



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 AM UTC

PDB ID : 2WW2 / pdb_00002ww2
Title : Structure of the Family GH92 Inverting Mannosidase BT2199 from Bacteroides
thetaiotaomicron VPI-5482
Authors : Suits, M.D.L.; Zhu, Y.; Thompson, A.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2009-10-21
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

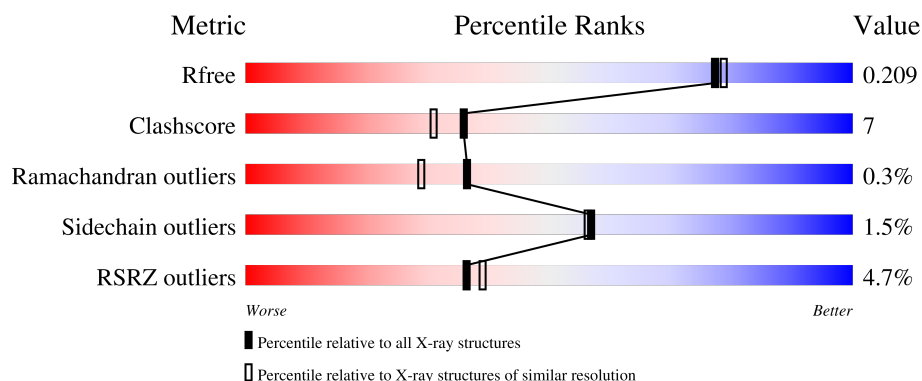
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	2% 88% 12%
1	B	737	6% 88% 11%
1	C	737	6% 87% 12%

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	MPD	A	759	-	-	X	-
4	GOL	A	804	-	-	X	-
4	GOL	A	805	-	-	X	-
4	GOL	A	806	-	-	X	-
4	GOL	A	807	-	-	X	-
4	GOL	B	802	-	-	X	-

2 Entry composition [i](#)

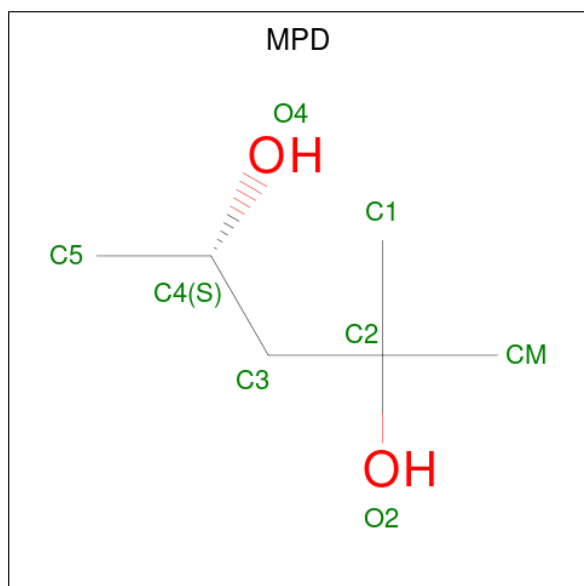
There are 6 unique types of molecules in this entry. The entry contains 19766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	9	0
			5882	3753	975	1124	30			
1	B	737	Total	C	N	O	S	0	8	0
			5843	3730	972	1111	30			
1	C	737	Total	C	N	O	S	0	4	0
			5851	3730	976	1116	29			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).

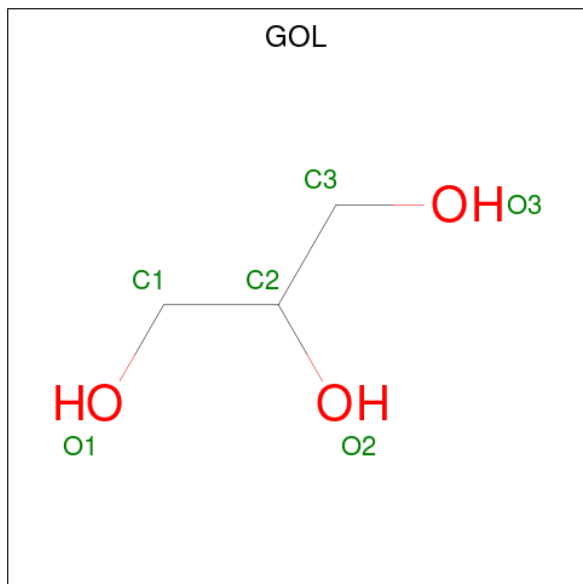


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



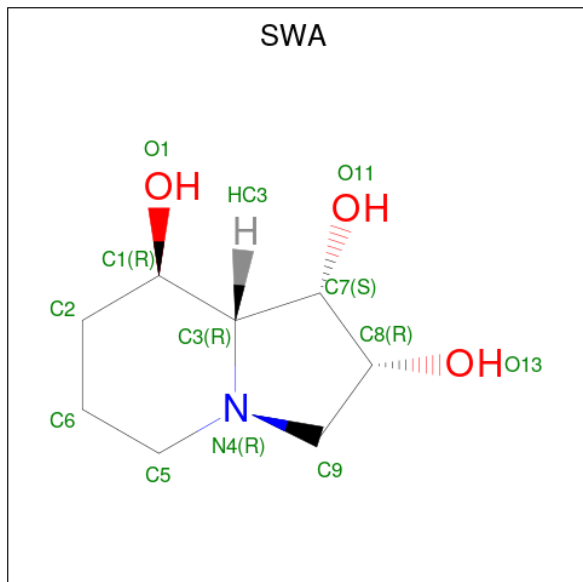
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is 1S-8AB-OCTAHYDRO-INDOLIZIDINE-1A,2A,8B-TRIOL (CCD ID: SWA) (formula: $C_8H_{15}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	1
			24	16	2	6		

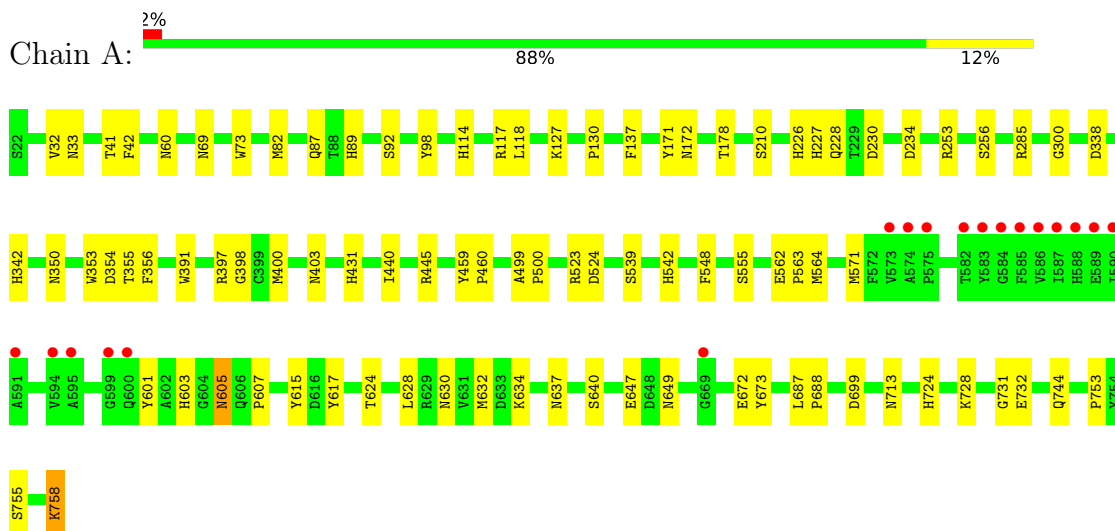
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	790	Total	O	0	0
			790	790		
6	B	653	Total	O	0	0
			653	653		
6	C	627	Total	O	0	0
			627	627		

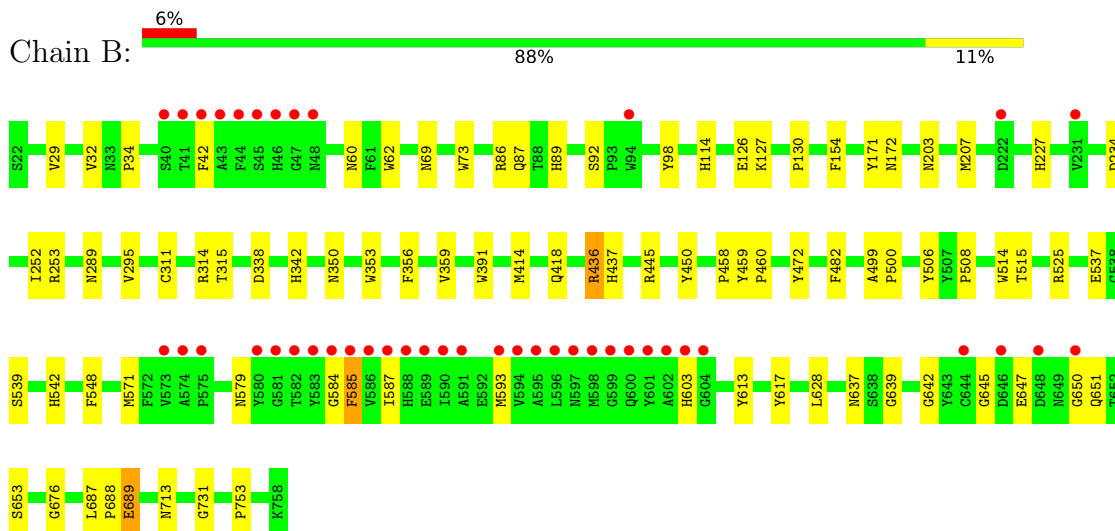
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

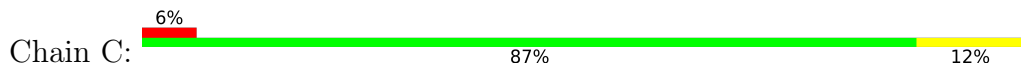
• Molecule 1: ALPHA-1,2-MANNOSIDASE

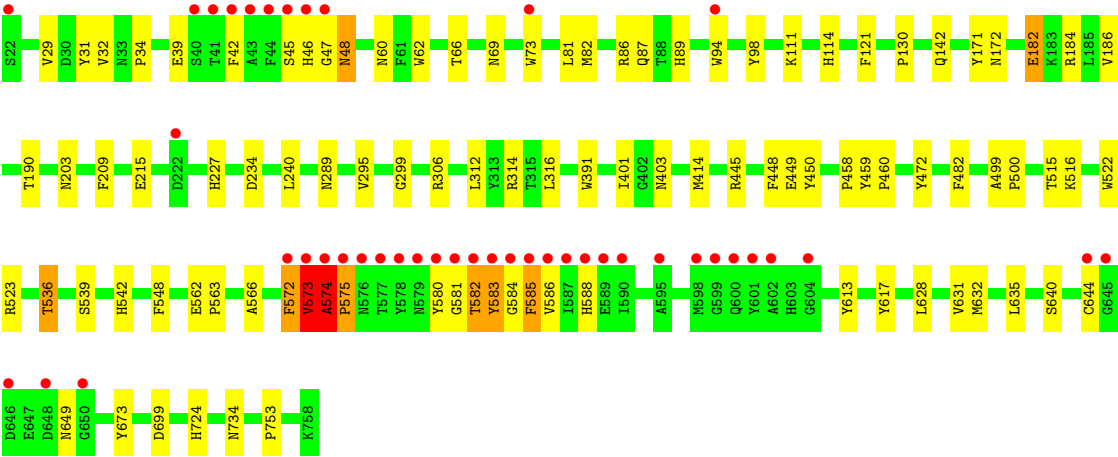


• Molecule 1: ALPHA-1,2-MANNOSIDASE



• Molecule 1: ALPHA-1,2-MANNOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.99Å 162.99Å 114.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.99 – 1.90 34.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.99-1.90) 99.9 (34.99-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.157 , 0.187 0.183 , 0.209	Depositor DCC
R_{free} test set	11455 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19766	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: NA, SWA, GOL, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/6094	0.76	0/8299
1	B	0.55	0/6051	0.77	1/8246 (0.0%)
1	C	0.53	0/6045	0.76	7/8233 (0.1%)
All	All	0.56	0/18190	0.77	8/24778 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	574	ALA	CA-C-N	7.07	128.68	119.84
1	C	574	ALA	C-N-CA	7.07	128.68	119.84
1	C	573	VAL	CB-CA-C	-6.34	100.90	111.29
1	C	644	CYS	N-CA-C	5.32	117.16	111.36
1	B	642	GLY	N-CA-C	5.29	120.56	114.16
1	C	582	THR	N-CA-C	5.27	117.02	111.28
1	C	295	VAL	CB-CA-C	-5.26	103.30	110.77
1	C	572	PHE	CB-CA-C	-5.17	109.63	117.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5882	0	5421	80	0
1	B	5843	0	5360	69	0
1	C	5851	0	5400	98	0
2	A	8	0	14	10	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	42	0	56	20	0
4	B	24	0	32	8	0
4	C	18	0	24	2	0
5	B	24	0	30	5	0
6	A	790	0	0	9	0
6	B	653	0	0	4	0
6	C	627	0	0	3	0
All	All	19766	0	16337	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:SER:HB3	2:A:759:MPD:HM3	1.25	1.13
4:A:804:GOL:H2	4:A:805:GOL:O2	1.48	1.13
1:B:253:ARG:HH22	4:B:802:GOL:H12	1.12	1.11
1:C:573:VAL:HG22	1:C:574:ALA:H	1.08	1.10
1:C:573:VAL:HG22	1:C:574:ALA:N	1.61	1.05
1:C:582:THR:N	1:C:583:TYR:CB	2.24	1.00
1:A:60:ASN:HD22	1:A:89:HIS:HE1	1.06	0.99
1:A:33:ASN:HD21	2:A:759:MPD:C1	1.76	0.98
1:C:539:SER:H	1:C:542:HIS:HD2	1.05	0.98
1:C:628[B]:LEU:CD2	1:C:632:MET:HE2	1.95	0.96
1:B:253:ARG:HH12	4:B:802:GOL:H32	1.27	0.95
1:C:60:ASN:HD22	1:C:89:HIS:HE1	1.06	0.93
1:A:628:LEU:CD1	1:A:632[A]:MET:HE2	1.99	0.92
1:B:585:PHE:HA	1:B:587:ILE:H	1.32	0.92
1:B:60:ASN:HD22	1:B:89:HIS:HE1	1.09	0.91
1:A:355:THR:CG2	4:A:805:GOL:H11	2.01	0.91
1:A:60:ASN:HD22	1:A:89:HIS:CE1	1.90	0.90
1:B:539:SER:H	1:B:542:HIS:HD2	1.17	0.90
1:C:60:ASN:HD22	1:C:89:HIS:CE1	1.90	0.88
1:C:82[B]:MET:HA	1:C:82[B]:MET:HE2	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:VAL:CG2	1:C:574:ALA:H	1.87	0.88
1:C:573:VAL:CG2	1:C:574:ALA:N	2.36	0.87
1:C:60:ASN:ND2	1:C:89:HIS:HE1	1.73	0.86
1:B:253:ARG:NH2	4:B:802:GOL:H12	1.92	0.85
1:C:628[B]:LEU:HD23	1:C:632:MET:HE2	1.57	0.85
1:A:33:ASN:HD21	2:A:759:MPD:H11	1.39	0.85
1:B:60:ASN:HD22	1:B:89:HIS:CE1	1.94	0.84
1:A:524:ASP:O	1:B:525[A]:ARG:NH2	2.10	0.84
1:A:60:ASN:ND2	1:A:89:HIS:HE1	1.76	0.84
1:C:66:THR:HG22	1:C:82[B]:MET:CE	2.08	0.84
1:A:355:THR:HG23	4:A:805:GOL:H11	1.60	0.83
1:A:398:GLY:H	4:A:807:GOL:C1	1.91	0.83
1:C:572:PHE:O	1:C:573:VAL:HB	1.75	0.82
1:A:539:SER:H	1:A:542:HIS:HD2	1.28	0.82
1:C:585:PHE:CD1	1:C:585:PHE:C	2.57	0.82
1:A:699[B]:ASP:OD1	6:A:2717:HOH:O	1.96	0.81
1:C:582:THR:H	1:C:583:TYR:CB	1.93	0.81
1:B:585:PHE:HA	1:B:587:ILE:N	1.95	0.81
1:B:60:ASN:ND2	1:B:89:HIS:HE1	1.77	0.81
1:B:637:ASN:HD22	1:B:639:GLY:H	1.28	0.81
1:A:403:ASN:HD21	1:A:445:ARG:HE	1.29	0.80
1:C:182:GLU:CD	1:C:182:GLU:H	1.87	0.80
1:A:398:GLY:H	4:A:807:GOL:H12	1.46	0.79
1:A:253:ARG:HH22	4:A:806:GOL:H31	1.46	0.79
1:C:582:THR:CA	1:C:583:TYR:CB	2.59	0.79
1:C:628[B]:LEU:HD21	1:C:632:MET:HE2	1.65	0.78
1:A:178[B]:THR:HG22	1:A:230:ASP:OD1	1.81	0.78
1:C:401:ILE:HD13	1:C:536:THR:HG21	1.63	0.78
1:B:253:ARG:NH1	4:B:802:GOL:H32	1.98	0.78
1:A:397:ARG:HA	4:A:807:GOL:H11	1.66	0.78
1:C:539:SER:H	1:C:542:HIS:CD2	1.97	0.77
1:A:562:GLU:HB3	1:A:563:PRO:HD3	1.70	0.73
1:B:253:ARG:HH22	4:B:802:GOL:C1	1.98	0.73
1:C:39:GLU:O	1:C:46:HIS:CD2	2.41	0.72
1:A:403:ASN:ND2	1:A:445:ARG:HE	1.87	0.72
1:C:403:ASN:HD21	1:C:445:ARG:HE	1.38	0.71
1:A:672:GLU:OE2	6:A:2696:HOH:O	2.09	0.70
1:B:584:GLY:O	1:B:585:PHE:CB	2.40	0.70
1:A:33:ASN:HD21	2:A:759:MPD:H12	1.56	0.70
1:C:39:GLU:O	1:C:46:HIS:HD2	1.75	0.69
1:C:66:THR:CG2	1:C:82[B]:MET:HE1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:PHE:O	1:C:573:VAL:CB	2.39	0.69
1:A:605:ASN:ND2	1:A:607:PRO:HD2	2.07	0.69
1:C:82[B]:MET:HA	1:C:82[B]:MET:CE	2.22	0.69
1:C:403:ASN:HD22	1:C:445:ARG:HH21	1.40	0.69
1:B:603:HIS:O	4:B:803:GOL:H31	1.93	0.68
1:A:403:ASN:HD22	1:A:445:ARG:HH21	1.43	0.66
1:A:253:ARG:HH22	4:A:806:GOL:C3	2.08	0.66
1:C:45:SER:OG	1:C:649:ASN:CB	2.44	0.66
1:C:66:THR:HG22	1:C:82[B]:MET:HE2	1.78	0.66
1:A:713:ASN:HD21	1:A:731:GLY:HA3	1.62	0.65
1:A:42:PHE:H	1:A:649:ASN:ND2	1.95	0.64
1:B:311:CYS:O	1:B:315:THR:HG23	1.98	0.63
1:A:628:LEU:HD11	1:A:632[A]:MET:HE2	1.79	0.63
1:C:403:ASN:ND2	1:C:445:ARG:HE	1.94	0.63
1:C:66:THR:CG2	1:C:82[B]:MET:CE	2.77	0.63
1:B:713:ASN:HD21	1:B:731:GLY:HA3	1.64	0.62
1:C:89:HIS:HD2	1:C:98:TYR:O	1.83	0.62
1:C:580:TYR:O	1:C:582:THR:N	2.27	0.62
1:A:637:ASN:HD22	1:B:579:ASN:HD21	1.46	0.62
1:B:154:PHE:HB2	1:B:252:ILE:HB	1.82	0.61
1:A:253:ARG:NH2	4:A:806:GOL:H31	2.15	0.61
1:C:582:THR:CB	1:C:583:TYR:CB	2.79	0.61
1:A:89:HIS:HD2	1:A:98:TYR:O	1.85	0.60
1:A:398:GLY:H	4:A:807:GOL:H11	1.63	0.60
1:C:574:ALA:O	1:C:588:HIS:CE1	2.55	0.60
1:C:539:SER:N	1:C:542:HIS:HD2	1.89	0.60
1:C:580:TYR:C	1:C:582:THR:H	2.10	0.59
1:C:34:PRO:O	1:C:314:ARG:NH2	2.35	0.59
1:A:33:ASN:ND2	2:A:759:MPD:C1	2.59	0.59
1:C:573:VAL:HG22	1:C:575:PRO:N	2.18	0.59
1:B:603:HIS:O	4:B:803:GOL:C3	2.51	0.59
1:B:539:SER:H	1:B:542:HIS:CD2	2.08	0.59
1:C:580:TYR:O	1:C:583:TYR:CB	2.50	0.59
1:B:89:HIS:HD2	1:B:98:TYR:O	1.86	0.58
1:C:215:GLU:OE1	1:C:227:HIS:HD2	1.86	0.58
1:B:353:TRP:CZ3	5:B:900[B]:SWA:HC7	2.38	0.58
1:C:94:TRP:HH2	6:C:2035:HOH:O	1.86	0.58
1:C:60:ASN:ND2	1:C:89:HIS:CE1	2.60	0.58
1:B:613:TYR:CE1	1:B:628:LEU:HD11	2.38	0.58
1:B:126:GLU:O	1:B:127[A]:LYS:HD2	2.04	0.57
1:C:673:TYR:OH	1:C:724:HIS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:GLU:HB3	1:C:563:PRO:HD3	1.86	0.57
2:A:759:MPD:H51	6:A:2782:HOH:O	2.04	0.57
1:C:47:GLY:HA2	1:C:649:ASN:C	2.28	0.57
1:B:172:ASN:HA	1:B:234:ASP:O	2.05	0.56
1:B:613:TYR:CZ	1:B:628:LEU:HD11	2.40	0.56
1:C:448:PHE:CE1	1:C:449:GLU:HG3	2.40	0.56
1:C:414:MET:CE	1:C:482:PHE:HA	2.36	0.56
1:A:523:ARG:HG2	1:B:525[A]:ARG:NH2	2.21	0.55
1:B:29:VAL:H	1:B:289:ASN:ND2	2.03	0.55
1:C:613:TYR:OH	1:C:628[B]:LEU:HD11	2.06	0.55
1:B:227:HIS:HD2	6:B:2207:HOH:O	1.88	0.55
1:A:33:ASN:ND2	2:A:759:MPD:H12	2.20	0.55
1:A:210:SER:HA	4:A:806:GOL:H2	1.89	0.55
1:A:673:TYR:OH	1:A:724:HIS:HD2	1.88	0.55
1:C:29:VAL:H	1:C:289:ASN:ND2	2.05	0.55
1:C:29:VAL:H	1:C:289:ASN:HD21	1.56	0.54
1:C:46:HIS:ND1	6:C:2033:HOH:O	2.09	0.54
1:A:73:TRP:CZ3	4:A:803:GOL:H31	2.43	0.54
1:C:574:ALA:O	1:C:575:PRO:CB	2.55	0.54
1:C:42:PHE:HA	1:C:73:TRP:CZ2	2.43	0.54
1:C:414:MET:HE1	1:C:482:PHE:HA	1.90	0.54
1:C:87:GLN:HE22	1:C:203:ASN:ND2	2.06	0.53
1:A:617:TYR:CE1	1:A:753:PRO:HB2	2.43	0.53
1:B:506:TYR:O	1:B:508:PRO:HD3	2.08	0.53
1:B:87:GLN:HE22	1:B:203:ASN:ND2	2.07	0.53
1:B:353:TRP:CZ3	5:B:900[A]:SWA:HC7	2.43	0.53
1:C:82[B]:MET:HE3	1:C:121:PHE:CE2	2.43	0.53
1:C:580:TYR:C	1:C:582:THR:N	2.68	0.52
1:B:29:VAL:H	1:B:289:ASN:HD21	1.56	0.52
1:A:355:THR:HG21	4:A:805:GOL:H11	1.86	0.52
1:B:414:MET:CE	1:B:482:PHE:HA	2.39	0.52
1:A:637:ASN:HD22	1:B:579:ASN:ND2	2.08	0.51
1:C:459:TYR:CG	1:C:460:PRO:HA	2.46	0.51
1:C:585:PHE:C	1:C:585:PHE:HD1	2.17	0.51
1:C:66:THR:HG23	1:C:82[B]:MET:HE1	1.93	0.51
1:A:628:LEU:HD13	1:A:632[A]:MET:HE2	1.87	0.51
1:B:60:ASN:ND2	1:B:89:HIS:CE1	2.66	0.50
1:C:82[B]:MET:CE	1:C:82[B]:MET:CA	2.86	0.50
1:A:60:ASN:ND2	1:A:89:HIS:CE1	2.63	0.50
1:A:354[B]:ASP:CG	4:A:804:GOL:H11	2.36	0.50
1:A:628:LEU:HD13	1:A:628:LEU:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:SER:HB2	1:A:758:LYS:HB3	1.94	0.49
1:B:637:ASN:ND2	1:B:639:GLY:H	2.05	0.49
1:A:440:ILE:HG12	4:A:807:GOL:H32	1.93	0.49
1:A:41:THR:HA	1:A:649:ASN:HD22	1.76	0.49
1:A:431:HIS:HE1	6:A:2518:HOH:O	1.96	0.49
1:C:459:TYR:CD1	1:C:460:PRO:HA	2.46	0.49
1:B:34:PRO:O	1:B:314:ARG:NH2	2.47	0.48
1:B:42:PHE:HB3	1:C:566:ALA:HB2	1.95	0.48
1:B:353:TRP:HZ3	5:B:900[B]:SWA:HC7	1.77	0.48
1:B:617:TYR:CE1	1:B:753:PRO:HB2	2.48	0.48
1:A:459:TYR:CG	1:A:460:PRO:HA	2.49	0.48
1:A:628:LEU:O	1:A:632[B]:MET:HG2	2.14	0.48
1:B:459:TYR:CG	1:B:460:PRO:HA	2.48	0.48
1:B:253:ARG:HH12	4:B:802:GOL:C3	2.12	0.48
1:B:418:GLN:NE2	6:B:2385:HOH:O	2.47	0.48
1:B:514:TRP:CG	1:B:515:THR:H	2.33	0.47
1:A:499:ALA:N	1:A:500:PRO:CD	2.77	0.47
1:B:42:PHE:HA	1:B:73:TRP:CZ2	2.49	0.47
1:B:687:LEU:HB3	1:B:688:PRO:HD2	1.95	0.47
1:B:688:PRO:C	1:B:689:GLU:HG2	2.40	0.47
1:C:69:ASN:H	1:C:114:HIS:CD2	2.32	0.47
1:C:617:TYR:CE1	1:C:753:PRO:HB2	2.50	0.47
1:A:300:GLY:HA2	4:A:801:GOL:H31	1.95	0.47
1:C:585:PHE:HD1	1:C:586:VAL:N	2.13	0.47
1:C:184:ARG:NH1	1:C:209:PHE:O	2.44	0.47
1:B:32:VAL:HG11	1:B:130:PRO:HG3	1.97	0.46
1:A:69:ASN:H	1:A:114:HIS:CD2	2.33	0.46
4:A:804:GOL:H2	4:A:805:GOL:C2	2.40	0.46
2:A:759:MPD:H31	6:A:2019:HOH:O	2.15	0.46
1:B:62:TRP:HA	1:B:86:ARG:O	2.16	0.46
1:B:69:ASN:H	1:B:114:HIS:CD2	2.35	0.46
1:A:117:ARG:C	1:A:118:LEU:HD22	2.41	0.45
1:B:92:SER:HB2	6:B:2548:HOH:O	2.16	0.45
1:B:414:MET:HE1	1:B:482:PHE:HA	1.99	0.45
1:B:647:GLU:OE2	1:B:650:GLY:HA2	2.16	0.45
1:C:573:VAL:HG13	1:C:574:ALA:N	2.26	0.45
1:C:94:TRP:HE3	4:C:802:GOL:H12	1.82	0.45
1:C:87:GLN:HE22	1:C:203:ASN:HD21	1.63	0.45
1:C:94:TRP:HD1	6:C:2043:HOH:O	2.00	0.45
1:A:539:SER:H	1:A:542:HIS:CD2	2.19	0.44
1:C:172:ASN:HA	1:C:234:ASP:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG11	1:A:130:PRO:HG3	1.99	0.44
2:A:759:MPD:H53	6:A:2151:HOH:O	2.16	0.44
1:B:445:ARG:HG3	1:B:472:TYR:CZ	2.53	0.44
4:A:804:GOL:C2	4:A:805:GOL:O2	2.40	0.44
1:B:450:TYR:HB3	1:B:458:PRO:HD3	2.00	0.44
1:C:66:THR:HG22	1:C:82[B]:MET:HE1	1.83	0.44
1:A:605:ASN:HD22	1:A:607:PRO:HD2	1.81	0.44
1:B:499:ALA:N	1:B:500:PRO:CD	2.81	0.44
1:B:436:ARG:HD2	1:B:437:HIS:O	2.18	0.43
1:C:584:GLY:HA3	1:C:585:PHE:HA	1.74	0.43
1:C:450:TYR:HB3	1:C:458:PRO:HD3	1.99	0.43
1:A:601:TYR:CE2	1:A:603:HIS:HB2	2.53	0.43
1:B:207:MET:HA	1:B:253:ARG:O	2.18	0.43
1:C:631:VAL:HG13	1:C:635:LEU:HD12	1.99	0.43
1:B:645:GLY:N	6:B:2544:HOH:O	2.51	0.43
1:A:555:SER:HA	1:A:564:MET:HE3	1.99	0.43
1:A:640:SER:N	2:A:759:MPD:H13	2.33	0.43
1:C:445:ARG:HG3	1:C:472:TYR:CZ	2.53	0.43
1:A:744:GLN:HG2	1:C:81:LEU:HD11	2.00	0.43
1:C:515:THR:HG23	1:C:523:ARG:HB2	2.01	0.43
1:A:127:LYS:CD	6:A:2059:HOH:O	2.66	0.43
1:C:574:ALA:O	1:C:588:HIS:NE2	2.52	0.43
1:B:593:MET:HE2	1:B:593:MET:HB3	1.92	0.43
1:C:48:ASN:HD21	1:C:73:TRP:HE1	1.66	0.43
1:B:338:ASP:OD1	1:B:342:HIS:HE1	2.01	0.42
1:A:356:PHE:CD1	1:A:356:PHE:C	2.97	0.42
1:A:555:SER:CA	1:A:564:MET:HE3	2.49	0.42
1:A:630:ASN:OD1	1:A:634:LYS:HD2	2.20	0.42
1:C:312:LEU:O	1:C:316:LEU:HG	2.19	0.42
1:B:359:VAL:HG23	1:B:651:GLN:HA	2.02	0.42
1:B:647:GLU:OE2	1:B:653:SER:OG	2.33	0.42
1:A:87:GLN:HE22	1:A:256:SER:CB	2.33	0.42
1:C:186:VAL:HG21	1:C:240:LEU:HD11	2.01	0.42
1:A:355:THR:HG21	4:A:805:GOL:C1	2.49	0.42
1:B:353:TRP:HZ3	5:B:900[A]:SWA:HC7	1.84	0.42
1:C:299:GLY:O	4:C:801:GOL:H32	2.20	0.42
1:A:338:ASP:OD1	1:A:342:HIS:HE1	2.03	0.42
1:B:356:PHE:CD1	1:B:356:PHE:C	2.98	0.42
1:C:585:PHE:CD1	1:C:586:VAL:N	2.85	0.42
1:C:516:LYS:HE3	1:C:522:TRP:CZ2	2.55	0.41
1:A:228:GLN:HE21	1:A:228:GLN:HB3	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:GLU:HG3	5:B:900[B]:SWA:HC8	2.01	0.41
1:A:172:ASN:HA	1:A:234:ASP:O	2.21	0.41
1:C:48:ASN:HD22	1:C:48:ASN:HA	1.62	0.41
1:C:573:VAL:CG2	1:C:575:PRO:N	2.83	0.41
1:A:687:LEU:HB3	1:A:688:PRO:HD2	2.01	0.41
1:C:32:VAL:HG11	1:C:130:PRO:HG3	2.02	0.41
1:C:734:ASN:OD1	1:C:734:ASN:C	2.62	0.41
1:A:226:HIS:O	1:A:227:HIS:HB2	2.21	0.41
1:A:353:TRP:CZ3	1:A:400:MET:HE2	2.56	0.41
1:C:62:TRP:HA	1:C:86:ARG:O	2.21	0.41
1:C:499:ALA:N	1:C:500:PRO:CD	2.84	0.41
1:A:398:GLY:N	4:A:807:GOL:H11	2.33	0.40
1:A:713:ASN:ND2	1:A:732:GLU:H	2.19	0.40
1:C:142:GLN:HE21	1:C:142:GLN:HB3	1.76	0.40
1:A:285:ARG:NH1	6:A:2388:HOH:O	2.37	0.40
1:A:571:MET:HE3	6:A:2624:HOH:O	2.21	0.40
1:C:39:GLU:HB2	1:C:640:SER:HB2	2.03	0.40
1:A:615:TYR:HB2	1:A:624:THR:HG1	1.86	0.40
1:B:628:LEU:CD1	1:B:676:GLY:HA3	2.51	0.40
1:A:82[B]:MET:HB3	1:A:137:PHE:HE1	1.86	0.40
1:C:31:TYR:HB3	1:C:306:ARG:HA	2.04	0.40
1:C:190:THR:HG23	1:C:203:ASN:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/737 (101%)	719 (97%)	25 (3%)	0	100	100
1	B	743/737 (101%)	714 (96%)	28 (4%)	1 (0%)	48	40
1	C	739/737 (100%)	703 (95%)	31 (4%)	5 (1%)	18	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2226/2211 (101%)	2136 (96%)	84 (4%)	6 (0%)	36	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	585	PHE
1	C	573	VAL
1	C	575	PRO
1	C	583	TYR
1	C	581	GLY
1	C	574	ALA

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	A	608/620 (98%)	599 (98%)	9 (2%)	57	56
1	B	596/620 (96%)	588 (99%)	8 (1%)	61	61
1	C	604/620 (97%)	594 (98%)	10 (2%)	53	52
All	All	1808/1860 (97%)	1781 (98%)	27 (2%)	57	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	171	TYR
1	A	350	ASN
1	A	391	TRP
1	A	548	PHE
1	A	605	ASN
1	A	647	GLU
1	A	728	LYS
1	A	758	LYS
1	B	171	TYR

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Mol	Chain	Res	Type
1	B	295	VAL
1	B	350	ASN
1	B	391	TRP
1	B	436	ARG
1	B	548	PHE
1	B	571	MET
1	B	689	GLU
1	C	48	ASN
1	C	111	LYS
1	C	171	TYR
1	C	182	GLU
1	C	391	TRP
1	C	536	THR
1	C	548	PHE
1	C	585	PHE
1	C	699[A]	ASP
1	C	699[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	ASN
1	A	87	GLN
1	A	89	HIS
1	A	114	HIS
1	A	203	ASN
1	A	228	GLN
1	A	340	ASN
1	A	342	HIS
1	A	376	GLN
1	A	403	ASN
1	A	431	HIS
1	A	521	ASN
1	A	542	HIS
1	A	605	ASN
1	A	649	ASN
1	A	713	ASN
1	A	715	GLN
1	A	724	HIS
1	A	748	GLN
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	89	HIS
1	B	90	GLN
1	B	114	HIS
1	B	203	ASN
1	B	227	HIS
1	B	289	ASN
1	B	330	ASN
1	B	342	HIS
1	B	376	GLN
1	B	404	ASN
1	B	418	GLN
1	B	434	GLN
1	B	521	ASN
1	B	542	HIS
1	B	579	ASN
1	B	637	ASN
1	B	713	ASN
1	C	48	ASN
1	C	60	ASN
1	C	89	HIS
1	C	114	HIS
1	C	142	GLN
1	C	203	ASN
1	C	227	HIS
1	C	289	ASN
1	C	342	HIS
1	C	350	ASN
1	C	376	GLN
1	C	403	ASN
1	C	418	GLN
1	C	431	HIS
1	C	434	GLN
1	C	504	ASN
1	C	542	HIS
1	C	724	HIS
1	C	748	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\# Z > 2$
4	GOL	B	802	-	5,5,5	0.34	0	5,5,5	0.39	0
4	GOL	A	804	-	5,5,5	0.39	0	5,5,5	0.55	0
4	GOL	B	801	-	5,5,5	0.36	0	5,5,5	0.66	0
4	GOL	A	803	-	5,5,5	0.34	0	5,5,5	0.41	0
4	GOL	A	806	-	5,5,5	0.42	0	5,5,5	0.46	0
4	GOL	C	801	-	5,5,5	0.33	0	5,5,5	0.79	0
5	SWA	B	900[B]	-	13,13,13	0.74	0	14,19,19	0.95	0
4	GOL	A	805	-	5,5,5	0.59	0	5,5,5	1.06	0
2	MPD	A	759	-	7,7,7	0.45	0	9,10,10	0.76	0
4	GOL	A	801	-	5,5,5	0.61	0	5,5,5	1.06	0
4	GOL	B	804	-	5,5,5	0.30	0	5,5,5	0.60	0
4	GOL	B	803	-	5,5,5	0.30	0	5,5,5	0.32	0
4	GOL	A	807	-	5,5,5	0.36	0	5,5,5	0.37	0
4	GOL	C	803	-	5,5,5	0.33	0	5,5,5	0.44	0
5	SWA	B	900[A]	-	13,13,13	0.82	0	14,19,19	0.91	1 (7%)
4	GOL	C	802	-	5,5,5	0.29	0	5,5,5	0.93	0
4	GOL	A	802	-	5,5,5	0.23	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	802	-	-	2/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-
4	GOL	B	801	-	-	4/4/4/4	-
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	A	806	-	-	2/4/4/4	-
4	GOL	C	801	-	-	4/4/4/4	-
5	SWA	B	900[B]	-	-	-	1/2/2/2
4	GOL	A	805	-	-	4/4/4/4	-
2	MPD	A	759	-	-	2/5/5/5	-
4	GOL	A	801	-	-	4/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
4	GOL	B	803	-	-	4/4/4/4	-
4	GOL	A	807	-	-	4/4/4/4	-
4	GOL	C	803	-	-	4/4/4/4	-
5	SWA	B	900[A]	-	-	-	0/2/2/2
4	GOL	C	802	-	-	4/4/4/4	-
4	GOL	A	802	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900[A]	SWA	C5-N4-C3	-2.02	110.17	112.14

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	GOL	O1-C1-C2-C3
4	A	802	GOL	C1-C2-C3-O3
4	A	803	GOL	C1-C2-C3-O3
4	A	804	GOL	O1-C1-C2-O2
4	A	804	GOL	O1-C1-C2-C3
4	A	804	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	A	807	GOL	O1-C1-C2-O2
4	A	807	GOL	O1-C1-C2-C3
4	B	801	GOL	O1-C1-C2-C3
4	B	801	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	B	803	GOL	O2-C2-C3-O3
4	C	801	GOL	O1-C1-C2-C3
4	C	802	GOL	O1-C1-C2-C3
4	C	802	GOL	C1-C2-C3-O3
4	C	803	GOL	O1-C1-C2-O2
4	C	803	GOL	O1-C1-C2-C3
4	C	803	GOL	C1-C2-C3-O3
4	A	801	GOL	O1-C1-C2-O2
4	A	806	GOL	O2-C2-C3-O3
4	B	801	GOL	O2-C2-C3-O3
4	A	801	GOL	C1-C2-C3-O3
4	A	802	GOL	O1-C1-C2-C3
4	A	803	GOL	O1-C1-C2-C3
4	A	805	GOL	C1-C2-C3-O3
4	A	806	GOL	C1-C2-C3-O3
4	A	807	GOL	C1-C2-C3-O3
4	C	801	GOL	C1-C2-C3-O3
4	A	801	GOL	O2-C2-C3-O3
4	A	802	GOL	O2-C2-C3-O3
4	A	803	GOL	O1-C1-C2-O2
4	A	803	GOL	O2-C2-C3-O3
4	A	804	GOL	O2-C2-C3-O3
4	A	805	GOL	O1-C1-C2-O2
4	B	801	GOL	O1-C1-C2-O2
4	B	803	GOL	O1-C1-C2-O2
4	C	802	GOL	O1-C1-C2-O2
4	C	802	GOL	O2-C2-C3-O3
4	A	805	GOL	O2-C2-C3-O3
4	C	803	GOL	O2-C2-C3-O3
4	C	801	GOL	O1-C1-C2-O2
4	B	802	GOL	O1-C1-C2-O2
4	C	801	GOL	O2-C2-C3-O3
4	B	802	GOL	O1-C1-C2-C3
4	A	807	GOL	O2-C2-C3-O3
4	A	802	GOL	O1-C1-C2-O2
2	A	759	MPD	C1-C2-C3-C4
2	A	759	MPD	CM-C2-C3-C4

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	900[B]	SWA	C1-C2-C3-C5-C6-N4

13 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	GOL	6	0
4	A	804	GOL	4	0
4	A	803	GOL	1	0
4	A	806	GOL	4	0
4	C	801	GOL	1	0
5	B	900[B]	SWA	3	0
4	A	805	GOL	7	0
2	A	759	MPD	10	0
4	A	801	GOL	1	0
4	B	803	GOL	2	0
4	A	807	GOL	6	0
5	B	900[A]	SWA	2	0
4	C	802	GOL	1	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	A	737/737 (100%)	-0.19	18 (2%)	59	63	6, 11, 24, 57	9 (1%)
1	B	737/737 (100%)	0.24	43 (5%)	29	30	6, 14, 27, 59	8 (1%)
1	C	737/737 (100%)	0.18	43 (5%)	29	30	8, 15, 34, 56	4 (0%)
All	All	2211/2211 (100%)	0.08	104 (4%)	36	39	6, 13, 30, 59	21 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	GLN	9.3
1	C	574	ALA	9.0
1	C	43	ALA	8.4
1	B	583	TYR	8.0
1	B	585	PHE	8.0
1	C	575	PRO	7.5
1	C	47	GLY	7.3
1	B	601	TYR	6.8
1	C	40	SER	6.5
1	C	585	PHE	6.5
1	C	580	TYR	6.4
1	B	586	VAL	6.1
1	B	595	ALA	6.1
1	C	41	THR	6.1
1	C	599	GLY	5.9
1	B	604	GLY	5.8
1	B	594	VAL	5.8
1	B	599	GLY	5.6
1	C	578	TYR	5.6
1	C	583	TYR	5.5
1	A	585	PHE	5.5
1	B	603	HIS	5.5
1	C	44	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	41	THR	5.3
1	C	586	VAL	5.3
1	B	44	PHE	5.3
1	C	582	THR	5.2
1	B	644[A]	CYS	5.1
1	B	596	LEU	5.1
1	B	597	ASN	5.1
1	C	600	GLN	5.0
1	C	42	PHE	4.9
1	C	573	VAL	4.9
1	B	43	ALA	4.8
1	B	42	PHE	4.8
1	B	582	THR	4.7
1	C	46	HIS	4.6
1	B	590	ILE	4.5
1	B	574	ALA	4.5
1	B	587	ILE	4.4
1	C	601	TYR	4.3
1	B	584	GLY	4.1
1	B	602	ALA	4.1
1	C	588	HIS	4.1
1	A	574	ALA	4.0
1	A	590	ILE	4.0
1	A	587	ILE	4.0
1	C	581	GLY	3.9
1	B	589	GLU	3.9
1	A	583	TYR	3.8
1	C	584	GLY	3.8
1	A	594	VAL	3.8
1	A	588	HIS	3.8
1	B	580	TYR	3.8
1	C	22	SER	3.8
1	B	598	MET	3.7
1	B	581	GLY	3.7
1	B	47	GLY	3.6
1	C	590	ILE	3.6
1	C	595	ALA	3.6
1	C	579	ASN	3.6
1	C	589	GLU	3.6
1	C	577	THR	3.5
1	A	586	VAL	3.5
1	B	573	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	576	ASN	3.3
1	B	46	HIS	3.2
1	A	595	ALA	3.1
1	C	222	ASP	3.1
1	B	40	SER	3.1
1	C	602	ALA	3.1
1	C	587	ILE	3.1
1	B	588	HIS	3.1
1	B	575	PRO	3.1
1	B	591	ALA	3.1
1	C	73	TRP	2.9
1	B	45	SER	2.9
1	A	584	GLY	2.9
1	B	650	GLY	2.9
1	A	575	PRO	2.8
1	A	591	ALA	2.8
1	B	648	ASP	2.8
1	A	600	GLN	2.8
1	A	582	THR	2.7
1	C	604	GLY	2.7
1	C	598	MET	2.6
1	B	222	ASP	2.6
1	C	646	ASP	2.6
1	A	589	GLU	2.5
1	C	45	SER	2.5
1	B	48	ASN	2.5
1	C	648	ASP	2.5
1	C	645	GLY	2.4
1	C	644	CYS	2.3
1	C	650	GLY	2.3
1	B	94	TRP	2.2
1	C	94	TRP	2.2
1	A	599	GLY	2.2
1	B	593	MET	2.2
1	C	572	PHE	2.1
1	B	646	ASP	2.1
1	A	573	VAL	2.1
1	A	669	GLY	2.0
1	B	231	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors($\text{\AA}^2$)	Q<0.9
5	SWA	B	900[A]	12/12	0.52	0.17	26,32,33,33	12
5	SWA	B	900[B]	12/12	0.52	0.17	31,36,37,37	12
4	GOL	C	803	6/6	0.65	0.21	50,51,52,52	0
4	GOL	C	802	6/6	0.70	0.22	52,53,53,53	0
4	GOL	B	803	6/6	0.77	0.14	43,45,46,46	0
4	GOL	A	807	6/6	0.79	0.19	48,49,49,49	0
2	MPD	A	759	8/8	0.80	0.18	28,33,35,36	0
4	GOL	B	804	6/6	0.80	0.13	26,29,30,31	0
4	GOL	B	802	6/6	0.80	0.13	49,49,50,50	0
4	GOL	A	802	6/6	0.83	0.13	33,34,36,37	0
4	GOL	A	804	6/6	0.84	0.15	35,40,41,44	0
4	GOL	A	803	6/6	0.86	0.15	29,34,35,37	0
4	GOL	A	806	6/6	0.86	0.15	36,36,37,39	0
4	GOL	A	805	6/6	0.87	0.24	26,33,34,35	0
4	GOL	A	801	6/6	0.89	0.12	12,21,24,30	0
4	GOL	C	801	6/6	0.90	0.10	17,21,23,27	0
4	GOL	B	801	6/6	0.92	0.11	16,19,22,23	0
3	NA	C	800	1/1	0.95	0.14	20,20,20,20	0
3	NA	B	800	1/1	0.96	0.05	17,17,17,17	0
3	NA	A	799	1/1	0.97	0.07	11,11,11,11	0
3	NA	A	800	1/1	0.98	0.09	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.