wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 19, 2023 – 11:39 PM EDT

PDB ID	:	5IJT
Title	:	Human Peroxiredoxin 2 Oxidized (SS)
Authors	:	Haynes, A.C.; Bolduc, J.A.; Lowther, W.T.
Deposited on	:	2016-03-02
Resolution	:	2.15 Å(reported)

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

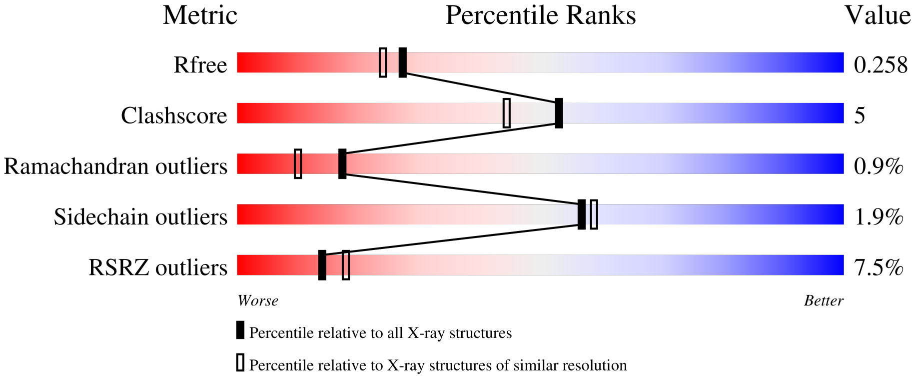
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

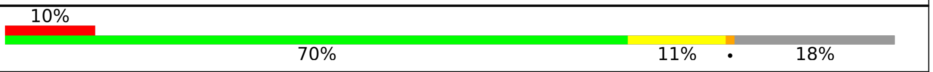
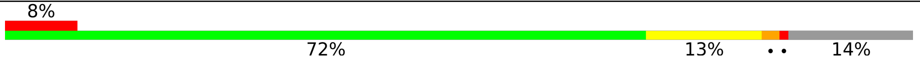
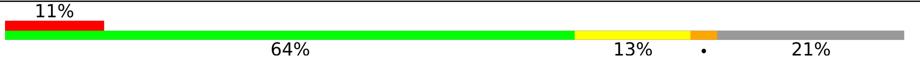
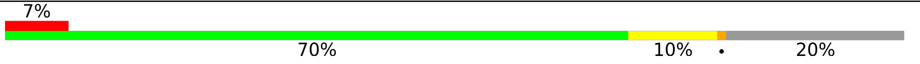
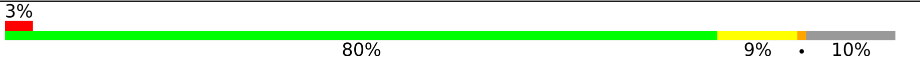
The reported resolution of this entry is 2.15 Å.

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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	198	
1	B	198	
1	C	198	
1	D	198	
1	E	198	

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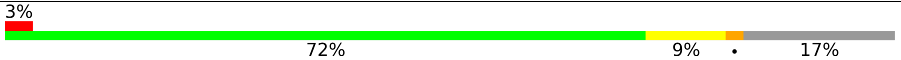
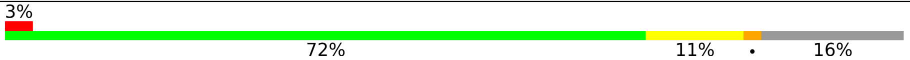
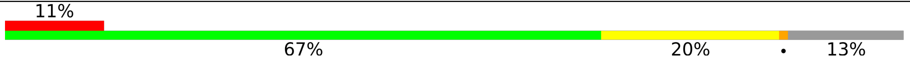
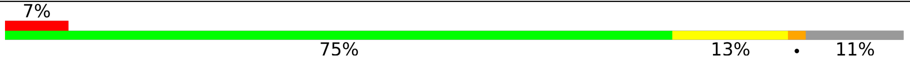
Mol	Chain	Length	Quality of chain
1	F	198	
1	G	198	
1	H	198	
1	I	198	
1	J	198	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26406 atoms, of which 13166 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-2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	162	Total C H N O S 2549 820 1281 214 232 2	0	0	0
1	B	171	Total C H N O S 2674 862 1343 225 241 3	0	0	0
1	C	157	Total C H N O S 2466 795 1236 206 227 2	0	0	0
1	D	158	Total C H N O S 2489 803 1250 207 227 2	0	0	0
1	E	178	Total C H N O S 2762 891 1377 234 257 3	0	0	0
1	F	177	Total C H N O S 2750 887 1373 233 254 3	0	0	0
1	G	164	Total C H N O S 2576 829 1291 216 238 2	0	0	0
1	H	167	Total C H N O S 2610 842 1304 218 243 3	0	0	0
1	I	173	Total C H N O S 2692 871 1343 226 249 3	0	0	0
1	J	176	Total C H N O S 2739 884 1368 232 252 3	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	F	2	Total Zn 2 2	0	0
2	H	1	Total Zn 1 1	0	0

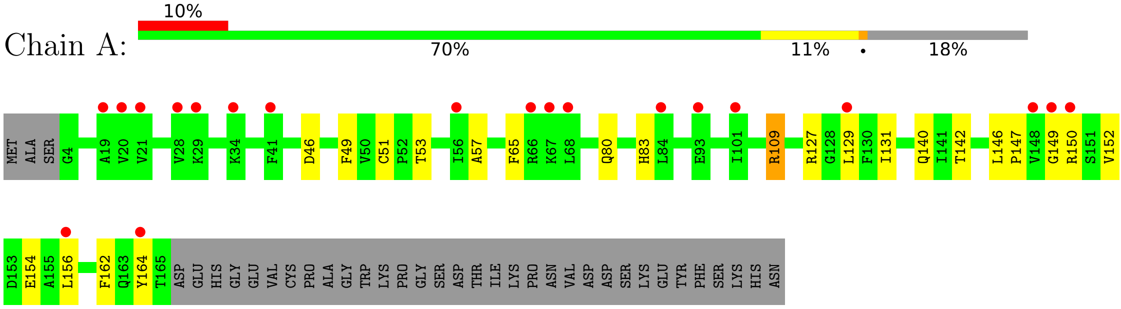
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	16	Total O 16 16	0	0
3	D	5	Total O 5 5	0	0
3	E	17	Total O 17 17	0	0
3	F	15	Total O 15 15	0	0
3	G	5	Total O 5 5	0	0
3	H	16	Total O 16 16	0	0
3	I	9	Total O 9 9	0	0
3	J	11	Total O 11 11	0	0

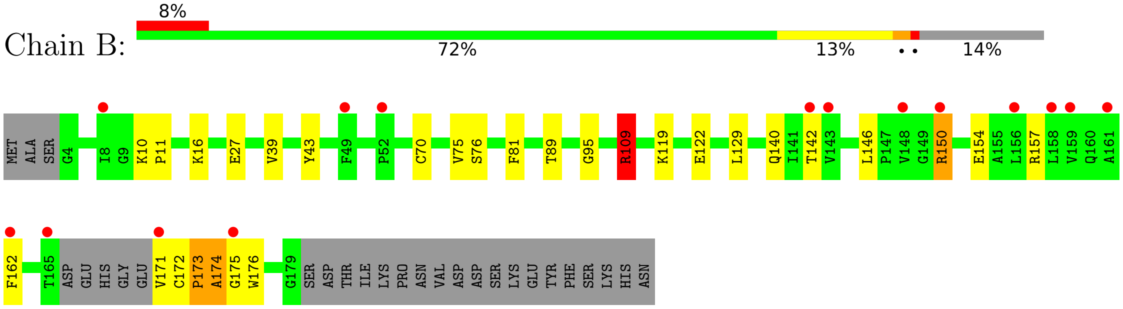
3 Residue-property plots ⓘ

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.

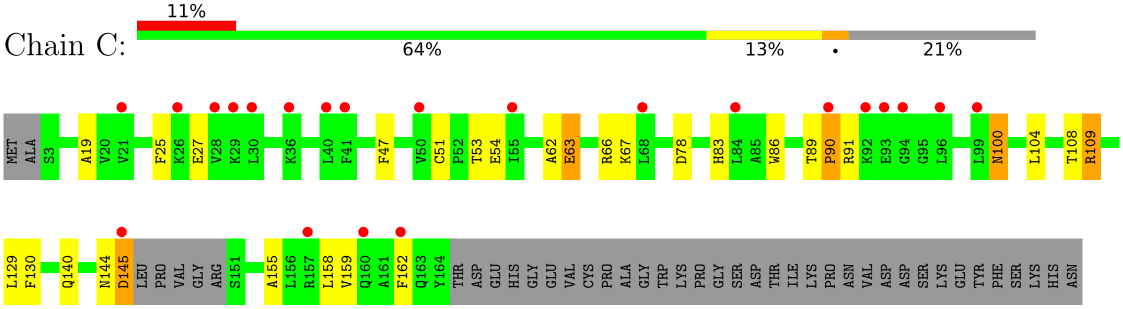
- Molecule 1: Peroxiredoxin-2



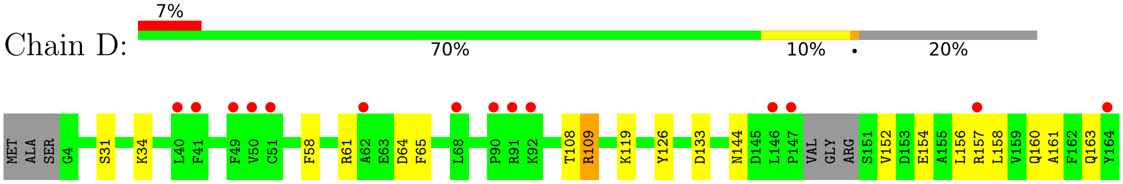
- Molecule 1: Peroxiredoxin-2



- Molecule 1: Peroxiredoxin-2

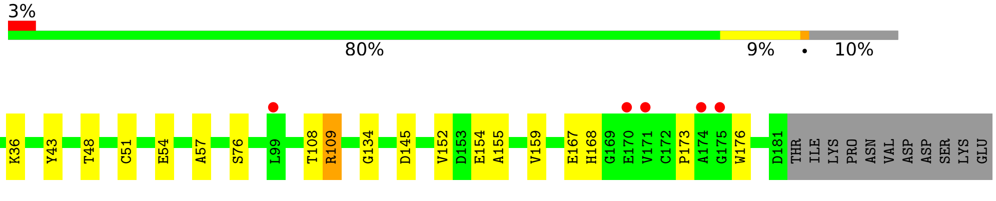


- Molecule 1: Peroxiredoxin-2



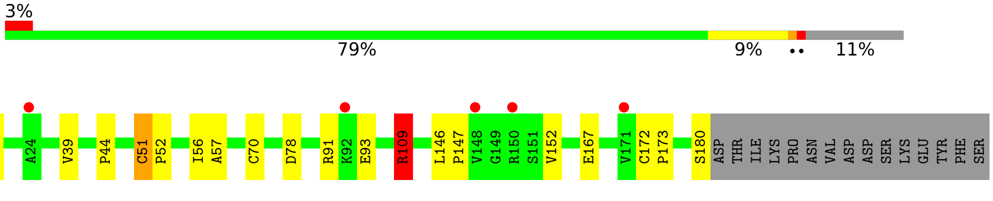
- Molecule 1: Peroxiredoxin-2

Chain E:



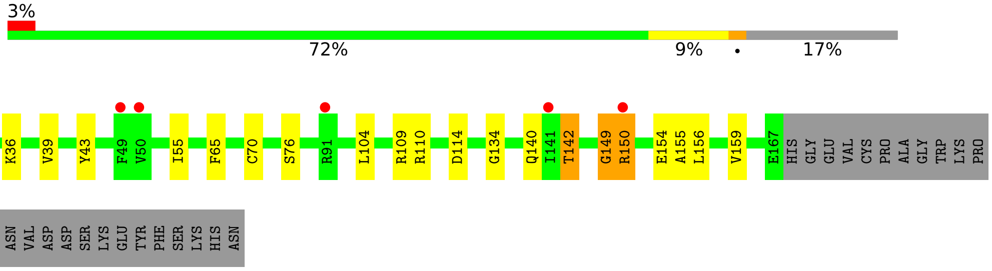
- Molecule 1: Peroxiredoxin-2

Chain F:



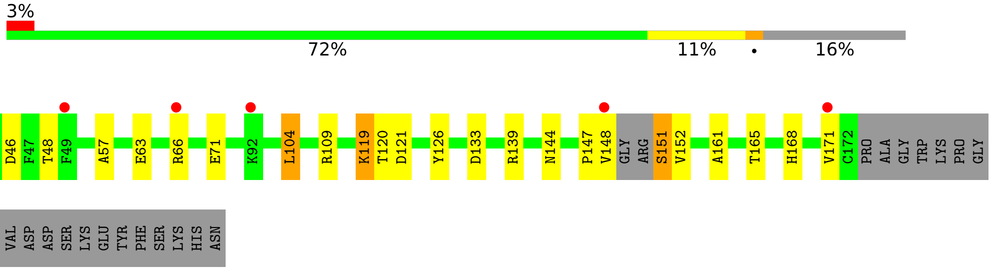
- Molecule 1: Peroxiredoxin-2

Chain G:



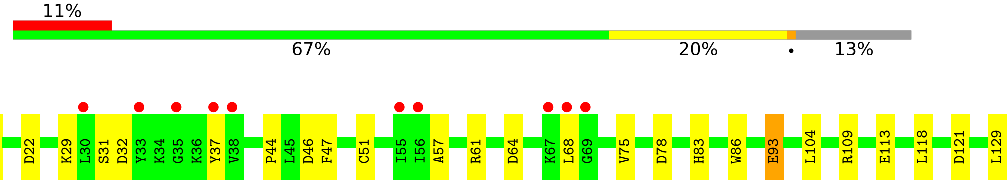
- Molecule 1: Peroxiredoxin-2

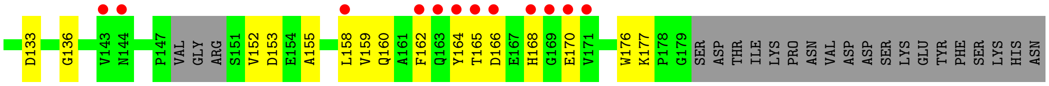
Chain H:



- Molecule 1: Peroxiredoxin-2

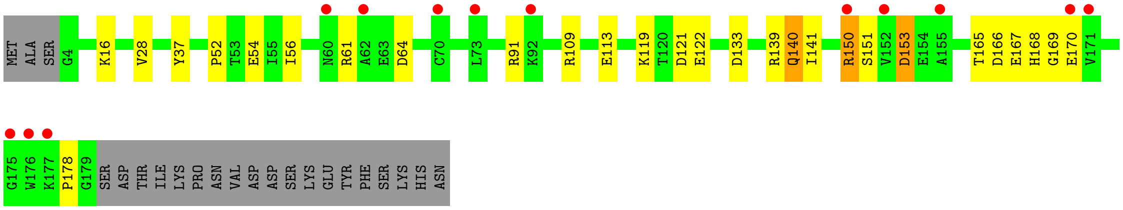
Chain I:





- Molecule 1: Peroxiredoxin-2

Chain J:



4 Data and refinement statistics

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.01Å 198.78Å 116.52Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	44.46 – 2.15 44.46 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.46-2.15) 94.0 (44.46-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.207 , 0.257 0.208 , 0.258	Depositor DCC
R_{free} test set	3612 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26406	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.60	0/1295	0.67	0/1755
1	B	0.79	1/1361 (0.1%)	0.82	1/1845 (0.1%)
1	C	0.61	0/1255	0.70	1/1698 (0.1%)
1	D	0.74	1/1265 (0.1%)	0.81	1/1713 (0.1%)
1	E	0.82	2/1417 (0.1%)	0.80	1/1922 (0.1%)
1	F	0.98	4/1409 (0.3%)	0.95	4/1911 (0.2%)
1	G	0.75	1/1312 (0.1%)	0.79	0/1778
1	H	0.91	0/1333	0.88	3/1806 (0.2%)
1	I	0.73	4/1380 (0.3%)	0.72	2/1871 (0.1%)
1	J	0.78	1/1403 (0.1%)	0.76	0/1903
All	All	0.78	14/13430 (0.1%)	0.79	13/18202 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	93	GLU	CG-CD	8.30	1.64	1.51
1	F	93	GLU	CB-CG	7.83	1.67	1.52
1	I	93	GLU	CB-CG	6.29	1.64	1.52
1	E	154	GLU	CG-CD	5.92	1.60	1.51
1	I	51	CYS	C-N	5.81	1.45	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	109	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	F	109	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	109	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	H	46	ASP	CB-CG-OD1	7.11	124.69	118.30
1	I	109	ARG	NE-CZ-NH1	6.87	123.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	151	SER	Peptide

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	1268	1281	1280	19	0
1	B	1331	1343	1341	24	0
1	C	1230	1236	1235	19	0
1	D	1239	1250	1248	14	0
1	E	1385	1377	1376	15	0
1	F	1377	1373	1372	13	0
1	G	1285	1291	1290	11	0
1	H	1306	1304	1303	10	1
1	I	1349	1343	1341	19	1
1	J	1371	1368	1367	18	0
2	B	1	0	0	0	1
2	F	2	0	0	0	1
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	16	0	0	0	0
3	D	5	0	0	1	0
3	E	17	0	0	0	0
3	F	15	0	0	0	0
3	G	5	0	0	0	0
3	H	16	0	0	1	0
3	I	9	0	0	1	0
3	J	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13240	13166	13153	141	2

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 5.

The worst 5 of 141 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:A:154:GLU:OE2	1:B:150:ARG:NH2	2.02	0.94
1:G:19:ALA:HB2	1:G:104:LEU:HD23	1.63	0.79
1:B:109:ARG:NH1	1:E:109:ARG:HD3	1.99	0.77
1:B:154:GLU:OE2	1:B:157:ARG:NH2	2.23	0.70
1:B:119:LYS:NZ	1:B:122:GLU:OE2	2.19	0.66

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:GLU:OE2	2:F:202:ZN:ZN[2_455]	1.56	0.64
1:H:168:HIS:HE2	2:B:201:ZN:ZN[2_555]	1.17	0.43

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	160/198 (81%)	149 (93%)	10 (6%)	1 (1%)	25	17
1	B	167/198 (84%)	158 (95%)	6 (4%)	3 (2%)	8	2
1	C	153/198 (77%)	141 (92%)	11 (7%)	1 (1%)	22	14
1	D	154/198 (78%)	140 (91%)	14 (9%)	0	100	100
1	E	176/198 (89%)	170 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	175/198 (88%)	168 (96%)	6 (3%)	1 (1%)	25	17
1	G	162/198 (82%)	154 (95%)	6 (4%)	2 (1%)	13	6
1	H	163/198 (82%)	156 (96%)	5 (3%)	2 (1%)	13	6
1	I	169/198 (85%)	159 (94%)	7 (4%)	3 (2%)	8	2
1	J	174/198 (88%)	163 (94%)	9 (5%)	2 (1%)	14	7
All	All	1653/1980 (84%)	1558 (94%)	80 (5%)	15 (1%)	17	10

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	ALA
1	C	90	PRO
1	G	150	ARG
1	J	168	HIS
1	B	175	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/166 (81%)	131 (97%)	4 (3%)	41	39
1	B	141/166 (85%)	139 (99%)	2 (1%)	67	70
1	C	131/166 (79%)	125 (95%)	6 (5%)	27	22
1	D	132/166 (80%)	132 (100%)	0	100	100
1	E	147/166 (89%)	147 (100%)	0	100	100
1	F	146/166 (88%)	143 (98%)	3 (2%)	53	54
1	G	137/166 (82%)	135 (98%)	2 (2%)	65	68
1	H	140/166 (84%)	136 (97%)	4 (3%)	42	40
1	I	143/166 (86%)	142 (99%)	1 (1%)	84	87
1	J	145/166 (87%)	141 (97%)	4 (3%)	43	42
All	All	1397/1660 (84%)	1371 (98%)	26 (2%)	57	59

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	180	SER
1	H	63	GLU
1	J	151	SER
1	G	142	THR
1	H	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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	162/198 (81%)	0.99	20 (12%)	4	5	55, 81, 108, 118	0
1	B	171/198 (86%)	0.73	15 (8%)	10	13	38, 58, 98, 131	0
1	C	157/198 (79%)	1.00	22 (14%)	2	3	54, 83, 113, 138	0
1	D	158/198 (79%)	0.65	14 (8%)	9	13	45, 69, 104, 132	0
1	E	178/198 (89%)	0.60	6 (3%)	45	52	41, 65, 105, 146	0
1	F	177/198 (89%)	0.36	5 (2%)	53	61	40, 59, 90, 108	0
1	G	164/198 (82%)	0.60	5 (3%)	50	58	41, 65, 98, 146	0
1	H	167/198 (84%)	0.60	5 (2%)	50	58	40, 57, 90, 112	0
1	I	173/198 (87%)	0.96	22 (12%)	3	4	46, 78, 125, 214	0
1	J	176/198 (88%)	0.81	13 (7%)	14	18	43, 63, 109, 135	0
All	All	1683/1980 (85%)	0.73	127 (7%)	14	18	38, 67, 107, 214	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	164	TYR	10.8
1	G	50	VAL	6.7
1	I	168	HIS	6.5
1	B	171	VAL	5.4
1	E	174	ALA	5.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	F	201	1/1	0.82	0.11	102,102,102,102	0
2	ZN	H	201	1/1	0.85	0.20	147,147,147,147	0
2	ZN	F	202	1/1	0.86	0.29	120,120,120,120	0
2	ZN	B	201	1/1	0.98	0.12	63,63,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.