



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 2WZS / pdb_00002wzs
Title : Structure of the Family GH92 Inverting Mannosidase BT3990 from Bacteroides
thetaiotaomicron VPI-5482 in complex with Mannoimidazole
Authors : Zhu, Y.; Suits, M.D.L.; Thompson, A.; Chavan, S.; Dinev, Z.; Dumon,
C.; Smith, N.; Moremen, K.W.; Xiang, Y.; Siriwardena, A.; Williams, S.J.;
Gilbert, H.J.; Davies, G.J.
Deposited on : 2009-12-02
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

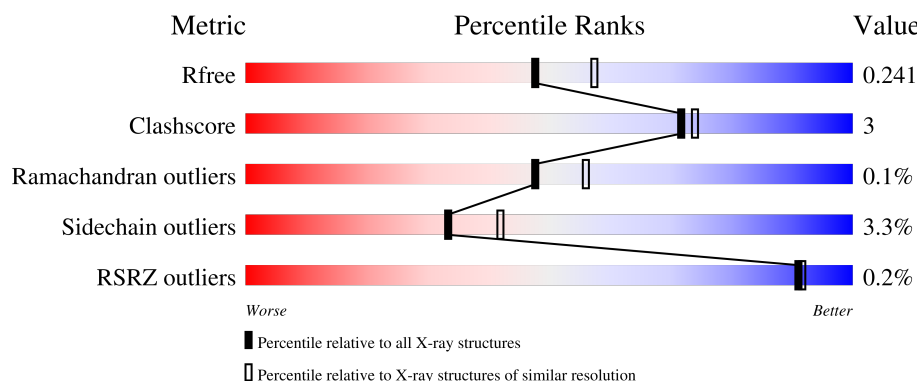
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	738	91% 8% .
1	B	738	92% 7% .
1	C	738	91% 8% .
1	D	738	94% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	738	 90% 8% •
1	F	738	 90% 9% •
1	G	738	 89% 10% •
1	H	738	 86% 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
4	GOL	B	805	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 49858 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	0	4	0
			5982	3837	985	1126	34			
1	B	736	Total	C	N	O	S	0	2	0
			5980	3835	984	1127	34			
1	C	736	Total	C	N	O	S	0	0	0
			5965	3824	983	1125	33			
1	D	738	Total	C	N	O	S	0	5	0
			6015	3862	987	1133	33			
1	E	736	Total	C	N	O	S	0	0	0
			5950	3816	982	1119	33			
1	F	735	Total	C	N	O	S	0	2	0
			5955	3820	981	1120	34			
1	G	736	Total	C	N	O	S	0	0	0
			5943	3810	977	1123	33			
1	H	736	Total	C	N	O	S	0	1	0
			5966	3825	982	1125	34			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

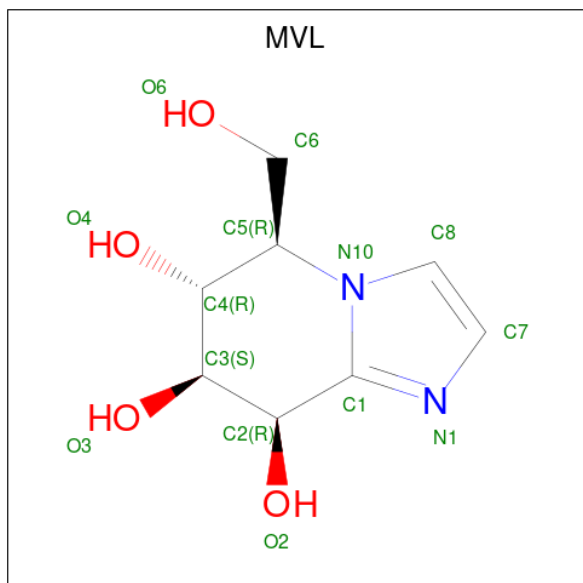
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (CCD ID: MVL) (formula: $C_8H_{12}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	2	4		
3	B	1	Total	C	N	O	0	0
			14	8	2	4		
3	C	1	Total	C	N	O	0	0
			14	8	2	4		
3	D	1	Total	C	N	O	0	0
			14	8	2	4		
3	E	1	Total	C	N	O	0	0
			14	8	2	4		
3	F	1	Total	C	N	O	0	0
			14	8	2	4		
3	G	1	Total	C	N	O	0	0
			14	8	2	4		
3	H	1	Total	C	N	O	0	0
			14	8	2	4		

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



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

Continued on next page...

Continued from previous page...

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

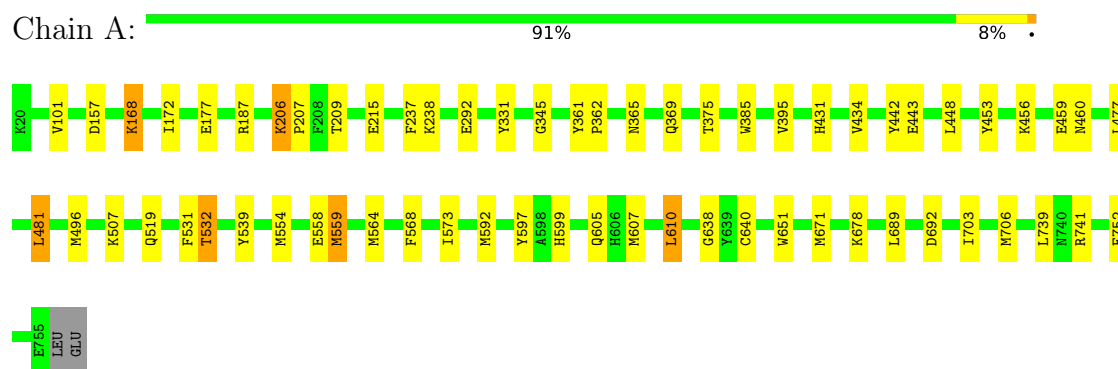
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	349	Total	O	0	0
			349	349		
5	B	320	Total	O	0	0
			320	320		
5	C	279	Total	O	0	0
			279	279		
5	D	323	Total	O	0	0
			323	323		
5	E	261	Total	O	0	0
			261	261		
5	F	179	Total	O	0	0
			179	179		
5	G	87	Total	O	0	0
			87	87		
5	H	70	Total	O	0	0
			70	70		

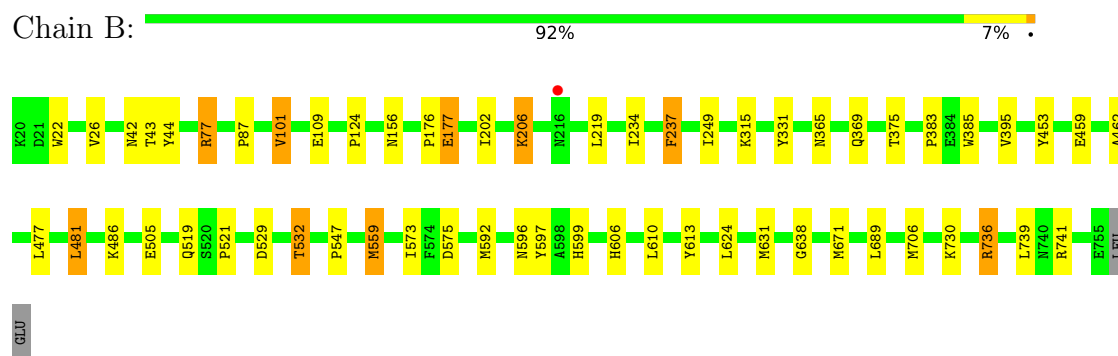
3 Residue-property plots

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.

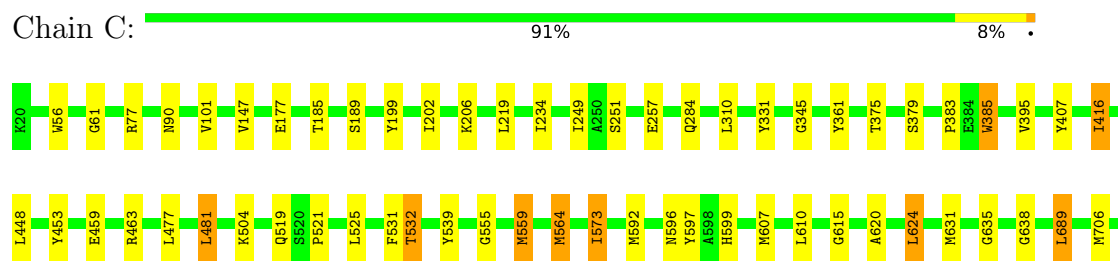
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

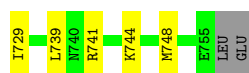


• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



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





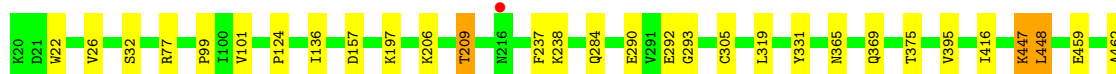
- Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain D: 94% 6%



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

Chain E: 90% 8%



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

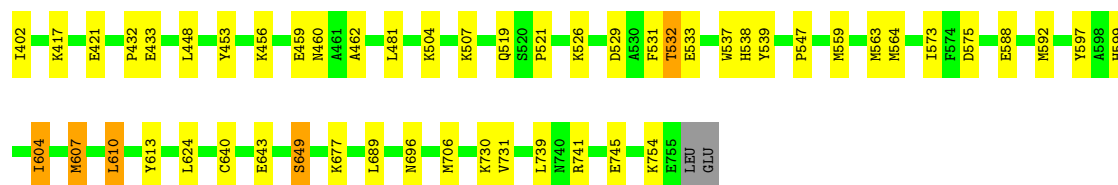
Chain F: 90% 9%



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

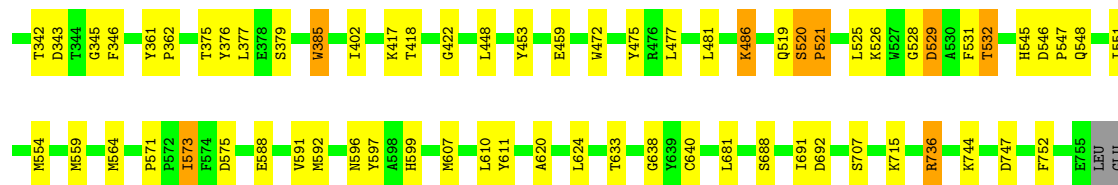
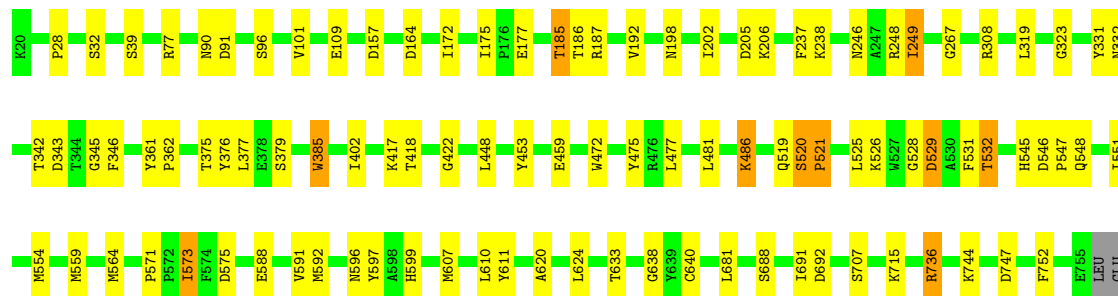
Chain G: 89% 10%





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

Chain H: 86% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.19Å 152.39Å 221.45Å 90.00° 94.21° 90.00°	Depositor
Resolution (Å)	218.22 – 2.25 218.22 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (218.22-2.25) 100.0 (218.22-2.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.242 0.201 , 0.241	Depositor DCC
R_{free} test set	17260 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49858	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MVL, CA, 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	0.60	0/6175	0.82	3/8376 (0.0%)
1	B	0.59	0/6167	0.81	1/8364 (0.0%)
1	C	0.57	0/6146	0.81	3/8338 (0.0%)
1	D	0.58	0/6213	0.80	1/8429 (0.0%)
1	E	0.60	0/6131	0.83	1/8320 (0.0%)
1	F	0.61	0/6142	0.82	3/8334 (0.0%)
1	G	0.61	0/6124	0.81	1/8314 (0.0%)
1	H	0.63	0/6150	0.83	4/8344 (0.0%)
All	All	0.60	0/49248	0.82	17/66819 (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
1	H	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	638	GLY	N-CA-C	6.99	122.93	113.99
1	C	638	GLY	N-CA-C	6.82	122.51	113.37
1	B	638	GLY	N-CA-C	6.59	121.20	112.77
1	F	638	GLY	N-CA-C	6.58	122.19	113.37
1	E	638	GLY	N-CA-C	6.33	121.85	113.37
1	H	175	ILE	CA-C-N	6.23	126.13	119.28
1	H	175	ILE	C-N-CA	6.23	126.13	119.28
1	H	638	GLY	N-CA-C	6.17	120.66	112.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	635	GLY	CA-C-N	5.89	126.03	119.32
1	C	635	GLY	C-N-CA	5.89	126.03	119.32
1	A	638	GLY	N-CA-C	5.49	120.73	113.37
1	H	323	GLY	N-CA-C	-5.43	107.52	115.72
1	A	460	ASN	N-CA-C	5.41	117.18	111.28
1	F	460	ASN	N-CA-C	5.36	117.54	111.11
1	G	607	MET	N-CA-C	5.17	116.92	111.28
1	A	605	GLN	N-CA-C	5.13	117.61	111.71
1	F	607	MET	N-CA-C	5.11	117.51	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	520	SER	Peptide

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	5982	0	5660	35	0
1	B	5980	0	5658	42	0
1	C	5965	0	5632	34	0
1	D	6015	0	5693	22	0
1	E	5950	0	5611	41	0
1	F	5955	0	5622	42	0
1	G	5943	0	5584	37	0
1	H	5966	0	5630	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	14	0	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	10	0	0
3	C	14	0	10	0	0
3	D	14	0	10	1	0
3	E	14	0	10	0	0
3	F	14	0	10	1	0
3	G	14	0	10	1	0
3	H	14	0	10	0	0
4	A	18	0	24	0	0
4	B	24	0	32	10	0
4	C	24	0	32	0	0
4	D	24	0	32	1	0
4	E	18	0	24	2	0
4	F	6	0	8	0	0
5	A	349	0	0	2	0
5	B	320	0	0	5	0
5	C	279	0	0	1	0
5	D	323	0	0	5	0
5	E	261	0	0	7	0
5	F	179	0	0	5	0
5	G	87	0	0	0	0
5	H	70	0	0	3	0
All	All	49858	0	45322	312	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 3.

All (312) 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:F:592[B]:MET:HA	1:F:592[B]:MET:CE	1.59	1.32
1:F:592[B]:MET:HE3	1:F:592[B]:MET:CA	1.70	1.18
1:H:592[B]:MET:HA	1:H:592[B]:MET:CE	1.75	1.16
1:G:706:MET:HE3	1:G:741:ARG:HH22	1.19	1.04
1:H:592[B]:MET:HA	1:H:592[B]:MET:HE2	1.42	0.96
1:C:706:MET:HE3	1:C:741:ARG:NH2	1.82	0.95
1:G:706:MET:HE3	1:G:741:ARG:NH2	1.83	0.93
1:B:42:ASN:O	4:B:805:GOL:H31	1.68	0.93
1:H:592[B]:MET:HA	1:H:592[B]:MET:HE3	1.51	0.92
1:B:42:ASN:O	4:B:805:GOL:C3	2.20	0.90
1:B:44:TYR:HD1	4:B:805:GOL:H2	1.37	0.89
1:F:592[B]:MET:HE2	1:F:631:MET:HE1	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:MET:HE3	1:C:741:ARG:HH22	1.36	0.85
1:E:706:MET:HE3	1:E:741:ARG:HH22	1.42	0.84
1:E:319:LEU:HG	5:E:2129:HOH:O	1.76	0.84
1:E:706:MET:HE3	1:E:741:ARG:NH2	1.94	0.82
1:D:459:GLU:HB3	1:D:532:THR:HG22	1.64	0.79
1:E:197:LYS:HE2	5:E:2086:HOH:O	1.84	0.77
1:D:558[A]:GLU:CD	1:D:558[A]:GLU:H	1.92	0.77
1:B:459:GLU:HB3	1:B:532:THR:HG22	1.65	0.76
1:H:459:GLU:HB3	1:H:532:THR:HG22	1.69	0.75
1:E:459:GLU:OE1	1:E:532:THR:HB	1.89	0.73
1:B:44:TYR:CD1	4:B:805:GOL:H2	2.25	0.71
1:A:558[B]:GLU:CD	1:A:558[B]:GLU:H	1.98	0.71
1:F:507:LYS:HB2	1:F:563:MET:HE2	1.73	0.71
1:B:453:TYR:CE1	1:B:519:GLN:HG3	2.26	0.71
1:F:209:THR:HG22	5:F:2031:HOH:O	1.91	0.69
1:F:526:LYS:HA	1:F:575:ASP:HB3	1.74	0.69
1:B:315:LYS:NZ	4:B:804:GOL:H32	2.06	0.69
1:H:453:TYR:CE1	1:H:519:GLN:HG3	2.27	0.69
1:A:706:MET:HE3	1:A:741:ARG:NH2	2.09	0.68
1:C:453:TYR:CE1	1:C:519:GLN:HG3	2.29	0.68
1:B:736:ARG:HB3	1:B:736:ARG:HH11	1.58	0.68
1:A:507:LYS:HZ1	1:A:559:MET:HE3	1.60	0.67
1:B:87:PRO:HD3	4:B:805:GOL:H32	1.77	0.67
1:F:408:MET:HE1	1:F:480:GLU:HB2	1.77	0.67
1:A:453:TYR:CE1	1:A:519:GLN:HG3	2.30	0.66
1:D:503:ASP:OD1	1:D:505:GLU:HG3	1.96	0.66
1:F:592[B]:MET:HA	1:F:592[B]:MET:HE3	0.75	0.66
1:A:157:ASP:HA	1:A:238:LYS:HG2	1.77	0.65
1:G:592:MET:HE2	1:G:640:CYS:HB2	1.77	0.65
1:C:257:GLU:HG3	5:C:2108:HOH:O	1.96	0.65
1:G:643:GLU:OE2	1:G:649:SER:OG	2.14	0.65
1:C:706:MET:CE	1:C:741:ARG:HH22	2.09	0.64
1:F:453:TYR:CE1	1:F:519:GLN:HG3	2.31	0.64
1:B:42:ASN:O	4:B:805:GOL:H32	1.98	0.64
1:B:453:TYR:CZ	1:B:519:GLN:HG3	2.33	0.63
1:F:459:GLU:HG2	1:F:531:PHE:O	1.98	0.63
1:B:315:LYS:HZ3	4:B:804:GOL:H32	1.60	0.63
1:D:519:GLN:HG2	5:D:2212:HOH:O	1.99	0.63
1:F:564:MET:HE1	1:F:607:MET:HG2	1.80	0.62
1:A:597:TYR:CE2	1:A:599:HIS:HB2	2.35	0.62
1:F:547:PRO:HG2	1:F:613:TYR:CE2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HA	4:B:805:GOL:H31	1.82	0.61
1:A:453:TYR:CZ	1:A:519:GLN:HG3	2.36	0.61
1:A:592[A]:MET:HE2	1:A:640:CYS:HB2	1.83	0.60
1:H:453:TYR:CZ	1:H:519:GLN:HG3	2.36	0.60
1:B:597:TYR:CE2	1:B:599:HIS:HB2	2.36	0.60
1:A:554:MET:O	1:A:559:MET:HE2	2.02	0.60
1:B:26:VAL:HG11	1:B:124:PRO:HG3	1.84	0.59
1:G:538:HIS:HA	1:G:604:ILE:HD12	1.84	0.59
1:H:157:ASP:HA	1:H:238:LYS:HG3	1.82	0.59
1:B:706:MET:HE3	1:B:741:ARG:NH2	2.19	0.58
1:F:568:PHE:CZ	1:F:607:MET:HE1	2.38	0.58
1:D:453:TYR:CZ	1:D:519:GLN:HG3	2.38	0.58
1:F:453:TYR:CZ	1:F:519:GLN:HG3	2.39	0.58
1:C:615:GLY:HA2	1:C:748:MET:HE1	1.85	0.58
1:D:20:LYS:N	5:D:2001:HOH:O	2.36	0.58
1:B:176:PRO:HD2	1:B:177:GLU:OE1	2.04	0.57
1:E:538:HIS:HA	1:E:604:ILE:HD12	1.86	0.57
1:G:597:TYR:CE2	1:G:599:HIS:HB2	2.40	0.57
1:G:607:MET:HA	1:G:610:LEU:HD22	1.86	0.57
1:A:459:GLU:OE1	1:A:532:THR:HB	2.05	0.57
1:E:462:ALA:CB	1:E:532:THR:HG22	2.34	0.57
1:E:32:SER:HB3	5:E:2012:HOH:O	2.04	0.56
1:G:453:TYR:CE1	1:G:519:GLN:HG3	2.40	0.56
1:G:453:TYR:CZ	1:G:519:GLN:HG3	2.41	0.56
1:C:459:GLU:OE1	1:C:532:THR:HB	2.05	0.56
1:C:395:VAL:HG21	1:C:532:THR:HG21	1.88	0.56
1:C:459:GLU:HB3	1:C:532:THR:HG22	1.87	0.56
1:C:564:MET:HE1	1:C:607:MET:HG2	1.88	0.55
1:H:715:LYS:HG3	1:H:747:ASP:HA	1.88	0.55
1:G:293:GLY:HA3	1:G:677:LYS:HB2	1.87	0.55
1:B:519:GLN:NE2	1:B:521:PRO:O	2.40	0.55
1:E:724:PHE:HE2	4:E:804:GOL:H11	1.71	0.55
1:H:377:LEU:HD21	1:H:418:THR:HG21	1.88	0.55
1:H:477:LEU:O	1:H:481:LEU:HB2	2.07	0.55
1:H:592[B]:MET:CE	1:H:592[B]:MET:CA	2.62	0.54
1:A:168:LYS:HG3	1:A:187:ARG:HG3	1.88	0.54
1:C:564:MET:CE	1:C:607:MET:HG2	2.37	0.54
1:A:507:LYS:NZ	1:A:559:MET:HE3	2.21	0.54
1:D:453:TYR:CE1	1:D:519:GLN:HG3	2.42	0.54
1:E:547:PRO:HG2	1:E:613:TYR:CE2	2.42	0.54
1:E:597:TYR:CE2	1:E:599:HIS:HB2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:ASP:OD1	1:F:409:LYS:NZ	2.36	0.54
1:G:507:LYS:NZ	1:G:559:MET:HE2	2.22	0.54
1:H:592[B]:MET:HE2	1:H:592[B]:MET:CA	2.23	0.54
1:E:26:VAL:HG11	1:E:124:PRO:HG3	1.90	0.54
1:G:462:ALA:CB	1:G:532:THR:HG22	2.38	0.54
1:B:477:LEU:HG	1:B:481:LEU:HD22	1.90	0.54
1:G:459:GLU:HG2	1:G:531:PHE:O	2.09	0.53
1:H:592[A]:MET:HE2	1:H:640:CYS:HB2	1.90	0.53
1:F:519:GLN:HG2	5:F:2142:HOH:O	2.09	0.53
1:F:564:MET:CE	1:F:607:MET:HG2	2.39	0.53
1:F:331:TYR:CZ	1:F:375:THR:HG23	2.43	0.52
1:H:528:GLY:HA2	1:H:531:PHE:O	2.10	0.52
1:H:157:ASP:OD1	1:H:238:LYS:HE3	2.09	0.52
1:G:533:GLU:OE2	3:G:801:MVL:O2	2.27	0.52
1:A:592[A]:MET:HE1	5:A:2282:HOH:O	2.09	0.52
1:H:248:ARG:NH2	1:H:267:GLY:O	2.38	0.52
1:E:395:VAL:HG21	1:E:532:THR:HG21	1.92	0.51
1:E:583:ILE:HD12	1:E:585:GLU:HB2	1.92	0.51
1:G:432:PRO:HB2	1:G:433:GLU:OE2	2.11	0.51
3:A:801:MVL:H7	5:A:2267:HOH:O	2.09	0.51
3:D:801:MVL:H7	5:D:2233:HOH:O	2.08	0.51
1:B:736:ARG:HB3	1:B:736:ARG:NH1	2.23	0.51
3:F:801:MVL:H7	5:F:2151:HOH:O	2.11	0.51
1:G:157:ASP:HA	1:G:238:LYS:HG3	1.91	0.51
1:F:408:MET:HE1	1:F:480:GLU:CB	2.40	0.51
1:G:547:PRO:HG2	1:G:613:TYR:CE2	2.45	0.51
1:H:486:LYS:CD	1:H:486:LYS:H	2.23	0.51
1:C:407:TYR:HE2	1:C:416:ILE:HD12	1.75	0.51
1:D:462:ALA:CB	1:D:532:THR:HG23	2.41	0.51
1:D:597:TYR:CE2	1:D:599:HIS:HB2	2.46	0.51
1:A:496:MET:HE2	1:A:752:PHE:CD2	2.46	0.51
1:B:77:ARG:HH21	1:B:109:GLU:HA	1.75	0.50
1:F:606:HIS:HB3	5:F:2175:HOH:O	2.10	0.50
1:B:206:LYS:HD2	1:B:237:PHE:CD1	2.46	0.50
1:E:209:THR:HB	1:E:237:PHE:HA	1.93	0.50
1:F:597:TYR:CE2	1:F:599:HIS:HB2	2.45	0.50
1:H:526:LYS:HA	1:H:575:ASP:HB3	1.94	0.50
1:E:617:PRO:HG2	5:E:2257:HOH:O	2.11	0.50
1:B:395:VAL:HG21	1:B:532:THR:HG21	1.94	0.49
1:C:620:ALA:O	1:C:624:LEU:HB2	2.12	0.49
1:G:677:LYS:HE3	1:G:696:ASN:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:ILE:HG12	1:H:249:ILE:HD13	1.95	0.49
1:B:22:TRP:CD1	5:B:2001:HOH:O	2.66	0.49
1:E:526:LYS:HA	1:E:575:ASP:HB3	1.95	0.49
1:E:462:ALA:HB3	1:E:532:THR:HG22	1.94	0.48
1:F:417:LYS:O	1:F:421:GLU:HG3	2.13	0.48
1:G:417:LYS:O	1:G:421:GLU:HG3	2.13	0.48
1:A:459:GLU:HG2	1:A:531:PHE:O	2.13	0.48
1:C:219:LEU:HD11	1:C:234:ILE:HD12	1.96	0.48
1:H:546:ASP:N	1:H:547:PRO:HD3	2.28	0.48
1:F:462:ALA:CB	1:F:532:THR:HG22	2.43	0.48
1:G:331:TYR:CZ	1:G:375:THR:HG23	2.48	0.48
1:E:157:ASP:HA	1:E:238:LYS:HG3	1.95	0.48
1:H:192:VAL:HG22	5:H:2022:HOH:O	2.14	0.48
1:A:331:TYR:CZ	1:A:375:THR:HG23	2.48	0.48
1:E:608:ILE:HG21	1:E:624:LEU:HD13	1.94	0.48
1:F:364:VAL:HG12	1:F:368:MET:HE3	1.95	0.48
1:H:331:TYR:HB3	1:H:379:SER:HB3	1.96	0.48
1:H:346:PHE:CD1	1:H:402:ILE:CD1	2.97	0.48
1:G:135:ASP:OD2	1:H:571:PRO:HB3	2.14	0.48
1:A:703:ILE:HD13	1:A:706:MET:HE2	1.96	0.48
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.95	0.48
1:E:459:GLU:HG2	1:E:531:PHE:O	2.14	0.48
1:C:597:TYR:CE2	1:C:599:HIS:HB2	2.49	0.47
1:F:206:LYS:HE3	1:F:237:PHE:HB2	1.97	0.47
1:G:316:PHE:CE2	1:G:330:PRO:HG3	2.49	0.47
1:F:219:LEU:HD11	1:F:234:ILE:HD12	1.96	0.47
1:H:185:THR:HG23	1:H:198:ASN:HB3	1.96	0.47
1:B:462:ALA:CB	1:B:532:THR:HG23	2.44	0.47
1:B:547:PRO:HG2	1:B:613:TYR:CE2	2.49	0.47
1:C:706:MET:CE	1:C:741:ARG:NH2	2.65	0.47
1:E:22:TRP:CZ2	1:E:290:GLU:HG2	2.49	0.47
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.95	0.47
1:D:86:SER:HB2	5:D:2260:HOH:O	2.15	0.47
1:E:293:GLY:HA3	1:E:677:LYS:HB2	1.96	0.47
1:E:592:MET:HE2	1:E:640:CYS:HB2	1.97	0.47
1:G:60:THR:O	1:G:77:ARG:NH1	2.44	0.47
1:B:101:VAL:HG13	1:B:156:ASN:ND2	2.29	0.47
1:C:61:GLY:O	1:C:77:ARG:HD3	2.15	0.47
1:C:519:GLN:NE2	1:C:521:PRO:O	2.48	0.47
1:E:608:ILE:CG2	1:E:624:LEU:HD13	2.45	0.47
1:B:671:MET:HG2	1:B:706:MET:HE1	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:TYR:CD1	1:A:519:GLN:HG3	2.49	0.46
1:C:689:LEU:HD11	1:C:729:ILE:HD12	1.97	0.46
1:E:447:LYS:HG3	1:E:448:LEU:HD13	1.97	0.46
1:F:519:GLN:NE2	1:F:521:PRO:O	2.49	0.46
1:E:331:TYR:CZ	1:E:375:THR:HG23	2.50	0.46
1:E:724:PHE:CE2	4:E:804:GOL:H31	2.50	0.46
1:F:177:GLU:H	1:F:177:GLU:CD	2.23	0.46
1:G:28:PRO:O	1:G:308:ARG:NH2	2.49	0.46
1:A:365:ASN:O	1:A:369:GLN:HG2	2.16	0.46
1:G:162:VAL:HG22	1:G:234:ILE:HG12	1.97	0.46
1:B:365:ASN:O	1:B:369:GLN:HG2	2.16	0.46
1:G:202:ILE:HG23	1:G:249:ILE:HG12	1.97	0.46
1:H:529:ASP:HB3	5:H:2043:HOH:O	2.16	0.46
1:D:395:VAL:HG21	1:D:532:THR:HG21	1.98	0.46
1:G:526:LYS:HA	1:G:575:ASP:HB3	1.98	0.45
1:C:56:TRP:CE2	1:C:147:VAL:HG11	2.51	0.45
1:F:26:VAL:HG11	1:F:124:PRO:HG3	1.98	0.45
1:G:86:SER:HB2	1:G:87:PRO:HD2	1.98	0.45
1:C:202:ILE:HG23	1:C:249:ILE:HG12	1.98	0.45
1:C:592:MET:HE3	1:C:631:MET:SD	2.56	0.45
1:A:361:TYR:N	1:A:362:PRO:CD	2.79	0.45
1:B:331:TYR:CZ	1:B:375:THR:HG23	2.51	0.45
1:C:555:GLY:HA3	1:C:559:MET:HE2	1.97	0.45
1:H:564:MET:HE3	1:H:607:MET:HG2	1.97	0.45
1:H:554:MET:O	1:H:559:MET:HE3	2.17	0.45
1:A:395:VAL:HG21	1:A:532:THR:HG21	1.98	0.45
1:A:607:MET:O	1:A:610:LEU:HB2	2.16	0.45
1:C:525:LEU:HD13	1:C:573:ILE:HG13	1.99	0.45
1:D:197:LYS:NZ	4:D:802:GOL:O3	2.50	0.45
1:E:565:ASP:OD2	1:E:619:LYS:NZ	2.49	0.45
1:F:592[B]:MET:HG3	1:F:631:MET:SD	2.57	0.45
1:G:537:TRP:CH2	1:G:563:MET:HE3	2.52	0.45
1:A:459:GLU:HB3	1:A:532:THR:HG22	1.99	0.45
1:F:707:SER:HB2	1:F:711:ALA:O	2.17	0.45
1:A:671:MET:HG2	1:A:706:MET:HE1	1.98	0.45
1:C:395:VAL:CG2	1:C:532:THR:HG21	2.46	0.45
1:B:559[B]:MET:HG3	5:B:2212:HOH:O	2.17	0.45
1:H:361:TYR:N	1:H:362:PRO:CD	2.80	0.45
1:H:681:LEU:O	1:H:688:SER:HA	2.17	0.45
1:C:459:GLU:O	1:C:463:ARG:HG3	2.17	0.45
1:E:292:GLU:HG3	1:E:678:LYS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:588:GLU:O	1:G:592:MET:HE3	2.17	0.45
1:E:209:THR:HG22	5:E:2091:HOH:O	2.16	0.44
1:F:592[A]:MET:HE2	1:F:640:CYS:HB2	1.98	0.44
1:H:332:ASN:OD1	1:H:332:ASN:C	2.60	0.44
1:B:592:MET:HG2	1:B:631:MET:SD	2.58	0.44
1:D:128:LYS:HA	1:D:138:THR:O	2.17	0.44
1:A:442:TYR:CE2	1:A:443:GLU:HG2	2.53	0.44
1:E:99:PRO:HB2	1:E:136:ILE:HD13	2.00	0.44
1:C:345:GLY:HA3	1:C:385:TRP:CE2	2.52	0.44
1:B:459:GLU:OE1	1:B:532:THR:HB	2.16	0.44
1:C:199:TYR:O	1:C:251:SER:HA	2.18	0.44
1:E:305:CYS:O	1:E:649:SER:HB3	2.18	0.44
1:E:462:ALA:CB	1:E:532:THR:CG2	2.95	0.44
1:F:744:LYS:HB2	1:F:747:ASP:OD2	2.17	0.44
1:C:90:ASN:HB3	1:C:189:SER:OG	2.18	0.44
1:F:431:HIS:HB3	1:F:434:VAL:O	2.18	0.44
1:F:510:ARG:HG3	1:F:522:PHE:CD1	2.53	0.44
1:G:330:PRO:HB3	1:G:388:PRO:HB2	1.99	0.44
1:G:519:GLN:NE2	1:G:521:PRO:O	2.49	0.44
1:H:611:TYR:HB2	1:H:620:ALA:HB2	2.00	0.44
1:D:459:GLU:HG2	1:D:531:PHE:O	2.18	0.43
1:F:706:MET:HB3	1:F:741:ARG:HH21	1.83	0.43
1:H:39:SER:HB3	1:H:588:GLU:OE2	2.18	0.43
1:H:376:TYR:CE1	1:H:422:GLY:HA2	2.52	0.43
1:E:546:ASP:N	1:E:547:PRO:HD3	2.33	0.43
1:F:592[B]:MET:CE	1:F:592[B]:MET:CA	2.46	0.43
1:H:525:LEU:HD13	1:H:573:ILE:HD11	2.00	0.43
1:B:315:LYS:HZ1	4:B:804:GOL:H32	1.81	0.43
1:H:331:TYR:CZ	1:H:375:THR:HG23	2.54	0.43
1:A:507:LYS:NZ	1:A:559:MET:CE	2.80	0.43
1:F:62:LYS:NZ	1:F:109:GLU:OE2	2.51	0.43
1:A:431:HIS:HB3	1:A:434:VAL:O	2.19	0.43
1:D:157:ASP:HA	1:D:238:LYS:HG2	2.01	0.43
1:C:375:THR:HG21	1:C:383:PRO:HD3	2.01	0.43
1:H:205:ASP:OD2	1:H:246:ASN:HB2	2.18	0.43
1:C:310:LEU:HD21	1:C:361:TYR:CE2	2.54	0.43
1:B:375:THR:HG21	1:B:383:PRO:HD3	2.01	0.42
1:D:519:GLN:NE2	1:D:521:PRO:O	2.44	0.42
1:G:387:SER:O	1:G:391:ARG:NH1	2.51	0.42
1:H:597:TYR:CE2	1:H:599:HIS:HB2	2.54	0.42
1:A:206:LYS:HA	1:A:207:PRO:HD3	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:HG3	1:A:678:LYS:HB3	2.01	0.42
1:A:345:GLY:HA3	1:A:385:TRP:CE2	2.55	0.42
1:H:486:LYS:H	1:H:486:LYS:HD2	1.84	0.42
1:B:519:GLN:HG2	5:B:2200:HOH:O	2.20	0.42
1:H:345:GLY:HA3	1:H:385:TRP:CE2	2.54	0.42
1:A:507:LYS:HZ1	1:A:559:MET:CE	2.31	0.42
1:A:568:PHE:CZ	1:A:607:MET:HE1	2.54	0.42
1:H:736:ARG:HB3	1:H:736:ARG:NH1	2.35	0.42
1:F:29:LEU:HD23	1:F:45:PRO:HG3	2.01	0.42
1:H:77:ARG:HH21	1:H:109:GLU:HG2	1.85	0.42
1:B:575:ASP:C	1:B:575:ASP:OD1	2.62	0.42
1:D:353:LEU:C	1:D:353:LEU:HD13	2.45	0.42
1:E:607:MET:O	1:E:610:LEU:HB2	2.19	0.42
1:F:592[A]:MET:HE1	5:F:2159:HOH:O	2.19	0.41
1:H:592[B]:MET:HE3	1:H:592[B]:MET:CA	2.36	0.41
1:E:571:PRO:HB2	1:E:573:ILE:HG23	2.02	0.41
1:G:564:MET:CE	1:G:607:MET:HE3	2.50	0.41
1:G:607:MET:O	1:G:610:LEU:HB2	2.20	0.41
1:H:591:VAL:O	1:H:592[B]:MET:HE3	2.20	0.41
1:H:96:SER:OG	1:H:164:ASP:HB3	2.20	0.41
1:H:186:THR:O	1:H:187:ARG:C	2.62	0.41
1:H:472:TRP:HB2	1:H:545:HIS:CD2	2.54	0.41
1:G:745:GLU:OE2	1:G:754:LYS:NZ	2.48	0.41
1:B:202:ILE:HG12	1:B:249:ILE:HG12	2.02	0.41
1:H:342:THR:O	1:H:343:ASP:HB2	2.19	0.41
1:D:86:SER:HB2	1:D:87:PRO:HD2	2.02	0.41
1:H:548:GLN:HA	1:H:551:ILE:HD12	2.02	0.41
1:D:725:LYS:HE2	5:D:2303:HOH:O	2.21	0.41
1:H:177:GLU:CD	1:H:177:GLU:H	2.29	0.41
1:E:365:ASN:O	1:E:369:GLN:HG2	2.20	0.41
1:E:592:MET:HE1	5:E:2221:HOH:O	2.20	0.41
1:H:346:PHE:CG	1:H:402:ILE:HD12	2.55	0.41
1:A:564:MET:HE3	1:A:607:MET:HE3	2.03	0.41
1:B:177:GLU:CD	1:B:177:GLU:H	2.29	0.41
1:B:606:HIS:HB3	5:B:2270:HOH:O	2.20	0.41
1:C:331:TYR:HB3	1:C:379:SER:HB3	2.03	0.41
1:C:459:GLU:HG2	1:C:531:PHE:O	2.21	0.41
1:E:609:TYR:CZ	1:E:660:TYR:HB2	2.56	0.41
1:H:475:TYR:CE1	1:H:752:PHE:CE1	3.08	0.41
1:B:219:LEU:HD11	1:B:234:ILE:HD12	2.03	0.41
1:F:352:CYS:HA	1:F:355:PRO:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ASN:OD1	1:H:91:ASP:N	2.53	0.41
1:D:365:ASN:O	1:D:369:GLN:HG2	2.21	0.40
1:H:28:PRO:O	1:H:308:ARG:NH2	2.54	0.40
1:H:32:SER:HB3	5:H:2001:HOH:O	2.21	0.40
1:B:529:ASP:HB3	5:B:2207:HOH:O	2.21	0.40
1:G:354:PHE:CD2	1:G:402:ILE:HD12	2.56	0.40
1:A:599:HIS:HE1	1:A:651:TRP:CE2	2.39	0.40
1:D:26:VAL:HG11	1:D:124:PRO:HG3	2.03	0.40
1:H:519:GLN:NE2	1:H:521:PRO:O	2.54	0.40
1:D:444:TYR:HB3	1:D:452:PRO:HD3	2.04	0.40
1:E:519:GLN:HG2	5:E:2198:HOH:O	2.21	0.40
1:F:462:ALA:HB1	1:F:532:THR:HG22	2.04	0.40
1:H:77:ARG:NH2	1:H:109:GLU:HG2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/738 (100%)	712 (96%)	26 (4%)	0	100	100
1	B	736/738 (100%)	708 (96%)	28 (4%)	0	100	100
1	C	734/738 (100%)	713 (97%)	21 (3%)	0	100	100
1	D	741/738 (100%)	715 (96%)	26 (4%)	0	100	100
1	E	734/738 (100%)	710 (97%)	23 (3%)	1 (0%)	48	56
1	F	735/738 (100%)	708 (96%)	27 (4%)	0	100	100
1	G	734/738 (100%)	699 (95%)	34 (5%)	1 (0%)	48	56
1	H	735/738 (100%)	699 (95%)	34 (5%)	2 (0%)	36	40
All	All	5887/5904 (100%)	5664 (96%)	219 (4%)	4 (0%)	48	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	521	PRO
1	G	529	ASP
1	H	529	ASP
1	E	529	ASP

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	637/637 (100%)	618 (97%)	19 (3%)	36	45
1	B	637/637 (100%)	617 (97%)	20 (3%)	35	44
1	C	634/637 (100%)	613 (97%)	21 (3%)	33	42
1	D	641/637 (101%)	619 (97%)	22 (3%)	32	40
1	E	630/637 (99%)	610 (97%)	20 (3%)	34	43
1	F	632/637 (99%)	611 (97%)	21 (3%)	33	42
1	G	629/637 (99%)	603 (96%)	26 (4%)	27	33
1	H	634/637 (100%)	611 (96%)	23 (4%)	31	39
All	All	5074/5096 (100%)	4902 (97%)	172 (3%)	33	40

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	A	168	LYS
1	A	172	ILE
1	A	177	GLU
1	A	206	LYS
1	A	209	THR
1	A	215	GLU
1	A	237	PHE
1	A	448	LEU
1	A	456	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	481	LEU
1	A	532	THR
1	A	539	TYR
1	A	559	MET
1	A	573	ILE
1	A	610	LEU
1	A	689	LEU
1	A	692	ASP
1	A	739	LEU
1	B	77	ARG
1	B	101	VAL
1	B	177	GLU
1	B	206	LYS
1	B	237	PHE
1	B	385	TRP
1	B	481	LEU
1	B	486	LYS
1	B	505	GLU
1	B	532	THR
1	B	559[A]	MET
1	B	559[B]	MET
1	B	573	ILE
1	B	596	ASN
1	B	610	LEU
1	B	624	LEU
1	B	689	LEU
1	B	730	LYS
1	B	736	ARG
1	B	739	LEU
1	C	101	VAL
1	C	177	GLU
1	C	185	THR
1	C	206	LYS
1	C	284	GLN
1	C	385	TRP
1	C	416	ILE
1	C	448	LEU
1	C	481	LEU
1	C	504	LYS
1	C	532	THR
1	C	539	TYR
1	C	559	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	564	MET
1	C	573	ILE
1	C	596	ASN
1	C	610	LEU
1	C	624	LEU
1	C	689	LEU
1	C	739	LEU
1	C	744	LYS
1	D	101	VAL
1	D	177	GLU
1	D	237	PHE
1	D	284	GLN
1	D	319	LEU
1	D	385	TRP
1	D	416[A]	ILE
1	D	416[B]	ILE
1	D	479	LYS
1	D	481	LEU
1	D	505	GLU
1	D	532	THR
1	D	558[A]	GLU
1	D	558[B]	GLU
1	D	573	ILE
1	D	633	THR
1	D	689	LEU
1	D	730[A]	LYS
1	D	730[B]	LYS
1	D	736	ARG
1	D	739	LEU
1	D	756	LEU
1	E	77	ARG
1	E	101	VAL
1	E	206	LYS
1	E	209	THR
1	E	284	GLN
1	E	416	ILE
1	E	447	LYS
1	E	448	LEU
1	E	481	LEU
1	E	520	SER
1	E	532	THR
1	E	573	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	604	ILE
1	E	610	LEU
1	E	624	LEU
1	E	678	LYS
1	E	689	LEU
1	E	692	ASP
1	E	695	ASN
1	E	739	LEU
1	F	77	ARG
1	F	101	VAL
1	F	177	GLU
1	F	206	LYS
1	F	209	THR
1	F	215	GLU
1	F	220	GLN
1	F	284	GLN
1	F	433	GLU
1	F	479	LYS
1	F	481	LEU
1	F	539	TYR
1	F	559	MET
1	F	564	MET
1	F	573	ILE
1	F	596	ASN
1	F	610	LEU
1	F	692	ASP
1	F	730	LYS
1	F	739	LEU
1	F	744	LYS
1	G	77	ARG
1	G	101	VAL
1	G	168	LYS
1	G	177	GLU
1	G	209	THR
1	G	220	GLN
1	G	237	PHE
1	G	238	LYS
1	G	277	LYS
1	G	385	TRP
1	G	448	LEU
1	G	456	LYS
1	G	460	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	481	LEU
1	G	504	LYS
1	G	532	THR
1	G	539	TYR
1	G	573	ILE
1	G	604	ILE
1	G	610	LEU
1	G	624	LEU
1	G	649	SER
1	G	689	LEU
1	G	730	LYS
1	G	731	VAL
1	G	739	LEU
1	H	101	VAL
1	H	172	ILE
1	H	185	THR
1	H	206	LYS
1	H	237	PHE
1	H	249	ILE
1	H	319	LEU
1	H	385	TRP
1	H	417	LYS
1	H	448	LEU
1	H	486	LYS
1	H	520	SER
1	H	532	THR
1	H	573	ILE
1	H	596	ASN
1	H	610	LEU
1	H	624	LEU
1	H	633	THR
1	H	691	ILE
1	H	692	ASP
1	H	707	SER
1	H	736	ARG
1	H	744	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	334	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	369	GLN
1	A	398	ASN
1	A	460	ASN
1	B	84	GLN
1	B	398	ASN
1	C	369	GLN
1	C	513	ASN
1	C	616	GLN
1	D	81	GLN
1	D	84	GLN
1	D	158	HIS
1	D	198	ASN
1	D	244	GLN
1	D	616	GLN
1	E	84	GLN
1	E	158	HIS
1	E	246	ASN
1	E	369	GLN
1	E	519	GLN
1	E	616	GLN
1	E	713	HIS
1	F	74	ASN
1	F	103	GLN
1	F	244	GLN
1	F	258	GLN
1	F	334	GLN
1	F	369	GLN
1	F	429	ASN
1	F	460	ASN
1	F	647	GLN
1	F	695	ASN
1	G	59	GLN
1	G	246	ASN
1	G	740	ASN
1	H	246	ASN
1	H	374	ASN
1	H	425	HIS
1	H	500	ASN
1	H	626	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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	A	804	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	C	802	-	5,5,5	0.28	0	5,5,5	0.33	0
4	GOL	D	804	-	5,5,5	0.37	0	5,5,5	0.34	0
4	GOL	B	803	-	5,5,5	0.41	0	5,5,5	0.52	0
4	GOL	D	802	-	5,5,5	0.35	0	5,5,5	0.76	0
4	GOL	A	802	-	5,5,5	0.48	0	5,5,5	0.35	0
4	GOL	C	803	-	5,5,5	0.45	0	5,5,5	0.47	0
3	MVL	F	801	2	14,15,15	1.36	3 (21%)	14,22,22	1.97	4 (28%)
4	GOL	B	805	-	5,5,5	0.55	0	5,5,5	0.98	0
3	MVL	H	801	2	14,15,15	1.53	3 (21%)	14,22,22	2.03	5 (35%)
4	GOL	E	804	-	5,5,5	0.33	0	5,5,5	0.21	0
4	GOL	C	805	-	5,5,5	0.42	0	5,5,5	0.29	0
3	MVL	D	801	2	14,15,15	1.36	2 (14%)	14,22,22	1.71	3 (21%)
4	GOL	D	803	-	5,5,5	0.36	0	5,5,5	0.37	0
3	MVL	E	801	2	14,15,15	1.36	3 (21%)	14,22,22	2.28	5 (35%)
3	MVL	C	801	2	14,15,15	1.39	3 (21%)	14,22,22	2.13	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	802	-	5,5,5	0.39	0	5,5,5	0.34	0
4	GOL	C	804	-	5,5,5	0.40	0	5,5,5	0.35	0
4	GOL	D	805	-	5,5,5	0.30	0	5,5,5	0.49	0
4	GOL	E	802	-	5,5,5	0.35	0	5,5,5	0.27	0
4	GOL	F	802	-	5,5,5	0.40	0	5,5,5	0.31	0
3	MVL	B	801	2	14,15,15	1.47	2 (14%)	14,22,22	2.06	5 (35%)
4	GOL	A	803	-	5,5,5	0.35	0	5,5,5	0.22	0
4	GOL	E	803	-	5,5,5	0.36	0	5,5,5	0.45	0
3	MVL	A	801	2	14,15,15	1.37	2 (14%)	14,22,22	2.05	4 (28%)
3	MVL	G	801	2	14,15,15	1.49	3 (21%)	14,22,22	2.15	5 (35%)
4	GOL	B	804	-	5,5,5	0.48	0	5,5,5	0.41	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	A	804	-	-	2/4/4/4	-
4	GOL	C	802	-	-	4/4/4/4	-
4	GOL	D	804	-	-	1/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
4	GOL	D	802	-	-	4/4/4/4	-
4	GOL	A	802	-	-	4/4/4/4	-
4	GOL	C	803	-	-	2/4/4/4	-
3	MVL	F	801	2	-	1/2/22/22	0/2/2/2
4	GOL	B	805	-	-	2/4/4/4	-
3	MVL	H	801	2	-	0/2/22/22	0/2/2/2
4	GOL	E	804	-	-	2/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
3	MVL	D	801	2	-	0/2/22/22	0/2/2/2
4	GOL	D	803	-	-	3/4/4/4	-
3	MVL	E	801	2	-	0/2/22/22	0/2/2/2
3	MVL	C	801	2	-	0/2/22/22	0/2/2/2
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	C	804	-	-	3/4/4/4	-
4	GOL	D	805	-	-	2/4/4/4	-
4	GOL	E	802	-	-	2/4/4/4	-
4	GOL	F	802	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MVL	B	801	2	-	0/2/22/22	0/2/2/2
4	GOL	A	803	-	-	2/4/4/4	-
4	GOL	E	803	-	-	4/4/4/4	-
3	MVL	A	801	2	-	0/2/22/22	0/2/2/2
3	MVL	G	801	2	-	0/2/22/22	0/2/2/2
4	GOL	B	804	-	-	0/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	MVL	C1-N1	3.51	1.36	1.32
3	H	801	MVL	C1-N1	3.30	1.36	1.32
3	E	801	MVL	C1-N1	3.20	1.36	1.32
3	G	801	MVL	C1-N1	3.03	1.36	1.32
3	F	801	MVL	C1-N1	2.75	1.35	1.32
3	C	801	MVL	C1-N1	2.64	1.35	1.32
3	D	801	MVL	C8-N10	-2.59	1.34	1.38
3	A	801	MVL	C8-N10	-2.59	1.34	1.38
3	G	801	MVL	C8-N10	-2.55	1.34	1.38
3	A	801	MVL	C1-N10	-2.54	1.33	1.36
3	D	801	MVL	C1-N1	2.51	1.35	1.32
3	H	801	MVL	C5-N10	2.49	1.50	1.47
3	G	801	MVL	C1-N10	-2.40	1.33	1.36
3	F	801	MVL	C8-N10	-2.40	1.34	1.38
3	H	801	MVL	C8-N10	-2.29	1.34	1.38
3	C	801	MVL	C8-N10	-2.28	1.34	1.38
3	E	801	MVL	C8-N10	-2.25	1.34	1.38
3	F	801	MVL	C1-N10	-2.23	1.33	1.36
3	E	801	MVL	C1-N10	-2.13	1.33	1.36
3	C	801	MVL	C1-N10	-2.03	1.34	1.36
3	B	801	MVL	C8-C7	2.02	1.39	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	801	MVL	N10-C1-N1	-5.26	108.33	111.52
3	F	801	MVL	C4-C3-C2	4.14	116.77	110.22
3	A	801	MVL	N10-C1-N1	-4.13	109.01	111.52
3	G	801	MVL	N10-C1-N1	-4.04	109.07	111.52
3	H	801	MVL	C4-C3-C2	4.01	116.56	110.22
3	C	801	MVL	C4-C3-C2	3.99	116.53	110.22
3	D	801	MVL	C4-C3-C2	3.92	116.42	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	MVL	C4-C3-C2	3.92	116.41	110.22
3	E	801	MVL	C4-C3-C2	3.89	116.37	110.22
3	F	801	MVL	N10-C1-N1	-3.89	109.16	111.52
3	B	801	MVL	N10-C1-N1	-3.83	109.19	111.52
3	G	801	MVL	C4-C3-C2	3.81	116.25	110.22
3	H	801	MVL	N10-C1-N1	-3.58	109.35	111.52
3	C	801	MVL	N10-C1-N1	-3.55	109.37	111.52
3	B	801	MVL	C4-C3-C2	3.42	115.63	110.22
3	D	801	MVL	N10-C1-N1	-3.30	109.52	111.52
3	B	801	MVL	C7-N1-C1	3.29	107.89	104.86
3	E	801	MVL	C7-N1-C1	3.28	107.89	104.86
3	B	801	MVL	C8-C7-N1	-3.11	106.67	110.74
3	A	801	MVL	C7-N1-C1	3.01	107.64	104.86
3	C	801	MVL	C7-N1-C1	3.00	107.62	104.86
3	G	801	MVL	C7-N1-C1	2.98	107.61	104.86
3	G	801	MVL	C8-C7-N1	-2.91	106.93	110.74
3	H	801	MVL	C7-N1-C1	2.86	107.50	104.86
3	C	801	MVL	C8-C7-N1	-2.82	107.05	110.74
3	E	801	MVL	C8-C7-N1	-2.74	107.15	110.74
3	H	801	MVL	C8-C7-N1	-2.72	107.18	110.74
3	F	801	MVL	C7-N1-C1	2.61	107.27	104.86
3	H	801	MVL	C7-C8-N10	2.60	108.08	106.18
3	A	801	MVL	C8-C7-N1	-2.60	107.34	110.74
3	B	801	MVL	C7-C8-N10	2.54	108.04	106.18
3	G	801	MVL	C7-C8-N10	2.46	107.98	106.18
3	C	801	MVL	C3-C4-C5	2.40	115.43	111.37
3	F	801	MVL	C8-C7-N1	-2.32	107.70	110.74
3	C	801	MVL	C7-C8-N10	2.30	107.86	106.18
3	E	801	MVL	O3-C3-C4	-2.13	105.36	110.38
3	D	801	MVL	C8-C7-N1	-2.03	108.08	110.74

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	801	MVL	C4-C5-C6-O6
4	A	802	GOL	O1-C1-C2-C3
4	A	802	GOL	C1-C2-C3-O3
4	A	802	GOL	O2-C2-C3-O3
4	A	804	GOL	O1-C1-C2-C3
4	B	803	GOL	O1-C1-C2-C3
4	C	802	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	802	GOL	1	0
3	F	801	MVL	1	0
4	B	805	GOL	7	0
4	E	804	GOL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	MVL	1	0
3	A	801	MVL	1	0
3	G	801	MVL	1	0
4	B	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	736/738 (99%)	-0.33	0 100 100	14, 22, 33, 41	4 (0%)
1	B	736/738 (99%)	-0.28	1 (0%) 92 92	13, 21, 32, 39	2 (0%)
1	C	736/738 (99%)	-0.30	0 100 100	13, 22, 33, 41	0
1	D	738/738 (100%)	-0.31	2 (0%) 90 90	10, 21, 32, 50	5 (0%)
1	E	736/738 (99%)	-0.24	2 (0%) 90 90	15, 23, 34, 43	0
1	F	735/738 (99%)	-0.06	3 (0%) 88 89	15, 24, 35, 41	2 (0%)
1	G	736/738 (99%)	-0.04	1 (0%) 92 92	17, 24, 35, 49	0
1	H	736/738 (99%)	0.10	0 100 100	16, 25, 35, 47	1 (0%)
All	All	5889/5904 (99%)	-0.18	9 (0%) 91 92	10, 23, 34, 50	14 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	216	ASN	3.5
1	B	216	ASN	2.7
1	D	756	LEU	2.6
1	F	407	TYR	2.3
1	F	441	GLY	2.3
1	E	736	ARG	2.1
1	G	224	ALA	2.1
1	F	489	SER	2.0
1	E	216	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 ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	803	6/6	0.74	0.16	51,51,51,52	0
4	GOL	C	804	6/6	0.77	0.20	64,64,64,65	0
4	GOL	A	802	6/6	0.78	0.21	52,53,53,54	0
4	GOL	B	803	6/6	0.79	0.15	44,45,45,47	0
4	GOL	A	804	6/6	0.81	0.16	45,45,46,47	0
4	GOL	A	803	6/6	0.83	0.17	56,57,57,57	0
4	GOL	D	802	6/6	0.83	0.16	40,41,41,43	0
4	GOL	B	804	6/6	0.84	0.13	37,39,39,40	0
4	GOL	D	803	6/6	0.84	0.15	49,50,51,52	0
4	GOL	B	805	6/6	0.85	0.19	29,31,32,34	0
4	GOL	E	804	6/6	0.85	0.21	40,41,42,44	0
4	GOL	E	802	6/6	0.86	0.14	49,50,51,51	0
4	GOL	E	803	6/6	0.87	0.12	48,48,49,49	0
4	GOL	F	802	6/6	0.88	0.15	53,53,54,54	0
4	GOL	C	805	6/6	0.91	0.09	38,39,40,40	0
4	GOL	D	804	6/6	0.91	0.10	38,40,40,41	0
4	GOL	B	802	6/6	0.91	0.12	39,40,41,41	0
3	MVL	H	801	14/14	0.92	0.10	33,34,34,36	0
4	GOL	C	802	6/6	0.92	0.11	36,37,37,38	0
4	GOL	D	805	6/6	0.93	0.08	32,33,34,34	0
3	MVL	G	801	14/14	0.95	0.07	27,31,32,33	0
3	MVL	B	801	14/14	0.96	0.06	9,14,15,16	0
3	MVL	C	801	14/14	0.96	0.07	17,19,21,22	0
3	MVL	F	801	14/14	0.96	0.07	21,25,29,29	0
3	MVL	D	801	14/14	0.97	0.05	14,17,18,20	0
3	MVL	E	801	14/14	0.97	0.05	13,15,17,18	0
3	MVL	A	801	14/14	0.97	0.06	12,15,16,17	0
2	CA	H	800	1/1	0.98	0.06	33,33,33,33	0
2	CA	C	800	1/1	0.98	0.03	22,22,22,22	0
2	CA	F	800	1/1	0.99	0.02	23,23,23,23	0
2	CA	G	800	1/1	0.99	0.03	28,28,28,28	0
2	CA	B	800	1/1	0.99	0.05	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	800	1/1	0.99	0.07	17,17,17,17	0
2	CA	E	800	1/1	0.99	0.02	18,18,18,18	0
2	CA	A	800	1/1	1.00	0.03	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.