Full wwPDB X-ray Structure Validation Report

Aug 21, 2020 – 05:21 AM BST

PDB ID	:	2WVX
Title	:	Structure of the Family GH92 Inverting Mannosidase BT3990 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 following versions of software and data (see references ①) were used in the production of this report:

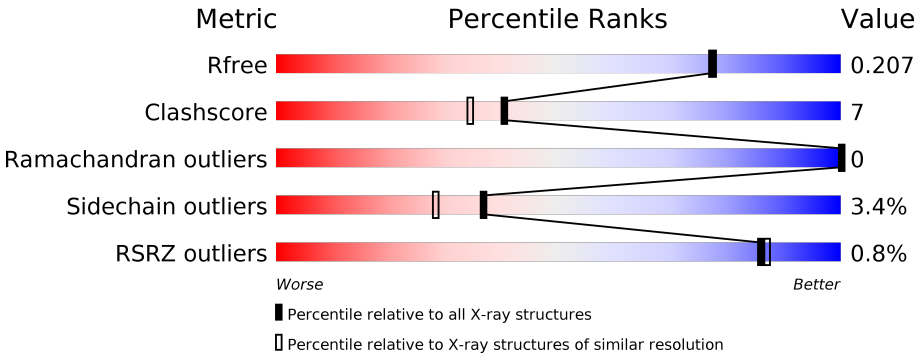
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 on 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	744	88% 10%
1	C	744	86% 12%
1	D	744	% 87% 11%
2	B	744	2% 86% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25973 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 PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	Se	0	2	0
			5932	3801	974	1124	6	27			
1	C	736	Total	C	N	O	S	Se	0	6	0
			5972	3831	976	1129	6	30			
1	D	736	Total	C	N	O	S	Se	0	4	0
			5973	3831	982	1126	6	28			

- Molecule 2 is a protein called PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	737	Total	C	N	O	S	Se	0	5	0
			5974	3833	982	1124	6	29			

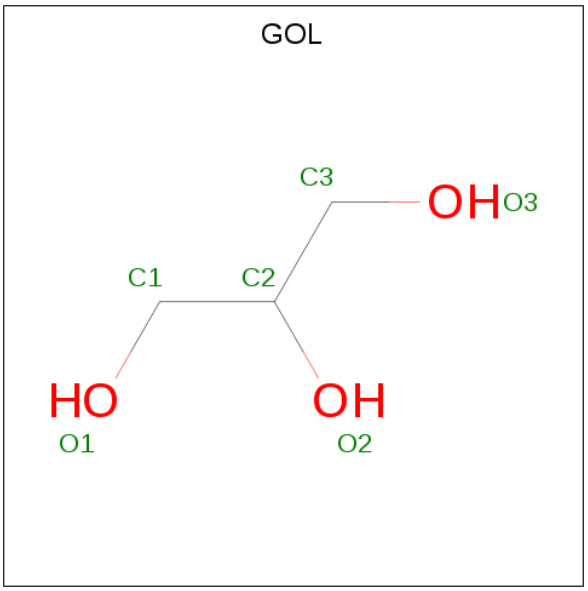
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	GLN	ASN	conflict	UNP Q8A0N1

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

- Molecule 5 is water.

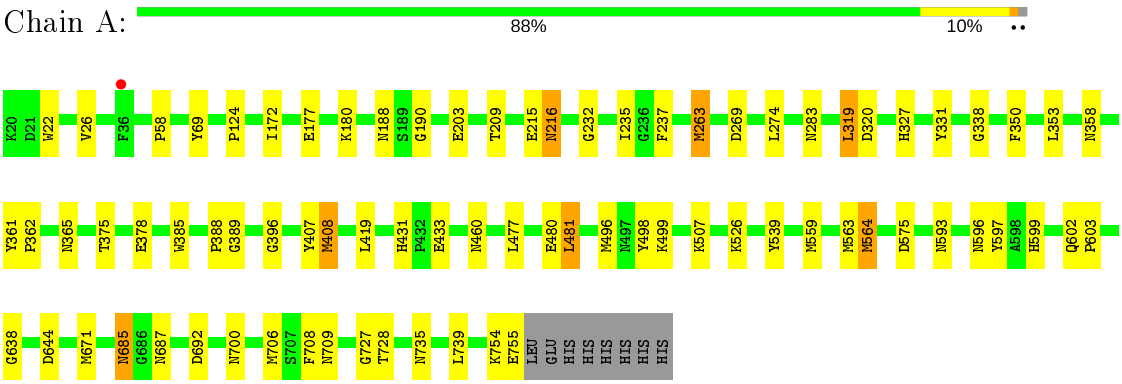
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	529	Total O 529 529	0	0
5	B	463	Total O 463 463	0	0
5	C	531	Total O 531 531	0	0
5	D	499	Total O 499 499	0	0

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.

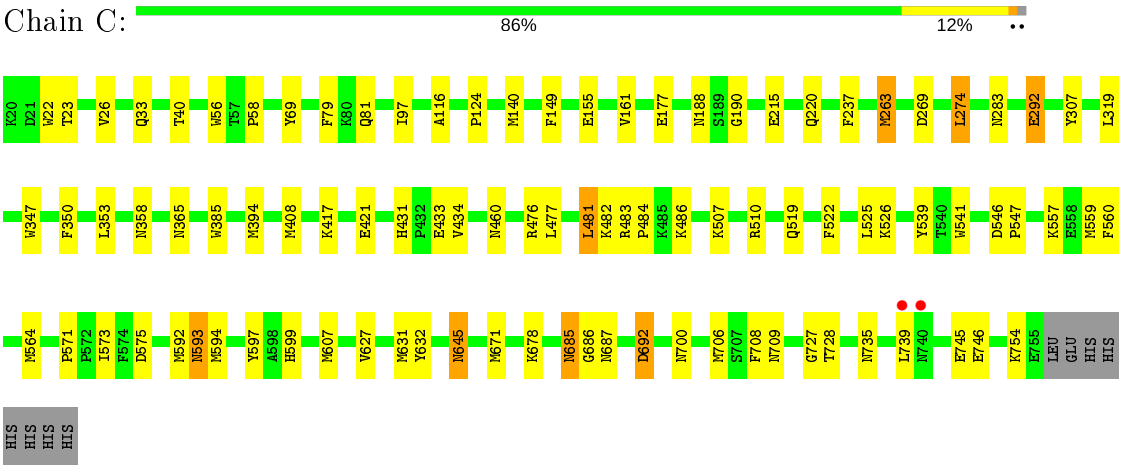
- Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain A:



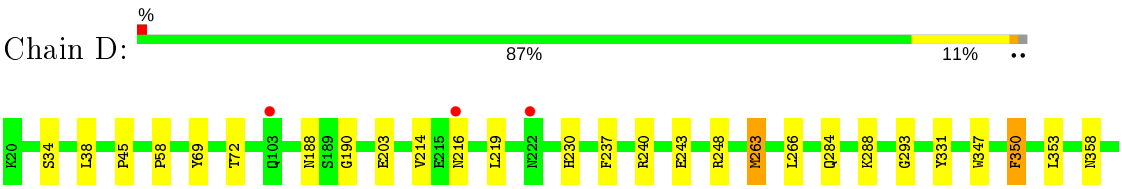
- Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

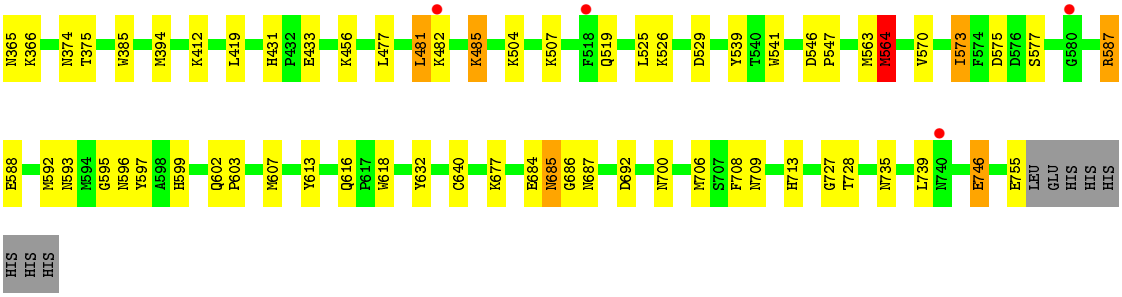
Chain C:



- Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

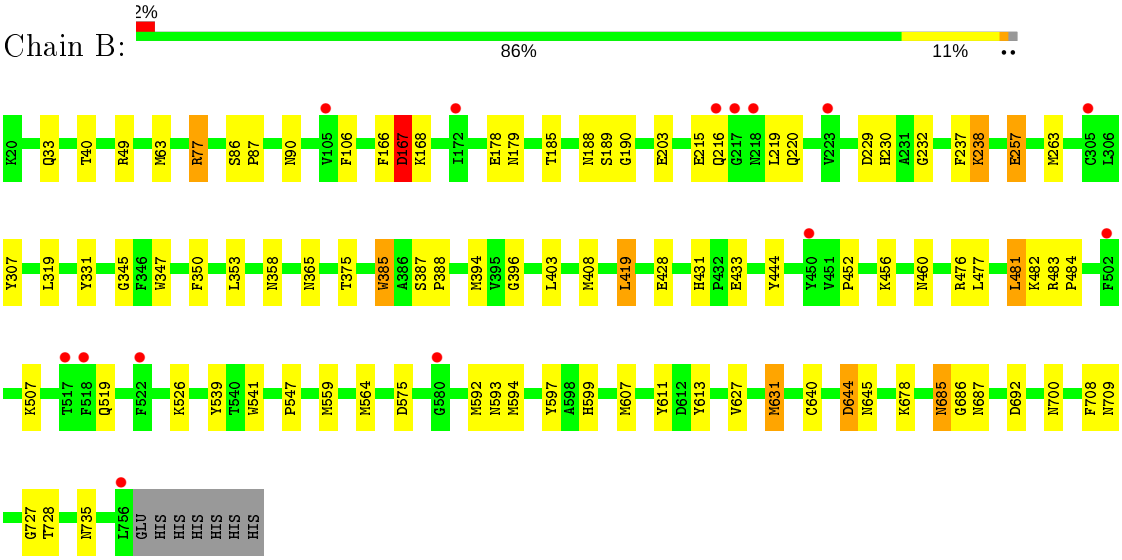
Chain D:





- Molecule 2: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.23Å 190.95Å 135.10Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	133.63 – 1.90 47.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (133.63-1.90) 97.5 (47.72-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.155 , 0.186 0.181 , 0.207	Depositor DCC
R_{free} test set	12380 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25973	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: GOL, CA

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	0.81	2/6086 (0.0%)	0.70	3/8226 (0.0%)
1	C	0.81	2/6141 (0.0%)	0.68	1/8292 (0.0%)
1	D	0.77	0/6136	0.69	2/8283 (0.0%)
2	B	0.74	3/6136 (0.0%)	0.67	3/8282 (0.0%)
All	All	0.78	7/24499 (0.0%)	0.68	9/33083 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	167	ASP	C-N	8.19	1.52	1.34
1	A	638	GLY	C-O	-6.14	1.13	1.23
1	C	116	ALA	CA-CB	-6.01	1.39	1.52
2	B	428	GLU	CB-CG	-5.86	1.41	1.52
2	B	396	GLY	C-O	-5.74	1.14	1.23
1	A	396	GLY	C-O	-5.56	1.14	1.23
1	C	215	GLU	CB-CG	-5.06	1.42	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	564	MSE	CG-SE-CE	-9.49	78.02	98.90
2	B	167	ASP	CA-C-N	-8.91	97.61	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	564	MSE	CG-SE-CE	-7.92	81.47	98.90
1	C	263	MSE	CG-SE-CE	-6.38	84.87	98.90
2	B	77	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	353	LEU	CB-CG-CD2	5.41	120.20	111.00
2	B	644	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	A	263	MSE	CG-SE-CE	-5.05	87.78	98.90
1	D	529	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	167	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5932	0	5528	80	0
1	C	5972	0	5606	86	0
1	D	5973	0	5627	74	0
2	B	5974	0	5623	94	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	32	0	0
4	B	24	0	32	0	0
4	C	24	0	32	0	0
4	D	24	0	32	3	0
5	A	529	0	0	4	0
5	B	463	0	0	5	0
5	C	531	0	0	6	0
5	D	499	0	0	6	0
All	All	25973	0	22512	334	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 (334) 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)
2:B:63:MSE:CE	2:B:166:PHE:HA	1.12	1.57
2:B:63:MSE:CE	2:B:166:PHE:CA	1.90	1.48
2:B:592:MSE:HE2	2:B:631[B]:MSE:SE	1.64	1.46
1:A:496:MSE:CE	1:A:499:LYS:HE3	1.41	1.44
2:B:63:MSE:HE1	2:B:166:PHE:CA	1.51	1.37
2:B:63:MSE:HE2	2:B:166:PHE:CB	1.55	1.35
1:A:507:LYS:CD	1:A:559:MSE:HE2	1.62	1.29
1:A:496:MSE:HE3	1:A:499:LYS:CE	1.74	1.17
1:A:496:MSE:CE	1:A:499:LYS:CE	2.20	1.17
1:C:671:MSE:HE3	1:C:706:MSE:SE	1.94	1.16
2:B:63:MSE:HE2	2:B:166:PHE:CG	1.78	1.16
1:A:407:TYR:CD1	1:A:408:MSE:HE3	1.83	1.13
1:A:507:LYS:HD2	1:A:559:MSE:HE2	1.25	1.12
2:B:63:MSE:HE3	2:B:166:PHE:HA	1.29	1.11
1:C:592:MSE:HE2	1:C:631[B]:MSE:HE3	1.32	1.11
1:D:587[A]:ARG:HH11	1:D:587[A]:ARG:HG2	1.03	1.09
1:A:408:MSE:HE2	1:A:408:MSE:HA	1.34	1.09
2:B:592:MSE:HE2	2:B:631[A]:MSE:CE	1.79	1.08
1:D:684:GLU:OE2	4:D:804:GOL:H11	1.54	1.07
1:A:407:TYR:HD1	1:A:408:MSE:CE	1.66	1.07
1:C:79:PHE:CD2	1:C:140[B]:MSE:CE	2.38	1.06
1:A:407:TYR:HD1	1:A:408:MSE:HE3	0.90	1.05
1:C:507:LYS:HD2	1:C:559:MSE:HE3	1.35	1.04
1:C:79:PHE:CD2	1:C:140[B]:MSE:HE1	1.91	1.04
2:B:63:MSE:CE	2:B:166:PHE:CG	2.41	1.02
2:B:592:MSE:CE	2:B:631[B]:MSE:SE	2.57	1.01
2:B:592:MSE:HE2	2:B:631[A]:MSE:HE3	1.38	0.95
1:C:592:MSE:HE2	1:C:631[B]:MSE:CE	1.83	0.93
2:B:188:ASN:HD22	2:B:190:GLY:H	1.05	0.92
2:B:63:MSE:CE	2:B:166:PHE:CB	2.28	0.91
1:A:358:ASN:HD21	1:A:365:ASN:HD22	1.19	0.90
2:B:631[B]:MSE:HG3	2:B:640:CYS:HB3	1.53	0.90
1:D:188:ASN:HD22	1:D:190:GLY:H	1.20	0.90
1:C:627:VAL:HG13	1:C:631[B]:MSE:HG3	1.54	0.90
2:B:63:MSE:HE2	2:B:166:PHE:HB3	1.52	0.89
1:C:79:PHE:HD2	1:C:140[B]:MSE:HE1	1.33	0.89
1:D:288:LYS:NZ	4:D:804:GOL:HO1	1.69	0.88
2:B:63:MSE:HE1	2:B:166:PHE:C	1.94	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:HD22	1:A:190:GLY:H	1.19	0.87
1:D:587[A]:ARG:CG	1:D:587[A]:ARG:HH11	1.86	0.87
2:B:419:LEU:C	2:B:419:LEU:HD13	1.94	0.87
1:C:358:ASN:HD21	1:C:365:ASN:HD22	1.23	0.86
1:A:507:LYS:HD3	1:A:559:MSE:HE2	1.55	0.85
1:D:587[A]:ARG:NH1	1:D:587[A]:ARG:HG2	1.84	0.84
1:D:203:GLU:CD	1:D:263[B]:MSE:CE	2.46	0.84
2:B:631[B]:MSE:HG3	2:B:640:CYS:CB	2.07	0.83
1:C:188:ASN:HD22	1:C:190:GLY:H	1.25	0.83
1:A:496:MSE:HE2	1:A:499:LYS:CE	2.09	0.82
1:A:496:MSE:HE2	1:A:499:LYS:NZ	1.93	0.82
1:A:407:TYR:CD1	1:A:408:MSE:CE	2.51	0.82
2:B:358:ASN:HD21	2:B:365:ASN:HD22	1.28	0.82
1:C:507:LYS:CD	1:C:559:MSE:HE3	2.09	0.82
1:C:507:LYS:HE3	1:C:559:MSE:HE2	1.60	0.81
2:B:63:MSE:HE1	2:B:166:PHE:HA	0.81	0.80
2:B:63:MSE:HE3	2:B:166:PHE:CD1	2.16	0.79
1:D:358:ASN:HD21	1:D:365:ASN:HD22	1.30	0.79
1:D:72[A]:THR:HG23	5:D:2052:HOH:O	1.82	0.79
1:A:358:ASN:ND2	1:A:365:ASN:HD22	1.81	0.78
1:A:507:LYS:CD	1:A:559:MSE:CE	2.56	0.78
1:C:79:PHE:HB3	1:C:140[B]:MSE:HE1	1.65	0.78
1:A:408:MSE:HA	1:A:408:MSE:CE	2.14	0.78
1:C:79:PHE:HD2	1:C:140[B]:MSE:CE	1.85	0.77
1:A:559:MSE:HE3	1:A:563:MSE:CG	2.16	0.76
1:C:507:LYS:CE	1:C:559:MSE:HE2	2.16	0.76
2:B:188:ASN:ND2	2:B:190:GLY:H	1.84	0.75
2:B:431:HIS:HD2	2:B:433:GLU:H	1.34	0.75
1:A:507:LYS:HD2	1:A:559:MSE:CE	2.12	0.74
2:B:594:MSE:SE	2:B:631[B]:MSE:HE1	2.37	0.74
1:D:477:LEU:HG	1:D:481:LEU:HD22	1.70	0.74
1:A:559:MSE:HE3	1:A:563:MSE:HG2	1.71	0.73
1:A:496:MSE:HE3	1:A:499:LYS:HE3	0.77	0.73
1:A:22:TRP:H	1:A:283:ASN:ND2	1.88	0.72
1:D:431:HIS:HD2	1:D:433:GLU:H	1.36	0.72
2:B:63:MSE:HE3	2:B:166:PHE:CG	2.26	0.71
1:C:709:ASN:HD21	1:C:727:GLY:HA3	1.55	0.71
1:A:709:ASN:ND2	1:A:728:THR:H	1.88	0.71
1:C:263:MSE:HG3	1:C:263:MSE:O	1.89	0.71
1:C:358:ASN:ND2	1:C:365:ASN:HD22	1.88	0.71
1:C:431:HIS:HD2	1:C:433:GLU:H	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:GLU:H	1:D:746:GLU:CD	1.94	0.71
2:B:263:MSE:HG3	2:B:263:MSE:O	1.91	0.70
2:B:431:HIS:CD2	2:B:433:GLU:H	2.09	0.70
1:C:507:LYS:HE3	1:C:559:MSE:CE	2.21	0.70
1:C:685:ASN:ND2	1:C:687:ASN:H	1.89	0.70
1:C:671:MSE:HE1	1:C:706:MSE:HE1	1.71	0.70
1:C:671:MSE:CE	1:C:706:MSE:HE1	2.22	0.70
1:C:431:HIS:CD2	1:C:433:GLU:H	2.09	0.70
1:C:594:MSE:SE	1:C:631[B]:MSE:SE	3.08	0.70
1:C:347:TRP:CZ3	1:C:394:MSE:HE2	2.27	0.69
1:D:216[A]:ASN:HD21	1:D:230:HIS:H	1.41	0.69
1:D:358:ASN:ND2	1:D:365:ASN:HD22	1.90	0.69
1:A:22:TRP:H	1:A:283:ASN:HD21	1.40	0.68
1:D:38:LEU:HD12	1:D:588:GLU:HG3	1.76	0.68
1:A:597:TYR:OH	1:A:599:HIS:HD2	1.76	0.68
1:D:431:HIS:CD2	1:D:433:GLU:H	2.12	0.67
2:B:358:ASN:ND2	2:B:365:ASN:HD22	1.92	0.67
1:D:263[A]:MSE:HE2	1:D:266:LEU:HD12	1.75	0.67
1:D:709:ASN:HD21	1:D:727:GLY:HA3	1.59	0.67
1:C:507:LYS:CE	1:C:559:MSE:CE	2.73	0.67
1:D:525:LEU:HD13	1:D:573:ILE:HG13	1.76	0.67
1:D:203:GLU:OE1	1:D:263[B]:MSE:HE3	1.94	0.67
2:B:419:LEU:C	2:B:419:LEU:CD1	2.64	0.66
1:C:155:GLU:OE1	5:C:2113:HOH:O	2.12	0.66
1:D:203:GLU:CD	1:D:263[B]:MSE:HE3	2.15	0.66
1:C:269:ASP:HB2	1:C:274:LEU:HD13	1.77	0.66
1:C:22:TRP:H	1:C:283:ASN:ND2	1.94	0.66
1:A:431:HIS:HD2	1:A:433[A]:GLU:H	1.42	0.66
1:C:269:ASP:CB	1:C:274:LEU:HD13	2.25	0.66
1:C:597:TYR:OH	1:C:599:HIS:HD2	1.79	0.66
1:C:564[A]:MSE:HE1	1:C:607:MSE:HG2	1.77	0.66
2:B:419:LEU:O	2:B:419:LEU:HD13	1.96	0.65
1:A:431:HIS:HD2	1:A:433[B]:GLU:H	1.42	0.65
2:B:63:MSE:HE1	2:B:167:ASP:N	2.12	0.65
1:C:79:PHE:CG	1:C:140[B]:MSE:HE1	2.32	0.65
1:A:644:ASP:CG	5:A:2454:HOH:O	2.34	0.64
1:A:203:GLU:CD	1:A:263:MSE:HE3	2.17	0.64
2:B:592:MSE:HE2	2:B:631[A]:MSE:HE1	1.75	0.63
1:A:559:MSE:HE3	1:A:563:MSE:SE	2.48	0.63
1:D:288:LYS:HZ2	4:D:804:GOL:HO1	1.31	0.63
2:B:685:ASN:ND2	2:B:687:ASN:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:LYS:HD2	1:C:559:MSE:CE	2.21	0.62
1:D:685:ASN:ND2	1:D:687:ASN:H	1.98	0.62
1:C:79:PHE:CB	1:C:140[B]:MSE:HE1	2.29	0.62
1:A:709:ASN:HD21	1:A:727:GLY:HA3	1.63	0.62
1:C:557[B]:LYS:HG3	5:C:2396:HOH:O	1.98	0.61
1:A:327:HIS:HE1	1:A:378:GLU:OE2	1.83	0.61
1:D:709:ASN:ND2	1:D:728:THR:H	1.97	0.61
1:C:560:PHE:CE1	1:C:564[B]:MSE:HE2	2.35	0.61
2:B:203:GLU:CD	2:B:263:MSE:HE3	2.20	0.61
2:B:216:GLN:OE1	2:B:216:GLN:N	2.33	0.61
1:D:72[A]:THR:HG22	5:D:2055:HOH:O	2.01	0.60
2:B:167:ASP:O	2:B:168[A]:LYS:O	2.19	0.60
1:C:671:MSE:CE	1:C:706:MSE:SE	2.87	0.60
1:A:507:LYS:HD3	1:A:559:MSE:CE	2.27	0.60
2:B:597:TYR:OH	2:B:599:HIS:HD2	1.85	0.60
2:B:631[B]:MSE:HG3	2:B:640:CYS:SG	2.41	0.60
1:D:700:ASN:ND2	1:D:735:ASN:HB3	2.18	0.59
1:A:709:ASN:HD21	1:A:728:THR:H	1.49	0.59
2:B:709:ASN:HD21	2:B:727:GLY:HA3	1.68	0.59
1:A:507:LYS:CE	1:A:559:MSE:HE2	2.30	0.59
1:C:685:ASN:HD22	1:C:685:ASN:C	2.04	0.59
1:C:507:LYS:CD	1:C:559:MSE:CE	2.80	0.58
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.85	0.58
1:A:431:HIS:CD2	1:A:433[A]:GLU:H	2.20	0.57
1:C:22:TRP:H	1:C:283:ASN:HD21	1.50	0.57
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.86	0.57
1:D:507:LYS:HB2	1:D:563:MSE:HE2	1.86	0.57
1:D:240:ARG:HG2	1:D:243:GLU:HB2	1.86	0.57
1:D:526:LYS:HA	1:D:575:ASP:HB3	1.87	0.57
1:A:431:HIS:CD2	1:A:433[B]:GLU:H	2.21	0.57
1:D:216[A]:ASN:H	1:D:216[A]:ASN:HD22	1.50	0.57
1:A:559:MSE:CE	1:A:563:MSE:SE	3.03	0.57
2:B:347:TRP:CZ3	2:B:394:MSE:HE2	2.40	0.57
1:D:755:GLU:HG2	5:D:2493:HOH:O	2.03	0.57
1:D:347:TRP:CZ3	1:D:394:MSE:HE2	2.39	0.56
1:C:177:GLU:OE1	1:C:177:GLU:N	2.27	0.56
1:C:678:LYS:HE2	1:C:692:ASP:OD1	2.06	0.56
1:D:485:LYS:HD3	5:D:2341:HOH:O	2.04	0.56
2:B:216:GLN:CD	2:B:216:GLN:N	2.59	0.56
1:C:347:TRP:CE3	1:C:394:MSE:HE2	2.41	0.56
1:C:417:LYS:HE2	1:C:421:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:CD2	1:C:140[B]:MSE:HE3	2.39	0.55
1:D:188:ASN:ND2	1:D:190:GLY:H	1.98	0.55
1:A:685:ASN:ND2	1:A:687:ASN:H	2.03	0.55
1:A:685:ASN:C	1:A:685:ASN:HD22	2.09	0.55
1:D:214:VAL:HG22	1:D:219:LEU:HD12	1.89	0.55
1:D:700:ASN:HD22	1:D:735:ASN:HB3	1.70	0.55
2:B:167:ASP:C	2:B:168[A]:LYS:O	2.44	0.54
1:A:177:GLU:CD	1:A:177:GLU:H	2.09	0.54
1:D:685:ASN:C	1:D:685:ASN:HD22	2.09	0.54
1:A:408:MSE:HE2	1:A:408:MSE:CA	2.23	0.54
1:A:203:GLU:CD	1:A:263:MSE:CE	2.75	0.54
1:A:431:HIS:HE1	5:A:2275:HOH:O	1.91	0.54
1:A:327:HIS:HD2	1:A:338:GLY:O	1.91	0.53
1:A:358:ASN:HD21	1:A:365:ASN:ND2	1.99	0.53
2:B:216:GLN:HE22	2:B:230:HIS:N	2.06	0.53
2:B:685:ASN:HD22	2:B:685:ASN:C	2.11	0.53
1:A:263:MSE:O	1:A:263:MSE:HG3	2.07	0.52
1:A:644:ASP:OD2	5:A:2453:HOH:O	2.19	0.52
2:B:678:LYS:HE2	2:B:692:ASP:OD1	2.08	0.52
2:B:645:ASN:HA	5:B:2059:HOH:O	2.10	0.52
1:D:203:GLU:OE2	1:D:263[B]:MSE:CE	2.58	0.52
1:C:685:ASN:HD22	1:C:686:GLY:N	2.08	0.52
1:D:597:TYR:OH	1:D:599:HIS:HD2	1.93	0.52
2:B:353:LEU:HD13	2:B:353:LEU:C	2.29	0.52
1:C:58:PRO:HG2	1:C:69:TYR:CD1	2.45	0.52
1:C:671:MSE:CE	1:C:706:MSE:CE	2.88	0.51
1:A:216:ASN:H	1:A:216:ASN:HD22	1.57	0.51
2:B:627:VAL:HG13	2:B:631[A]:MSE:HG3	1.92	0.51
1:C:671:MSE:HE3	1:C:706:MSE:CE	2.39	0.51
1:D:504:LYS:HG3	5:D:2346:HOH:O	2.11	0.51
2:B:700:ASN:HD22	2:B:735:ASN:HB3	1.76	0.51
1:D:216[A]:ASN:ND2	1:D:230:HIS:H	2.07	0.51
1:D:746:GLU:N	1:D:746:GLU:CD	2.64	0.51
2:B:526:LYS:HA	2:B:575:ASP:HB3	1.93	0.50
1:A:496:MSE:HE2	1:A:499:LYS:HZ2	1.74	0.50
1:A:671:MSE:SE	1:A:706:MSE:HE1	2.62	0.50
2:B:631[B]:MSE:CG	2:B:640:CYS:SG	2.99	0.50
1:A:203:GLU:OE1	1:A:263:MSE:HE3	2.12	0.50
2:B:33:GLN:O	2:B:40:THR:OG1	2.29	0.50
2:B:709:ASN:ND2	2:B:728:THR:H	2.10	0.50
1:D:564:MSE:HE1	1:D:607:MSE:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:MSE:HE3	1:D:640:CYS:HB2	1.94	0.50
1:A:408:MSE:CA	1:A:408:MSE:CE	2.88	0.49
1:C:745:GLU:OE2	1:C:754:LYS:HE2	2.11	0.49
2:B:627:VAL:O	2:B:631[A]:MSE:HG2	2.12	0.49
1:D:248:ARG:C	1:D:263[A]:MSE:HE1	2.32	0.49
1:C:353:LEU:HD13	1:C:353:LEU:C	2.33	0.49
2:B:63:MSE:CE	2:B:166:PHE:CD1	2.82	0.49
1:C:292:GLU:HG3	1:C:678:LYS:HB3	1.95	0.49
2:B:168[A]:LYS:O	2:B:229:ASP:O	2.30	0.49
2:B:331:TYR:CZ	2:B:375:THR:HG23	2.48	0.49
2:B:685:ASN:HD22	2:B:686:GLY:N	2.11	0.49
1:C:593:ASN:ND2	5:C:2424:HOH:O	2.44	0.49
1:A:180:LYS:HE2	1:A:203:GLU:HG2	1.95	0.48
1:D:203:GLU:OE2	1:D:263[B]:MSE:HE2	2.13	0.48
1:A:188:ASN:ND2	1:A:190:GLY:H	1.98	0.48
1:A:754:LYS:O	1:A:755:GLU:C	2.51	0.48
2:B:90:ASN:HB3	2:B:189:SER:OG	2.13	0.48
1:C:746:GLU:HG2	5:C:2517:HOH:O	2.12	0.48
1:D:546:ASP:N	1:D:547:PRO:HD3	2.29	0.48
2:B:700:ASN:ND2	2:B:735:ASN:HB3	2.28	0.48
1:C:23:THR:H	1:C:283:ASN:HD21	1.61	0.48
1:D:547:PRO:HG2	1:D:613:TYR:CE2	2.49	0.48
1:A:526:LYS:HA	1:A:575:ASP:HB3	1.96	0.48
2:B:477:LEU:HG	2:B:481:LEU:HD22	1.96	0.48
1:C:709:ASN:ND2	1:C:728:THR:H	2.10	0.48
1:D:587[A]:ARG:CG	1:D:587[A]:ARG:NH1	2.57	0.48
2:B:644:ASP:O	2:B:645:ASN:HB2	2.14	0.47
1:C:507:LYS:HE3	1:C:559:MSE:HG2	1.96	0.47
1:D:353:LEU:HD13	1:D:353:LEU:C	2.34	0.47
1:A:408:MSE:HE1	1:A:480:GLU:HG2	1.97	0.47
1:D:706:MSE:HE2	1:D:713:HIS:ND1	2.29	0.47
2:B:63:MSE:HE2	2:B:166:PHE:CD2	2.43	0.47
1:C:358:ASN:HD21	1:C:365:ASN:ND2	2.02	0.46
1:A:26:VAL:HG11	1:A:124:PRO:HG3	1.97	0.46
1:C:685:ASN:HD22	1:C:687:ASN:H	1.60	0.46
2:B:63:MSE:CE	2:B:167:ASP:N	2.78	0.46
1:C:220:GLN:HG3	5:C:2162:HOH:O	2.15	0.46
1:D:602:GLN:N	1:D:603:PRO:CD	2.79	0.46
2:B:547:PRO:HG2	2:B:613:TYR:CE2	2.50	0.46
2:B:408:MSE:HE3	2:B:476:ARG:HB3	1.98	0.46
2:B:631[B]:MSE:HB2	2:B:631[B]:MSE:HE2	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:MSE:HE2	1:A:706:MSE:SE	2.66	0.46
1:C:79:PHE:HB3	1:C:140[B]:MSE:CE	2.43	0.46
1:C:347:TRP:CH2	1:C:394:MSE:HE2	2.51	0.45
1:C:431:HIS:HD2	1:C:433:GLU:N	2.11	0.45
1:D:293:GLY:HA3	1:D:677:LYS:HB2	1.99	0.45
2:B:564:MSE:HE3	2:B:564:MSE:HB2	1.92	0.45
1:D:570:VAL:O	1:D:595:GLY:HA2	2.17	0.45
2:B:592:MSE:CE	2:B:631[A]:MSE:HE3	2.29	0.45
1:D:203:GLU:CD	1:D:263[B]:MSE:HE1	2.34	0.45
1:D:366:LYS:HE2	1:D:412:LYS:O	2.17	0.44
1:D:541:TRP:CG	1:D:607:MSE:HG3	2.52	0.44
1:A:331:TYR:CZ	1:A:375:THR:HG23	2.52	0.44
2:B:203:GLU:CD	2:B:263:MSE:CE	2.85	0.44
2:B:49:ARG:HD3	5:B:2034:HOH:O	2.17	0.44
1:A:216:ASN:N	1:A:216:ASN:HD22	2.14	0.43
1:A:327:HIS:CE1	1:A:378:GLU:OE2	2.68	0.43
1:A:709:ASN:HD21	1:A:727:GLY:CA	2.31	0.43
1:A:361:TYR:N	1:A:362:PRO:CD	2.81	0.43
2:B:257:GLU:HG2	5:B:2149:HOH:O	2.19	0.43
2:B:106:PHE:CE1	2:B:232:GLY:HA3	2.54	0.43
1:C:33:GLN:O	1:C:40:THR:OG1	2.37	0.43
1:D:599:HIS:HE1	1:D:632:TYR:OH	2.01	0.43
1:C:571:PRO:O	1:C:573:ILE:HG12	2.18	0.43
1:A:172:ILE:HG21	1:A:232:GLY:O	2.19	0.43
2:B:594:MSE:SE	2:B:631[B]:MSE:CE	3.13	0.43
1:C:564[A]:MSE:CE	1:C:607:MSE:HG2	2.48	0.42
2:B:345:GLY:HA3	2:B:385:TRP:CE2	2.53	0.42
2:B:403:LEU:HB3	2:B:419:LEU:HD21	2.02	0.42
1:C:97:ILE:HD11	1:C:161:VAL:HG11	2.01	0.42
1:A:235:ILE:C	1:A:235:ILE:HD12	2.40	0.42
2:B:219:LEU:HD23	2:B:219:LEU:C	2.39	0.42
1:C:685:ASN:ND2	1:C:685:ASN:C	2.72	0.42
1:C:140[B]:MSE:HE2	1:C:149:PHE:HE2	1.85	0.42
1:C:599:HIS:HE1	1:C:632:TYR:OH	2.03	0.42
1:A:320:ASP:HB2	5:A:2240:HOH:O	2.20	0.42
2:B:541:TRP:CG	2:B:607:MSE:HG3	2.54	0.42
2:B:709:ASN:HD21	2:B:728:THR:H	1.66	0.42
1:C:408:MSE:HE2	1:C:476:ARG:HB3	2.01	0.42
2:B:507:LYS:HZ2	2:B:559[A]:MSE:HG2	1.85	0.42
1:C:546:ASP:N	1:C:547:PRO:HD3	2.35	0.42
1:D:350:PHE:CD2	1:D:350:PHE:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ASN:HD22	1:A:735:ASN:HB3	1.85	0.42
2:B:631[A]:MSE:HB3	2:B:631[A]:MSE:HE2	1.41	0.42
1:A:58:PRO:HG2	1:A:69:TYR:CD1	2.55	0.41
2:B:178:GLU:O	2:B:179:ASN:C	2.56	0.41
1:D:575:ASP:OD1	1:D:577:SER:OG	2.24	0.41
1:D:706:MSE:HE2	1:D:713:HIS:HD1	1.85	0.41
2:B:216:GLN:HE22	2:B:230:HIS:H	1.68	0.41
1:A:709:ASN:HD21	1:A:728:THR:N	2.17	0.41
1:C:483:ARG:HB3	1:C:484:PRO:HD2	2.01	0.41
1:D:374:ASN:HA	1:D:374:ASN:HD22	1.69	0.41
1:D:547:PRO:HB2	1:D:613:TYR:CD2	2.55	0.41
2:B:188:ASN:HD22	2:B:190:GLY:N	1.90	0.41
2:B:216:GLN:NE2	2:B:216:GLN:HA	2.34	0.41
1:C:431:HIS:HD2	1:C:434:VAL:H	1.68	0.41
1:C:645[B]:ASN:HB2	5:C:2263:HOH:O	2.20	0.41
1:A:180:LYS:HE3	1:A:180:LYS:HB2	1.85	0.41
2:B:431:HIS:HE1	5:B:2230:HOH:O	2.03	0.41
1:D:685:ASN:HD22	1:D:687:ASN:H	1.66	0.41
1:A:388:PRO:CD	1:A:389:GLY:H	2.34	0.41
1:A:407:TYR:CD1	1:A:408:MSE:HE1	2.49	0.41
1:C:709:ASN:HD21	1:C:728:THR:H	1.69	0.41
2:B:387:SER:HA	2:B:388:PRO:HA	1.82	0.41
2:B:444:TYR:HB3	2:B:452:PRO:HD3	2.02	0.41
1:D:331:TYR:CZ	1:D:375:THR:HG23	2.55	0.41
2:B:483:ARG:HB3	2:B:484:PRO:HD2	2.03	0.41
1:C:26:VAL:HG11	1:C:124:PRO:HG3	2.02	0.41
1:C:56:TRP:CZ2	1:C:81:GLN:HB2	2.56	0.41
1:C:541:TRP:CG	1:C:607:MSE:HG3	2.56	0.41
1:A:496:MSE:HE1	1:A:498:TYR:OH	2.21	0.40
2:B:86:SER:HB2	2:B:87:PRO:HD2	2.02	0.40
1:C:700:ASN:HD22	1:C:735:ASN:HB3	1.86	0.40
1:A:602:GLN:N	1:A:603:PRO:CD	2.84	0.40
2:B:167:ASP:HB2	5:B:2104:HOH:O	2.20	0.40
2:B:564:MSE:HG2	2:B:611:TYR:CZ	2.55	0.40
1:D:685:ASN:ND2	1:D:685:ASN:C	2.74	0.40
1:C:510:ARG:HG3	1:C:522:PHE:CD1	2.57	0.40
1:C:525:LEU:HD13	1:C:573:ILE:HG13	2.02	0.40
1:C:526:LYS:HA	1:C:575:ASP:HB3	2.04	0.40
1:D:685:ASN:HD22	1:D:686:GLY:N	2.18	0.40
1:D:58:PRO:HG2	1:D:69:TYR:CD1	2.57	0.40
1:A:269:ASP:HB3	1:A:274:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.90	0.40
2:B:238:LYS:HE2	2:B:238:LYS:HB3	1.51	0.40
2:B:627:VAL:HG13	2:B:631[A]:MSE:CG	2.51	0.40
1:D:431:HIS:HE1	5:D:2275:HOH:O	2.04	0.40
1:D:616:GLN:HG2	1:D:618:TRP:CZ2	2.57	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	736/744 (99%)	716 (97%)	20 (3%)	0	100	100
1	C	740/744 (100%)	719 (97%)	21 (3%)	0	100	100
1	D	738/744 (99%)	718 (97%)	20 (3%)	0	100	100
2	B	740/744 (100%)	722 (98%)	18 (2%)	0	100	100
All	All	2954/2976 (99%)	2875 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	623/616 (101%)	604 (97%)	19 (3%)	41	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	632/616 (103%)	612 (97%)	20 (3%)	39 30
1	D	633/616 (103%)	607 (96%)	26 (4%)	30 21
2	B	631/616 (102%)	608 (96%)	23 (4%)	35 26
All	All	2519/2464 (102%)	2431 (96%)	88 (4%)	37 27

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	THR
1	A	215	GLU
1	A	216	ASN
1	A	237	PHE
1	A	319	LEU
1	A	350	PHE
1	A	385	TRP
1	A	408	MSE
1	A	419	LEU
1	A	460	ASN
1	A	481	LEU
1	A	539	TYR
1	A	564	MSE
1	A	593	ASN
1	A	596	ASN
1	A	685	ASN
1	A	692	ASP
1	A	708	PHE
1	A	739	LEU
2	B	77	ARG
2	B	185	THR
2	B	215	GLU
2	B	220	GLN
2	B	237	PHE
2	B	238	LYS
2	B	257	GLU
2	B	307	TYR
2	B	319	LEU
2	B	350	PHE
2	B	385	TRP
2	B	419	LEU
2	B	456	LYS
2	B	460	ASN

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Mol	Chain	Res	Type
2	B	481	LEU
2	B	482	LYS
2	B	519	GLN
2	B	539	TYR
2	B	593	ASN
2	B	631[A]	MSE
2	B	631[B]	MSE
2	B	685	ASN
2	B	708	PHE
1	C	237	PHE
1	C	274	LEU
1	C	292	GLU
1	C	307	TYR
1	C	319	LEU
1	C	350	PHE
1	C	385	TRP
1	C	460	ASN
1	C	481	LEU
1	C	482	LYS
1	C	486	LYS
1	C	519	GLN
1	C	539	TYR
1	C	593	ASN
1	C	645[A]	ASN
1	C	645[B]	ASN
1	C	685	ASN
1	C	692	ASP
1	C	708	PHE
1	C	739	LEU
1	D	34	SER
1	D	45	PRO
1	D	237	PHE
1	D	263[A]	MSE
1	D	263[B]	MSE
1	D	284	GLN
1	D	350	PHE
1	D	385	TRP
1	D	419	LEU
1	D	456	LYS
1	D	481	LEU
1	D	482	LYS
1	D	485	LYS

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Mol	Chain	Res	Type
1	D	519	GLN
1	D	539	TYR
1	D	564	MSE
1	D	573	ILE
1	D	587[A]	ARG
1	D	587[B]	ARG
1	D	593	ASN
1	D	596	ASN
1	D	685	ASN
1	D	692	ASP
1	D	708	PHE
1	D	739	LEU
1	D	746	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	216	ASN
1	A	226	GLN
1	A	264	ASN
1	A	283	ASN
1	A	327	HIS
1	A	358	ASN
1	A	374	ASN
1	A	431	HIS
1	A	446	ASN
1	A	593	ASN
1	A	599	HIS
1	A	601	ASN
1	A	685	ASN
1	A	700	ASN
1	A	709	ASN
1	A	716	ASN
2	B	188	ASN
2	B	222	ASN
2	B	258	GLN
2	B	262	ASN
2	B	264	ASN
2	B	358	ASN
2	B	374	ASN
2	B	431	HIS

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Mol	Chain	Res	Type
2	B	446	ASN
2	B	460	ASN
2	B	593	ASN
2	B	599	HIS
2	B	601	ASN
2	B	685	ASN
2	B	700	ASN
2	B	709	ASN
2	B	716	ASN
2	B	740	ASN
1	C	59	GLN
1	C	188	ASN
1	C	220	GLN
1	C	226	GLN
1	C	262	ASN
1	C	264	ASN
1	C	283	ASN
1	C	284	GLN
1	C	358	ASN
1	C	374	ASN
1	C	431	HIS
1	C	446	ASN
1	C	593	ASN
1	C	599	HIS
1	C	601	ASN
1	C	616	GLN
1	C	685	ASN
1	C	695	ASN
1	C	700	ASN
1	C	709	ASN
1	C	716	ASN
1	D	59	GLN
1	D	188	ASN
1	D	258	GLN
1	D	264	ASN
1	D	358	ASN
1	D	374	ASN
1	D	431	HIS
1	D	446	ASN
1	D	593	ASN
1	D	599	HIS
1	D	601	ASN

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Mol	Chain	Res	Type
1	D	685	ASN
1	D	700	ASN
1	D	709	ASN
1	D	716	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	C	803	-	5,5,5	0.42	0	5,5,5	0.54	0
4	GOL	B	805	-	5,5,5	0.31	0	5,5,5	0.43	0
4	GOL	A	803	-	5,5,5	0.37	0	5,5,5	0.20	0
4	GOL	D	805	-	5,5,5	0.36	0	5,5,5	0.60	0
4	GOL	B	802	-	5,5,5	0.25	0	5,5,5	0.58	0
4	GOL	D	806	-	5,5,5	0.26	0	5,5,5	0.64	0
4	GOL	C	802	-	5,5,5	0.22	0	5,5,5	0.52	0
4	GOL	A	805	-	5,5,5	0.27	0	5,5,5	0.57	0
4	GOL	A	802	-	5,5,5	0.35	0	5,5,5	0.41	0
4	GOL	C	805	-	5,5,5	0.43	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	D	803	-	5,5,5	0.35	0	5,5,5	0.08	0
4	GOL	B	803	-	5,5,5	0.42	0	5,5,5	0.95	0
4	GOL	B	804	-	5,5,5	0.35	0	5,5,5	0.50	0
4	GOL	A	804	-	5,5,5	0.53	0	5,5,5	0.42	0
4	GOL	D	804	1	5,5,5	0.23	0	5,5,5	0.62	0
4	GOL	C	804	-	5,5,5	0.29	0	5,5,5	0.70	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	C	803	-	-	0/4/4/4	-
4	GOL	B	805	-	-	0/4/4/4	-
4	GOL	A	803	-	-	0/4/4/4	-
4	GOL	D	805	-	-	2/4/4/4	-
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	D	806	-	-	2/4/4/4	-
4	GOL	C	802	-	-	0/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	A	802	-	-	2/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
4	GOL	D	803	-	-	0/4/4/4	-
4	GOL	B	803	-	-	3/4/4/4	-
4	GOL	B	804	-	-	1/4/4/4	-
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	D	804	1	-	2/4/4/4	-
4	GOL	C	804	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	805	GOL	O1-C1-C2-C3
4	D	806	GOL	O1-C1-C2-C3
4	A	805	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	804	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	B	803	GOL	O1-C1-C2-O2
4	A	802	GOL	C1-C2-C3-O3
4	D	805	GOL	O1-C1-C2-O2
4	D	806	GOL	O1-C1-C2-O2
4	D	804	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	C	804	GOL	O2-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	C	804	GOL	C1-C2-C3-O3
4	A	802	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	804	GOL	3	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	709/744 (95%)	-0.35	1 (0%)	95	95	2, 7, 16, 26	0
1	C	709/744 (95%)	-0.28	2 (0%)	94	94	2, 7, 15, 26	0
1	D	709/744 (95%)	-0.26	7 (0%)	82	84	2, 7, 17, 28	0
2	B	710/744 (95%)	0.07	14 (1%)	65	68	3, 8, 15, 25	0
All	All	2837/2976 (95%)	-0.21	24 (0%)	86	87	2, 7, 16, 28	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	580	GLY	3.5
1	A	36	PHE	3.2
2	B	105	VAL	3.2
2	B	517	THR	2.7
2	B	217	GLY	2.7
2	B	518	PHE	2.6
2	B	218	ASN	2.6
1	C	740	ASN	2.6
2	B	216	GLN	2.5
1	D	216[A]	ASN	2.4
2	B	223	VAL	2.4
2	B	450	TYR	2.3
2	B	172	ILE	2.2
1	D	222	ASN	2.2
1	C	739	LEU	2.2
1	D	482	LYS	2.2
2	B	502	PHE	2.2
1	D	103	GLN	2.2
2	B	756	LEU	2.1
2	B	522	PHE	2.1
2	B	305	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	580	GLY	2.1
1	D	518	PHE	2.0
1	D	740	ASN	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	D	804	6/6	0.84	0.15	18,19,23,26	0
4	GOL	D	806	6/6	0.85	0.14	23,24,25,25	0
4	GOL	A	805	6/6	0.88	0.19	21,22,22,23	0
4	GOL	C	804	6/6	0.88	0.14	14,21,23,25	0
4	GOL	B	804	6/6	0.92	0.14	14,18,19,20	0
4	GOL	A	804	6/6	0.92	0.15	11,12,14,19	0
4	GOL	C	805	6/6	0.93	0.12	9,14,16,20	0
4	GOL	B	805	6/6	0.93	0.12	13,14,15,15	0
4	GOL	D	805	6/6	0.93	0.11	9,11,14,20	0
4	GOL	D	803	6/6	0.93	0.10	10,14,16,17	0
4	GOL	C	803	6/6	0.93	0.10	11,14,16,17	0
4	GOL	B	802	6/6	0.94	0.09	14,15,15,17	0
4	GOL	A	803	6/6	0.95	0.07	15,16,17,17	0
4	GOL	C	802	6/6	0.96	0.09	9,12,13,14	0
3	CA	D	801	1/1	0.96	0.06	25,25,25,25	0
4	GOL	B	803	6/6	0.96	0.11	12,13,15,19	0
3	CA	A	801	1/1	0.97	0.05	23,23,23,23	0
4	GOL	A	802	6/6	0.97	0.08	7,12,14,15	0
3	CA	B	801	1/1	0.98	0.05	26,26,26,26	0
3	CA	C	801	1/1	0.99	0.06	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.