Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 01:34 PM EDT

PDB ID	:	2ZWS
Title	:	Crystal Structure Analysis of neutral ceramidase from Pseudomonas aeruginosa
Authors	:	Kakuta, Y.; Okino, N.; Inoue, T.; Okano, H.; Ito, M.
Deposited on	:	2008-12-17
Resolution	:	1.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

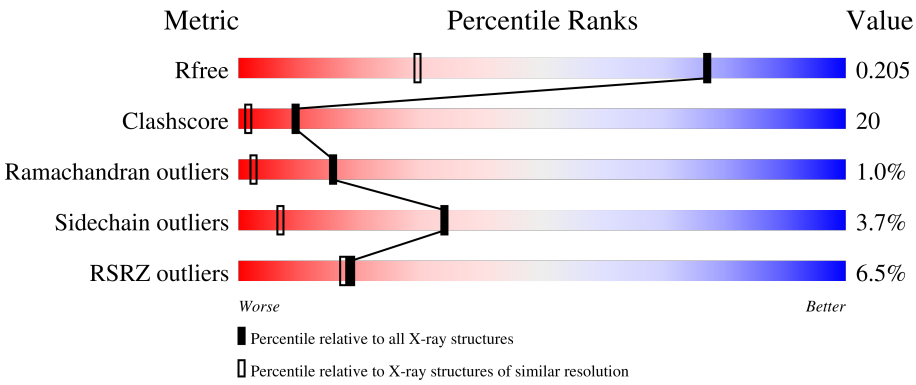
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

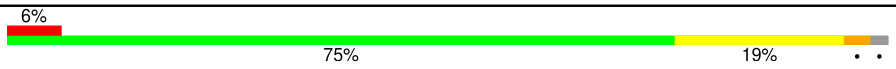
The reported resolution of this entry is 1.40 Å.

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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	646	

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	FMT	A	650	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	653	-	-	-	X
6	GOL	A	654	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6020 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 Neutral ceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	630	5236	3331	906	976	23	0	60	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	SER	ASN	SEE REMARK 999	UNP Q9I596
A	172	ALA	VAL	SEE REMARK 999	UNP Q9I596
A	574	VAL	GLU	SEE REMARK 999	UNP Q9I596

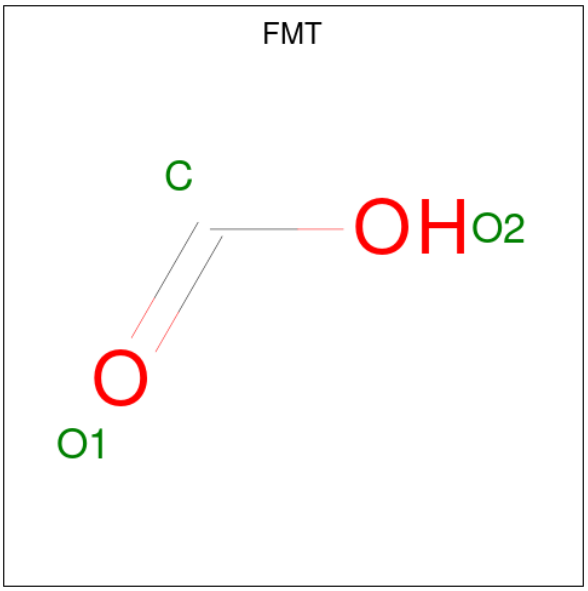
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

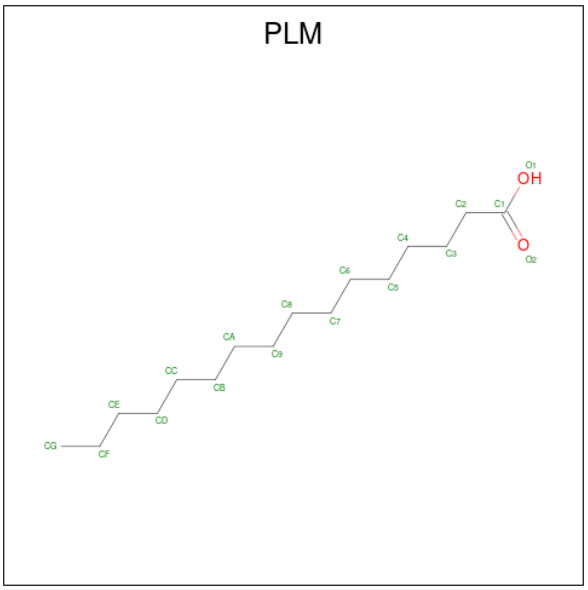
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



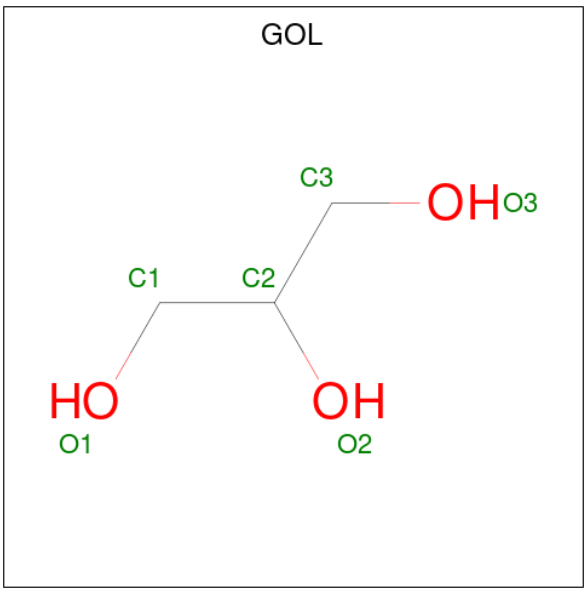
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	3	1	2	0	0
			Total	C	O		
4	A	1	3	1	2	0	0
			Total	C	O		
4	A	1	3	1	2	0	0

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	18	16	2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 7 is water.

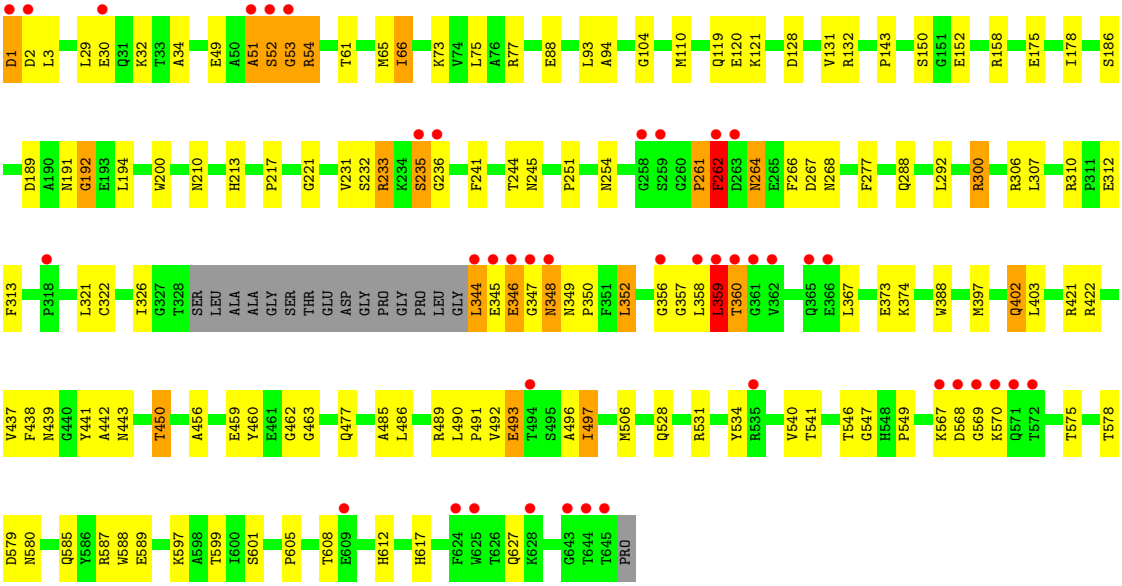
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	653	653	653	0	0

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: Neutral ceramidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.18Å 59.29Å 70.98Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	22.60 – 1.40 22.60 – 1.40	Depositor EDS
% Data completeness (in resolution range)	90.7 (22.60-1.40) 90.7 (22.60-1.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.206 0.173 , 0.205	Depositor DCC
R_{free} test set	6630 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6020	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, MG, GOL, PLM, ZN

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	0.61	0/5496	0.80	9/7449 (0.1%)

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	A	1	7

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	497	ILE	N-CA-C	-8.28	88.64	111.00
1	A	262	PHE	N-CA-C	8.07	132.78	111.00
1	A	233	ARG	N-CA-C	6.78	129.30	111.00
1	A	261	PRO	N-CA-C	6.71	129.55	112.10
1	A	51	ALA	N-CA-C	6.64	128.93	111.00
1	A	450	THR	OG1-CB-CG2	6.18	124.22	110.00
1	A	261	PRO	C-N-CA	5.74	136.05	121.70
1	A	450	THR	N-CA-CB	-5.50	99.86	110.30
1	A	132	ARG	NE-CZ-NH2	-5.13	117.74	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	450	THR	CB

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ASN	Peptide
1	A	232	SER	Peptide
1	A	235[B]	SER	Peptide
1	A	261	PRO	Peptide
1	A	496	ALA	Peptide
1	A	51	ALA	Peptide
1	A	53	GLY	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	5236	0	5240	211	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	9	0	3	2	0
5	A	18	0	31	3	0
6	A	102	0	136	6	0
7	A	653	0	0	23	0
All	All	6020	0	5410	212	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 20.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73[A]:LYS:HE2	1:A:77[A]:ARG:NH1	1.34	1.43
1:A:344:LEU:N	1:A:346:GLU:HG3	1.29	1.39
1:A:344:LEU:C	1:A:346:GLU:HG2	1.47	1.35
1:A:110[B]:MET:SD	1:A:326:ILE:HD11	1.67	1.32
1:A:345:GLU:N	1:A:346:GLU:CG	1.97	1.27
1:A:73[A]:LYS:CE	1:A:77[A]:ARG:HH12	1.46	1.26
1:A:344:LEU:C	1:A:346:GLU:CG	2.08	1.20
1:A:346:GLU:HB2	1:A:347:GLY:O	1.41	1.20
1:A:346:GLU:HB3	1:A:347:GLY:HA3	1.22	1.19
1:A:346:GLU:HB2	1:A:347:GLY:C	1.65	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:CB	1:A:347:GLY:HA3	1.74	1.14
1:A:346:GLU:CB	1:A:347:GLY:CA	2.26	1.12
1:A:344:LEU:N	1:A:346:GLU:CG	2.10	1.12
1:A:569:GLY:HA3	1:A:570:LYS:HB2	1.29	1.11
1:A:1:ASP:HB3	1:A:2:ASP:HA	1.27	1.11
1:A:346:GLU:HB2	1:A:347:GLY:CA	1.81	1.10
1:A:344:LEU:CA	1:A:346:GLU:HG3	1.80	1.10
1:A:345:GLU:N	1:A:346:GLU:HG2	1.64	1.09
1:A:489[A]:ARG:O	1:A:490[A]:LEU:HB2	1.48	1.05
1:A:345:GLU:N	1:A:346:GLU:CB	2.20	1.04
1:A:345:GLU:N	1:A:347:GLY:O	1.90	1.04
1:A:587[B]:ARG:HH11	1:A:587[B]:ARG:HG3	1.21	1.03
1:A:346:GLU:CB	1:A:347:GLY:O	2.10	0.99
1:A:568:ASP:HB2	1:A:569:GLY:HA2	1.41	0.99
1:A:348:ASN:HD22	1:A:349:ASN:HA	1.25	0.98
1:A:345:GLU:N	1:A:346:GLU:HB2	1.79	0.97
1:A:110[B]:MET:SD	1:A:326:ILE:CD1	2.52	0.97
1:A:73[A]:LYS:CE	1:A:77[A]:ARG:NH1	2.14	0.95
1:A:49:GLU:HB3	1:A:52:SER:CB	1.97	0.94
1:A:345:GLU:H	1:A:346:GLU:HB2	1.32	0.94
1:A:73[A]:LYS:HE2	1:A:77[A]:ARG:CZ	1.96	0.93
1:A:1:ASP:CB	1:A:2:ASP:HA	1.95	0.92
1:A:241:PHE:H	4:A:650:FMT:H	1.34	0.92
1:A:402:GLN:HE21	1:A:402:GLN:H	1.17	0.92
1:A:585:GLN:HE22	1:A:587[B]:ARG:HH22	1.17	0.91
1:A:491:PRO:HB3	5:A:652:PLM:H42	1.54	0.89
1:A:373:GLU:HG3	1:A:456:ALA:HA	1.55	0.89
1:A:310:ARG:H	1:A:477:GLN:HE22	1.18	0.87
1:A:175[A]:GLU:OE2	7:A:939:HOH:O	1.92	0.87
1:A:158[B]:ARG:HA	1:A:178:ILE:HD11	1.58	0.85
1:A:546[A]:THR:HG22	1:A:547:GLY:H	1.40	0.85
1:A:52:SER:HB3	1:A:53:GLY:HA2	1.60	0.84
1:A:49:GLU:HB3	1:A:52:SER:HB3	1.58	0.83
1:A:1:ASP:HB3	1:A:2:ASP:CA	2.09	0.83
1:A:578[A]:THR:CG2	7:A:775:HOH:O	2.25	0.82
1:A:373:GLU:CG	1:A:456:ALA:HA	2.10	0.82
1:A:568:ASP:HB2	1:A:569:GLY:CA	2.08	0.82
1:A:321:LEU:N	7:A:932:HOH:O	2.13	0.81
1:A:348:ASN:ND2	1:A:349:ASN:HA	1.95	0.80
1:A:344:LEU:C	1:A:345:GLU:HG2	2.01	0.80
1:A:585:GLN:HE21	1:A:587[B]:ARG:HH12	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158[A]:ARG:HA	1:A:178:ILE:HD11	1.66	0.77
1:A:344:LEU:CA	1:A:346:GLU:CG	2.49	0.77
1:A:345:GLU:CA	1:A:346:GLU:CB	2.62	0.77
1:A:568:ASP:CB	1:A:569:GLY:HA2	2.14	0.76
1:A:52:SER:HB3	1:A:53:GLY:CA	2.16	0.76
1:A:359[A]:LEU:HB3	1:A:360:THR:HA	1.67	0.75
1:A:66[A]:ILE:HD11	1:A:441:TYR:O	1.85	0.75
1:A:493:GLU:OE2	7:A:973:HOH:O	2.05	0.74
1:A:73[A]:LYS:HE3	1:A:77[A]:ARG:HH12	1.47	0.74
1:A:344:LEU:C	1:A:346:GLU:HG3	1.94	0.74
1:A:359[B]:LEU:HB3	1:A:360:THR:HA	1.68	0.74
1:A:345:GLU:N	1:A:346:GLU:HG3	1.99	0.73
1:A:587[B]:ARG:HH11	1:A:587[B]:ARG:CG	2.00	0.73
1:A:75[B]:LEU:CD2	1:A:88[B]:GLU:HG3	2.18	0.73
1:A:585:GLN:NE2	1:A:587[B]:ARG:HH22	1.85	0.73
1:A:485:ALA:O	1:A:489[A]:ARG:O	2.07	0.73
1:A:310:ARG:H	1:A:477:GLN:NE2	1.87	0.72
1:A:73[A]:LYS:HE2	1:A:77[A]:ARG:HH12	0.93	0.71
1:A:29:LEU:HD12	1:A:344:LEU:HA	1.73	0.71
1:A:344:LEU:N	1:A:346:GLU:OE1	2.23	0.71
1:A:587[B]:ARG:NH2	7:A:1137:HOH:O	2.23	0.70
1:A:345:GLU:CA	1:A:346:GLU:HB2	2.20	0.70
1:A:345:GLU:H	1:A:346:GLU:CG	2.04	0.69
1:A:585:GLN:HE21	1:A:587[B]:ARG:NH1	1.90	0.69
1:A:348:ASN:HD22	1:A:349:ASN:CA	2.04	0.69
1:A:569:GLY:CA	1:A:570:LYS:HB2	2.17	0.68
1:A:546[A]:THR:HG21	7:A:678:HOH:O	1.92	0.67
1:A:75[B]:LEU:HD21	1:A:88[B]:GLU:HG3	1.75	0.67
1:A:77[B]:ARG:NH2	7:A:781:HOH:O	2.27	0.67
1:A:49:GLU:HB3	1:A:52:SER:HB2	1.76	0.67
1:A:358:LEU:O	1:A:359[B]:LEU:HB2	1.94	0.67
1:A:546[A]:THR:HG22	1:A:547:GLY:N	2.08	0.66
1:A:605:PRO:O	1:A:608[B]:THR:HG23	1.94	0.66
1:A:569:GLY:HA3	1:A:570:LYS:CB	2.07	0.66
1:A:158[B]:ARG:CA	1:A:178:ILE:HD11	2.26	0.66
1:A:359[A]:LEU:CB	1:A:360:THR:HA	2.24	0.66
1:A:344:LEU:O	1:A:345:GLU:HG2	1.95	0.65
1:A:110[A]:MET:CE	1:A:388:TRP:HE3	2.10	0.65
1:A:52:SER:CB	1:A:53:GLY:HA2	2.21	0.65
1:A:53:GLY:HA2	1:A:54:ARG:HB2	1.79	0.64
1:A:251:PRO:HD2	6:A:658:GOL:H32	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110[A]:MET:HE2	1:A:388:TRP:HE3	1.62	0.64
1:A:587[B]:ARG:HG3	1:A:587[B]:ARG:NH1	2.02	0.64
1:A:345:GLU:H	1:A:347:GLY:C	1.96	0.64
1:A:262:PHE:CD1	1:A:262:PHE:N	2.55	0.64
1:A:66[A]:ILE:CD1	1:A:441:TYR:O	2.45	0.63
1:A:585:GLN:HE22	1:A:587[B]:ARG:NH2	1.92	0.63
1:A:344:LEU:O	1:A:345:GLU:CG	2.47	0.62
1:A:345:GLU:HA	1:A:346:GLU:C	2.19	0.62
1:A:358:LEU:O	1:A:359[A]:LEU:HB2	1.98	0.62
1:A:344:LEU:N	1:A:346:GLU:CD	2.53	0.61
1:A:460:TYR:HH	6:A:656:GOL:C1	2.13	0.61
1:A:585:GLN:NE2	1:A:587[B]:ARG:NH2	2.48	0.61
1:A:612:HIS:HD2	7:A:785:HOH:O	1.83	0.61
1:A:292:LEU:H	1:A:402:GLN:HE22	1.49	0.60
1:A:546[A]:THR:HG23	1:A:617:HIS:NE2	2.15	0.60
1:A:578[A]:THR:HG22	1:A:580:ASN:H	1.67	0.60
1:A:348:ASN:HB2	1:A:350:PRO:HD3	1.84	0.60
1:A:627[B]:GLN:NE2	7:A:1011:HOH:O	2.15	0.60
1:A:344:LEU:O	1:A:346:GLU:HG2	1.97	0.60
1:A:531[B]:ARG:HG2	1:A:534:TYR:CZ	2.37	0.60
1:A:373:GLU:HG3	1:A:456:ALA:CA	2.31	0.59
1:A:346:GLU:CG	1:A:347:GLY:O	2.50	0.59
1:A:345:GLU:H	1:A:346:GLU:CB	1.94	0.57
1:A:30[B]:GLU:O	7:A:817:HOH:O	2.17	0.57
1:A:189:ASP:O	1:A:192:GLY:HA2	2.04	0.57
1:A:75[B]:LEU:HD23	1:A:88[B]:GLU:HG3	1.87	0.56
1:A:34:ALA:HB2	6:A:665:GOL:H2	1.87	0.56
1:A:77[B]:ARG:HG2	1:A:131:VAL:HG21	1.87	0.56
1:A:241:PHE:H	4:A:650:FMT:C	2.11	0.56
1:A:200:TRP:HE1	1:A:439:ASN:ND2	2.04	0.55
1:A:528:GLN:NE2	1:A:541[A]:THR:HG23	2.22	0.55
1:A:110[A]:MET:HE2	1:A:388:TRP:CE3	2.42	0.55
1:A:66[A]:ILE:HD11	1:A:442:ALA:HA	1.88	0.55
1:A:93:LEU:H	1:A:443:ASN:HD21	1.55	0.55
1:A:254:ASN:HD22	1:A:268:ASN:HD22	1.53	0.54
1:A:93:LEU:H	1:A:443:ASN:ND2	2.05	0.54
1:A:300:ARG:CZ	1:A:493:GLU:HG2	2.37	0.54
1:A:568:ASP:CB	1:A:569:GLY:CA	2.78	0.54
1:A:344:LEU:C	1:A:345:GLU:CG	2.75	0.54
1:A:200:TRP:HE1	1:A:439:ASN:HD22	1.55	0.54
1:A:152[A]:GLU:HG2	7:A:1042:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489[A]:ARG:O	1:A:490[A]:LEU:CB	2.26	0.54
1:A:359[A]:LEU:HB3	1:A:360:THR:CA	2.37	0.54
1:A:402:GLN:HE21	1:A:402:GLN:N	1.98	0.54
1:A:402:GLN:H	1:A:402:GLN:NE2	1.98	0.54
1:A:217:PRO:HB2	1:A:221:GLY:HA3	1.90	0.53
1:A:459:GLU:O	1:A:462[A]:GLY:O	2.27	0.52
1:A:345:GLU:HB3	1:A:349:ASN:HB2	1.91	0.52
1:A:120[B]:GLU:HG3	1:A:121:LYS:N	2.25	0.52
1:A:158[A]:ARG:CA	1:A:178:ILE:HD11	2.30	0.52
1:A:359[B]:LEU:HB3	1:A:360:THR:CA	2.39	0.52
1:A:345:GLU:CA	1:A:346:GLU:HG2	2.39	0.52
1:A:345:GLU:HA	1:A:346:GLU:HB2	1.90	0.52
1:A:264:ASN:HD21	1:A:266:PHE:HB2	1.75	0.52
1:A:403[B]:LEU:HD11	1:A:437:VAL:HG23	1.91	0.52
1:A:345:GLU:C	1:A:346:GLU:HG2	2.30	0.51
1:A:29:LEU:HG	1:A:344:LEU:HD13	1.92	0.51
1:A:605:PRO:HD2	1:A:608[B]:THR:HG21	1.93	0.51
1:A:66[A]:ILE:HA	7:A:1241:HOH:O	2.11	0.51
1:A:605:PRO:O	1:A:608[B]:THR:CG2	2.59	0.51
1:A:29:LEU:H	1:A:344:LEU:HD21	1.76	0.51
5:A:652:PLM:H41	7:A:782:HOH:O	2.11	0.50
1:A:578[A]:THR:HG21	7:A:775:HOH:O	2.04	0.50
1:A:1:ASP:CB	1:A:2:ASP:CA	2.78	0.50
1:A:346:GLU:CB	1:A:347:GLY:C	2.49	0.50
1:A:356:GLY:HA3	7:A:829:HOH:O	2.11	0.50
1:A:585:GLN:NE2	1:A:587[B]:ARG:HH12	2.04	0.50
1:A:312[A]:GLU:HG3	1:A:313:PHE:CE1	2.47	0.49
1:A:346:GLU:HG3	1:A:347:GLY:O	2.11	0.49
1:A:359[B]:LEU:CB	1:A:360:THR:HA	2.30	0.49
1:A:34:ALA:CB	6:A:665:GOL:H2	2.42	0.49
1:A:589[A]:GLU:CD	1:A:597[A]:LYS:HE2	2.33	0.49
1:A:73[A]:LYS:HE2	1:A:77[A]:ARG:NH2	2.25	0.49
1:A:506:MET:HE2	6:A:655:GOL:H11	1.95	0.48
1:A:150:SER:H	1:A:288:GLN:HE22	1.62	0.48
1:A:306[A]:ARG:HA	7:A:932:HOH:O	2.12	0.48
1:A:66[A]:ILE:CD1	1:A:94:ALA:HA	2.45	0.47
1:A:374:LYS:HE2	1:A:463[A]:GLY:HA2	1.96	0.47
1:A:578[A]:THR:CG2	1:A:579:ASP:N	2.78	0.46
1:A:307:LEU:N	7:A:932:HOH:O	2.47	0.46
1:A:352:LEU:HD22	1:A:357[B]:GLY:HA3	1.98	0.46
1:A:546[A]:THR:CG2	1:A:617:HIS:NE2	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422[B]:ARG:NH2	7:A:1267:HOH:O	2.45	0.46
1:A:29:LEU:HD22	1:A:348:ASN:HD21	1.80	0.46
1:A:421[B]:ARG:HD3	1:A:438:PHE:HB2	1.99	0.45
1:A:322[B]:CYS:SG	1:A:367:LEU:HD12	2.56	0.45
1:A:77[B]:ARG:HD2	7:A:886:HOH:O	2.16	0.45
1:A:585:GLN:NE2	1:A:587[B]:ARG:NH1	2.62	0.45
1:A:397[B]:MET:SD	1:A:486:LEU:HD12	2.57	0.45
1:A:66[A]:ILE:HD11	1:A:94:ALA:HA	1.98	0.45
1:A:345:GLU:HA	1:A:346:GLU:CB	2.46	0.44
1:A:32:LYS:O	1:A:213:HIS:HD2	2.00	0.44
1:A:497:ILE:HD13	1:A:497:ILE:HA	1.86	0.44
1:A:244:THR:HA	1:A:438:PHE:O	2.17	0.44
1:A:352:LEU:HD22	1:A:357[A]:GLY:HA3	1.98	0.44
1:A:61:THR:OG1	1:A:66[B]:ILE:HD11	2.18	0.44
1:A:492:VAL:O	5:A:652:PLM:HC1	2.18	0.44
1:A:104:GLY:HA3	1:A:119:GLN:HG2	2.00	0.43
1:A:460:TYR:OH	6:A:656:GOL:C1	2.67	0.43
1:A:587[B]:ARG:CG	1:A:587[B]:ARG:NH1	2.66	0.43
1:A:345:GLU:CD	1:A:349:ASN:HD22	2.22	0.43
1:A:597[B]:LYS:NZ	1:A:599:THR:OG1	2.48	0.43
1:A:150:SER:H	1:A:288:GLN:NE2	2.16	0.43
1:A:77[B]:ARG:NH1	1:A:128:ASP:OD1	2.48	0.42
1:A:264:ASN:ND2	1:A:267:ASP:H	2.16	0.42
1:A:541[A]:THR:HG21	7:A:1201:HOH:O	2.20	0.42
1:A:346:GLU:HB3	1:A:347:GLY:CA	2.06	0.42
1:A:186[A]:SER:HB2	1:A:194:LEU:CD1	2.50	0.42
1:A:549:PRO:HD3	1:A:588:TRP:CD1	2.54	0.42
1:A:3:LEU:HD12	1:A:143:PRO:HB2	2.01	0.42
1:A:54:ARG:NH1	7:A:909:HOH:O	2.53	0.42
1:A:531[A]:ARG:NH1	7:A:830:HOH:O	2.52	0.41
1:A:29:LEU:H	1:A:344:LEU:CD2	2.32	0.41
1:A:235[A]:SER:HA	1:A:236[A]:GLY:HA2	1.82	0.41
1:A:347:GLY:H	1:A:348:ASN:C	2.23	0.41
1:A:120[B]:GLU:HG3	1:A:121:LYS:H	1.86	0.41
1:A:540:VAL:O	1:A:601:SER:HA	2.21	0.41
1:A:300:ARG:HD2	7:A:749:HOH:O	2.21	0.40
1:A:300:ARG:NH1	1:A:493:GLU:HG2	2.35	0.40
1:A:231:VAL:HG21	1:A:277:PHE:CZ	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	686/646 (106%)	644 (94%)	35 (5%)	7 (1%)	15 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ARG
1	A	262	PHE
1	A	192	GLY
1	A	54	ARG
1	A	359[A]	LEU
1	A	359[B]	LEU
1	A	52	SER

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	565/520 (109%)	543 (96%)	22 (4%)	32 6

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	65	MET
1	A	66[A]	ILE
1	A	66[B]	ILE

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	245	ASN
1	A	262	PHE
1	A	264	ASN
1	A	300	ARG
1	A	344	LEU
1	A	346	GLU
1	A	348	ASN
1	A	352	LEU
1	A	359[A]	LEU
1	A	359[B]	LEU
1	A	360	THR
1	A	402	GLN
1	A	450	THR
1	A	493	GLU
1	A	567	LYS
1	A	575[A]	THR
1	A	575[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	112	ASN
1	A	119	GLN
1	A	124	ASN
1	A	138	GLN
1	A	181	GLN
1	A	210	ASN
1	A	213	HIS
1	A	264	ASN
1	A	268	ASN
1	A	288	GLN
1	A	348	ASN
1	A	365	GLN
1	A	382	ASN
1	A	402	GLN
1	A	439	ASN
1	A	443	ASN
1	A	477	GLN
1	A	585	GLN
1	A	612	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
6	GOL	A	655	-	5,5,5	0.33	0	5,5,5	0.68	0
4	FMT	A	650	-	2,2,2	0.78	0	1,1,1	0.44	0
6	GOL	A	665	-	5,5,5	0.30	0	5,5,5	0.49	0
5	PLM	A	652	-	17,17,17	0.50	0	17,17,17	0.98	1 (5%)
6	GOL	A	664	-	5,5,5	0.54	0	5,5,5	0.61	0
6	GOL	A	656	-	5,5,5	0.42	0	5,5,5	0.31	0
6	GOL	A	662	-	5,5,5	0.31	0	5,5,5	0.58	0
6	GOL	A	658	-	5,5,5	0.53	0	5,5,5	0.36	0
6	GOL	A	653	-	5,5,5	0.36	0	5,5,5	0.31	0
6	GOL	A	668	-	5,5,5	0.18	0	5,5,5	0.49	0
6	GOL	A	667	-	5,5,5	0.32	0	5,5,5	0.40	0
4	FMT	A	649	-	2,2,2	0.67	0	1,1,1	0.24	0
6	GOL	A	657	-	5,5,5	0.67	0	5,5,5	0.73	0
6	GOL	A	666	-	5,5,5	0.39	0	5,5,5	0.28	0
4	FMT	A	651	-	2,2,2	0.68	0	1,1,1	0.10	0
6	GOL	A	660	-	5,5,5	0.38	0	5,5,5	0.30	0
6	GOL	A	659	-	5,5,5	0.31	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	A	661	-	5,5,5	0.40	0	5,5,5	0.11	0
6	GOL	A	669	-	5,5,5	0.30	0	5,5,5	0.54	0
6	GOL	A	663	-	5,5,5	0.40	0	5,5,5	0.26	0
6	GOL	A	654	-	5,5,5	0.34	0	5,5,5	0.25	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
5	PLM	A	652	-	-	10/15/15/15	-
6	GOL	A	660	-	-	2/4/4/4	-
6	GOL	A	655	-	-	2/4/4/4	-
6	GOL	A	667	-	-	0/4/4/4	-
6	GOL	A	657	-	-	0/4/4/4	-
6	GOL	A	659	-	-	2/4/4/4	-
6	GOL	A	664	-	-	4/4/4/4	-
6	GOL	A	666	-	-	2/4/4/4	-
6	GOL	A	661	-	-	0/4/4/4	-
6	GOL	A	669	-	-	0/4/4/4	-
6	GOL	A	656	-	-	2/4/4/4	-
6	GOL	A	662	-	-	2/4/4/4	-
6	GOL	A	663	-	-	2/4/4/4	-
6	GOL	A	665	-	-	2/4/4/4	-
6	GOL	A	654	-	-	2/4/4/4	-
6	GOL	A	658	-	-	2/4/4/4	-
6	GOL	A	653	-	-	0/4/4/4	-
6	GOL	A	668	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	652	PLM	O1-C1-C2	2.08	120.58	114.00

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	654	GOL	O1-C1-C2-O2
6	A	654	GOL	O1-C1-C2-C3
6	A	656	GOL	C1-C2-C3-O3
6	A	658	GOL	O1-C1-C2-O2
6	A	658	GOL	O1-C1-C2-C3
6	A	659	GOL	O1-C1-C2-C3
6	A	662	GOL	C1-C2-C3-O3
6	A	666	GOL	C1-C2-C3-O3
6	A	664	GOL	O1-C1-C2-O2
6	A	665	GOL	O2-C2-C3-O3
6	A	655	GOL	O1-C1-C2-C3
6	A	660	GOL	C1-C2-C3-O3
6	A	663	GOL	O1-C1-C2-C3
6	A	664	GOL	O1-C1-C2-C3
6	A	665	GOL	C1-C2-C3-O3
6	A	655	GOL	O1-C1-C2-O2
6	A	659	GOL	O1-C1-C2-O2
6	A	663	GOL	O1-C1-C2-O2
6	A	666	GOL	O2-C2-C3-O3
5	A	652	PLM	C5-C6-C7-C8
5	A	652	PLM	CA-CB-CC-CD
5	A	652	PLM	C7-C8-C9-CA
5	A	652	PLM	C4-C5-C6-C7
6	A	656	GOL	O2-C2-C3-O3
6	A	662	GOL	O2-C2-C3-O3
5	A	652	PLM	C8-C9-CA-CB
5	A	652	PLM	C9-CA-CB-CC
5	A	652	PLM	CC-CD-CE-CF
6	A	660	GOL	O2-C2-C3-O3
6	A	664	GOL	C1-C2-C3-O3
5	A	652	PLM	O2-C1-C2-C3
5	A	652	PLM	CD-CE-CF-CG
5	A	652	PLM	O1-C1-C2-C3
6	A	664	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	655	GOL	1	0
4	A	650	FMT	2	0
6	A	665	GOL	2	0
5	A	652	PLM	3	0

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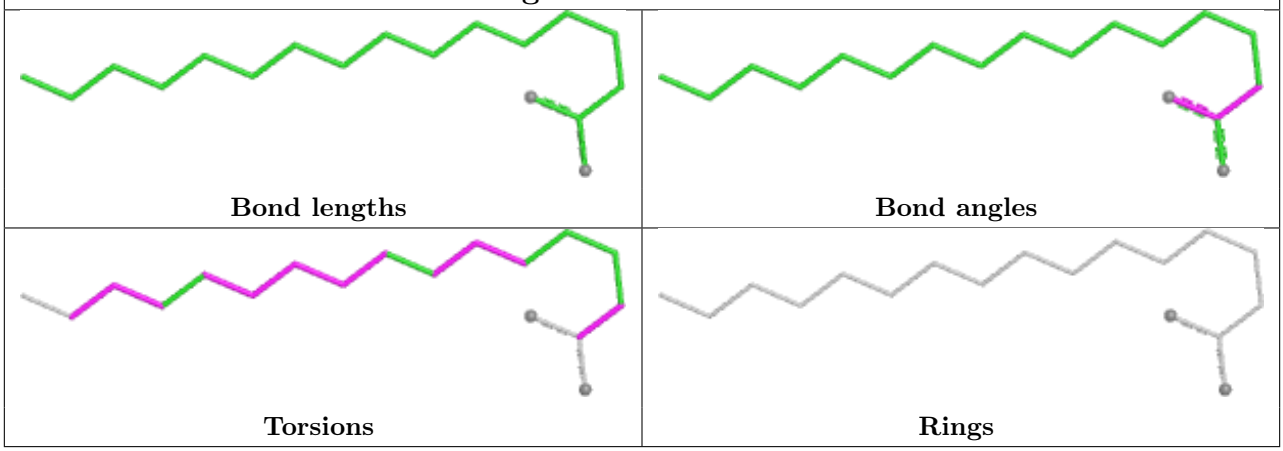
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	656	GOL	2	0
6	A	658	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PLM A 652



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	630/646 (97%)	0.10	41 (6%) 18 17	10, 17, 33, 44	7 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	LEU	13.2
1	A	644	THR	12.9
1	A	360	THR	11.1
1	A	348	ASN	9.6
1	A	645	THR	9.2
1	A	51	ALA	8.7
1	A	1	ASP	8.1
1	A	625[A]	TRP	7.8
1	A	361	GLY	6.9
1	A	262	PHE	6.7
1	A	359[A]	LEU	6.4
1	A	52	SER	6.4
1	A	362	VAL	6.3
1	A	568	ASP	6.2
1	A	2	ASP	6.2
1	A	643	GLY	5.5
1	A	346	GLU	4.8
1	A	570	LYS	4.5
1	A	347	GLY	4.2
1	A	345	GLU	3.7
1	A	235[A]	SER	3.3
1	A	365	GLN	3.3
1	A	358	LEU	3.1
1	A	535	ARG	2.9
1	A	318	PRO	2.9
1	A	494[A]	THR	2.7
1	A	30[A]	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	356	GLY	2.6
1	A	572[A]	THR	2.5
1	A	366	GLU	2.5
1	A	567	LYS	2.4
1	A	236[A]	GLY	2.4
1	A	569	GLY	2.4
1	A	259	SER	2.3
1	A	258	GLY	2.3
1	A	609	GLU	2.3
1	A	263	ASP	2.2
1	A	571	GLN	2.2
1	A	624	PHE	2.2
1	A	53	GLY	2.2
1	A	628[A]	LYS	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, 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
6	GOL	A	664	6/6	0.29	0.27	34,47,48,55	0
6	GOL	A	654	6/6	0.32	0.42	47,50,55,58	0
6	GOL	A	663	6/6	0.47	0.35	46,52,57,59	0
5	PLM	A	652	18/18	0.52	0.38	43,45,48,59	0
6	GOL	A	656	6/6	0.62	0.26	31,36,36,46	0
6	GOL	A	665	6/6	0.63	0.37	38,39,40,41	0
6	GOL	A	659	6/6	0.64	0.18	38,46,52,54	0
6	GOL	A	669	6/6	0.64	0.23	32,35,40,40	0
6	GOL	A	666	6/6	0.65	0.17	41,45,46,49	0

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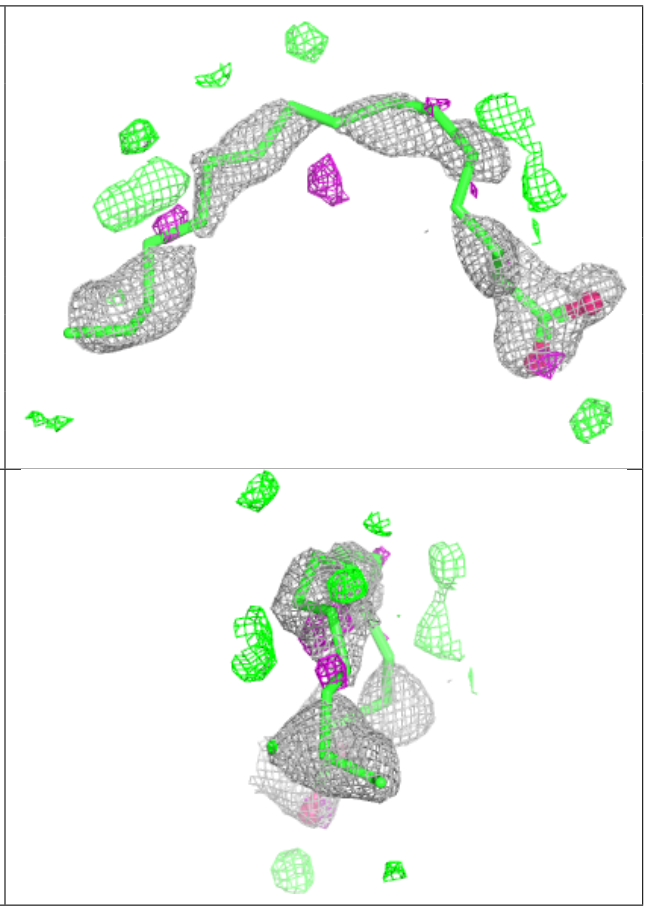
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	660	6/6	0.66	0.23	38,41,43,44	0
6	GOL	A	653	6/6	0.67	0.54	52,54,56,56	0
6	GOL	A	661	6/6	0.69	0.14	49,52,54,56	0
4	FMT	A	651	3/3	0.79	0.12	41,41,41,41	0
6	GOL	A	658	6/6	0.81	0.26	32,37,38,39	0
6	GOL	A	662	6/6	0.85	0.28	31,37,38,41	0
6	GOL	A	657	6/6	0.85	0.22	32,34,36,37	0
4	FMT	A	650	3/3	0.86	0.14	22,22,22,24	0
6	GOL	A	655	6/6	0.94	0.14	22,30,32,32	0
6	GOL	A	668	6/6	0.96	0.10	13,13,14,14	6
6	GOL	A	667	6/6	0.96	0.11	23,31,31,39	6
4	FMT	A	649	3/3	0.98	0.05	13,13,13,14	0
3	MG	A	648	1/1	1.00	0.04	13,13,13,13	0
2	ZN	A	647	1/1	1.00	0.02	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PLM A 652:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.