O2-C2-C1	2.89	115.06	109.18
8	M	1527	SO4	O4-S-O3	2.93	122.18	108.96
4	M	1510	BMA	C2-C3-C4	3.04	116.17	110.88
2	M	1523	NAG	O5-C1-C2	3.11	115.80	111.47
5	M	1511	XYP	C1B-C2B-C3B	3.26	113.78	109.65
2	M	1520	NAG	O4-C4-C3	3.43	117.82	110.36
4	M	1515	BMA	C3-C4-C5	3.66	116.67	110.22
2	M	1506	NAG	C3-C4-C5	3.92	117.13	110.22
6	M	1518	MAN	O6-C6-C5	4.36	126.02	111.34
2	M	1505	NAG	O3-C3-C4	4.40	119.92	110.36
8	M	1532	SO4	O4-S-O3	4.51	129.27	108.96
2	M	1505	NAG	O5-C1-C2	5.21	118.72	111.47
6	M	1517	MAN	C1-C2-C3	5.26	116.31	109.65
6	M	1518	MAN	C1-C2-C3	5.43	116.53	109.65
4	M	1515	BMA	C6-C5-C4	6.00	127.05	113.00
2	M	1521	NAG	O7-C7-N2	6.33	134.11	121.92
2	M	1512	NAG	O5-C1-C2	6.54	120.57	111.47
2	M	1519	NAG	C1-O5-C5	8.30	123.61	112.17
6	M	1518	MAN	O4-C4-C5	8.61	130.98	109.28
2	M	1505	NAG	C3-C4-C5	9.13	126.30	110.22
4	M	1515	BMA	O4-C4-C5	9.87	134.15	109.28
6	M	1518	MAN	C6-C5-C4	12.88	143.14	113.00
2	M	1506	NAG	C8-C7-N2	13.51	140.50	116.11
2	M	1506	NAG	O5-C1-C2	16.62	134.59	111.47
2	M	1506	NAG	C2-N2-C7	21.07	153.68	122.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	1518	MAN	C5
2	M	1519	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1502	NAG	5	0
2	M	1503	NAG	3	0
2	M	1504	NAG	3	0
2	M	1506	NAG	8	0
4	M	1515	BMA	7	0
6	M	1518	MAN	8	0
2	M	1519	NAG	2	0
2	M	1522	NAG	1	0
8	M	1526	SO4	2	0
8	M	1527	SO4	5	0
8	M	1532	SO4	7	0
9	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, 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%)	3.17	437 (87%) 0 0	9, 13, 27, 54	3 (0%)

All (437) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	212	PRO	8.3
1	M	23	SER	7.2
1	M	376	ALA	7.1
1	M	378	SER	6.9
1	M	345	THR	6.7
1	M	469	PHE	6.3
1	M	419	ASN	6.2
1	M	417	ASP	6.2
1	M	380	ASP	6.2
1	M	420	ARG	6.1
1	M	375	LYS	6.0
1	M	390	TYR	5.7
1	M	17	THR	5.7
1	M	366[A]	TYR	5.7
1	M	481	ASN	5.6
1	M	206	CYS	5.6
1	M	339	PRO	5.6
1	M	360[A]	ILE	5.4
1	M	78	TYR	5.4
1	M	482	ASN	5.4
1	M	79	TRP	5.4
1	M	457	TRP	5.3
1	M	138	THR	5.3
1	M	480	TRP	5.3
1	M	374	ASP	5.2
1	M	497	THR	5.2
1	M	209	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	M	18	ASP	5.1
1	M	83	ILE	5.1
1	M	471	VAL	5.1
1	M	10	LEU	5.0
1	M	4	ILE	5.0
1	M	197	GLY	5.0
1	M	196	TYR	4.9
1	M	421	ASN	4.9
1	M	144	LEU	4.9
1	M	283	LEU	4.8
1	M	3	GLU	4.8
1	M	152	TYR	4.8
1	M	112	GLY	4.8
1	M	449[A]	VAL	4.8
1	M	213[A]	SER	4.7
1	M	167	TYR	4.7
1	M	478	ILE	4.6
1	M	12	PHE	4.6
1	M	245	TYR	4.6
1	M	458	ALA	4.6
1	M	55	THR	4.6
1	M	80	GLN	4.6
1	M	30[A]	ILE	4.6
1	M	444	ILE	4.6
1	M	305[A]	GLU	4.6
1	M	362	ALA	4.6
1	M	89	LEU	4.6
1	M	434	CYS	4.6
1	M	371	PHE	4.6
1	M	73	CYS	4.5
1	M	300	ILE	4.5
1	M	51	TRP	4.5
1	M	36	SER	4.5
1	M	142	TRP	4.5
1	M	424	MET	4.5
1	M	219	SER	4.5
1	M	25	PHE	4.5
1	M	20[A]	LEU	4.4
1	M	363[A]	SER	4.4
1	M	9	ASN	4.4
1	M	99	ALA	4.4
1	M	50	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	M	16	ASN	4.4
1	M	208	PRO	4.4
1	M	415	PRO	4.4
1	M	488	LEU	4.4
1	M	128	LEU	4.4
1	M	364	GLY	4.3
1	M	147	THR	4.3
1	M	183	LEU	4.3
1	M	418	GLU	4.3
1	M	113	VAL	4.3
1	M	71	THR	4.3
1	M	379	THR	4.3
1	M	465	PHE	4.3
1	M	377	ASP	4.3
1	M	97	SER	4.3
1	M	223	PRO	4.2
1	M	210	VAL	4.2
1	M	203	PRO	4.2
1	M	388	GLY	4.2
1	M	470	THR	4.1
1	M	154	GLY	4.1
1	M	160	ILE	4.1
1	M	13	THR	4.1
1	M	330	TYR	4.1
1	M	27	SER	4.1
1	M	215	TYR	4.1
1	M	48	LEU	4.1
1	M	313	GLU	4.1
1	M	94	TYR	4.1
1	M	344[A]	SER	4.0
1	M	140	PHE	4.0
1	M	433	LEU	4.0
1	M	43	THR	4.0
1	M	349	ALA	4.0
1	M	359	TYR	4.0
1	M	54	PHE	4.0
1	M	257	ILE	4.0
1	M	317	LEU	4.0
1	M	459	LEU	4.0
1	M	485	ASP	3.9
1	M	404	LEU	3.9
1	M	396	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	M	334	TYR	3.9
1	M	400	TYR	3.9
1	M	45	GLY	3.9
1	M	342[A]	VAL	3.9
1	M	59	PRO	3.9
1	M	338[A]	SER	3.9
1	M	432	TYR	3.9
1	M	484	THR	3.9
1	M	129	ILE	3.9
1	M	298	ILE	3.9
1	M	93	GLY	3.9
1	M	191	VAL	3.9
1	M	281	PHE	3.9
1	M	492	GLY	3.9
1	M	401	TYR	3.9
1	M	24	SER	3.8
1	M	101[A]	SER	3.8
1	M	132	GLY	3.8
1	M	326	GLY	3.8
1	M	115	GLU	3.8
1	M	430	ILE	3.8
1	M	499	ILE	3.8
1	M	500	SER	3.8
1	M	370	LEU	3.8
1	M	318	VAL	3.8
1	M	474	GLY	3.8
1	M	90	ASN	3.7
1	M	308	PRO	3.7
1	M	29	PHE	3.7
1	M	164	PHE	3.7
1	M	425	LEU	3.7
1	M	143	ASP	3.7
1	M	490	LYS	3.7
1	M	335	ALA	3.7
1	M	38	TYR	3.7
1	M	365	HIS	3.6
1	M	53	GLY	3.6
1	M	169[A]	ASP	3.6
1	M	63	GLY	3.6
1	M	170	LEU	3.6
1	M	88[A]	GLU	3.6
1	M	479	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	310	PHE	3.6
1	M	139	LEU	3.5
1	M	493	GLN	3.5
1	M	428	THR	3.5
1	M	200	LEU	3.5
1	M	249	GLY	3.5
1	M	414	THR	3.5
1	M	177	ASP	3.5
1	M	11	PRO	3.5
1	M	357	LEU	3.5
1	M	395	TYR	3.5
1	M	315	SER	3.5
1	M	409	GLU	3.4
1	M	60	ASN	3.4
1	M	103	ILE	3.4
1	M	350	MET	3.4
1	M	106	ARG	3.4
1	M	264	TYR	3.4
1	M	52	ASP	3.4
1	M	66	HIS	3.4
1	M	278	MET	3.4
1	M	211	ASP	3.4
1	M	274	ALA	3.4
1	M	157	ASP	3.4
1	M	260	TRP	3.4
1	M	285	TRP	3.4
1	M	148	LEU	3.4
1	M	275	THR	3.4
1	M	204	GLY	3.4
1	M	324	PHE	3.4
1	M	498	PHE	3.4
1	M	192	PRO	3.4
1	M	151	GLU	3.4
1	M	304	GLY	3.4
1	M	368	GLY	3.4
1	M	81	LYS	3.3
1	M	58	TYR	3.3
1	M	5	THR	3.3
1	M	118[A]	ILE	3.3
1	M	62[A]	SER	3.3
1	M	68	ASN	3.3
1	M	441	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	141	HIS	3.3
1	M	240	LEU	3.3
1	M	77	SER	3.3
1	M	258	THR	3.3
1	M	341	PRO	3.3
1	M	69	GLY	3.3
1	M	443	VAL	3.3
1	M	122	HIS	3.2
1	M	124	LEU	3.2
1	M	121	TYR	3.2
1	M	149	GLN	3.2
1	M	290	LEU	3.2
1	M	491	SER	3.2
1	M	120	TYR	3.2
1	M	49	ASN	3.2
1	M	57	ARG	3.2
1	M	347	HIS	3.2
1	M	156	LEU	3.2
1	M	296	PRO	3.2
1	M	271[A]	SER	3.2
1	M	311	SER	3.2
1	M	84	ASP	3.2
1	M	56	HIS	3.1
1	M	26	SER	3.1
1	M	146	GLN	3.1
1	M	294	THR	3.1
1	M	489	LYS	3.1
1	M	31	PHE	3.1
1	M	104	ILE	3.1
1	M	172	PHE	3.1
1	M	422	GLN	3.1
1	M	382	ILE	3.1
1	M	426	ASP	3.1
1	M	85	VAL	3.1
1	M	184	THR	3.1
1	M	75	SER	3.1
1	M	295	TYR	3.1
1	M	150	ASP	3.1
1	M	381	ASN	3.1
1	M	423	SER	3.1
1	M	28	ASP	3.1
1	M	76	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	33	VAL	3.1
1	M	226	VAL	3.1
1	M	272	ILE	3.1
1	M	329	TYR	3.1
1	M	406	TYR	3.1
1	M	42	GLY	3.0
1	M	220[A]	SER	3.0
1	M	224	TYR	3.0
1	M	403	PRO	3.0
1	M	126[A]	SER	3.0
1	M	95	ARG	3.0
1	M	448	ASP	3.0
1	M	47	GLY	3.0
1	M	214	CYS	3.0
1	M	353	ALA	3.0
1	M	162	ASP	3.0
1	M	452	LYS	3.0
1	M	145	PRO	3.0
1	M	22	SER	3.0
1	M	384	TYR	3.0
1	M	332	THR	3.0
1	M	117	GLY	3.0
1	M	373	LYS	3.0
1	M	237	VAL	2.9
1	M	171	CYS	2.9
1	M	445	LYS	2.9
1	M	487	ASP	2.9
1	M	494	TRP	2.9
1	M	297	GLN	2.9
1	M	286	PHE	2.9
1	M	450	ASN	2.9
1	M	217	GLY	2.9
1	M	72	THR	2.9
1	M	187	GLN	2.9
1	M	182	TRP	2.9
1	M	327	LEU	2.9
1	M	346	ASN	2.9
1	M	451	VAL	2.9
1	M	399	LYS	2.9
1	M	46	ARG	2.9
1	M	218	ASN	2.9
1	M	466	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	195	GLY	2.8
1	M	181	TYR	2.8
1	M	161	ILE	2.8
1	M	265	ASN	2.8
1	M	405	ILE	2.8
1	M	383	TYR	2.8
1	M	64	PRO	2.8
1	M	343	ASN	2.8
1	M	14	CYS	2.8
1	M	185	ILE	2.8
1	M	225	ILE	2.8
1	M	252	ILE	2.8
1	M	108	LYS	2.8
1	M	32	GLY	2.8
1	M	468	GLY	2.8
1	M	235	ALA	2.8
1	M	98	ILE	2.8
1	M	175	PHE	2.8
1	M	301	ASP	2.8
1	M	86	LEU	2.8
1	M	437	LEU	2.8
1	M	216	ALA	2.7
1	M	114	ASN	2.7
1	M	221	THR	2.7
1	M	229	HIS	2.7
1	M	386	PRO	2.7
1	M	100	TRP	2.7
1	M	439	PHE	2.7
1	M	6	CYS	2.7
1	M	463	TYR	2.7
1	M	486	ARG	2.7
1	M	105	PRO	2.7
1	M	233	ALA	2.7
1	M	385	TYR	2.7
1	M	134	THR	2.7
1	M	238	VAL	2.7
1	M	287	MET	2.7
1	M	116	LYS	2.7
1	M	91	ALA	2.7
1	M	322	TYR	2.7
1	M	455	LEU	2.7
1	M	67	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	37	ALA	2.7
1	M	193	THR	2.7
1	M	427	TYR	2.7
1	M	391	SER	2.7
1	M	123	GLY	2.7
1	M	356	LYS	2.7
1	M	496	GLN	2.7
1	M	316	ASN	2.7
1	M	303	VAL	2.6
1	M	309[A]	SER	2.6
1	M	125	ILE	2.6
1	M	133	ILE	2.6
1	M	501	PRO	2.6
1	M	70	ASP	2.6
1	M	389	ILE	2.6
1	M	188	LEU	2.6
1	M	436	HIS	2.6
1	M	107	GLY	2.6
1	M	186	ASN	2.6
1	M	467	LYS	2.6
1	M	246	THR	2.6
1	M	130	LYS	2.6
1	M	35	SER	2.6
1	M	201	ASP	2.6
1	M	284	GLY	2.6
1	M	153	GLU	2.6
1	M	228	HIS	2.5
1	M	293	GLY	2.5
1	M	7	GLN	2.5
1	M	266	ASP	2.5
1	M	198	SER	2.5
1	M	280	GLU	2.5
1	M	158	PRO	2.5
1	M	96	PHE	2.5
1	M	178	SER	2.5
1	M	331	PHE	2.5
1	M	413	SER	2.5
1	M	21	ASN	2.5
1	M	15	GLY	2.5
1	M	429	ARG	2.5
1	M	456	ALA	2.5
1	M	477	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	473	PHE	2.5
1	M	464	GLU	2.5
1	M	351	MET	2.5
1	M	179	VAL	2.5
1	M	110	SER	2.5
1	M	262	LEU	2.4
1	M	472	ARG	2.4
1	M	119	ASP	2.4
1	M	207	SER	2.4
1	M	241	TYR	2.4
1	M	232	LEU	2.4
1	M	398	ASN	2.4
1	M	454	TYR	2.4
1	M	168	ALA	2.4
1	M	92	THR	2.4
1	M	136	PHE	2.4
1	M	476	SER	2.4
1	M	253	GLY	2.4
1	M	407	VAL	2.4
1	M	307	LEU	2.4
1	M	462[A]	ASN	2.4
1	M	205	ARG	2.4
1	M	250	GLY	2.4
1	M	261	PHE	2.4
1	M	461	ASP	2.4
1	M	392	VAL	2.4
1	M	410	ASN	2.4
1	M	34	ALA	2.4
1	M	227	ALA	2.4
1	M	242	ARG	2.4
1	M	65	ASP	2.4
1	M	194	ARG	2.3
1	M	255	THR	2.3
1	M	314	GLU	2.3
1	M	40	ILE	2.3
1	M	431	ASP	2.3
1	M	247	HIS	2.3
1	M	263	PRO	2.3
1	M	483	VAL	2.3
1	M	352	ASP	2.3
1	M	159	GLN	2.3
1	M	137	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	438	CYS	2.2
1	M	127	GLY	2.2
1	M	74	ASP	2.2
1	M	416	GLY	2.2
1	M	102	ARG	2.2
1	M	475	LEU	2.2
1	M	165	LYS	2.2
1	M	236	LYS	2.2
1	M	495	TYR	2.2
1	M	292	ASN	2.2
1	M	202	ALA	2.2
1	M	166	ASP	2.1
1	M	19	ALA	2.1
1	M	44	ILE	2.1
1	M	325	LEU	2.1
1	M	447	LYS	2.1
1	M	222	GLU	2.1
1	M	189	TYR	2.1
1	M	397	LYS	2.1
1	M	267	THR	2.1
1	M	412	ILE	2.1
1	M	340	ASN	2.1
1	M	109	ARG	2.1
1	M	234	HIS	2.1
1	M	354	GLY	2.1
1	M	355	ALA	2.0
1	M	8	GLU	2.0
1	M	155	PHE	2.0
1	M	289	PRO	2.0
1	M	270	HIS	2.0
1	M	288	GLY	2.0
1	M	394	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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, 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	SO4	M	1532	5/5	0.52	0.58	10.36	36,38,44,57	1
9	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
9	GOL	M	1534	6/6	0.53	0.42	3.10	3,12,16,16	1
8	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
2	NAG	M	1505	14/15	0.49	0.46	0.33	35,43,55,57	0
2	NAG	M	1507	14/15	0.64	0.34	0.18	13,20,25,25	0
2	NAG	M	1521	14/15	0.65	0.31	-0.11	7,14,19,21	0
8	SO4	M	1527	5/5	0.77	0.27	-0.17	12,26,28,32	5
2	NAG	M	1504	14/15	0.63	0.31	-0.23	17,21,30,35	0
9	GOL	M	1537	6/6	0.65	0.28	-0.68	13,14,20,20	0
9	GOL	M	1535	6/6	0.74	0.23	-1.34	9,19,24,29	6
7	ZN	M	1524	1/1	0.84	0.19	-	34,34,34,34	0
2	NAG	M	1520	14/15	0.57	0.40	-	54,62,68,68	0
4	BMA	M	1515	11/12	0.53	0.27	-	23,28,33,45	0
8	SO4	M	1530	5/5	0.76	0.34	-	11,31,32,35	5
5	XYP	M	1516	9/10	0.48	0.42	-	30,36,41,61	0
8	SO4	M	1528	5/5	0.72	0.31	-	15,19,24,27	0
8	SO4	M	1531	5/5	0.74	0.33	-	31,33,36,37	5
6	MAN	M	1518	11/12	0.54	0.56	-	31,41,52,53	0
3	FUC	M	1508	10/11	0.59	0.38	-	22,30,37,46	0
2	NAG	M	1522	14/15	0.57	0.36	-	24,29,47,54	0
2	NAG	M	1503	14/15	0.64	0.31	-	22,25,34,43	0
8	SO4	M	1529	5/5	0.78	0.49	-	24,28,32,33	5
2	NAG	M	1512	14/15	0.75	0.27	-	15,18,24,27	0
6	MAN	M	1517	11/12	0.42	0.47	-	23,37,49,54	0
3	FUC	M	1513	10/11	0.64	0.30	-	17,19,31,31	0
2	NAG	M	1509	14/15	0.71	0.30	-	19,25,31,36	0
2	NAG	M	1514	14/15	0.79	0.24	-	18,21,26,30	0
9	GOL	M	1536	6/6	0.52	0.57	-	29,29,41,43	6
8	SO4	M	1526	5/5	0.60	0.53	-	23,26,33,34	5
5	XYP	M	1511	9/10	0.54	0.34	-	39,46,50,52	0
2	NAG	M	1523	14/15	0.35	0.66	-	32,38,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BMA	M	1510	11/12	0.34	0.51	-	36,41,46,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.