



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:53 AM UTC

PDB ID : 6IV2 / pdb_00006iv2
Title : Crystal structure of a bacterial Bestrophin homolog from *Klebsiella pneumoniae* with a mutation Y211A
Authors : Kittredge, A.; Chen, S.; Yang, T.
Deposited on : 2018-12-02
Resolution : 2.62 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

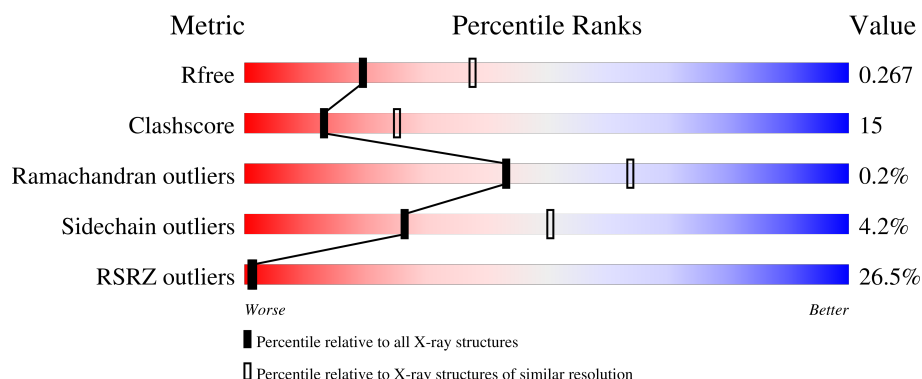
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	296	21% 67% 21% 10%
1	B	296	22% 66% 21% 10%
1	C	296	22% 68% 19% 11%
1	D	296	18% 70% 19% 9%
1	E	296	37% 60% 25% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10448 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 Bestrophin homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2099	1356	358	376	9			
1	B	267	Total	C	N	O	S	0	0	0
			2089	1348	355	377	9			
1	C	262	Total	C	N	O	S	0	0	0
			2045	1319	349	368	9			
1	D	268	Total	C	N	O	S	0	0	0
			2093	1349	359	376	9			
1	E	265	Total	C	N	O	S	0	0	0
			2074	1337	354	374	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP W1ELP7
A	0	ALA	-	expression tag	UNP W1ELP7
A	211	ALA	TYR	engineered mutation	UNP W1ELP7
B	-1	ASN	-	expression tag	UNP W1ELP7
B	0	ALA	-	expression tag	UNP W1ELP7
B	211	ALA	TYR	engineered mutation	UNP W1ELP7
C	-1	ASN	-	expression tag	UNP W1ELP7
C	0	ALA	-	expression tag	UNP W1ELP7
C	211	ALA	TYR	engineered mutation	UNP W1ELP7
D	-1	ASN	-	expression tag	UNP W1ELP7
D	0	ALA	-	expression tag	UNP W1ELP7
D	211	ALA	TYR	engineered mutation	UNP W1ELP7
E	-1	ASN	-	expression tag	UNP W1ELP7
E	0	ALA	-	expression tag	UNP W1ELP7
E	211	ALA	TYR	engineered mutation	UNP W1ELP7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Zn 4	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	3	Total 3	Zn 3	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0

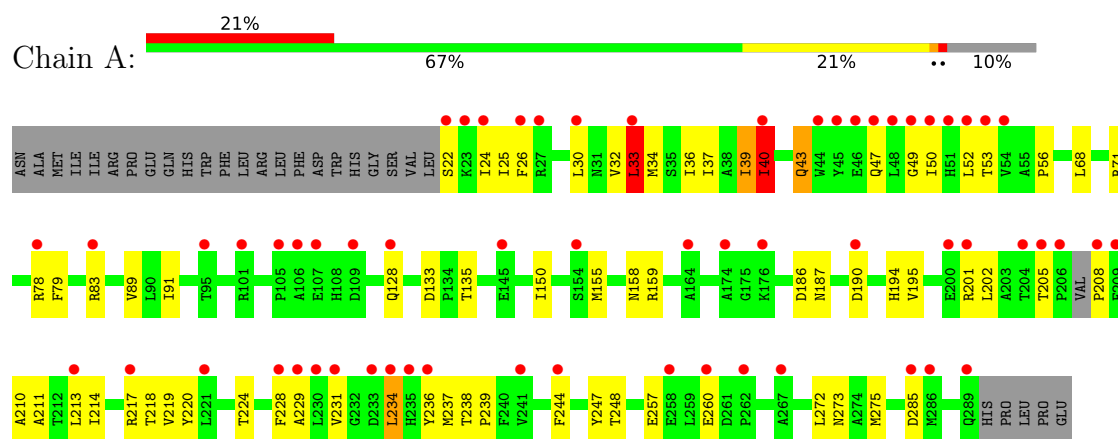
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0
3	B	5	Total 5	O 5	0	0
3	C	9	Total 9	O 9	0	0
3	D	10	Total 10	O 10	0	0
3	E	3	Total 3	O 3	0	0

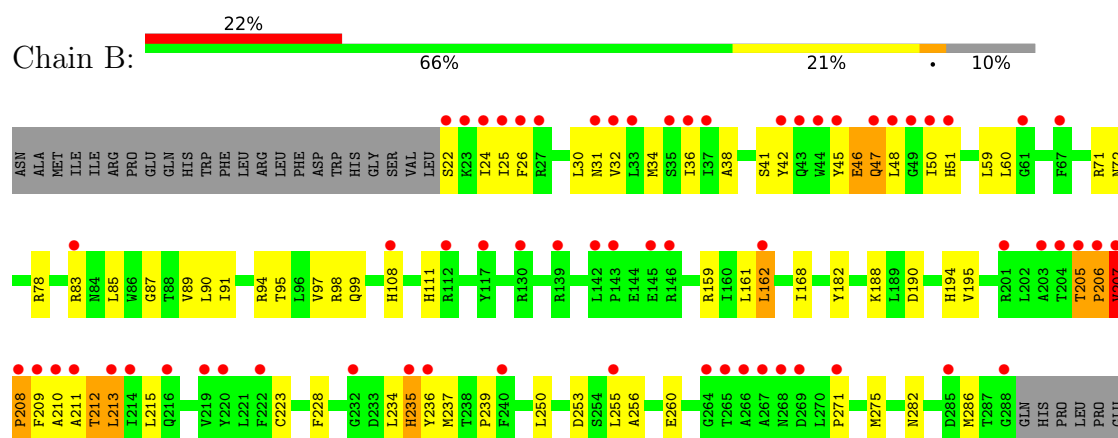
3 Residue-property plots [i](#)

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

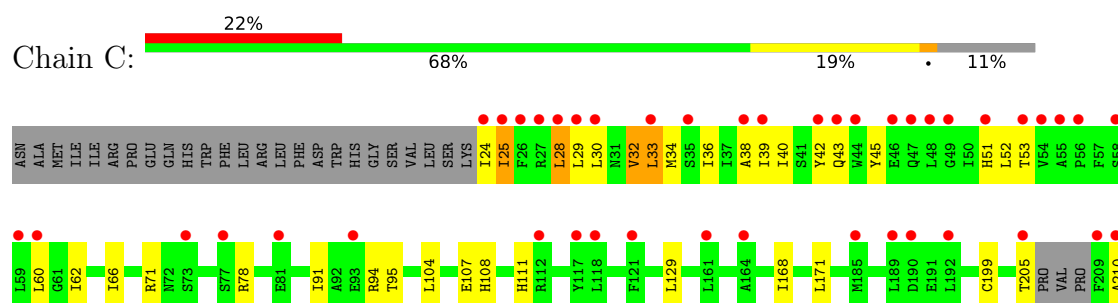
• Molecule 1: Bestrophin homolog

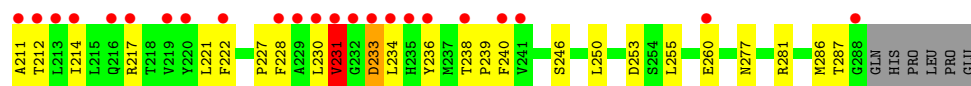


• Molecule 1: Bestrophin homolog

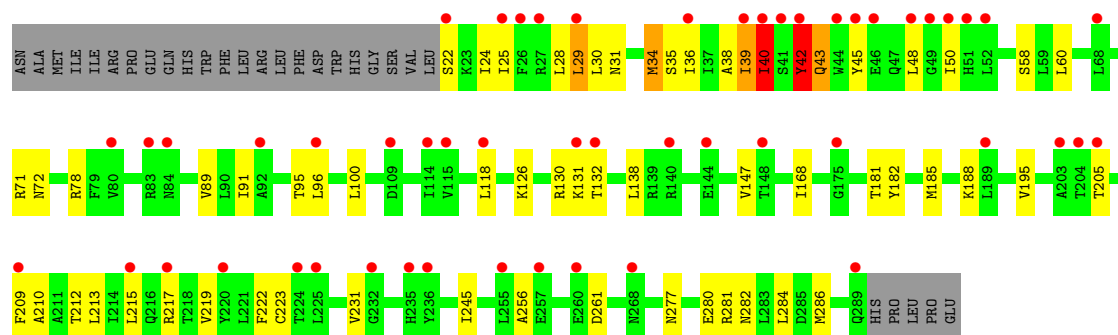


• Molecule 1: Bestrophin homolog

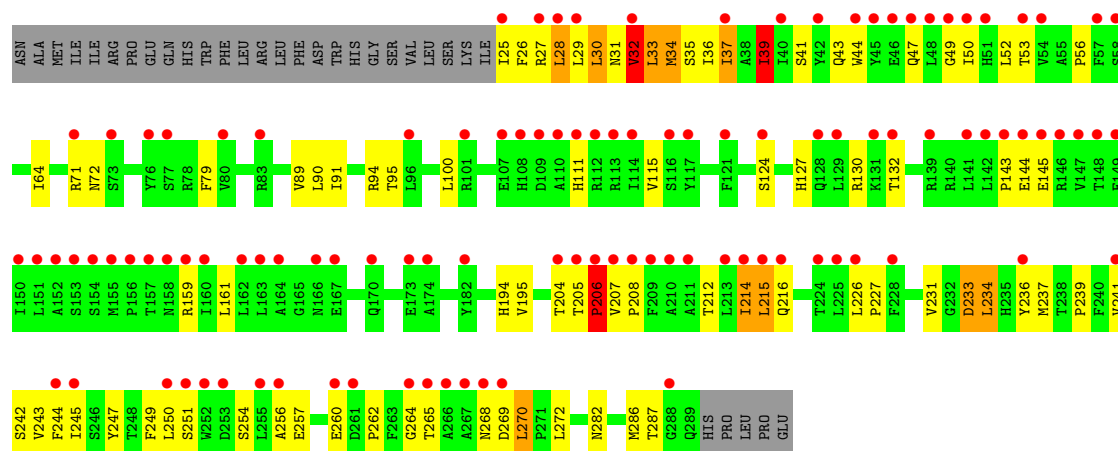




• Molecule 1: Bestrophin homolog



• Molecule 1: Bestrophin homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.16Å 160.11Å 162.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.77 – 2.62 71.77 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.2 (71.77-2.62) 97.2 (71.77-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.224 , 0.263 0.239 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	2/2142 (0.1%)	0.61	1/2914 (0.0%)
1	B	0.48	0/2131	0.71	5/2903 (0.2%)
1	C	0.37	0/2084	0.63	2/2836 (0.1%)
1	D	0.46	2/2135 (0.1%)	0.70	5/2908 (0.2%)
1	E	0.61	3/2116 (0.1%)	0.87	3/2882 (0.1%)
All	All	0.48	7/10608 (0.1%)	0.71	16/14443 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	37	ILE	C-O	-7.66	1.15	1.24
1	E	41	SER	C-O	-6.53	1.16	1.24
1	D	43	GLN	C-O	6.28	1.31	1.24
1	A	39	ILE	C-O	6.14	1.31	1.24
1	D	39	ILE	C-O	5.91	1.30	1.24
1	A	40	ILE	C-O	5.28	1.30	1.24
1	E	39	ILE	C-O	5.11	1.29	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	PRO	N-CA-C	-9.96	99.68	113.53
1	D	48	LEU	N-CA-C	8.76	120.60	111.14
1	D	42	TYR	CA-C-N	-6.63	111.40	120.28
1	D	42	TYR	C-N-CA	-6.63	111.40	120.28
1	E	32	VAL	N-CA-CB	6.03	117.61	110.55
1	B	212	THR	CA-CB-OG1	-6.03	100.56	109.60
1	B	235	HIS	CB-CA-C	-5.95	109.73	116.63
1	D	39	ILE	N-CA-CB	-5.45	104.17	110.55
1	C	231	VAL	CA-C-N	5.33	126.81	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	VAL	C-N-CA	5.33	126.81	120.14
1	B	209	PHE	N-CA-C	-5.33	106.28	112.89
1	A	33	LEU	N-CA-C	-5.31	105.49	111.28
1	E	206	PRO	CA-C-N	5.25	123.55	120.24
1	E	206	PRO	C-N-CA	5.25	123.55	120.24
1	B	208	PRO	N-CA-C	-5.21	101.75	112.47
1	D	40	ILE	N-CA-CB	-5.10	104.58	110.55

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	2099	0	2131	68	0
1	B	2089	0	2126	81	0
1	C	2045	0	2071	57	0
1	D	2093	0	2126	46	0
1	E	2074	0	2101	92	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	9	0	0	3	0
3	B	5	0	0	0	0
3	C	9	0	0	0	0
3	D	10	0	0	1	0
3	E	3	0	0	1	0
All	All	10448	0	10555	313	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 15.

All (313) 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:B:207:VAL:HB	1:B:208:PRO:CD	1.36	1.51
1:E:71:ARG:NH1	1:E:212:THR:HG22	1.25	1.48
1:D:45:TYR:CB	1:D:50:ILE:HD11	1.62	1.29
1:C:236:TYR:O	1:C:239:PRO:HD2	1.39	1.23
1:B:207:VAL:CB	1:B:208:PRO:CD	2.21	1.18
1:B:71:ARG:HH11	1:B:212:THR:HG22	1.01	1.17
1:B:71:ARG:NH1	1:B:212:THR:HG22	1.60	1.14
1:E:71:ARG:HH11	1:E:212:THR:CG2	1.63	1.11
1:E:236:TYR:O	1:E:239:PRO:HD2	1.52	1.09
1:E:71:ARG:NH1	1:E:212:THR:CG2	2.16	1.09
1:B:71:ARG:HH11	1:B:212:THR:CG2	1.64	1.08
1:B:207:VAL:HB	1:B:208:PRO:HD2	1.07	1.05
1:B:207:VAL:HB	1:B:208:PRO:HD3	1.35	1.04
1:D:45:TYR:CB	1:D:50:ILE:CD1	2.36	1.04
1:E:208:PRO:HG2	1:E:260:GLU:OE2	1.63	0.99
1:B:207:VAL:CG1	1:B:208:PRO:HD3	1.92	0.98
1:D:100:LEU:HG	1:D:185:MET:HE1	1.46	0.96
1:B:207:VAL:CB	1:B:208:PRO:HD3	1.89	0.94
1:E:208:PRO:HB2	1:E:260:GLU:OE2	1.67	0.94
1:B:71:ARG:NH1	1:B:212:THR:CG2	2.25	0.94
1:B:210:ALA:HA	1:B:213:LEU:HB3	1.50	0.93
1:E:208:PRO:CB	1:E:260:GLU:OE2	2.17	0.92
1:E:208:PRO:CG	1:E:260:GLU:OE2	2.18	0.91
1:A:83:ARG:NH1	1:E:205:THR:CB	2.34	0.91
1:E:207:VAL:CG1	1:E:208:PRO:HD3	2.01	0.90
1:E:264:GLY:HA3	1:E:269:ASP:OD2	1.73	0.89
1:C:227:PRO:O	1:C:231:VAL:HG22	1.73	0.89
1:A:237:MET:HE3	1:E:50:ILE:HA	1.56	0.88
1:E:208:PRO:HB2	1:E:260:GLU:CD	1.99	0.88
1:E:207:VAL:HG13	1:E:208:PRO:HD3	1.54	0.87
1:A:194:HIS:HA	1:B:91:ILE:HD13	1.58	0.85
1:D:30:LEU:O	1:D:30:LEU:HD23	1.78	0.83
1:C:236:TYR:O	1:C:239:PRO:CD	2.26	0.83
1:C:30:LEU:HD23	1:C:30:LEU:O	1.78	0.83
1:A:210:ALA:HB3	1:B:255:LEU:HD13	1.61	0.82
1:E:71:ARG:HH11	1:E:212:THR:HG22	0.77	0.82
1:A:52:LEU:HD11	1:B:237:MET:HG2	1.62	0.82
1:C:25:ILE:HD12	1:C:25:ILE:O	1.78	0.82
1:A:237:MET:HE1	1:E:49:GLY:O	1.80	0.81
1:B:59:LEU:HD12	1:D:58:SER:HA	1.59	0.81
1:E:30:LEU:HD12	1:E:30:LEU:O	1.80	0.81
1:B:94:ARG:NH1	1:B:282:ASN:OD1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASP:OD1	1:C:233:ASP:N	2.10	0.79
1:A:237:MET:CE	1:E:50:ILE:HA	2.12	0.79
1:B:159:ARG:HD3	1:B:162:LEU:HD23	1.64	0.79
1:E:33:LEU:O	1:E:36:ILE:HB	1.81	0.79
1:C:33:LEU:O	1:C:36:ILE:N	2.15	0.78
1:B:47:GLN:OE1	1:B:47:GLN:HA	1.85	0.77
1:E:100:LEU:HG	1:E:111:HIS:CD2	2.20	0.77
1:A:247:TYR:OH	1:E:214:ILE:HD11	1.86	0.75
1:A:205:THR:OG1	1:B:83:ARG:NE	2.20	0.74
1:E:236:TYR:O	1:E:239:PRO:CD	2.35	0.74
1:E:30:LEU:HD12	1:E:30:LEU:C	2.11	0.73
1:C:30:LEU:CD2	1:C:34:MET:HG2	2.18	0.73
1:D:30:LEU:HD23	1:D:30:LEU:C	2.14	0.73
1:B:83:ARG:NH2	1:B:275:MET:SD	2.62	0.72
1:A:53:THR:HG23	1:A:56:PRO:CD	2.20	0.72
1:B:25:ILE:HD12	1:B:26:PHE:N	2.05	0.72
1:A:210:ALA:HA	1:A:213:LEU:HB3	1.70	0.71
1:E:264:GLY:CA	1:E:269:ASP:OD2	2.39	0.71
1:B:97:VAL:HG23	1:B:286:MET:CE	2.20	0.70
1:D:25:ILE:HG23	1:D:29:LEU:HG	1.71	0.70
1:C:228:PHE:HA	1:C:231:VAL:CG2	2.20	0.70
1:A:201:ARG:HD2	1:B:83:ARG:HG3	1.74	0.70
1:A:34:MET:CE	1:A:228:PHE:CE1	2.75	0.69
1:B:207:VAL:HG12	1:B:208:PRO:HD3	1.72	0.69
1:D:40:ILE:HD13	1:D:40:ILE:N	2.06	0.69
1:E:34:MET:HE2	1:E:37:ILE:HD12	1.75	0.69
1:D:215:LEU:O	1:D:219:VAL:HG12	1.93	0.69
1:E:233:ASP:N	1:E:233:ASP:OD1	2.26	0.68
1:B:97:VAL:HG23	1:B:286:MET:HE2	1.75	0.68
1:B:25:ILE:HD12	1:B:26:PHE:H	1.59	0.67
1:C:30:LEU:HD23	1:C:30:LEU:C	2.20	0.67
1:B:282:ASN:O	1:B:286:MET:HB2	1.94	0.67
1:A:53:THR:HG23	1:A:56:PRO:HD3	1.78	0.66
1:D:24:ILE:HD12	1:D:25:ILE:HG13	1.77	0.66
1:E:282:ASN:O	1:E:286:MET:HG3	1.96	0.65
1:B:210:ALA:HA	1:B:213:LEU:HD23	1.79	0.65
1:A:285:ASP:OD1	1:E:159:ARG:NH2	2.28	0.64
1:A:257:GLU:HA	1:A:260:GLU:HB2	1.78	0.64
1:D:29:LEU:HD23	1:D:29:LEU:N	2.11	0.64
1:C:217:ARG:NH2	1:E:247:TYR:OH	2.31	0.64
1:C:227:PRO:O	1:C:231:VAL:CG2	2.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:THR:C	1:B:207:VAL:HG23	2.23	0.64
1:B:71:ARG:NH2	1:B:253:ASP:OD1	2.31	0.63
1:C:30:LEU:HD23	1:C:34:MET:HG2	1.80	0.63
1:D:78:ARG:NH1	1:D:205:THR:O	2.33	0.62
1:D:181:THR:O	1:D:185:MET:HG3	1.99	0.62
1:E:115:VAL:HG21	1:E:287:THR:HG21	1.80	0.62
1:A:34:MET:CE	1:A:228:PHE:HE1	2.11	0.62
1:A:83:ARG:CZ	1:E:205:THR:CB	2.79	0.61
1:D:25:ILE:CG2	1:D:29:LEU:HG	2.29	0.61
1:E:50:ILE:HD12	1:E:50:ILE:O	2.00	0.61
1:A:83:ARG:HH11	1:E:205:THR:CB	2.13	0.61
1:C:38:ALA:O	1:C:231:VAL:HG11	2.00	0.61
1:C:227:PRO:HA	1:C:230:LEU:HB2	1.81	0.61
1:C:228:PHE:O	1:C:231:VAL:HG23	2.01	0.61
1:E:207:VAL:HG12	1:E:208:PRO:HD3	1.83	0.61
1:A:237:MET:CE	1:E:49:GLY:O	2.48	0.60
1:B:236:TYR:O	1:B:239:PRO:HD2	2.02	0.60
1:A:91:ILE:HD13	1:E:194:HIS:HA	1.84	0.60
1:E:31:ASN:OD1	1:E:242:SER:OG	2.18	0.60
1:A:190:ASP:OD1	3:A:401:HOH:O	2.17	0.59
1:E:207:VAL:HG13	1:E:208:PRO:CD	2.28	0.59
1:B:91:ILE:O	1:B:95:THR:HG23	2.02	0.59
1:C:60:LEU:HD21	1:E:244:PHE:CE2	2.38	0.59
1:A:30:LEU:O	1:A:34:MET:HG2	2.01	0.59
1:C:32:VAL:O	1:C:36:ILE:HG13	2.02	0.59
1:C:78:ARG:NH1	1:C:205:THR:O	2.35	0.59
1:E:226:LEU:H	1:E:227:PRO:HD2	1.68	0.59
1:D:42:TYR:HB3	1:D:231:VAL:HG11	1.85	0.59
1:B:108:HIS:ND1	1:B:111:HIS:HB2	2.18	0.58
1:C:30:LEU:HD21	1:C:34:MET:HG2	1.85	0.58
1:A:128:GLN:OE1	3:A:402:HOH:O	2.18	0.57
1:D:96:LEU:HD23	1:D:118:LEU:HD11	1.86	0.57
1:E:71:ARG:HH12	1:E:212:THR:HG22	1.55	0.57
1:B:50:ILE:O	1:B:50:ILE:HD12	2.03	0.57
1:D:277:ASN:O	1:D:281:ARG:HG2	2.03	0.57
1:C:234:LEU:HB2	1:C:238:THR:OG1	2.05	0.57
1:A:40:ILE:O	1:A:43:GLN:HG3	2.04	0.57
1:E:30:LEU:HD11	1:E:34:MET:HE3	1.86	0.57
1:A:273:ASN:HB2	3:A:406:HOH:O	2.05	0.56
1:B:205:THR:N	1:B:206:PRO:HD3	2.19	0.56
1:C:227:PRO:O	1:C:231:VAL:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:O	1:A:239:PRO:HD2	2.05	0.56
1:A:68:LEU:HD11	1:A:219:VAL:HG21	1.88	0.56
1:D:91:ILE:O	1:D:95:THR:HG23	2.06	0.56
1:A:22:SER:HB2	1:A:24:ILE:HG22	1.88	0.56
1:B:78:ARG:NH1	1:B:260:GLU:O	2.39	0.56
1:E:34:MET:HE2	1:E:34:MET:HA	1.88	0.56
1:B:90:LEU:O	1:B:94:ARG:HG3	2.05	0.56
1:E:127:HIS:ND1	1:E:132:THR:HG23	2.21	0.56
1:B:205:THR:O	1:B:207:VAL:HG23	2.06	0.55
1:C:39:ILE:HD11	1:C:236:TYR:HA	1.86	0.55
1:A:24:ILE:HG23	1:A:25:ILE:HD12	1.88	0.55
1:E:237:MET:O	1:E:241:VAL:HG12	2.06	0.55
1:B:31:ASN:ND2	1:B:223:CYS:O	2.39	0.55
1:C:108:HIS:CD2	1:C:111:HIS:HB2	2.42	0.55
1:E:130:ARG:HG3	1:E:130:ARG:HH11	1.71	0.55
1:E:64:ILE:HD11	1:E:249:PHE:CE2	2.42	0.55
1:C:108:HIS:NE2	1:C:287:THR:HB	2.22	0.54
1:D:213:LEU:HD21	1:D:217:ARG:NH2	2.23	0.54
1:B:85:LEU:HD22	1:B:195:VAL:HA	1.90	0.54
1:C:62:ILE:O	1:C:66:ILE:HG13	2.07	0.54
1:B:34:MET:HE3	1:B:228:PHE:HE1	1.71	0.54
1:E:26:PHE:CD1	1:E:26:PHE:C	2.84	0.54
1:E:91:ILE:O	1:E:95:THR:HG23	2.08	0.54
1:B:168:ILE:HG22	1:B:182:TYR:CD2	2.43	0.54
1:C:228:PHE:C	1:C:231:VAL:HG23	2.33	0.54
1:B:24:ILE:HD12	1:B:250:LEU:HB3	1.90	0.53
1:A:155:MET:HG2	1:A:158:ASN:HB2	1.90	0.53
1:C:25:ILE:HD12	1:C:25:ILE:C	2.33	0.53
1:A:34:MET:CE	1:A:228:PHE:CZ	2.92	0.53
1:C:60:LEU:HD13	1:E:245:ILE:HG22	1.90	0.53
1:E:208:PRO:CB	1:E:260:GLU:CD	2.75	0.52
1:B:89:VAL:HG23	1:B:195:VAL:HG11	1.89	0.52
1:B:95:THR:O	1:B:99:GLN:HG3	2.09	0.52
1:C:38:ALA:HB1	1:C:231:VAL:CG2	2.39	0.52
1:E:39:ILE:HA	1:E:231:VAL:HG21	1.91	0.52
1:A:91:ILE:HG21	1:E:194:HIS:ND1	2.24	0.52
1:A:150:ILE:HA	1:A:159:ARG:HG2	1.92	0.52
1:A:210:ALA:HB3	1:B:255:LEU:CD1	2.35	0.52
1:A:34:MET:HE2	1:A:228:PHE:HE1	1.74	0.52
1:C:129:LEU:HD11	1:C:199:CYS:HB3	1.91	0.52
1:C:104:LEU:HB3	1:C:107:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:O	1:A:218:THR:HG23	2.11	0.52
1:B:207:VAL:CB	1:B:208:PRO:HD2	2.03	0.52
1:A:52:LEU:HB3	1:A:229:ALA:HA	1.91	0.51
1:B:38:ALA:O	1:B:42:TYR:HB2	2.10	0.51
1:B:32:VAL:O	1:B:36:ILE:HG13	2.11	0.51
1:B:206:PRO:O	1:B:207:VAL:C	2.54	0.51
1:A:208:PRO:O	1:A:211:ALA:HB3	2.09	0.51
1:C:277:ASN:O	1:C:281:ARG:HG2	2.11	0.51
1:D:29:LEU:N	1:D:29:LEU:CD2	2.73	0.51
1:A:210:ALA:HB1	1:A:214:ILE:HD11	1.92	0.51
1:B:50:ILE:C	1:B:51:HIS:CD2	2.90	0.50
1:D:30:LEU:C	1:D:30:LEU:CD2	2.85	0.49
1:C:40:ILE:O	1:C:43:GLN:HG2	2.12	0.49
1:D:45:TYR:CB	1:D:50:ILE:HD12	2.38	0.49
1:B:22:SER:O	1:B:22:SER:OG	2.29	0.49
1:C:30:LEU:CD2	1:C:30:LEU:C	2.85	0.49
1:A:220:TYR:O	1:A:224:THR:HG23	2.12	0.49
1:B:60:LEU:HD13	1:D:245:ILE:HG12	1.95	0.48
1:B:71:ARG:HD3	1:B:212:THR:HG22	1.95	0.48
1:D:138:LEU:HB3	1:D:147:VAL:HG22	1.94	0.48
1:A:237:MET:N	1:A:237:MET:HE2	2.28	0.48
1:E:270:LEU:HB3	1:E:272:LEU:CD1	2.43	0.48
1:E:143:PRO:HB2	1:E:145:GLU:HG2	1.96	0.48
1:A:187:ASN:O	1:A:190:ASP:HB3	2.14	0.48
1:C:168:ILE:HA	1:C:171:LEU:HD12	1.95	0.48
1:A:272:LEU:HD23	1:A:275:MET:CE	2.44	0.48
1:E:234:LEU:HD23	1:E:241:VAL:CG1	2.42	0.48
1:E:33:LEU:C	1:E:33:LEU:HD12	2.39	0.48
1:D:126:LYS:NZ	3:D:402:HOH:O	2.36	0.47
1:A:71:ARG:NH1	1:A:211:ALA:O	2.46	0.47
1:C:246:SER:O	1:C:250:LEU:HD12	2.15	0.47
1:E:234:LEU:CD2	1:E:241:VAL:HG11	2.45	0.47
1:A:34:MET:HE3	1:A:228:PHE:CE1	2.49	0.47
1:B:34:MET:HE3	1:B:228:PHE:CE1	2.48	0.47
1:B:89:VAL:CG2	1:B:195:VAL:HG11	2.43	0.47
1:B:210:ALA:CA	1:B:213:LEU:HB3	2.32	0.47
1:A:234:LEU:HD22	1:E:52:LEU:HD23	1.97	0.47
1:B:205:THR:N	1:B:206:PRO:CD	2.78	0.47
1:B:46:GLU:C	1:B:46:GLU:CD	2.83	0.47
1:C:51:HIS:O	1:C:53:THR:N	2.48	0.47
1:C:221:LEU:HD12	1:E:244:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:C	1:E:30:LEU:CD1	2.84	0.47
1:C:30:LEU:CD2	1:C:34:MET:CG	2.89	0.46
1:C:78:ARG:NH2	1:C:260:GLU:O	2.39	0.46
1:E:34:MET:HE3	1:E:34:MET:HB2	1.54	0.46
1:A:89:VAL:CG2	1:A:195:VAL:HG11	2.45	0.46
1:A:50:ILE:HB	1:B:237:MET:HE2	1.96	0.46
1:E:270:LEU:HB3	1:E:272:LEU:HD13	1.98	0.46
1:A:78:ARG:HG3	1:A:202:LEU:HD22	1.98	0.45
1:A:244:PHE:O	1:A:248:THR:HG23	2.16	0.45
1:C:91:ILE:O	1:C:95:THR:HG23	2.15	0.45
1:B:210:ALA:HA	1:B:213:LEU:CB	2.34	0.45
1:D:280:GLU:O	1:D:284:LEU:HG	2.16	0.45
1:A:26:PHE:CE1	1:A:30:LEU:HG	2.51	0.45
1:B:72:ASN:ND2	1:B:256:ALA:HB2	2.31	0.45
1:D:22:SER:C	1:D:24:ILE:H	2.24	0.45
1:D:282:ASN:O	1:D:286:MET:HG3	2.17	0.45
1:E:52:LEU:HD23	1:E:52:LEU:HA	1.71	0.45
1:D:130:ARG:HB2	1:D:132:THR:HG22	1.98	0.45
1:E:44:TRP:CD1	1:E:44:TRP:O	2.69	0.45
1:E:53:THR:HG23	1:E:56:PRO:CD	2.47	0.45
1:C:60:LEU:HD23	1:C:222:PHE:HD1	1.81	0.45
1:D:31:ASN:ND2	1:D:223:CYS:O	2.50	0.45
1:B:50:ILE:O	1:B:51:HIS:HD2	2.00	0.45
1:E:79:PHE:CD2	1:E:262:PRO:HB3	2.52	0.45
1:A:217:ARG:HB3	1:A:217:ARG:NH1	2.32	0.45
1:C:71:ARG:NH2	1:C:253:ASP:OD1	2.32	0.45
1:A:158:ASN:OD1	1:B:94:ARG:HD2	2.16	0.44
1:E:64:ILE:HD11	1:E:249:PHE:HE2	1.82	0.44
1:B:71:ARG:HH11	1:B:212:THR:HG21	1.68	0.44
1:C:71:ARG:HH11	1:C:212:THR:HG22	1.82	0.44
1:E:28:LEU:H	1:E:28:LEU:HG	1.42	0.44
1:E:44:TRP:O	1:E:44:TRP:CG	2.70	0.44
1:A:89:VAL:HG22	1:A:195:VAL:HG11	1.98	0.44
1:C:36:ILE:O	1:C:39:ILE:HB	2.18	0.44
1:C:38:ALA:HB1	1:C:231:VAL:HG22	1.99	0.44
1:E:130:ARG:HG3	1:E:130:ARG:NH1	2.31	0.44
1:D:188:LYS:HA	1:D:188:LYS:HD3	1.75	0.44
1:B:190:ASP:O	1:B:194:HIS:HD2	2.00	0.44
1:C:228:PHE:CA	1:C:231:VAL:CG2	2.93	0.44
1:C:240:PHE:N	1:C:240:PHE:CD1	2.86	0.44
1:D:50:ILE:HD12	1:D:50:ILE:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:OH	1:E:214:ILE:CD1	2.63	0.44
1:E:89:VAL:CG2	1:E:195:VAL:HG11	2.47	0.44
1:A:272:LEU:HD23	1:A:275:MET:HE3	2.00	0.43
1:E:30:LEU:CD1	1:E:34:MET:HE3	2.47	0.43
1:E:72:ASN:OD1	1:E:256:ALA:HB2	2.19	0.43
1:A:217:ARG:HB3	1:A:217:ARG:CZ	2.48	0.43
1:D:168:ILE:HG22	1:D:182:TYR:CD1	2.54	0.43
1:D:60:LEU:HD23	1:D:222:PHE:HD1	1.84	0.43
1:E:32:VAL:O	1:E:35:SER:OG	2.32	0.43
1:E:33:LEU:O	1:E:36:ILE:N	2.52	0.43
1:A:47:GLN:C	1:A:49:GLY:N	2.76	0.43
1:C:228:PHE:HA	1:C:231:VAL:HG21	1.96	0.43
1:E:207:VAL:N	1:E:208:PRO:CD	2.82	0.43
1:A:133:ASP:OD1	1:A:135:THR:HG23	2.19	0.43
1:B:30:LEU:HD23	1:B:34:MET:HG2	2.01	0.43
1:C:94:ARG:O	1:C:286:MET:HE1	2.18	0.43
1:E:35:SER:HA	1:E:227:PRO:CB	2.48	0.42
1:E:239:PRO:O	1:E:243:VAL:HG12	2.19	0.42
1:B:271:PRO:O	1:B:275:MET:HG3	2.20	0.42
1:D:28:LEU:HD23	1:D:28:LEU:HA	1.81	0.42
1:B:41:SER:O	1:B:45:TYR:N	2.53	0.42
1:B:208:PRO:O	1:B:208:PRO:HG2	2.18	0.42
1:D:30:LEU:HD23	1:D:34:MET:HG2	2.01	0.42
1:B:168:ILE:HG22	1:B:182:TYR:CE2	2.54	0.42
1:C:255:LEU:HD13	1:D:210:ALA:HB3	2.02	0.42
1:D:71:ARG:NH1	1:D:212:THR:HA	2.35	0.42
1:A:32:VAL:O	1:A:33:LEU:C	2.62	0.42
1:A:34:MET:HE2	1:A:228:PHE:CE1	2.52	0.42
1:C:42:TYR:HA	1:C:45:TYR:CD1	2.55	0.42
1:D:96:LEU:HD12	1:D:185:MET:HE2	2.02	0.42
1:A:79:PHE:CE2	1:E:207:VAL:HB	2.55	0.41
1:B:87:GLY:O	1:B:91:ILE:HG13	2.20	0.41
1:C:30:LEU:HD21	1:C:34:MET:CG	2.47	0.41
1:D:209:PHE:CE2	1:D:213:LEU:HD12	2.55	0.41
1:E:71:ARG:HH12	1:E:212:THR:CG2	2.21	0.41
1:B:210:ALA:O	1:B:211:ALA:C	2.63	0.41
1:D:35:SER:O	1:D:38:ALA:HB3	2.20	0.41
1:E:254:SER:O	1:E:257:GLU:HB3	2.21	0.41
1:C:214:ILE:HG12	1:E:251:SER:HB3	2.03	0.41
1:D:25:ILE:HA	1:D:28:LEU:HB2	2.01	0.41
1:D:72:ASN:OD1	1:D:256:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ASP:CG	1:D:261:ASP:O	2.64	0.41
1:E:144:GLU:O	1:E:144:GLU:HG3	2.21	0.41
1:B:188:LYS:HA	1:B:188:LYS:HD3	1.90	0.41
1:B:234:LEU:O	1:B:235:HIS:HB2	2.20	0.41
1:C:210:ALA:O	1:C:211:ALA:C	2.64	0.41
1:E:215:LEU:HD12	1:E:215:LEU:HA	1.77	0.41
1:E:226:LEU:N	1:E:227:PRO:HD2	2.34	0.41
1:A:231:VAL:HA	1:A:238:THR:OG1	2.21	0.41
1:B:78:ARG:NH2	1:B:205:THR:OG1	2.53	0.41
1:C:28:LEU:HA	1:C:28:LEU:HD13	1.85	0.41
1:D:131:LYS:HE3	1:D:131:LYS:HB2	1.92	0.41
1:E:27:ARG:CB	1:E:250:LEU:HD13	2.51	0.41
1:E:124:SER:O	3:E:401:HOH:O	2.22	0.41
1:A:36:ILE:HA	1:A:39:ILE:HD12	2.04	0.41
1:A:47:GLN:O	1:A:49:GLY:N	2.54	0.41
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.79	0.40
1:B:50:ILE:O	1:B:50:ILE:CG1	2.69	0.40
1:A:186:ASP:OD2	1:B:98:ARG:NH2	2.52	0.40
1:B:50:ILE:O	1:B:50:ILE:CD1	2.69	0.40
1:D:89:VAL:CG2	1:D:195:VAL:HG11	2.51	0.40
1:E:205:THR:HA	1:E:206:PRO:HD3	1.97	0.40
1:A:237:MET:HE2	1:A:237:MET:H	1.86	0.40
1:B:210:ALA:CA	1:B:213:LEU:HD23	2.50	0.40
1:E:90:LEU:O	1:E:94:ARG:HG3	2.21	0.40
1:E:161:LEU:HD23	1:E:161:LEU:HA	1.79	0.40

There are no symmetry-related clashes.

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	263/296 (89%)	260 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	265/296 (90%)	256 (97%)	8 (3%)	1 (0%)	30	49
1	C	258/296 (87%)	250 (97%)	7 (3%)	1 (0%)	30	49
1	D	266/296 (90%)	261 (98%)	5 (2%)	0	100	100
1	E	263/296 (89%)	259 (98%)	3 (1%)	1 (0%)	30	49
All	All	1315/1480 (89%)	1286 (98%)	26 (2%)	3 (0%)	43	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	VAL
1	C	52	LEU
1	E	206	PRO

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	226/258 (88%)	221 (98%)	5 (2%)	45	70
1	B	226/258 (88%)	218 (96%)	8 (4%)	32	57
1	C	218/258 (84%)	210 (96%)	8 (4%)	30	55
1	D	225/258 (87%)	218 (97%)	7 (3%)	35	61
1	E	223/258 (86%)	204 (92%)	19 (8%)	10	21
All	All	1118/1290 (87%)	1071 (96%)	47 (4%)	26	50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	37	ILE
1	A	40	ILE
1	A	43	GLN
1	A	234	LEU

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Mol	Chain	Res	Type
1	B	46	GLU
1	B	47	GLN
1	B	48	LEU
1	B	162	LEU
1	B	205	THR
1	B	207	VAL
1	B	213	LEU
1	B	215	LEU
1	C	24	ILE
1	C	25	ILE
1	C	28	LEU
1	C	29	LEU
1	C	32	VAL
1	C	33	LEU
1	C	231	VAL
1	C	233	ASP
1	D	29	LEU
1	D	34	MET
1	D	36	ILE
1	D	39	ILE
1	D	40	ILE
1	D	42	TYR
1	D	43	GLN
1	E	25	ILE
1	E	28	LEU
1	E	29	LEU
1	E	30	LEU
1	E	32	VAL
1	E	33	LEU
1	E	34	MET
1	E	39	ILE
1	E	43	GLN
1	E	47	GLN
1	E	204	THR
1	E	214	ILE
1	E	215	LEU
1	E	216	GLN
1	E	233	ASP
1	E	234	LEU
1	E	265	THR
1	E	268	ASN
1	E	270	LEU

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

Mol	Chain	Res	Type
1	A	31	ASN
1	A	84	ASN
1	A	166	ASN
1	A	187	ASN
1	B	51	HIS
1	B	84	ASN
1	B	128	GLN
1	B	187	ASN
1	C	31	ASN
1	C	43	GLN
1	C	51	HIS
1	C	72	ASN
1	C	99	GLN
1	D	43	GLN
1	D	99	GLN
1	D	187	ASN
1	E	102	ASN
1	E	108	HIS
1	E	128	GLN
1	E	216	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	267/296 (90%)	1.23	61 (22%) 2 1	58, 83, 133, 163	0
1	B	267/296 (90%)	1.17	64 (23%) 2 1	50, 81, 145, 175	0
1	C	262/296 (88%)	1.37	66 (25%) 1 1	53, 88, 142, 174	0
1	D	268/296 (90%)	1.00	52 (19%) 3 2	53, 77, 136, 167	0
1	E	265/296 (89%)	2.18	109 (41%) 0 0	58, 95, 157, 190	0
All	All	1329/1480 (89%)	1.39	352 (26%) 1 1	50, 85, 145, 190	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	ILE	10.6
1	E	131	LYS	9.4
1	E	154	SER	9.4
1	E	146	ARG	9.2
1	E	153	SER	8.2
1	A	209	PHE	7.9
1	A	204	THR	7.7
1	E	204	THR	7.1
1	A	47	GLN	7.1
1	C	24	ILE	7.0
1	E	166	ASN	6.9
1	E	149	GLU	6.7
1	B	288	GLY	6.6
1	D	41	SER	6.6
1	B	204	THR	6.6
1	B	48	LEU	6.5
1	B	208	PRO	6.4
1	E	129	LEU	6.3
1	E	269	ASP	6.3
1	E	50	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	117	TYR	6.1
1	E	209	PHE	6.0
1	C	47	GLN	5.9
1	E	49	GLY	5.8
1	E	128	GLN	5.8
1	A	107	GLU	5.6
1	A	206	PRO	5.6
1	C	44	TRP	5.6
1	E	116	SER	5.6
1	E	266	ALA	5.5
1	B	285	ASP	5.4
1	E	28	LEU	5.4
1	C	288	GLY	5.4
1	A	235	HIS	5.3
1	C	220	TYR	5.3
1	E	159	ARG	5.3
1	C	77	SER	5.3
1	B	209	PHE	5.3
1	B	206	PRO	5.2
1	C	192	LEU	5.2
1	E	51	HIS	5.2
1	C	235	HIS	5.1
1	E	265	THR	5.1
1	C	25	ILE	5.1
1	C	30	LEU	5.1
1	A	285	ASP	5.1
1	B	267	ALA	5.0
1	E	160	ILE	4.9
1	E	44	TRP	4.9
1	C	58	SER	4.8
1	E	150	ILE	4.7
1	B	236	TYR	4.7
1	B	50	ILE	4.7
1	E	163	LEU	4.7
1	E	264	GLY	4.7
1	C	209	PHE	4.7
1	C	232	GLY	4.7
1	E	208	PRO	4.7
1	D	236	TYR	4.7
1	A	213	LEU	4.6
1	A	106	ALA	4.6
1	C	214	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	207	VAL	4.5
1	C	236	TYR	4.5
1	E	152	ALA	4.5
1	E	164	ALA	4.5
1	E	211	ALA	4.5
1	B	44	TRP	4.5
1	C	59	LEU	4.5
1	E	147	VAL	4.5
1	A	51	HIS	4.5
1	A	260	GLU	4.4
1	E	158	ASN	4.4
1	E	142	LEU	4.4
1	D	42	TYR	4.4
1	C	205	THR	4.4
1	B	210	ALA	4.4
1	C	211	ALA	4.4
1	E	267	ALA	4.4
1	A	208	PRO	4.4
1	C	190	ASP	4.3
1	A	289	GLN	4.3
1	E	253	ASP	4.3
1	E	155	MET	4.3
1	E	48	LEU	4.3
1	E	148	THR	4.2
1	B	207	VAL	4.2
1	C	27	ARG	4.2
1	E	210	ALA	4.2
1	A	49	GLY	4.2
1	E	58	SER	4.2
1	E	236	TYR	4.2
1	E	252	TRP	4.2
1	E	261	ASP	4.2
1	B	203	ALA	4.2
1	A	176	LYS	4.2
1	C	51	HIS	4.2
1	B	268	ASN	4.1
1	D	209	PHE	4.1
1	E	111	HIS	4.1
1	A	50	ILE	4.0
1	E	101	ARG	4.0
1	C	230	LEU	4.0
1	D	80	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	112	ARG	3.9
1	E	27	ARG	3.9
1	E	255	LEU	3.9
1	D	39	ILE	3.9
1	E	42	TYR	3.9
1	E	109	ASP	3.9
1	E	206	PRO	3.9
1	B	36	ILE	3.9
1	B	33	LEU	3.8
1	B	45	TYR	3.8
1	A	26	PHE	3.8
1	E	83	ARG	3.8
1	B	211	ALA	3.8
1	A	101	ARG	3.8
1	E	151	LEU	3.8
1	E	214	ILE	3.8
1	D	26	PHE	3.8
1	D	51	HIS	3.7
1	B	23	LYS	3.7
1	A	22	SER	3.7
1	B	269	ASP	3.7
1	E	77	SER	3.7
1	B	201	ARG	3.7
1	E	45	TYR	3.7
1	E	224	THR	3.6
1	A	45	TYR	3.6
1	A	286	MET	3.6
1	E	156	PRO	3.6
1	E	144	GLU	3.6
1	A	48	LEU	3.6
1	C	121	PHE	3.6
1	E	173	GLU	3.6
1	E	215	LEU	3.6
1	D	204	THR	3.6
1	B	145	GLU	3.6
1	C	33	LEU	3.6
1	D	224	THR	3.6
1	B	83	ARG	3.5
1	E	112	ARG	3.5
1	E	256	ALA	3.5
1	E	57	PHE	3.5
1	B	32	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	265	THR	3.5
1	E	143	PRO	3.5
1	E	108	HIS	3.5
1	C	117	TYR	3.5
1	E	157	THR	3.5
1	B	146	ARG	3.5
1	D	175	GLY	3.4
1	D	144	GLU	3.4
1	D	40	ILE	3.4
1	A	234	LEU	3.4
1	E	170	GLN	3.4
1	B	162	LEU	3.4
1	C	38	ALA	3.4
1	B	26	PHE	3.4
1	D	115	VAL	3.4
1	E	162	LEU	3.3
1	C	228	PHE	3.3
1	A	105	PRO	3.3
1	B	108	HIS	3.3
1	C	210	ALA	3.3
1	D	260	GLU	3.3
1	E	145	GLU	3.3
1	B	266	ALA	3.3
1	A	52	LEU	3.2
1	D	45	TYR	3.2
1	D	114	ILE	3.2
1	D	48	LEU	3.2
1	A	205	THR	3.2
1	B	47	GLN	3.2
1	D	36	ILE	3.2
1	A	46	GLU	3.2
1	B	143	PRO	3.2
1	E	37	ILE	3.2
1	A	217	ARG	3.2
1	D	215	LEU	3.2
1	C	189	LEU	3.1
1	A	154	SER	3.1
1	C	29	LEU	3.1
1	A	128	GLN	3.1
1	D	232	GLY	3.1
1	C	26	PHE	3.1
1	C	48	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	141	LEU	3.1
1	B	61	GLY	3.1
1	D	44	TRP	3.1
1	A	236	TYR	3.1
1	C	161	LEU	3.1
1	A	145	GLU	3.1
1	B	264	GLY	3.1
1	B	112	ARG	3.1
1	E	251	SER	3.0
1	C	73	SER	3.0
1	C	93	GLU	3.0
1	B	214	ILE	3.0
1	E	268	ASN	3.0
1	B	235	HIS	2.9
1	E	174	ALA	2.9
1	A	30	LEU	2.9
1	D	52	LEU	2.9
1	D	84	ASN	2.9
1	C	54	VAL	2.9
1	E	225	LEU	2.9
1	C	46	GLU	2.9
1	A	40	ILE	2.9
1	B	37	ILE	2.9
1	E	110	ALA	2.9
1	A	54	VAL	2.9
1	A	231	VAL	2.9
1	E	73	SER	2.8
1	B	42	TYR	2.8
1	B	25	ILE	2.8
1	A	109	ASP	2.8
1	E	213	LEU	2.8
1	D	148	THR	2.8
1	D	203	ALA	2.8
1	E	132	THR	2.8
1	C	240	PHE	2.8
1	E	241	VAL	2.8
1	E	205	THR	2.8
1	D	83	ARG	2.8
1	B	43	GLN	2.8
1	B	22	SER	2.7
1	B	35	SER	2.7
1	B	51	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	78	ARG	2.7
1	E	46	GLU	2.7
1	B	205	THR	2.7
1	C	231	VAL	2.7
1	E	139	ARG	2.7
1	B	213	LEU	2.7
1	D	132	THR	2.7
1	C	42	TYR	2.7
1	B	24	ILE	2.7
1	A	23	LYS	2.7
1	C	241	VAL	2.7
1	D	131	LYS	2.7
1	D	205	THR	2.7
1	A	24	ILE	2.6
1	E	260	GLU	2.6
1	C	118	LEU	2.6
1	B	27	ARG	2.6
1	E	71	ARG	2.6
1	A	200	GLU	2.6
1	D	96	LEU	2.6
1	C	81	GLU	2.6
1	C	164	ALA	2.6
1	C	222	PHE	2.6
1	E	245	ILE	2.5
1	D	217	ARG	2.5
1	D	49	GLY	2.5
1	B	219	VAL	2.5
1	B	216	GLN	2.5
1	A	233	ASP	2.5
1	C	234	LEU	2.5
1	E	167	GLU	2.5
1	C	217	ARG	2.5
1	D	50	ILE	2.5
1	D	235	HIS	2.5
1	C	49	GLY	2.5
1	A	228	PHE	2.5
1	A	229	ALA	2.5
1	E	244	PHE	2.5
1	D	225	LEU	2.5
1	C	39	ILE	2.4
1	D	189	LEU	2.4
1	D	289	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	244	PHE	2.4
1	E	228	PHE	2.4
1	B	142	LEU	2.4
1	E	114	ILE	2.4
1	E	250	LEU	2.4
1	B	222	PHE	2.4
1	A	230	LEU	2.4
1	C	212	THR	2.4
1	B	49	GLY	2.4
1	E	288	GLY	2.4
1	E	47	GLN	2.4
1	A	241	VAL	2.4
1	E	113	ARG	2.4
1	E	121	PHE	2.4
1	E	226	LEU	2.3
1	D	22	SER	2.3
1	A	164	ALA	2.3
1	C	53	THR	2.3
1	B	240	PHE	2.3
1	C	213	LEU	2.3
1	D	92	ALA	2.3
1	B	139	ARG	2.3
1	E	32	VAL	2.3
1	D	255	LEU	2.3
1	E	96	LEU	2.3
1	C	229	ALA	2.3
1	D	25	ILE	2.3
1	B	220	TYR	2.3
1	A	258	GLU	2.3
1	D	27	ARG	2.3
1	C	216	GLN	2.3
1	C	219	VAL	2.3
1	D	29	LEU	2.3
1	C	185	MET	2.2
1	E	53	THR	2.2
1	D	46	GLU	2.2
1	A	201	ARG	2.2
1	C	233	ASP	2.2
1	A	95	THR	2.2
1	D	257	GLU	2.2
1	A	27	ARG	2.2
1	A	83	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	60	LEU	2.2
1	C	56	PRO	2.2
1	A	221	LEU	2.2
1	E	124	SER	2.2
1	C	43	GLN	2.1
1	A	33	LEU	2.1
1	C	28	LEU	2.1
1	C	35	SER	2.1
1	C	55	ALA	2.1
1	C	260	GLU	2.1
1	B	31	ASN	2.1
1	B	117	TYR	2.1
1	D	68	LEU	2.1
1	D	220	TYR	2.1
1	E	182	TYR	2.1
1	B	232	GLY	2.1
1	A	190	ASP	2.1
1	A	174	ALA	2.1
1	A	53	THR	2.1
1	C	238	THR	2.1
1	B	271	PRO	2.1
1	B	67	PHE	2.1
1	A	267	ALA	2.1
1	D	140	ARG	2.1
1	A	44	TRP	2.1
1	E	216	GLN	2.1
1	E	29	LEU	2.1
1	E	40	ILE	2.1
1	B	130	ARG	2.0
1	D	109	ASP	2.0
1	A	262	PRO	2.0
1	B	255	LEU	2.0
1	D	118	LEU	2.0
1	E	54	VAL	2.0
1	E	80	VAL	2.0
1	E	107	GLU	2.0
1	D	268	ASN	2.0
1	E	76	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	ZN	E	301	1/1	0.50	0.28	188,188,188,188	0
2	ZN	B	301	1/1	0.79	0.18	162,162,162,162	0
2	ZN	A	304	1/1	0.92	0.39	30,30,30,30	0
2	ZN	A	301	1/1	0.96	0.15	79,79,79,79	0
2	ZN	B	303	1/1	0.97	0.14	84,84,84,84	0
2	ZN	A	302	1/1	0.98	0.04	87,87,87,87	0
2	ZN	C	303	1/1	0.98	0.08	81,81,81,81	0
2	ZN	A	303	1/1	0.98	0.06	85,85,85,85	0
2	ZN	C	302	1/1	0.99	0.03	81,81,81,81	0
2	ZN	B	302	1/1	0.99	0.05	78,78,78,78	0
2	ZN	D	301	1/1	0.99	0.05	86,86,86,86	0
2	ZN	C	301	1/1	0.99	0.04	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.