



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 10:46 am BST

PDB ID : 6COF
Title : AtHNL enantioselectivity mutant At-A9-H7 Apo, Y13C,Y121L,P126F,L128
W,C131T,A209I
Authors : Jones, B.J.; Kazlauskas, R.J.; Desrouleaux, R.
Deposited on : 2018-03-12
Resolution : 1.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

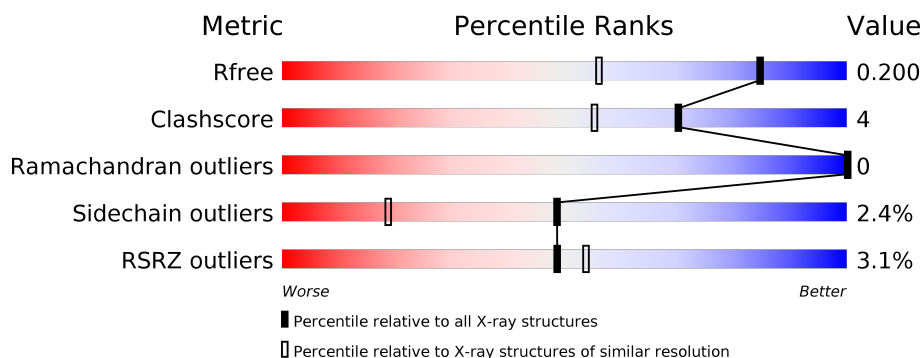
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	260	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	260	<div> <div>3%</div> <div>82%</div> <div>17%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	5	0
			2103	1353	348	386	16			
1	B	259	Total	C	N	O	S	0	7	0
			2111	1358	345	391	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	TYR	engineered mutation	UNP Q9LFT6
A	122	LEU	TYR	engineered mutation	UNP Q9LFT6
A	126	PHE	PRO	engineered mutation	UNP Q9LFT6
A	129	TRP	LEU	engineered mutation	UNP Q9LFT6
A	132	THR	CYS	engineered mutation	UNP Q9LFT6
A	210	ILE	ALA	engineered mutation	UNP Q9LFT6
A	259	GLY	-	expression tag	UNP Q9LFT6
A	260	LEU	-	expression tag	UNP Q9LFT6
B	14	CYS	TYR	engineered mutation	UNP Q9LFT6
B	122	LEU	TYR	engineered mutation	UNP Q9LFT6
B	126	PHE	PRO	engineered mutation	UNP Q9LFT6
B	129	TRP	LEU	engineered mutation	UNP Q9LFT6
B	132	THR	CYS	engineered mutation	UNP Q9LFT6
B	210	ILE	ALA	engineered mutation	UNP Q9LFT6
B	259	GLY	-	expression tag	UNP Q9LFT6
B	260	LEU	-	expression tag	UNP Q9LFT6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

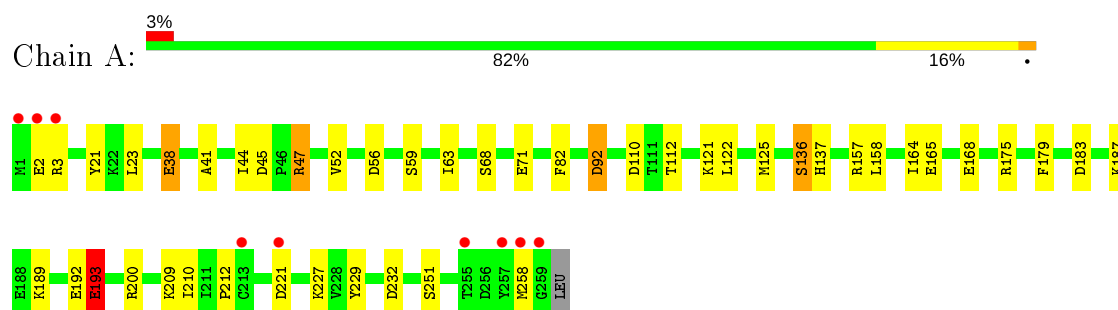
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	B	188	Total	O	0	0
			188	188		

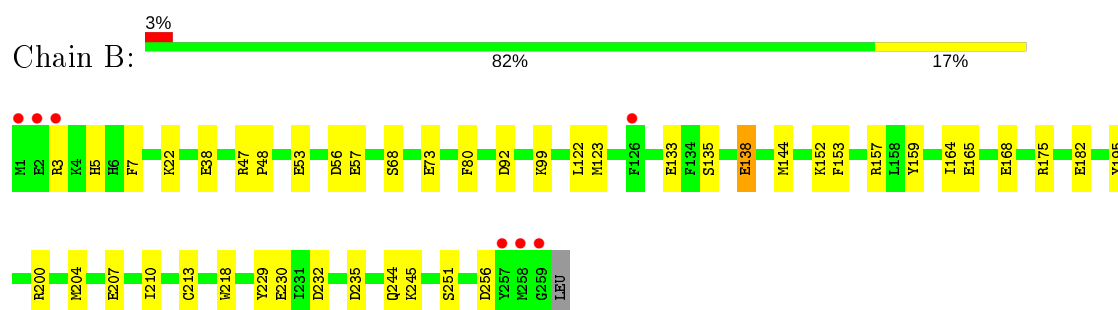
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alpha-hydroxynitrile lyase



- Molecule 1: Alpha-hydroxynitrile lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.84Å 87.09Å 123.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.52 35.55 – 1.52	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-1.52) 99.0 (35.55-1.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.158 , 0.191 0.171 , 0.200	Depositor DCC
R_{free} test set	4180 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4587	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: GOL, CL

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	1.69	17/2161 (0.8%)	1.58	20/2917 (0.7%)
1	B	1.68	28/2169 (1.3%)	1.52	21/2927 (0.7%)
All	All	1.69	45/4330 (1.0%)	1.55	41/5844 (0.7%)

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	0	1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CD-OE2	10.49	1.37	1.25
1	A	136	SER	CB-OG	-9.36	1.30	1.42
1	B	168	GLU	CD-OE2	9.27	1.35	1.25
1	B	182	GLU	CD-OE1	9.24	1.35	1.25
1	B	53	GLU	CD-OE2	-9.05	1.15	1.25
1	B	207	GLU	CD-OE2	8.22	1.34	1.25
1	A	38	GLU	CD-OE2	-7.88	1.17	1.25
1	B	38	GLU	CD-OE1	-7.45	1.17	1.25
1	B	22	LYS	CD-CE	-7.34	1.32	1.51
1	B	47	ARG	CZ-NH1	7.17	1.42	1.33
1	B	165	GLU	CD-OE2	7.07	1.33	1.25
1	B	182	GLU	CG-CD	6.71	1.62	1.51
1	B	53	GLU	CD-OE1	6.68	1.32	1.25
1	B	138[A]	GLU	CD-OE2	6.64	1.32	1.25
1	B	138[B]	GLU	CD-OE2	6.64	1.32	1.25
1	A	221	ASP	CB-CG	-6.60	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	SER	CB-OG	-6.55	1.33	1.42
1	A	193	GLU	CG-CD	6.44	1.61	1.51
1	B	135	SER	CB-OG	-6.18	1.34	1.42
1	A	52	VAL	C-N	-6.03	1.20	1.34
1	B	159	TYR	CE2-CZ	-6.01	1.30	1.38
1	A	47[A]	ARG	CD-NE	5.99	1.56	1.46
1	A	47[B]	ARG	CD-NE	5.99	1.56	1.46
1	A	165	GLU	CD-OE1	5.96	1.32	1.25
1	A	45	ASP	CB-CG	5.95	1.64	1.51
1	B	256	ASP	CB-CG	-5.91	1.39	1.51
1	B	195	TYR	CB-CG	-5.64	1.43	1.51
1	A	47[A]	ARG	CZ-NH1	5.62	1.40	1.33
1	A	47[B]	ARG	CZ-NH1	5.62	1.40	1.33
1	B	48	PRO	N-CA	-5.47	1.38	1.47
1	B	256	ASP	N-CA	5.44	1.57	1.46
1	B	195	TYR	CE1-CZ	5.40	1.45	1.38
1	B	218	TRP	CG-CD1	5.40	1.44	1.36
1	B	251[A]	SER	C-O	5.39	1.33	1.23
1	B	251[B]	SER	C-O	5.39	1.33	1.23
1	A	251	SER	CA-CB	-5.30	1.45	1.52
1	B	152	LYS	CE-NZ	5.26	1.62	1.49
1	B	80	PHE	CG-CD1	5.23	1.46	1.38
1	B	230	GLU	CG-CD	5.19	1.59	1.51
1	B	73	GLU	CD-OE2	-5.19	1.20	1.25
1	A	38	GLU	CD-OE1	-5.17	1.20	1.25
1	A	187	LYS	CD-CE	-5.15	1.38	1.51
1	A	23	LEU	C-O	5.13	1.33	1.23
1	B	210	ILE	CB-CG1	-5.10	1.39	1.54
1	B	210	ILE	CA-CB	5.04	1.66	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	B	175	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	38	GLU	OE1-CD-OE2	10.80	136.26	123.30
1	A	200	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	B	144	MET	CG-SD-CE	-10.08	84.07	100.20
1	A	47[A]	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	A	47[B]	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	B	232	ASP	CB-CG-OD2	-9.46	109.79	118.30
1	B	157	ARG	NE-CZ-NH1	8.99	124.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	A	136	SER	CB-CA-C	-7.90	95.09	110.10
1	B	232	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	183	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	175	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	80	PHE	CB-CG-CD2	7.26	125.88	120.80
1	B	3	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	56	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	92	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	45	ASP	CA-C-O	6.57	133.89	120.10
1	B	123	MET	CG-SD-CE	6.45	110.52	100.20
1	A	179	PHE	CB-CG-CD1	6.35	125.24	120.80
1	A	125	MET	CG-SD-CE	-6.23	90.23	100.20
1	A	232	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	110	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	157[A]	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	157[B]	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	38	GLU	CG-CD-OE1	-6.02	106.25	118.30
1	A	82	PHE	CB-CG-CD2	6.02	125.02	120.80
1	A	56	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	235	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	B	200	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	193	GLU	OE1-CD-OE2	-5.78	116.37	123.30
1	B	229	TYR	CG-CD2-CE2	-5.67	116.76	121.30
1	B	122	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	153	PHE	CZ-CE2-CD2	-5.56	113.43	120.10
1	A	158	LEU	CB-CG-CD2	5.47	120.31	111.00
1	B	7	PHE	CB-CG-CD2	5.42	124.59	120.80
1	A	21	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	B	256	ASP	N-CA-C	5.17	124.95	111.00
1	B	133[A]	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	B	133[B]	GLU	CG-CD-OE2	-5.09	108.12	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ILE	Mainchain

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	2103	0	2088	20	0
1	B	2111	0	2088	10	0
2	A	12	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	171	0	0	6	0
4	B	188	0	0	6	0
All	All	4587	0	4192	30	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 4.

All (30) 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:47[B]:ARG:CG	1:A:47[B]:ARG:HH21	1.14	1.47
1:A:47[B]:ARG:CB	1:A:47[B]:ARG:HH21	1.69	1.06
1:A:47[B]:ARG:NH2	1:A:47[B]:ARG:HG2	1.27	1.05
1:A:209:LYS:NZ	4:A:401:HOH:O	2.00	0.91
1:A:47[B]:ARG:HG2	1:A:47[B]:ARG:HH21	0.77	0.88
1:A:47[B]:ARG:NH2	1:A:47[B]:ARG:CG	1.93	0.88
1:B:138[B]:GLU:HG2	4:B:487:HOH:O	1.74	0.86
1:A:68:SER:OG	4:A:402:HOH:O	2.04	0.74
1:B:57[B]:GLU:OE2	4:B:401:HOH:O	2.07	0.72
1:A:136:SER:HB3	4:A:430:HOH:O	1.91	0.70
1:B:68:SER:OG	4:B:402:HOH:O	2.10	0.70
1:A:47[B]:ARG:HB3	1:A:47[B]:ARG:NH2	2.06	0.69
1:B:244:GLN:OE1	4:B:403:HOH:O	2.14	0.65
1:A:193:GLU:H	1:A:193:GLU:CD	2.01	0.64
1:A:210:ILE:O	1:A:212:PRO:HD3	2.01	0.61
1:A:192:GLU:HB2	1:A:193:GLU:OE2	2.06	0.54
1:A:164:ILE:CD1	4:A:513:HOH:O	2.59	0.50
1:A:193:GLU:N	1:A:193:GLU:CD	2.66	0.47
1:B:5:HIS:HD2	1:B:99:LYS:NZ	2.13	0.47
1:A:137:HIS:HE1	4:A:404:HOH:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HE3	1:A:229:TYR:CZ	2.51	0.46
1:B:204:MET:CE	1:B:213[B]:CYS:SG	3.04	0.46
1:A:164:ILE:HD11	4:A:415:HOH:O	2.15	0.45
1:B:164:ILE:HD11	4:B:409:HOH:O	2.16	0.45
1:A:47[B]:ARG:CB	1:A:47[B]:ARG:NH2	2.46	0.45
1:B:99:LYS:HE2	1:B:99:LYS:HB2	1.57	0.45
1:A:112:THR:O	1:A:189:LYS:HE3	2.17	0.44
1:B:164:ILE:CD1	4:B:499:HOH:O	2.66	0.44
1:A:41:ALA:HA	1:A:47[B]:ARG:O	2.19	0.41
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.97	0.41

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	262/260 (101%)	259 (99%)	3 (1%)	0	100	100
1	B	264/260 (102%)	260 (98%)	4 (2%)	0	100	100
All	All	526/520 (101%)	519 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	231/227 (102%)	221 (96%)	10 (4%)	29 5
1	B	233/227 (103%)	232 (100%)	1 (0%)	91 82
All	All	464/454 (102%)	453 (98%)	11 (2%)	49 19

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ARG
1	A	38	GLU
1	A	63	ILE
1	A	71	GLU
1	A	92	ASP
1	A	121	LYS
1	A	122	LEU
1	A	193	GLU
1	A	258	MET
1	B	92	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	HIS
1	B	141	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	301	-	5,5,5	1.27	1 (20%)	5,5,5	0.59	0
2	GOL	A	302	-	5,5,5	0.47	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GOL	O1-C1	2.27	1.52	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	GOL	O1-C1-C2-O2
2	A	302	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:VAL	C	53:GLU	N	1.20

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	259/260 (99%)	0.02	9 (3%) 44 48	12, 23, 42, 97	0
1	B	259/260 (99%)	-0.14	7 (2%) 54 59	11, 20, 41, 78	0
All	All	518/520 (99%)	-0.06	16 (3%) 49 54	11, 21, 41, 97	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLY	12.1
1	B	259	GLY	9.8
1	A	258	MET	6.6
1	A	1	MET	4.9
1	A	257	TYR	4.4
1	B	1	MET	4.1
1	A	2	GLU	4.0
1	B	258	MET	3.7
1	B	126	PHE	3.0
1	A	213	CYS	3.0
1	B	257	TYR	2.8
1	A	3	ARG	2.7
1	B	3	ARG	2.6
1	A	255	THR	2.5
1	A	221	ASP	2.2
1	B	2	GLU	2.1

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 carbohydrates in this entry.

6.4 Ligands

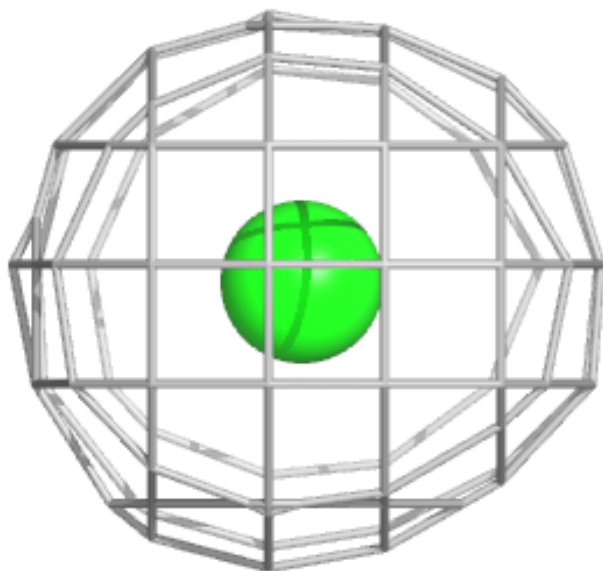
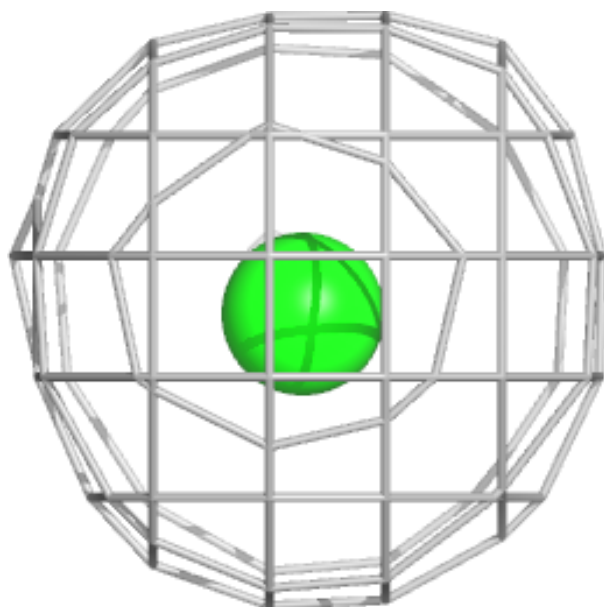
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	302	6/6	0.83	0.28	38,44,49,52	0
2	GOL	A	301	6/6	0.93	0.09	23,29,31,38	0
3	CL	A	303	1/1	0.99	0.07	18,18,18,18	0
3	CL	B	301	1/1	1.00	0.06	17,17,17,17	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.

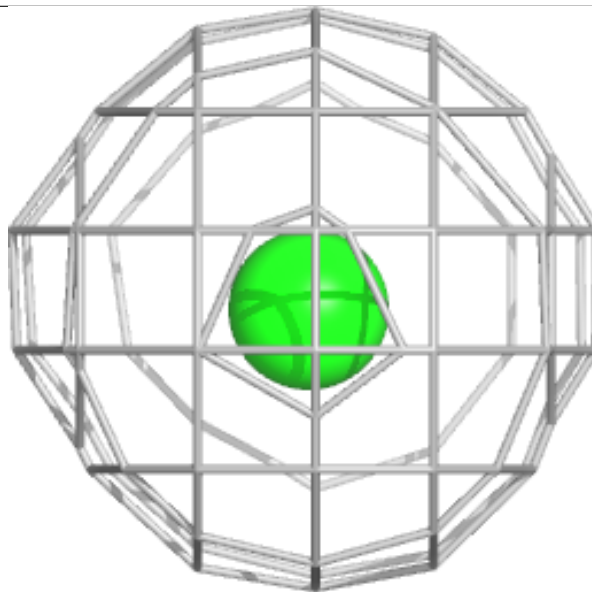
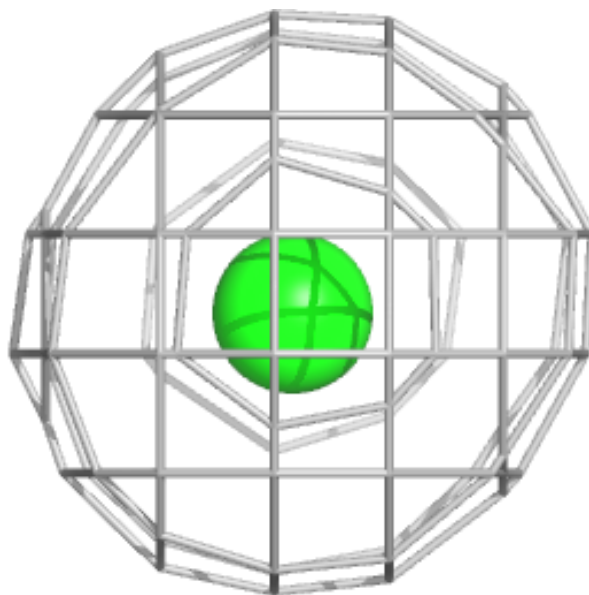
Electron density around CL A 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL B 301:

$2mF_o-DF_c$ (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.