Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:46 pm BST

PDB ID	:	5GT7
Title	:	Crystal Structure of Arg-bound CASTOR1
Authors	:	Guo, L.; Deng, D.
Deposited on	:	2016-08-18
Resolution	:	2.05 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:

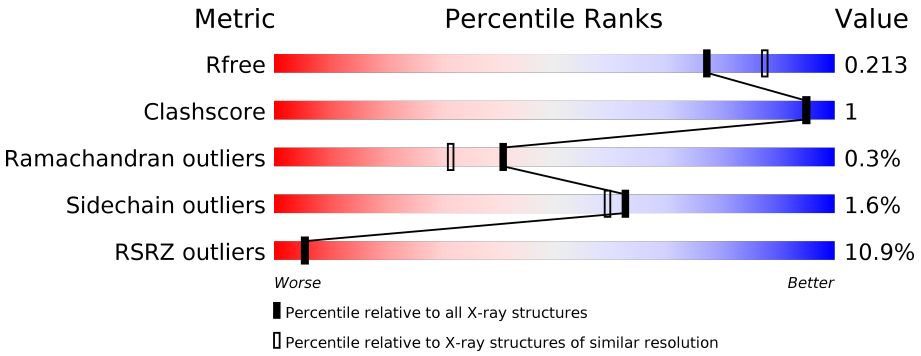
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	335	13% 89% • 9%
1	B	335	10% 84% • 12%
1	C	335	8% 89% 5% • 5%
1	D	335	8% 84% 5% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19732 atoms, of which 9594 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 GATS-like protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	H	N	O	S	0	2	0
			4767	1542	2384	392	440	9			
1	B	296	Total	C	H	N	O	S	0	4	0
			4666	1510	2335	381	432	8			
1	C	318	Total	C	H	N	O	S	0	3	0
			4946	1596	2467	409	465	9			
1	D	300	Total	C	H	N	O	S	0	2	0
			4695	1515	2345	389	438	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP Q8WTX7
A	-4	GLY	-	expression tag	UNP Q8WTX7
A	-3	SER	-	expression tag	UNP Q8WTX7
A	-2	GLY	-	expression tag	UNP Q8WTX7
A	-1	HIS	-	expression tag	UNP Q8WTX7
A	0	MET	-	expression tag	UNP Q8WTX7
A	324	GLN	-	expression tag	UNP Q8WTX7
A	325	GLU	-	expression tag	UNP Q8WTX7
A	326	GLY	-	expression tag	UNP Q8WTX7
A	327	LEU	-	expression tag	UNP Q8WTX7
A	328	ALA	-	expression tag	UNP Q8WTX7
A	329	SER	-	expression tag	UNP Q8WTX7
B	-5	ALA	-	expression tag	UNP Q8WTX7
B	-4	GLY	-	expression tag	UNP Q8WTX7
B	-3	SER	-	expression tag	UNP Q8WTX7
B	-2	GLY	-	expression tag	UNP Q8WTX7
B	-1	HIS	-	expression tag	UNP Q8WTX7
B	0	MET	-	expression tag	UNP Q8WTX7
B	324	GLN	-	expression tag	UNP Q8WTX7
B	325	GLU	-	expression tag	UNP Q8WTX7
B	326	GLY	-	expression tag	UNP Q8WTX7

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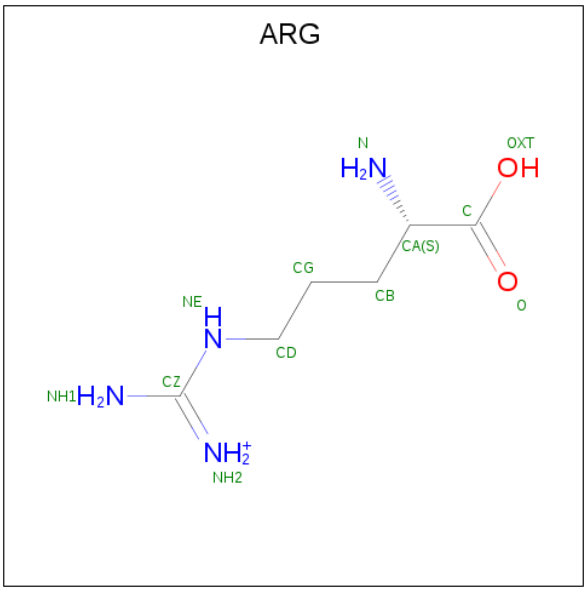
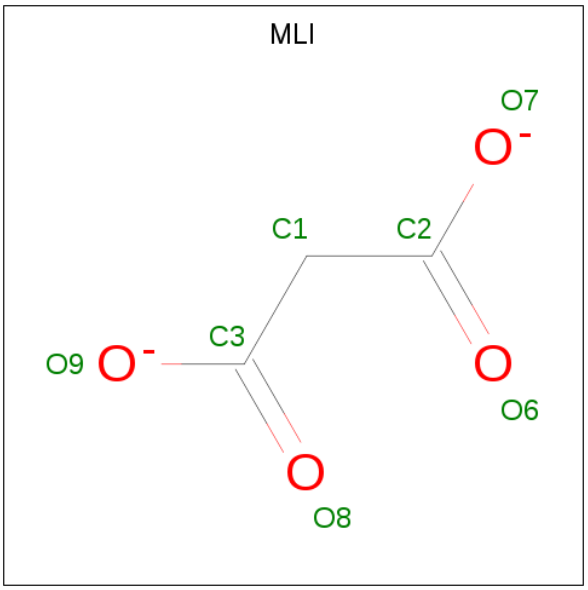
Chain	Residue	Modelled	Actual	Comment	Reference
B	327	LEU	-	expression tag	UNP Q8WTX7
B	328	ALA	-	expression tag	UNP Q8WTX7
B	329	SER	-	expression tag	UNP Q8WTX7
C	-5	ALA	-	expression tag	UNP Q8WTX7
C	-4	GLY	-	expression tag	UNP Q8WTX7
C	-3	SER	-	expression tag	UNP Q8WTX7
C	-2	GLY	-	expression tag	UNP Q8WTX7
C	-1	HIS	-	expression tag	UNP Q8WTX7
C	0	MET	-	expression tag	UNP Q8WTX7
C	324	GLN	-	expression tag	UNP Q8WTX7
C	325	GLU	-	expression tag	UNP Q8WTX7
C	326	GLY	-	expression tag	UNP Q8WTX7
C	327	LEU	-	expression tag	UNP Q8WTX7
C	328	ALA	-	expression tag	UNP Q8WTX7
C	329	SER	-	expression tag	UNP Q8WTX7
D	-5	ALA	-	expression tag	UNP Q8WTX7
D	-4	GLY	-	expression tag	UNP Q8WTX7
D	-3	SER	-	expression tag	UNP Q8WTX7
D	-2	GLY	-	expression tag	UNP Q8WTX7
D	-1	HIS	-	expression tag	UNP Q8WTX7
D	0	MET	-	expression tag	UNP Q8WTX7
D	324	GLN	-	expression tag	UNP Q8WTX7
D	325	GLU	-	expression tag	UNP Q8WTX7
D	326	GLY	-	expression tag	UNP Q8WTX7
D	327	LEU	-	expression tag	UNP Q8WTX7
D	328	ALA	-	expression tag	UNP Q8WTX7
D	329	SER	-	expression tag	UNP Q8WTX7

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	6	15	4	2		
2	B	1	Total	C	H	N	O	0	0
			24	6	12	4	2		
2	C	1	Total	C	H	N	O	0	0
			24	6	12	4	2		
2	D	1	Total	C	H	N	O	0	0
			24	6	12	4	2		

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 9 3 2 4	0	0
3	A	1	Total C H O 9 3 2 4	0	0
3	A	1	Total C H O 9 3 2 4	0	0
3	C	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0
3	D	1	Total C H O 9 3 2 4	0	0

- Molecule 4 is water.

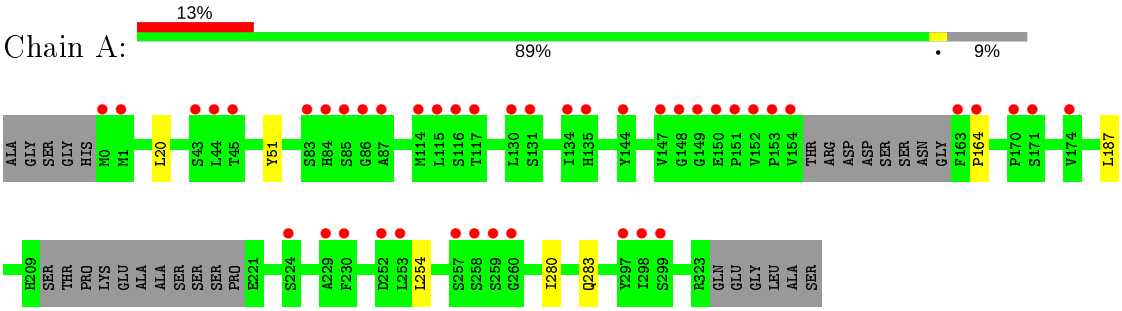
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 115 115	0	0
4	B	104	Total O 104 104	0	0
4	C	158	Total O 158 158	0	0
4	D	128	Total O 128 128	0	0

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.

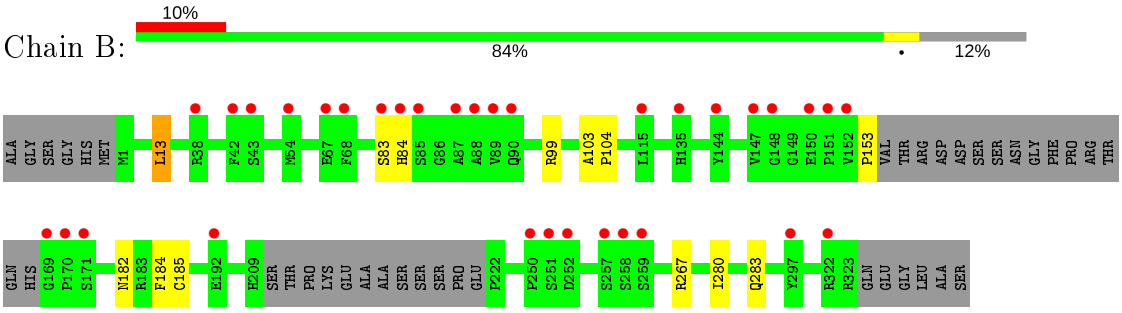
- Molecule 1: GATS-like protein 3

Chain A:



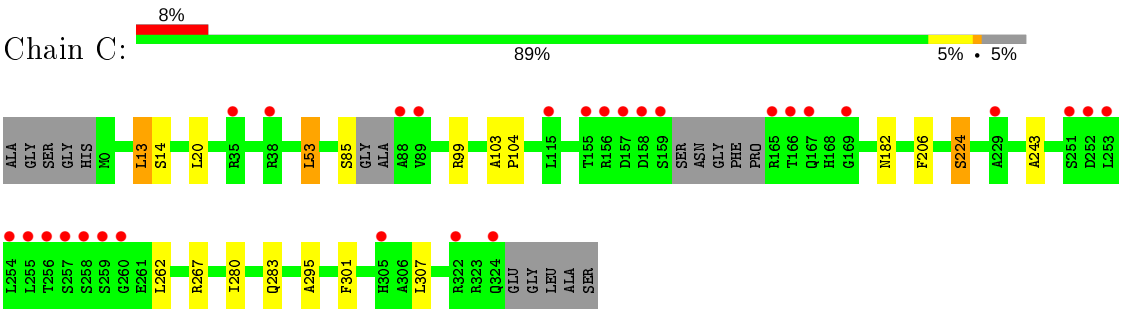
- Molecule 1: GATS-like protein 3

Chain B:



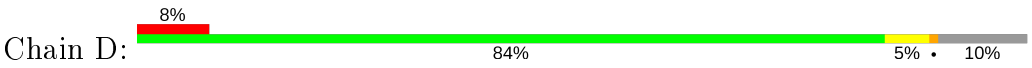
- Molecule 1: GATS-like protein 3

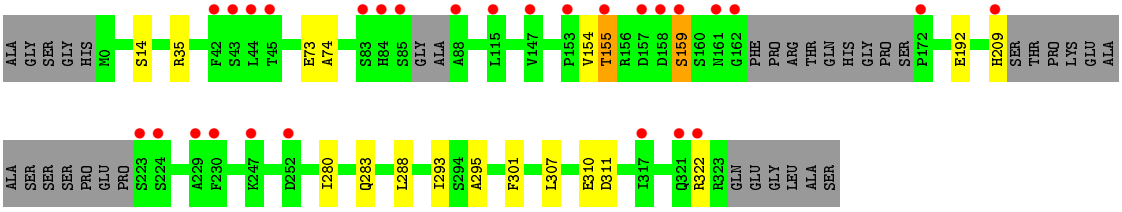
Chain C:



- Molecule 1: GATS-like protein 3

Chain D:




ALA GLY SER GLY HIS MO S14 R35 F42 S43 L44 T45 E73 A74 S83 H84 S85 GLY ALA A88 L115 V147 P153 V154 T155 R156 D157 D158 S159 S160 N161 G162 PHE PRO ARG THR GLN HIS GLY PRO SER P172 E192 H209 SER THR PRO LYS GLU ALA
ALA SER SER SER PRO GLU PRO S223 S224 A229 F230 K247 D252 I260 Q283 L288 I293 S294 A295 F301 L307 E310 D311 I317 Q321 R322 R323 GLN GLU GLY LEU ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.83Å 83.15Å 97.29Å 90.00° 116.39° 90.00°	Depositor
Resolution (Å)	33.03 – 2.05 33.03 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.03-2.05) 94.4 (33.03-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.185 , 0.211 0.187 , 0.213	Depositor DCC
R_{free} test set	4521 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19732	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: MLI

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	0.26	0/2447	0.47	0/3338
1	B	0.26	0/2399	0.48	1/3270 (0.0%)
1	C	0.27	0/2548	0.51	2/3476 (0.1%)
1	D	0.26	0/2409	0.49	0/3280
All	All	0.26	0/9803	0.48	3/13364 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	153	PRO	N-CA-CB	5.95	110.44	103.30
1	C	13	LEU	CA-CB-CG	5.69	128.40	115.30
1	C	53	LEU	CA-CB-CG	5.60	128.18	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2383	2384	2380	3	0
1	B	2331	2335	2340	4	0
1	C	2479	2467	2465	7	0
1	D	2350	2345	2336	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	15	12	0	0
2	B	12	12	12	0	0
2	C	12	12	12	0	0
2	D	12	12	12	0	0
3	A	21	6	6	0	0
3	C	7	2	2	0	0
3	D	14	4	4	0	0
4	A	115	0	0	0	0
4	B	104	0	0	0	1
4	C	158	0	0	0	0
4	D	128	0	0	0	1
All	All	10138	9594	9581	22	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 1.

All (22) 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:187:LEU:HD13	1:A:254:LEU:HB3	1.92	0.51
1:C:280:ILE:O	1:C:283:GLN:HG2	2.13	0.48
1:D:155:THR:O	1:D:155:THR:HG23	2.13	0.48
1:B:13:LEU:HD23	1:B:13:LEU:N	2.29	0.47
1:C:182:ASN:OD1	1:C:224:SER:HA	2.16	0.45
1:A:280:ILE:O	1:A:283:GLN:HG2	2.17	0.45
1:D:154:VAL:O	1:D:155:THR:HB	2.15	0.45
1:D:280:ILE:O	1:D:283:GLN:HG2	2.17	0.44
1:D:295:ALA:HA	1:D:307:LEU:O	2.18	0.43
1:D:14:SER:HB2	1:D:301:PHE:CG	2.54	0.43
1:C:295:ALA:HA	1:C:307:LEU:O	2.19	0.43
1:D:288:LEU:HD22	1:D:293:ILE:HB	2.00	0.43
1:B:182:ASN:HB2	1:B:184:PHE:CE2	2.54	0.42
1:C:103:ALA:HB3	1:C:104:PRO:HD3	2.00	0.42
1:C:14:SER:HB2	1:C:301:PHE:CG	2.54	0.42
1:D:310:GLU:HG3	1:D:311:ASP:N	2.35	0.41
1:A:20:LEU:HD22	1:A:51:TYR:CZ	2.56	0.41
1:B:103:ALA:HB3	1:B:104:PRO:HD3	2.03	0.41
1:B:280:ILE:O	1:B:283:GLN:HG2	2.20	0.41
1:D:73:GLU:O	1:D:74:ALA:HB3	2.20	0.41
1:C:20:LEU:HD21	1:C:206:PHE:HD1	1.86	0.40
1:C:243:ALA:HB2	1:C:262:LEU:HD13	2.03	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)
4:B:600:HOH:O	4:D:623:HOH:O[1_655]	2.11	0.09

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	301/335 (90%)	294 (98%)	6 (2%)	1 (0%)	41 31
1	B	294/335 (88%)	286 (97%)	8 (3%)	0	100 100
1	C	315/335 (94%)	312 (99%)	3 (1%)	0	100 100
1	D	294/335 (88%)	283 (96%)	9 (3%)	2 (1%)	22 12
All	All	1204/1340 (90%)	1175 (98%)	26 (2%)	3 (0%)	41 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	155	THR
1	A	164	PRO
1	D	159	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	264/289 (91%)	264 (100%)	0	100	100
1	B	260/289 (90%)	254 (98%)	6 (2%)	50	44
1	C	277/289 (96%)	271 (98%)	6 (2%)	52	46
1	D	259/289 (90%)	254 (98%)	5 (2%)	57	53
All	All	1060/1156 (92%)	1043 (98%)	17 (2%)	62	59

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
1	B	83	SER
1	B	84	HIS
1	B	99	ARG
1	B	185	CYS
1	B	267	ARG
1	C	13	LEU
1	C	53	LEU
1	C	85	SER
1	C	99	ARG
1	C	224	SER
1	C	267	ARG
1	D	35	ARG
1	D	159	SER
1	D	192	GLU
1	D	209	HIS
1	D	322	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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	MLI	C	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	D	403	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	404	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	402	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	A	403	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	D	402	-	0,6,6	0.00	-	0,7,7	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
3	MLI	C	402	-	-	0/0/4/4	-
3	MLI	D	403	-	-	0/0/4/4	-
3	MLI	A	404	-	-	0/0/4/4	-
3	MLI	A	402	-	-	0/0/4/4	-
3	MLI	A	403	-	-	0/0/4/4	-
3	MLI	D	402	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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)

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	305/335 (91%)	0.69	44 (14%) 2 2	27, 42, 72, 89	0
1	B	296/335 (88%)	0.50	33 (11%) 5 5	27, 42, 74, 96	0
1	C	318/335 (94%)	0.28	28 (8%) 10 10	21, 32, 67, 94	0
1	D	300/335 (89%)	0.36	28 (9%) 8 9	25, 38, 75, 91	0
All	All	1219/1340 (90%)	0.45	133 (10%) 5 5	21, 39, 73, 96	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	SER	11.2
1	B	147	VAL	7.7
1	B	84	HIS	7.5
1	C	260	GLY	7.0
1	A	148	GLY	6.5
1	A	163	PHE	6.4
1	A	87	ALA	6.1
1	D	88	ALA	6.0
1	D	84	HIS	6.0
1	A	260	GLY	5.7
1	A	147	VAL	5.5
1	D	85	SER	5.4
1	C	159	SER	5.3
1	D	158	ASP	5.1
1	B	258	SER	4.9
1	D	223	SER	4.9
1	A	84	HIS	4.7
1	A	85	SER	4.6
1	D	155	THR	4.6
1	A	152	VAL	4.5
1	C	157	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	257	SER	4.3
1	A	252	ASP	4.3
1	B	85	SER	4.3
1	D	321	GLN	4.2
1	D	83	SER	4.1
1	C	257	SER	4.1
1	A	154	VAL	4.1
1	A	144	TYR	4.0
1	C	324	GLN	3.8
1	D	322	ARG	3.8
1	B	252	ASP	3.8
1	B	87	ALA	3.8
1	A	115	LEU	3.8
1	A	86	GLY	3.7
1	B	38	ARG	3.6
1	C	258	SER	3.6
1	A	259	SER	3.5
1	D	159	SER	3.5
1	D	209	HIS	3.5
1	A	150	GLU	3.4
1	A	153	PRO	3.3
1	B	135	HIS	3.3
1	D	147	VAL	3.3
1	A	298	ILE	3.3
1	A	174	VAL	3.3
1	C	165	ARG	3.3
1	A	297	TYR	3.3
1	C	88	ALA	3.3
1	B	67	GLU	3.2
1	D	172	PRO	3.1
1	A	0	MET	3.1
1	A	171	SER	3.1
1	C	166	THR	3.0
1	C	89	VAL	2.9
1	A	1	MET	2.9
1	A	258	SER	2.9
1	D	44	LEU	2.9
1	D	252	ASP	2.9
1	A	151	PRO	2.9
1	B	171	SER	2.8
1	C	251	SER	2.8
1	B	148	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	83	SER	2.8
1	A	170	PRO	2.8
1	B	88	ALA	2.8
1	A	116	SER	2.7
1	B	83	SER	2.7
1	B	251	SER	2.7
1	B	259	SER	2.7
1	B	89	VAL	2.7
1	B	144	TYR	2.7
1	C	255	LEU	2.7
1	A	130	LEU	2.7
1	B	169	GLY	2.6
1	D	43	SER	2.6
1	C	158	ASP	2.6
1	D	153	PRO	2.6
1	C	35	ARG	2.6
1	B	322	ARG	2.6
1	D	247	LYS	2.6
1	D	161	ASN	2.6
1	A	253	LEU	2.6
1	D	157	ASP	2.5
1	D	230	PHE	2.5
1	A	134	ILE	2.5
1	A	299	SER	2.5
1	D	224	SER	2.5
1	C	252	ASP	2.5
1	B	90	GLN	2.5
1	A	45	THR	2.4
1	A	114	MET	2.4
1	B	151	PRO	2.4
1	B	115	LEU	2.4
1	D	115	LEU	2.4
1	A	43	SER	2.4
1	A	149	GLY	2.4
1	C	115	LEU	2.3
1	C	38	ARG	2.3
1	B	152	VAL	2.3
1	C	169	GLY	2.3
1	B	43	SER	2.3
1	B	297	TYR	2.3
1	B	68	PHE	2.2
1	A	229	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	257	SER	2.2
1	B	150	GLU	2.2
1	C	156	ARG	2.2
1	D	162	GLY	2.2
1	D	229	ALA	2.2
1	A	131	SER	2.2
1	B	250	PRO	2.2
1	D	42	PHE	2.1
1	D	45	THR	2.1
1	B	170	PRO	2.1
1	A	230	PHE	2.1
1	A	117	THR	2.1
1	B	192	GLU	2.1
1	D	317	ILE	2.1
1	C	253	LEU	2.1
1	C	254	LEU	2.1
1	A	224	SER	2.1
1	B	54	MET	2.1
1	A	164	PRO	2.1
1	B	42	PHE	2.1
1	C	167	GLN	2.1
1	A	44	LEU	2.0
1	C	155	THR	2.0
1	C	305	HIS	2.0
1	C	322	ARG	2.0
1	C	229	ALA	2.0
1	A	135	HIS	2.0
1	C	256	THR	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
3	MLI	A	402	7/7	0.85	0.26	60,64,79,84	0
3	MLI	A	404	7/7	0.86	0.29	40,56,66,67	0
3	MLI	A	403	7/7	0.86	0.22	56,68,78,80	0
3	MLI	D	403	7/7	0.89	0.27	53,57,73,73	0
3	MLI	D	402	7/7	0.91	0.16	47,54,58,62	0
3	MLI	C	402	7/7	0.93	0.14	41,46,65,68	0
2	ARG	B	401	12/12	0.95	0.12	28,34,41,41	0
2	ARG	A	401	12/12	0.97	0.09	27,32,36,38	0
2	ARG	C	401	12/12	0.98	0.12	18,25,30,30	0
2	ARG	D	401	12/12	0.98	0.08	27,32,39,39	0

6.5 Other polymers

There are no such residues in this entry.