



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:09 AM UTC

PDB ID : 9SOH / pdb\_00009soh  
Title : CTLH-CRA domains of the Maea-RanBP10 mutant (Q519G, F543L, Y548F and V556F) complex  
Authors : van gen Hassend, P.M.; Schindelin, H.  
Deposited on : 2025-09-12  
Resolution : 3.54 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.

The types of validation reports are described at

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

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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

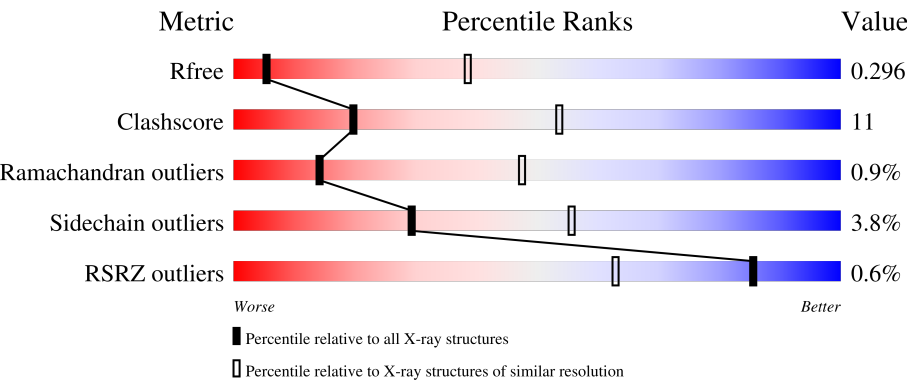
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.54 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 <sub>free</sub>	180053	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

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 of 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	146	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>79%17%..</div></div>
1	C	146	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>67%27%..</div></div>
1	E	146	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>71%24%..</div></div>
1	G	146	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>58%31%5%7%</div></div>
2	B	126	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>67%25%•6%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	126	<div> <div> <div></div> <div>2%</div> </div> <div> <div></div> <div>51%</div> </div> <div> <div></div> <div>41%</div> </div> <div> <div></div> <div>6%</div> </div> </div>
2	F	126	<div> <div></div> <div>78%</div> </div> <div> <div></div> <div>17%</div> </div> <div> <div></div> <div>5%</div> </div>
2	H	126	<div> <div></div> <div>56%</div> </div> <div> <div></div> <div>33%</div> </div> <div> <div></div> <div>10%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8379 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 Ran-binding protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1124	703	200	215	6			
1	C	140	Total	C	N	O	S	0	0	0
			1104	693	197	208	6			
1	E	140	Total	C	N	O	S	0	0	0
			1105	692	197	210	6			
1	G	136	Total	C	N	O	S	0	0	0
			1069	671	190	202	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLY	GLN	engineered mutation	UNP Q6VN19
A	109	LEU	PHE	engineered mutation	UNP Q6VN19
A	114	PHE	TYR	engineered mutation	UNP Q6VN19
A	122	PHE	VAL	engineered mutation	UNP Q6VN19
C	85	GLY	GLN	engineered mutation	UNP Q6VN19
C	109	LEU	PHE	engineered mutation	UNP Q6VN19
C	114	PHE	TYR	engineered mutation	UNP Q6VN19
C	122	PHE	VAL	engineered mutation	UNP Q6VN19
E	85	GLY	GLN	engineered mutation	UNP Q6VN19
E	109	LEU	PHE	engineered mutation	UNP Q6VN19
E	114	PHE	TYR	engineered mutation	UNP Q6VN19
E	122	PHE	VAL	engineered mutation	UNP Q6VN19
G	85	GLY	GLN	engineered mutation	UNP Q6VN19
G	109	LEU	PHE	engineered mutation	UNP Q6VN19
G	114	PHE	TYR	engineered mutation	UNP Q6VN19
G	122	PHE	VAL	engineered mutation	UNP Q6VN19

- Molecule 2 is a protein called E3 ubiquitin-protein transferase MAEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	S	0	0	0
			1004	627	191	179	7			
2	D	118	Total	C	N	O	S	0	0	0
			995	625	187	176	7			
2	H	114	Total	C	N	O	S	0	0	0
			965	604	185	169	7			
2	F	120	Total	C	N	O	S	0	0	0
			1013	636	191	178	8			

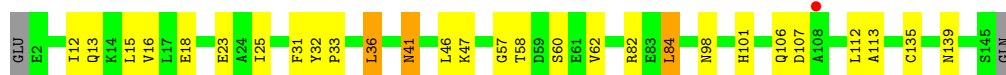
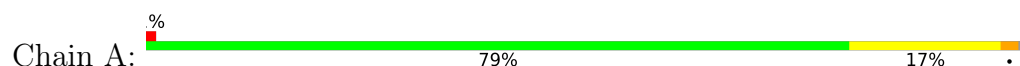
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP Q4VC33
B	2	PRO	-	expression tag	UNP Q4VC33
D	1	GLY	-	expression tag	UNP Q4VC33
D	2	PRO	-	expression tag	UNP Q4VC33
H	1	GLY	-	expression tag	UNP Q4VC33
H	2	PRO	-	expression tag	UNP Q4VC33
F	1	GLY	-	expression tag	UNP Q4VC33
F	2	PRO	-	expression tag	UNP Q4VC33

### 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.

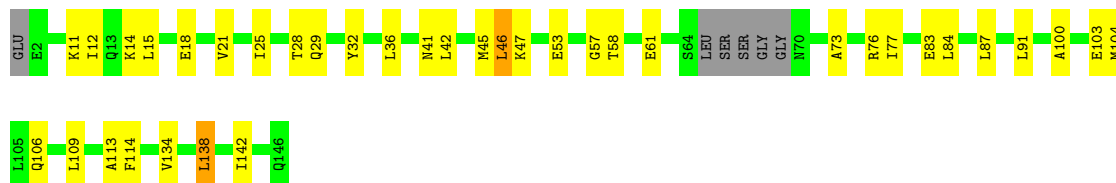
- Molecule 1: Ran-binding protein 10



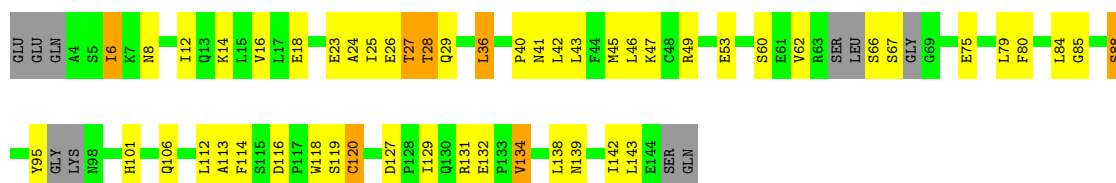
- Molecule 1: Ran-binding protein 10



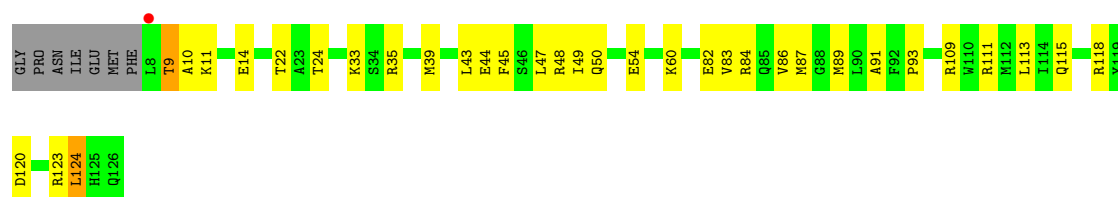
- Molecule 1: Ran-binding protein 10



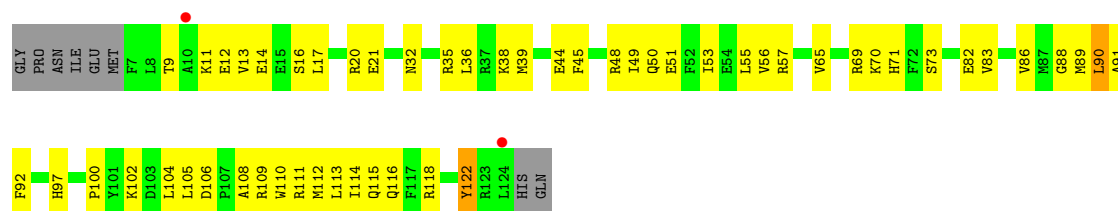
- Molecule 1: Ran-binding protein 10



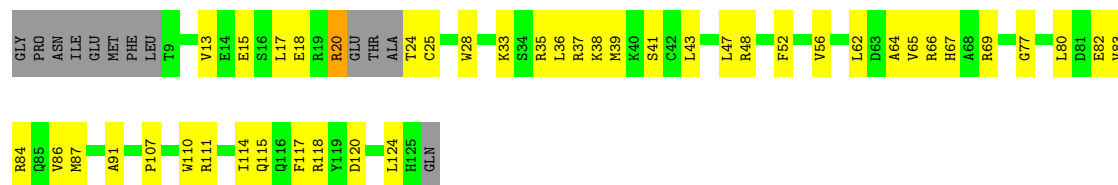
## • Molecule 2: E3 ubiquitin-protein transferase MAEA



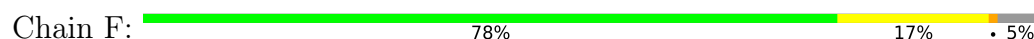
## • Molecule 2: E3 ubiquitin-protein transferase MAEA



## • Molecule 2: E3 ubiquitin-protein transferase MAEA



## • Molecule 2: E3 ubiquitin-protein transferase MAEA



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	359.82Å 359.82Å 359.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.85 – 3.54 46.85 – 3.54	Depositor EDS
% Data completeness (in resolution range)	87.7 (46.85-3.54) 88.4 (46.85-3.54)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.282 , 0.295 0.282 , 0.296	Depositor DCC
$R_{free}$ test set	1143 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	166.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 218.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0606e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.19	0/1142	0.43	0/1540
1	C	0.18	0/1121	0.42	0/1511
1	E	0.18	0/1122	0.36	0/1512
1	G	0.20	0/1084	0.43	0/1459
2	B	0.21	0/1024	0.52	0/1373
2	D	0.20	0/1015	0.54	0/1362
2	F	0.22	0/1034	0.51	0/1387
2	H	0.22	0/984	0.55	0/1318
All	All	0.20	0/8526	0.47	0/11462

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1124	0	1119	21	0
1	C	1104	0	1104	28	0
1	E	1105	0	1099	25	0
1	G	1069	0	1062	38	0
2	B	1004	0	1000	25	0
2	D	995	0	994	35	0
2	F	1013	0	1010	15	0
2	H	965	0	962	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8379	0	8350	192	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 11.

All (192) 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:E:29:GLN:HG2	1:E:36:LEU:HD11	1.70	0.73
1:G:46:LEU:HD11	1:G:138:LEU:HD21	1.72	0.71
1:G:40:PRO:HG2	1:G:95:TYR:HE2	1.56	0.71
1:A:31:PHE:O	1:A:33:PRO:HD3	1.93	0.69
1:C:112:LEU:O	1:C:114:PHE:N	2.26	0.68
1:G:23:GLU:HG3	1:G:60:SER:HB3	1.74	0.68
2:H:17:LEU:O	2:H:20:ARG:NH1	2.26	0.68
1:C:36:LEU:HD22	1:C:43:LEU:HD13	1.77	0.67
2:D:53:ILE:HG23	2:D:89:MET:HE1	1.77	0.67
1:C:18:GLU:HG2	1:G:18:GLU:HG2	1.78	0.66
1:E:106:GLN:HB3	2:F:84:ARG:HG2	1.76	0.65
2:D:50:GLN:HG2	2:D:113:LEU:HD11	1.79	0.65
1:A:23:GLU:HG3	1:A:60:SER:HB3	1.81	0.62
2:D:17:LEU:HD13	2:D:114:ILE:HG12	1.82	0.61
1:E:14:LYS:NZ	1:E:18:GLU:OE2	2.28	0.60
2:D:49:ILE:HD12	2:D:86:VAL:HG21	1.82	0.60
2:D:109:ARG:NH1	2:D:112:MET:SD	2.74	0.60
1:A:18:GLU:HG2	1:E:18:GLU:HG2	1.82	0.60
1:A:36:LEU:H	1:A:36:LEU:HD22	1.67	0.60
1:A:106:GLN:HB3	2:B:84:ARG:HG2	1.82	0.60
1:C:85:GLY:HA3	2:D:91:ALA:HB1	1.84	0.59
2:D:16:SER:HB2	2:D:21:GLU:HB2	1.84	0.58
1:C:82:ARG:HA	2:D:91:ALA:HA	1.84	0.58
2:D:97:HIS:HB3	2:D:102:LYS:HD2	1.87	0.57
1:G:24:ALA:O	1:G:28:THR:OG1	2.21	0.57
2:H:120:ASP:O	2:H:124:LEU:N	2.37	0.56
2:D:83:VAL:HA	2:D:86:VAL:HG22	1.86	0.56
2:B:39:MET:SD	2:B:123:ARG:HD2	2.46	0.56
1:G:41:ASN:OD1	1:G:101:HIS:NE2	2.36	0.56
1:G:106:GLN:HB3	2:H:84:ARG:HG2	1.88	0.56
1:G:23:GLU:HG3	1:G:60:SER:CB	2.36	0.55
1:C:53:GLU:OE2	1:C:131:ARG:NE	2.39	0.55
1:E:41:ASN:O	1:E:45:MET:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:LEU:HA	2:H:39:MET:HE2	1.88	0.55
1:C:9:ARG:NH1	1:C:139:ASN:OD1	2.40	0.55
2:H:65:VAL:O	2:H:69:ARG:HG3	2.07	0.55
1:G:8:ASN:O	1:G:12:ILE:HG12	2.07	0.55
1:E:61:GLU:HB3	1:E:76:ARG:HH21	1.71	0.54
1:C:105:LEU:O	1:C:109:LEU:HG	2.06	0.54
2:B:83:VAL:HA	2:B:86:VAL:HG22	1.90	0.54
2:B:14:GLU:OE2	2:B:118:ARG:NH2	2.39	0.54
1:C:131:ARG:HH22	1:G:14:LYS:HE2	1.73	0.54
2:D:65:VAL:O	2:D:69:ARG:HG3	2.08	0.54
1:G:43:LEU:O	1:G:47:LYS:HG2	2.08	0.53
2:H:117:PHE:CD2	2:H:118:ARG:HG3	2.43	0.53
2:F:83:VAL:HA	2:F:86:VAL:HG22	1.89	0.53
2:B:47:LEU:HD23	2:B:113:LEU:HD13	1.90	0.53
1:E:45:MET:HG2	1:E:104:MET:HE1	1.90	0.53
1:A:47:LYS:HB3	1:A:84:LEU:HD21	1.90	0.52
1:C:132:GLU:HG3	1:G:132:GLU:CD	2.33	0.52
1:G:127:ASP:OD1	1:G:129:ILE:HG22	2.09	0.52
2:H:111:ARG:O	2:H:115:GLN:HG3	2.09	0.52
1:G:23:GLU:O	1:G:27:THR:OG1	2.25	0.52
2:B:50:GLN:O	2:B:54:GLU:HG2	2.10	0.52
2:H:39:MET:HE1	2:H:124:LEU:HD11	1.91	0.52
2:B:111:ARG:O	2:B:115:GLN:HG2	2.10	0.52
2:H:82:GLU:O	2:H:86:VAL:HG13	2.10	0.52
1:A:107:ASP:OD1	2:B:84:ARG:NH1	2.43	0.52
1:A:41:ASN:OD1	1:A:41:ASN:N	2.42	0.51
2:B:22:THR:O	2:B:24:THR:N	2.42	0.51
1:C:5:SER:HA	1:C:32:TYR:OH	2.10	0.51
2:F:61:ARG:O	2:F:65:VAL:HG23	2.11	0.51
1:A:12:ILE:O	1:A:16:VAL:HG23	2.11	0.51
1:E:21:VAL:O	1:E:25:ILE:HG13	2.10	0.51
1:G:25:ILE:HG13	1:G:26:GLU:N	2.26	0.51
1:G:85:GLY:HA3	2:H:91:ALA:O	2.11	0.50
2:D:14:GLU:OE2	2:D:118:ARG:NH2	2.45	0.50
1:G:40:PRO:HG2	1:G:95:TYR:CE2	2.43	0.50
2:D:51:GLU:O	2:D:55:LEU:HG	2.12	0.50
1:C:112:LEU:C	1:C:114:PHE:H	2.19	0.50
1:C:41:ASN:OD1	1:C:42:LEU:N	2.45	0.49
2:F:47:LEU:HD23	2:F:113:LEU:HD13	1.93	0.49
2:D:56:VAL:HG11	2:D:89:MET:HG3	1.93	0.49
1:G:114:PHE:O	2:H:69:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLU:O	2:B:48:ARG:HG2	2.12	0.49
1:E:138:LEU:O	1:E:142:ILE:HG12	2.13	0.49
1:A:82:ARG:HH22	2:B:93:PRO:HA	1.77	0.48
1:G:45:MET:HE2	1:G:134:VAL:HG12	1.96	0.48
2:D:38:LYS:HD3	2:D:38:LYS:HA	1.65	0.48
2:D:32:ASN:HB3	2:D:35:ARG:HE	1.77	0.48
2:D:90:LEU:C	2:D:92:PHE:H	2.20	0.48
1:G:139:ASN:O	1:G:143:LEU:HG	2.13	0.48
1:G:113:ALA:O	2:H:69:ARG:HA	2.14	0.48
1:E:109:LEU:HD12	2:F:88:GLY:HA2	1.95	0.47
2:H:48:ARG:HD2	2:H:67:HIS:CE1	2.49	0.47
2:D:111:ARG:O	2:D:115:GLN:HG3	2.15	0.47
1:E:47:LYS:HB3	1:E:84:LEU:HD11	1.96	0.47
1:G:53:GLU:OE2	1:G:131:ARG:HD3	2.15	0.47
2:H:13:VAL:HG22	2:H:25:CYS:HB2	1.97	0.47
2:H:28:TRP:CZ3	2:H:36:LEU:HD13	2.49	0.47
2:F:109:ARG:O	2:F:113:LEU:HG	2.15	0.47
1:C:41:ASN:O	1:C:45:MET:HG3	2.14	0.47
1:C:47:LYS:HE3	1:C:84:LEU:HD11	1.96	0.47
2:D:20:ARG:HG2	2:D:110:TRP:CE2	2.49	0.47
2:D:44:GLU:O	2:D:48:ARG:HG2	2.14	0.47
1:E:45:MET:CE	1:E:134:VAL:HG12	2.45	0.47
1:G:116:ASP:HB3	1:G:119:SER:OG	2.14	0.47
1:E:83:GLU:O	1:E:87:LEU:HG	2.15	0.47
2:B:9:THR:HG22	2:B:10:ALA:H	1.80	0.47
2:D:9:THR:HG22	2:D:11:LYS:H	1.79	0.47
2:D:82:GLU:O	2:D:86:VAL:HG13	2.15	0.46
2:B:45:PHE:HZ	2:B:83:VAL:HG23	1.80	0.46
2:B:39:MET:HB3	2:B:123:ARG:NH1	2.30	0.46
2:D:32:ASN:O	2:D:36:LEU:HG	2.15	0.46
1:A:25:ILE:HG12	1:A:46:LEU:HD13	1.97	0.46
1:G:75:GLU:O	1:G:79:LEU:HD23	2.15	0.46
2:B:109:ARG:O	2:B:113:LEU:HG	2.16	0.46
1:G:42:LEU:HD11	1:G:138:LEU:HD22	1.97	0.46
2:D:45:PHE:O	2:D:49:ILE:HG12	2.16	0.46
1:E:11:LYS:O	1:E:15:LEU:HD13	2.16	0.46
1:G:138:LEU:O	1:G:142:ILE:HG13	2.15	0.46
2:H:124:LEU:HA	2:H:124:LEU:HD23	1.73	0.45
1:C:83:GLU:O	1:C:87:LEU:HG	2.16	0.45
2:D:100:PRO:O	2:D:104:LEU:HG	2.16	0.45
2:H:83:VAL:HA	2:H:86:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HB2	2:B:87:MET:SD	2.56	0.45
2:B:49:ILE:HG23	2:B:86:VAL:HG11	1.98	0.45
1:A:57:GLY:HA2	1:A:62:VAL:HG21	1.99	0.45
1:C:29:GLN:HG2	1:C:36:LEU:HD11	1.99	0.45
2:B:82:GLU:O	2:B:86:VAL:HG13	2.16	0.45
1:C:82:ARG:HD2	2:D:91:ALA:HA	1.99	0.45
1:A:112:LEU:HB2	2:B:87:MET:HE2	1.99	0.45
2:F:82:GLU:O	2:F:86:VAL:HG13	2.17	0.45
1:A:47:LYS:HB3	1:A:84:LEU:CD2	2.47	0.44
1:G:84:LEU:O	1:G:88:SER:OG	2.36	0.44
2:B:120:ASP:O	2:B:124:LEU:HD12	2.18	0.44
1:C:49:ARG:HE	1:C:134:VAL:HG21	1.82	0.44
2:D:13:VAL:O	2:D:17:LEU:HD12	2.17	0.44
2:H:28:TRP:HZ3	2:H:36:LEU:HD13	1.81	0.44
2:D:17:LEU:HD23	2:D:110:TRP:HE3	1.82	0.44
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.81	0.44
1:G:114:PHE:CG	1:G:120:CYS:HB2	2.53	0.44
1:G:112:LEU:C	1:G:114:PHE:H	2.24	0.44
2:F:13:VAL:HG11	2:F:117:PHE:CZ	2.53	0.44
1:C:70:ASN:CG	1:C:71:GLN:H	2.25	0.44
2:H:52:PHE:O	2:H:56:VAL:HG23	2.17	0.43
1:G:25:ILE:HD13	1:G:47:LYS:NZ	2.33	0.43
1:C:34:GLY:O	1:C:38:HIS:ND1	2.50	0.43
2:D:106:ASP:C	2:D:108:ALA:H	2.26	0.43
2:H:33:LYS:O	2:H:37:ARG:N	2.40	0.43
1:C:107:ASP:O	1:C:111:LEU:HG	2.19	0.43
2:H:39:MET:HE3	2:H:39:MET:HB2	1.76	0.43
2:F:51:GLU:O	2:F:55:LEU:HG	2.18	0.43
1:C:49:ARG:NE	1:C:134:VAL:HG21	2.33	0.43
1:E:12:ILE:HD13	1:E:28:THR:HG22	1.99	0.43
2:F:32:ASN:O	2:F:33:LYS:C	2.61	0.43
2:D:70:LYS:HD3	2:D:71:HIS:CE1	2.54	0.43
2:D:109:ARG:O	2:D:113:LEU:HG	2.19	0.43
2:B:35:ARG:O	2:B:39:MET:HG3	2.19	0.43
1:C:13:GLN:HA	1:C:16:VAL:HG22	2.00	0.43
2:H:107:PRO:O	2:H:110:TRP:HD1	2.02	0.43
1:C:53:GLU:O	1:C:57:GLY:N	2.52	0.43
2:H:52:PHE:CE2	2:H:64:ALA:HB1	2.53	0.42
1:C:6:ILE:HG23	1:C:9:ARG:HH21	1.85	0.42
1:G:36:LEU:H	1:G:36:LEU:HG	1.50	0.42
2:H:87:MET:HE3	2:H:87:MET:HB2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:CD2	2:D:88:GLY:HA2	2.48	0.42
1:E:45:MET:HE2	1:E:134:VAL:HG12	2.01	0.42
1:G:47:LYS:HE3	1:G:80:PHE:CZ	2.54	0.42
2:D:9:THR:HB	2:D:12:GLU:HG3	2.01	0.42
2:H:110:TRP:O	2:H:114:ILE:HG13	2.20	0.42
2:D:35:ARG:HG2	2:D:39:MET:HE2	2.01	0.42
1:G:47:LYS:HB3	1:G:84:LEU:HD11	2.01	0.42
1:A:13:GLN:NE2	1:A:139:ASN:OD1	2.53	0.42
1:A:98:ASN:HB3	1:A:101:HIS:CD2	2.55	0.42
1:E:42:LEU:O	1:E:46:LEU:HD13	2.19	0.42
1:G:49:ARG:HA	1:G:49:ARG:HD2	1.86	0.42
2:H:62:LEU:O	2:H:66:ARG:HG3	2.19	0.42
1:E:32:TYR:CD2	1:E:142:ILE:HD12	2.55	0.42
1:G:66:SER:OG	1:G:67:SER:N	2.51	0.42
2:H:17:LEU:C	2:H:20:ARG:H	2.27	0.42
2:H:36:LEU:HG	2:H:41:SER:HB3	2.01	0.42
1:E:113:ALA:O	2:F:69:ARG:HA	2.20	0.42
2:D:57:ARG:NH2	2:D:105:LEU:O	2.53	0.41
1:G:29:GLN:HG2	1:G:36:LEU:HD23	2.01	0.41
2:H:43:LEU:O	2:H:47:LEU:HB2	2.20	0.41
1:C:7:LYS:HE2	1:G:118:TRP:HB2	2.03	0.41
1:E:53:GLU:O	1:E:57:GLY:N	2.54	0.41
1:A:82:ARG:NH2	2:B:93:PRO:HA	2.35	0.41
2:B:43:LEU:O	2:B:47:LEU:HG	2.21	0.41
2:B:45:PHE:O	2:B:49:ILE:HG12	2.19	0.41
1:E:109:LEU:HD11	2:F:91:ALA:HB2	2.02	0.41
1:E:100:ALA:O	1:E:104:MET:HG3	2.21	0.41
1:E:109:LEU:CD1	2:F:88:GLY:HA2	2.51	0.41
1:A:82:ARG:HA	2:B:91:ALA:HA	2.02	0.40
1:E:73:ALA:O	1:E:77:ILE:HG13	2.21	0.40
1:A:16:VAL:HB	1:A:135:CYS:SG	2.61	0.40
2:H:35:ARG:HA	2:H:38:LYS:HD2	2.02	0.40
2:F:119:TYR:HE2	2:F:123:ARG:HH21	1.68	0.40
1:E:114:PHE:O	2:F:69:ARG:NH1	2.55	0.40
1:G:6:ILE:H	1:G:6:ILE:HG12	1.70	0.40
2:H:77:GLY:H	2:H:80:LEU:HD12	1.86	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	142/146 (97%)	134 (94%)	7 (5%)	1 (1%)	18	52
1	C	136/146 (93%)	130 (96%)	3 (2%)	3 (2%)	5	30
1	E	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
1	G	128/146 (88%)	123 (96%)	5 (4%)	0	100	100
2	B	117/126 (93%)	108 (92%)	8 (7%)	1 (1%)	14	47
2	D	116/126 (92%)	107 (92%)	6 (5%)	3 (3%)	4	27
2	F	118/126 (94%)	114 (97%)	3 (2%)	1 (1%)	16	50
2	H	110/126 (87%)	103 (94%)	7 (6%)	0	100	100
All	All	1003/1088 (92%)	953 (95%)	41 (4%)	9 (1%)	14	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	113	ALA
2	F	33	LYS
1	A	32	TYR
2	B	33	LYS
1	C	34	GLY
1	C	33	PRO
2	D	90	LEU
2	D	73	SER
2	D	122	TYR

### 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	122/124 (98%)	118 (97%)	4 (3%)	33	58
1	C	120/124 (97%)	116 (97%)	4 (3%)	33	58
1	E	120/124 (97%)	115 (96%)	5 (4%)	26	52
1	G	116/124 (94%)	107 (92%)	9 (8%)	11	37
2	B	109/115 (95%)	104 (95%)	5 (5%)	24	50
2	D	108/115 (94%)	106 (98%)	2 (2%)	50	67
2	F	110/115 (96%)	108 (98%)	2 (2%)	51	69
2	H	105/115 (91%)	101 (96%)	4 (4%)	29	56
All	All	910/956 (95%)	875 (96%)	35 (4%)	29	56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	41	ASN
1	A	58	THR
1	A	84	LEU
2	B	9	THR
2	B	11	LYS
2	B	60	LYS
2	B	89	MET
2	B	124	LEU
1	C	6	ILE
1	C	58	THR
1	C	62	VAL
1	C	143	LEU
2	D	116	GLN
2	D	122	TYR
1	E	46	LEU
1	E	58	THR
1	E	91	LEU
1	E	103	GLU
1	E	138	LEU
1	G	6	ILE
1	G	16	VAL
1	G	27	THR
1	G	28	THR
1	G	36	LEU

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Mol	Chain	Res	Type
1	G	62	VAL
1	G	88	SER
1	G	120	CYS
1	G	134	VAL
2	H	15	GLU
2	H	18	GLU
2	H	20	ARG
2	H	24	THR
2	F	20	ARG
2	F	25	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	101	HIS
2	B	67	HIS
2	B	71	HIS
1	C	29	GLN
2	D	97	HIS
1	E	8	ASN
1	E	13	GLN
1	E	130	GLN
1	G	71	GLN
1	G	90	GLN
2	H	30	HIS
2	H	50	GLN
2	H	74	GLN
2	F	32	ASN
2	F	71	HIS

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	144/146 (98%)	-0.42	1 (0%) 84 60	100, 151, 215, 226	0
1	C	140/146 (95%)	-0.13	2 (1%) 73 45	152, 200, 244, 272	0
1	E	140/146 (95%)	-0.45	0 100 100	96, 140, 196, 211	0
1	G	136/146 (93%)	-0.12	0 100 100	131, 188, 237, 252	0
2	B	119/126 (94%)	-0.22	1 (0%) 82 57	111, 155, 205, 239	0
2	D	118/126 (93%)	-0.09	2 (1%) 69 40	173, 216, 254, 272	0
2	F	120/126 (95%)	-0.33	0 100 100	98, 144, 189, 214	0
2	H	114/126 (90%)	-0.15	0 100 100	180, 218, 257, 272	0
All	All	1031/1088 (94%)	-0.25	6 (0%) 85 63	96, 180, 243, 272	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	CYS	3.2
2	D	124	LEU	2.5
2	D	10	ALA	2.3
1	C	51	PHE	2.3
2	B	8	LEU	2.1
1	A	108	ALA	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.