



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:01 am BST

PDB ID : 3KUR  
Title : Crystal structure of the MLLE domain of poly(A)-binding protein  
Authors : Kozlov, G.; Gehring, K.  
Deposited on : 2009-11-27  
Resolution : 2.50 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](mailto: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.

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

MolProbity	:	4.02b-467
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

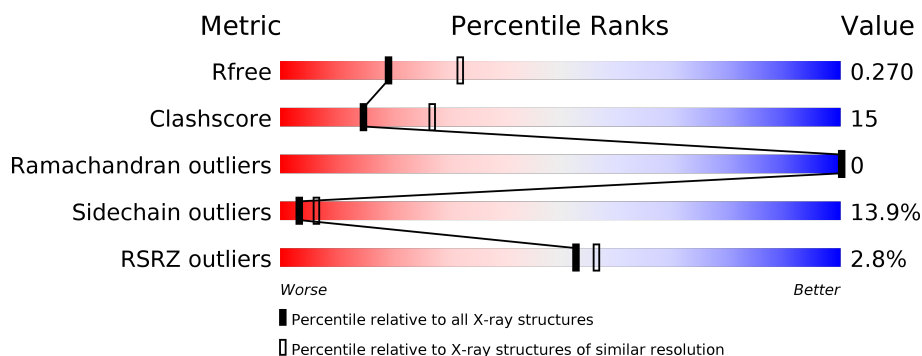
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	79	<div> <div></div> <div>63%24%5%8%</div> </div>
1	B	79	<div> <div></div> <div>71%20%8%</div> </div>
1	C	79	<div> <div></div> <div>68%20%9%</div> </div>
1	D	79	<div> <div>8%</div> <div>59%25%5%10%</div> </div>
1	E	79	<div> <div></div> <div>66%22%9%</div> </div>
1	F	79	<div> <div>4%</div> <div>43%43%5%9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	79	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>9%</div> </div> </div>
1	H	79	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>6%</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	G	1	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4501 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 Polyadenylate-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	0	0
			552	349	92	106	5			
1	B	73	Total	C	N	O	S	0	1	0
			557	352	92	108	5			
1	C	72	Total	C	N	O	S	0	0	0
			547	346	91	105	5			
1	D	71	Total	C	N	O	S	0	0	0
			540	341	90	104	5			
1	E	72	Total	C	N	O	S	0	0	0
			547	346	91	105	5			
1	F	72	Total	C	N	O	S	0	0	0
			547	346	91	105	5			
1	G	72	Total	C	N	O	S	0	0	0
			547	346	91	105	5			
1	H	73	Total	C	N	O	S	0	0	0
			552	349	92	106	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	539	GLY	-	EXPRESSION TAG	UNP P11940
A	540	PRO	-	EXPRESSION TAG	UNP P11940
A	541	LEU	-	EXPRESSION TAG	UNP P11940
A	542	GLY	-	EXPRESSION TAG	UNP P11940
A	543	SER	-	EXPRESSION TAG	UNP P11940
B	539	GLY	-	EXPRESSION TAG	UNP P11940
B	540	PRO	-	EXPRESSION TAG	UNP P11940
B	541	LEU	-	EXPRESSION TAG	UNP P11940
B	542	GLY	-	EXPRESSION TAG	UNP P11940
B	543	SER	-	EXPRESSION TAG	UNP P11940
C	539	GLY	-	EXPRESSION TAG	UNP P11940
C	540	PRO	-	EXPRESSION TAG	UNP P11940
C	541	LEU	-	EXPRESSION TAG	UNP P11940

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Chain	Residue	Modelled	Actual	Comment	Reference
C	542	GLY	-	EXPRESSION TAG	UNP P11940
C	543	SER	-	EXPRESSION TAG	UNP P11940
D	539	GLY	-	EXPRESSION TAG	UNP P11940
D	540	PRO	-	EXPRESSION TAG	UNP P11940
D	541	LEU	-	EXPRESSION TAG	UNP P11940
D	542	GLY	-	EXPRESSION TAG	UNP P11940
D	543	SER	-	EXPRESSION TAG	UNP P11940
E	539	GLY	-	EXPRESSION TAG	UNP P11940
E	540	PRO	-	EXPRESSION TAG	UNP P11940
E	541	LEU	-	EXPRESSION TAG	UNP P11940
E	542	GLY	-	EXPRESSION TAG	UNP P11940
E	543	SER	-	EXPRESSION TAG	UNP P11940
F	539	GLY	-	EXPRESSION TAG	UNP P11940
F	540	PRO	-	EXPRESSION TAG	UNP P11940
F	541	LEU	-	EXPRESSION TAG	UNP P11940
F	542	GLY	-	EXPRESSION TAG	UNP P11940
F	543	SER	-	EXPRESSION TAG	UNP P11940
G	539	GLY	-	EXPRESSION TAG	UNP P11940
G	540	PRO	-	EXPRESSION TAG	UNP P11940
G	541	LEU	-	EXPRESSION TAG	UNP P11940
G	542	GLY	-	EXPRESSION TAG	UNP P11940
G	543	SER	-	EXPRESSION TAG	UNP P11940
H	539	GLY	-	EXPRESSION TAG	UNP P11940
H	540	PRO	-	EXPRESSION TAG	UNP P11940
H	541	LEU	-	EXPRESSION TAG	UNP P11940
H	542	GLY	-	EXPRESSION TAG	UNP P11940
H	543	SER	-	EXPRESSION TAG	UNP P11940

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	15	Total	O	0	0
			15	15		
3	C	15	Total	O	0	0
			15	15		
3	D	5	Total	O	0	0
			5	5		
3	E	16	Total	O	0	0
			16	16		
3	F	16	Total	O	0	0
			16	16		
3	G	12	Total	O	0	0
			12	12		
3	H	10	Total	O	0	0
			10	10		

### 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: Polyadenylate-binding protein 1

Chain A: 



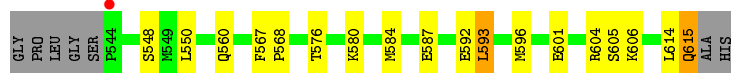
#### • Molecule 1: Polyadenylate-binding protein 1

Chain B: 



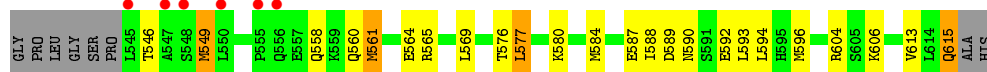
#### • Molecule 1: Polyadenylate-binding protein 1

Chain C: 



#### • Molecule 1: Polyadenylate-binding protein 1

Chain D: 

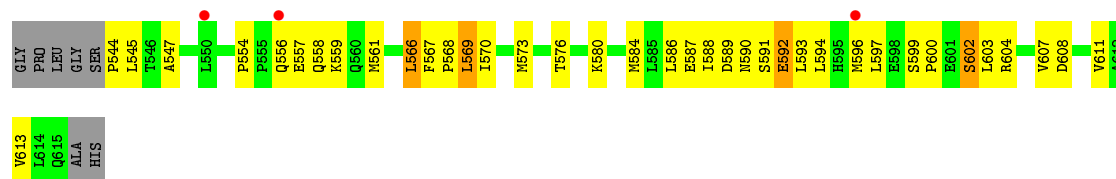


#### • Molecule 1: Polyadenylate-binding protein 1

Chain E: 



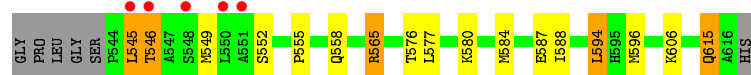
#### • Molecule 1: Polyadenylate-binding protein 1



- Molecule 1: Polyadenylate-binding protein 1



- Molecule 1: Polyadenylate-binding protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.98 Å   146.98 Å   83.06 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-2.50) 96.7 (39.96-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.216   ,   0.272 0.214   ,   0.270	Depositor DCC
$R_{free}$ test set	1558 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.77	0/560	0.80	0/757
1	B	0.77	0/568	0.87	0/768
1	C	0.70	0/555	0.83	0/750
1	D	0.67	1/547 (0.2%)	0.76	1/739 (0.1%)
1	E	0.76	1/555 (0.2%)	0.82	0/750
1	F	0.68	0/555	0.81	0/750
1	G	0.64	0/555	0.79	0/750
1	H	0.67	0/560	0.77	0/757
All	All	0.71	2/4455 (0.0%)	0.81	1/6021 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	598	GLU	CG-CD	5.25	1.59	1.51
1	D	561	MET	SD-CE	5.13	2.06	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	561	MET	CG-SD-CE	-7.00	89.00	100.20

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	552	0	574	18	0
1	B	557	0	578	9	0
1	C	547	0	569	21	0
1	D	540	0	561	24	0
1	E	547	0	569	22	0
1	F	547	0	569	37	0
1	G	547	0	569	14	0
1	H	552	0	574	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	2	0
2	H	1	0	0	0	0
3	A	18	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
3	E	16	0	0	1	0
3	F	16	0	0	2	0
3	G	12	0	0	2	0
3	H	10	0	0	0	0
All	All	4501	0	4563	136	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 (136) 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:D:561:MET:SD	1:D:561:MET:CE	2.06	1.41
1:C:584:MET:HE3	1:D:584:MET:HE3	1.16	1.14
1:A:592:GLU:HG3	1:A:596:MET:CE	1.80	1.11
1:E:592:GLU:HG3	1:E:596:MET:HE3	1.37	1.05
1:G:584:MET:HE3	1:H:584:MET:HE3	1.38	1.05
1:C:593:LEU:HD12	1:C:596:MET:HE3	1.43	1.01
1:C:593:LEU:HA	1:C:596:MET:HE3	1.42	0.99
1:C:584:MET:HE3	1:D:584:MET:CE	1.95	0.95
1:A:592:GLU:HG3	1:A:596:MET:HE2	1.52	0.89
1:A:592:GLU:HG3	1:A:596:MET:HE3	1.56	0.86
2:G:1:CL:CL	3:G:75:HOH:O	2.31	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:GLU:HG3	1:E:596:MET:CE	2.07	0.85
1:G:598:GLU:O	1:G:600:PRO:HD3	1.77	0.84
1:C:593:LEU:HD12	1:C:596:MET:CE	2.07	0.83
1:A:584:MET:HE3	1:B:584:MET:HE3	1.59	0.83
1:C:584:MET:CE	1:D:584:MET:HE3	2.07	0.80
1:A:592:GLU:CG	1:A:596:MET:CE	2.62	0.75
1:D:593:LEU:HA	1:D:596:MET:HE3	1.70	0.74
1:F:569:LEU:CD2	1:F:573:MET:HE2	2.17	0.73
1:C:593:LEU:CD1	1:C:596:MET:CE	2.66	0.73
1:C:593:LEU:HA	1:C:596:MET:CE	2.19	0.72
1:D:593:LEU:HD23	1:D:596:MET:HE1	1.73	0.70
1:F:554:PRO:HB2	1:F:556:GLN:HE22	1.57	0.69
1:F:607:VAL:O	1:F:611:VAL:HG23	1.93	0.68
1:C:593:LEU:CD1	1:C:596:MET:HE3	2.19	0.68
1:E:614:LEU:O	1:E:615:GLN:HB2	1.94	0.67
1:G:614:LEU:O	1:G:615:GLN:HB2	1.94	0.66
1:A:580:LYS:O	1:A:584:MET:HG3	1.94	0.66
1:C:584:MET:CE	1:D:584:MET:CE	2.71	0.66
1:D:596:MET:SD	1:D:606:LYS:HG3	2.37	0.65
1:F:559:LYS:NZ	1:F:590:ASN:OD1	2.30	0.64
1:D:558:GLN:HE21	1:D:590:ASN:ND2	1.96	0.64
1:F:599:SER:O	1:F:602:SER:HB2	1.96	0.64
1:A:605:SER:O	1:A:609:GLU:HG2	1.98	0.64
1:F:569:LEU:HD23	1:F:573:MET:HE2	1.79	0.63
1:H:565:ARG:HH11	1:H:565:ARG:CG	2.12	0.63
1:G:571:GLN:O	1:G:575:PRO:HG3	1.99	0.62
1:C:593:LEU:HD13	1:C:596:MET:HE1	1.81	0.62
1:C:614:LEU:O	1:C:615:GLN:HB2	1.99	0.62
1:E:584:MET:HE3	1:F:584:MET:CE	2.28	0.62
1:D:615:GLN:CA	1:D:615:GLN:HE21	2.13	0.62
1:E:584:MET:CE	1:F:584:MET:CE	2.77	0.61
1:C:593:LEU:CD1	1:C:596:MET:HE1	2.31	0.61
1:H:615:GLN:HA	1:H:615:GLN:HE21	1.65	0.61
1:H:615:GLN:CA	1:H:615:GLN:HE21	2.14	0.60
1:A:584:MET:CE	1:B:584:MET:HE3	2.29	0.60
1:C:592:GLU:HG3	1:C:596:MET:HE2	1.83	0.60
1:G:580:LYS:HD2	1:H:587:GLU:O	2.02	0.60
1:G:576:THR:OG1	2:G:1:CL:CL	2.55	0.60
1:D:561:MET:CG	1:D:561:MET:CE	2.79	0.60
1:A:550:LEU:HD22	1:A:558:GLN:HG2	1.82	0.59
1:A:606:LYS:HD2	1:A:609:GLU:OE1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:589:ASP:HA	3:F:116:HOH:O	2.01	0.59
1:F:586:LEU:HA	1:F:593:LEU:HD11	1.83	0.59
1:E:545:LEU:HA	1:E:549:MET:HE1	1.84	0.59
1:E:588:ILE:HD13	1:E:596:MET:HE1	1.83	0.59
1:E:584:MET:HG2	1:F:587:GLU:HG3	1.83	0.59
1:A:592:GLU:CG	1:A:596:MET:HE2	2.27	0.58
1:E:584:MET:HE3	1:F:584:MET:HE2	1.84	0.58
1:F:588:ILE:HB	1:F:593:LEU:HG	1.84	0.58
1:G:577:LEU:N	3:G:75:HOH:O	2.30	0.58
1:F:569:LEU:HD22	1:F:573:MET:HE2	1.85	0.57
1:F:558:GLN:OE1	1:F:590:ASN:ND2	2.38	0.57
1:H:546:THR:HG23	1:H:549:MET:HB2	1.86	0.57
1:C:560:GLN:HE22	1:F:544:PRO:HB3	1.70	0.56
1:D:592:GLU:HG3	1:D:596:MET:HE2	1.87	0.56
1:F:566:LEU:HD22	1:F:570:ILE:HG12	1.88	0.56
1:E:573:MET:HE1	1:E:604:ARG:HA	1.88	0.56
1:A:580:LYS:HD2	1:B:587:GLU:O	2.06	0.55
1:H:588:ILE:HG21	1:H:596:MET:HE1	1.90	0.54
1:E:584:MET:CE	1:F:584:MET:HE3	2.38	0.53
1:B:593:LEU:HA	1:B:596:MET:HE3	1.90	0.53
1:D:558:GLN:HB3	1:D:590:ASN:HD21	1.74	0.53
1:E:584:MET:CE	1:F:584:MET:HE2	2.37	0.52
1:F:547:ALA:HA	1:F:594:LEU:HD21	1.92	0.52
1:F:569:LEU:HD23	1:F:573:MET:CE	2.40	0.52
1:G:580:LYS:O	1:G:584:MET:HG3	2.10	0.51
1:H:545:LEU:HD12	1:H:565:ARG:HG2	1.91	0.51
1:C:567:PHE:HB3	1:C:568:PRO:HD3	1.93	0.51
1:C:606:LYS:HE3	1:D:613:VAL:O	2.11	0.51
1:D:615:GLN:N	1:D:615:GLN:HE21	2.09	0.50
1:F:569:LEU:CD2	1:F:573:MET:CE	2.89	0.50
1:D:577:LEU:HD12	1:D:577:LEU:N	2.28	0.49
1:A:580:LYS:NZ	1:B:589[B]:ASP:OD1	2.46	0.48
1:A:613:VAL:O	1:B:606:LYS:NZ	2.45	0.48
1:A:601:GLU:OE2	1:A:601:GLU:HA	2.13	0.48
1:D:593:LEU:CD2	1:D:596:MET:HE1	2.44	0.48
1:B:592:GLU:O	1:B:596:MET:HE3	2.14	0.47
1:E:587:GLU:HG3	1:F:580:LYS:HG2	1.96	0.47
1:B:553:ALA:HB1	1:B:557:GLU:HB3	1.95	0.47
1:E:584:MET:HE3	1:F:584:MET:HE3	1.95	0.46
1:G:587:GLU:HG2	1:H:580:LYS:O	2.15	0.46
1:G:584:MET:CE	1:H:584:MET:HE3	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:PRO:N	3:E:20:HOH:O	2.49	0.46
1:A:588:ILE:HG21	1:A:596:MET:HE3	1.98	0.46
1:C:587:GLU:HG2	1:D:580:LYS:O	2.17	0.45
1:G:615:GLN:HG2	1:H:606:LYS:HZ1	1.81	0.45
1:G:553:ALA:CB	1:G:561:MET:SD	3.05	0.45
1:B:554:PRO:HD2	1:B:557:GLU:OE1	2.17	0.45
1:F:557:GLU:O	1:F:561:MET:HG3	2.16	0.45
1:F:567:PHE:N	1:F:568:PRO:HD2	2.31	0.45
1:H:565:ARG:HH11	1:H:565:ARG:HG3	1.81	0.45
1:F:600:PRO:HA	3:F:72:HOH:O	2.17	0.45
1:F:604:ARG:O	1:F:608:ASP:OD2	2.35	0.44
1:F:556:GLN:NE2	1:F:557:GLU:H	2.16	0.44
1:G:615:GLN:HG2	1:H:606:LYS:NZ	2.33	0.44
1:F:603:LEU:HD12	1:F:603:LEU:HA	1.81	0.44
1:A:588:ILE:HD13	1:A:596:MET:HE1	1.99	0.44
1:E:545:LEU:HD23	1:E:549:MET:CE	2.48	0.43
1:E:550:LEU:HD22	1:E:558:GLN:HG2	1.99	0.43
1:C:604:ARG:HA	1:C:604:ARG:HD2	1.93	0.43
1:H:615:GLN:N	1:H:615:GLN:HE21	2.17	0.43
1:D:606:LYS:HA	1:D:606:LYS:HD3	1.70	0.43
1:E:592:GLU:CG	1:E:596:MET:CE	2.88	0.43
1:F:596:MET:HB3	1:F:603:LEU:HD13	2.01	0.43
1:H:565:ARG:NH1	1:H:565:ARG:CG	2.77	0.42
1:H:555:PRO:O	1:H:558:GLN:HB2	2.20	0.42
1:D:549:MET:HE2	1:D:549:MET:HB3	1.77	0.42
1:F:597:LEU:HA	1:F:597:LEU:HD23	1.83	0.42
1:F:596:MET:HG2	1:F:602:SER:HB3	2.01	0.42
1:E:584:MET:HE3	1:F:584:MET:HB3	2.01	0.42
1:F:584:MET:HE1	1:F:613:VAL:HB	2.02	0.42
1:A:586:LEU:HA	1:A:586:LEU:HD23	1.89	0.42
1:E:571:GLN:HA	1:E:578:ALA:HB2	2.02	0.41
1:F:589:ASP:HB3	1:F:592:GLU:HB2	2.02	0.41
1:C:593:LEU:HD13	1:C:596:MET:CE	2.43	0.41
1:G:588:ILE:HG22	1:G:589:ASP:N	2.35	0.41
1:C:580:LYS:HD3	1:D:587:GLU:O	2.21	0.41
1:D:593:LEU:HD23	1:D:596:MET:CE	2.45	0.41
1:F:588:ILE:HG22	1:F:589:ASP:N	2.35	0.41
1:D:588:ILE:HG22	1:D:589:ASP:N	2.35	0.41
1:H:584:MET:HB3	1:H:584:MET:HE3	1.95	0.41
1:E:588:ILE:HG21	1:E:596:MET:HE3	2.03	0.41
1:E:545:LEU:HD23	1:E:549:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:GLN:CA	1:D:615:GLN:NE2	2.82	0.40
1:H:594:LEU:HD22	1:H:594:LEU:HA	1.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/79 (90%)	71 (100%)	0	0	100	100
1	B	72/79 (91%)	71 (99%)	1 (1%)	0	100	100
1	C	70/79 (89%)	69 (99%)	1 (1%)	0	100	100
1	D	69/79 (87%)	64 (93%)	5 (7%)	0	100	100
1	E	70/79 (89%)	70 (100%)	0	0	100	100
1	F	70/79 (89%)	65 (93%)	5 (7%)	0	100	100
1	G	70/79 (89%)	69 (99%)	1 (1%)	0	100	100
1	H	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
All	All	563/632 (89%)	549 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/66 (94%)	48 (77%)	14 (23%)	1	1
1	B	63/66 (96%)	54 (86%)	9 (14%)	3	6
1	C	62/66 (94%)	55 (89%)	7 (11%)	6	11
1	D	61/66 (92%)	50 (82%)	11 (18%)	1	3
1	E	62/66 (94%)	56 (90%)	6 (10%)	8	16
1	F	62/66 (94%)	55 (89%)	7 (11%)	6	11
1	G	62/66 (94%)	54 (87%)	8 (13%)	4	8
1	H	62/66 (94%)	54 (87%)	8 (13%)	4	8
All	All	496/528 (94%)	426 (86%)	70 (14%)	3	6

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545	LEU
1	A	546	THR
1	A	550	LEU
1	A	552	SER
1	A	556	GLN
1	A	560	GLN
1	A	585	LEU
1	A	587	GLU
1	A	591	SER
1	A	593	LEU
1	A	601	GLU
1	A	604	ARG
1	A	605	SER
1	A	606	LYS
1	B	548	SER
1	B	564	GLU
1	B	565	ARG
1	B	576	THR
1	B	585	LEU
1	B	589[A]	ASP
1	B	589[B]	ASP
1	B	604	ARG
1	B	615	GLN
1	C	548	SER
1	C	550	LEU
1	C	576	THR
1	C	593	LEU

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Mol	Chain	Res	Type
1	C	601	GLU
1	C	605	SER
1	C	615	GLN
1	D	546	THR
1	D	549	MET
1	D	560	GLN
1	D	564	GLU
1	D	565	ARG
1	D	569	LEU
1	D	576	THR
1	D	577	LEU
1	D	594	LEU
1	D	604	ARG
1	D	615	GLN
1	E	545	LEU
1	E	548	SER
1	E	550	LEU
1	E	556	GLN
1	E	593	LEU
1	E	598	GLU
1	F	545	LEU
1	F	566	LEU
1	F	569	LEU
1	F	576	THR
1	F	591	SER
1	F	592	GLU
1	F	602	SER
1	G	545	LEU
1	G	550	LEU
1	G	556	GLN
1	G	560	GLN
1	G	585	LEU
1	G	593	LEU
1	G	604	ARG
1	G	606	LYS
1	H	545	LEU
1	H	546	THR
1	H	552	SER
1	H	565	ARG
1	H	576	THR
1	H	577	LEU
1	H	594	LEU

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Mol	Chain	Res	Type
1	H	615	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	HIS
1	B	590	ASN
1	B	615	GLN
1	C	560	GLN
1	C	595	HIS
1	D	558	GLN
1	D	615	GLN
1	E	595	HIS
1	F	556	GLN
1	G	556	GLN
1	G	615	GLN
1	H	560	GLN
1	H	615	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	73/79 (92%)	-0.04	0 100 100	19, 27, 39, 41	0
1	B	73/79 (92%)	-0.17	0 100 100	15, 26, 42, 44	0
1	C	72/79 (91%)	-0.08	1 (1%) 75 77	22, 28, 36, 44	0
1	D	71/79 (89%)	0.49	6 (8%) 10 10	27, 40, 80, 81	0
1	E	72/79 (91%)	-0.24	0 100 100	17, 26, 32, 35	0
1	F	72/79 (91%)	0.24	3 (4%) 36 39	26, 37, 47, 48	0
1	G	72/79 (91%)	-0.06	1 (1%) 75 77	20, 33, 41, 44	0
1	H	73/79 (92%)	0.27	5 (6%) 17 17	20, 32, 68, 69	0
All	All	578/632 (91%)	0.05	16 (2%) 53 56	15, 31, 52, 81	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	548	SER	5.1
1	H	546	THR	5.0
1	D	550	LEU	4.2
1	D	545	LEU	3.6
1	F	596	MET	2.9
1	H	545	LEU	2.6
1	G	576	THR	2.5
1	H	551	ALA	2.4
1	H	550	LEU	2.4
1	D	555	PRO	2.3
1	D	548	SER	2.3
1	F	556	GLN	2.3
1	F	550	LEU	2.2
1	D	547	ALA	2.2
1	C	544	PRO	2.1
1	D	556	GLN	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CL	B	5	1/1	0.91	0.19	62,62,62,62	0
2	CL	E	2	1/1	0.92	0.09	62,62,62,62	0
2	CL	G	1	1/1	0.93	0.08	67,67,67,67	0
2	CL	A	3	1/1	0.95	0.07	53,53,53,53	0
2	CL	H	4	1/1	0.97	0.08	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.