



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WW2  
Title : STRUCTURE OF THE FAMILY GH92 INVERTING MANNOSIDASE  
BT2199 FROM BACTEROIDES THETA IOTAOMICRON 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

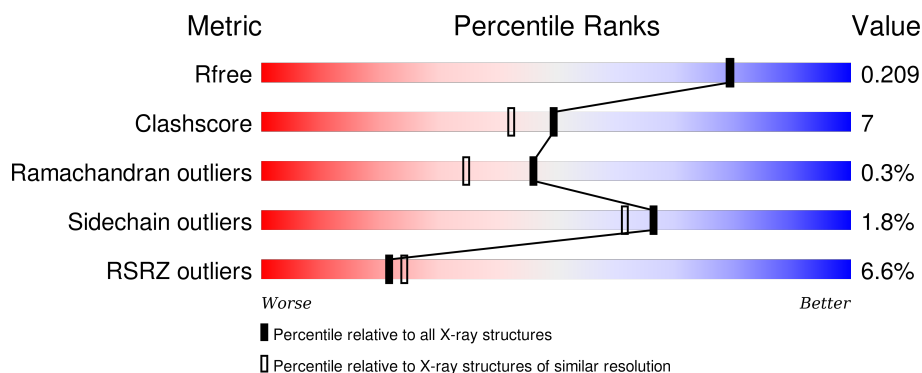
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	737	<div> <div>4%</div> <div>88%</div> <div>11%</div> </div>
1	B	737	<div> <div>8%</div> <div>89%</div> <div>11%</div> </div>
1	C	737	<div> <div>8%</div> <div>87%</div> <div>12%</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	MPD	A	759	-	-	X	X
4	GOL	A	801	-	-	-	X
4	GOL	A	803	-	-	-	X
4	GOL	A	804	-	-	X	X
4	GOL	A	805	-	-	X	X
4	GOL	A	806	-	-	X	X
4	GOL	A	807	-	-	X	X
4	GOL	B	801	-	-	-	X
4	GOL	B	802	-	-	X	X
4	GOL	C	802	-	-	-	X
5	SWA	B	900[A]	-	-	-	X
5	SWA	B	900[B]	-	-	-	X

## 2 Entry composition [i](#)

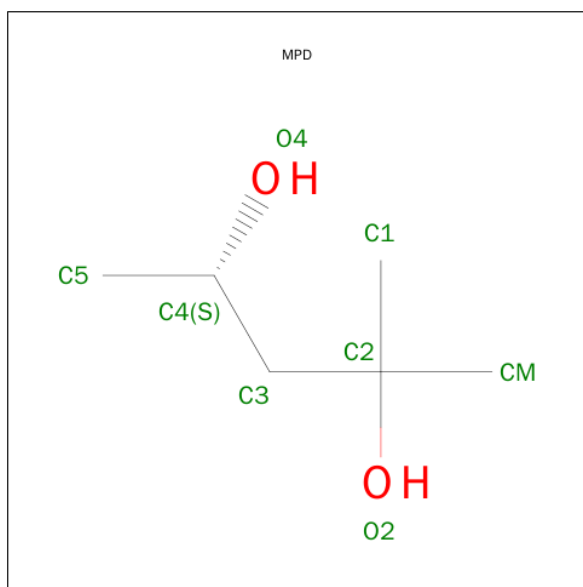
There are 6 unique types of molecules in this entry. The entry contains 19766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



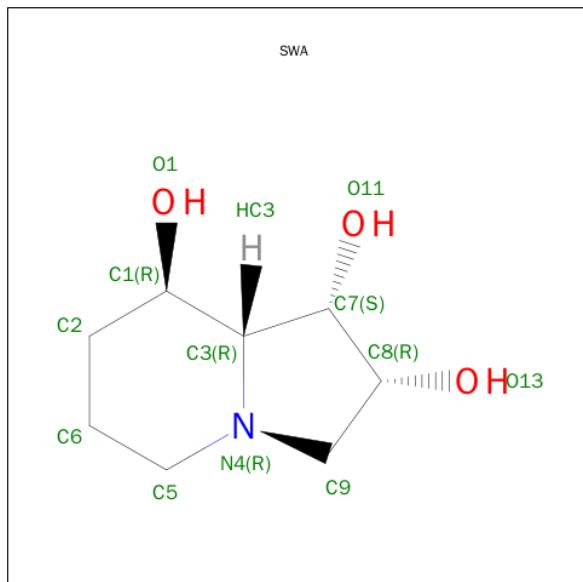
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

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 (three-letter code: 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		

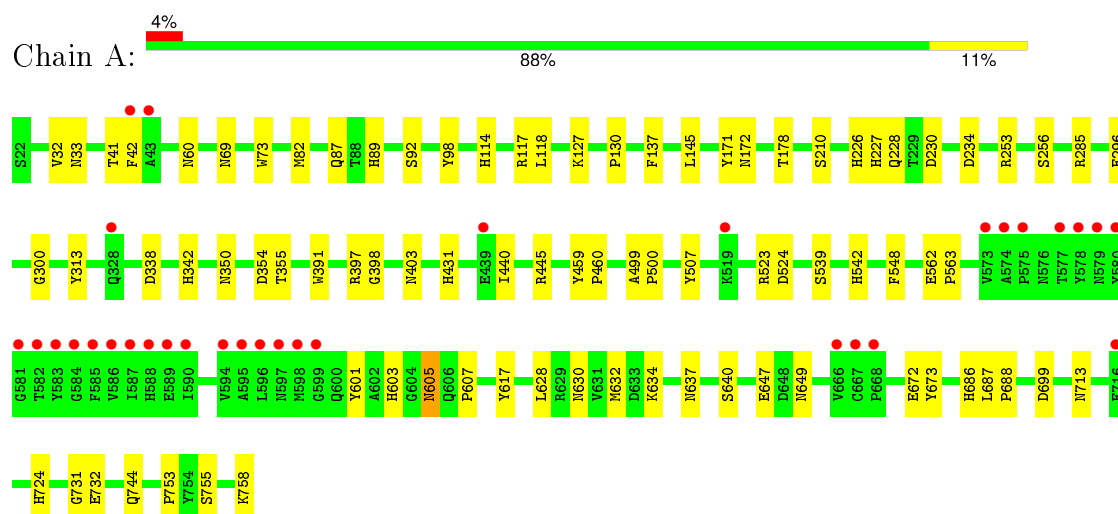
- Molecule 6 is water.

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		

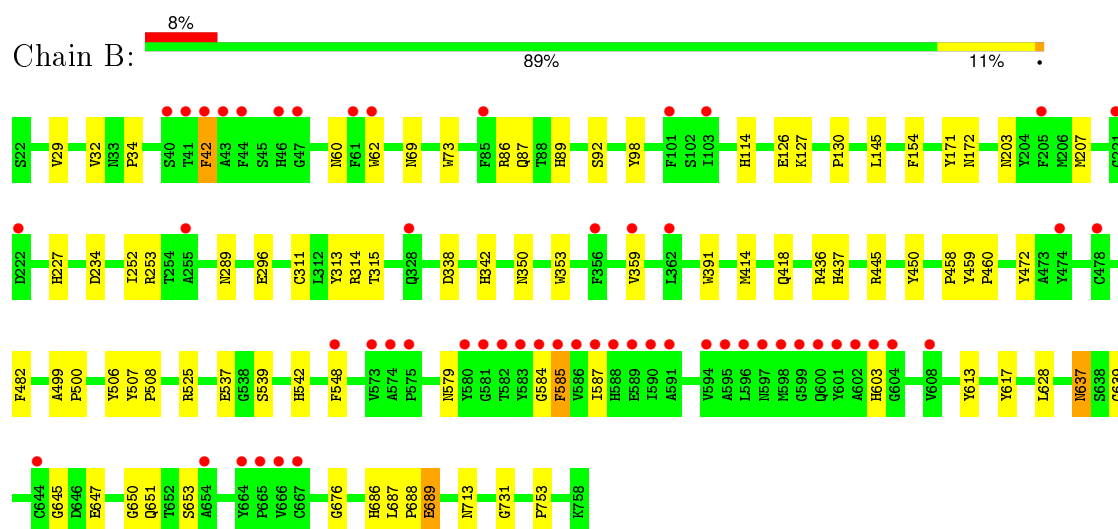
### 3 Residue-property plots

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.

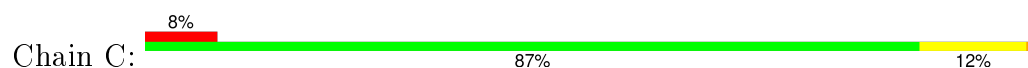
#### • Molecule 1: ALPHA-1,2-MANNOSIDASE

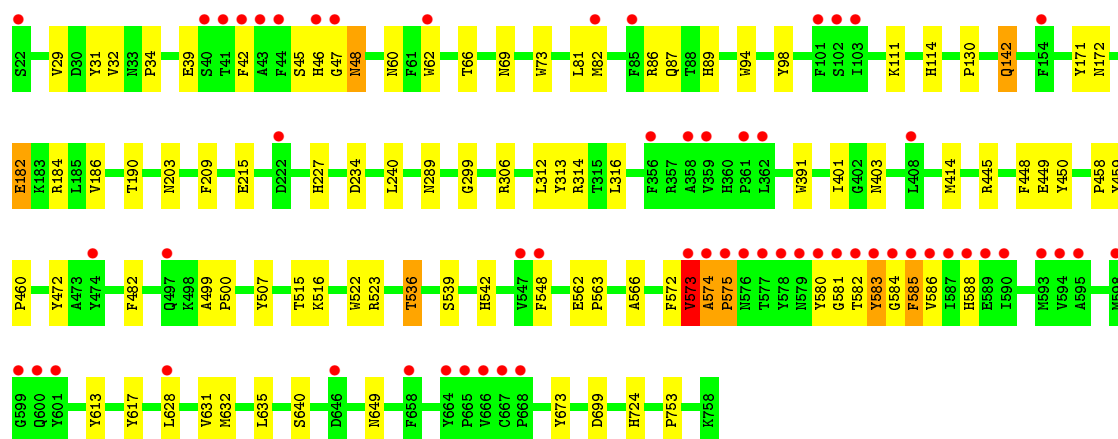


#### • Molecule 1: ALPHA-1,2-MANNOSIDASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.157 , 0.187 0.184 , 0.209	Depositor DCC
$R_{free}$ test set	11455 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.5	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 227941 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SWA, GOL, MPD, NA

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	0.52	0/6094	0.59	0/8299
1	B	0.48	0/6051	0.58	0/8246
1	C	0.45	0/6045	0.56	1/8233 (0.0%)
All	All	0.48	0/18190	0.58	1/24778 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	573	VAL	CB-CA-C	-5.53	100.90	111.40

There are no chirality outliers.

There are no planarity outliers.

### 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	A	5882	0	5421	73	0
1	B	5843	0	5360	67	0
1	C	5851	0	5400	101	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	42	0	56	21	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	8	0
6	B	653	0	0	4	0
6	C	627	0	0	3	0
All	All	19766	0	16337	242	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 (242) 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: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: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: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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:582:THR:H	1:C:583:TYR:CB	1.93	0.81
1:A:699[B]:ASP:OD1	6:A:2717:HOH:O	1.96	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:582:THR:CA	1:C:583:TYR:CB	2.59	0.79
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: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:585:PHE:C	1:C:585:PHE:CD1	2.57	0.77
1:C:539:SER:H	1:C:542:HIS:CD2	1.97	0.77
1:C:182:GLU:H	1:C:182:GLU:CD	1.87	0.76
1:C:66:THR:HG22	1:C:82[B]:MET:HE2	1.67	0.74
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:572:PHE:O	1:C:573:VAL:CB	2.39	0.69
1:C:82[B]:MET:CE	1:C:82[B]:MET:HA	2.22	0.69
1:C:403:ASN:HD22	1:C:445:ARG:HH21	1.40	0.69
1:A:605:ASN:ND2	1:A:607:PRO:HD2	2.07	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:A:713:ASN:HD21	1:A:731:GLY:HA3	1.62	0.65
1:C:628[B]:LEU:HD23	1:C:632:MET:HE2	1.80	0.64
1:C:82[B]:MET:HE2	1:C:82[B]:MET:HA	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:628[B]:LEU:HD21	1:C:632:MET:HE1	1.80	0.64
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: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:C:582:THR:CB	1:C:583:TYR:CB	2.79	0.61
1:A:253:ARG:NH2	4:A:806:GOL:H31	2.15	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: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:C:580:TYR:O	1:C:583:TYR:CB	2.50	0.59
1:B:539:SER:H	1:B:542:HIS:CD2	2.08	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:C:94:TRP:HH2	6:C:2035:HOH:O	1.86	0.58
1:B:353:TRP:CZ3	5:B:900[B]:SWA:HC7	2.38	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:C:673:TYR:OH	1:C:724:HIS:HD2	1.87	0.57
1:B:126:GLU:O	1:B:127[A]:LYS:HD2	2.04	0.57
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: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:C:66:THR:CG2	1:C:82[B]:MET:HE2	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:HIS:ND1	6:C:2033:HOH:O	2.09	0.54
1:C:29:VAL:H	1:C:289:ASN:HD21	1.56	0.54
1:C:574:ALA:O	1:C:575:PRO:CB	2.55	0.54
1:A:73:TRP:CZ3	4:A:803:GOL:H31	2.43	0.54
1:C:42:PHE:HA	1:C:73:TRP:CZ2	2.43	0.54
1:C:628[B]:LEU:CD2	1:C:632:MET:CE	2.86	0.53
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:353:TRP:CZ3	5:B:900[A]:SWA:HC7	2.43	0.53
1:B:87:GLN:HE22	1:B:203:ASN:ND2	2.07	0.53
1:C:66:THR:CG2	1:C:82[B]:MET:HE1	2.39	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:C:47:GLY:HA2	1:C:649:ASN:C	2.28	0.52
1:C:628[B]:LEU:CD2	1:C:632:MET:HE1	2.40	0.52
1:C:414:MET:HE1	1:C:482:PHE:HA	1.92	0.52
1:C:580:TYR:C	1:C:582:THR:H	2.10	0.51
1:A:637:ASN:HD22	1:B:579:ASN:ND2	2.08	0.51
1:A:296:GLU:OE1	1:A:686:HIS:NE2	2.43	0.51
1:C:459:TYR:CG	1:C:460:PRO:HA	2.46	0.51
1:C:573:VAL:HG13	1:C:574:ALA:N	2.26	0.50
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:C:82[B]:MET:HE3	1:C:82[B]:MET:CA	2.42	0.49
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:C:459:TYR:CD1	1:C:460:PRO:HA	2.46	0.49
1:A:431:HIS:HE1	6:A:2518:HOH:O	1.96	0.49
1:B:42:PHE:HB3	1:C:566:ALA:HB2	1.95	0.48
1:B:34:PRO:O	1:B:314:ARG:NH2	2.47	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:TYR:CG	1:A:460:PRO:HA	2.49	0.48
1:C:580:TYR:C	1:C:582:THR:N	2.68	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:C:182:GLU:N	1:C:182:GLU:CD	2.64	0.48
1:B:418:GLN:NE2	6:B:2385:HOH:O	2.47	0.48
1:B:42:PHE:HA	1:B:73:TRP:CZ2	2.49	0.47
1:A:499:ALA:N	1:A:500:PRO:CD	2.77	0.47
1:B:687:LEU:HB3	1:B:688:PRO:HD2	1.95	0.47
1:B:414:MET:HE1	1:B:482:PHE:HA	1.96	0.47
1:C:617:TYR:CE1	1:C:753:PRO:HB2	2.50	0.47
1:C:69:ASN:H	1:C:114:HIS:CD2	2.32	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
4:A:804:GOL:H2	4:A:805:GOL:HO2	1.72	0.47
1:C:184:ARG:NH1	1:C:209:PHE:O	2.44	0.47
1:C:585:PHE:C	1:C:585:PHE:HD1	2.17	0.46
1:B:32:VAL:HG11	1:B:130:PRO:HG3	1.97	0.46
1:C:628[B]:LEU:HD21	1:C:632:MET:CE	2.45	0.46
4:A:804:GOL:H2	4:A:805:GOL:C2	2.40	0.46
1:A:69:ASN:H	1:A:114:HIS:CD2	2.33	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:B:92:SER:HB2	6:B:2548:HOH:O	2.16	0.45
1:A:354[B]:ASP:CG	4:A:804:GOL:H11	2.36	0.45
1:B:647:GLU:OE2	1:B:650:GLY:HA2	2.16	0.45
1:A:628:LEU:C	1:A:628:LEU:HD13	2.37	0.45
1:C:94:TRP:HE3	4:C:802:GOL:H12	1.82	0.45
1:C:94:TRP:HD1	6:C:2043:HOH:O	2.00	0.45
1:C:87:GLN:HE22	1:C:203:ASN:HD21	1.63	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
2:A:759:MPD:H53	6:A:2151:HOH:O	2.16	0.44
1:A:628:LEU:CD1	1:A:632[A]:MET:CE	2.96	0.44
1:A:32:VAL:HG11	1:A:130:PRO:HG3	1.99	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:A:605:ASN:HD22	1:A:607:PRO:HD2	1.81	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:601:TYR:CE2	1:A:603:HIS:HB2	2.53	0.43
1:B:645:GLY:N	6:B:2544:HOH:O	2.51	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:C:574:ALA:O	1:C:588:HIS:NE2	2.52	0.43
1:A:127:LYS:CD	6:A:2059:HOH:O	2.66	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:B:688:PRO:C	1:B:689:GLU:HG2	2.40	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:647:GLU:OE2	1:B:653:SER:OG	2.33	0.42
1:B:359:VAL:HG23	1:B:651:GLN:HA	2.02	0.42
1:C:66:THR:HG22	1:C:82[B]:MET:HE1	1.96	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:C:628[B]:LEU:HD23	1:C:632:MET:CE	2.46	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:C:585:PHE:CD1	1:C:586:VAL:N	2.85	0.42
1:B:296:GLU:OE2	1:B:686:HIS:NE2	2.53	0.42
1:A:338:ASP:OD1	1:A:342:HIS:HE1	2.03	0.42
1:C:516:LYS:HE3	1:C:522:TRP:CZ2	2.55	0.41
1:B:537:GLU:HG3	5:B:900[B]:SWA:HC8	2.01	0.41
1:A:228:GLN:HE21	1:A:228:GLN:HB3	1.64	0.41
1:C:573:VAL:CG2	1:C:575:PRO:N	2.83	0.41
1:C:48:ASN:HA	1:C:48:ASN:HD22	1.62	0.41
1:A:172:ASN:HA	1:A:234:ASP:O	2.21	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:A:226:HIS:O	1:A:227:HIS:HB2	2.21	0.41
1:C:499:ALA:N	1:C:500:PRO:CD	2.84	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:TRP:HA	1:C:86:ARG:O	2.21	0.41
1:A:117:ARG:C	1:A:118:LEU:HD22	2.41	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:HB3	1:C:142:GLN:HE21	1.76	0.40
1:C:39:GLU:HB2	1:C:640:SER:HB2	2.03	0.40
1:A:285:ARG:NH1	6:A:2388:HOH:O	2.37	0.40
1:B:628:LEU:CD1	1:B:676:GLY:HA3	2.51	0.40
1:C:190:THR:HG23	1:C:203:ASN:HB3	2.04	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

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%)	56	46
1	C	739/737 (100%)	703 (95%)	31 (4%)	5 (1%)	26	14
All	All	2226/2211 (101%)	2136 (96%)	84 (4%)	6 (0%)	46	35

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%)	598 (98%)	10 (2%)	70	66
1	B	596/620 (96%)	586 (98%)	10 (2%)	68	64
1	C	604/620 (97%)	591 (98%)	13 (2%)	60	53
All	All	1808/1860 (97%)	1775 (98%)	33 (2%)	66	61

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	145	LEU
1	A	171	TYR
1	A	313	TYR
1	A	350	ASN
1	A	391	TRP
1	A	507	TYR
1	A	548	PHE
1	A	605	ASN
1	A	647	GLU
1	B	42	PHE
1	B	145	LEU
1	B	171	TYR
1	B	313	TYR
1	B	350	ASN
1	B	391	TRP
1	B	507	TYR
1	B	548	PHE
1	B	637	ASN
1	B	689	GLU
1	C	48	ASN
1	C	111	LYS
1	C	142	GLN
1	C	171	TYR
1	C	182	GLU
1	C	313	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	391	TRP
1	C	507	TYR
1	C	536	THR
1	C	548	PHE
1	C	585	PHE
1	C	699[A]	ASP
1	C	699[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	87	GLN
1	A	89	HIS
1	A	114	HIS
1	A	132	ASN
1	A	203	ASN
1	A	228	GLN
1	A	342	HIS
1	A	403	ASN
1	A	404	ASN
1	A	431	HIS
1	A	494	GLN
1	A	542	HIS
1	A	605	ASN
1	A	649	ASN
1	A	713	ASN
1	A	724	HIS
1	B	60	ASN
1	B	89	HIS
1	B	114	HIS
1	B	132	ASN
1	B	203	ASN
1	B	227	HIS
1	B	289	ASN
1	B	328	GLN
1	B	330	ASN
1	B	342	HIS
1	B	404	ASN
1	B	418	GLN
1	B	431	HIS
1	B	542	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	132	ASN
1	C	142	GLN
1	C	203	ASN
1	C	227	HIS
1	C	287	GLN
1	C	289	ASN
1	C	342	HIS
1	C	350	ASN
1	C	403	ASN
1	C	404	ASN
1	C	418	GLN
1	C	431	HIS
1	C	504	ASN
1	C	542	HIS
1	C	724	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 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
2	MPD	A	759	-	6,7,7	0.35	0	7,10,10	1.05	1 (14%)
4	GOL	A	801	-	5,5,5	0.62	0	5,5,5	0.96	0
4	GOL	A	802	-	5,5,5	0.17	0	5,5,5	0.44	0
4	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.38	0
4	GOL	A	804	-	5,5,5	0.36	0	5,5,5	0.47	0
4	GOL	A	805	-	5,5,5	0.58	0	5,5,5	0.90	0
4	GOL	A	806	-	5,5,5	0.41	0	5,5,5	0.46	0
4	GOL	A	807	-	5,5,5	0.33	0	5,5,5	0.37	0
4	GOL	B	801	-	5,5,5	0.35	0	5,5,5	0.61	0
4	GOL	B	802	-	5,5,5	0.31	0	5,5,5	0.30	0
4	GOL	B	803	-	5,5,5	0.27	0	5,5,5	0.25	0
4	GOL	B	804	-	5,5,5	0.22	0	5,5,5	0.52	0
5	SWA	B	900[A]	-	13,13,13	0.85	0	13,19,19	0.95	1 (7%)
5	SWA	B	900[B]	-	13,13,13	0.78	0	13,19,19	0.91	0
4	GOL	C	801	-	5,5,5	0.33	0	5,5,5	0.75	0
4	GOL	C	802	-	5,5,5	0.28	0	5,5,5	0.81	0
4	GOL	C	803	-	5,5,5	0.29	0	5,5,5	0.40	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
2	MPD	A	759	-	-	0/5/5/5	0/0/0/0
4	GOL	A	801	-	-	0/4/4/4	0/0/0/0
4	GOL	A	802	-	-	0/4/4/4	0/0/0/0
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
4	GOL	A	806	-	-	0/4/4/4	0/0/0/0
4	GOL	A	807	-	-	0/4/4/4	0/0/0/0
4	GOL	B	801	-	-	0/4/4/4	0/0/0/0
4	GOL	B	802	-	-	0/4/4/4	0/0/0/0
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	GOL	B	804	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SWA	B	900[A]	-	-	0/0/26/26	0/2/2/2
5	SWA	B	900[B]	-	-	0/0/26/26	1/2/2/2
4	GOL	C	801	-	-	0/4/4/4	0/0/0/0
4	GOL	C	802	-	-	0/4/4/4	0/0/0/0
4	GOL	C	803	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	B	900[A]	SWA	C5-N4-C3	-2.24	110.17	111.85
2	A	759	MPD	C2-C3-C4	-2.20	106.28	116.66

There are no chirality outliers.

There are no torsion outliers.

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 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	759	MPD	10	0
4	A	801	GOL	1	0
4	A	803	GOL	1	0
4	A	804	GOL	5	0
4	A	805	GOL	8	0
4	A	806	GOL	4	0
4	A	807	GOL	6	0
4	B	802	GOL	6	0
4	B	803	GOL	2	0
5	B	900[A]	SWA	2	0
5	B	900[B]	SWA	3	0
4	C	801	GOL	1	0
4	C	802	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	737/737 (100%)	0.05	32 (4%)	39 42	6, 11, 24, 57	0
1	B	737/737 (100%)	0.40	56 (7%)	17 18	8, 14, 27, 59	0
1	C	737/737 (100%)	0.44	59 (8%)	15 17	9, 15, 34, 56	0
All	All	2211/2211 (100%)	0.30	147 (6%)	22 24	6, 13, 30, 59	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	PHE	11.3
1	B	585	PHE	11.0
1	C	43	ALA	9.0
1	C	575	PRO	8.9
1	C	583	TYR	8.8
1	B	583	TYR	8.6
1	C	585	PHE	8.5
1	A	584	GLY	8.0
1	B	600	GLN	7.7
1	A	574	ALA	7.7
1	C	582	THR	7.7
1	B	599	GLY	7.6
1	C	574	ALA	7.4
1	C	580	TYR	6.9
1	C	586	VAL	6.6
1	C	599	GLY	6.6
1	A	586	VAL	6.0
1	B	596	LEU	6.0
1	C	47	GLY	5.9
1	B	595	ALA	5.9
1	B	586	VAL	5.8
1	B	598	MET	5.5
1	C	581	GLY	5.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	44	PHE	5.3
1	C	44	PHE	5.2
1	B	582	THR	5.2
1	C	590	ILE	5.1
1	C	40	SER	5.1
1	C	41	THR	5.0
1	A	583	TYR	5.0
1	A	575	PRO	4.9
1	B	601	TYR	4.8
1	A	582	THR	4.8
1	A	580	TYR	4.6
1	C	578	TYR	4.6
1	B	644[A]	CYS	4.6
1	B	41	THR	4.5
1	C	577	THR	4.5
1	B	587	ILE	4.5
1	B	42	PHE	4.5
1	C	666	VAL	4.4
1	B	584	GLY	4.4
1	C	46	HIS	4.3
1	B	590	ILE	4.3
1	C	588	HIS	4.3
1	C	42	PHE	4.3
1	A	594	VAL	4.2
1	B	43	ALA	4.2
1	B	574	ALA	4.2
1	C	584	GLY	4.1
1	A	599	GLY	4.1
1	C	576	ASN	4.0
1	B	594	VAL	4.0
1	B	581	GLY	3.9
1	B	580	TYR	3.8
1	B	597	ASN	3.8
1	A	573	VAL	3.7
1	C	664	TYR	3.7
1	C	667	CYS	3.7
1	C	579	ASN	3.6
1	A	595	ALA	3.6
1	A	581	GLY	3.6
1	A	598	MET	3.6
1	B	575	PRO	3.5
1	A	577	THR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	600	GLN	3.4
1	A	588	HIS	3.4
1	A	590	ILE	3.3
1	C	22	SER	3.3
1	B	103	ILE	3.3
1	C	548	PHE	3.2
1	C	598	MET	3.2
1	A	587	ILE	3.2
1	C	601	TYR	3.2
1	C	665	PRO	3.2
1	C	573	VAL	3.1
1	C	103	ILE	3.1
1	C	356	PHE	3.1
1	C	222	ASP	3.1
1	B	604	GLY	3.0
1	B	589	GLU	2.9
1	B	603	HIS	2.9
1	C	101	PHE	2.9
1	B	46	HIS	2.9
1	C	587	ILE	2.8
1	B	62	TRP	2.8
1	C	595	ALA	2.8
1	A	42	PHE	2.8
1	B	573	VAL	2.7
1	A	597	ASN	2.7
1	B	222	ASP	2.7
1	B	665	PRO	2.7
1	C	362	LEU	2.7
1	C	646	ASP	2.7
1	C	668	PRO	2.7
1	B	474	TYR	2.7
1	C	85	PHE	2.7
1	B	664	TYR	2.6
1	C	474	TYR	2.6
1	B	356	PHE	2.6
1	B	666	VAL	2.6
1	C	589	GLU	2.6
1	B	328	GLN	2.6
1	B	602	ALA	2.6
1	B	548	PHE	2.5
1	C	658	PHE	2.5
1	A	328	GLN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	85	PHE	2.5
1	A	578	TYR	2.5
1	C	358	ALA	2.5
1	A	668	PRO	2.5
1	C	62	TRP	2.5
1	A	666	VAL	2.5
1	C	593	MET	2.4
1	A	519	LYS	2.4
1	B	591	ALA	2.4
1	B	47	GLY	2.4
1	A	589	GLU	2.4
1	B	359	VAL	2.3
1	B	40	SER	2.3
1	A	667	CYS	2.2
1	B	608	VAL	2.2
1	C	359	VAL	2.2
1	B	101	PHE	2.2
1	A	579	ASN	2.2
1	A	596	LEU	2.2
1	B	221	GLY	2.2
1	C	102	SER	2.2
1	C	154	PHE	2.2
1	C	628[A]	LEU	2.2
1	C	408	LEU	2.2
1	C	547	VAL	2.2
1	B	654	ALA	2.1
1	A	439	GLU	2.1
1	C	497	GLN	2.1
1	C	361	PRO	2.1
1	B	588	HIS	2.1
1	C	594	VAL	2.1
1	B	205	PHE	2.1
1	B	667	CYS	2.1
1	A	716	GLU	2.1
1	B	362	LEU	2.0
1	B	478	CYS	2.0
1	C	82[A]	MET	2.0
1	B	255	ALA	2.0
1	B	61	PHE	2.0
1	A	43	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	A	807	6/6	0.67	0.23	15.08	48,49,49,49	0
2	MPD	A	759	8/8	0.83	0.26	12.04	28,33,35,36	0
4	GOL	B	802	6/6	0.86	0.40	7.63	49,49,50,50	0
4	GOL	A	806	6/6	0.85	0.26	6.64	36,36,37,39	0
5	SWA	B	900[B]	12/12	0.74	0.28	5.51	31,36,37,37	12
5	SWA	B	900[A]	12/12	0.74	0.28	4.70	26,32,33,33	12
4	GOL	A	804	6/6	0.81	0.27	4.65	35,40,41,44	0
4	GOL	C	802	6/6	0.77	0.25	4.12	52,53,53,53	0
4	GOL	A	805	6/6	0.92	0.22	3.84	26,33,34,35	0
4	GOL	A	803	6/6	0.86	0.21	3.80	29,34,35,37	0
4	GOL	B	801	6/6	0.93	0.15	3.71	16,19,22,23	0
4	GOL	A	801	6/6	0.90	0.14	2.97	12,21,24,30	0
4	GOL	B	804	6/6	0.84	0.15	1.28	26,29,30,31	0
4	GOL	C	803	6/6	0.74	0.29	1.24	50,51,52,52	0
4	GOL	A	802	6/6	0.88	0.15	1.14	33,34,36,37	0
4	GOL	C	801	6/6	0.91	0.12	1.01	17,21,23,27	0
4	GOL	B	803	6/6	0.77	0.21	-0.52	43,45,46,46	0
3	NA	A	800	1/1	0.99	0.10	-0.62	13,13,13,13	0
3	NA	B	800	1/1	0.99	0.05	-2.84	17,17,17,17	0
3	NA	C	800	1/1	0.97	0.17	-	20,20,20,20	0
3	NA	A	799	1/1	0.99	0.09	-	11,11,11,11	0

## 6.5 Other polymers

There are no such residues in this entry.