Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2024 – 12:57 PM JST

PDB ID	:	8YJ7
Title	:	Characerization of a novel format scFvXVHH single-chain Biparatopic antibody 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:

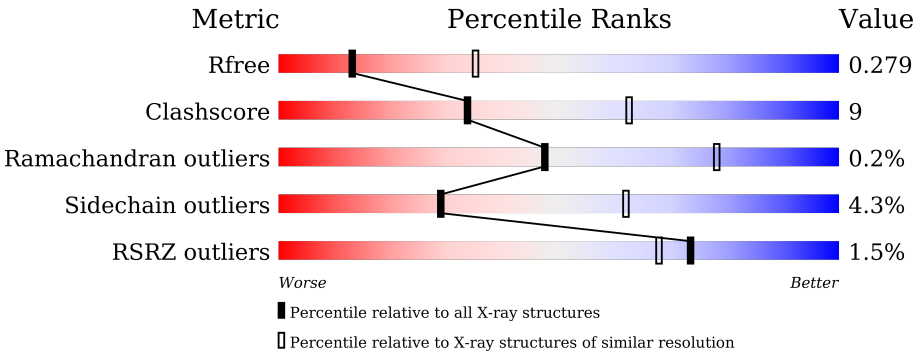
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	85% 14%
1	B	279	86% 13%
1	C	279	% 78% 21%
1	D	279	85% 14%
2	E	253	2% 60% 24% 15%
2	F	253	2% 64% 20% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	253	2% 60% 24% 15%
2	H	253	4% 62% 22% 14%

2 Entry composition (i)

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 (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

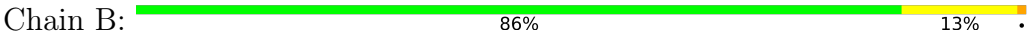
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

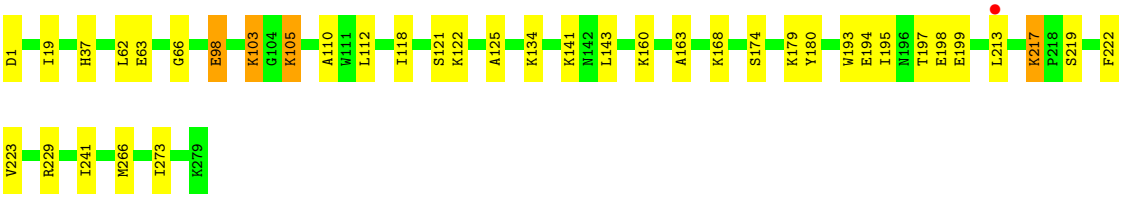
3 Residue-property plots (i)

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

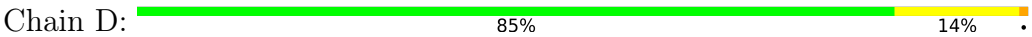
Chain B:

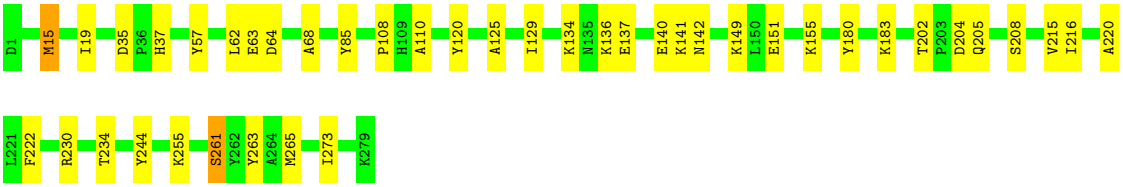




• Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA

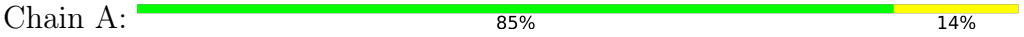
Chain D:

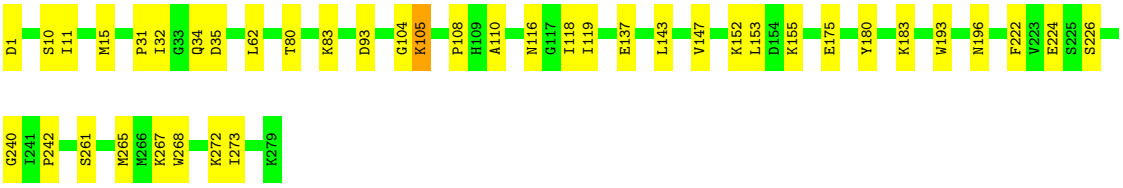




• Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA

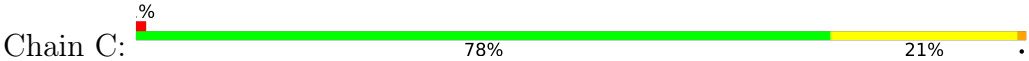
Chain A:

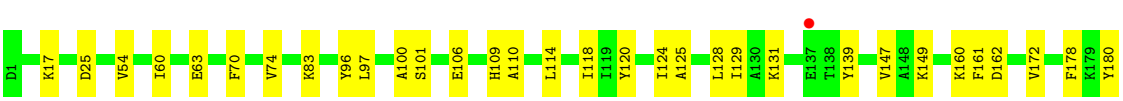


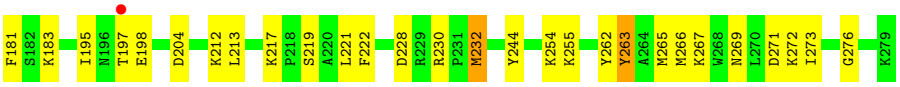


• Molecule 1: Iron ABC transporter substrate-binding lipoprotein MtsA

Chain C:

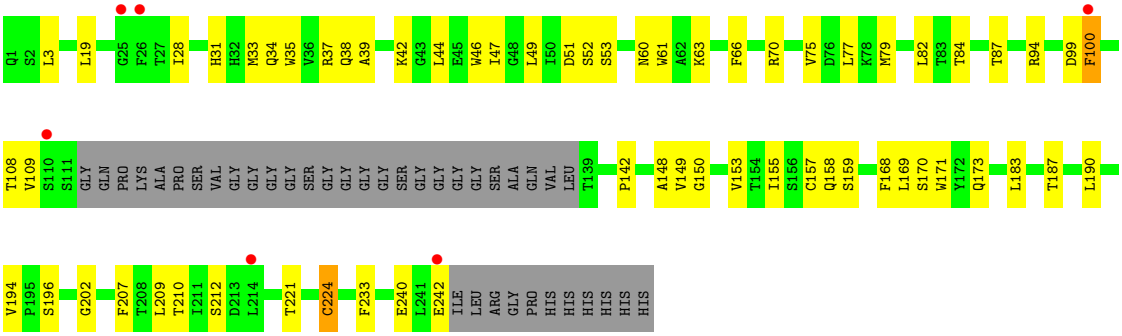






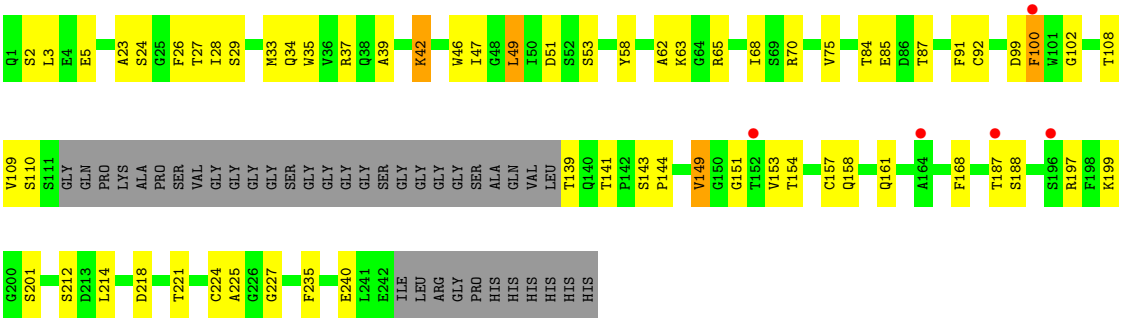
• Molecule 2: scFv13

Chain G:



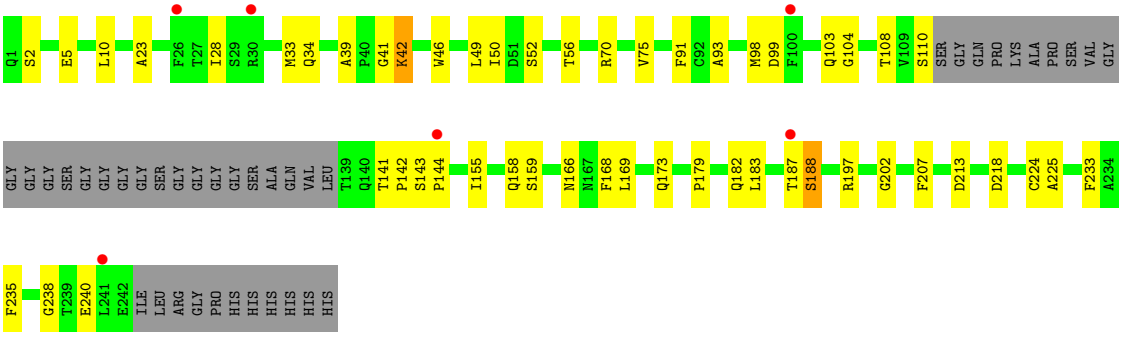
• Molecule 2: scFv13

Chain E:



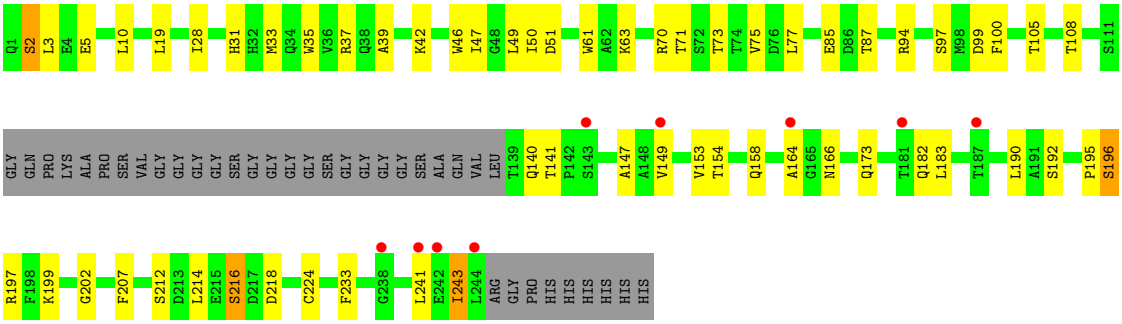
• Molecule 2: scFv13

Chain F:



• Molecule 2: scFv13

Chain H:


Q1 S2 L3 E4 E5 L10 L19 I28 H31 H32 M33 Q34 W35 V36 R37 Q38 A39 K42 W46 I47 G48 L49 I50 D51 W61 A62 K63 R70 T71 S72 T73 T74 V75 D76 L77 E85 D86 T87 R94 S97 M98 D99 F100 T105 T108 S111
GLY GLN PRO LYS ALA PRO SER VAL GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY GLY SER ALA GLN VAL LEU T139 Q140 T141 P142 S143 A147 A148 V149 V153 T154 Q158 A164 G165 N166 Q173 T181 Q182 L183 T187 L190 A191 S192 P195 S196
R197 F198 K199 G202 F207 S212 D213 L214 E215 S216 D217 D218 C224 F233 G238 L241 E242 I243 L244 ARG GLY PRO HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.276 0.225 , 0.279	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 , 29.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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	0.44	0/2239	0.47	0/3020
1	B	0.45	0/2239	0.47	0/3020
1	C	0.38	0/2231	0.45	0/3012
1	D	0.40	0/2235	0.46	0/3016
2	E	0.43	0/1641	0.59	0/2232
2	F	0.44	0/1619	0.59	0/2204
2	G	0.45	0/1629	0.63	0/2216
2	H	0.47	0/1645	0.60	0/2238
All	All	0.43	0/15478	0.53	0/20958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2196	0	2213	25	0
1	B	2196	0	2213	25	0
1	C	2188	0	2191	37	0
1	D	2192	0	2202	20	0
2	E	1604	0	1527	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1583	0	1502	34	0
2	G	1593	0	1518	40	0
2	H	1609	0	1540	45	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	256	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 (256) 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:94:ARG:NH2	2:G:99:ASP:OD2	2.12	0.82
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
1:C:272:LYS:HE3	2:E:63:LYS:HD2	1.68	0.75
2:E:51:ASP:OD2	2:E:53:SER:OG	2.03	0.74
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:G:94:ARG:HH21	2:G:99:ASP:CG	2.08	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:D:15:MET:HE1	1:D:120:TYR:HD2	1.76	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1:ASP:OD1	1:A:1:ASP:N	2.40	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:B:98:GLU:CD	1:B:179:LYS:HE3	2.34	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
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
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
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:F:166:ASN:OD1	2:F:166:ASN:C	2.53	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:109:HIS:CE1	1:C:195:ILE:HD11	2.50	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
1:C:221:LEU:C	1:C:222:PHE:CD1	2.88	0.46
2:G:190:LEU:HD11	2:G:196:SER:HA	1.98	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
1:C:263:TYR:CD1	1:C:263:TYR:C	2.89	0.45
2:E:143:SER:HB2	2:E:144:PRO:HD3	1.98	0.45
2:F:5:GLU:CD	2:F:104:GLY:H	2.20	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
1:C:172:VAL:HG12	1:C:232:MET:HE1	1.99	0.44
2:E:35:TRP:HE1	2:E:75:VAL:HG12	1.82	0.44
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
2:F:28:ILE:HG23	2:F:33:MET:HE3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:70:ARG:HG2	2:H:71:THR:N	2.33	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: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: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:B:134:LYS:HD3	1:B:134:LYS:C	2.40	0.42
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: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
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
2:H:164:ALA:C	2:H:166:ASN:H	2.22	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:E:158:GLN:CD	2:E:224:CYS:SG	2.98	0.41
2:H:37:ARG:HB3	2:H:47:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:61:TRP:O	2:G:63:LYS:HG2	2.20	0.41
2:G:79:MET:CE	2:G:82:LEU:HD21	2.50	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
1:D:220:ALA:HB1	1:D:244:TYR:HB2	2.01	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: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
1:C:172:VAL:HG12	1:C:232:MET:CE	2.52	0.40
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	11 34
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%)	47 78

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 (i)

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%)	236 (98%)	4 (2%)	60 87
1	B	240/240 (100%)	231 (96%)	9 (4%)	33 67
1	C	238/240 (99%)	225 (94%)	13 (6%)	21 52
1	D	239/240 (100%)	232 (97%)	7 (3%)	42 76
2	E	173/194 (89%)	161 (93%)	12 (7%)	15 41
2	F	170/194 (88%)	161 (95%)	9 (5%)	22 54
2	G	172/194 (89%)	163 (95%)	9 (5%)	23 55
2	H	174/194 (90%)	164 (94%)	10 (6%)	20 50
All	All	1646/1736 (95%)	1573 (96%)	73 (4%)	29 61

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	ASP
1	B	63	GLU
1	B	98	GLU
1	B	103	LYS
1	B	105	LYS
1	B	141	LYS
1	B	160	LYS
1	B	199	GLU
1	B	217	LYS
1	D	15	MET
1	D	134	LYS
1	D	151	GLU
1	D	155	LYS
1	D	183	LYS
1	D	255	LYS
1	D	261	SER
2	G	49	LEU
2	G	70	ARG
2	G	100	PHE
2	G	157	CYS
2	G	159	SER
2	G	168[A]	PHE
2	G	168[C]	PHE
2	G	187	THR
2	G	224	CYS
1	A	93	ASP
1	A	105	LYS
1	A	183	LYS
1	A	226	SER
1	C	17	LYS
1	C	25	ASP
1	C	63	GLU
1	C	83	LYS
1	C	160	LYS
1	C	183	LYS
1	C	204	ASP
1	C	212	LYS
1	C	217	LYS
1	C	232	MET
1	C	254	LYS
1	C	255	LYS
1	C	263	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2	SER
2	E	24	SER
2	E	42	LYS
2	E	49	LEU
2	E	99	ASP
2	E	100	PHE
2	E	110	SER
2	E	141	THR
2	E	157	CYS
2	E	187	THR
2	E	199	LYS
2	E	201	SER
2	F	2	SER
2	F	42	LYS
2	F	49	LEU
2	F	110	SER
2	F	141	THR
2	F	168[A]	PHE
2	F	168[C]	PHE
2	F	188	SER
2	F	240	GLU
2	H	2	SER
2	H	49	LEU
2	H	51	ASP
2	H	73	THR
2	H	141	THR
2	H	192	SER
2	H	196	SER
2	H	199	LYS
2	H	216	SER
2	H	243	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	158	GLN
1	C	127	GLN
2	F	103	GLN
2	F	140	GLN
2	F	158	GLN
2	H	140	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

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, 95^{th} 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%)	-0.21	0 100 100	24, 39, 63, 92	0
1	B	279/279 (100%)	-0.21	1 (0%) 92 91	21, 35, 59, 71	0
1	C	279/279 (100%)	0.05	2 (0%) 87 84	34, 63, 90, 106	0
1	D	279/279 (100%)	-0.13	0 100 100	28, 45, 74, 86	0
2	E	215/253 (84%)	0.16	5 (2%) 60 51	32, 51, 73, 105	0
2	F	214/253 (84%)	0.36	6 (2%) 53 43	32, 56, 80, 104	0
2	G	215/253 (84%)	0.10	6 (2%) 53 43	24, 41, 70, 81	0
2	H	217/253 (85%)	0.06	9 (4%) 37 27	22, 40, 77, 101	0
All	All	1977/2128 (92%)	0.00	29 (1%) 73 68	21, 46, 77, 106	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	100	PHE	3.7
2	H	181	THR	3.5
2	F	26	PHE	3.3
2	F	187	THR	3.2
2	H	143	SER	3.0
1	C	197	THR	2.9
2	F	30	ARG	2.7
2	H	149	VAL	2.7
2	G	242	GLU	2.6
2	G	25	GLY	2.6
2	F	144	PRO	2.6
2	G	100	PHE	2.4
2	E	164	ALA	2.4
2	G	214	LEU	2.4
2	H	244	LEU	2.3
2	E	152	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	100	PHE	2.3
2	E	187	THR	2.3
2	H	242	GLU	2.2
2	H	241	LEU	2.2
2	G	26	PHE	2.1
2	F	241	LEU	2.1
2	H	187	THR	2.1
2	H	164	ALA	2.1
2	H	238	GLY	2.0
1	C	137	GLU	2.0
2	E	196	SER	2.0
1	B	213	LEU	2.0
2	G	110	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

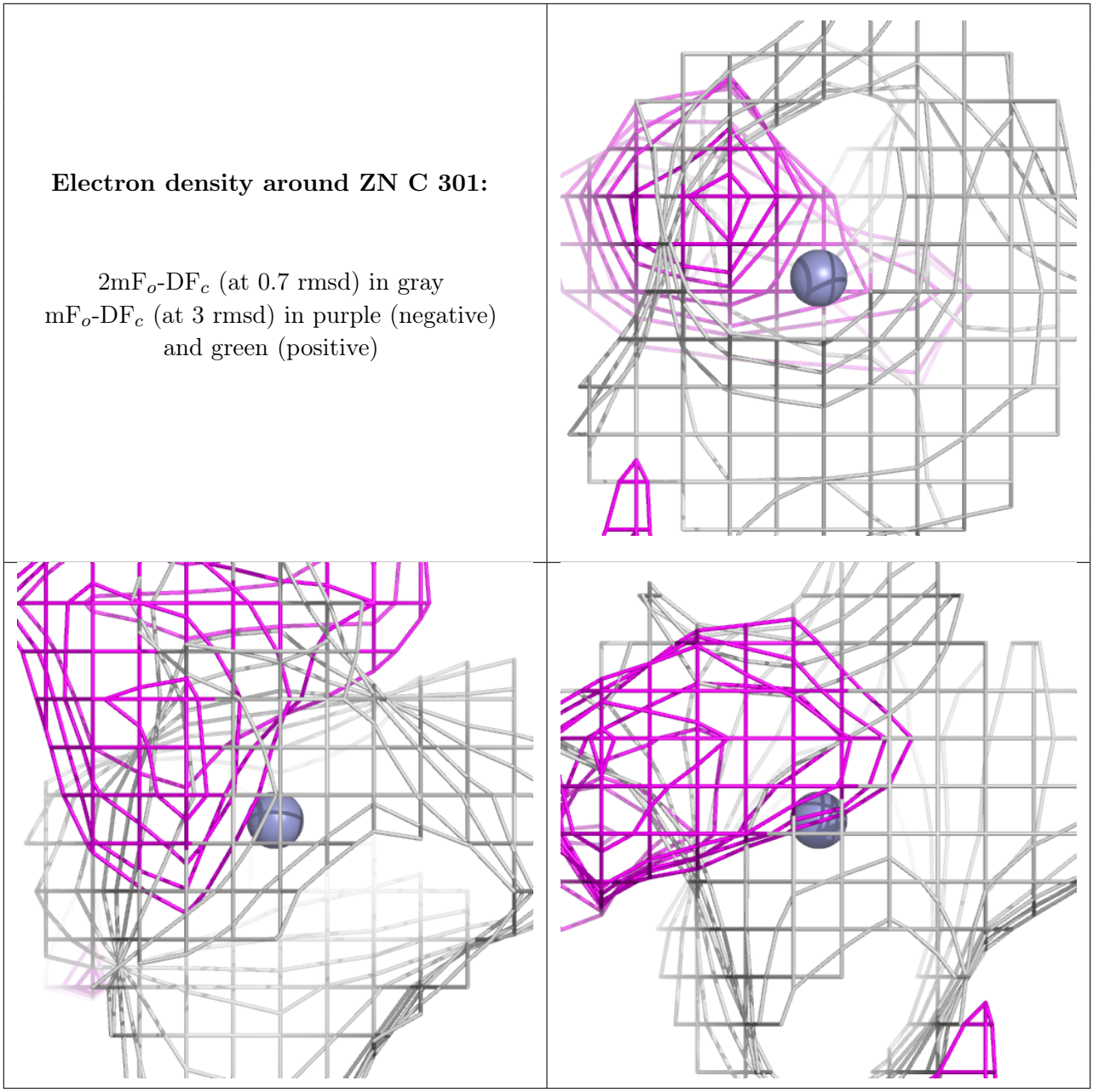
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	C	301	1/1	0.83	0.11	91,91,91,91	0
3	ZN	D	301	1/1	0.89	0.18	84,84,84,84	0
3	ZN	B	301	1/1	0.92	0.09	67,67,67,67	0
3	ZN	A	301	1/1	0.97	0.03	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.

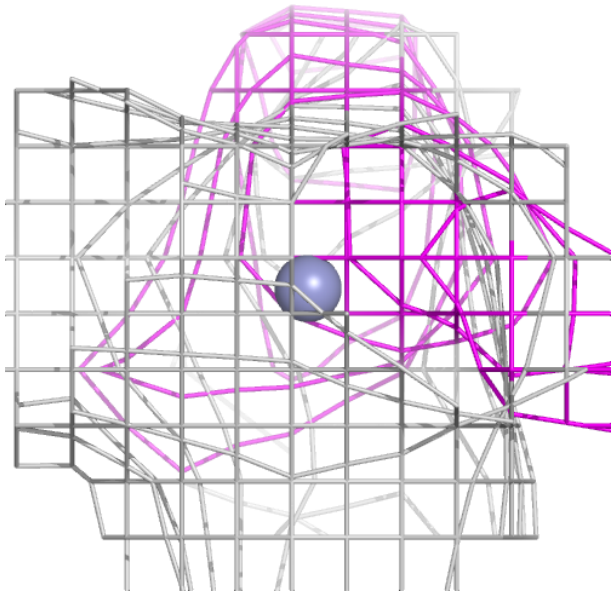
Electron density around ZN C 301:

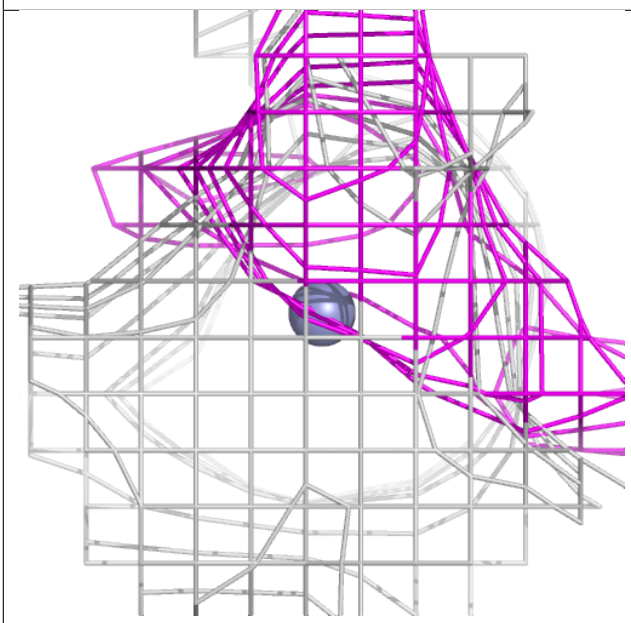
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

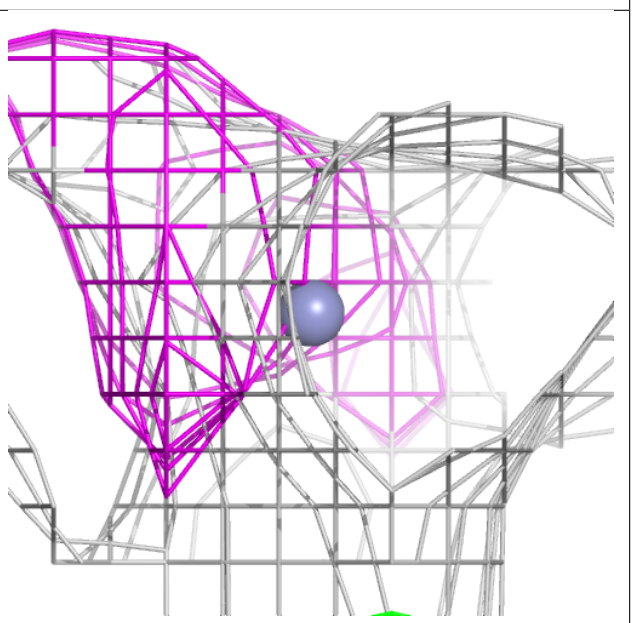


Electron density around ZN D 301:

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

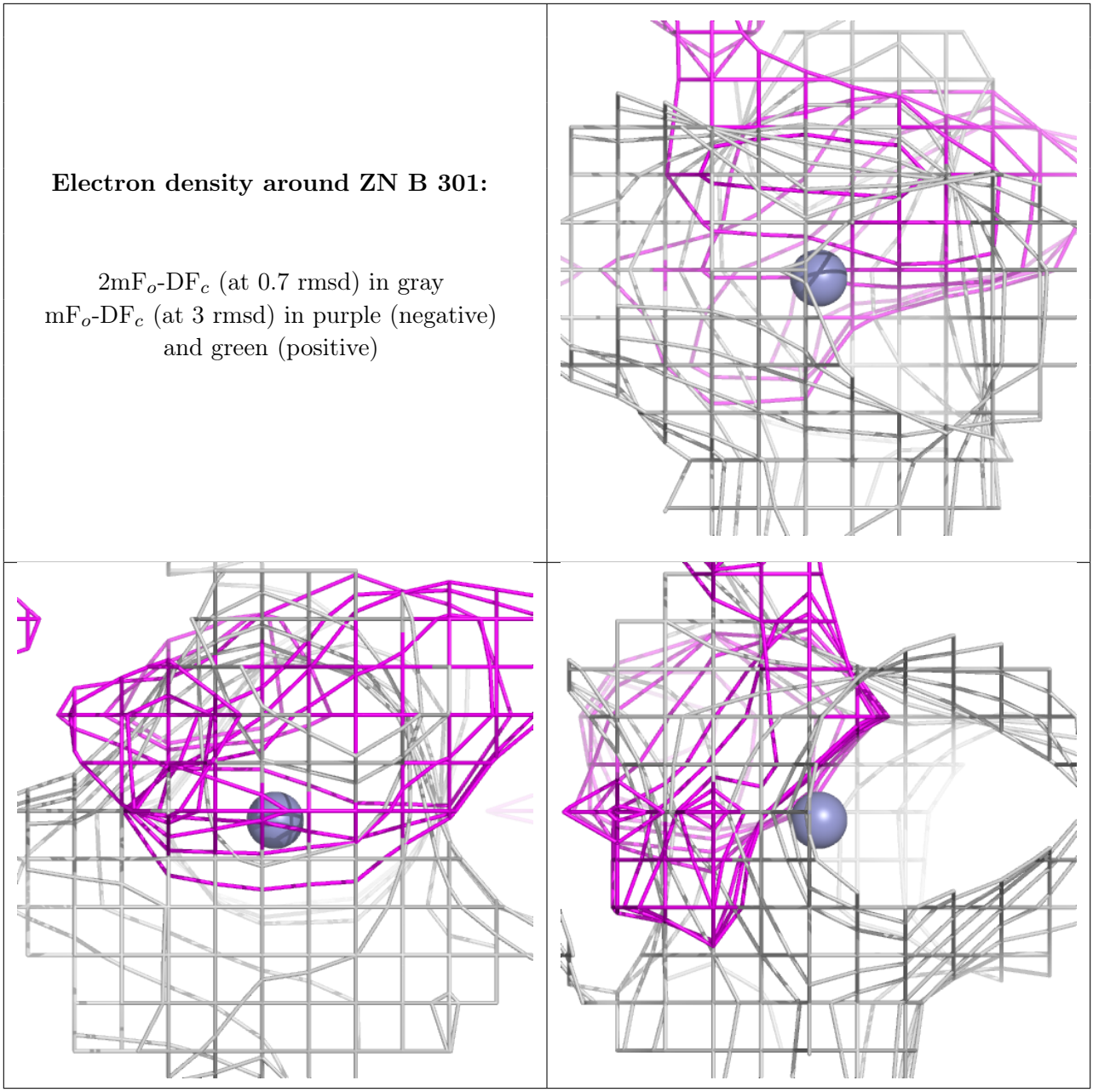






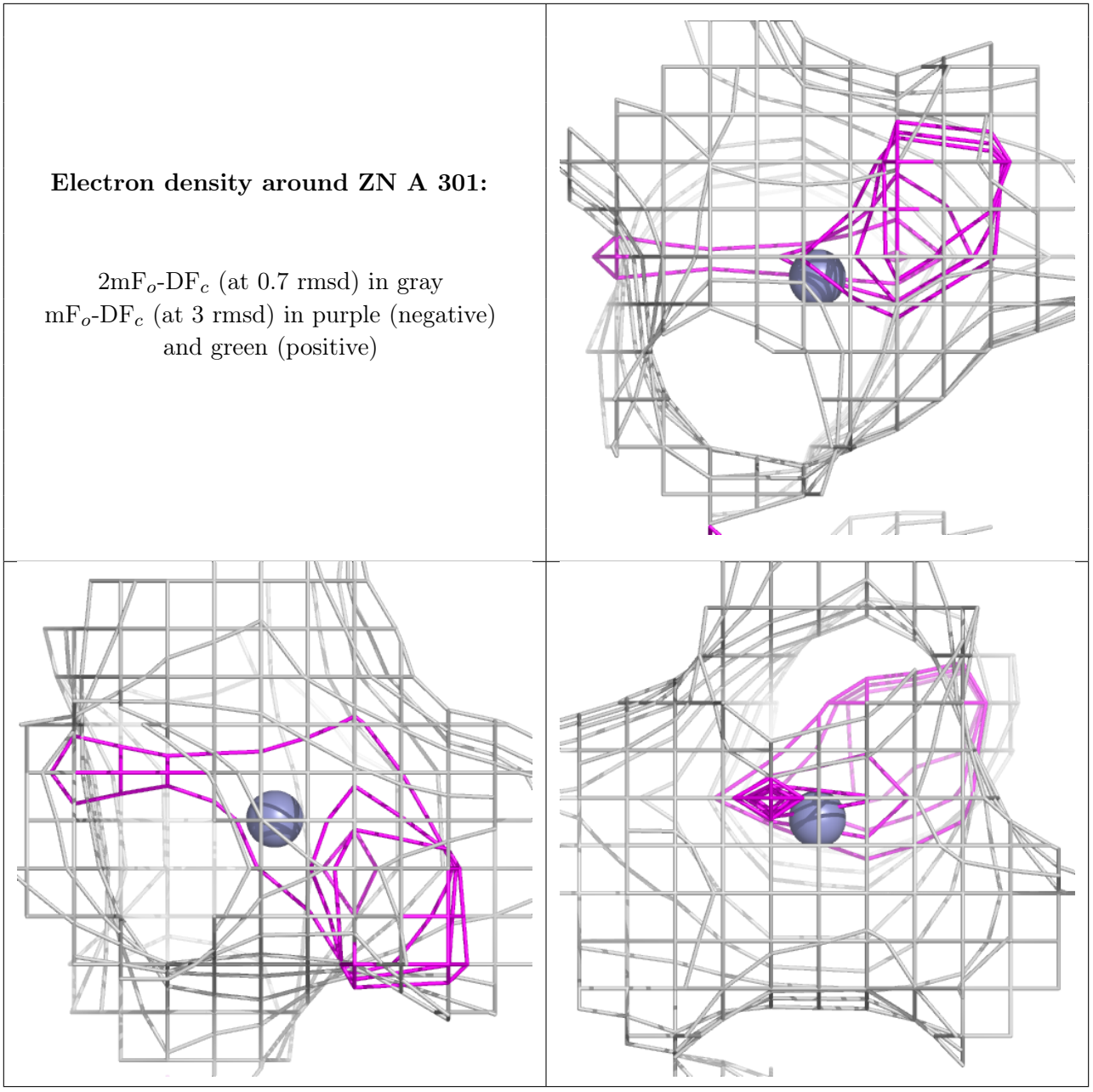
Electron density around ZN B 301:

$2mF_o$-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.