



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:09 am BST

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)

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 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

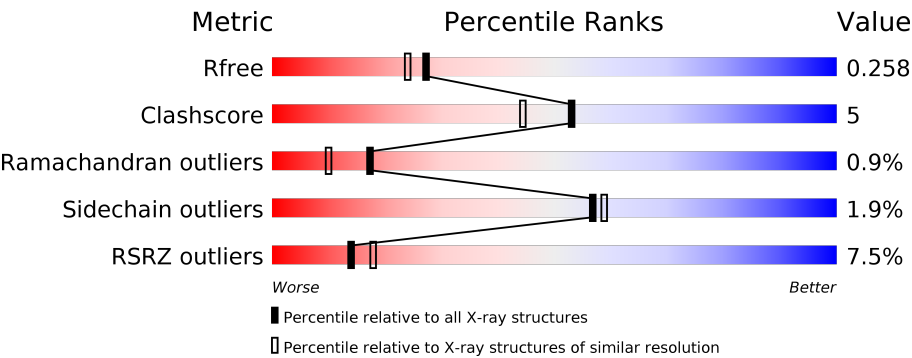
# 1 Overall quality at a glance i

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 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	198	<div><div>10%</div><div><div></div><div>70%</div><div>11%</div><div>•</div><div>18%</div></div></div>
1	B	198	<div><div>8%</div><div><div></div><div>72%</div><div>13%</div><div>••</div><div>14%</div></div></div>
1	C	198	<div><div>11%</div><div><div></div><div>64%</div><div>13%</div><div>•</div><div>21%</div></div></div>
1	D	198	<div><div>7%</div><div><div></div><div>70%</div><div>10%</div><div>•</div><div>20%</div></div></div>
1	E	198	<div><div>3%</div><div><div></div><div>80%</div><div>9%</div><div>•</div><div>10%</div></div></div>
1	F	198	<div><div>3%</div><div><div></div><div>79%</div><div>9%</div><div>••</div><div>11%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	198	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>72%</div><div>9%</div><div>•</div><div>17%</div></div></div>
1	H	198	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>72%</div><div>11%</div><div>•</div><div>16%</div></div></div>
1	I	198	<div><div><div></div><div></div><div></div></div><div><div>11%</div><div>67%</div><div>20%</div><div>•</div><div>13%</div></div></div>
1	J	198	<div><div><div></div><div></div><div></div></div><div><div>7%</div><div>75%</div><div>13%</div><div>•</div><div>11%</div></div></div>

## 2 Entry composition [i](#)

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

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

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

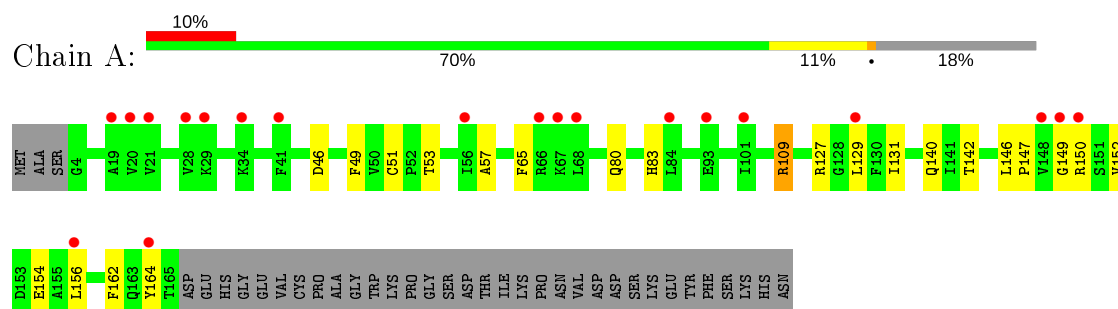
- Molecule 3 is water.

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

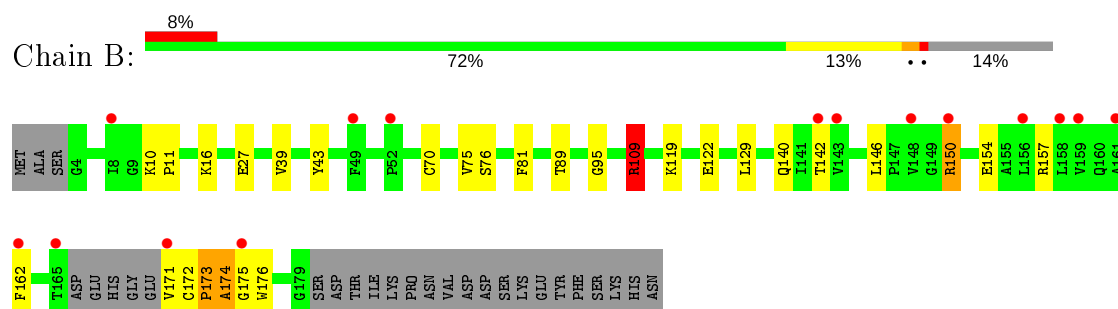
### 3 Residue-property plots [i](#)

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.

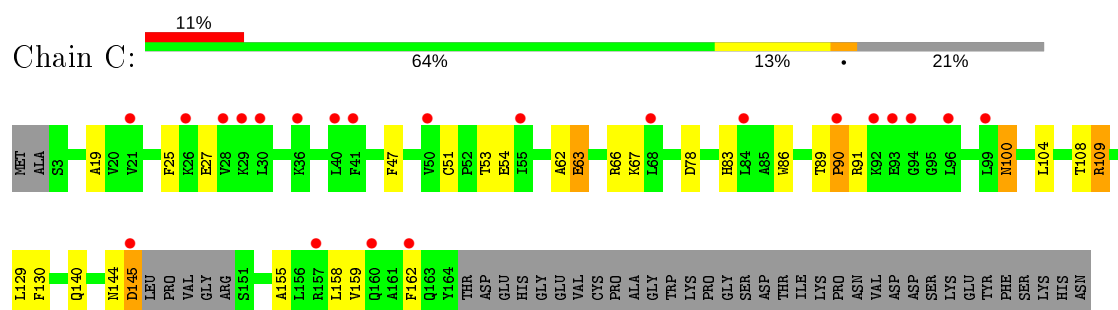
#### • Molecule 1: Peroxiredoxin-2



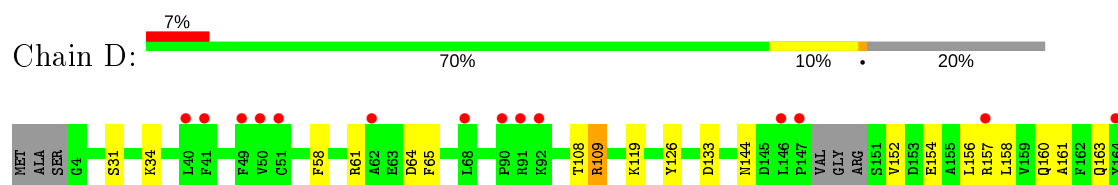
#### • Molecule 1: Peroxiredoxin-2



#### • Molecule 1: Peroxiredoxin-2



#### • Molecule 1: Peroxiredoxin-2



THR ASP  
GLU HIS  
GLY VAL  
CYS PRO  
ALA GLY  
TRP LYS  
PRO GLY  
SER ASP  
THR ILE  
LYS LYS  
PRO VAL  
ASN ASP  
SER ASP  
LYS LYS  
TYR PHE  
SER LYS  
HIS ASN

• Molecule 1: Peroxiredoxin-2

Chain E: 3% 80% 9% 10%

MET ALA G4 G23 K36 Y43 Y48 C51 E54 A57 S76 L99 T108 R109 G134 D145 V152 D153 A155 V159 E167 H168 G169 V171 C172 P173 A174 G175 W176 D181 THR ILE LYS PRO ASP VAL ASP ASP LYS SER LYS GLU

TYR PHE SER LYS HIS ASN

• Molecule 1: Peroxiredoxin-2

Chain F: 3% 79% 9% 11%

MET ALA G4 V20 V21 A24 V39 P44 C51 P52 I56 A57 C70 D78 R91 R92 E93 R109 L146 P147 V148 G149 R150 S151 V152 E167 V171 C172 P173 S180 ASP THR ILE LYS PRO ASN VAL ASP ASP ASP LYS SER LYS GLU TYR PHE SER

LYS HIS ASN

• Molecule 1: Peroxiredoxin-2

Chain G: 3% 72% 9% 17%

MET ALA G4 A19 K36 V39 Y43 F49 F50 I55 F65 C70 S76 R91 L104 R109 R110 D114 G134 Q140 I141 T142 G149 R150 E154 A155 L156 V159 E167 HIS GLY VAL CYS PRO ASP GLY TRP PRO

GLY SER ASP THR ILE LYS PRO ASN VAL ASP ASP ASP LYS LYS GLU TYR PHE SER LYS HIS ASN

• Molecule 1: Peroxiredoxin-2

Chain H: 3% 72% 11% 16%

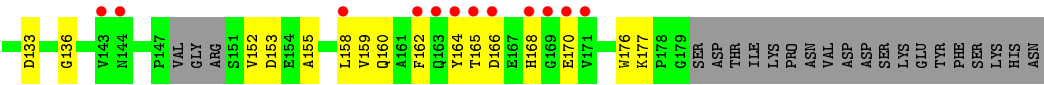
MET ALA G4 P44 L45 D46 F47 F48 F49 A57 E63 R66 E71 R92 L104 R109 R119 T120 D121 Y126 D133 R139 N144 P147 V148 ARG S151 V152 A161 T165 H168 V171 C172 PRO ALA GLY TRP LYS PRO GLY

SER ASP THR ILE LYS PRO ASN VAL ASP ASP ASP LYS LYS GLU TYR PHE SER LYS HIS ASN

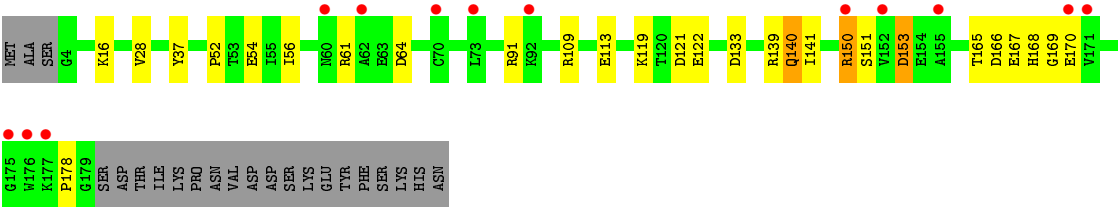
• Molecule 1: Peroxiredoxin-2

Chain I: 11% 67% 20% 13%

MET ALA G4 P11 D22 K29 L30 S31 D32 T33 K34 G35 K36 Y37 Y38 P44 L45 D46 F47 C51 F55 F56 A57 R61 D64 R67 L68 G69 V75 D78 H83 W86 E93 L104 R109 E113 L118 D121 L129



● Molecule 1: Peroxiredoxin-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<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: 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

All (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
1	J	54	GLU	CB-CG	5.79	1.63	1.52
1	F	20	VAL	CB-CG2	5.75	1.65	1.52
1	G	154	GLU	CB-CG	5.62	1.62	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	75	VAL	CB-CG1	5.56	1.64	1.52
1	D	109	ARG	CB-CG	5.54	1.67	1.52
1	F	51	CYS	C-N	5.33	1.44	1.34
1	I	93	GLU	CD-OE2	5.09	1.31	1.25
1	B	75	VAL	CB-CG1	5.08	1.63	1.52
1	E	54	GLU	CD-OE1	5.08	1.31	1.25

All (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
1	I	109	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	H	104	LEU	CA-CB-CG	5.83	128.72	115.30
1	E	109	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	133	ASP	CB-CG-OD1	5.66	123.39	118.30
1	F	78	ASP	CB-CG-OD1	5.58	123.33	118.30
1	C	78	ASP	CB-CG-OD1	5.39	123.16	118.30
1	F	93	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	H	46	ASP	CB-CG-OD2	-5.26	113.56	118.30

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:J:119:LYS:NZ	1:J:122:GLU:OE2	2.30	0.64
1:J:167:GLU:O	1:J:169:GLY:N	2.26	0.63
1:I:61:ARG:NH2	1:I:153:ASP:OD1	2.33	0.62
1:A:109:ARG:HD3	1:C:109:ARG:CZ	2.29	0.62
1:B:174:ALA:O	1:B:176:TRP:N	2.34	0.60
1:D:108:THR:OG1	3:D:201:HOH:O	2.17	0.59
1:I:155:ALA:O	1:I:159:VAL:HG23	2.03	0.59
1:H:66:ARG:NH1	1:H:71:GLU:OE2	2.35	0.58
1:G:110:ARG:NH1	1:G:114:ASP:OD1	2.37	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:LYS:O	1:J:121:ASP:O	2.22	0.58
1:A:127:ARG:NH2	1:A:149:GLY:HA3	2.19	0.57
1:C:140:GLN:HG2	1:D:144:ASN:HB3	1.88	0.56
1:A:51:CYS:SG	1:B:173:PRO:CD	2.93	0.56
1:C:62:ALA:O	1:C:66:ARG:HG3	2.06	0.56
1:C:155:ALA:O	1:C:159:VAL:HG23	2.05	0.56
1:J:133:ASP:OD2	1:J:139:ARG:NH1	2.39	0.55
1:J:16:LYS:HA	1:J:28:VAL:O	2.07	0.55
1:B:129:LEU:HB3	1:B:142:THR:OG1	2.07	0.55
1:J:121:ASP:O	1:J:122:GLU:HB2	2.07	0.55
1:A:142:THR:HG23	1:B:142:THR:HG22	1.89	0.55
1:A:51:CYS:SG	1:B:173:PRO:HD3	2.47	0.55
1:H:119:LYS:HG3	1:H:126:TYR:CZ	2.42	0.55
1:I:22:ASP:OD2	3:I:201:HOH:O	2.18	0.54
1:B:171:VAL:HG12	1:B:172:CYS:H	1.73	0.53
1:C:66:ARG:NH2	1:C:100:ASN:O	2.42	0.53
1:B:16:LYS:HD2	1:B:27:GLU:OE2	2.08	0.53
1:D:58:PHE:CE2	1:D:152:VAL:HG22	2.44	0.52
1:I:164:TYR:O	1:I:168:HIS:HB2	2.09	0.52
1:D:160:GLN:O	1:D:163:GLN:N	2.40	0.52
1:B:140:GLN:HE21	1:B:142:THR:HG23	1.74	0.52
1:B:173:PRO:O	1:B:174:ALA:O	2.26	0.52
1:G:65:PHE:CZ	1:G:156:LEU:HG	2.45	0.52
1:B:140:GLN:HE21	1:B:142:THR:CG2	2.24	0.51
1:A:51:CYS:SG	1:B:173:PRO:HD2	2.51	0.50
1:G:140:GLN:OE1	1:G:142:THR:HG22	2.12	0.50
1:D:58:PHE:CD2	1:D:152:VAL:HG22	2.47	0.49
1:C:129:LEU:HD23	1:C:130:PHE:N	2.27	0.49
1:G:155:ALA:O	1:G:159:VAL:HG23	2.12	0.49
1:A:146:LEU:HG	1:B:162:PHE:CE1	2.47	0.49
1:I:11:PRO:HA	1:I:136:GLY:O	2.12	0.49
1:I:57:ALA:HB3	1:I:152:VAL:HG21	1.95	0.49
1:F:146:LEU:HB3	1:F:147:PRO:HD2	1.95	0.49
1:F:21:VAL:HG23	1:F:21:VAL:O	2.12	0.48
1:H:148:VAL:HG11	1:H:151:SER:OG	2.13	0.48
1:F:52:PRO:O	1:F:56:ILE:HG12	2.13	0.48
1:I:165:THR:O	1:I:165:THR:HG22	2.13	0.48
1:C:158:LEU:O	1:C:162:PHE:CD2	2.67	0.48
1:E:57:ALA:HB3	1:E:152:VAL:HG21	1.96	0.48
1:F:57:ALA:HB3	1:F:152:VAL:HG21	1.95	0.48
1:J:119:LYS:CE	1:J:122:GLU:OE2	2.61	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:GLN:HG3	1:J:141:ILE:N	2.28	0.48
1:J:37:TYR:CD2	1:J:133:ASP:HA	2.49	0.47
1:E:145:ASP:OD1	1:E:145:ASP:N	2.44	0.47
1:A:109:ARG:N	1:A:109:ARG:HD2	2.30	0.47
1:E:51:CYS:SG	1:F:173:PRO:CD	3.03	0.47
1:I:162:PHE:O	1:I:166:ASP:OD2	2.33	0.47
1:D:61:ARG:O	1:D:64:ASP:HB2	2.15	0.47
1:E:51:CYS:SG	1:F:173:PRO:HD3	2.55	0.47
1:G:149:GLY:O	1:G:150:ARG:HB2	2.15	0.46
1:D:109:ARG:HD3	1:J:109:ARG:CZ	2.45	0.46
1:E:155:ALA:O	1:E:159:VAL:HG23	2.15	0.46
1:H:57:ALA:HB3	1:H:152:VAL:HG21	1.96	0.46
1:H:161:ALA:O	1:H:165:THR:HG23	2.16	0.46
1:J:165:THR:HG23	1:J:170:GLU:HG2	1.97	0.46
1:I:129:LEU:C	1:I:129:LEU:HD23	2.35	0.46
1:J:150:ARG:HD3	1:J:153:ASP:CG	2.36	0.46
1:A:65:PHE:CZ	1:A:156:LEU:HG	2.51	0.46
1:B:81:PHE:CD1	1:E:48:THR:HA	2.51	0.45
1:I:61:ARG:HD2	1:I:64:ASP:OD2	2.17	0.45
1:A:80:GLN:N	1:A:80:GLN:OE1	2.45	0.45
1:D:161:ALA:C	1:D:163:GLN:H	2.20	0.45
1:A:46:ASP:OD2	1:A:83:HIS:ND1	2.41	0.45
1:C:63:GLU:O	1:C:67:LYS:HG3	2.17	0.45
1:A:127:ARG:HH21	1:A:149:GLY:HA3	1.82	0.45
1:D:65:PHE:CZ	1:D:156:LEU:HG	2.52	0.45
1:I:113:GLU:HG3	1:I:118:LEU:HD22	1.98	0.45
1:I:68:LEU:HD21	1:I:160:GLN:HG2	1.99	0.45
1:C:83:HIS:NE2	1:C:104:LEU:O	2.50	0.44
1:E:173:PRO:CD	1:F:51:CYS:SG	3.06	0.44
1:J:169:GLY:O	1:J:170:GLU:HG2	2.16	0.44
1:C:89:THR:HG23	1:C:90:PRO:HD2	1.99	0.44
1:E:108:THR:O	1:E:109:ARG:HB2	2.17	0.44
1:J:61:ARG:HD2	1:J:64:ASP:OD2	2.18	0.44
1:E:167:GLU:OE1	1:E:168:HIS:CE1	2.70	0.44
1:C:47:PHE:CZ	1:C:86:TRP:HA	2.53	0.44
1:D:154:GLU:O	1:D:158:LEU:HG	2.18	0.44
1:E:36:LYS:O	1:E:134:GLY:HA2	2.18	0.44
1:G:43:TYR:CZ	1:G:55:ILE:HD11	2.53	0.44
1:D:31:SER:O	1:D:34:LYS:HE2	2.18	0.44
1:F:172:CYS:SG	1:F:173:PRO:HD2	2.58	0.43
1:H:133:ASP:OD2	1:H:139:ARG:HD3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:LYS:HG3	1:I:32:ASP:OD1	2.19	0.43
1:E:176:TRP:HA	1:F:91:ARG:O	2.19	0.43
1:E:173:PRO:HD2	1:F:51:CYS:SG	2.59	0.43
1:A:127:ARG:NH2	1:A:149:GLY:CA	2.82	0.43
1:G:36:LYS:O	1:G:134:GLY:HA2	2.19	0.43
1:J:56:ILE:HD12	1:J:91:ARG:CZ	2.48	0.43
1:B:43:TYR:CZ	1:B:76:SER:HB3	2.54	0.43
1:I:46:ASP:N	1:I:78:ASP:OD2	2.46	0.42
1:C:144:ASN:O	1:C:145:ASP:CB	2.67	0.42
1:C:129:LEU:C	1:C:129:LEU:HD23	2.39	0.42
1:H:168:HIS:HB3	1:H:171:VAL:CG2	2.49	0.42
1:B:10:LYS:HB3	1:B:11:PRO:HD2	2.01	0.42
1:A:131:ILE:HB	1:A:140:GLN:HB3	2.00	0.42
1:E:43:TYR:CZ	1:E:76:SER:HB3	2.54	0.42
1:J:109:ARG:O	1:J:113:GLU:HG3	2.18	0.42
1:C:90:PRO:O	1:C:91:ARG:CG	2.68	0.42
1:G:39:VAL:HG23	1:G:70:CYS:SG	2.59	0.42
1:I:158:LEU:O	1:I:162:PHE:HD2	2.03	0.42
1:F:109:ARG:HD2	1:H:109:ARG:NH2	2.35	0.42
1:H:48:THR:HG21	3:H:304:HOH:O	2.20	0.42
1:I:176:TRP:O	1:I:177:LYS:HD3	2.20	0.42
1:I:47:PHE:CZ	1:I:86:TRP:HA	2.55	0.42
1:A:57:ALA:HB3	1:A:152:VAL:HG21	2.01	0.41
1:F:39:VAL:HG23	1:F:70:CYS:SG	2.59	0.41
1:D:154:GLU:HA	1:D:157:ARG:HD2	2.02	0.41
1:J:139:ARG:NH2	1:J:166:ASP:OD1	2.52	0.41
1:C:53:THR:OG1	1:C:54:GLU:N	2.53	0.41
1:I:83:HIS:NE2	1:I:104:LEU:O	2.54	0.41
1:A:53:THR:HG21	1:B:171:VAL:O	2.20	0.41
1:H:120:THR:HG23	1:H:121:ASP:N	2.35	0.41
1:A:162:PHE:CE1	1:B:146:LEU:HG	2.56	0.41
1:D:154:GLU:HA	1:D:157:ARG:CD	2.51	0.41
1:E:51:CYS:SG	1:F:173:PRO:HD2	2.60	0.41
1:I:37:TYR:CE1	1:I:133:ASP:HB2	2.55	0.41
1:J:52:PRO:O	1:J:56:ILE:HG12	2.20	0.41
1:B:39:VAL:HG23	1:B:70:CYS:SG	2.60	0.41
1:A:49:PHE:O	1:B:176:TRP:HH2	2.04	0.41
1:D:119:LYS:HG3	1:D:126:TYR:CZ	2.56	0.41
1:B:89:THR:O	1:B:95:GLY:HA3	2.22	0.40
1:C:19:ALA:O	1:C:25:PHE:HA	2.21	0.40
1:G:43:TYR:CZ	1:G:76:SER:HB3	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLU:O	1:C:67:LYS:N	2.45	0.40
1:C:90:PRO:HB2	1:C:91:ARG:H	1.74	0.40
1:G:140:GLN:HB2	1:G:140:GLN:HE21	1.72	0.40
1:C:108:THR:O	1:C:109:ARG:HB2	2.22	0.40

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 ⓘ

### 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	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
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



All (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
1	G	149	GLY
1	I	31	SER
1	J	178	PRO
1	H	147	PRO
1	I	170	GLU
1	A	147	PRO
1	B	173	PRO
1	I	44	PRO
1	F	44	PRO
1	H	44	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	129	LEU
1	A	150	ARG
1	A	164	TYR
1	B	109	ARG
1	B	150	ARG
1	C	27	GLU
1	C	51	CYS
1	C	63	GLU
1	C	100	ASN
1	C	109	ARG
1	C	145	ASP
1	F	109	ARG
1	F	167	GLU
1	F	180	SER
1	G	109	ARG
1	G	142	THR
1	H	63	GLU
1	H	104	LEU
1	H	119	LYS
1	H	144	ASN
1	I	121	ASP
1	J	140	GLN
1	J	150	ARG
1	J	151	SER
1	J	153	ASP

Some 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [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, 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	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

All (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
1	C	68	LEU	5.2
1	E	171	VAL	5.0
1	G	150	ARG	4.9
1	A	164	TYR	4.6
1	D	50	VAL	4.5
1	J	175	GLY	4.1
1	G	49	PHE	4.0
1	D	146	LEU	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	68	LEU	3.9
1	C	21	VAL	3.9
1	H	92	LYS	3.8
1	C	92	LYS	3.7
1	C	90	PRO	3.7
1	D	51	CYS	3.7
1	F	171	VAL	3.6
1	I	162	PHE	3.6
1	E	170	GLU	3.4
1	J	171	VAL	3.3
1	A	20	VAL	3.3
1	I	37	TYR	3.3
1	I	169	GLY	3.2
1	C	26	LYS	3.2
1	C	30	LEU	3.2
1	H	49	PHE	3.2
1	I	171	VAL	3.2
1	C	55	ILE	3.1
1	I	170	GLU	3.1
1	D	147	PRO	3.1
1	I	67	LYS	3.1
1	C	93	GLU	3.1
1	C	50	VAL	3.1
1	A	156	LEU	3.0
1	D	92	LYS	3.0
1	A	93	GLU	3.0
1	I	35	GLY	3.0
1	J	170	GLU	3.0
1	I	163	GLN	3.0
1	I	56	ILE	2.9
1	J	70	CYS	2.9
1	D	90	PRO	2.8
1	C	84	LEU	2.8
1	D	68	LEU	2.8
1	I	166	ASP	2.8
1	A	84	LEU	2.8
1	D	49	PHE	2.8
1	A	68	LEU	2.8
1	A	148	VAL	2.7
1	F	150	ARG	2.7
1	A	19	ALA	2.7
1	B	159	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	2.6
1	I	69	GLY	2.6
1	D	41	PHE	2.6
1	A	150	ARG	2.6
1	F	148	VAL	2.6
1	I	30	LEU	2.6
1	B	148	VAL	2.5
1	B	161	ALA	2.5
1	C	94	GLY	2.5
1	C	96	LEU	2.5
1	A	67	LYS	2.5
1	J	176	TRP	2.5
1	B	143	VAL	2.4
1	J	150	ARG	2.4
1	I	33	TYR	2.4
1	B	150	ARG	2.4
1	B	175	GLY	2.4
1	C	157	ARG	2.4
1	D	91	ARG	2.4
1	E	23	GLY	2.4
1	J	177	LYS	2.4
1	D	164	TYR	2.4
1	A	34	LYS	2.4
1	B	142	THR	2.4
1	B	156	LEU	2.3
1	I	38	VAL	2.3
1	C	145	ASP	2.3
1	B	162	PHE	2.3
1	C	41	PHE	2.3
1	C	160	GLN	2.3
1	H	148	VAL	2.3
1	I	165	THR	2.3
1	I	144	ASN	2.3
1	D	157	ARG	2.3
1	I	55	ILE	2.3
1	B	49	PHE	2.3
1	D	62	ALA	2.3
1	G	91	ARG	2.3
1	F	92	LYS	2.3
1	D	40	LEU	2.2
1	J	155	ALA	2.2
1	C	28	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	99	LEU	2.2
1	J	62	ALA	2.2
1	J	60	ASN	2.2
1	B	165	THR	2.2
1	I	158	LEU	2.2
1	A	28	VAL	2.2
1	A	41	PHE	2.2
1	C	162	PHE	2.2
1	C	99	LEU	2.2
1	H	66	ARG	2.2
1	A	101	ILE	2.1
1	C	40	LEU	2.1
1	I	143	VAL	2.1
1	C	29	LYS	2.1
1	A	66	ARG	2.1
1	J	152	VAL	2.1
1	C	36	LYS	2.1
1	B	8	ILE	2.1
1	F	24	ALA	2.1
1	A	129	LEU	2.0
1	A	21	VAL	2.0
1	H	171	VAL	2.0
1	E	175	GLY	2.0
1	B	52	PRO	2.0
1	J	92	LYS	2.0
1	B	158	LEU	2.0
1	J	73	LEU	2.0
1	A	56	ILE	2.0
1	G	141	ILE	2.0
1	A	29	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	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 [i](#)

There are no such residues in this entry.