



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:12 AM BST

PDB ID : 6KHX
Title : Crystal structure of Prx from Akkermansia muciniphila
Authors : Li, M.; Wang, J.; Xu, W.; Wang, Y.; Zhang, M.; Wang, M.
Deposited on : 2019-07-16
Resolution : 2.58 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
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

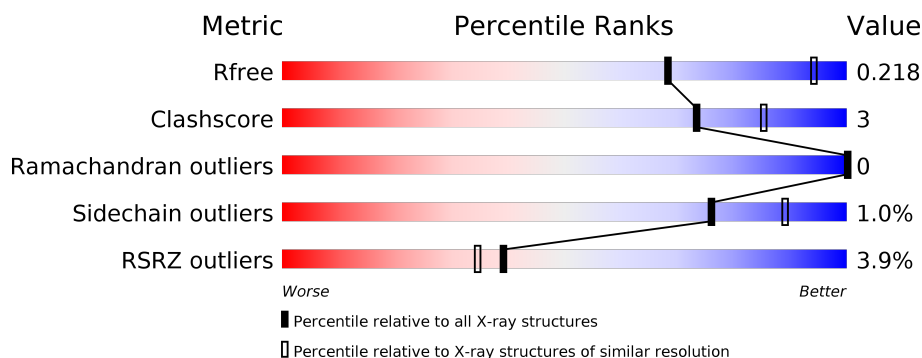
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	215	<div> <div>5%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	B	215	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	C	215	<div> <div>6%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	D	215	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	E	215	<div> <div>5%</div> <div>86%</div> <div>9%</div> <div>..</div> </div>
1	F	215	<div> <div>3%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	215	<div><div></div><div>5%</div><div>85%</div><div>12%</div><div></div><div></div></div>
1	H	215	<div><div></div><div>4%</div><div>87%</div><div>8%</div><div>6%</div><div></div></div>
1	I	215	<div><div></div><div>5%</div><div>90%</div><div>7%</div><div></div><div></div></div>
1	J	215	<div><div></div><div>2%</div><div>87%</div><div>9%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16954 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1640	1054	268	313	5			
1	B	211	Total	C	N	O	S	0	0	0
			1650	1060	271	314	5			
1	C	211	Total	C	N	O	S	0	0	0
			1650	1060	271	314	5			
1	D	208	Total	C	N	O	S	0	0	0
			1629	1049	268	307	5			
1	E	208	Total	C	N	O	S	0	0	0
			1621	1043	264	309	5			
1	F	211	Total	C	N	O	S	0	0	0
			1650	1060	271	314	5			
1	G	209	Total	C	N	O	S	0	0	0
			1630	1048	265	312	5			
1	H	203	Total	C	N	O	S	0	0	0
			1584	1022	259	298	5			
1	I	211	Total	C	N	O	S	0	0	0
			1650	1060	271	314	5			
1	J	207	Total	C	N	O	S	0	0	0
			1621	1045	267	304	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	LEU	-	expression tag	UNP A0A2N8HPY4
A	209	GLU	-	expression tag	UNP A0A2N8HPY4
A	210	HIS	-	expression tag	UNP A0A2N8HPY4
A	211	HIS	-	expression tag	UNP A0A2N8HPY4
A	212	HIS	-	expression tag	UNP A0A2N8HPY4
A	213	HIS	-	expression tag	UNP A0A2N8HPY4
A	214	HIS	-	expression tag	UNP A0A2N8HPY4
A	215	HIS	-	expression tag	UNP A0A2N8HPY4
B	208	LEU	-	expression tag	UNP A0A2N8HPY4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	209	GLU	-	expression tag	UNP A0A2N8HPY4
B	210	HIS	-	expression tag	UNP A0A2N8HPY4
B	211	HIS	-	expression tag	UNP A0A2N8HPY4
B	212	HIS	-	expression tag	UNP A0A2N8HPY4
B	213	HIS	-	expression tag	UNP A0A2N8HPY4
B	214	HIS	-	expression tag	UNP A0A2N8HPY4
B	215	HIS	-	expression tag	UNP A0A2N8HPY4
C	208	LEU	-	expression tag	UNP A0A2N8HPY4
C	209	GLU	-	expression tag	UNP A0A2N8HPY4
C	210	HIS	-	expression tag	UNP A0A2N8HPY4
C	211	HIS	-	expression tag	UNP A0A2N8HPY4
C	212	HIS	-	expression tag	UNP A0A2N8HPY4
C	213	HIS	-	expression tag	UNP A0A2N8HPY4
C	214	HIS	-	expression tag	UNP A0A2N8HPY4
C	215	HIS	-	expression tag	UNP A0A2N8HPY4
D	208	LEU	-	expression tag	UNP A0A2N8HPY4
D	209	GLU	-	expression tag	UNP A0A2N8HPY4
D	210	HIS	-	expression tag	UNP A0A2N8HPY4
D	211	HIS	-	expression tag	UNP A0A2N8HPY4
D	212	HIS	-	expression tag	UNP A0A2N8HPY4
D	213	HIS	-	expression tag	UNP A0A2N8HPY4
D	214	HIS	-	expression tag	UNP A0A2N8HPY4
D	215	HIS	-	expression tag	UNP A0A2N8HPY4
E	208	LEU	-	expression tag	UNP A0A2N8HPY4
E	209	GLU	-	expression tag	UNP A0A2N8HPY4
E	210	HIS	-	expression tag	UNP A0A2N8HPY4
E	211	HIS	-	expression tag	UNP A0A2N8HPY4
E	212	HIS	-	expression tag	UNP A0A2N8HPY4
E	213	HIS	-	expression tag	UNP A0A2N8HPY4
E	214	HIS	-	expression tag	UNP A0A2N8HPY4
E	215	HIS	-	expression tag	UNP A0A2N8HPY4
F	208	LEU	-	expression tag	UNP A0A2N8HPY4
F	209	GLU	-	expression tag	UNP A0A2N8HPY4
F	210	HIS	-	expression tag	UNP A0A2N8HPY4
F	211	HIS	-	expression tag	UNP A0A2N8HPY4
F	212	HIS	-	expression tag	UNP A0A2N8HPY4
F	213	HIS	-	expression tag	UNP A0A2N8HPY4
F	214	HIS	-	expression tag	UNP A0A2N8HPY4
F	215	HIS	-	expression tag	UNP A0A2N8HPY4
G	208	LEU	-	expression tag	UNP A0A2N8HPY4
G	209	GLU	-	expression tag	UNP A0A2N8HPY4
G	210	HIS	-	expression tag	UNP A0A2N8HPY4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	211	HIS	-	expression tag	UNP A0A2N8HPY4
G	212	HIS	-	expression tag	UNP A0A2N8HPY4
G	213	HIS	-	expression tag	UNP A0A2N8HPY4
G	214	HIS	-	expression tag	UNP A0A2N8HPY4
G	215	HIS	-	expression tag	UNP A0A2N8HPY4
H	208	LEU	-	expression tag	UNP A0A2N8HPY4
H	209	GLU	-	expression tag	UNP A0A2N8HPY4
H	210	HIS	-	expression tag	UNP A0A2N8HPY4
H	211	HIS	-	expression tag	UNP A0A2N8HPY4
H	212	HIS	-	expression tag	UNP A0A2N8HPY4
H	213	HIS	-	expression tag	UNP A0A2N8HPY4
H	214	HIS	-	expression tag	UNP A0A2N8HPY4
H	215	HIS	-	expression tag	UNP A0A2N8HPY4
I	208	LEU	-	expression tag	UNP A0A2N8HPY4
I	209	GLU	-	expression tag	UNP A0A2N8HPY4
I	210	HIS	-	expression tag	UNP A0A2N8HPY4
I	211	HIS	-	expression tag	UNP A0A2N8HPY4
I	212	HIS	-	expression tag	UNP A0A2N8HPY4
I	213	HIS	-	expression tag	UNP A0A2N8HPY4
I	214	HIS	-	expression tag	UNP A0A2N8HPY4
I	215	HIS	-	expression tag	UNP A0A2N8HPY4
J	208	LEU	-	expression tag	UNP A0A2N8HPY4
J	209	GLU	-	expression tag	UNP A0A2N8HPY4
J	210	HIS	-	expression tag	UNP A0A2N8HPY4
J	211	HIS	-	expression tag	UNP A0A2N8HPY4
J	212	HIS	-	expression tag	UNP A0A2N8HPY4
J	213	HIS	-	expression tag	UNP A0A2N8HPY4
J	214	HIS	-	expression tag	UNP A0A2N8HPY4
J	215	HIS	-	expression tag	UNP A0A2N8HPY4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 1	0	0

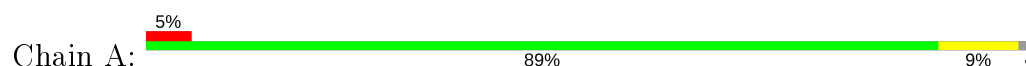
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	68	Total 68	O 68	0	0
3	C	56	Total 56	O 56	0	0
3	D	58	Total 58	O 58	0	0
3	E	55	Total 55	O 55	0	0
3	F	52	Total 52	O 52	0	0
3	G	39	Total 39	O 39	0	0
3	H	62	Total 62	O 62	0	0
3	I	81	Total 81	O 81	0	0
3	J	81	Total 81	O 81	0	0

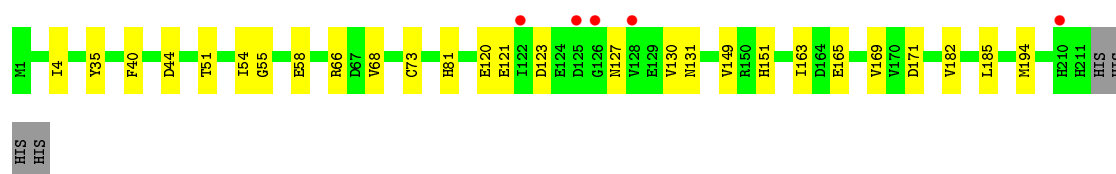
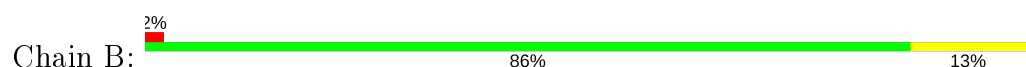
3 Residue-property plots [i](#)

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.

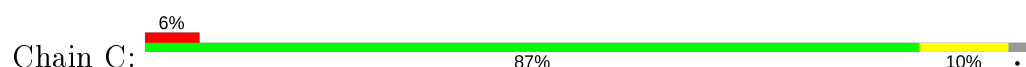
- Molecule 1: Peroxiredoxin



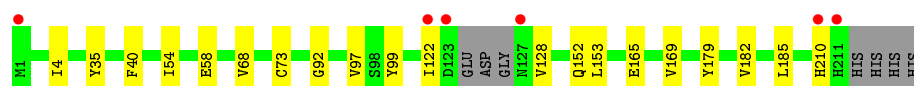
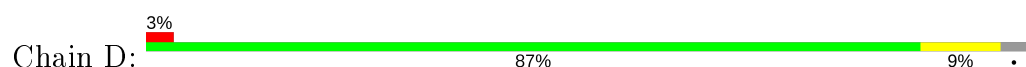
- Molecule 1: Peroxiredoxin



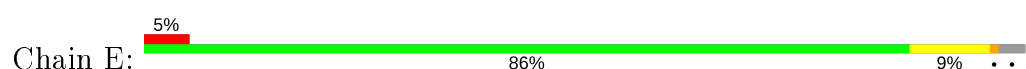
- Molecule 1: Peroxiredoxin



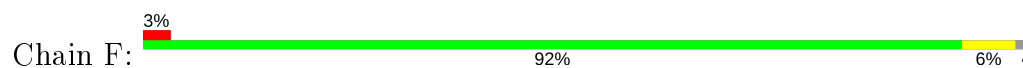
- Molecule 1: Peroxiredoxin



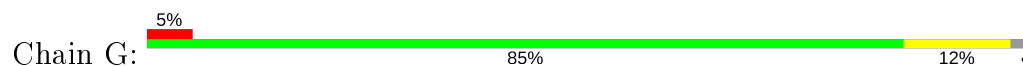
- Molecule 1: Peroxiredoxin



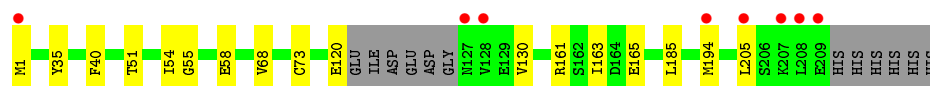
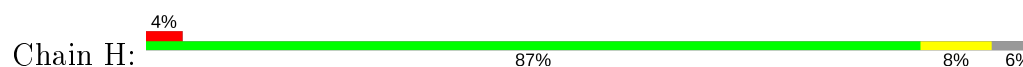
- Molecule 1: Peroxiredoxin



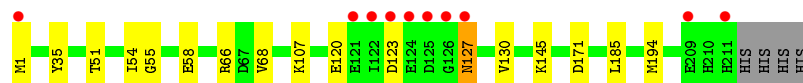
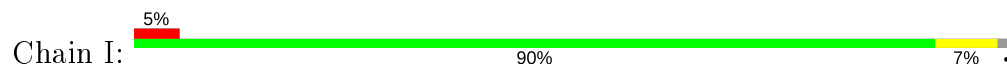
- Molecule 1: Peroxiredoxin



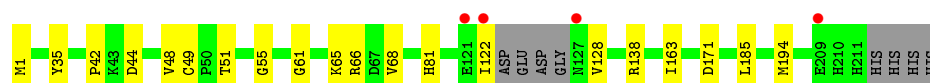
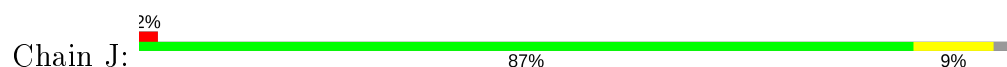
- Molecule 1: Peroxiredoxin



- Molecule 1: Peroxiredoxin



- Molecule 1: Peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.73 Å 211.37 Å 92.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.58 49.10 – 2.58	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.09-2.58) 96.1 (49.10-2.58)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.58 Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.177 , 0.218 0.177 , 0.218	Depositor DCC
R_{free} test set	3986 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16954	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: CA

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	0.30	0/1682	0.49	0/2285
1	B	0.30	0/1693	0.50	0/2300
1	C	0.30	0/1693	0.49	0/2300
1	D	0.29	0/1671	0.48	0/2269
1	E	0.29	0/1662	0.47	0/2258
1	F	0.29	0/1693	0.48	0/2300
1	G	0.29	0/1671	0.49	0/2270
1	H	0.30	0/1624	0.50	0/2205
1	I	0.32	0/1693	0.50	0/2300
1	J	0.31	0/1663	0.49	0/2258
All	All	0.30	0/16745	0.49	0/22745

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 ⓘ

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	1640	0	1582	14	0
1	B	1650	0	1589	17	0
1	C	1650	0	1589	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1629	0	1575	12	0
1	E	1621	0	1569	13	0
1	F	1650	0	1589	9	0
1	G	1630	0	1575	21	0
1	H	1584	0	1540	16	0
1	I	1650	0	1589	14	0
1	J	1621	0	1571	12	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	69	0	0	0	0
3	B	68	0	0	0	0
3	C	56	0	0	0	0
3	D	58	0	0	1	0
3	E	55	0	0	0	0
3	F	52	0	0	0	0
3	G	39	0	0	0	0
3	H	62	0	0	0	0
3	I	81	0	0	1	0
3	J	81	0	0	0	0
All	All	16954	0	15768	107	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 3.

All (107) 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:J:122:ILE:HG13	1:J:128:VAL:HG22	1.75	0.67
1:D:4:ILE:HD11	1:D:152:GLN:HG2	1.77	0.65
1:G:121:GLU:OE2	1:G:131:ASN:ND2	2.31	0.63
1:E:203:SER:OG	1:E:207:LYS:NZ	2.32	0.63
1:A:122:ILE:HG12	1:A:128:VAL:HG22	1.79	0.62
1:J:42:PRO:HD2	1:J:49:CYS:SG	2.41	0.61
1:E:35:TYR:HB2	1:E:68:VAL:HG22	1.83	0.61
1:J:35:TYR:HB2	1:J:68:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:MET:HE1	1:J:51:THR:HG21	1.82	0.60
1:E:153:LEU:HD12	1:F:153:LEU:HD12	1.82	0.59
1:I:185:LEU:HD21	1:J:163:ILE:HG13	1.85	0.58
1:A:185:LEU:HD21	1:B:163:ILE:HG13	1.86	0.58
1:D:122:ILE:HG12	1:D:128:VAL:HG22	1.86	0.57
1:F:112:ASP:OD1	1:I:127:ASN:ND2	2.37	0.57
1:D:179:TYR:O	3:D:401:HOH:O	2.17	0.56
1:H:120:GLU:HG2	1:H:130:VAL:HG22	1.88	0.56
1:C:1:MET:SD	1:C:2:LEU:N	2.80	0.55
1:B:35:TYR:HB2	1:B:68:VAL:HG22	1.88	0.55
1:C:35:TYR:HB2	1:C:68:VAL:HG22	1.88	0.55
1:G:194:MET:HE1	1:H:51:THR:HG21	1.90	0.54
1:A:35:TYR:HB2	1:A:68:VAL:HG22	1.89	0.54
1:I:35:TYR:HB2	1:I:68:VAL:HG22	1.91	0.53
1:G:165:GLU:HG2	1:H:165:GLU:HG2	1.91	0.52
1:G:50:PRO:HB2	1:H:205:LEU:HD11	1.91	0.52
1:E:205:LEU:HD12	1:F:92:GLY:HA2	1.92	0.52
1:E:120:GLU:HG2	1:E:130:VAL:HG22	1.92	0.51
1:F:120:GLU:HG2	1:F:130:VAL:HG22	1.92	0.51
1:C:158:PRO:HB3	1:D:182:VAL:HG12	1.92	0.51
1:G:35:TYR:HB2	1:G:68:VAL:HG22	1.91	0.51
1:A:51:THR:HG21	1:B:194:MET:HE1	1.93	0.50
1:I:120:GLU:HG2	1:I:130:VAL:HG22	1.93	0.50
1:G:54:ILE:O	1:G:58:GLU:HG2	2.12	0.50
1:I:123:ASP:N	1:I:127:ASN:O	2.32	0.49
1:B:54:ILE:O	1:B:58:GLU:HG2	2.13	0.49
1:B:121:GLU:OE2	1:B:131:ASN:ND2	2.45	0.48
1:B:120:GLU:HG2	1:B:130:VAL:HG22	1.95	0.48
1:G:163:ILE:HG13	1:H:185:LEU:HD21	1.94	0.48
1:H:35:TYR:HB2	1:H:68:VAL:HG22	1.96	0.48
1:G:185:LEU:HD21	1:H:163:ILE:HG13	1.96	0.48
1:G:124:GLU:HG3	1:G:125:ASP:H	1.78	0.48
1:A:194:MET:HE1	1:B:51:THR:HG21	1.95	0.48
1:B:40:PHE:HA	1:B:73:CYS:O	2.14	0.47
1:J:61:GLY:O	1:J:65:LYS:HG3	2.14	0.47
1:J:66:ARG:HD3	1:J:171:ASP:OD1	2.14	0.47
1:A:48:VAL:HB	1:A:138:ARG:NH2	2.30	0.47
1:I:35:TYR:CE1	1:I:145:LYS:HE3	2.49	0.47
1:C:163:ILE:HG13	1:D:185:LEU:HD21	1.96	0.47
1:F:35:TYR:HB2	1:F:68:VAL:HG22	1.97	0.47
1:G:51:THR:HG21	1:H:194:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ARG:NE	1:E:157:PHE:O	2.39	0.46
1:C:130:VAL:HG11	1:C:134:LEU:HG	1.96	0.46
1:G:122:ILE:HA	1:G:127:ASN:O	2.15	0.46
1:B:4:ILE:HD13	1:B:149:VAL:HG12	1.98	0.45
1:A:181:GLU:OE1	1:A:193:ALA:HB3	2.16	0.45
1:B:66:ARG:HD3	1:B:171:ASP:OD1	2.16	0.45
1:D:40:PHE:HA	1:D:73:CYS:O	2.16	0.45
1:I:51:THR:HG21	1:J:194:MET:HE1	1.99	0.45
1:I:66:ARG:HD3	1:I:171:ASP:OD1	2.17	0.45
1:F:54:ILE:O	1:F:58:GLU:HG2	2.17	0.45
1:C:122:ILE:HA	1:C:127:ASN:O	2.16	0.45
1:D:35:TYR:HB2	1:D:68:VAL:HG22	1.99	0.45
1:C:153:LEU:HD12	1:D:153:LEU:HD12	2.00	0.44
1:G:142:LEU:HB3	1:G:151:HIS:HB3	1.99	0.44
1:G:185:LEU:CD2	1:H:55:GLY:HA3	2.47	0.44
1:C:48:VAL:HB	1:C:138:ARG:NH2	2.33	0.44
1:G:85:VAL:HA	1:G:94:ILE:HG13	2.00	0.44
1:A:161:ARG:O	1:B:185:LEU:HD12	2.18	0.44
1:I:185:LEU:CD2	1:J:55:GLY:HA3	2.48	0.43
1:J:48:VAL:HB	1:J:138:ARG:NH2	2.33	0.43
1:C:40:PHE:HA	1:C:73:CYS:O	2.18	0.43
1:G:55:GLY:HA3	1:H:185:LEU:CD2	2.48	0.43
1:C:151:HIS:CG	1:C:169:VAL:HG11	2.54	0.43
1:E:123:ASP:OD1	1:E:127:ASN:N	2.52	0.43
1:E:158:PRO:HB3	1:F:182:VAL:HG12	2.00	0.43
1:G:1:MET:HB2	1:G:2:LEU:H	1.55	0.42
1:E:1:MET:HG2	1:E:114:GLY:HA3	2.01	0.42
1:E:62:GLU:HB3	1:E:66:ARG:HH21	1.84	0.42
1:J:44:ASP:OD2	1:J:81:HIS:ND1	2.43	0.42
1:I:1:MET:HE2	3:I:401:HOH:O	2.18	0.42
1:A:158:PRO:HB3	1:B:182:VAL:HG12	2.01	0.42
1:H:40:PHE:HA	1:H:73:CYS:O	2.19	0.42
1:E:151:HIS:CG	1:E:169:VAL:HG11	2.55	0.42
1:E:54:ILE:O	1:E:58:GLU:HG3	2.19	0.42
1:F:107:LYS:HE2	1:I:107:LYS:HE2	2.02	0.42
1:I:55:GLY:HA3	1:J:185:LEU:CD2	2.50	0.42
1:B:44:ASP:OD2	1:B:81:HIS:ND1	2.39	0.42
1:G:52:GLU:HA	1:H:185:LEU:HB2	2.01	0.42
1:G:55:GLY:HA3	1:H:185:LEU:HD23	2.01	0.42
1:E:36:VAL:HB	1:E:143:ILE:HB	2.02	0.42
1:G:151:HIS:CG	1:G:169:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:LEU:HD12	1:H:161:ARG:O	2.20	0.41
1:H:54:ILE:O	1:H:58:GLU:HG2	2.20	0.41
1:D:165:GLU:O	1:D:169:VAL:HG23	2.21	0.41
1:F:194:MET:HE2	1:F:194:MET:HB2	1.90	0.41
1:A:55:GLY:HA3	1:B:185:LEU:CD2	2.50	0.41
1:C:97:VAL:HG13	1:C:99:TYR:CE2	2.56	0.41
1:A:40:PHE:HA	1:A:73:CYS:O	2.21	0.41
1:D:54:ILE:O	1:D:58:GLU:HG2	2.20	0.41
1:A:165:GLU:HG2	1:B:165:GLU:HG2	2.02	0.41
1:C:66:ARG:HD3	1:C:171:ASP:OD1	2.21	0.41
1:A:194:MET:HB2	1:A:194:MET:HE2	1.82	0.41
1:C:205:LEU:HD12	1:D:92:GLY:HA2	2.02	0.41
1:B:151:HIS:CG	1:B:169:VAL:HG11	2.56	0.40
1:A:185:LEU:CD2	1:B:55:GLY:HA3	2.51	0.40
1:G:185:LEU:HD23	1:H:55:GLY:HA3	2.03	0.40
1:I:54:ILE:O	1:I:58:GLU:HG2	2.21	0.40
1:D:97:VAL:HG13	1:D:99:TYR:CE2	2.56	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	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
1	B	209/215 (97%)	200 (96%)	9 (4%)	0	100	100
1	C	209/215 (97%)	202 (97%)	7 (3%)	0	100	100
1	D	204/215 (95%)	198 (97%)	6 (3%)	0	100	100
1	E	206/215 (96%)	197 (96%)	9 (4%)	0	100	100
1	F	209/215 (97%)	199 (95%)	10 (5%)	0	100	100
1	G	207/215 (96%)	199 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	199/215 (93%)	193 (97%)	6 (3%)	0	100	100
1	I	209/215 (97%)	201 (96%)	8 (4%)	0	100	100
1	J	203/215 (94%)	196 (97%)	7 (3%)	0	100	100
All	All	2063/2150 (96%)	1986 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	176/181 (97%)	174 (99%)	2 (1%)	73	88
1	B	177/181 (98%)	175 (99%)	2 (1%)	73	88
1	C	177/181 (98%)	175 (99%)	2 (1%)	73	88
1	D	175/181 (97%)	174 (99%)	1 (1%)	86	94
1	E	174/181 (96%)	171 (98%)	3 (2%)	60	79
1	F	177/181 (98%)	176 (99%)	1 (1%)	86	94
1	G	175/181 (97%)	172 (98%)	3 (2%)	60	79
1	H	170/181 (94%)	169 (99%)	1 (1%)	86	94
1	I	177/181 (98%)	176 (99%)	1 (1%)	86	94
1	J	174/181 (96%)	173 (99%)	1 (1%)	86	94
All	All	1752/1810 (97%)	1735 (99%)	17 (1%)	76	89

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	210	HIS
1	B	123	ASP
1	B	127	ASN
1	C	1	MET

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Mol	Chain	Res	Type
1	C	120	GLU
1	D	210	HIS
1	E	1	MET
1	E	62	GLU
1	E	127	ASN
1	F	127	ASN
1	G	1	MET
1	G	123	ASP
1	G	207	LYS
1	H	1	MET
1	I	127	ASN
1	J	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	127	ASN
1	E	127	ASN
1	F	127	ASN
1	I	91	GLN
1	J	188	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	210/215 (97%)	-0.18	11 (5%) 27 23	26, 38, 76, 103	0
1	B	211/215 (98%)	-0.17	5 (2%) 59 55	24, 39, 80, 122	0
1	C	211/215 (98%)	-0.01	12 (5%) 23 20	27, 38, 83, 129	0
1	D	208/215 (96%)	-0.25	6 (2%) 51 47	29, 43, 70, 106	0
1	E	208/215 (96%)	-0.03	10 (4%) 30 26	28, 45, 70, 117	0
1	F	211/215 (98%)	-0.13	6 (2%) 53 49	24, 42, 78, 112	0
1	G	209/215 (97%)	0.02	10 (4%) 30 26	30, 44, 73, 127	0
1	H	203/215 (94%)	-0.20	8 (3%) 39 34	22, 36, 64, 100	0
1	I	211/215 (98%)	-0.14	10 (4%) 31 28	20, 31, 72, 125	0
1	J	207/215 (96%)	-0.39	4 (1%) 66 64	22, 32, 60, 108	0
All	All	2089/2150 (97%)	-0.15	82 (3%) 39 34	20, 39, 75, 129	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	ASP	7.1
1	B	125	ASP	6.2
1	J	122	ILE	5.9
1	C	211	HIS	5.8
1	I	125	ASP	5.6
1	A	126	GLY	5.5
1	I	211	HIS	5.1
1	A	210	HIS	5.0
1	E	125	ASP	4.7
1	F	211	HIS	4.6
1	I	126	GLY	4.6
1	G	126	GLY	4.5
1	I	122	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	127	ASN	4.3
1	C	124	GLU	4.2
1	C	1	MET	4.2
1	D	1	MET	4.0
1	G	125	ASP	3.9
1	H	127	ASN	3.9
1	D	122	ILE	3.7
1	I	1	MET	3.7
1	J	209	GLU	3.6
1	C	123	ASP	3.6
1	A	209	GLU	3.6
1	G	127	ASN	3.5
1	D	211	HIS	3.5
1	E	124	GLU	3.5
1	E	1	MET	3.5
1	I	209	GLU	3.4
1	F	210	HIS	3.4
1	B	122	ILE	3.4
1	I	123	ASP	3.3
1	B	126	GLY	3.3
1	G	122	ILE	3.2
1	I	124	GLU	3.2
1	D	127	ASN	3.2
1	E	127	ASN	3.2
1	F	1	MET	3.1
1	G	124	GLU	3.1
1	H	208	LEU	3.1
1	G	123	ASP	3.1
1	A	128	VAL	3.1
1	C	126	GLY	3.0
1	A	208	LEU	3.0
1	E	126	GLY	3.0
1	H	205	LEU	3.0
1	G	209	GLU	3.0
1	E	122	ILE	2.9
1	C	210	HIS	2.9
1	C	127	ASN	2.8
1	F	209	GLU	2.8
1	A	122	ILE	2.7
1	J	121	GLU	2.6
1	A	207	LYS	2.6
1	C	122	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	123	ASP	2.5
1	E	192	ALA	2.5
1	J	127	ASN	2.5
1	G	208	LEU	2.4
1	F	179	TYR	2.4
1	D	123	ASP	2.4
1	C	121	GLU	2.4
1	F	124	GLU	2.4
1	H	207	LYS	2.4
1	I	121	GLU	2.4
1	A	125	ASP	2.4
1	C	209	GLU	2.4
1	E	207	LYS	2.3
1	E	206	SER	2.3
1	H	209	GLU	2.2
1	B	128	VAL	2.2
1	G	128	VAL	2.2
1	H	1	MET	2.2
1	B	210	HIS	2.2
1	I	127	ASN	2.1
1	H	194	MET	2.1
1	C	192	ALA	2.1
1	D	210	HIS	2.1
1	G	199	GLU	2.1
1	E	193	ALA	2.0
1	A	1	MET	2.0
1	H	128	VAL	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 monosaccharides 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	CA	D	301	1/1	0.71	0.11	78,78,78,78	0
2	CA	G	301	1/1	0.73	0.09	74,74,74,74	0
2	CA	B	301	1/1	0.75	0.10	81,81,81,81	0
2	CA	F	301	1/1	0.78	0.10	84,84,84,84	0
2	CA	H	301	1/1	0.84	0.10	80,80,80,80	0
2	CA	C	301	1/1	0.86	0.08	76,76,76,76	0
2	CA	I	301	1/1	0.96	0.08	69,69,69,69	0
2	CA	J	301	1/1	0.98	0.07	70,70,70,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.