wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2024 – 10:45 pm BST

PDB ID	:	2WZS
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 wwPDB X-ray Structure Validation Summary 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:

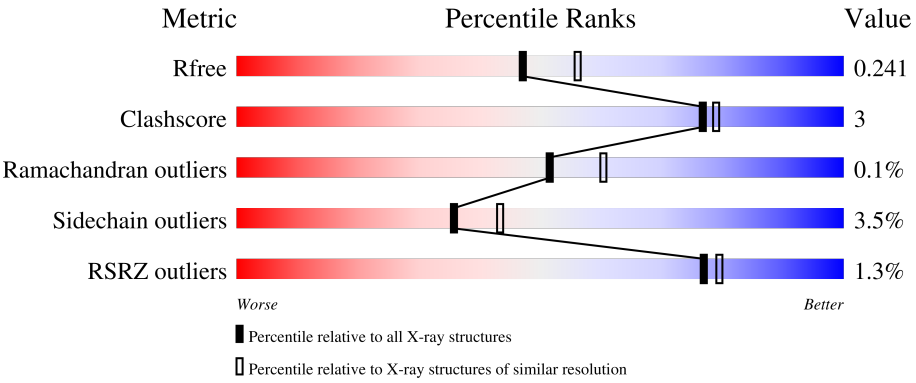
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 <=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	93% 6% •
1	B	738	92% 7% •
1	C	738	91% 7% •
1	D	738	94% 6%

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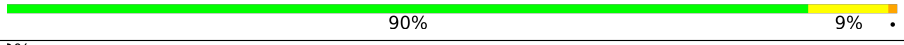
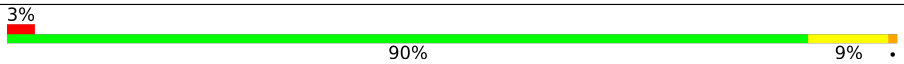
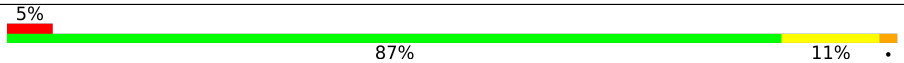
Mol	Chain	Length	Quality of chain
1	E	738	
1	F	738	
1	G	738	
1	H	738	

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 (i)

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 (three-letter code: 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		

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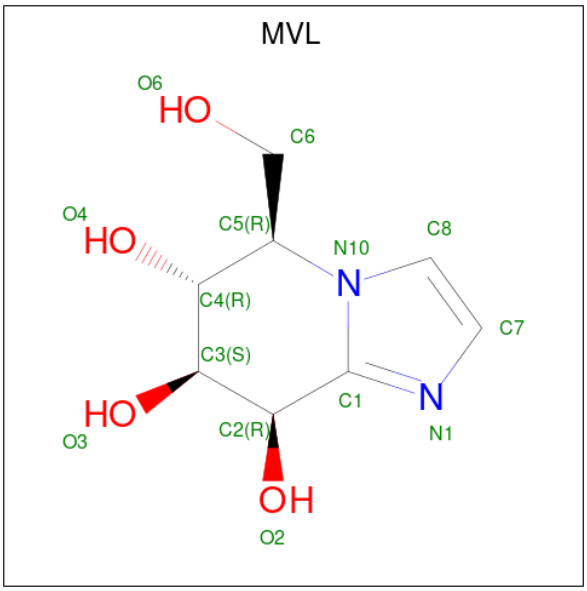
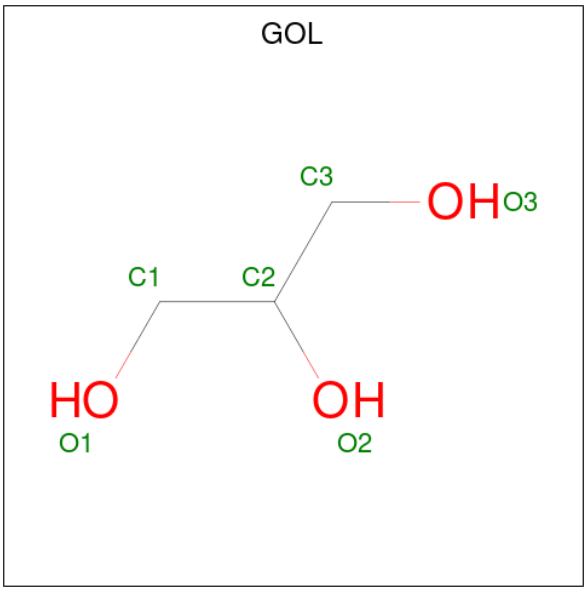
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 2 4	0	0
3	B	1	Total C N O 14 8 2 4	0	0
3	C	1	Total C N O 14 8 2 4	0	0
3	D	1	Total C N O 14 8 2 4	0	0
3	E	1	Total C N O 14 8 2 4	0	0
3	F	1	Total C N O 14 8 2 4	0	0
3	G	1	Total C N O 14 8 2 4	0	0
3	H	1	Total C N O 14 8 2 4	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	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
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	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

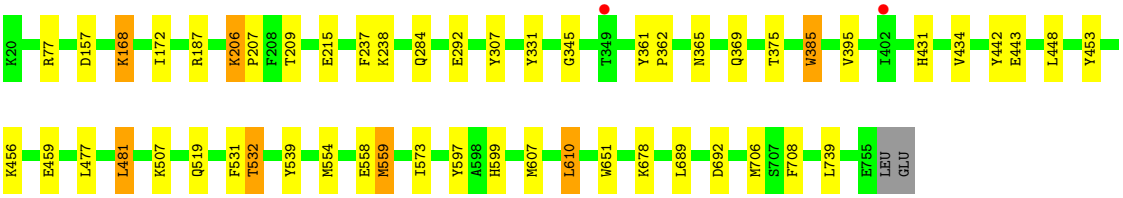
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	349	Total O 349 349	0	0
5	B	320	Total O 320 320	0	0
5	C	279	Total O 279 279	0	0
5	D	323	Total O 323 323	0	0
5	E	261	Total O 261 261	0	0
5	F	179	Total O 179 179	0	0
5	G	87	Total O 87 87	0	0
5	H	70	Total O 70 70	0	0

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.

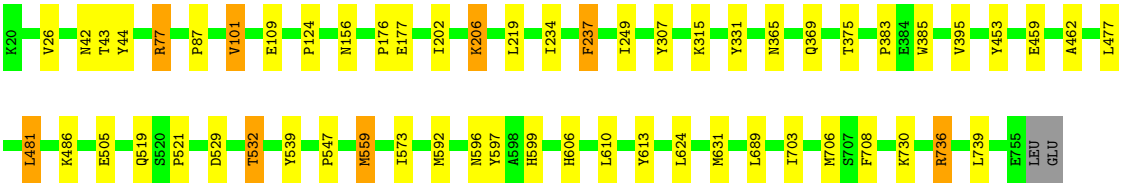
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain A:



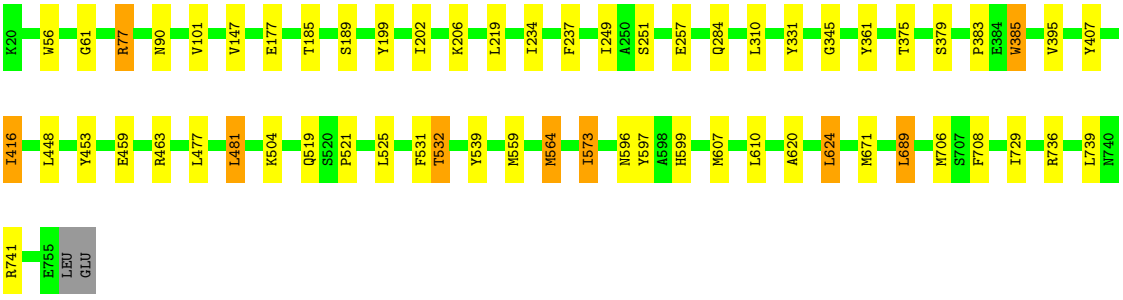
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain B:



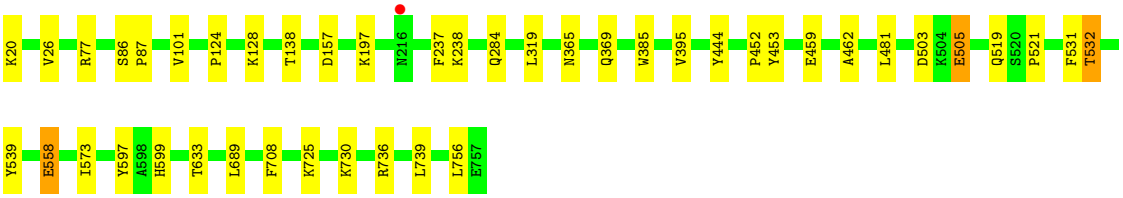
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain C:



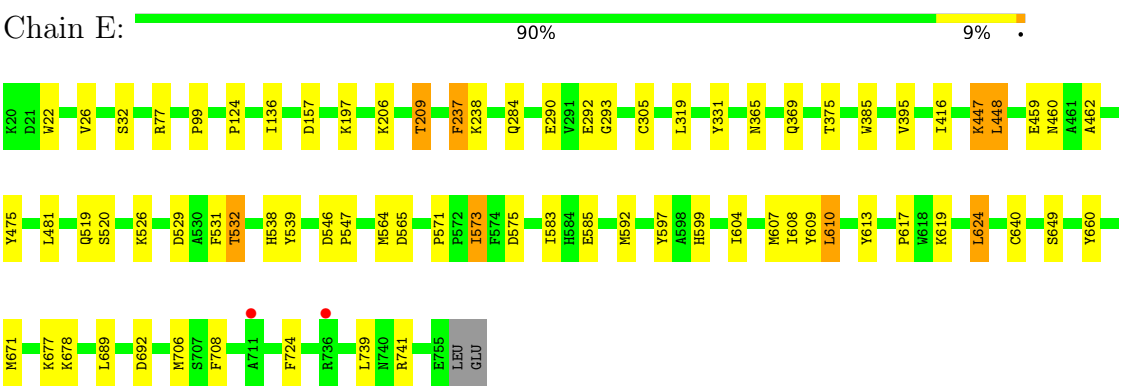
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain D:



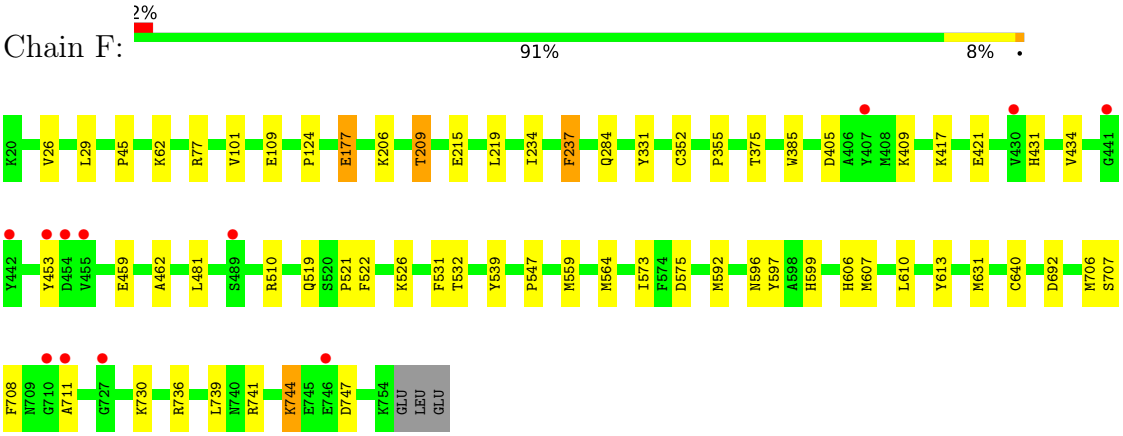
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain E:



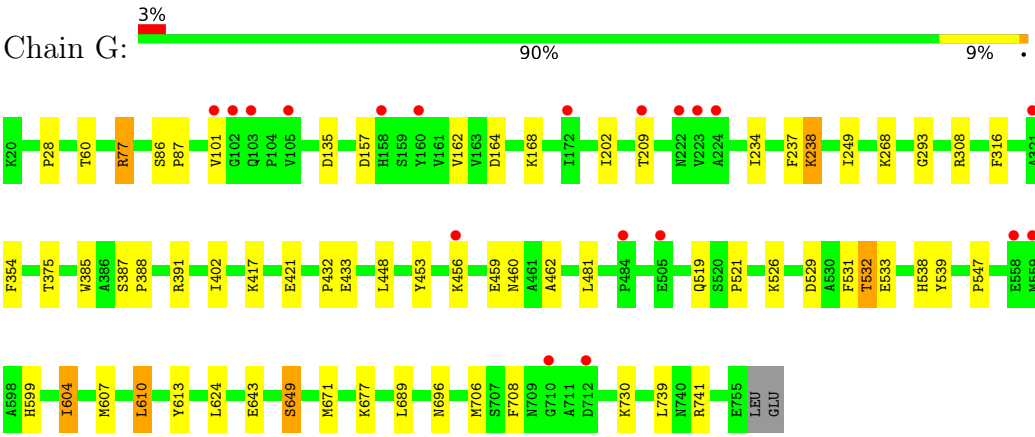
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain F:



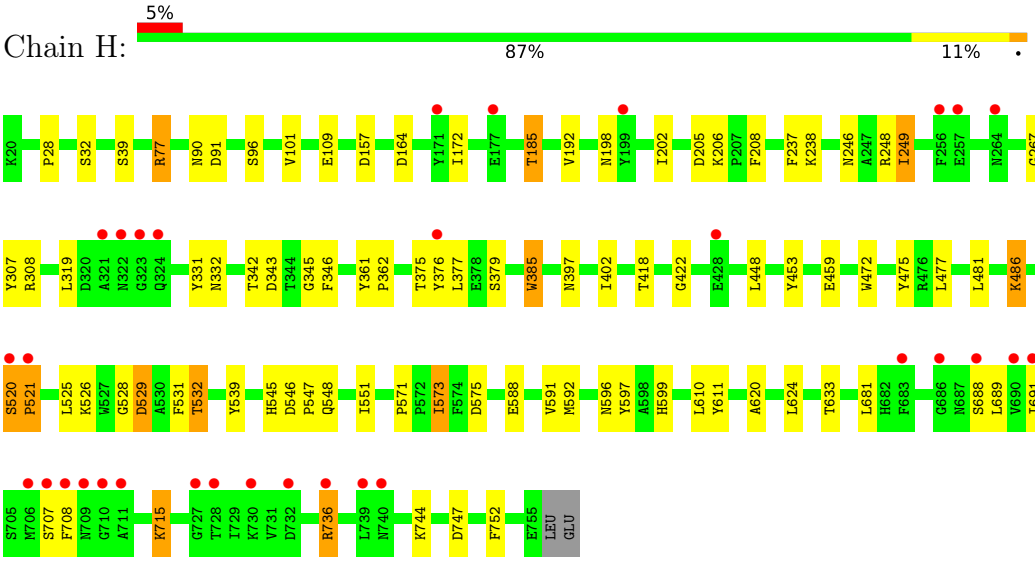
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain G:



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

Chain H:


5%
87%
11%
K20 P28 S32 S39 R77 N90 D91 S96 V101 E109 D157 D164 Y171 I172 E177 T185 V192 N198 Y199 I202 D205 K206 P207 F208 F237 K238 N246 A247 R248 I249 F256 E257 N264 G267 K268 G293
Y307 R308 L319 D320 A321 N322 G323 Q324 Y331 N332 T342 D343 T344 G345 F346 Y361 P362 T375 Y376 L377 E378 S379 W385 N397 I402 T418 G422 E428 L448 Y453 E459 W472 Y475 R476 L477 L481 K486 K504 F518 Q519
S520 P521 L525 K526 W527 G528 D529 A530 F531 T532 Y539 H545 D546 P547 Q548 I551 P571 P572 I573 F574 D575 E588 V591 M592 N596 Y597 A598 H599 L610 Y611 A620 L624 T633 L681 H682 F683 C686 N687 S688 L689 V690 I691 D692 A693 D704
S705 M706 S707 F708 N709 G710 A711 K715 G727 T728 I729 K730 V731 D732 R736 L739 N740 K744 D747 F752 E755 LEU GLU

4 Data and refinement statistics (i)

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 45.40 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (218.22-2.25) 100.0 (45.40-2.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.33 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[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: 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	0.49	0/6175	0.58	0/8376
1	B	0.47	0/6167	0.57	0/8364
1	C	0.46	0/6146	0.57	0/8338
1	D	0.47	0/6213	0.57	0/8429
1	E	0.50	0/6131	0.58	0/8320
1	F	0.52	0/6142	0.58	0/8334
1	G	0.54	0/6124	0.57	1/8314 (0.0%)
1	H	0.56	0/6150	0.57	1/8344 (0.0%)
All	All	0.50	0/49248	0.57	2/66819 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	164	ASP	CB-CG-OD1	5.45	123.21	118.30
1	H	689	LEU	CA-CB-CG	5.27	127.42	115.30

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 (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	5982	0	5660	27	0
1	B	5980	0	5658	39	0
1	C	5965	0	5632	32	0
1	D	6015	0	5693	21	0
1	E	5950	0	5611	42	0
1	F	5955	0	5622	36	0
1	G	5943	0	5584	34	0
1	H	5966	0	5630	51	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
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	1	0
5	B	320	0	0	4	0
5	C	279	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	323	0	0	5	0
5	E	261	0	0	6	0
5	F	179	0	0	4	0
5	G	87	0	0	0	0
5	H	70	0	0	3	0
All	All	49858	0	45322	284	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.

The worst 5 of 284 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:H:592[B]:MET:HA	1:H:592[B]:MET:CE	1.75	1.16
1:H:592[B]:MET:HA	1:H:592[B]:MET:HE3	1.35	1.06
1:F:592[B]:MET:HA	1:F:592[B]:MET:HE3	0.99	0.98
1:B:42:ASN:O	4:B:805:GOL:H31	1.68	0.93

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	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%)	51	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	735/738 (100%)	708 (96%)	27 (4%)	0	100 100
1	G	734/738 (100%)	699 (95%)	34 (5%)	1 (0%)	51 60
1	H	735/738 (100%)	699 (95%)	34 (5%)	2 (0%)	41 46
All	All	5887/5904 (100%)	5664 (96%)	219 (4%)	4 (0%)	51 60

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 (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	637/637 (100%)	615 (96%)	22 (4%)	36 43
1	B	637/637 (100%)	615 (96%)	22 (4%)	36 43
1	C	634/637 (100%)	610 (96%)	24 (4%)	33 39
1	D	641/637 (101%)	620 (97%)	21 (3%)	38 46
1	E	630/637 (99%)	608 (96%)	22 (4%)	36 43
1	F	632/637 (99%)	612 (97%)	20 (3%)	39 47
1	G	629/637 (99%)	607 (96%)	22 (4%)	36 43
1	H	634/637 (100%)	605 (95%)	29 (5%)	27 30
All	All	5074/5096 (100%)	4892 (96%)	182 (4%)	36 42

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	215	GLU
1	G	532	THR

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Mol	Chain	Res	Type
1	F	481	LEU
1	F	744	LYS
1	G	708	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	713	HIS
1	F	74	ASN
1	G	548	GLN
1	G	740	ASN
1	H	398	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 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	802	-	5,5,5	0.47	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	D	802	-	5,5,5	0.35	0	5,5,5	0.71	0
4	GOL	F	802	-	5,5,5	0.39	0	5,5,5	0.27	0
4	GOL	B	804	-	5,5,5	0.47	0	5,5,5	0.41	0
4	GOL	D	804	-	5,5,5	0.36	0	5,5,5	0.31	0
4	GOL	A	803	-	5,5,5	0.35	0	5,5,5	0.19	0
4	GOL	A	804	-	5,5,5	0.36	0	5,5,5	0.28	0
3	MVL	E	801	2	13,15,15	0.76	0	11,22,22	1.53	2 (18%)
4	GOL	B	805	-	5,5,5	0.53	0	5,5,5	0.94	0
3	MVL	C	801	2	13,15,15	0.93	1 (7%)	11,22,22	1.76	3 (27%)
4	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	C	805	-	5,5,5	0.41	0	5,5,5	0.25	0
4	GOL	E	802	-	5,5,5	0.35	0	5,5,5	0.24	0
3	MVL	D	801	2	13,15,15	0.94	0	11,22,22	1.46	1 (9%)
4	GOL	C	802	-	5,5,5	0.28	0	5,5,5	0.30	0
3	MVL	F	801	2	13,15,15	0.84	0	11,22,22	1.61	1 (9%)
4	GOL	E	803	-	5,5,5	0.35	0	5,5,5	0.42	0
4	GOL	C	803	-	5,5,5	0.43	0	5,5,5	0.46	0
4	GOL	D	803	-	5,5,5	0.35	0	5,5,5	0.34	0
3	MVL	A	801	2	13,15,15	0.86	0	11,22,22	1.48	1 (9%)
3	MVL	B	801	2	13,15,15	0.74	0	11,22,22	1.38	1 (9%)
3	MVL	G	801	2	13,15,15	0.84	0	11,22,22	1.69	2 (18%)
4	GOL	C	804	-	5,5,5	0.40	0	5,5,5	0.30	0
4	GOL	D	805	-	5,5,5	0.29	0	5,5,5	0.45	0
3	MVL	H	801	2	13,15,15	0.81	0	11,22,22	1.57	1 (9%)
4	GOL	E	804	-	5,5,5	0.33	0	5,5,5	0.22	0
4	GOL	B	803	-	5,5,5	0.41	0	5,5,5	0.48	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	802	-	-	4/4/4/4	-
4	GOL	D	802	-	-	4/4/4/4	-
4	GOL	F	802	-	-	0/4/4/4	-
4	GOL	B	804	-	-	1/4/4/4	-
4	GOL	D	804	-	-	2/4/4/4	-
4	GOL	A	803	-	-	3/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MVL	E	801	2	-	0/2/22/22	0/1/2/2
4	GOL	B	805	-	-	2/4/4/4	-
3	MVL	C	801	2	-	0/2/22/22	0/1/2/2
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	C	805	-	-	0/4/4/4	-
4	GOL	E	802	-	-	2/4/4/4	-
3	MVL	D	801	2	-	0/2/22/22	0/1/2/2
4	GOL	C	802	-	-	3/4/4/4	-
3	MVL	F	801	2	-	1/2/22/22	0/1/2/2
4	GOL	E	803	-	-	4/4/4/4	-
4	GOL	C	803	-	-	2/4/4/4	-
4	GOL	D	803	-	-	3/4/4/4	-
3	MVL	A	801	2	-	0/2/22/22	0/1/2/2
3	MVL	B	801	2	-	0/2/22/22	0/1/2/2
3	MVL	G	801	2	-	0/2/22/22	0/1/2/2
4	GOL	C	804	-	-	4/4/4/4	-
4	GOL	D	805	-	-	2/4/4/4	-
3	MVL	H	801	2	-	0/2/22/22	0/1/2/2
4	GOL	E	804	-	-	3/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	MVL	C1-C2	-2.01	1.48	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	801	MVL	C4-C3-C2	4.30	116.77	110.24
3	H	801	MVL	C4-C3-C2	4.16	116.56	110.24
3	C	801	MVL	C4-C3-C2	4.14	116.53	110.24
3	D	801	MVL	C4-C3-C2	4.07	116.42	110.24
3	A	801	MVL	C4-C3-C2	4.06	116.41	110.24

There are no chirality outliers.

5 of 44 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

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
4	B	804	GOL	3	0
4	B	805	GOL	7	0
3	D	801	MVL	1	0
3	F	801	MVL	1	0
3	A	801	MVL	1	0
3	G	801	MVL	1	0
4	E	804	GOL	2	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	736/738 (99%)	-0.15	2 (0%) 94 94	14, 22, 33, 41	0
1	B	736/738 (99%)	-0.19	0 100 100	13, 21, 32, 39	0
1	C	736/738 (99%)	-0.25	0 100 100	13, 22, 33, 41	0
1	D	738/738 (100%)	-0.19	1 (0%) 95 96	13, 21, 32, 50	0
1	E	736/738 (99%)	-0.20	2 (0%) 94 94	15, 23, 34, 43	0
1	F	735/738 (99%)	-0.09	12 (1%) 72 74	15, 24, 35, 41	0
1	G	736/738 (99%)	-0.05	19 (2%) 56 59	17, 24, 35, 49	0
1	H	736/738 (99%)	0.20	39 (5%) 26 29	17, 25, 35, 47	0
All	All	5889/5904 (99%)	-0.12	75 (1%) 77 79	13, 23, 34, 50	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	710	GLY	5.3
1	H	321	ALA	4.1
1	H	520	SER	3.6
1	H	739	LEU	3.5
1	H	711	ALA	3.4

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

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

6.3 Carbohydrates

There are no 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	803	6/6	0.72	0.19	56,57,57,57	0
4	GOL	C	803	6/6	0.72	0.20	51,51,51,52	0
4	GOL	B	803	6/6	0.77	0.17	44,45,45,47	0
4	GOL	A	804	6/6	0.80	0.17	45,45,46,47	0
4	GOL	C	804	6/6	0.80	0.19	64,64,64,65	0
4	GOL	D	802	6/6	0.81	0.20	40,41,41,43	0
4	GOL	D	803	6/6	0.83	0.20	49,50,51,52	0
4	GOL	B	804	6/6	0.84	0.17	37,39,39,40	0
4	GOL	E	803	6/6	0.84	0.14	48,48,49,49	0
4	GOL	B	805	6/6	0.86	0.26	29,31,32,34	0
4	GOL	E	804	6/6	0.87	0.32	40,41,42,44	0
4	GOL	F	802	6/6	0.87	0.17	53,53,54,54	0
3	MVL	H	801	14/14	0.89	0.18	33,34,34,36	0
4	GOL	C	805	6/6	0.89	0.13	38,39,40,40	0
4	GOL	E	802	6/6	0.89	0.17	49,50,51,51	0
4	GOL	C	802	6/6	0.90	0.16	36,37,37,38	0
4	GOL	B	802	6/6	0.90	0.16	39,40,41,41	0
4	GOL	A	802	6/6	0.91	0.23	52,53,53,54	0
4	GOL	D	804	6/6	0.91	0.16	38,40,40,41	0
3	MVL	F	801	14/14	0.95	0.11	21,25,29,29	0
4	GOL	D	805	6/6	0.95	0.08	32,33,34,34	0
3	MVL	G	801	14/14	0.96	0.12	27,31,32,33	0
3	MVL	C	801	14/14	0.96	0.12	17,19,21,22	0
3	MVL	B	801	14/14	0.96	0.17	9,14,15,16	0
3	MVL	D	801	14/14	0.97	0.14	14,17,18,20	0
3	MVL	E	801	14/14	0.97	0.12	13,15,17,18	0
3	MVL	A	801	14/14	0.97	0.12	12,15,16,17	0
2	CA	H	800	1/1	0.98	0.18	33,33,33,33	0
2	CA	F	800	1/1	0.98	0.11	23,23,23,23	0
2	CA	B	800	1/1	0.99	0.19	17,17,17,17	0
2	CA	E	800	1/1	0.99	0.10	18,18,18,18	0
2	CA	A	800	1/1	0.99	0.13	20,20,20,20	0
2	CA	G	800	1/1	0.99	0.13	28,28,28,28	0
2	CA	D	800	1/1	1.00	0.18	17,17,17,17	0
2	CA	C	800	1/1	1.00	0.13	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.