Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 06:37 pm GMT

PDB ID	:	2WW2
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 (i) 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 (i)) were used in the production of this report:

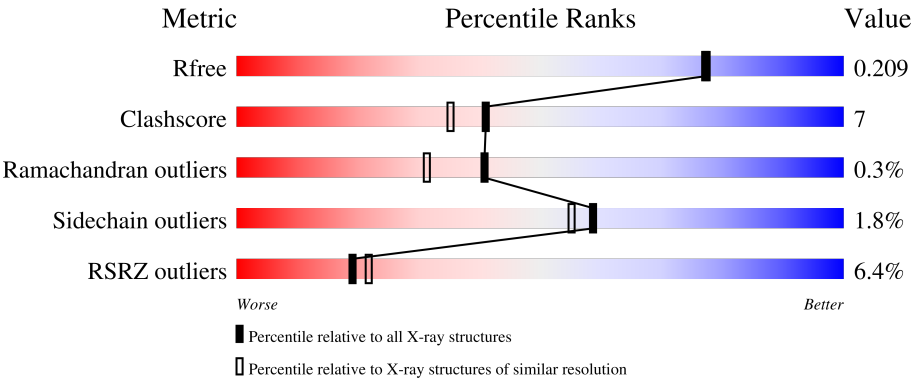
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	4% 88% 11%
1	B	737	7% 89% 11%
1	C	737	8% 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)

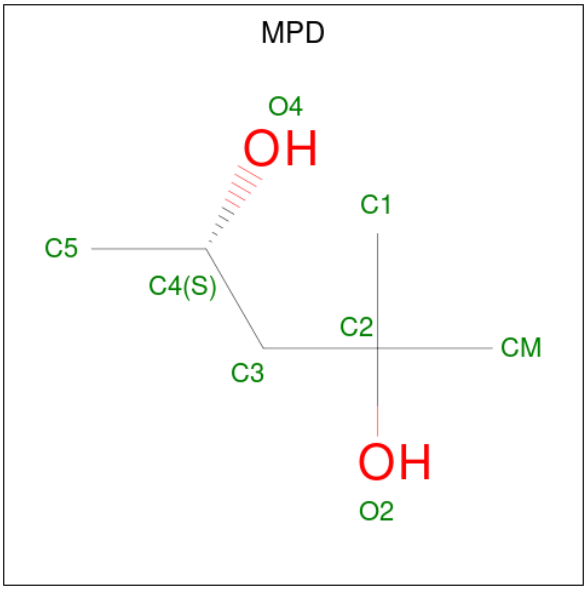
There are 6 unique types of molecules in this entry. The entry contains 19766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

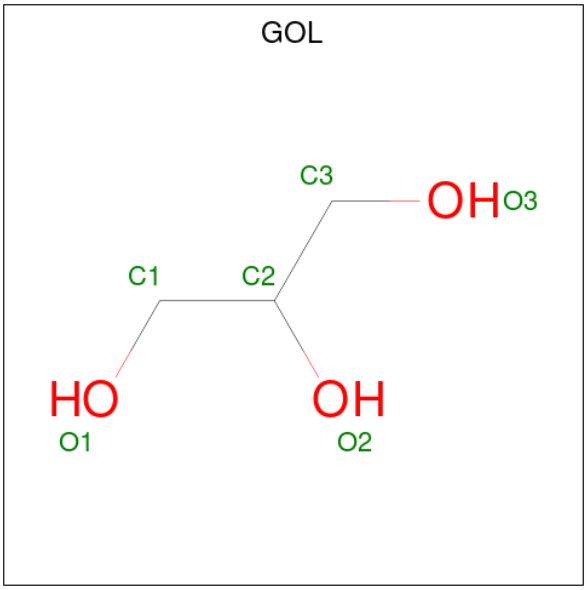


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

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

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

- 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 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

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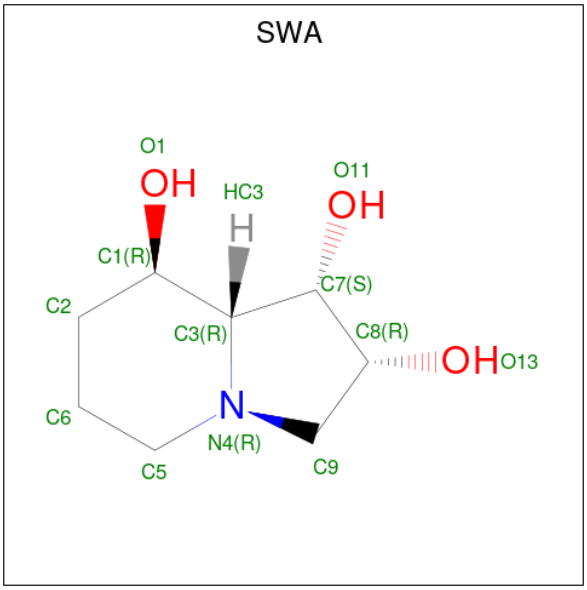
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- 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 24 16 2 6	0	1

- Molecule 6 is water.

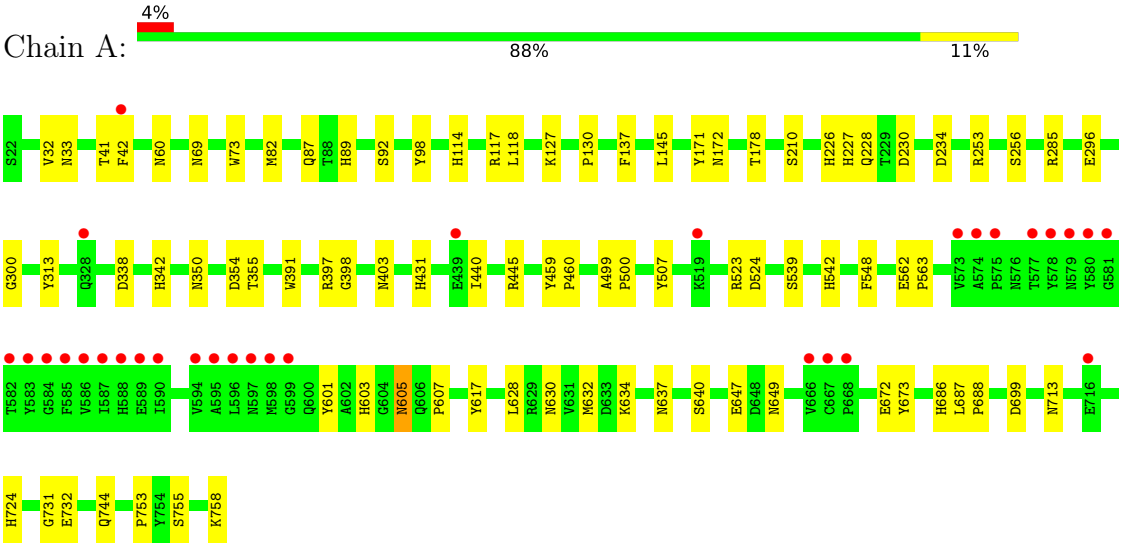
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	790	Total O 790 790	0	0
6	B	653	Total O 653 653	0	0
6	C	627	Total O 627 627	0	0

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.

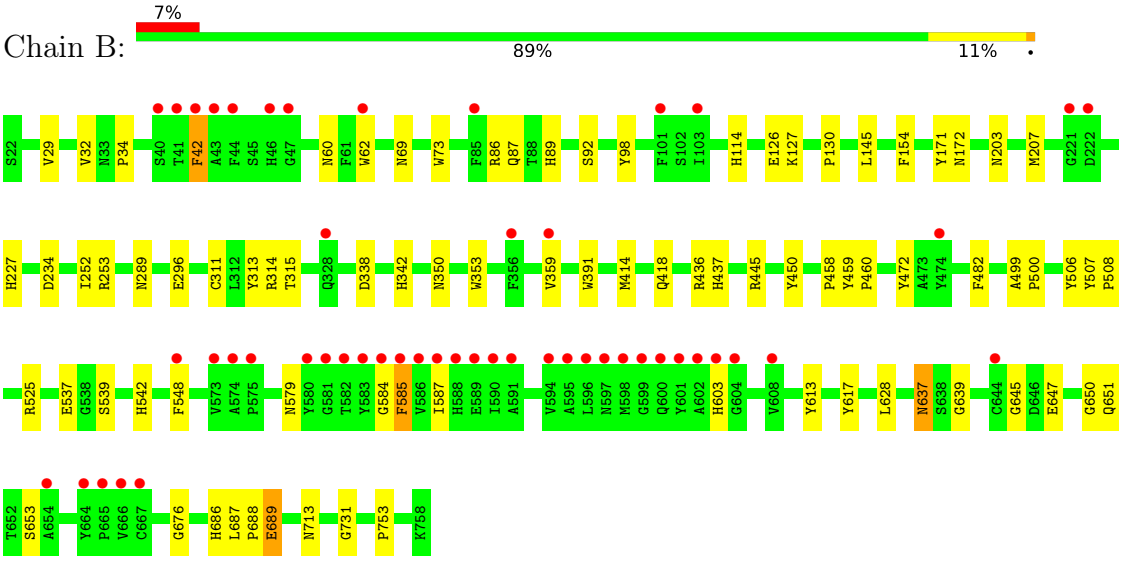
• Molecule 1: ALPHA-1,2-MANNOSIDASE

Chain A:



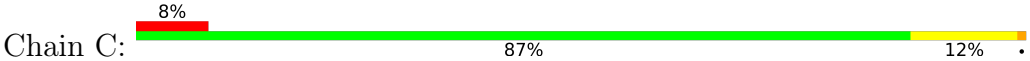
• Molecule 1: ALPHA-1,2-MANNOSIDASE

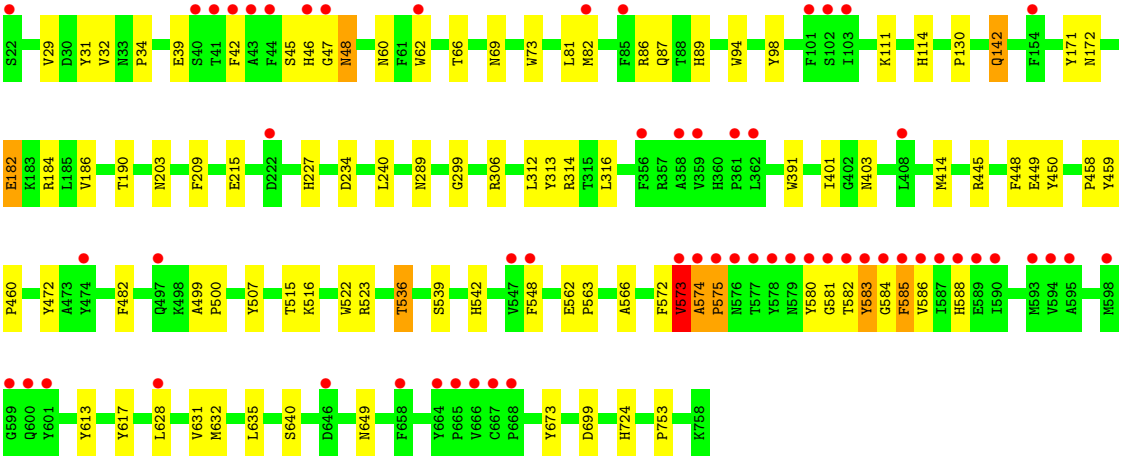
Chain B:



• Molecule 1: ALPHA-1,2-MANNOSIDASE

Chain C:




S22 V29 D30 Y31 V32 N33 P34 E39 S40 T41 F42 A43 F44 S45 H46 G47 N48 N60 F61 W62 T66 N69 W73 L81 M82 F85 R86 Q87 T88 H89 W94 Y98 F101 S102 I103 K111 H114 P130 Q142 F154 Y171 N172
E182 K183 R184 L185 V186 T190 N203 F209 E215 D222 H227 D234 L240 N289 G299 R306 L312 Y313 R314 T315 L316 F356 R357 A358 V359 H360 P361 L362 W391 I401 G402 N403 L408 M414 R445 F448 E449 Y450 P458 Y459
P460 Y472 A473 Y474 F482 Q497 K498 A499 P500 Y507 T515 K516 W522 R523 T536 S539 H542 V547 F548 E562 P563 A566 F572 V573 A574 P575 N576 T577 Y578 N579 Y580 G581 T582 Y583 G584 F585 V586 I587 H588 E589 I590 M593 V594 A595 M598
G599 Q600 Y601 Y613 Y617 L628 V631 M632 L635 S640 D646 N649 F658 Y664 P665 V666 C667 P668 Y673 D699 H724 P753 K758

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	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 (5.03%)	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 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SWA, MPD, NA, GOL

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(^{o})	Ideal(^{o})
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

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

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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

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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: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: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:CD1	1:C:585:PHE:C	2.57	0.77
1:C:539:SER:H	1:C:542:HIS:CD2	1.97	0.77
1:C:182:GLU:CD	1:C:182:GLU:H	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:A:605:ASN:ND2	1:A:607:PRO:HD2	2.07	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: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

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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: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: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
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

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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: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: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: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:B:29:VAL:H	1:B:289:ASN:HD21	1.56	0.52
1:C:66:THR:CG2	1:C:82[B]:MET:HE1	2.39	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:A:637:ASN:HD22	1:B:579:ASN:ND2	2.08	0.51
1:C:580:TYR:C	1:C:582:THR:H	2.10	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:CA	1:C:82[B]:MET:HE3	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: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

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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: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:C:580:TYR:C	1:C:582:THR:N	2.68	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:C:182:GLU:CD	1:C:182:GLU:N	2.64	0.48
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:414:MET:HE1	1:B:482:PHE:HA	1.96	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
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
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: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: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
1:A:32:VAL:HG11	1:A:130:PRO:HG3	1.99	0.44
1:A:628:LEU:CD1	1:A:632[A]:MET:CE	2.96	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:A:605:ASN:HD22	1:A:607:PRO:HD2	1.81	0.44

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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: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: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: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:630:ASN:OD1	1:A:634:LYS:HD2	2.20	0.42
1:B:688:PRO:C	1:B:689:GLU:HG2	2.40	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:66:THR:HG22	1:C:82[B]:MET:HE1	1.96	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:C:628[B]:LEU:HD23	1:C:632:MET:CE	2.46	0.42
1:A:338:ASP:OD1	1:A:342:HIS:HE1	2.03	0.42
1:B:296:GLU:OE2	1:B:686:HIS:NE2	2.53	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
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:A:226:HIS:O	1:A:227:HIS:HB2	2.21	0.41
1:C:62:TRP:HA	1:C:86:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ALA:N	1:C:500:PRO:CD	2.84	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: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:C:39:GLU:HB2	1:C:640:SER:HB2	2.03	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%)	51	42
1	C	739/737 (100%)	703 (95%)	31 (4%)	5 (1%)	22	12
All	All	2226/2211 (101%)	2136 (96%)	84 (4%)	6 (0%)	41	31

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 (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	A	608/620 (98%)	598 (98%)	10 (2%)	62	60
1	B	596/620 (96%)	586 (98%)	10 (2%)	60	57
1	C	604/620 (97%)	591 (98%)	13 (2%)	52	47
All	All	1808/1860 (97%)	1775 (98%)	33 (2%)	59	55

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

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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

Sometimes 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

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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 monosaccharides 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	-	7,7,7	0.42	0	9,10,10	0.74	0
4	GOL	C	803	-	5,5,5	0.33	0	5,5,5	0.40	0
4	GOL	A	801	-	5,5,5	0.60	0	5,5,5	0.99	0
5	SWA	B	900[B]	-	13,13,13	0.76	0	13,19,19	0.92	0
4	GOL	A	803	-	5,5,5	0.33	0	5,5,5	0.39	0
4	GOL	A	805	-	5,5,5	0.58	0	5,5,5	0.97	0
4	GOL	A	807	-	5,5,5	0.35	0	5,5,5	0.35	0
4	GOL	B	801	-	5,5,5	0.36	0	5,5,5	0.61	0
4	GOL	C	802	-	5,5,5	0.29	0	5,5,5	0.85	0
4	GOL	B	802	-	5,5,5	0.33	0	5,5,5	0.35	0
4	GOL	B	803	-	5,5,5	0.30	0	5,5,5	0.29	0
4	GOL	A	802	-	5,5,5	0.23	0	5,5,5	0.46	0
4	GOL	B	804	-	5,5,5	0.29	0	5,5,5	0.56	0
4	GOL	A	806	-	5,5,5	0.41	0	5,5,5	0.43	0
4	GOL	A	804	-	5,5,5	0.38	0	5,5,5	0.50	0
5	SWA	B	900[A]	-	13,13,13	0.83	0	13,19,19	0.89	0
4	GOL	C	801	-	5,5,5	0.32	0	5,5,5	0.73	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	-	-	2/5/5/5	-
4	GOL	C	803	-	-	4/4/4/4	-
4	GOL	A	801	-	-	4/4/4/4	-
5	SWA	B	900[B]	-	-	-	0/2/2/2
4	GOL	A	803	-	-	4/4/4/4	-
4	GOL	A	805	-	-	4/4/4/4	-
4	GOL	A	807	-	-	4/4/4/4	-
4	GOL	B	801	-	-	4/4/4/4	-
4	GOL	C	802	-	-	4/4/4/4	-
4	GOL	B	802	-	-	2/4/4/4	-
4	GOL	B	803	-	-	4/4/4/4	-

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

There are no bond length outliers.

There are no bond angle outliers.

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	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
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	803	GOL	O1-C1-C2-C3
4	A	805	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	806	GOL	C1-C2-C3-O3
4	A	807	GOL	C1-C2-C3-O3
4	B	802	GOL	O1-C1-C2-C3
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	A	807	GOL	O2-C2-C3-O3
2	A	759	MPD	O2-C2-C3-C4
4	A	802	GOL	O1-C1-C2-O2
2	A	759	MPD	C2-C3-C4-C5

There are no ring outliers.

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
5	B	900[B]	SWA	3	0
4	A	803	GOL	1	0
4	A	805	GOL	8	0
4	A	807	GOL	6	0
4	C	802	GOL	1	0
4	B	802	GOL	6	0
4	B	803	GOL	2	0
4	A	806	GOL	4	0
4	A	804	GOL	5	0
5	B	900[A]	SWA	2	0
4	C	801	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	737/737 (100%)	0.01	31 (4%)	36 39	6, 11, 24, 57	0
1	B	737/737 (100%)	0.36	51 (6%)	16 19	8, 14, 27, 59	0
1	C	737/737 (100%)	0.40	59 (8%)	12 13	9, 15, 34, 56	0
All	All	2211/2211 (100%)	0.26	141 (6%)	19 22	6, 13, 30, 59	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	PHE	11.3
1	B	585	PHE	10.6
1	C	43	ALA	8.8
1	C	575	PRO	8.7
1	C	583	TYR	8.7
1	B	583	TYR	8.5
1	C	585	PHE	8.4
1	A	584	GLY	8.0
1	B	600	GLN	7.7
1	A	574	ALA	7.6
1	C	582	THR	7.5
1	B	599	GLY	7.4
1	C	574	ALA	7.2
1	C	580	TYR	6.8
1	C	599	GLY	6.6
1	C	586	VAL	6.4
1	A	586	VAL	6.0
1	C	47	GLY	5.9
1	B	596	LEU	5.8
1	B	595	ALA	5.7
1	B	586	VAL	5.6
1	B	598	MET	5.5
1	C	581	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	44	PHE	5.2
1	B	582	THR	5.1
1	C	44	PHE	5.1
1	C	590	ILE	5.0
1	C	40	SER	5.0
1	C	41	THR	4.9
1	A	583	TYR	4.9
1	A	575	PRO	4.8
1	A	582	THR	4.7
1	B	601	TYR	4.7
1	C	578	TYR	4.6
1	B	644[A]	CYS	4.6
1	A	580	TYR	4.5
1	B	41	THR	4.4
1	C	577	THR	4.4
1	B	42	PHE	4.3
1	C	666	VAL	4.3
1	B	587	ILE	4.3
1	B	590	ILE	4.2
1	C	46	HIS	4.2
1	C	588	HIS	4.2
1	B	584	GLY	4.2
1	A	594	VAL	4.2
1	C	42	PHE	4.1
1	B	574	ALA	4.1
1	B	43	ALA	4.1
1	A	599	GLY	4.0
1	C	584	GLY	4.0
1	C	576	ASN	3.9
1	B	594	VAL	3.9
1	B	581	GLY	3.8
1	B	580	TYR	3.8
1	B	597	ASN	3.7
1	C	664	TYR	3.6
1	A	573	VAL	3.6
1	A	598	MET	3.6
1	C	667	CYS	3.6
1	C	579	ASN	3.5
1	A	595	ALA	3.5
1	A	581	GLY	3.5
1	C	600	GLN	3.4
1	B	575	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	577	THR	3.3
1	A	588	HIS	3.3
1	A	590	ILE	3.3
1	C	22	SER	3.3
1	C	601	TYR	3.2
1	A	587	ILE	3.2
1	B	103	ILE	3.2
1	C	598	MET	3.2
1	C	548	PHE	3.1
1	C	665	PRO	3.1
1	C	573	VAL	3.1
1	C	103	ILE	3.1
1	C	222	ASP	3.0
1	C	356	PHE	3.0
1	B	604	GLY	3.0
1	B	589	GLU	2.9
1	B	603	HIS	2.9
1	B	46	HIS	2.8
1	C	101	PHE	2.8
1	B	62	TRP	2.7
1	C	595	ALA	2.7
1	C	587	ILE	2.7
1	A	597	ASN	2.7
1	A	42	PHE	2.6
1	C	646	ASP	2.6
1	B	573	VAL	2.6
1	B	665	PRO	2.6
1	B	222	ASP	2.6
1	B	474	TYR	2.6
1	C	668	PRO	2.6
1	C	85	PHE	2.6
1	B	664	TYR	2.6
1	C	362	LEU	2.6
1	C	589	GLU	2.6
1	B	356	PHE	2.5
1	C	474	TYR	2.5
1	B	328	GLN	2.5
1	B	666	VAL	2.5
1	B	602	ALA	2.5
1	A	328	GLN	2.5
1	B	548	PHE	2.5
1	C	658	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	62	TRP	2.4
1	A	578	TYR	2.4
1	B	85	PHE	2.4
1	A	668	PRO	2.4
1	C	358	ALA	2.4
1	C	593	MET	2.4
1	B	47	GLY	2.4
1	A	519	LYS	2.4
1	B	591	ALA	2.4
1	A	666	VAL	2.4
1	A	589	GLU	2.3
1	B	40	SER	2.3
1	B	359	VAL	2.2
1	A	579	ASN	2.2
1	A	667	CYS	2.2
1	A	596	LEU	2.2
1	B	221	GLY	2.2
1	B	608	VAL	2.2
1	C	359	VAL	2.2
1	B	101	PHE	2.1
1	C	102	SER	2.1
1	C	154	PHE	2.1
1	A	439	GLU	2.1
1	B	654	ALA	2.1
1	C	497	GLN	2.1
1	C	408	LEU	2.1
1	C	628[A]	LEU	2.1
1	C	547	VAL	2.1
1	C	361	PRO	2.1
1	A	716	GLU	2.0
1	B	588	HIS	2.0
1	C	82[A]	MET	2.0
1	C	594	VAL	2.0
1	B	667	CYS	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	807	6/6	0.67	0.24	48,49,49,49	0
4	GOL	C	803	6/6	0.74	0.29	50,51,52,52	0
5	SWA	B	900[A]	12/12	0.74	0.28	26,32,33,33	12
5	SWA	B	900[B]	12/12	0.74	0.28	31,36,37,37	12
4	GOL	C	802	6/6	0.77	0.25	52,53,53,53	0
4	GOL	B	803	6/6	0.77	0.21	43,45,46,46	0
4	GOL	A	804	6/6	0.81	0.27	35,40,41,44	0
2	MPD	A	759	8/8	0.83	0.26	28,33,35,36	0
4	GOL	B	804	6/6	0.84	0.15	26,29,30,31	0
4	GOL	A	806	6/6	0.85	0.26	36,36,37,39	0
4	GOL	A	803	6/6	0.85	0.21	29,34,35,37	0
4	GOL	B	802	6/6	0.85	0.40	49,49,50,50	0
4	GOL	A	802	6/6	0.88	0.15	33,34,36,37	0
4	GOL	A	801	6/6	0.90	0.14	12,21,24,30	0
4	GOL	C	801	6/6	0.91	0.12	17,21,23,27	0
4	GOL	A	805	6/6	0.92	0.22	26,33,34,35	0
4	GOL	B	801	6/6	0.93	0.15	16,19,22,23	0
3	NA	C	800	1/1	0.97	0.18	20,20,20,20	0
3	NA	B	800	1/1	0.99	0.05	17,17,17,17	0
3	NA	A	799	1/1	0.99	0.09	11,11,11,11	0
3	NA	A	800	1/1	0.99	0.10	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.