



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:06 am BST

PDB ID : 5XX1
Title : Crystal structure of Arginine decarboxylase (AdiA) from *Salmonella typhimurium*
Authors : Deka, G.; Bharath, S.R.; Shavithri, H.S.; Murthy, M.R.N.
Deposited on : 2017-06-30
Resolution : 3.10 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

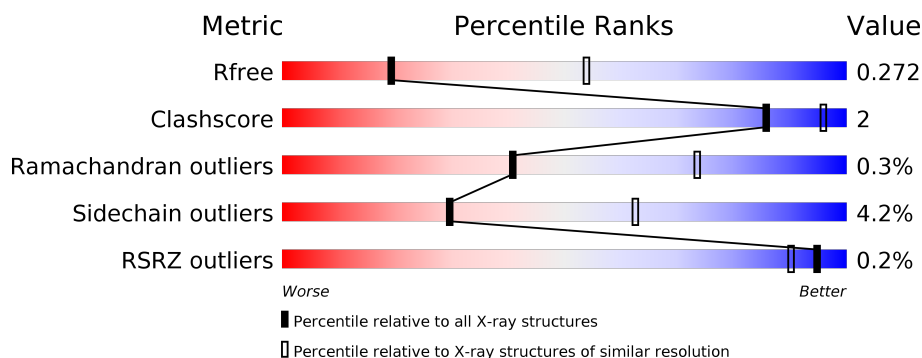
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	756	<div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	B	756	<div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	C	756	<div> <div>%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	D	756	<div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	E	756	<div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	F	756	<div> <div>89%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	756	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>89%</div><div>8%</div><div>• •</div></div></div>
1	H	756	<div><div><div></div><div></div><div></div></div><div>90%</div><div>7%</div><div>• •</div></div>
1	I	756	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>90%</div><div>7%</div><div>•</div></div></div>
1	J	756	<div><div><div></div><div></div><div></div></div><div>89%</div><div>8%</div><div>•</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 57533 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 Arginine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5607	3558	950	1061	38			
1	B	732	Total	C	N	O	S	0	0	0
			5543	3516	940	1049	38			
1	C	733	Total	C	N	O	S	0	0	0
			5526	3504	938	1047	37			
1	D	731	Total	C	N	O	S	0	1	0
			5531	3505	935	1055	36			
1	E	732	Total	C	N	O	S	0	0	0
			5566	3526	940	1063	37			
1	F	732	Total	C	N	O	S	0	0	0
			5597	3549	952	1058	38			
1	G	735	Total	C	N	O	S	0	0	0
			5684	3597	967	1082	38			
1	H	733	Total	C	N	O	S	0	0	0
			5697	3601	974	1084	38			
1	I	735	Total	C	N	O	S	0	0	0
			5665	3584	968	1076	37			
1	J	734	Total	C	N	O	S	0	0	0
			5682	3595	970	1079	38			

There are 10 discrepancies between the modelled and reference sequences:

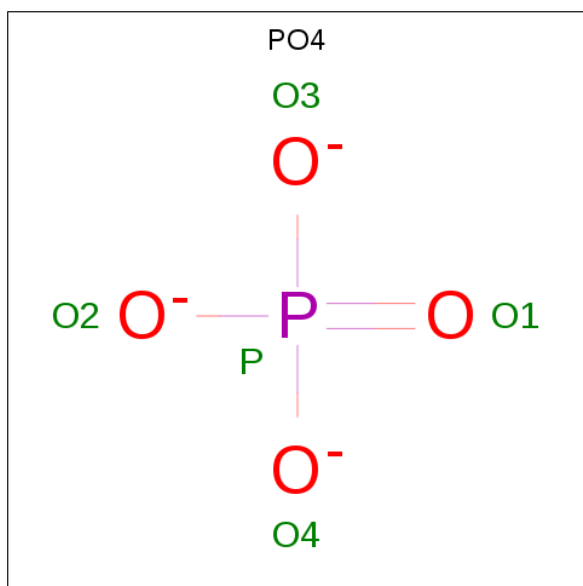
Chain	Residue	Modelled	Actual	Comment	Reference
A	174	SER	ALA	engineered mutation	UNP Q8Z1P1
B	174	SER	ALA	engineered mutation	UNP Q8Z1P1
C	174	SER	ALA	engineered mutation	UNP Q8Z1P1
D	174	SER	ALA	engineered mutation	UNP Q8Z1P1
E	174	SER	ALA	engineered mutation	UNP Q8Z1P1
F	174	SER	ALA	engineered mutation	UNP Q8Z1P1
G	174	SER	ALA	engineered mutation	UNP Q8Z1P1
H	174	SER	ALA	engineered mutation	UNP Q8Z1P1
I	174	SER	ALA	engineered mutation	UNP Q8Z1P1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	174	SER	ALA	engineered mutation	UNP Q8Z1P1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

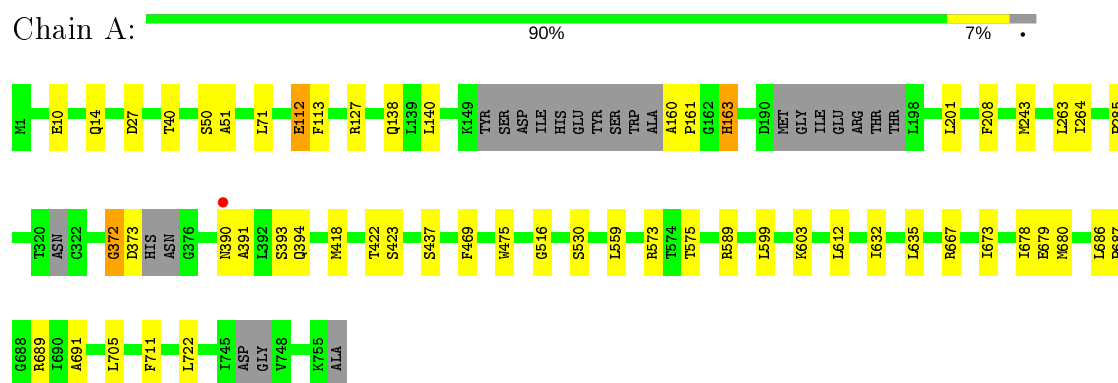
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	118	Total 118	O 118	0	0
3	C	112	Total 112	O 112	0	0
3	D	137	Total 137	O 137	0	0
3	E	134	Total 134	O 134	0	0
3	F	119	Total 119	O 119	0	0
3	G	154	Total 154	O 154	0	0
3	H	160	Total 160	O 160	0	0
3	I	137	Total 137	O 137	0	0
3	J	151	Total 151	O 151	0	0

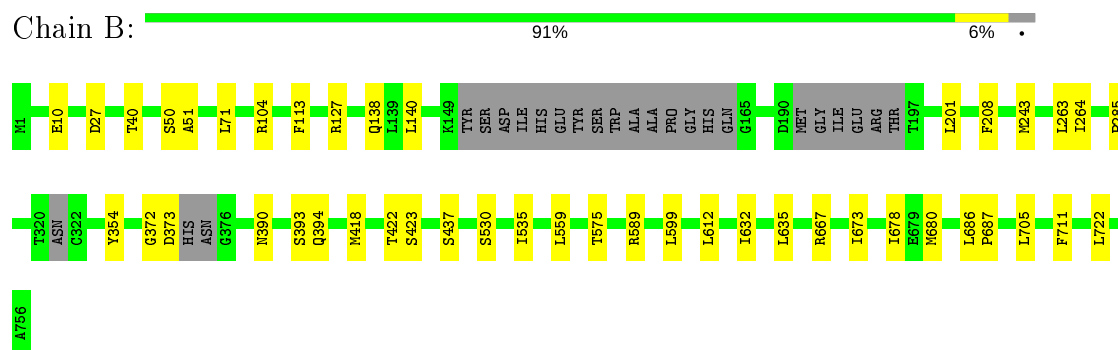
3 Residue-property plots

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.

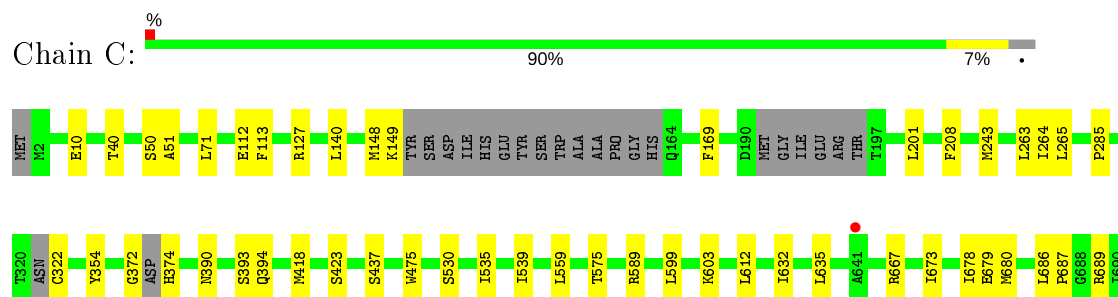
- Molecule 1: Arginine decarboxylase

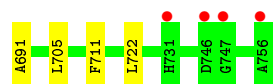


- Molecule 1: Arginine decarboxylase



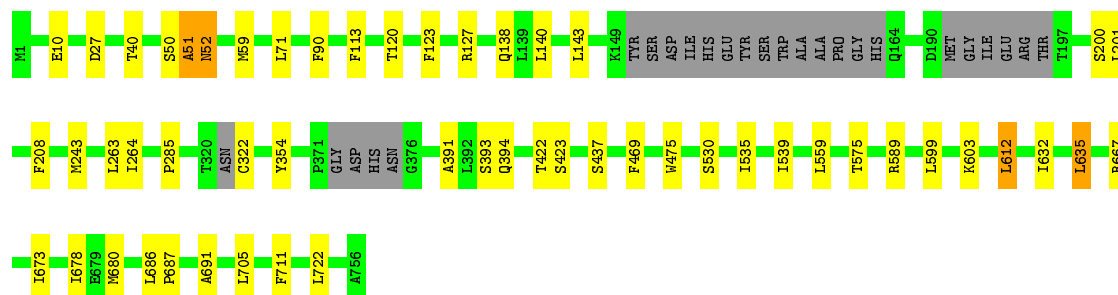
- Molecule 1: Arginine decarboxylase





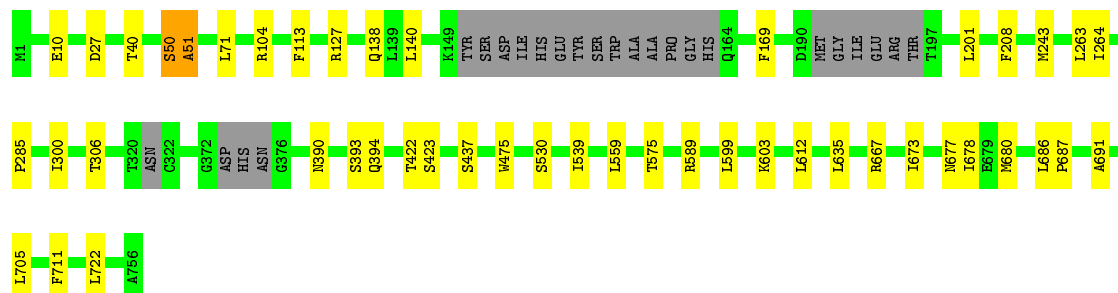
- Molecule 1: Arginine decarboxylase

Chain D: 90% 7% ..



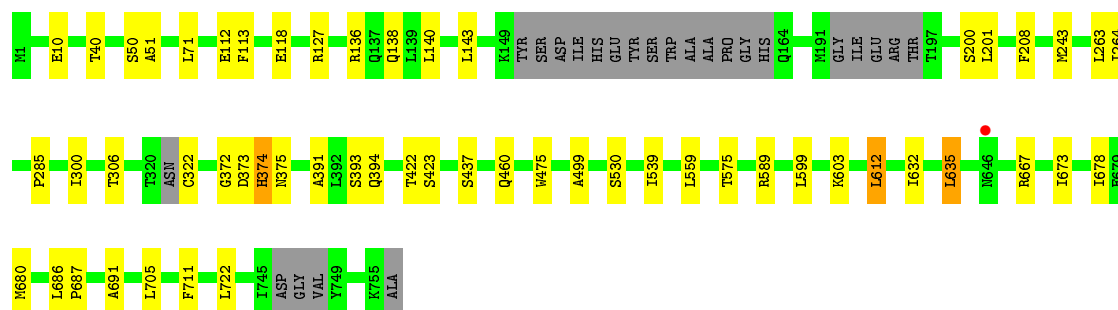
- Molecule 1: Arginine decarboxylase

Chain E: 91% 6% .



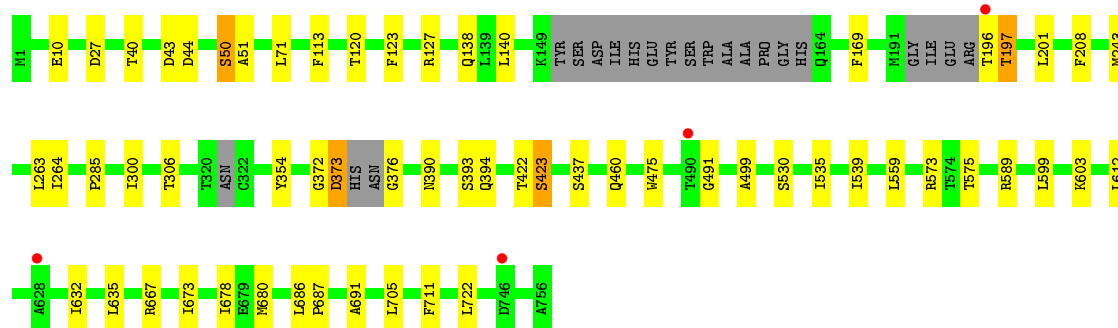
- Molecule 1: Arginine decarboxylase

Chain F: 89% 7% .



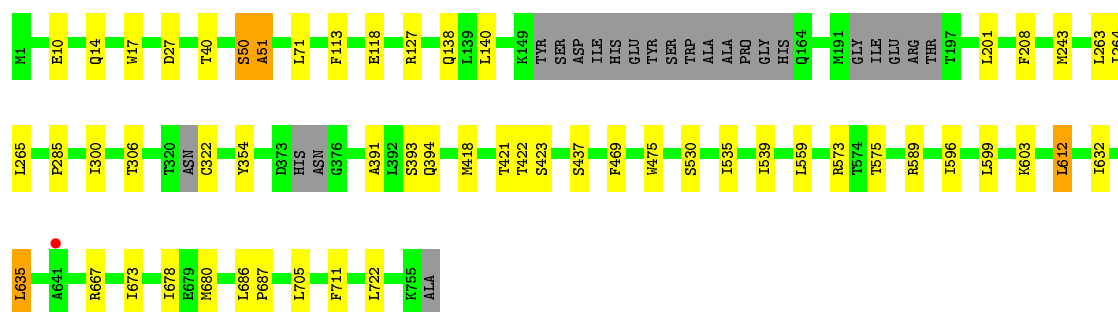
- Molecule 1: Arginine decarboxylase

Chain G: 89% 8% ..



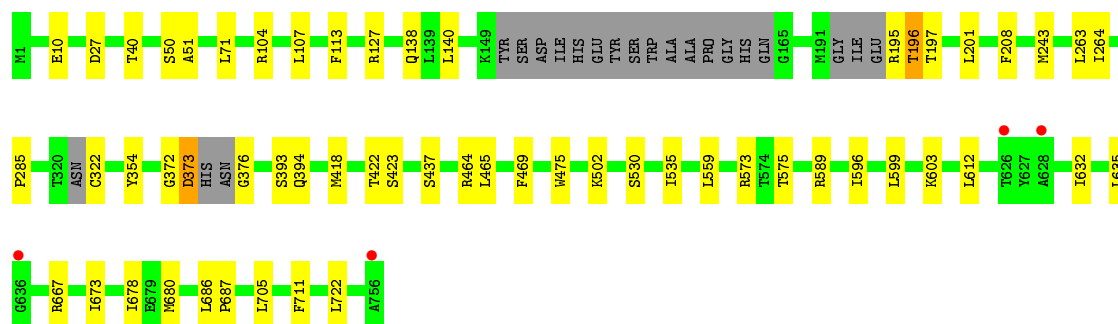
• Molecule 1: Arginine decarboxylase

Chain H: 90% 7% . .



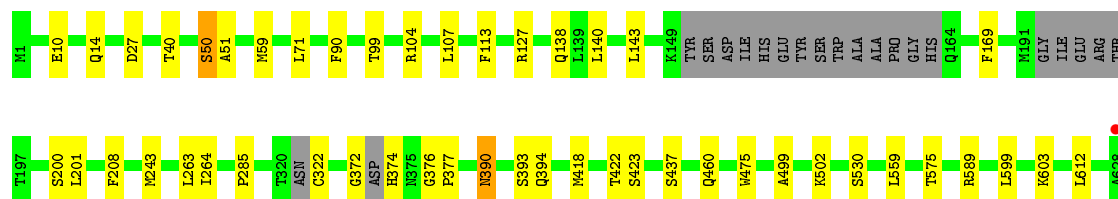
• Molecule 1: Arginine decarboxylase

Chain I: 90% 7% .



• Molecule 1: Arginine decarboxylase

Chain J: 89% 8% .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	179.36Å 193.25Å 280.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.12 – 3.10 57.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (57.12-3.10) 90.8 (57.12-3.10)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.241 , 0.272 0.240 , 0.272	Depositor DCC
R_{free} test set	7890 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	57533	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: CME, PO4

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	0.29	0/5735	0.50	0/7809
1	B	0.30	0/5671	0.50	0/7730
1	C	0.30	0/5652	0.50	0/7703
1	D	0.30	0/5660	0.50	0/7715
1	E	0.30	0/5693	0.50	0/7757
1	F	0.30	0/5726	0.51	0/7797
1	G	0.30	0/5811	0.50	0/7901
1	H	0.31	0/5825	0.51	0/7919
1	I	0.30	0/5792	0.51	0/7879
1	J	0.32	0/5810	0.52	2/7899 (0.0%)
All	All	0.30	0/57375	0.51	2/78109 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	376	GLY	C-N-CD	6.59	142.25	128.40
1	J	377	PRO	CA-N-CD	-5.03	104.46	111.50

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	5607	0	5290	26	1
1	B	5543	0	5171	23	0
1	C	5526	0	5133	22	0
1	D	5531	0	5148	26	0
1	E	5566	0	5210	17	0
1	F	5597	0	5261	29	0
1	G	5684	0	5419	25	1
1	H	5697	0	5443	39	0
1	I	5665	0	5386	30	0
1	J	5682	0	5420	34	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
3	A	163	0	0	0	0
3	B	118	0	0	1	0
3	C	112	0	0	0	0
3	D	137	0	0	0	0
3	E	134	0	0	2	0
3	F	119	0	0	1	0
3	G	154	0	0	0	0
3	H	160	0	0	0	0
3	I	137	0	0	0	0
3	J	151	0	0	0	0
All	All	57533	0	52881	242	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 2.

All (242) 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:372:GLY:C	1:C:374:HIS:N	2.07	1.07
1:H:705:LEU:HD22	1:H:711:PHE:CE1	1.92	1.05
1:B:705:LEU:HD22	1:B:711:PHE:CE1	1.95	1.02
1:I:705:LEU:HD22	1:I:711:PHE:CE1	1.98	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD11	1:D:208:PHE:CE1	1.99	0.98
1:H:686:LEU:HB3	1:H:711:PHE:HD2	1.29	0.97
1:J:372:GLY:C	1:J:374:HIS:N	2.16	0.97
1:F:143:LEU:HD11	1:F:208:PHE:CE1	2.01	0.95
1:J:143:LEU:HD11	1:J:208:PHE:CE1	2.00	0.95
1:D:143:LEU:HD11	1:D:208:PHE:CD1	2.07	0.90
1:B:686:LEU:HD22	1:B:711:PHE:HE2	1.38	0.89
1:I:686:LEU:HD22	1:I:711:PHE:HE2	1.35	0.89
1:F:143:LEU:HD11	1:F:208:PHE:CD1	2.07	0.89
1:D:143:LEU:CD1	1:D:208:PHE:CD1	2.57	0.86
1:F:143:LEU:CD1	1:F:208:PHE:CD1	2.58	0.86
1:J:143:LEU:CD1	1:J:208:PHE:CD1	2.58	0.86
1:J:143:LEU:HD11	1:J:208:PHE:CD1	2.09	0.86
1:B:686:LEU:HB3	1:B:711:PHE:HD2	1.41	0.85
1:H:705:LEU:HD22	1:H:711:PHE:HE1	1.37	0.85
1:I:686:LEU:HB3	1:I:711:PHE:HD2	1.42	0.85
1:H:686:LEU:HB3	1:H:711:PHE:CD2	2.13	0.84
1:H:686:LEU:HD22	1:H:711:PHE:HE2	1.42	0.84
1:I:686:LEU:HB3	1:I:711:PHE:CD2	2.16	0.80
1:B:705:LEU:HD22	1:B:711:PHE:HE1	1.46	0.80
1:I:686:LEU:HD22	1:I:711:PHE:CE2	2.16	0.80
1:B:686:LEU:HB3	1:B:711:PHE:CD2	2.17	0.79
1:B:686:LEU:HD22	1:B:711:PHE:CE2	2.18	0.79
1:H:686:LEU:HD22	1:H:711:PHE:CE2	2.19	0.76
1:I:705:LEU:HD22	1:I:711:PHE:HE1	1.48	0.75
1:H:705:LEU:HD22	1:H:711:PHE:CD1	2.21	0.75
1:A:163:HIS:HB3	1:J:390:ASN:HD22	1.53	0.73
1:D:143:LEU:HD13	1:D:208:PHE:HD1	1.54	0.72
1:D:143:LEU:CD1	1:D:208:PHE:HD1	2.04	0.71
1:C:372:GLY:O	1:C:374:HIS:N	2.23	0.71
1:B:705:LEU:HD22	1:B:711:PHE:CD1	2.25	0.71
1:J:143:LEU:HD13	1:J:208:PHE:HD1	1.56	0.70
1:H:705:LEU:CD2	1:H:711:PHE:CD1	2.75	0.70
1:F:143:LEU:HD13	1:F:208:PHE:HD1	1.57	0.68
1:B:705:LEU:CD2	1:B:711:PHE:CD1	2.78	0.67
1:F:143:LEU:CD1	1:F:208:PHE:HD1	2.07	0.65
1:I:705:LEU:HD22	1:I:711:PHE:CD1	2.30	0.65
1:A:160:ALA:HB3	1:A:161:PRO:CD	2.28	0.64
1:D:200:SER:C	1:D:208:PHE:HD2	2.02	0.63
1:F:373:ASP:C	1:F:375:ASN:N	2.50	0.62
1:I:705:LEU:CD2	1:I:711:PHE:CD1	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:LEU:HD13	1:C:711:PHE:CE2	2.35	0.62
1:J:200:SER:C	1:J:208:PHE:HD2	2.03	0.62
1:F:200:SER:C	1:F:208:PHE:HD2	2.04	0.61
1:F:373:ASP:O	1:F:375:ASN:N	2.34	0.61
1:E:686:LEU:HD13	1:E:711:PHE:CE2	2.36	0.60
1:D:686:LEU:HD13	1:D:711:PHE:CE2	2.38	0.59
1:J:686:LEU:HD13	1:J:711:PHE:CE2	2.37	0.59
1:H:469:PHE:CZ	1:I:104:ARG:HD3	2.37	0.58
1:A:686:LEU:HD13	1:A:711:PHE:CE2	2.39	0.58
1:F:686:LEU:HD13	1:F:711:PHE:CE2	2.39	0.58
1:A:163:HIS:N	1:J:390:ASN:HB2	2.19	0.57
1:H:705:LEU:HD21	1:H:711:PHE:HD1	1.69	0.57
1:F:285:PRO:HG3	1:F:530:SER:OG	2.05	0.56
1:D:285:PRO:HG3	1:D:530:SER:OG	2.06	0.55
1:A:285:PRO:HG3	1:A:530:SER:OG	2.07	0.55
1:I:469:PHE:CZ	1:J:104:ARG:HD3	2.42	0.55
1:B:285:PRO:HG3	1:B:530:SER:OG	2.05	0.55
1:G:686:LEU:HD13	1:G:711:PHE:CE2	2.42	0.54
1:D:201:LEU:N	1:D:208:PHE:CD2	2.75	0.54
1:J:285:PRO:HG3	1:J:530:SER:OG	2.08	0.54
1:J:201:LEU:N	1:J:208:PHE:CD2	2.76	0.54
1:I:285:PRO:HG3	1:I:530:SER:OG	2.08	0.54
1:H:285:PRO:HG3	1:H:530:SER:OG	2.09	0.53
1:E:285:PRO:HG3	1:E:530:SER:OG	2.09	0.53
1:G:43:ASP:HB3	1:H:17:TRP:CD2	2.44	0.53
1:F:373:ASP:O	1:F:375:ASN:CB	2.57	0.53
1:G:113:PHE:O	1:G:127:ARG:NH2	2.42	0.53
1:G:285:PRO:HG3	1:G:530:SER:OG	2.08	0.52
1:A:160:ALA:HB3	1:A:161:PRO:HD3	1.91	0.52
1:F:201:LEU:N	1:F:208:PHE:CD2	2.77	0.52
1:G:43:ASP:CB	1:H:17:TRP:CD2	2.93	0.52
1:H:113:PHE:O	1:H:127:ARG:NH2	2.42	0.52
1:C:285:PRO:HG3	1:C:530:SER:OG	2.09	0.52
1:A:163:HIS:CB	1:J:390:ASN:HD22	2.21	0.52
1:D:469:PHE:CZ	1:E:104:ARG:HD3	2.46	0.51
1:H:686:LEU:HD13	1:H:711:PHE:CE2	2.45	0.51
1:H:705:LEU:CD2	1:H:711:PHE:HD1	2.19	0.51
1:H:705:LEU:HD21	1:H:711:PHE:CD1	2.45	0.50
1:C:113:PHE:O	1:C:127:ARG:NH2	2.45	0.50
1:E:677:ASN:ND2	3:E:901:HOH:O	2.45	0.50
1:E:113:PHE:O	1:E:127:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:PHE:O	1:F:127:ARG:NH2	2.41	0.50
1:G:43:ASP:HB2	1:H:17:TRP:CE3	2.47	0.49
1:I:195:ARG:O	1:I:196:THR:CB	2.61	0.49
1:B:113:PHE:O	1:B:127:ARG:NH2	2.43	0.49
1:B:705:LEU:HD21	1:B:711:PHE:CD1	2.48	0.49
1:E:169:PHE:CZ	1:F:391:ALA:HA	2.48	0.48
1:H:673:ILE:HA	1:H:678:ILE:HG13	1.96	0.48
1:J:113:PHE:O	1:J:127:ARG:NH2	2.46	0.48
1:G:705:LEU:HD22	1:G:711:PHE:CE1	2.48	0.48
1:D:51:ALA:O	1:D:52:ASN:CG	2.52	0.48
1:F:691:ALA:HB2	1:F:711:PHE:HE1	1.78	0.48
1:H:201:LEU:HB2	1:H:208:PHE:CE2	2.49	0.48
1:D:143:LEU:HD11	1:D:208:PHE:HE1	1.71	0.48
1:E:686:LEU:N	1:E:687:PRO:CD	2.77	0.48
1:F:673:ILE:HA	1:F:678:ILE:HG13	1.95	0.48
1:J:691:ALA:HB2	1:J:711:PHE:HE1	1.78	0.48
1:J:673:ILE:HA	1:J:678:ILE:HG13	1.96	0.48
1:B:705:LEU:HD21	1:B:711:PHE:HD1	1.79	0.48
1:F:475:TRP:O	1:F:603:LYS:HE3	2.14	0.48
1:G:673:ILE:HA	1:G:678:ILE:HG13	1.96	0.48
1:C:691:ALA:HB2	1:C:711:PHE:HE1	1.79	0.47
1:I:673:ILE:HA	1:I:678:ILE:HG13	1.95	0.47
1:G:196:THR:O	1:G:197:THR:CB	2.62	0.47
1:A:691:ALA:HB2	1:A:711:PHE:HE1	1.79	0.47
1:E:673:ILE:HA	1:E:678:ILE:HG13	1.95	0.47
1:G:691:ALA:HB2	1:G:711:PHE:HE1	1.78	0.47
1:C:705:LEU:HD22	1:C:711:PHE:CE1	2.49	0.47
1:H:596:ILE:HG21	1:I:107:LEU:HD21	1.95	0.47
1:D:673:ILE:HA	1:D:678:ILE:HG13	1.95	0.47
1:H:264:ILE:HG23	1:H:667:ARG:HA	1.96	0.47
1:I:113:PHE:O	1:I:127:ARG:NH2	2.46	0.47
1:A:201:LEU:HB2	1:A:208:PHE:CE2	2.50	0.47
1:A:686:LEU:N	1:A:687:PRO:CD	2.78	0.47
1:B:673:ILE:HA	1:B:678:ILE:HG13	1.96	0.47
1:I:201:LEU:HB2	1:I:208:PHE:CE2	2.49	0.47
1:B:127:ARG:NH1	3:B:902:HOH:O	2.47	0.47
1:G:201:LEU:HB2	1:G:208:PHE:CE2	2.50	0.47
1:A:113:PHE:O	1:A:127:ARG:NH2	2.46	0.47
1:C:169:PHE:CZ	1:H:391:ALA:HA	2.50	0.47
1:D:691:ALA:HB2	1:D:711:PHE:HE1	1.79	0.47
1:E:691:ALA:HB2	1:E:711:PHE:HE1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:475:TRP:O	1:H:603:LYS:HE3	2.16	0.46
1:B:201:LEU:HB2	1:B:208:PHE:CE2	2.50	0.46
1:E:264:ILE:HG23	1:E:667:ARG:HA	1.97	0.46
1:J:264:ILE:HG23	1:J:667:ARG:HA	1.97	0.46
1:J:705:LEU:HD22	1:J:711:PHE:CE1	2.50	0.46
1:F:686:LEU:N	1:F:687:PRO:CD	2.79	0.46
1:F:705:LEU:HD22	1:F:711:PHE:CE1	2.51	0.46
1:A:163:HIS:HA	1:J:390:ASN:HD22	1.81	0.46
1:C:673:ILE:HA	1:C:678:ILE:HG13	1.98	0.46
1:F:264:ILE:HG23	1:F:667:ARG:HA	1.97	0.46
1:B:705:LEU:CD2	1:B:711:PHE:HD1	2.28	0.46
1:C:201:LEU:HB2	1:C:208:PHE:CE2	2.50	0.46
1:G:686:LEU:N	1:G:687:PRO:CD	2.79	0.46
1:A:705:LEU:HD22	1:A:711:PHE:CE1	2.50	0.46
1:C:686:LEU:N	1:C:687:PRO:CD	2.79	0.46
1:D:391:ALA:HA	1:G:169:PHE:CZ	2.51	0.46
1:A:393:SER:O	1:A:394:GLN:HB2	2.16	0.46
1:B:264:ILE:HG23	1:B:667:ARG:HA	1.98	0.46
1:I:705:LEU:HD21	1:I:711:PHE:CD1	2.51	0.46
1:A:673:ILE:HA	1:A:678:ILE:HG13	1.96	0.46
1:D:705:LEU:HD22	1:D:711:PHE:CE1	2.51	0.46
1:J:475:TRP:O	1:J:603:LYS:HE3	2.16	0.46
1:J:686:LEU:N	1:J:687:PRO:CD	2.78	0.46
1:C:393:SER:O	1:C:394:GLN:HB2	2.16	0.45
1:G:44:ASP:HA	1:H:17:TRP:HB2	1.98	0.45
1:I:393:SER:O	1:I:394:GLN:HB2	2.16	0.45
1:D:686:LEU:N	1:D:687:PRO:CD	2.79	0.45
1:G:475:TRP:O	1:G:603:LYS:HE3	2.17	0.45
1:A:112:GLU:HG3	3:E:905:HOH:O	2.16	0.45
1:A:160:ALA:CB	1:A:161:PRO:CD	2.94	0.45
1:D:113:PHE:O	1:D:127:ARG:NH2	2.49	0.45
1:I:686:LEU:N	1:I:687:PRO:CD	2.80	0.45
1:C:475:TRP:O	1:C:603:LYS:HE3	2.17	0.45
1:H:393:SER:O	1:H:394:GLN:HB2	2.17	0.45
1:H:469:PHE:CE1	1:I:104:ARG:HD3	2.52	0.45
1:I:475:TRP:O	1:I:603:LYS:HE3	2.16	0.45
1:B:393:SER:O	1:B:394:GLN:HB2	2.17	0.45
1:A:264:ILE:HG23	1:A:667:ARG:HA	1.99	0.44
1:D:264:ILE:HG23	1:D:667:ARG:HA	1.99	0.44
1:E:393:SER:O	1:E:394:GLN:HB2	2.18	0.44
1:A:163:HIS:HB3	1:J:390:ASN:ND2	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:ASP:OD1	1:G:376:GLY:N	2.50	0.44
1:B:686:LEU:N	1:B:687:PRO:CD	2.79	0.44
1:F:393:SER:O	1:F:394:GLN:HB2	2.17	0.44
1:H:686:LEU:N	1:H:687:PRO:CD	2.80	0.44
1:I:264:ILE:HG23	1:I:667:ARG:HA	1.99	0.44
1:E:705:LEU:HD22	1:E:711:PHE:CE1	2.51	0.44
1:I:469:PHE:CE1	1:J:104:ARG:HD3	2.53	0.44
1:A:163:HIS:CA	1:J:390:ASN:HD22	2.31	0.44
1:D:393:SER:O	1:D:394:GLN:HB2	2.18	0.44
1:I:596:ILE:HG21	1:J:107:LEU:HD21	2.00	0.44
1:J:460:GLN:NE2	1:J:499:ALA:O	2.51	0.44
1:F:673:ILE:HA	1:F:678:ILE:CG1	2.48	0.43
1:B:686:LEU:HD13	1:B:711:PHE:CE2	2.54	0.43
1:G:354:TYR:CZ	1:G:535:ILE:HD11	2.53	0.43
1:C:418:MET:HE2	1:H:265:LEU:CD2	2.48	0.43
1:C:265:LEU:CD2	1:H:418:MET:HE2	2.48	0.43
1:G:264:ILE:HG23	1:G:667:ARG:HA	2.00	0.43
1:H:354:TYR:CZ	1:H:535:ILE:HD11	2.54	0.43
1:H:300:ILE:HG23	1:H:306:THR:HB	2.01	0.43
1:E:673:ILE:HA	1:E:678:ILE:CG1	2.49	0.42
1:F:373:ASP:O	1:F:374:HIS:C	2.57	0.42
1:G:393:SER:O	1:G:394:GLN:HB2	2.18	0.42
1:J:393:SER:O	1:J:394:GLN:HB2	2.18	0.42
1:I:705:LEU:HD21	1:I:711:PHE:HD1	1.85	0.42
1:C:265:LEU:HD21	1:H:418:MET:HE2	2.01	0.42
1:E:201:LEU:HB2	1:E:208:PHE:CE2	2.54	0.42
1:D:354:TYR:CZ	1:D:535:ILE:HD11	2.54	0.42
1:F:143:LEU:HD13	1:F:208:PHE:CD1	2.35	0.42
1:C:394:GLN:HG2	1:H:421:THR:HG21	2.02	0.42
1:I:373:ASP:OD1	1:I:376:GLY:N	2.52	0.42
1:A:391:ALA:HA	1:J:169:PHE:CZ	2.55	0.42
1:C:264:ILE:HG23	1:C:667:ARG:HA	1.99	0.42
1:G:460:GLN:NE2	1:G:499:ALA:O	2.52	0.42
1:B:673:ILE:HA	1:B:678:ILE:CG1	2.50	0.42
1:G:673:ILE:HA	1:G:678:ILE:CG1	2.49	0.42
1:H:612:LEU:HD21	1:H:635:LEU:HD12	2.02	0.42
1:A:475:TRP:O	1:A:603:LYS:HE3	2.20	0.42
1:E:475:TRP:O	1:E:603:LYS:HE3	2.20	0.42
1:J:673:ILE:HA	1:J:678:ILE:CG1	2.50	0.42
1:B:354:TYR:CZ	1:B:535:ILE:HD11	2.54	0.41
1:C:148:MET:O	1:C:149:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:673:ILE:HA	1:I:678:ILE:CG1	2.50	0.41
1:A:372:GLY:O	1:A:373:ASP:CB	2.68	0.41
1:A:679:GLU:OE1	1:A:689:ARG:NH2	2.53	0.41
1:D:475:TRP:O	1:D:603:LYS:HE3	2.20	0.41
1:J:200:SER:C	1:J:208:PHE:CD2	2.89	0.41
1:A:673:ILE:HA	1:A:678:ILE:CG1	2.51	0.41
1:D:120:THR:HB	1:D:123:PHE:CD2	2.56	0.41
1:D:673:ILE:HA	1:D:678:ILE:CG1	2.50	0.41
1:F:136:ARG:NE	3:F:901:HOH:O	2.54	0.41
1:F:300:ILE:HG23	1:F:306:THR:HB	2.03	0.41
2:D:801:PO4:O2	1:G:423:SER:OG	2.38	0.41
1:H:705:LEU:CD2	1:H:711:PHE:CE1	2.81	0.41
1:H:673:ILE:HA	1:H:678:ILE:CG1	2.50	0.41
1:A:469:PHE:CZ	1:B:104:ARG:HD3	2.56	0.41
1:D:612:LEU:HD21	1:D:635:LEU:HD12	2.03	0.41
1:I:686:LEU:HD13	1:I:711:PHE:CE2	2.56	0.41
1:G:120:THR:HB	1:G:123:PHE:CD2	2.56	0.40
1:I:354:TYR:CZ	1:I:535:ILE:HD11	2.55	0.40
1:F:118:GLU:HA	1:J:50:SER:HB3	2.03	0.40
1:J:59:MET:HG2	1:J:90:PHE:HB2	2.02	0.40
1:C:372:GLY:CA	1:C:374:HIS:N	2.80	0.40
1:C:679:GLU:OE1	1:C:689:ARG:NH2	2.55	0.40
1:F:460:GLN:NE2	1:F:499:ALA:O	2.54	0.40
1:F:612:LEU:HD21	1:F:635:LEU:HD12	2.03	0.40
1:D:59:MET:HG2	1:D:90:PHE:HB2	2.02	0.40
1:E:50:SER:C	1:E:51:ALA:O	2.60	0.40
1:G:300:ILE:HG23	1:G:306:THR:HB	2.02	0.40
1:G:50:SER:HB3	1:H:118:GLU:HA	2.04	0.40
1:C:354:TYR:CZ	1:C:535:ILE:HD11	2.56	0.40
1:E:300:ILE:HG23	1:E:306:THR:HB	2.04	0.40
1:H:50:SER:C	1:H:51:ALA:O	2.60	0.40
1:J:390:ASN:CG	1:J:390:ASN:O	2.60	0.40
1:I:464:ARG:NH1	1:J:99:THR:O	2.55	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:516:GLY:O	1:G:491:GLY:O[3_545]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	720/756 (95%)	695 (96%)	23 (3%)	2 (0%)	41	73
1	B	721/756 (95%)	695 (96%)	24 (3%)	2 (0%)	41	73
1	C	722/756 (96%)	699 (97%)	22 (3%)	1 (0%)	51	83
1	D	721/756 (95%)	698 (97%)	21 (3%)	2 (0%)	41	73
1	E	721/756 (95%)	697 (97%)	23 (3%)	1 (0%)	51	83
1	F	721/756 (95%)	692 (96%)	26 (4%)	3 (0%)	34	69
1	G	724/756 (96%)	698 (96%)	23 (3%)	3 (0%)	34	69
1	H	722/756 (96%)	696 (96%)	25 (4%)	1 (0%)	51	83
1	I	724/756 (96%)	695 (96%)	25 (4%)	4 (1%)	25	59
1	J	723/756 (96%)	693 (96%)	29 (4%)	1 (0%)	51	83
All	All	7219/7560 (96%)	6958 (96%)	241 (3%)	20 (0%)	41	73

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	51	ALA
1	D	52	ASN
1	F	374	HIS
1	I	196	THR
1	I	197	THR
1	A	51	ALA
1	G	197	THR
1	H	51	ALA
1	J	51	ALA
1	B	51	ALA
1	C	51	ALA
1	E	51	ALA
1	F	51	ALA
1	G	51	ALA

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Mol	Chain	Res	Type
1	I	51	ALA
1	A	372	GLY
1	B	372	GLY
1	G	372	GLY
1	I	372	GLY
1	F	372	GLY

5.3.2 Protein sidechains ⓘ

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	575/633 (91%)	548 (95%)	27 (5%)	26	59
1	B	559/633 (88%)	535 (96%)	24 (4%)	29	62
1	C	554/633 (88%)	532 (96%)	22 (4%)	31	65
1	D	558/633 (88%)	535 (96%)	23 (4%)	30	64
1	E	569/633 (90%)	547 (96%)	22 (4%)	32	65
1	F	571/633 (90%)	548 (96%)	23 (4%)	31	65
1	G	595/633 (94%)	570 (96%)	25 (4%)	30	62
1	H	601/633 (95%)	576 (96%)	25 (4%)	30	62
1	I	589/633 (93%)	562 (95%)	27 (5%)	27	59
1	J	596/633 (94%)	570 (96%)	26 (4%)	28	61
All	All	5767/6330 (91%)	5523 (96%)	244 (4%)	30	62

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	14	GLN
1	A	27	ASP
1	A	40	THR
1	A	50	SER
1	A	71	LEU
1	A	112	GLU

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Mol	Chain	Res	Type
1	A	138	GLN
1	A	140	LEU
1	A	163	HIS
1	A	243	MET
1	A	263	LEU
1	A	390	ASN
1	A	418	MET
1	A	422	THR
1	A	423	SER
1	A	437	SER
1	A	559	LEU
1	A	573	ARG
1	A	575	THR
1	A	589	ARG
1	A	599	LEU
1	A	612	LEU
1	A	632	ILE
1	A	635	LEU
1	A	680	MET
1	A	722	LEU
1	B	10	GLU
1	B	27	ASP
1	B	40	THR
1	B	50	SER
1	B	71	LEU
1	B	138	GLN
1	B	140	LEU
1	B	243	MET
1	B	263	LEU
1	B	373	ASP
1	B	390	ASN
1	B	418	MET
1	B	422	THR
1	B	423	SER
1	B	437	SER
1	B	559	LEU
1	B	575	THR
1	B	589	ARG
1	B	599	LEU
1	B	612	LEU
1	B	632	ILE
1	B	635	LEU

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Mol	Chain	Res	Type
1	B	680	MET
1	B	722	LEU
1	C	10	GLU
1	C	40	THR
1	C	50	SER
1	C	71	LEU
1	C	112	GLU
1	C	140	LEU
1	C	243	MET
1	C	263	LEU
1	C	322	CYS
1	C	390	ASN
1	C	423	SER
1	C	437	SER
1	C	539	ILE
1	C	559	LEU
1	C	575	THR
1	C	589	ARG
1	C	599	LEU
1	C	612	LEU
1	C	632	ILE
1	C	635	LEU
1	C	680	MET
1	C	722	LEU
1	D	10	GLU
1	D	27	ASP
1	D	40	THR
1	D	50	SER
1	D	71	LEU
1	D	138	GLN
1	D	140	LEU
1	D	243	MET
1	D	263	LEU
1	D	322	CYS
1	D	422	THR
1	D	423	SER
1	D	437	SER
1	D	539	ILE
1	D	559	LEU
1	D	575	THR
1	D	589	ARG
1	D	599	LEU

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Mol	Chain	Res	Type
1	D	612	LEU
1	D	632	ILE
1	D	635	LEU
1	D	680	MET
1	D	722	LEU
1	E	10	GLU
1	E	27	ASP
1	E	40	THR
1	E	50	SER
1	E	71	LEU
1	E	138	GLN
1	E	140	LEU
1	E	243	MET
1	E	263	LEU
1	E	390	ASN
1	E	422	THR
1	E	423	SER
1	E	437	SER
1	E	539	ILE
1	E	559	LEU
1	E	575	THR
1	E	589	ARG
1	E	599	LEU
1	E	612	LEU
1	E	635	LEU
1	E	680	MET
1	E	722	LEU
1	F	10	GLU
1	F	40	THR
1	F	50	SER
1	F	71	LEU
1	F	112	GLU
1	F	138	GLN
1	F	140	LEU
1	F	243	MET
1	F	263	LEU
1	F	322	CYS
1	F	422	THR
1	F	423	SER
1	F	437	SER
1	F	539	ILE
1	F	559	LEU

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Mol	Chain	Res	Type
1	F	575	THR
1	F	589	ARG
1	F	599	LEU
1	F	612	LEU
1	F	632	ILE
1	F	635	LEU
1	F	680	MET
1	F	722	LEU
1	G	10	GLU
1	G	27	ASP
1	G	40	THR
1	G	50	SER
1	G	71	LEU
1	G	138	GLN
1	G	140	LEU
1	G	243	MET
1	G	263	LEU
1	G	373	ASP
1	G	390	ASN
1	G	422	THR
1	G	423	SER
1	G	437	SER
1	G	539	ILE
1	G	559	LEU
1	G	573	ARG
1	G	575	THR
1	G	589	ARG
1	G	599	LEU
1	G	612	LEU
1	G	632	ILE
1	G	635	LEU
1	G	680	MET
1	G	722	LEU
1	H	10	GLU
1	H	14	GLN
1	H	27	ASP
1	H	40	THR
1	H	50	SER
1	H	71	LEU
1	H	138	GLN
1	H	140	LEU
1	H	243	MET

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Mol	Chain	Res	Type
1	H	263	LEU
1	H	322	CYS
1	H	422	THR
1	H	423	SER
1	H	437	SER
1	H	539	ILE
1	H	559	LEU
1	H	573	ARG
1	H	575	THR
1	H	589	ARG
1	H	599	LEU
1	H	612	LEU
1	H	632	ILE
1	H	635	LEU
1	H	680	MET
1	H	722	LEU
1	I	10	GLU
1	I	27	ASP
1	I	40	THR
1	I	50	SER
1	I	71	LEU
1	I	138	GLN
1	I	140	LEU
1	I	243	MET
1	I	263	LEU
1	I	322	CYS
1	I	373	ASP
1	I	418	MET
1	I	422	THR
1	I	423	SER
1	I	437	SER
1	I	465	LEU
1	I	502	LYS
1	I	559	LEU
1	I	573	ARG
1	I	575	THR
1	I	589	ARG
1	I	599	LEU
1	I	612	LEU
1	I	632	ILE
1	I	635	LEU
1	I	680	MET

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Mol	Chain	Res	Type
1	I	722	LEU
1	J	10	GLU
1	J	14	GLN
1	J	27	ASP
1	J	40	THR
1	J	50	SER
1	J	71	LEU
1	J	138	GLN
1	J	140	LEU
1	J	243	MET
1	J	263	LEU
1	J	322	CYS
1	J	390	ASN
1	J	418	MET
1	J	422	THR
1	J	423	SER
1	J	437	SER
1	J	502	LYS
1	J	559	LEU
1	J	575	THR
1	J	589	ARG
1	J	599	LEU
1	J	612	LEU
1	J	632	ILE
1	J	635	LEU
1	J	680	MET
1	J	722	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	20	ASN
1	A	70	HIS
1	A	84	GLN
1	A	204	HIS
1	A	240	GLN
1	A	383	HIS
1	B	13	HIS
1	B	20	ASN
1	B	70	HIS
1	B	204	HIS

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Mol	Chain	Res	Type
1	B	383	HIS
1	B	508	GLN
1	B	750	HIS
1	C	13	HIS
1	C	20	ASN
1	C	70	HIS
1	C	84	GLN
1	C	204	HIS
1	C	383	HIS
1	C	508	GLN
1	C	750	HIS
1	D	13	HIS
1	D	20	ASN
1	D	70	HIS
1	D	84	GLN
1	D	204	HIS
1	D	383	HIS
1	D	386	HIS
1	D	508	GLN
1	D	604	HIS
1	D	750	HIS
1	E	13	HIS
1	E	20	ASN
1	E	70	HIS
1	E	84	GLN
1	E	204	HIS
1	E	383	HIS
1	E	508	GLN
1	E	677	ASN
1	F	13	HIS
1	F	70	HIS
1	F	84	GLN
1	F	204	HIS
1	F	383	HIS
1	F	508	GLN
1	F	750	HIS
1	G	13	HIS
1	G	20	ASN
1	G	31	GLN
1	G	70	HIS
1	G	84	GLN
1	G	204	HIS

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Mol	Chain	Res	Type
1	G	383	HIS
1	G	508	GLN
1	G	750	HIS
1	H	13	HIS
1	H	14	GLN
1	H	70	HIS
1	H	84	GLN
1	H	204	HIS
1	H	383	HIS
1	H	508	GLN
1	H	730	HIS
1	H	750	HIS
1	I	13	HIS
1	I	20	ASN
1	I	70	HIS
1	I	84	GLN
1	I	137	GLN
1	I	204	HIS
1	I	508	GLN
1	I	750	HIS
1	J	13	HIS
1	J	14	GLN
1	J	20	ASN
1	J	63	GLN
1	J	70	HIS
1	J	84	GLN
1	J	204	HIS
1	J	246	ASN
1	J	383	HIS
1	J	390	ASN
1	J	508	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	B	600	1	8,9,10	0.82	0	5,9,11	0.82	0
1	CME	D	600	1	8,9,10	0.79	0	5,9,11	0.86	0
1	CME	I	600	1	8,9,10	0.79	0	5,9,11	0.99	0
1	CME	E	600	1	8,9,10	0.79	0	5,9,11	0.93	0
1	CME	H	600	1	8,9,10	0.75	0	5,9,11	0.93	0
1	CME	G	600	1	8,9,10	0.83	0	5,9,11	0.95	0
1	CME	A	600	1	8,9,10	0.87	0	5,9,11	1.02	0
1	CME	C	600	1	8,9,10	0.85	0	5,9,11	0.93	0
1	CME	J	600	1	8,9,10	0.86	0	5,9,11	1.06	0
1	CME	F	600	1	8,9,10	0.82	0	5,9,11	0.93	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
1	CME	B	600	1	-	1/5/8/10	-
1	CME	D	600	1	-	1/5/8/10	-
1	CME	I	600	1	-	1/5/8/10	-
1	CME	E	600	1	-	1/5/8/10	-
1	CME	H	600	1	-	1/5/8/10	-
1	CME	G	600	1	-	1/5/8/10	-
1	CME	A	600	1	-	1/5/8/10	-
1	CME	C	600	1	-	1/5/8/10	-
1	CME	J	600	1	-	1/5/8/10	-
1	CME	F	600	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	600	CME	SD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
1	D	600	CME	SD-CE-CZ-OH
1	I	600	CME	SD-CE-CZ-OH
1	E	600	CME	SD-CE-CZ-OH
1	H	600	CME	SD-CE-CZ-OH
1	G	600	CME	SD-CE-CZ-OH
1	A	600	CME	SD-CE-CZ-OH
1	C	600	CME	SD-CE-CZ-OH
1	J	600	CME	SD-CE-CZ-OH
1	F	600	CME	SD-CE-CZ-OH

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
2	PO4	E	801	-	4,4,4	0.89	0	6,6,6	0.32	0
2	PO4	C	801	-	4,4,4	0.90	0	6,6,6	0.46	0
2	PO4	I	801	-	4,4,4	0.90	0	6,6,6	0.56	0
2	PO4	B	801	-	4,4,4	0.87	0	6,6,6	0.51	0
2	PO4	F	801	-	4,4,4	0.89	0	6,6,6	0.43	0
2	PO4	D	801	-	4,4,4	0.95	0	6,6,6	0.37	0
2	PO4	J	801	-	4,4,4	0.93	0	6,6,6	0.49	0
2	PO4	G	801	-	4,4,4	0.87	0	6,6,6	0.46	0
2	PO4	H	801	-	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	A	801	-	4,4,4	0.95	0	6,6,6	0.40	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	PO4	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, 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	732/756 (96%)	-0.13	1 (0%) 95 92	15, 29, 45, 60	0
1	B	731/756 (96%)	-0.13	0 100 100	15, 29, 46, 57	0
1	C	732/756 (96%)	-0.11	5 (0%) 87 75	15, 29, 48, 62	0
1	D	730/756 (96%)	-0.14	0 100 100	16, 29, 46, 65	0
1	E	731/756 (96%)	-0.20	0 100 100	16, 28, 46, 60	0
1	F	731/756 (96%)	-0.18	1 (0%) 95 92	16, 26, 42, 61	0
1	G	734/756 (97%)	-0.13	4 (0%) 91 81	15, 27, 45, 62	0
1	H	732/756 (96%)	-0.18	1 (0%) 95 92	13, 25, 42, 59	0
1	I	734/756 (97%)	-0.16	4 (0%) 91 81	15, 28, 46, 62	0
1	J	733/756 (96%)	-0.12	1 (0%) 95 92	16, 28, 48, 67	0
All	All	7320/7560 (96%)	-0.15	17 (0%) 95 90	13, 28, 45, 67	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	746	ASP	2.8
1	C	756	ALA	2.8
1	J	628	ALA	2.7
1	I	628	ALA	2.5
1	G	196	THR	2.2
1	G	746	ASP	2.2
1	G	628	ALA	2.2
1	I	626	THR	2.2
1	A	390	ASN	2.2
1	C	641	ALA	2.1
1	F	646	ASN	2.1
1	H	641	ALA	2.1
1	I	756	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	731	HIS	2.0
1	C	747	GLY	2.0
1	G	490	THR	2.0
1	I	636	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	D	600	10/11	0.91	0.27	36,39,44,44	0
1	CME	H	600	10/11	0.92	0.21	22,23,25,25	0
1	CME	G	600	10/11	0.92	0.25	34,36,41,41	0
1	CME	C	600	10/11	0.92	0.28	37,40,47,47	0
1	CME	J	600	10/11	0.92	0.25	40,43,48,49	0
1	CME	I	600	10/11	0.93	0.23	29,31,34,35	0
1	CME	E	600	10/11	0.94	0.27	34,36,38,38	0
1	CME	A	600	10/11	0.94	0.21	32,33,36,36	0
1	CME	F	600	10/11	0.94	0.22	27,28,32,32	0
1	CME	B	600	10/11	0.96	0.21	32,33,35,35	0

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, 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
2	PO4	B	801	5/5	0.80	0.28	60,61,62,62	0
2	PO4	F	801	5/5	0.85	0.26	77,78,79,80	0
2	PO4	D	801	5/5	0.86	0.24	71,71,72,74	0
2	PO4	G	801	5/5	0.88	0.26	55,56,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	H	801	5/5	0.91	0.21	72,74,75,75	0
2	PO4	I	801	5/5	0.92	0.22	65,66,67,68	0
2	PO4	E	801	5/5	0.92	0.18	57,58,58,59	0
2	PO4	C	801	5/5	0.92	0.17	62,63,63,63	0
2	PO4	A	801	5/5	0.92	0.17	64,64,65,66	0
2	PO4	J	801	5/5	0.94	0.18	59,60,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.