Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:42 pm BST

PDB ID	:	5G5N
Title	:	Structure of the snake adenovirus 1 hexon-interlacing LH3 protein, methylmercury chloride derivative
Authors	:	Nguyen, T.H.; Singh, A.K.; Albala-Perez, B.; van Raaij, M.J.
Deposited on	:	2016-05-26
Resolution	:	2.30 Å(reported)

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

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

The following versions of software and data (see references ①) were used in the production of this report:

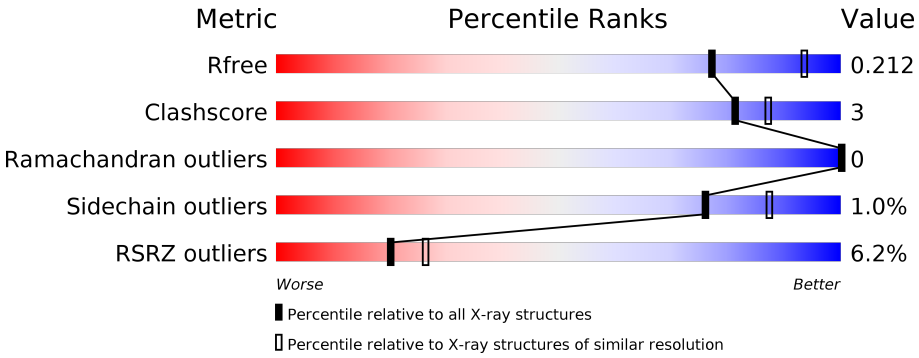
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	353	8% 90% 6%
1	B	353	6% 89% 7%
1	C	353	4% 90% 6%

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
3	MMC	B	1375	-	-	X	-
3	MMC	C	1375	-	-	X	-
4	CL	C	1381	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8019 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 LH3 HEXON-INTERLACING CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2561	1617	448	479	17			
1	B	341	Total	C	N	O	S	0	0	0
			2581	1630	451	483	17			
1	C	343	Total	C	N	O	S	0	0	0
			2596	1638	456	485	17			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	ALA	conflict	UNP A9CB85
A	22	LEU	PHE	conflict	UNP A9CB85
A	23	PRO	LEU	conflict	UNP A9CB85
A	24	VAL	TYR	conflict	UNP A9CB85
A	26	SER	LEU	conflict	UNP A9CB85
A	28	PRO	ARG	conflict	UNP A9CB85
A	71	ASN	GLU	conflict	UNP A9CB85
A	72	GLY	ARG	conflict	UNP A9CB85
A	73	ALA	CYS	conflict	UNP A9CB85
A	74	THR	HIS	conflict	UNP A9CB85
A	75	VAL	GLY	conflict	UNP A9CB85
A	76	LYS	GLU	conflict	UNP A9CB85
A	77	THR	ASP	conflict	UNP A9CB85
A	78	SER	PHE	conflict	UNP A9CB85
A	79	GLY	ARG	conflict	UNP A9CB85
A	80	LEU	PRO	conflict	UNP A9CB85
A	81	GLY	ARG	conflict	UNP A9CB85
A	82	PRO	ALA	conflict	UNP A9CB85
B	21	GLY	ALA	conflict	UNP A9CB85
B	22	LEU	PHE	conflict	UNP A9CB85
B	23	PRO	LEU	conflict	UNP A9CB85
B	24	VAL	TYR	conflict	UNP A9CB85
B	26	SER	LEU	conflict	UNP A9CB85

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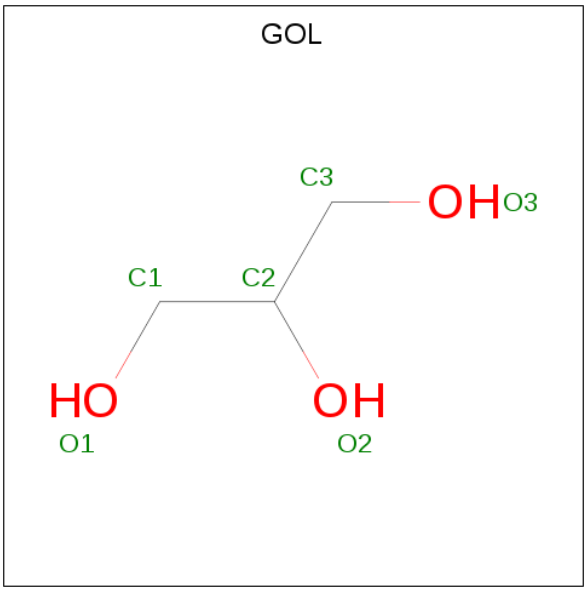
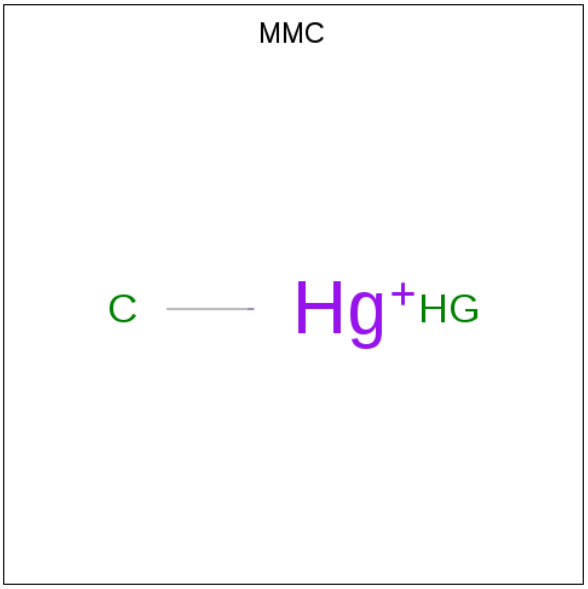
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	PRO	ARG	conflict	UNP A9CB85
B	71	ASN	GLU	conflict	UNP A9CB85
B	72	GLY	ARG	conflict	UNP A9CB85
B	73	ALA	CYS	conflict	UNP A9CB85
B	74	THR	HIS	conflict	UNP A9CB85
B	75	VAL	GLY	conflict	UNP A9CB85
B	76	LYS	GLU	conflict	UNP A9CB85
B	77	THR	ASP	conflict	UNP A9CB85
B	78	SER	PHE	conflict	UNP A9CB85
B	79	GLY	ARG	conflict	UNP A9CB85
B	80	LEU	PRO	conflict	UNP A9CB85
B	81	GLY	ARG	conflict	UNP A9CB85
B	82	PRO	ALA	conflict	UNP A9CB85
C	21	GLY	ALA	conflict	UNP A9CB85
C	22	LEU	PHE	conflict	UNP A9CB85
C	23	PRO	LEU	conflict	UNP A9CB85
C	24	VAL	TYR	conflict	UNP A9CB85
C	26	SER	LEU	conflict	UNP A9CB85
C	28	PRO	ARG	conflict	UNP A9CB85
C	71	ASN	GLU	conflict	UNP A9CB85
C	72	GLY	ARG	conflict	UNP A9CB85
C	73	ALA	CYS	conflict	UNP A9CB85
C	74	THR	HIS	conflict	UNP A9CB85
C	75	VAL	GLY	conflict	UNP A9CB85
C	76	LYS	GLU	conflict	UNP A9CB85
C	77	THR	ASP	conflict	UNP A9CB85
C	78	SER	PHE	conflict	UNP A9CB85
C	79	GLY	ARG	conflict	UNP A9CB85
C	80	LEU	PRO	conflict	UNP A9CB85
C	81	GLY	ARG	conflict	UNP A9CB85
C	82	PRO	ALA	conflict	UNP A9CB85

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is METHYL MERCURY ION (three-letter code: MMC) (formula: CH_3Hg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Hg 2 1 1	0	0
3	A	1	Total C Hg 2 1 1	0	0
3	A	1	Total C Hg 2 1 1	0	0
3	B	1	Total C Hg 2 1 1	0	0
3	B	1	Total C Hg 2 1 1	0	0
3	B	1	Total C Hg 2 1 1	0	0
3	B	1	Total C Hg 2 1 1	0	0
3	C	1	Total C Hg 2 1 1	0	0
3	C	1	Total C Hg 2 1 1	0	0
3	C	1	Total C Hg 2 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total Cl 5 5	0	0
4	A	5	Total Cl 5 5	0	0
4	C	4	Total Cl 4 4	0	0

- Molecule 5 is water.

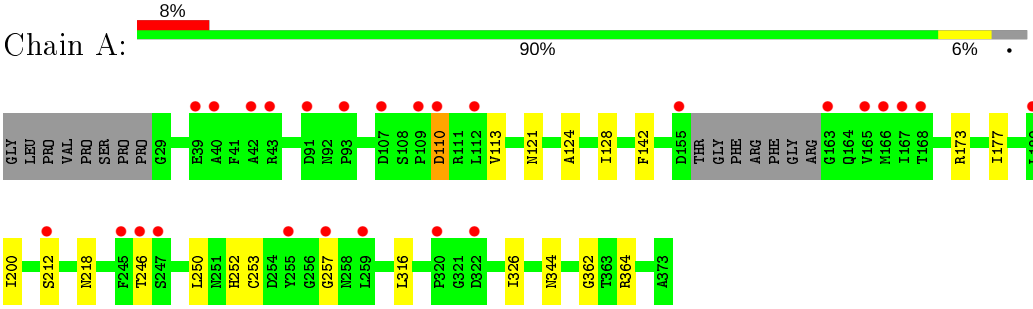
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	79	Total O 79 79	0	0
5	B	75	Total O 75 75	0	0
5	C	63	Total O 63 63	0	0

3 Residue-property plots

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.

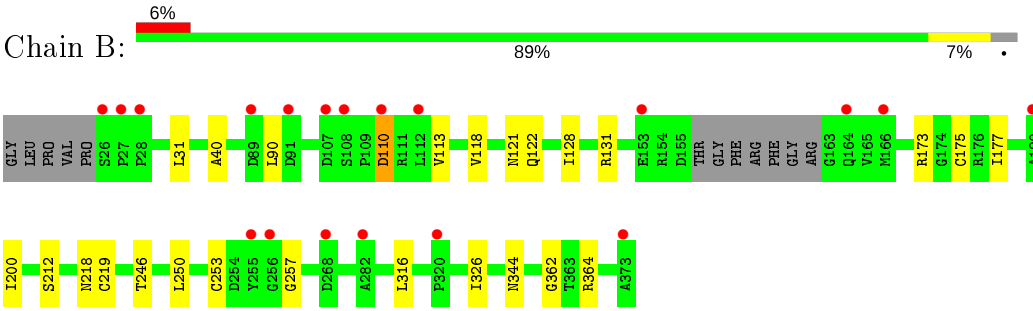
- Molecule 1: LH3 HEXON-INTERLACING CAPSID PROTEIN

Chain A:



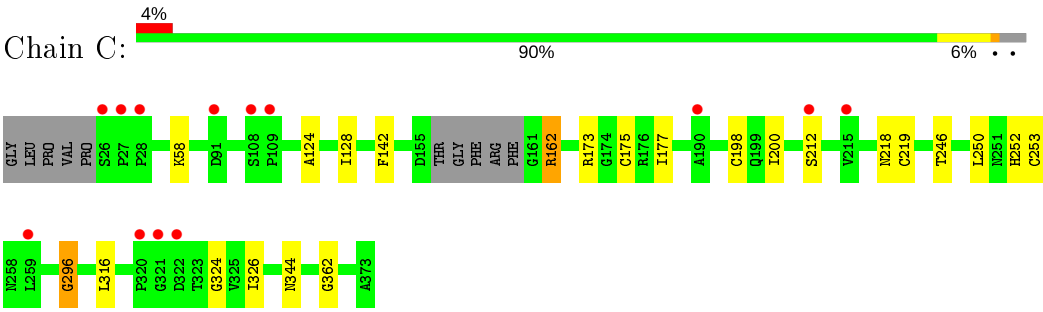
- Molecule 1: LH3 HEXON-INTERLACING CAPSID PROTEIN

Chain B:



- Molecule 1: LH3 HEXON-INTERLACING CAPSID PROTEIN

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	149.26Å 149.26Å 108.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.00 – 2.30 38.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.00-2.30) 100.0 (38.69-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.172 , 0.205 0.179 , 0.212	Depositor DCC
R_{free} test set	2691 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MMC, 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	0.64	0/2624	0.77	2/3571 (0.1%)
1	B	0.64	0/2646	0.75	1/3603 (0.0%)
1	C	0.66	0/2661	0.78	1/3622 (0.0%)
All	All	0.65	0/7931	0.77	4/10796 (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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	364	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	364	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	162	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	296	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	2561	0	2455	10	1
1	B	2581	0	2474	15	0
1	C	2596	0	2490	14	1
2	A	18	0	24	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
3	A	6	0	0	2	0
3	B	8	0	0	3	0
3	C	6	0	0	3	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	4	0	0	1	0
5	A	79	0	0	0	0
5	B	75	0	0	0	0
5	C	63	0	0	0	0
All	All	8019	0	7459	39	1

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 (39) 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:C:253:CYS:SG	3:C:1375:MMC:HG	1.74	1.06
1:B:253:CYS:SG	3:B:1375:MMC:HG	1.86	0.92
1:A:253:CYS:SG	3:A:1377:MMC:HG	1.89	0.89
1:C:296:GLY:O	1:C:324:GLY:HA2	1.73	0.89
1:B:118:VAL:O	1:B:121:ASN:ND2	2.12	0.83
1:A:252:HIS:ND1	4:A:1381:CL:CL	2.55	0.76
1:B:121:ASN:OD1	1:B:122:GLN:OE1	2.09	0.70
1:B:253:CYS:HG	3:B:1375:MMC:HG	1.31	0.70
1:A:128:ILE:HB	3:A:1379:MMC:C	2.26	0.66
1:C:253:CYS:HG	3:C:1375:MMC:HG	0.63	0.63
1:C:252:HIS:ND1	4:C:1379:CL:CL	2.76	0.55
1:B:128:ILE:HG22	3:B:1377:MMC:C	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASN:O	1:A:362:GLY:HA2	2.15	0.47
1:A:110:ASP:HB3	1:A:113:VAL:HG23	1.97	0.47
1:B:344:ASN:O	1:B:362:GLY:HA2	2.15	0.47
1:C:344:ASN:O	1:C:362:GLY:HA2	2.15	0.46
1:B:110:ASP:HB3	1:B:113:VAL:HG23	1.99	0.45
1:C:177:ILE:HA	1:C:200:ILE:O	2.16	0.45
1:B:90:LEU:O	1:B:131:ARG:NH2	2.49	0.45
1:A:177:ILE:HA	1:A:200:ILE:O	2.17	0.44
1:B:212:SER:HA	1:B:246:THR:O	2.17	0.44
1:B:177:ILE:HA	1:B:200:ILE:O	2.17	0.43
1:B:316:LEU:HD22	1:B:326:ILE:HD11	2.00	0.43
1:C:212:SER:HA	1:C:246:THR:O	2.19	0.43
1:B:31:LEU:HD13	1:B:40:ALA:HB2	2.00	0.43
1:A:316:LEU:HD22	1:A:326:ILE:HD11	2.00	0.43
1:C:124:ALA:HB2	1:C:142:PHE:CZ	2.54	0.43
1:A:218:ASN:OD1	1:A:257:GLY:HA3	2.19	0.42
1:C:218:ASN:OD1	1:C:257:GLY:HA3	2.18	0.42
1:A:212:SER:HA	1:A:246:THR:O	2.19	0.42
1:B:218:ASN:OD1	1:B:257:GLY:HA3	2.19	0.42
1:C:316:LEU:HD22	1:C:326:ILE:HD11	2.01	0.42
1:B:175:CYS:O	1:B:198:CYS:HA	2.21	0.41
1:B:219:CYS:O	1:B:253:CYS:HA	2.20	0.41
1:C:175:CYS:O	1:C:198:CYS:HA	2.21	0.41
1:C:296:GLY:O	1:C:324:GLY:CA	2.57	0.41
1:A:124:ALA:HB2	1:A:142:PHE:CZ	2.56	0.40
1:C:128:ILE:HB	3:C:1377:MMC:C	2.51	0.40
1:C:219:CYS:O	1:C:253:CYS:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:OD1	1:C:58:LYS:NZ[4_565]	2.10	0.10

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	334/353 (95%)	323 (97%)	11 (3%)	0	100	100
1	B	337/353 (96%)	326 (97%)	11 (3%)	0	100	100
1	C	339/353 (96%)	329 (97%)	10 (3%)	0	100	100
All	All	1010/1059 (95%)	978 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/279 (96%)	265 (99%)	2 (1%)	84	92
1	B	270/279 (97%)	267 (99%)	3 (1%)	73	86
1	C	271/279 (97%)	268 (99%)	3 (1%)	73	86
All	All	808/837 (96%)	800 (99%)	8 (1%)	76	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	250	LEU
1	B	110	ASP
1	B	173	ARG
1	B	250	LEU
1	C	162	ARG
1	C	173	ARG
1	C	250	LEU

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

Mol	Chain	Res	Type
1	A	239	ASN
1	B	208	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 29 ligands modelled in this entry, 14 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
3	MMC	C	1377	4	0,1,1	0.00	-	-		
3	MMC	A	1378	1	0,1,1	0.00	-	-		
3	MMC	B	1378	-	0,1,1	0.00	-	-		
2	GOL	A	1376	-	5,5,5	0.73	0	5,5,5	0.61	0
3	MMC	C	1375	1	0,1,1	0.00	-	-		
3	MMC	B	1376	1	0,1,1	0.00	-	-		
3	MMC	B	1375	1	0,1,1	0.00	-	-		
3	MMC	A	1379	4	0,1,1	0.00	-	-		
2	GOL	A	1374	-	5,5,5	1.38	1 (20%)	5,5,5	1.29	1 (20%)
2	GOL	A	1375	-	5,5,5	0.35	0	5,5,5	0.72	0
3	MMC	C	1376	1	0,1,1	0.00	-	-		
2	GOL	C	1374	-	5,5,5	0.28	0	5,5,5	0.27	0
2	GOL	B	1374	-	5,5,5	0.18	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MMC	B	1377	4	0,1,1	0.00	-	-		
3	MMC	A	1377	1	0,1,1	0.00	-	-		

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	1375	-	-	0/4/4/4	-
2	GOL	C	1374	-	-	4/4/4/4	-
2	GOL	B	1374	-	-	2/4/4/4	-
2	GOL	A	1374	-	-	2/4/4/4	-
2	GOL	A	1376	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1374	GOL	O2-C2	-2.02	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1374	GOL	C3-C2-C1	2.31	120.69	111.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1374	GOL	C1-C2-C3-O3
2	B	1374	GOL	O1-C1-C2-C3
2	A	1376	GOL	O1-C1-C2-C3
2	A	1374	GOL	O1-C1-C2-C3
2	B	1374	GOL	O1-C1-C2-O2
2	C	1374	GOL	O2-C2-C3-O3
2	A	1374	GOL	O1-C1-C2-O2
2	A	1376	GOL	O1-C1-C2-O2
2	C	1374	GOL	O1-C1-C2-C3
2	C	1374	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1377	MMC	1	0
3	C	1375	MMC	2	0
3	B	1375	MMC	2	0
3	A	1379	MMC	1	0
3	B	1377	MMC	1	0
3	A	1377	MMC	1	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	338/353 (95%)	0.13	28 (8%)	11	15	24, 39, 68, 97	0
1	B	341/353 (96%)	0.01	20 (5%)	22	28	22, 39, 70, 98	0
1	C	343/353 (97%)	0.05	15 (4%)	34	41	25, 41, 77, 124	0
All	All	1022/1059 (96%)	0.06	63 (6%)	20	26	22, 40, 74, 124	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	SER	6.5
1	C	28	PRO	5.2
1	B	26	SER	5.1
1	B	89	ASP	4.7
1	C	27	PRO	4.7
1	C	255	TYR	4.7
1	B	27	PRO	4.4
1	C	91	ASP	4.4
1	C	321	GLY	4.3
1	A	110	ASP	4.0
1	B	255	TYR	3.9
1	B	268	ASP	3.9
1	A	320	PRO	3.7
1	A	257	GLY	3.6
1	C	322	ASP	3.5
1	A	112	LEU	3.4
1	A	166	MET	3.4
1	A	91	ASP	3.4
1	C	320	PRO	3.3
1	A	255	TYR	3.3
1	C	109	PRO	3.2
1	A	167	ILE	3.1
1	A	163	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	212	SER	3.0
1	A	165	VAL	2.9
1	A	259	LEU	2.9
1	B	28	PRO	2.7
1	A	189	LEU	2.7
1	C	190	ALA	2.7
1	A	43	ARG	2.7
1	A	39	GLU	2.6
1	A	168	THR	2.6
1	B	166	MET	2.6
1	B	373	ALA	2.6
1	B	107	ASP	2.5
1	B	153	GLU	2.5
1	B	320	PRO	2.5
1	A	107	ASP	2.5
1	B	108	SER	2.4
1	A	40	ALA	2.4
1	A	155	ASP	2.4
1	B	110	ASP	2.4
1	A	190	ALA	2.4
1	B	190	ALA	2.4
1	A	245	PHE	2.4
1	B	282	ALA	2.4
1	B	191	SER	2.4
1	C	257	GLY	2.3
1	A	246	THR	2.3
1	A	212	SER	2.3
1	B	112	LEU	2.3
1	A	42	ALA	2.3
1	A	109	PRO	2.2
1	B	256	GLY	2.2
1	A	93	PRO	2.2
1	B	91	ASP	2.2
1	C	259	LEU	2.1
1	A	192	GLN	2.1
1	B	164	GLN	2.1
1	A	247	SER	2.1
1	C	108	SER	2.1
1	A	322	ASP	2.1
1	C	215	VAL	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 carbohydrates 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	CL	C	1381	1/1	0.61	1.42	88,88,88,88	0
4	CL	B	1381	1/1	0.74	0.11	81,81,81,81	0
2	GOL	A	1376	6/6	0.79	0.20	55,67,70,75	0
4	CL	C	1380	1/1	0.86	0.08	70,70,70,70	0
2	GOL	A	1374	6/6	0.89	0.21	34,43,46,51	0
4	CL	A	1384	1/1	0.89	0.13	78,78,78,78	0
4	CL	B	2000	1/1	0.90	0.07	83,83,83,83	0
2	GOL	B	1374	6/6	0.91	0.28	60,64,68,71	0
4	CL	B	2001	1/1	0.91	1.06	93,93,93,93	0
2	GOL	A	1375	6/6	0.91	0.20	53,65,66,66	0
4	CL	A	1383	1/1	0.93	0.06	83,83,83,83	0
4	CL	C	1379	1/1	0.93	0.08	62,62,62,62	0
2	GOL	C	1374	6/6	0.95	0.14	49,69,72,83	0
4	CL	B	1380	1/1	0.96	0.09	79,79,79,79	0
3	MMC	C	1377	2/2	0.97	0.13	73,73,73,88	2
3	MMC	C	1376	2/2	0.97	0.09	71,71,71,74	2
3	MMC	A	1378	2/2	0.97	0.14	76,76,76,88	2
3	MMC	B	1377	2/2	0.97	0.14	82,82,82,98	0
3	MMC	A	1379	2/2	0.98	0.10	57,57,57,67	2
3	MMC	B	1378	2/2	0.98	0.14	84,84,84,95	2
4	CL	A	1382	1/1	0.98	0.04	86,86,86,86	0
3	MMC	B	1376	2/2	0.98	0.22	68,68,68,77	2
4	CL	A	1381	1/1	0.99	0.06	54,54,54,54	0
4	CL	B	1379	1/1	0.99	0.11	30,30,30,30	0
3	MMC	B	1375	2/2	1.00	0.04	38,38,38,47	2
4	CL	A	1380	1/1	1.00	0.14	31,31,31,31	0
3	MMC	C	1375	2/2	1.00	0.03	39,39,39,43	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	C	1378	1/1	1.00	0.13	31,31,31,31	0
3	MMC	A	1377	2/2	1.00	0.04	38,38,38,51	2

6.5 Other polymers (i)

There are no such residues in this entry.