



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 11:06 am GMT

PDB ID : 5C7F
Title : Crystal structure of the rice Topless related protein 2 (TPR2) N-terminal domain (1-209) in complex with Arabidopsis IAA1 peptide
Authors : Ke, J.; Ma, H.; Gu, X.; Brunzelle, J.S.; Xu, H.E.; Melcher, K.
Deposited on : 2015-06-24
Resolution : 2.70 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

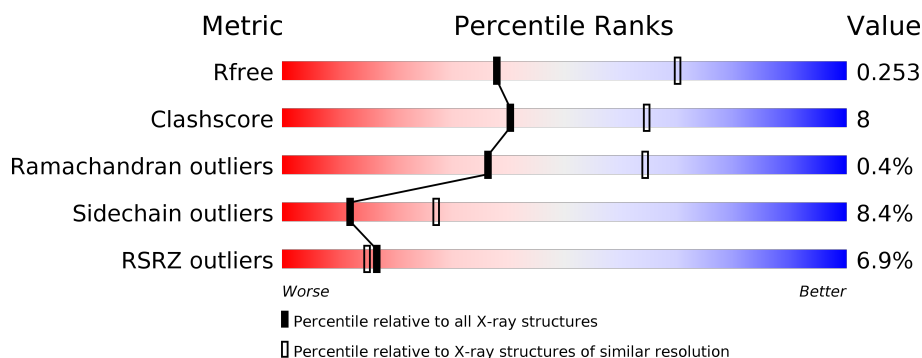
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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. 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	209	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>6%</div> </div> </div>
1	B	209	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>5%</div> </div> </div>
1	C	209	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>6%</div> </div> </div>
1	D	209	<div> <div>11%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
2	E	11	<div> <div>9%</div> <div> <div>36%</div> <div>9%</div> <div>36%</div> <div>18%</div> </div> </div>
2	F	11	<div> <div>27%</div> <div> <div>9%</div> <div>36%</div> <div>27%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	11	<div><div></div><div></div><div></div><div></div></div> <div>9%9%45%18%27%</div>
2	H	11	<div><div></div><div></div><div></div><div></div></div> <div>27%27%9%36%27%</div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6841 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 ASPR2 protein.

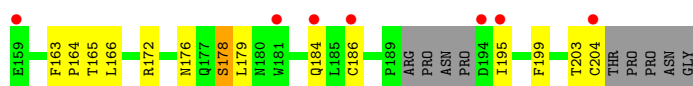
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1639	1059	271	305	4			
1	B	199	Total	C	N	O	S	0	0	0
			1643	1061	269	308	5			
1	C	197	Total	C	N	O	S	0	0	0
			1656	1068	277	306	5			
1	D	200	Total	C	N	O	S	0	0	0
			1662	1073	272	311	6			

- Molecule 2 is a protein called Auxin-responsive protein IAA1.

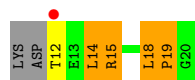
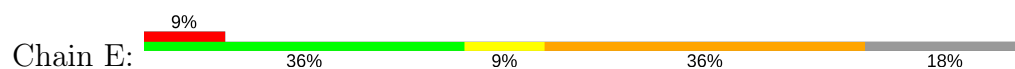
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			66	42	12	12			
2	F	8	Total	C	N	O	0	0	0
			59	38	11	10			
2	G	8	Total	C	N	O	0	0	0
			59	37	11	11			
2	H	8	Total	C	N	O	0	0	0
			55	36	11	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

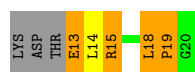
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		



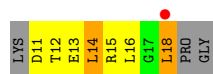
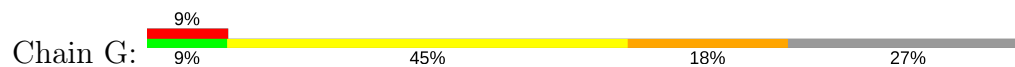
- Molecule 2: Auxin-responsive protein IAA1



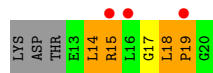
- Molecule 2: Auxin-responsive protein IAA1



- Molecule 2: Auxin-responsive protein IAA1



- Molecule 2: Auxin-responsive protein IAA1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.51Å 129.28Å 79.17Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	41.86 – 2.70 48.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.86-2.70) 99.9 (48.78-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.256 0.225 , 0.253	Depositor DCC
R_{free} test set	1567 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6841	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: 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	0.43	0/1670	0.65	0/2241
1	B	0.37	0/1674	0.61	0/2249
1	C	0.40	0/1687	0.62	1/2260 (0.0%)
1	D	0.41	1/1694 (0.1%)	0.58	0/2275
2	E	0.70	0/66	1.29	1/88 (1.1%)
2	F	0.46	0/59	0.98	0/78
2	G	0.49	0/58	1.20	0/77
2	H	0.50	0/55	1.24	0/73
All	All	0.41	1/6963 (0.0%)	0.64	2/9341 (0.0%)

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
2	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	204	CYS	CB-SG	-8.30	1.68	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	14	LEU	CB-CG-CD2	-6.91	99.26	111.00
1	C	4	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	LEU	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	1639	0	1632	29	0
1	B	1643	0	1621	23	0
1	C	1656	0	1661	33	0
1	D	1662	0	1644	24	0
2	E	66	0	71	16	0
2	F	59	0	64	9	0
2	G	59	0	61	10	0
2	H	55	0	60	7	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
All	All	6841	0	6814	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 8.

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)
2:E:12:THR:HA	2:E:15:ARG:HB2	1.38	1.03
2:H:17:GLY:C	2:H:19:PRO:HD3	1.95	0.86
1:A:4:LEU:HD12	1:B:198:LEU:HD11	1.55	0.86
1:A:67:ARG:HG3	2:E:14:LEU:HD22	1.65	0.77
1:C:111:LEU:HD11	2:G:14:LEU:HB2	1.67	0.76
1:A:67:ARG:CZ	2:E:14:LEU:HD21	2.16	0.76
1:C:186:CYS:HB2	1:C:204:CYS:HB2	1.68	0.75
1:D:111:LEU:O	1:D:115:ILE:HG13	1.88	0.74
1:B:130:LEU:HD23	2:F:19:PRO:HD3	1.68	0.73
1:D:130:LEU:HD21	2:H:18:LEU:HD22	1.69	0.73
1:A:183:HIS:O	1:A:185:LEU:HA	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ARG:NH2	1:C:134:GLY:O	2.26	0.69
2:H:14:LEU:HD23	2:H:15:ARG:N	2.08	0.68
1:D:125:ARG:NH2	1:D:134:GLY:O	2.28	0.66
2:F:13:GLU:N	2:F:15:ARG:HG2	2.10	0.66
1:C:183:HIS:O	1:C:186:CYS:N	2.21	0.65
1:D:78:LYS:HE2	2:H:18:LEU:HD23	1.80	0.64
2:H:18:LEU:N	2:H:19:PRO:HD3	2.10	0.64
1:C:184:GLN:NE2	1:D:184:GLN:OE1	2.26	0.64
1:D:186:CYS:SG	1:D:203:THR:HA	2.38	0.64
2:E:18:LEU:H	2:E:18:LEU:HD12	1.63	0.63
1:D:179:LEU:HD13	1:D:195:ILE:HD13	1.82	0.62
1:A:94:VAL:HG11	1:C:90:ARG:HD2	1.82	0.62
1:D:71:LYS:HD2	2:H:14:LEU:O	2.00	0.61
1:A:71:LYS:HD3	2:E:14:LEU:HA	1.81	0.61
1:C:71:LYS:HD3	2:G:18:LEU:HB2	1.82	0.61
2:G:13:GLU:CB	2:G:14:LEU:HA	2.31	0.61
1:A:4:LEU:CD1	1:B:198:LEU:HD11	2.30	0.60
1:B:78:LYS:HE2	2:F:18:LEU:HB3	1.83	0.60
1:C:172:ARG:HH22	1:D:5:SER:HB3	1.68	0.59
1:C:67:ARG:HD2	2:G:18:LEU:HD21	1.85	0.58
1:C:7:GLU:HG2	1:D:199:PHE:CZ	2.39	0.57
1:A:7:GLU:HG2	1:B:199:PHE:CZ	2.39	0.57
1:C:186:CYS:HB2	1:C:187:LYS:HA	1.87	0.57
1:A:76:ILE:HA	1:A:143:MET:CE	2.35	0.56
1:B:76:ILE:HA	1:B:143:MET:CE	2.36	0.56
1:C:5:SER:HB3	1:D:172:ARG:HH22	1.71	0.56
1:C:130:LEU:HD21	2:G:13:GLU:O	2.05	0.56
1:A:199:PHE:CZ	1:B:7:GLU:HG2	2.40	0.55
1:A:130:LEU:HD23	2:E:19:PRO:HD3	1.89	0.55
1:C:186:CYS:CB	1:C:187:LYS:HA	2.37	0.55
1:C:7:GLU:HG2	1:D:199:PHE:CE1	2.42	0.54
1:A:67:ARG:CG	2:E:14:LEU:HD22	2.35	0.54
1:B:78:LYS:NZ	2:F:18:LEU:HA	2.22	0.54
2:G:14:LEU:H	2:G:14:LEU:HD22	1.72	0.54
1:C:76:ILE:HA	1:C:143:MET:CE	2.39	0.53
1:D:69:SER:HA	1:D:72:ILE:HD12	1.91	0.53
1:C:179:LEU:O	1:C:183:HIS:ND1	2.41	0.53
1:C:111:LEU:CD1	2:G:14:LEU:HB2	2.38	0.52
1:B:76:ILE:HA	1:B:143:MET:HE1	1.91	0.52
1:A:67:ARG:HB2	2:E:14:LEU:HD13	1.91	0.52
1:A:78:LYS:NZ	2:E:19:PRO:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:O	1:C:176:ASN:HB3	2.10	0.51
1:D:76:ILE:HA	1:D:143:MET:CE	2.41	0.51
1:B:78:LYS:HZ1	2:F:18:LEU:HA	1.75	0.51
1:A:76:ILE:HA	1:A:143:MET:HE1	1.93	0.50
1:A:11:LEU:HD21	1:A:174:LEU:HD12	1.93	0.50
1:A:90:ARG:HD2	1:C:94:VAL:HG11	1.94	0.50
1:B:188:ASN:CB	1:B:189:PRO:HD2	2.44	0.47
1:A:104:PHE:O	1:A:108:ASN:HB2	2.15	0.47
1:D:165:THR:O	1:D:166:LEU:HD23	2.15	0.46
1:A:138:SER:O	1:A:142:ILE:HG12	2.16	0.46
1:D:69:SER:HB3	1:D:154:ASN:HD21	1.80	0.46
1:B:78:LYS:HZ3	2:F:19:PRO:HA	1.80	0.46
2:H:14:LEU:HD23	2:H:15:ARG:CA	2.45	0.46
1:A:78:LYS:HZ3	2:E:19:PRO:HA	1.80	0.46
1:A:51:ASP:O	1:A:55:LYS:HB2	2.17	0.45
2:F:14:LEU:O	2:F:14:LEU:HD12	2.17	0.45
1:A:178:SER:HB3	1:B:177:GLN:HB2	1.98	0.45
1:C:177:GLN:HB2	1:D:178:SER:HB3	1.97	0.45
1:C:76:ILE:HA	1:C:143:MET:HE1	1.99	0.44
2:E:18:LEU:N	2:E:18:LEU:HD12	2.30	0.44
1:B:71:LYS:HE2	2:F:13:GLU:O	2.17	0.44
1:C:71:LYS:CD	2:G:18:LEU:HB2	2.47	0.44
1:A:67:ARG:NE	2:E:14:LEU:HD21	2.33	0.44
1:C:49:GLU:O	1:C:53:VAL:HG23	2.18	0.43
1:B:44:LYS:HD2	1:B:49:GLU:HG3	1.99	0.43
1:C:198:LEU:HD11	1:D:4:LEU:CD1	2.48	0.43
1:C:24:THR:HG21	1:D:28:LEU:HB2	2.00	0.43
1:A:44:LYS:HD2	1:A:49:GLU:HG3	2.00	0.43
1:D:112:TYR:HA	1:D:115:ILE:HD12	1.99	0.43
1:A:125:ARG:NH2	1:A:133:TYR:HD1	2.16	0.43
1:C:154:ASN:HB3	1:C:157:PHE:HD2	1.83	0.43
1:C:69:SER:HA	1:C:72:ILE:HD12	2.00	0.43
2:E:12:THR:HA	2:E:15:ARG:CB	2.28	0.43
2:F:18:LEU:HA	2:F:19:PRO:HA	1.64	0.43
2:G:18:LEU:HA	2:G:18:LEU:HD22	1.88	0.43
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.91	0.43
1:B:124:PHE:HZ	1:B:133:TYR:CE1	2.36	0.43
1:C:198:LEU:HD11	1:D:4:LEU:HD12	2.00	0.43
1:C:199:PHE:CZ	1:D:7:GLU:HG2	2.54	0.43
1:A:7:GLU:HG2	1:B:199:PHE:CE1	2.53	0.43
1:C:172:ARG:HH22	1:D:5:SER:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLN:HE22	1:B:133:TYR:HE2	1.66	0.42
1:B:69:SER:HA	1:B:72:ILE:HD12	2.01	0.42
1:A:67:ARG:NE	2:E:14:LEU:CD2	2.83	0.42
1:A:179:LEU:O	1:A:183:HIS:ND1	2.51	0.42
1:B:184:GLN:HG2	1:B:184:GLN:O	2.20	0.41
1:C:51:ASP:O	1:C:55:LYS:HB2	2.21	0.41
1:D:163:PHE:HA	1:D:164:PRO:HD3	1.88	0.41
2:E:18:LEU:HA	2:E:19:PRO:HA	1.76	0.41
1:B:135:ASP:HB3	1:B:138:SER:H	1.86	0.41
2:G:14:LEU:HD13	2:G:14:LEU:N	2.36	0.41
2:E:14:LEU:O	2:E:14:LEU:HD12	2.21	0.40
1:B:51:ASP:O	1:B:55:LYS:HB2	2.21	0.40
1:C:38:MET:SD	1:C:148:LYS:HG2	2.62	0.40
1:B:97:LEU:HD21	1:B:116:THR:HG23	2.04	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	192/209 (92%)	190 (99%)	2 (1%)	0	100	100
1	B	195/209 (93%)	194 (100%)	1 (0%)	0	100	100
1	C	193/209 (92%)	193 (100%)	0	0	100	100
1	D	196/209 (94%)	195 (100%)	1 (0%)	0	100	100
2	E	7/11 (64%)	6 (86%)	0	1 (14%)	0	0
2	F	6/11 (54%)	5 (83%)	0	1 (17%)	0	0
2	G	6/11 (54%)	6 (100%)	0	0	100	100
2	H	6/11 (54%)	5 (83%)	0	1 (17%)	0	0
All	All	801/880 (91%)	794 (99%)	4 (0%)	3 (0%)	36	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	19	PRO
2	F	19	PRO
2	H	19	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	180/197 (91%)	168 (93%)	12 (7%)	18	40
1	B	179/197 (91%)	166 (93%)	13 (7%)	15	36
1	C	183/197 (93%)	170 (93%)	13 (7%)	16	38
1	D	183/197 (93%)	171 (93%)	12 (7%)	18	41
2	E	7/9 (78%)	5 (71%)	2 (29%)	0	1
2	F	6/9 (67%)	4 (67%)	2 (33%)	0	0
2	G	6/9 (67%)	0	6 (100%)	0	0
2	H	5/9 (56%)	2 (40%)	3 (60%)	0	0
All	All	749/824 (91%)	686 (92%)	63 (8%)	12	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5	SER
1	A	38	MET
1	A	39	LYS
1	A	55	LYS
1	A	106	THR
1	A	143	MET
1	A	144	LEU
1	A	147	LEU
1	A	175	ILE
1	A	178	SER

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Mol	Chain	Res	Type
1	A	204	CYS
1	B	3	SER
1	B	5	SER
1	B	22	LYS
1	B	86	ASP
1	B	135	ASP
1	B	143	MET
1	B	144	LEU
1	B	167	LYS
1	B	175	ILE
1	B	176	ASN
1	B	178	SER
1	B	184	GLN
1	B	196	LYS
1	C	3	SER
1	C	5	SER
1	C	39	LYS
1	C	69	SER
1	C	70	MET
1	C	86	ASP
1	C	143	MET
1	C	144	LEU
1	C	147	LEU
1	C	178	SER
1	C	186	CYS
1	C	187	LYS
1	C	204	CYS
1	D	2	SER
1	D	3	SER
1	D	5	SER
1	D	38	MET
1	D	39	LYS
1	D	86	ASP
1	D	133	TYR
1	D	135	ASP
1	D	143	MET
1	D	144	LEU
1	D	176	ASN
1	D	178	SER
2	E	15	ARG
2	E	18	LEU
2	F	13	GLU

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Mol	Chain	Res	Type
2	F	15	ARG
2	G	11	ASP
2	G	12	THR
2	G	14	LEU
2	G	15	ARG
2	G	16	LEU
2	G	18	LEU
2	H	14	LEU
2	H	15	ARG
2	H	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	196/209 (93%)	0.21	7 (3%) 42 42	44, 62, 103, 125	0
1	B	199/209 (95%)	0.42	13 (6%) 19 17	46, 66, 112, 151	0
1	C	197/209 (94%)	0.30	10 (5%) 28 26	40, 54, 103, 163	0
1	D	200/209 (95%)	0.62	22 (11%) 5 4	48, 74, 110, 132	0
2	E	9/11 (81%)	0.77	1 (11%) 5 4	68, 76, 91, 92	0
2	F	8/11 (72%)	0.60	0 100 100	71, 83, 89, 91	0
2	G	8/11 (72%)	1.13	1 (12%) 4 3	49, 58, 72, 72	0
2	H	8/11 (72%)	1.68	3 (37%) 0 0	83, 88, 101, 107	0
All	All	825/880 (93%)	0.42	57 (6%) 17 15	40, 65, 108, 163	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	ARG	4.4
1	A	195	ILE	4.4
1	C	185	LEU	4.2
1	C	186	CYS	4.1
1	D	194	ASP	4.1
1	D	184	GLN	3.9
1	D	115	ILE	3.9
1	D	90	ARG	3.8
1	D	159	GLU	3.8
1	D	157	PHE	3.7
1	C	184	GLN	3.6
2	H	19	PRO	3.6
1	A	4	LEU	3.5
1	C	176	ASN	3.4
1	D	81	TYR	3.4
1	B	186	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	16	LEU	3.2
1	C	204	CYS	3.0
1	D	84	ALA	3.0
1	D	195	ILE	2.9
1	B	189	PRO	2.7
2	E	12	THR	2.7
1	C	183	HIS	2.7
1	A	204	CYS	2.7
1	D	68	TYR	2.7
1	A	183	HIS	2.7
1	A	158	ARG	2.6
1	B	107	PHE	2.6
1	D	204	CYS	2.6
1	B	184	GLN	2.6
1	C	1	MET	2.5
1	D	117	GLN	2.5
1	B	204	CYS	2.5
1	D	4	LEU	2.5
1	A	203	THR	2.5
1	B	182	GLN	2.5
1	D	181	TRP	2.5
1	C	181	TRP	2.4
1	C	196	LYS	2.4
1	C	180	ASN	2.4
1	B	187	LYS	2.4
1	D	186	CYS	2.4
1	D	107	PHE	2.3
1	B	188	ASN	2.3
1	B	175	ILE	2.3
1	B	115	ILE	2.3
1	B	99	LYS	2.2
1	D	1	MET	2.2
1	B	183	HIS	2.2
1	D	94	VAL	2.1
1	D	153	ALA	2.1
1	B	112	TYR	2.1
2	H	15	ARG	2.1
1	D	139	ALA	2.1
2	G	18	LEU	2.0
1	D	112	TYR	2.0
1	A	6	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	ZN	A	401	1/1	0.55	0.10	178,178,178,178	0
3	ZN	D	401	1/1	0.63	0.17	116,116,116,116	1

6.5 Other polymers [i](#)

There are no such residues in this entry.