



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:28 AM UTC

PDB ID : 8YJ7 / pdb_00008yj7
Title : Characterization of a novel format scFvXVHH single-chain Biparatopic anti-body against a metal binding protein, MtsA
Authors : Ito, S.; Nagatoishi, S.; Nakakido, M.; Tsumoto, K.
Deposited on : 2024-03-01
Resolution : 2.80 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

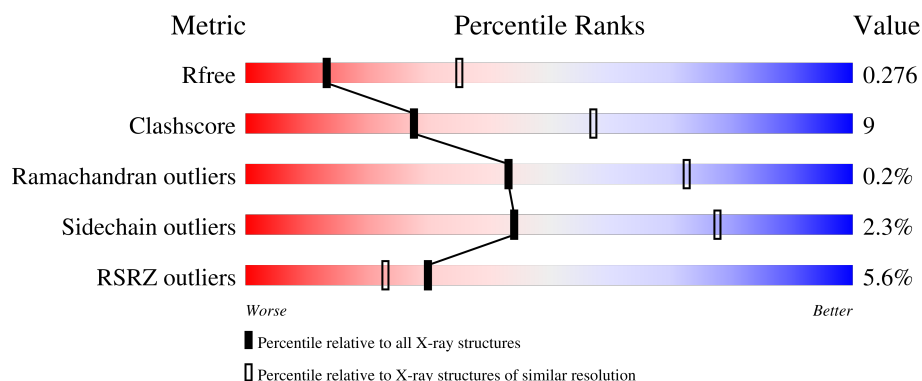
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	279	
1	B	279	
1	C	279	
1	D	279	
2	E	253	

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Mol	Chain	Length	Quality of chain
2	F	253	8% 64% 19% 15%
2	G	253	8% 60% 24% 15%
2	H	253	8% 61% 23% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15165 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 Iron ABC transporter substrate-binding lipoprotein MtsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	279	Total	C	N	O	S	0	0	0
			2196	1406	352	433	5			
1	D	279	Total	C	N	O	S	0	0	0
			2192	1403	351	433	5			
1	A	279	Total	C	N	O	S	0	0	0
			2196	1406	352	433	5			
1	C	279	Total	C	N	O	S	0	0	0
			2188	1400	350	433	5			

- Molecule 2 is a protein called scFv13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	215	Total	C	N	O	S	0	1	0
			1593	995	267	324	7			
2	E	215	Total	C	N	O	S	0	1	0
			1604	1004	268	325	7			
2	F	214	Total	C	N	O	S	0	1	0
			1583	989	265	322	7			
2	H	217	Total	C	N	O	S	0	1	0
			1609	1007	269	326	7			

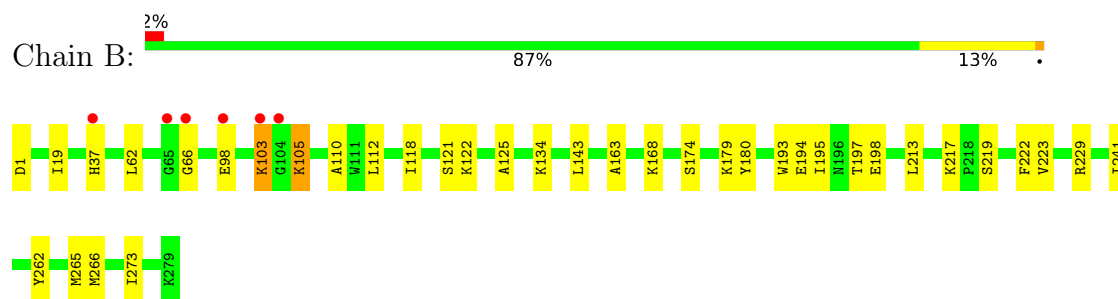
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

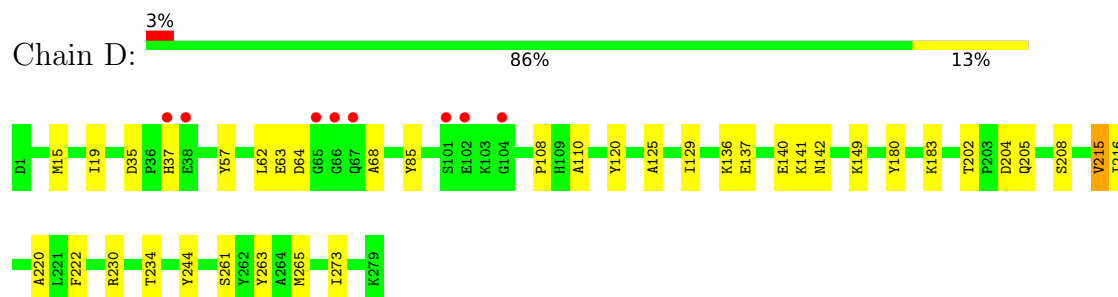
3 Residue-property plots [i](#)

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.

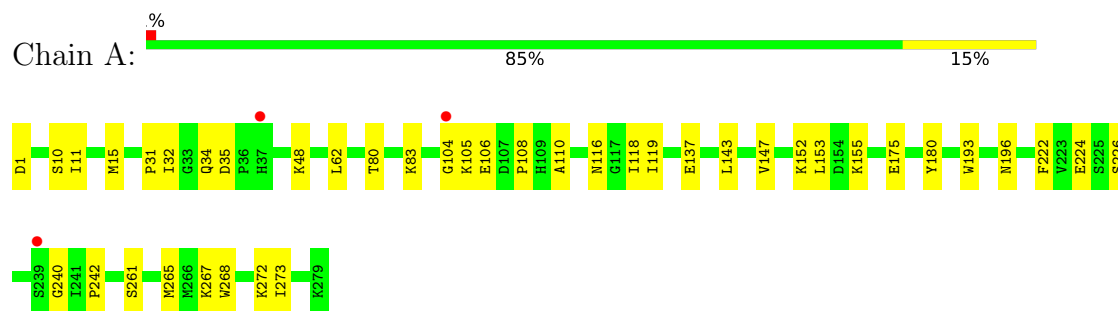
- Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA



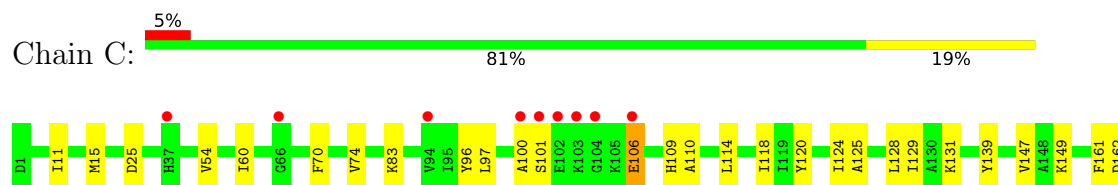
- Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA



- Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA

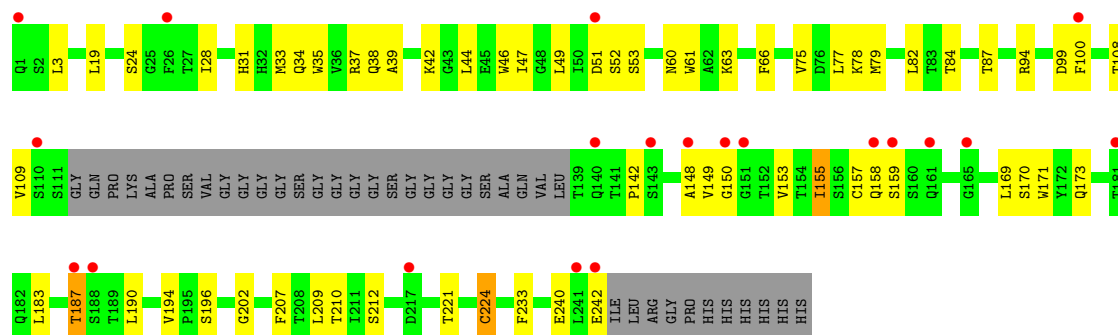


- Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA

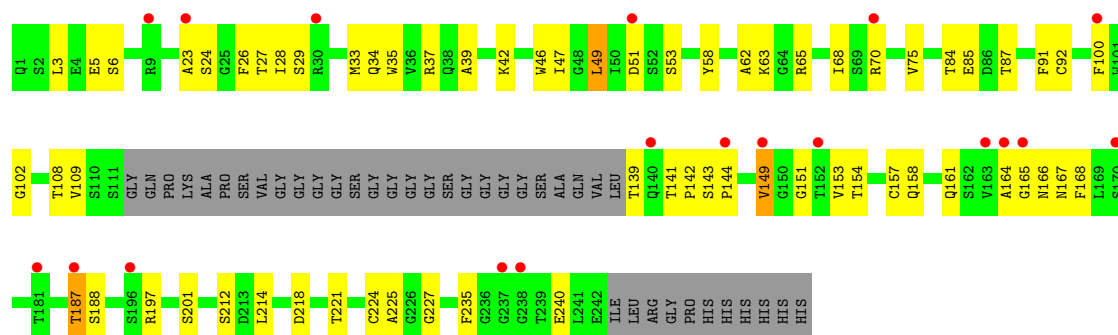




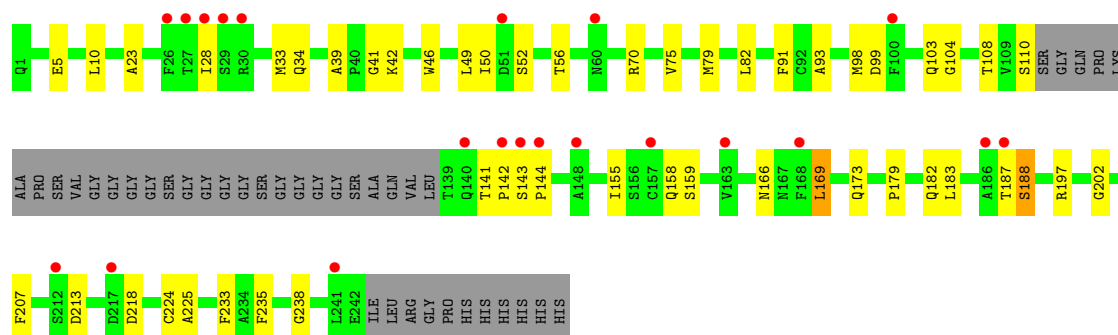
• Molecule 2: scFv13



• Molecule 2: scFv13

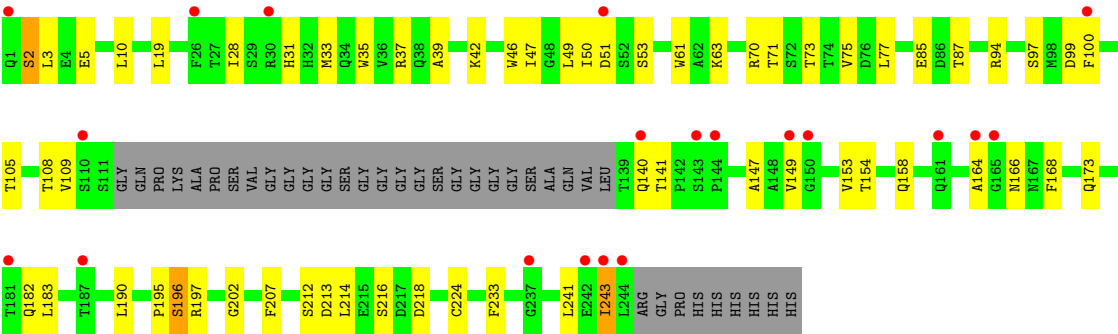


• Molecule 2: scFv13



• Molecule 2: scFv13





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.59Å 129.27Å 245.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 2.80 48.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.27-2.80) 99.9 (48.27-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.276 0.222 , 0.276	Depositor DCC
R_{free} test set	2893 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15165	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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	0.37	0/2239	0.36	0/3020
1	B	0.37	0/2239	0.37	0/3020
1	C	0.30	0/2231	0.35	0/3012
1	D	0.32	0/2235	0.36	0/3016
2	E	0.39	0/1641	0.54	2/2232 (0.1%)
2	F	0.38	0/1619	0.47	0/2204
2	G	0.41	0/1629	0.57	1/2216 (0.0%)
2	H	0.43	0/1645	0.51	0/2238
All	All	0.37	0/15478	0.44	3/20958 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	187	THR	CA-CB-OG1	-6.95	99.17	109.60
2	E	187	THR	CA-CB-OG1	-6.76	99.45	109.60
2	E	142	PRO	N-CA-C	-6.07	100.26	110.21

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	2196	0	2213	25	0
1	B	2196	0	2213	28	0
1	C	2188	0	2191	38	0
1	D	2192	0	2202	20	0
2	E	1604	0	1527	41	0
2	F	1583	0	1502	36	0
2	G	1593	0	1518	42	0
2	H	1609	0	1540	50	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	15165	0	14906	271	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 9.

All (271) 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:F:158:GLN:NE2	2:F:224:CYS:SG	2.42	0.92
2:G:158:GLN:NE2	2:G:224:CYS:SG	2.45	0.90
2:G:79:MET:HE2	2:G:82:LEU:HD21	1.56	0.86
2:G:94:ARG:NH2	2:G:99:ASP:OD2	2.12	0.82
1:C:172:VAL:HG12	1:C:232:MET:HE1	1.59	0.81
1:C:219:SER:OG	1:C:276:GLY:O	2.02	0.78
2:E:39:ALA:HB3	2:E:42:LYS:HB2	1.66	0.76
2:E:51:ASP:OD2	2:E:53:SER:OG	2.03	0.76
1:C:272:LYS:HE3	2:E:63:LYS:HD2	1.68	0.75
2:E:70:ARG:HG3	2:E:75:VAL:HG22	1.71	0.71
1:B:223:VAL:HG21	1:B:229:ARG:HG2	1.72	0.71
2:H:140:GLN:HB3	2:H:158:GLN:NE2	2.06	0.71
2:E:33:MET:HG3	2:E:75:VAL:HG21	1.72	0.70
1:A:116:ASN:HA	1:A:119:ILE:HD12	1.73	0.70
2:F:23:ALA:HB2	2:F:28:ILE:HD11	1.72	0.70
1:B:217:LYS:HD3	1:B:241:ILE:HD11	1.71	0.70
1:C:114:LEU:HD21	1:C:266:MET:HG3	1.74	0.69
2:H:158:GLN:OE1	2:H:224:CYS:SG	2.50	0.69
2:H:97:SER:HB2	2:H:182:GLN:HE22	1.55	0.69
2:E:5:GLU:OE2	2:E:91:PHE:HA	1.93	0.67
2:E:28:ILE:HD13	2:E:75:VAL:HG23	1.78	0.66
2:H:50:ILE:HG23	2:H:70:ARG:NH2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:HG2	1:C:263:TYR:CE2	2.32	0.65
2:G:51:ASP:OD2	2:G:53:SER:OG	2.13	0.65
2:H:140:GLN:HB3	2:H:158:GLN:HE21	1.61	0.65
1:D:261:SER:O	1:D:265:MET:HG2	1.96	0.65
2:E:158:GLN:OE1	2:E:224:CYS:SG	2.55	0.64
2:H:173:GLN:HB3	2:H:183:LEU:HD21	1.80	0.63
1:D:215:VAL:HG23	1:D:216:ILE:HG12	1.81	0.63
2:G:34:GLN:HG2	2:G:46:TRP:HE1	1.64	0.63
1:A:118:ILE:HG23	1:A:147:VAL:HG13	1.80	0.62
2:H:87:THR:HG23	2:H:108:THR:HA	1.80	0.62
2:E:158:GLN:NE2	2:E:224:CYS:SG	2.72	0.62
2:G:153:VAL:HG22	2:G:212:SER:HA	1.81	0.62
2:F:197:ARG:NH1	2:F:218:ASP:OD2	2.33	0.62
1:A:137:GLU:HG3	1:C:162:ASP:HB3	1.82	0.61
1:C:222:PHE:CE2	1:C:273:ILE:HA	2.36	0.61
1:B:98:GLU:OE1	1:B:194:GLU:OE2	2.18	0.61
2:H:154:THR:HG21	2:H:241:LEU:HD11	1.82	0.61
2:F:28:ILE:HG23	2:F:33:MET:HE3	1.81	0.60
2:E:85:GLU:N	2:E:85:GLU:OE1	2.32	0.60
2:F:34:GLN:HG2	2:F:46:TRP:HE1	1.66	0.60
2:E:3:LEU:HG	2:E:100:PHE:CZ	2.37	0.59
2:F:41:GLY:H	2:F:42:LYS:NZ	2.00	0.59
2:F:197:ARG:HD3	2:F:213:ASP:HB2	1.85	0.59
2:E:149:VAL:HG23	2:E:214:LEU:HD22	1.82	0.59
2:H:50:ILE:HD13	2:H:70:ARG:HB3	1.84	0.58
2:G:149:VAL:HG12	2:G:150:GLY:N	2.18	0.58
1:C:118:ILE:HD12	1:C:147:VAL:HG13	1.85	0.58
2:E:87:THR:HG23	2:E:108:THR:HA	1.86	0.58
1:A:35:ASP:OD1	1:A:196:ASN:ND2	2.31	0.58
2:G:94:ARG:HH21	2:G:99:ASP:CG	2.08	0.58
1:C:70:PHE:O	1:C:74:VAL:HG22	2.04	0.58
1:C:269:ASN:O	1:C:273:ILE:HG13	2.03	0.58
2:H:190:LEU:HD11	2:H:196:SER:HA	1.85	0.57
2:H:33:MET:HG3	2:H:75:VAL:HG21	1.86	0.57
2:H:149:VAL:HG22	2:H:154:THR:HG22	1.86	0.57
2:G:149:VAL:HG12	2:G:150:GLY:H	1.69	0.57
2:E:62:ALA:O	2:E:65:ARG:HG3	2.05	0.57
1:B:213:LEU:O	1:B:217:LYS:HG2	2.05	0.57
2:F:41:GLY:H	2:F:42:LYS:HZ3	1.50	0.56
1:C:267:LYS:HD2	1:C:271:ASP:OD2	2.04	0.56
2:F:91:PHE:HE2	2:F:179:PRO:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ILE:HD13	2:H:70:ARG:CB	2.36	0.55
2:G:84:THR:HA	2:G:109:VAL:HB	1.88	0.55
1:C:97:LEU:HD21	1:C:195:ILE:HD13	1.88	0.55
1:D:204:ASP:O	1:D:208:SER:OG	2.23	0.55
2:H:35:TRP:HE1	2:H:75:VAL:HG12	1.73	0.54
1:B:105:LYS:HD3	1:A:105:LYS:HG2	1.87	0.54
2:F:173:GLN:HB2	2:F:183:LEU:HD11	1.88	0.54
2:F:42:LYS:HD3	2:F:42:LYS:N	2.22	0.54
2:F:158:GLN:HG3	2:F:159:SER:N	2.22	0.54
1:C:178:PHE:HD1	1:C:181:PHE:HB3	1.71	0.54
2:H:97:SER:O	2:H:182:GLN:NE2	2.41	0.54
2:G:66:PHE:CE2	2:G:79:MET:HG2	2.42	0.54
1:A:261:SER:O	1:A:265:MET:HG2	2.08	0.54
1:A:143:LEU:O	1:A:147:VAL:HG23	2.09	0.53
1:C:109:HIS:HE1	1:C:195:ILE:CD1	2.20	0.53
2:G:28:ILE:HD13	2:G:75:VAL:HG23	1.91	0.53
1:B:98:GLU:CD	1:B:179:LYS:HE3	2.34	0.53
2:E:153:VAL:HG22	2:E:212:SER:HA	1.92	0.52
1:B:19:ILE:HD11	1:B:121:SER:HB3	1.91	0.52
1:C:109:HIS:HE1	1:C:195:ILE:HD11	1.75	0.52
2:F:5:GLU:OE1	2:F:5:GLU:N	2.42	0.52
2:G:19:LEU:HD12	2:G:77:LEU:HD23	1.91	0.52
2:G:173:GLN:HB2	2:G:183:LEU:HD11	1.90	0.52
2:F:166:ASN:OD1	2:F:166:ASN:C	2.53	0.52
2:H:214:LEU:HD11	2:H:241:LEU:HD21	1.92	0.52
1:D:149:LYS:HE2	1:D:263:TYR:CE2	2.45	0.52
2:G:87:THR:HG23	2:G:108:THR:HA	1.92	0.52
2:H:153:VAL:HG22	2:H:212:SER:HA	1.92	0.52
2:G:142:PRO:HG3	2:G:158:GLN:HE22	1.76	0.51
1:D:62:LEU:HB2	1:D:108:PRO:HB2	1.92	0.51
2:E:34:GLN:HG2	2:E:46:TRP:HE1	1.76	0.51
2:H:19:LEU:HD12	2:H:77:LEU:HD23	1.91	0.51
1:B:125:ALA:HB3	1:B:143:LEU:HD22	1.92	0.51
2:F:169:LEU:HD22	2:F:207:PHE:CG	2.45	0.51
2:H:61:TRP:HA	2:H:63:LYS:HE3	1.91	0.51
2:F:79:MET:HE3	2:F:82:LEU:HD21	1.90	0.51
1:C:221:LEU:C	1:C:222:PHE:CD1	2.88	0.51
2:E:3:LEU:HG	2:E:100:PHE:CE2	2.45	0.51
2:H:2:SER:HA	2:H:100:PHE:HZ	1.74	0.51
1:B:134:LYS:O	1:B:134:LYS:HD3	2.11	0.50
2:G:31:HIS:CG	2:G:94:ARG:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TYR:HD1	1:B:265:MET:HE2	1.76	0.50
2:G:169:LEU:HD13	2:G:170:SER:N	2.27	0.50
2:E:37:ARG:HB3	2:E:47:ILE:HD11	1.93	0.50
2:F:158:GLN:HE22	2:F:224:CYS:CB	2.24	0.50
2:E:34:GLN:HG3	2:E:49:LEU:HB2	1.93	0.50
2:F:10:LEU:HD22	2:F:108:THR:HB	1.92	0.50
2:G:190:LEU:HD22	2:G:194:VAL:HB	1.92	0.50
1:A:110:ALA:HA	1:A:180:TYR:CG	2.46	0.50
1:C:263:TYR:CD1	1:C:263:TYR:C	2.89	0.50
2:F:5:GLU:CD	2:F:104:GLY:H	2.20	0.49
1:A:152:LYS:HA	1:A:155:LYS:HE3	1.94	0.49
1:C:272:LYS:HE3	2:E:63:LYS:CD	2.41	0.49
2:E:149:VAL:HG22	2:E:154:THR:HG22	1.94	0.49
1:D:141:LYS:HE2	1:D:142:ASN:OD1	2.13	0.49
1:A:11:ILE:O	1:A:15:MET:HG3	2.12	0.49
1:C:195:ILE:HG23	1:C:197:THR:H	1.77	0.49
2:H:28:ILE:HG22	2:H:70:ARG:HH11	1.77	0.49
2:H:195:PRO:HG2	2:H:197:ARG:HH21	1.76	0.49
1:D:110:ALA:HA	1:D:180:TYR:CG	2.47	0.49
2:F:50:ILE:HD12	2:F:56:THR:HG22	1.95	0.49
1:B:66:GLY:H	1:A:104:GLY:CA	2.26	0.48
1:C:172:VAL:HG21	1:C:213:LEU:HD21	1.96	0.48
2:H:19:LEU:HD22	2:H:105:THR:HG21	1.96	0.48
2:G:202:GLY:HA3	2:G:207:PHE:HA	1.95	0.48
2:H:28:ILE:CG2	2:H:70:ARG:NH1	2.76	0.48
1:C:195:ILE:O	1:C:198:GLU:HG3	2.14	0.48
2:F:39:ALA:CB	2:F:42:LYS:HE2	2.43	0.48
1:B:195:ILE:HG23	1:B:197:THR:H	1.79	0.48
1:D:136:LYS:O	1:D:140:GLU:HG3	2.13	0.48
1:B:105:LYS:HD3	1:A:105:LYS:HD3	1.95	0.48
2:E:221:THR:HA	2:E:240:GLU:HA	1.94	0.48
1:D:35:ASP:OD1	1:D:37:HIS:ND1	2.30	0.48
1:A:31:PRO:HG2	1:A:34:GLN:HG3	1.96	0.48
1:D:15:MET:HE1	1:D:120:TYR:HD2	1.78	0.47
2:E:27:THR:HG22	2:E:29:SER:H	1.77	0.47
2:F:52:SER:O	2:F:70:ARG:NH2	2.46	0.47
1:B:112:LEU:HA	1:B:266:MET:HE1	1.97	0.47
2:H:39:ALA:HB3	2:H:42:LYS:HB2	1.95	0.47
2:H:197:ARG:NH1	2:H:218:ASP:OD2	2.48	0.47
1:D:129:ILE:HG12	1:D:136:LYS:HG3	1.97	0.47
2:G:37:ARG:HB3	2:G:47:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:GLU:OE1	2:E:102:GLY:HA3	2.15	0.47
2:F:10:LEU:CD2	2:F:108:THR:HB	2.44	0.47
2:H:46:TRP:CE2	2:H:233:PHE:HB2	2.49	0.47
1:D:230:ARG:O	1:D:234:THR:HG23	2.15	0.47
2:G:221:THR:HA	2:G:240:GLU:HA	1.97	0.47
2:G:35:TRP:HE1	2:G:75:VAL:HG12	1.79	0.47
1:C:120:TYR:O	1:C:124:ILE:HG13	2.15	0.47
2:H:10:LEU:HD23	2:H:108:THR:HB	1.96	0.47
2:H:31:HIS:ND1	2:H:94:ARG:HD3	2.29	0.47
1:B:134:LYS:HD3	1:B:134:LYS:C	2.40	0.46
1:C:128:LEU:HB3	1:C:139:TYR:CE2	2.50	0.46
2:E:139:THR:N	2:E:161:GLN:HG2	2.30	0.46
2:H:94:ARG:NH1	2:H:99:ASP:OD2	2.48	0.46
1:A:118:ILE:CG2	1:A:147:VAL:HG13	2.46	0.46
2:F:70:ARG:HG3	2:F:75:VAL:HG22	1.97	0.46
2:F:225:ALA:HB2	2:F:235:PHE:CE1	2.50	0.46
2:H:164:ALA:C	2:H:166:ASN:H	2.22	0.46
1:B:118:ILE:HG22	1:B:122:LYS:HE2	1.96	0.46
1:B:195:ILE:O	1:B:198:GLU:HG3	2.14	0.46
1:C:248:PHE:HB3	1:C:265:MET:HE3	1.97	0.46
1:C:109:HIS:CE1	1:C:195:ILE:HD11	2.50	0.46
2:E:158:GLN:CD	2:E:224:CYS:SG	2.98	0.46
2:E:197:ARG:NH1	2:E:218:ASP:OD2	2.49	0.46
2:G:158:GLN:OE1	2:G:171:TRP:CH2	2.69	0.46
2:F:143:SER:OG	2:F:144:PRO:HD3	2.15	0.46
2:G:79:MET:HE2	2:G:82:LEU:CD2	2.38	0.46
2:G:190:LEU:HD11	2:G:196:SER:HA	1.98	0.46
1:A:1:ASP:OD1	1:A:1:ASP:N	2.40	0.46
2:F:202:GLY:HA3	2:F:207:PHE:HA	1.97	0.45
1:B:222:PHE:CZ	1:B:273:ILE:HA	2.51	0.45
1:D:57:TYR:CE1	1:D:85:TYR:HD2	2.34	0.45
1:A:80:THR:HB	1:A:83:LYS:HB3	1.98	0.45
1:B:103:LYS:H	1:B:103:LYS:HG3	1.38	0.45
1:B:103:LYS:O	1:A:105:LYS:NZ	2.50	0.45
1:A:268:TRP:O	1:A:272:LYS:HG2	2.17	0.45
2:E:143:SER:HB2	2:E:144:PRO:HD3	1.98	0.45
2:F:93:ALA:CB	2:F:98:MET:HG2	2.47	0.45
1:C:161:PHE:N	1:C:161:PHE:CD1	2.85	0.45
1:A:62:LEU:HB2	1:A:108:PRO:HB2	1.99	0.45
2:G:60:ASN:OD1	2:G:60:ASN:N	2.49	0.44
2:E:35:TRP:HE1	2:E:75:VAL:HG12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ALA:HA	1:C:180:TYR:CG	2.53	0.44
2:G:169:LEU:HG	2:G:207:PHE:CG	2.53	0.44
2:F:93:ALA:HB3	2:F:98:MET:HG2	1.99	0.44
1:D:222:PHE:CZ	1:D:273:ILE:HA	2.53	0.44
2:G:66:PHE:CD2	2:G:79:MET:HG2	2.52	0.44
1:B:163:ALA:HA	2:F:155:ILE:HG21	2.00	0.44
2:H:154:THR:HG23	2:H:214:LEU:HD13	2.00	0.44
2:G:31:HIS:ND1	2:G:94:ARG:HD2	2.33	0.44
1:A:175:GLU:HA	1:A:193:TRP:O	2.17	0.44
2:G:46:TRP:CE2	2:G:233:PHE:HB2	2.52	0.44
2:E:84:THR:HA	2:E:109:VAL:HB	1.99	0.44
1:D:202:THR:OG1	1:D:205:GLN:HG3	2.18	0.44
1:A:224:GLU:OE1	1:A:224:GLU:N	2.49	0.43
1:C:54:VAL:HB	1:C:131:LYS:HD2	2.00	0.43
1:C:100:ALA:O	1:C:101:SER:OG	2.34	0.43
2:E:23:ALA:HB2	2:E:28:ILE:HG13	2.00	0.43
2:F:46:TRP:CE2	2:F:233:PHE:HB2	2.53	0.43
1:B:168:LYS:HE2	1:B:219:SER:OG	2.18	0.43
1:D:64:ASP:O	1:D:68:ALA:HB3	2.18	0.43
2:E:34:GLN:O	2:E:92:CYS:HA	2.18	0.43
1:B:110:ALA:HA	1:B:180:TYR:CG	2.53	0.43
2:G:78:LYS:HD3	2:G:78:LYS:C	2.44	0.43
2:G:155:ILE:HG12	2:G:210:THR:HG23	1.99	0.43
1:B:112:LEU:HA	1:B:266:MET:CE	2.49	0.43
2:G:148:ALA:CB	2:G:242:GLU:HB2	2.49	0.43
2:E:3:LEU:HD21	2:E:26:PHE:HZ	1.84	0.43
2:H:173:GLN:CB	2:H:183:LEU:HD21	2.47	0.43
2:H:212:SER:O	2:H:213:ASP:C	2.62	0.43
2:G:171:TRP:CD2	2:G:209:LEU:HB2	2.54	0.43
1:A:240:GLY:O	1:A:242:PRO:HD3	2.19	0.43
2:H:158:GLN:OE1	2:H:224:CYS:CB	2.67	0.43
2:E:154:THR:HG23	2:E:214:LEU:HD13	2.01	0.43
1:C:244:TYR:O	2:E:65:ARG:HD3	2.20	0.42
1:D:57:TYR:HD2	1:D:63:GLU:OE2	2.03	0.42
1:B:262:TYR:CD1	1:B:265:MET:HE2	2.54	0.42
2:H:168[B]:PHE:CD1	2:H:168[B]:PHE:C	2.97	0.42
1:D:137:GLU:O	1:D:141:LYS:HG2	2.19	0.42
2:E:168[C]:PHE:HD1	2:E:227:GLY:H	1.67	0.42
2:H:85:GLU:OE1	2:H:85:GLU:N	2.45	0.42
2:H:216:SER:HA	2:H:243:ILE:HG21	2.00	0.42
2:F:187:THR:HG23	2:F:188:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:ILE:HG22	2:H:70:ARG:NH1	2.35	0.42
2:G:39:ALA:HB3	2:G:42:LYS:HB2	2.02	0.42
2:E:225:ALA:HB2	2:E:235:PHE:CE1	2.55	0.42
2:H:50:ILE:CD1	2:H:70:ARG:HB3	2.49	0.42
1:C:149:LYS:HG2	1:C:263:TYR:HE2	1.80	0.42
2:F:103:GLN:HA	2:F:179:PRO:HG3	2.01	0.42
1:C:125:ALA:O	1:C:129:ILE:HG13	2.20	0.42
1:C:262:TYR:O	1:C:265:MET:HG2	2.20	0.42
1:B:37:HIS:HA	1:B:62:LEU:O	2.20	0.42
1:B:118:ILE:CG2	1:B:122:LYS:HE2	2.50	0.41
1:A:222:PHE:CZ	1:A:273:ILE:HA	2.55	0.41
2:E:58:TYR:HE1	2:E:68:ILE:HG13	1.84	0.41
2:H:37:ARG:HB3	2:H:47:ILE:HD11	2.01	0.41
2:H:70:ARG:HG2	2:H:71:THR:N	2.33	0.41
2:H:164:ALA:C	2:H:166:ASN:N	2.78	0.41
2:G:61:TRP:O	2:G:63:LYS:HG2	2.20	0.41
2:H:168[B]:PHE:C	2:H:168[B]:PHE:HD1	2.28	0.41
1:C:96:TYR:HA	1:C:106:GLU:HA	2.03	0.41
2:E:158:GLN:OE1	2:E:224:CYS:HB2	2.20	0.41
1:C:228:ASP:OD2	1:C:230:ARG:HG3	2.21	0.41
2:F:142:PRO:HG2	2:F:238:GLY:H	1.85	0.41
2:F:158:GLN:CD	2:F:224:CYS:SG	3.01	0.41
1:D:220:ALA:HB1	1:D:244:TYR:HB2	2.01	0.41
2:E:165:GLY:C	2:E:167:ASN:H	2.28	0.41
2:H:51:ASP:OD2	2:H:53:SER:OG	2.32	0.41
1:C:11:ILE:HG22	1:C:15:MET:HE3	2.02	0.41
1:B:174:SER:HB3	1:B:193:TRP:CH2	2.56	0.41
2:G:158:GLN:OE1	2:G:171:TRP:HH2	2.04	0.41
2:F:99:ASP:HA	2:F:182:GLN:OE1	2.21	0.41
2:H:147:ALA:O	2:H:241:LEU:HD12	2.20	0.41
2:H:46:TRP:CD2	2:H:233:PHE:HB2	2.56	0.41
1:D:19:ILE:HD13	1:D:125:ALA:HB2	2.03	0.40
2:G:38:GLN:HB2	2:G:44:LEU:HD23	2.02	0.40
1:A:10:SER:HB3	1:A:32:ILE:CD1	2.52	0.40
1:C:222:PHE:HE2	1:C:273:ILE:HA	1.85	0.40
2:E:164:ALA:C	2:E:166:ASN:N	2.79	0.40
2:H:3:LEU:HG	2:H:100:PHE:CE2	2.56	0.40
2:H:5:GLU:OE1	2:H:5:GLU:N	2.53	0.40
2:G:3:LEU:HG	2:G:100:PHE:CZ	2.56	0.40
2:G:33:MET:HG3	2:G:75:VAL:HG21	2.02	0.40
2:G:51:ASP:OD1	2:G:52:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:202:GLY:HA3	2:H:207:PHE:HA	2.03	0.40
1:A:153:LEU:HD11	1:A:267:LYS:HD2	2.03	0.40
1:C:60:ILE:HG22	1:C:106:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

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	277/279 (99%)	263 (95%)	14 (5%)	0	100	100
1	B	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	C	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
1	D	277/279 (99%)	267 (96%)	10 (4%)	0	100	100
2	E	213/253 (84%)	200 (94%)	10 (5%)	3 (1%)	9	30
2	F	211/253 (83%)	195 (92%)	16 (8%)	0	100	100
2	G	212/253 (84%)	196 (92%)	16 (8%)	0	100	100
2	H	214/253 (85%)	195 (91%)	19 (9%)	0	100	100
All	All	1958/2128 (92%)	1848 (94%)	107 (6%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	188	SER
2	E	149	VAL
2	E	151	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	240/240 (100%)	237 (99%)	3 (1%)	61	86
1	B	240/240 (100%)	237 (99%)	3 (1%)	61	86
1	C	238/240 (99%)	235 (99%)	3 (1%)	61	86
1	D	239/240 (100%)	237 (99%)	2 (1%)	73	90
2	E	173/194 (89%)	166 (96%)	7 (4%)	28	63
2	F	170/194 (88%)	165 (97%)	5 (3%)	37	73
2	G	172/194 (89%)	165 (96%)	7 (4%)	27	62
2	H	174/194 (90%)	167 (96%)	7 (4%)	28	63
All	All	1646/1736 (95%)	1609 (98%)	37 (2%)	44	78

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	ASP
1	B	103	LYS
1	B	105	LYS
1	D	183	LYS
1	D	215	VAL
2	G	24	SER
2	G	49	LEU
2	G	155	ILE
2	G	157	CYS
2	G	159	SER
2	G	187	THR
2	G	224	CYS
1	A	48	LYS
1	A	106	GLU
1	A	226	SER
1	C	25	ASP
1	C	83	LYS
1	C	106	GLU
2	E	6	SER

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Mol	Chain	Res	Type
2	E	24	SER
2	E	49	LEU
2	E	141	THR
2	E	157	CYS
2	E	187	THR
2	E	201	SER
2	F	49	LEU
2	F	110	SER
2	F	141	THR
2	F	169	LEU
2	F	188	SER
2	H	2	SER
2	H	49	LEU
2	H	73	THR
2	H	109	VAL
2	H	141	THR
2	H	196	SER
2	H	243	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	51	ASN
2	G	140	GLN
2	G	158	GLN
1	A	51	ASN
1	A	113	ASN
1	C	51	ASN
1	C	67	GLN
1	C	127	GLN
1	C	205	GLN
2	F	103	GLN
2	H	103	GLN
2	H	182	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 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	279/279 (100%)	-0.08	3 (1%) 78 70	24, 39, 63, 92	0
1	B	279/279 (100%)	-0.16	6 (2%) 62 52	21, 35, 59, 71	0
1	C	279/279 (100%)	0.55	13 (4%) 36 29	34, 63, 90, 106	0
1	D	279/279 (100%)	0.16	8 (2%) 53 43	28, 45, 74, 86	0
2	E	215/253 (84%)	0.61	19 (8%) 15 11	16, 51, 73, 105	1 (0%)
2	F	214/253 (84%)	0.71	21 (9%) 13 9	19, 56, 80, 104	1 (0%)
2	G	215/253 (84%)	0.43	20 (9%) 14 10	13, 41, 70, 81	1 (0%)
2	H	217/253 (85%)	0.40	20 (9%) 14 10	18, 40, 77, 101	1 (0%)
All	All	1977/2128 (92%)	0.30	110 (5%) 30 23	13, 46, 77, 106	4 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	187	THR	5.3
2	H	242	GLU	4.9
2	G	165	GLY	4.7
2	H	165	GLY	4.7
2	F	144	PRO	4.5
1	C	37	HIS	4.3
2	E	165	GLY	4.3
2	E	164	ALA	4.3
2	H	164	ALA	4.2
2	G	158	GLN	4.1
2	G	150	GLY	3.9
2	E	100	PHE	3.8
2	H	140	GLN	3.7
1	D	66	GLY	3.7
1	C	101	SER	3.6
2	F	30	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	51	ASP	3.5
1	D	37	HIS	3.5
2	E	187	THR	3.4
2	G	100	PHE	3.4
1	C	197	THR	3.4
2	F	26	PHE	3.3
2	E	140	GLN	3.2
2	H	51	ASP	3.1
2	H	181	THR	3.1
1	D	65	GLY	3.0
2	E	70	ARG	3.0
2	F	186	ALA	3.0
1	D	38	GLU	3.0
1	D	104	GLY	3.0
2	H	243	ILE	3.0
2	F	140	GLN	2.9
2	G	161	GLN	2.9
2	F	143	SER	2.9
2	H	143	SER	2.9
2	H	144	PRO	2.9
2	E	51	ASP	2.9
2	E	237	GLY	2.8
2	H	100	PHE	2.8
2	G	143	SER	2.8
2	F	212	SER	2.8
1	D	67	GLN	2.8
2	E	149	VAL	2.8
1	C	104	GLY	2.8
2	H	30	ARG	2.8
1	B	103	LYS	2.8
2	E	163	VAL	2.8
1	D	102	GLU	2.7
2	F	27	THR	2.7
2	F	29	SER	2.7
2	H	1	GLN	2.7
2	H	110	SER	2.7
2	F	148	ALA	2.6
2	F	100	PHE	2.6
2	F	157	CYS	2.6
1	C	66	GLY	2.6
2	G	242	GLU	2.6
2	F	163	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	9	ARG	2.5
1	D	101	SER	2.5
2	G	140	GLN	2.5
2	E	152	THR	2.5
2	E	170	SER	2.4
2	E	238	GLY	2.4
2	F	168[A]	PHE	2.4
1	B	66	GLY	2.4
2	G	181	THR	2.4
2	G	187	THR	2.4
2	F	60	ASN	2.4
1	C	183	LYS	2.4
2	G	151	GLY	2.4
2	E	196	SER	2.4
2	E	181	THR	2.4
2	F	217	ASP	2.3
2	H	244	LEU	2.3
1	C	102	GLU	2.3
1	A	37	HIS	2.3
2	F	241	LEU	2.3
2	E	30	ARG	2.3
2	F	142	PRO	2.3
2	G	1	GLN	2.3
2	H	161	GLN	2.3
2	H	149	VAL	2.3
2	G	51	ASP	2.2
2	H	150	GLY	2.2
1	C	106	GLU	2.2
1	C	103	LYS	2.2
2	G	110	SER	2.2
1	B	104	GLY	2.2
2	G	241	LEU	2.2
1	A	239	SER	2.2
2	F	28	ILE	2.1
1	B	65	GLY	2.1
2	G	188	SER	2.1
2	H	187	THR	2.1
2	H	237	GLY	2.1
1	B	37	HIS	2.1
1	C	279	LYS	2.1
2	G	26	PHE	2.1
1	A	104	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	23	ALA	2.1
1	B	98	GLU	2.1
2	H	26	PHE	2.0
1	C	100	ALA	2.0
1	C	94	VAL	2.0
1	C	236	SER	2.0
2	G	159	SER	2.0
2	E	144	PRO	2.0
2	G	148	ALA	2.0
2	G	217	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

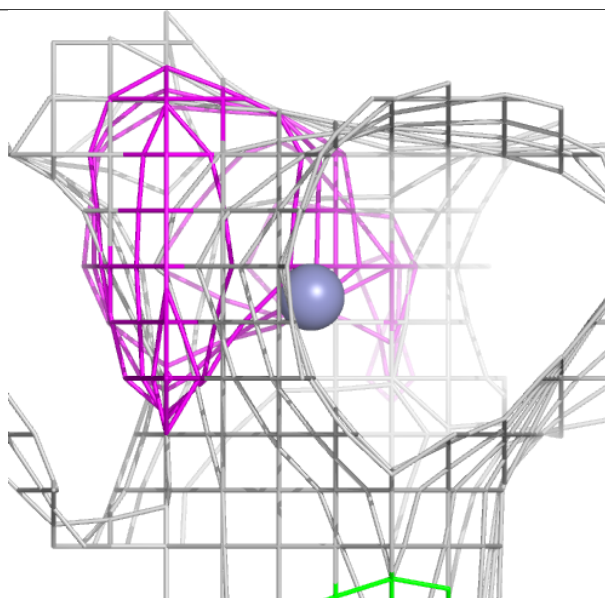
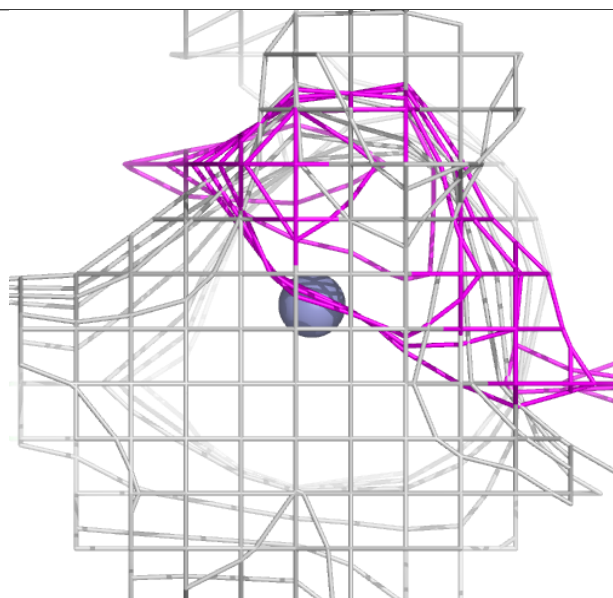
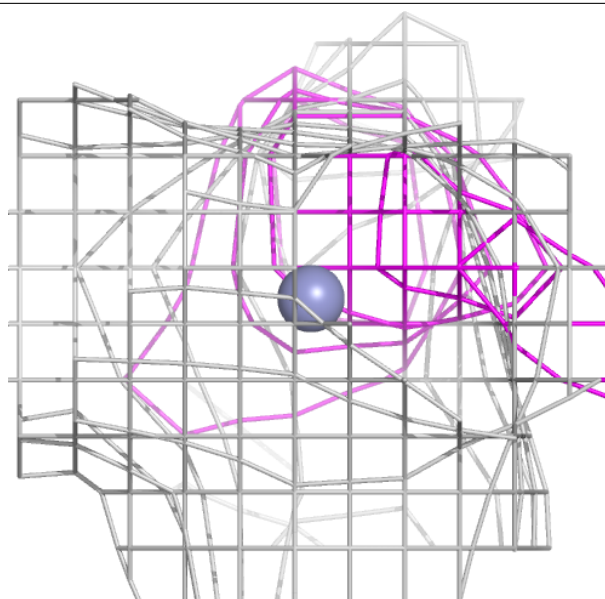
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	D	301	1/1	0.89	0.15	84,84,84,84	0
3	ZN	C	301	1/1	0.91	0.13	91,91,91,91	0
3	ZN	B	301	1/1	0.94	0.10	67,67,67,67	0
3	ZN	A	301	1/1	0.99	0.09	61,61,61,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

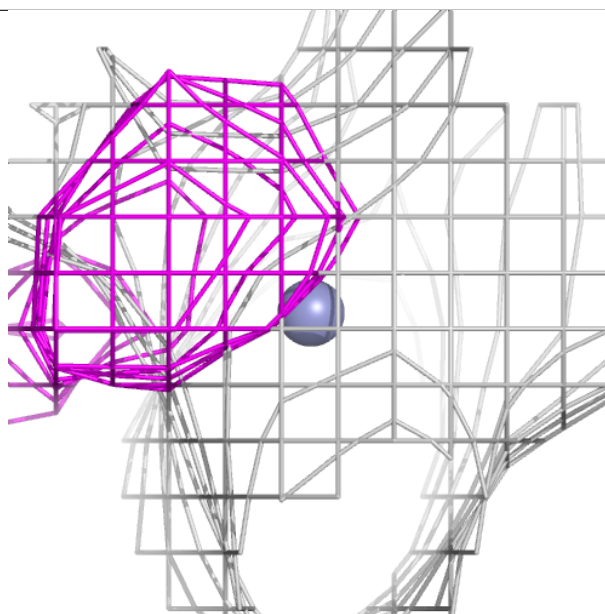
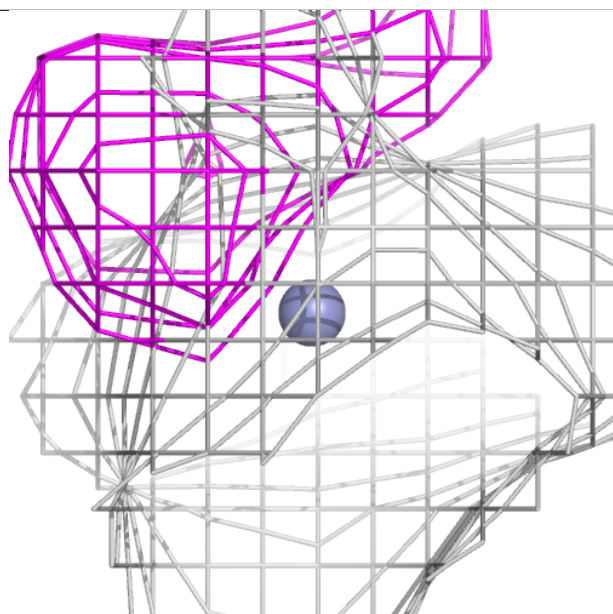
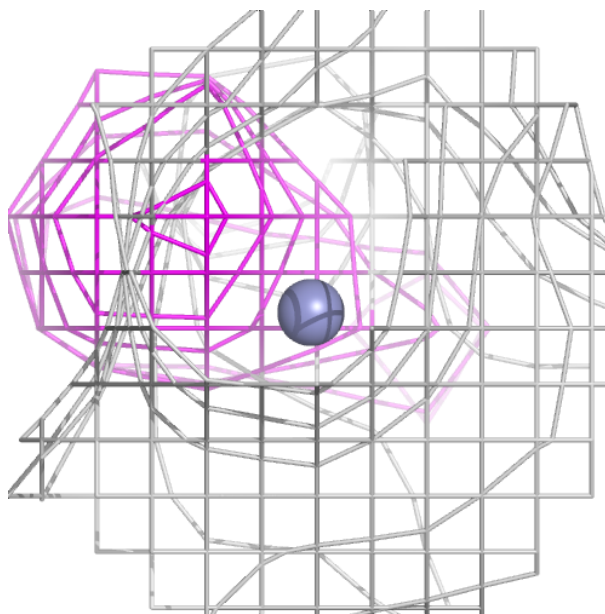
Electron density around ZN D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



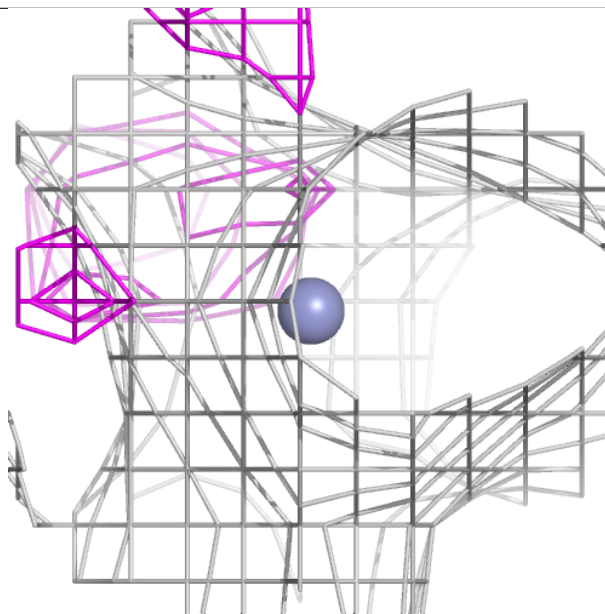
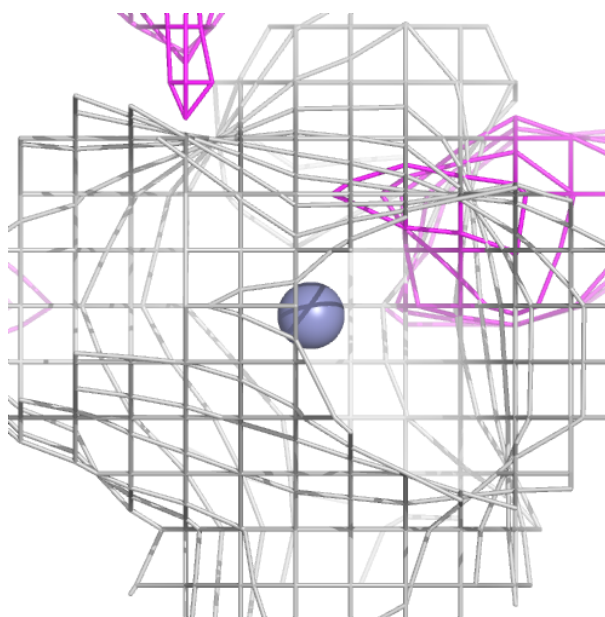
Electron density around ZN C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.