



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:54 AM UTC

PDB ID : 8VWL / pdb_00008vwl
Title : Crystal structure of Vibrio cholerae NFeoB in the apo form
Authors : Lee, M.; Smith, A.T.
Deposited on : 2024-02-01
Resolution : 3.67 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

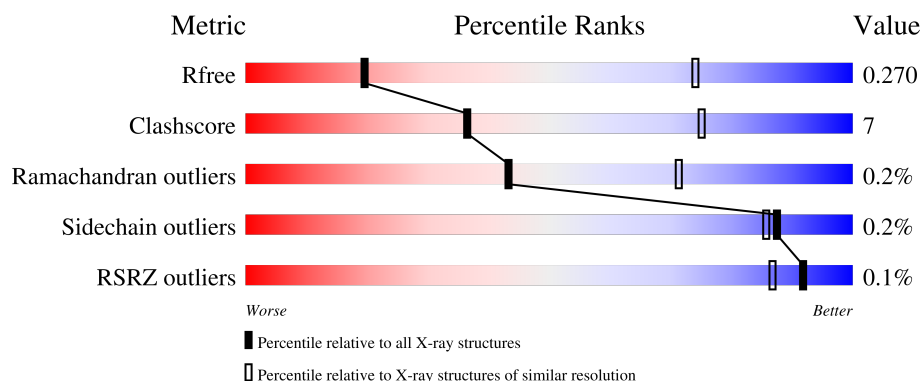
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.67 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	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	285	
1	B	285	
1	C	285	
1	D	285	
1	E	285	

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Mol	Chain	Length	Quality of chain
1	F	285	 73% 15% 12%
1	G	285	 73% 15% 12%
1	H	285	 63% 19% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15757 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 Ferrous iron transport protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2001	1255	360	377	9			
1	B	251	Total	C	N	O	S	0	0	0
			1983	1250	356	368	9			
1	C	255	Total	C	N	O	S	0	0	0
			2014	1265	363	377	9			
1	D	248	Total	C	N	O	S	0	0	0
			1962	1233	354	366	9			
1	E	247	Total	C	N	O	S	0	0	0
			1949	1223	351	367	8			
1	F	251	Total	C	N	O	S	0	0	0
			1993	1256	360	368	9			
1	G	251	Total	C	N	O	S	0	0	0
			1981	1243	357	373	8			
1	H	234	Total	C	N	O	S	0	0	0
			1868	1178	333	348	9			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	LYS	-	expression tag	UNP A0A655NVH2
A	274	LEU	-	expression tag	UNP A0A655NVH2
A	275	ALA	-	expression tag	UNP A0A655NVH2
A	276	ALA	-	expression tag	UNP A0A655NVH2
A	277	ALA	-	expression tag	UNP A0A655NVH2
A	278	LEU	-	expression tag	UNP A0A655NVH2
A	279	GLU	-	expression tag	UNP A0A655NVH2
A	280	HIS	-	expression tag	UNP A0A655NVH2
A	281	HIS	-	expression tag	UNP A0A655NVH2
A	282	HIS	-	expression tag	UNP A0A655NVH2
A	283	HIS	-	expression tag	UNP A0A655NVH2
A	284	HIS	-	expression tag	UNP A0A655NVH2
A	285	HIS	-	expression tag	UNP A0A655NVH2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	273	LYS	-	expression tag	UNP A0A655NVH2
B	274	LEU	-	expression tag	UNP A0A655NVH2
B	275	ALA	-	expression tag	UNP A0A655NVH2
B	276	ALA	-	expression tag	UNP A0A655NVH2
B	277	ALA	-	expression tag	UNP A0A655NVH2
B	278	LEU	-	expression tag	UNP A0A655NVH2
B	279	GLU	-	expression tag	UNP A0A655NVH2
B	280	HIS	-	expression tag	UNP A0A655NVH2
B	281	HIS	-	expression tag	UNP A0A655NVH2
B	282	HIS	-	expression tag	UNP A0A655NVH2
B	283	HIS	-	expression tag	UNP A0A655NVH2
B	284	HIS	-	expression tag	UNP A0A655NVH2
B	285	HIS	-	expression tag	UNP A0A655NVH2
C	273	LYS	-	expression tag	UNP A0A655NVH2
C	274	LEU	-	expression tag	UNP A0A655NVH2
C	275	ALA	-	expression tag	UNP A0A655NVH2
C	276	ALA	-	expression tag	UNP A0A655NVH2
C	277	ALA	-	expression tag	UNP A0A655NVH2
C	278	LEU	-	expression tag	UNP A0A655NVH2
C	279	GLU	-	expression tag	UNP A0A655NVH2
C	280	HIS	-	expression tag	UNP A0A655NVH2
C	281	HIS	-	expression tag	UNP A0A655NVH2
C	282	HIS	-	expression tag	UNP A0A655NVH2
C	283	HIS	-	expression tag	UNP A0A655NVH2
C	284	HIS	-	expression tag	UNP A0A655NVH2
C	285	HIS	-	expression tag	UNP A0A655NVH2
D	273	LYS	-	expression tag	UNP A0A655NVH2
D	274	LEU	-	expression tag	UNP A0A655NVH2
D	275	ALA	-	expression tag	UNP A0A655NVH2
D	276	ALA	-	expression tag	UNP A0A655NVH2
D	277	ALA	-	expression tag	UNP A0A655NVH2
D	278	LEU	-	expression tag	UNP A0A655NVH2
D	279	GLU	-	expression tag	UNP A0A655NVH2
D	280	HIS	-	expression tag	UNP A0A655NVH2
D	281	HIS	-	expression tag	UNP A0A655NVH2
D	282	HIS	-	expression tag	UNP A0A655NVH2
D	283	HIS	-	expression tag	UNP A0A655NVH2
D	284	HIS	-	expression tag	UNP A0A655NVH2
D	285	HIS	-	expression tag	UNP A0A655NVH2
E	273	LYS	-	expression tag	UNP A0A655NVH2
E	274	LEU	-	expression tag	UNP A0A655NVH2
E	275	ALA	-	expression tag	UNP A0A655NVH2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	276	ALA	-	expression tag	UNP A0A655NVH2
E	277	ALA	-	expression tag	UNP A0A655NVH2
E	278	LEU	-	expression tag	UNP A0A655NVH2
E	279	GLU	-	expression tag	UNP A0A655NVH2
E	280	HIS	-	expression tag	UNP A0A655NVH2
E	281	HIS	-	expression tag	UNP A0A655NVH2
E	282	HIS	-	expression tag	UNP A0A655NVH2
E	283	HIS	-	expression tag	UNP A0A655NVH2
E	284	HIS	-	expression tag	UNP A0A655NVH2
E	285	HIS	-	expression tag	UNP A0A655NVH2
F	273	LYS	-	expression tag	UNP A0A655NVH2
F	274	LEU	-	expression tag	UNP A0A655NVH2
F	275	ALA	-	expression tag	UNP A0A655NVH2
F	276	ALA	-	expression tag	UNP A0A655NVH2
F	277	ALA	-	expression tag	UNP A0A655NVH2
F	278	LEU	-	expression tag	UNP A0A655NVH2
F	279	GLU	-	expression tag	UNP A0A655NVH2
F	280	HIS	-	expression tag	UNP A0A655NVH2
F	281	HIS	-	expression tag	UNP A0A655NVH2
F	282	HIS	-	expression tag	UNP A0A655NVH2
F	283	HIS	-	expression tag	UNP A0A655NVH2
F	284	HIS	-	expression tag	UNP A0A655NVH2
F	285	HIS	-	expression tag	UNP A0A655NVH2
G	273	LYS	-	expression tag	UNP A0A655NVH2
G	274	LEU	-	expression tag	UNP A0A655NVH2
G	275	ALA	-	expression tag	UNP A0A655NVH2
G	276	ALA	-	expression tag	UNP A0A655NVH2
G	277	ALA	-	expression tag	UNP A0A655NVH2
G	278	LEU	-	expression tag	UNP A0A655NVH2
G	279	GLU	-	expression tag	UNP A0A655NVH2
G	280	HIS	-	expression tag	UNP A0A655NVH2
G	281	HIS	-	expression tag	UNP A0A655NVH2
G	282	HIS	-	expression tag	UNP A0A655NVH2
G	283	HIS	-	expression tag	UNP A0A655NVH2
G	284	HIS	-	expression tag	UNP A0A655NVH2
G	285	HIS	-	expression tag	UNP A0A655NVH2
H	273	LYS	-	expression tag	UNP A0A655NVH2
H	274	LEU	-	expression tag	UNP A0A655NVH2
H	275	ALA	-	expression tag	UNP A0A655NVH2
H	276	ALA	-	expression tag	UNP A0A655NVH2
H	277	ALA	-	expression tag	UNP A0A655NVH2
H	278	LEU	-	expression tag	UNP A0A655NVH2

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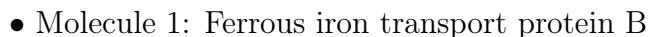
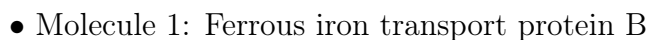
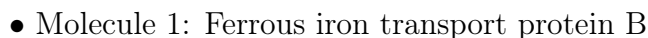
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Chain	Residue	Modelled	Actual	Comment	Reference
H	279	GLU	-	expression tag	UNP A0A655NVH2
H	280	HIS	-	expression tag	UNP A0A655NVH2
H	281	HIS	-	expression tag	UNP A0A655NVH2
H	282	HIS	-	expression tag	UNP A0A655NVH2
H	283	HIS	-	expression tag	UNP A0A655NVH2
H	284	HIS	-	expression tag	UNP A0A655NVH2
H	285	HIS	-	expression tag	UNP A0A655NVH2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	1	Total Mg 1 1	0	0
2	C	2	Total Mg 2 2	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 1: Ferrous iron transport protein B

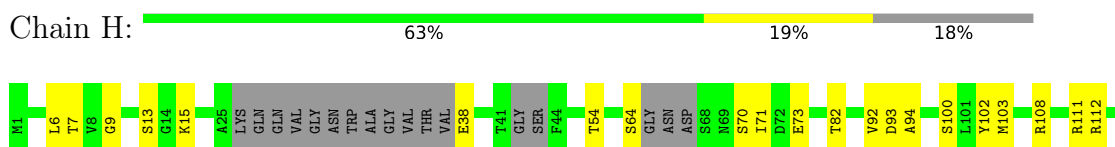


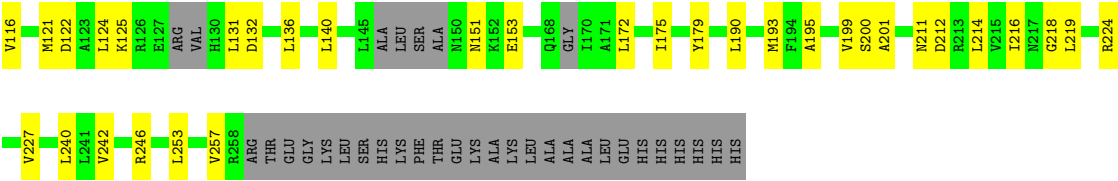
- Molecule 1: Ferrous iron transport protein B

- Molecule 1: Ferrous iron transport protein B

- Molecule 1: Ferrous iron transport protein B

- Molecule 1: Ferrous iron transport protein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.35Å 84.12Å 158.03Å 76.17° 83.91° 74.51°	Depositor
Resolution (Å)	77.57 – 3.67 77.57 – 3.67	Depositor EDS
% Data completeness (in resolution range)	94.9 (77.57-3.67) 95.1 (77.57-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.270 0.208 , 0.270	Depositor DCC
R_{free} test set	1204 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	131.2	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 117.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.067 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15757	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.15	0/2027	0.35	0/2737
1	B	0.20	0/2009	0.37	0/2712
1	C	0.14	0/2042	0.38	0/2759
1	D	0.13	0/1987	0.34	0/2681
1	E	0.16	0/1974	0.41	0/2666
1	F	0.16	0/2019	0.35	0/2720
1	G	0.13	0/2008	0.34	0/2714
1	H	0.13	0/1889	0.36	0/2542
All	All	0.15	0/15955	0.36	0/21531

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 [i](#)

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	2001	0	2039	30	0
1	B	1983	0	2024	25	0
1	C	2014	0	2049	34	0
1	D	1962	0	2006	28	0
1	E	1949	0	1977	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1993	0	2041	27	0
1	G	1981	0	2010	31	0
1	H	1868	0	1903	37	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	15757	0	16049	228	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 7.

All (228) 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:C:65:GLY:HA2	1:C:74:SER:HB2	1.58	0.83
1:A:35:VAL:HG11	1:A:75:ILE:HG13	1.63	0.80
1:E:180:GLY:O	1:E:184:GLU:HB2	1.85	0.75
1:D:153:GLU:HB3	1:D:157:ARG:HH21	1.54	0.72
1:C:238:ILE:H	1:C:238:ILE:HD12	1.55	0.72
1:C:64:SER:HA	1:C:214:LEU:HD22	1.72	0.71
1:E:122:ASP:OD2	1:E:126:ARG:NH2	2.22	0.71
1:H:7:THR:HG22	1:H:15:LYS:HG3	1.74	0.70
1:H:132:ASP:HB2	1:H:257:VAL:HA	1.75	0.68
1:E:130:HIS:H	1:E:259:ARG:HB2	1.59	0.68
1:A:59:ILE:HG22	1:A:73:GLU:HG3	1.77	0.66
1:G:9:GLY:HA2	1:G:103:MET:HE1	1.78	0.66
1:E:141:GLY:HA2	1:E:173:LYS:HE2	1.79	0.65
1:C:68:SER:HA	1:E:68:SER:HA	1.78	0.65
1:B:190:LEU:HD13	1:B:227:VAL:HG22	1.79	0.65
1:G:197:GLN:HG3	1:G:198:ALA:H	1.62	0.65
1:F:2:LYS:HA	1:F:50:GLU:HB2	1.79	0.64
1:E:112:ARG:HD2	1:E:199:VAL:HG12	1.79	0.64
1:B:78:ARG:HD3	1:G:75:ILE:HD11	1.80	0.64
1:F:240:LEU:HG	1:G:247:TYR:HB2	1.79	0.64
1:G:35:VAL:HG11	1:G:75:ILE:HG13	1.80	0.63
1:A:179:TYR:HA	1:A:245:VAL:HG11	1.79	0.63
1:G:35:VAL:HG23	1:G:39:LYS:HB2	1.81	0.63
1:E:194:PHE:HB3	1:E:204:LEU:HD12	1.81	0.62
1:D:134:LYS:H	1:D:134:LYS:HD2	1.64	0.62
1:B:74:SER:OG	1:B:78:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:HB2	1:C:57:PRO:HA	1.82	0.62
1:H:151:ASN:ND2	1:H:153:GLU:OE1	2.33	0.62
1:H:195:ALA:HA	1:H:201:ALA:HB2	1.85	0.59
1:B:140:LEU:HA	1:B:175:ILE:HD11	1.84	0.58
1:F:132:ASP:OD2	1:F:259:ARG:NH2	2.36	0.58
1:G:94:ALA:HB1	1:G:124:LEU:HD22	1.85	0.58
1:E:7:THR:HG22	1:E:15:LYS:HG3	1.85	0.57
1:D:80:VAL:O	1:D:112:ARG:NH1	2.38	0.57
1:F:92:VAL:HG13	1:F:100:SER:HB2	1.87	0.57
1:C:153:GLU:OE2	1:C:156:ARG:NE	2.36	0.57
1:D:140:LEU:HA	1:D:175:ILE:HD11	1.86	0.57
1:H:136:LEU:HD13	1:H:253:LEU:HD21	1.86	0.56
1:C:197:GLN:NE2	1:H:38:GLU:OE1	2.28	0.56
1:D:108:ARG:HD3	1:D:114:MET:HE2	1.88	0.56
1:B:45:VAL:HG11	1:C:167:VAL:HG21	1.88	0.56
1:E:94:ALA:HB1	1:E:124:LEU:HD22	1.87	0.56
1:H:94:ALA:HB1	1:H:124:LEU:HD22	1.86	0.56
1:G:164:LYS:HE2	1:G:168:GLN:HG3	1.86	0.56
1:A:62:LEU:HD12	1:A:106:GLN:HB3	1.88	0.55
1:F:98:GLU:HB3	1:G:235:GLN:O	2.06	0.55
1:F:179:TYR:HA	1:F:245:VAL:HG11	1.88	0.55
1:C:33:ALA:HB2	1:H:82:THR:HG21	1.88	0.55
1:G:67:ASP:HB2	1:G:70:SER:HB3	1.89	0.55
1:H:121:MET:O	1:H:125:LYS:HG3	2.07	0.55
1:D:6:LEU:HD23	1:D:54:THR:HB	1.88	0.54
1:D:96:CYS:SG	1:D:99:ARG:NH2	2.80	0.54
1:A:108:ARG:HB3	1:A:175:ILE:HD12	1.89	0.54
1:C:124:LEU:HG	1:C:129:VAL:HB	1.90	0.54
1:A:35:VAL:HG23	1:A:39:LYS:HB2	1.89	0.54
1:C:179:TYR:HA	1:C:245:VAL:HG11	1.89	0.53
1:B:32:TRP:HB3	1:G:193:MET:O	2.07	0.53
1:C:7:THR:HG23	1:C:55:ASP:HA	1.90	0.53
1:G:59:ILE:HG13	1:G:103:MET:SD	2.49	0.53
1:D:95:THR:HA	1:D:124:LEU:HD13	1.91	0.53
1:H:211:ASN:HA	1:H:216:ILE:HD11	1.91	0.53
1:C:34:GLY:HA2	1:H:218:GLY:N	2.24	0.53
1:F:254:CYS:O	1:F:258:ARG:HB2	2.09	0.53
1:G:65:GLY:HA2	1:G:74:SER:OG	2.09	0.52
1:G:148:SER:HB3	1:G:150:ASN:HD21	1.74	0.52
1:A:47:ALA:HB3	1:A:163:HIS:CE1	2.45	0.52
1:F:94:ALA:HB1	1:F:124:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:ASN:HB3	1:G:154:GLN:HG3	1.90	0.52
1:G:148:SER:HB3	1:G:150:ASN:ND2	2.24	0.52
1:A:118:LEU:HD12	1:A:133:LEU:HD22	1.91	0.52
1:A:111:ARG:HB2	1:A:200:SER:HB2	1.93	0.51
1:H:111:ARG:HH12	1:H:172:LEU:HB3	1.74	0.51
1:D:92:VAL:HG13	1:D:100:SER:HB2	1.93	0.51
1:G:213:ARG:HA	1:G:216:ILE:HB	1.93	0.51
1:C:158:PHE:HA	1:C:161:LYS:HD2	1.93	0.51
1:D:122:ASP:OD1	1:D:122:ASP:N	2.42	0.50
1:G:84:PRO:HA	1:G:112:ARG:HH22	1.76	0.50
1:A:108:ARG:HD3	1:A:142:CYS:HB3	1.93	0.50
1:E:103:MET:HE3	1:E:107:LEU:HD11	1.93	0.50
1:E:62:LEU:HB2	1:E:207:ARG:NH2	2.26	0.50
1:E:62:LEU:HD12	1:E:63:ASP:H	1.76	0.50
1:F:59:ILE:HG13	1:F:103:MET:HE1	1.94	0.50
1:F:140:LEU:HA	1:F:175:ILE:HD11	1.92	0.50
1:E:197:GLN:HG3	1:E:198:ALA:H	1.77	0.49
1:H:116:VAL:HG21	1:H:140:LEU:HD13	1.93	0.49
1:B:136:LEU:HD23	1:B:144:VAL:HG11	1.94	0.49
1:D:78:ARG:HH22	1:E:74:SER:HB3	1.76	0.49
1:H:9:GLY:HA2	1:H:103:MET:HE1	1.94	0.49
1:C:39:LYS:O	1:C:39:LYS:HG3	2.13	0.49
1:A:109:GLU:OE2	1:A:179:TYR:OH	2.28	0.49
1:H:70:SER:O	1:H:73:GLU:N	2.43	0.49
1:E:96:CYS:SG	1:E:99:ARG:NH2	2.86	0.48
1:A:194:PHE:HB3	1:A:204:LEU:HD12	1.95	0.48
1:G:103:MET:HE2	1:G:103:MET:HB3	1.68	0.48
1:C:15:LYS:HA	1:C:91:VAL:HG21	1.95	0.48
1:E:247:TYR:HB2	1:H:240:LEU:HG	1.94	0.48
1:C:122:ASP:OD1	1:C:122:ASP:N	2.46	0.48
1:G:32:TRP:CG	1:G:39:LYS:HG2	2.48	0.48
1:F:95:THR:HA	1:F:124:LEU:HD13	1.94	0.48
1:D:71:ILE:HD13	1:E:217:ASN:HB3	1.96	0.48
1:B:113:PRO:HA	1:B:172:LEU:HD11	1.96	0.47
1:C:69:ASN:CG	1:C:70:SER:H	2.22	0.47
1:A:38:GLU:CB	1:A:57:PRO:HA	2.45	0.47
1:H:122:ASP:HA	1:H:125:LYS:HE2	1.96	0.47
1:A:8:VAL:HG21	1:A:103:MET:HE1	1.96	0.47
1:D:59:ILE:HD11	1:D:103:MET:HE1	1.96	0.47
1:G:152:LYS:HA	1:G:155:VAL:HB	1.95	0.47
1:C:94:ALA:HB1	1:C:124:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:HIS:HB3	1:D:51:PHE:HE2	1.79	0.47
1:B:87:VAL:HG11	1:B:166:LEU:HD11	1.95	0.47
1:A:183:PHE:CD2	1:A:187:ILE:HD11	2.50	0.47
1:A:217:ASN:ND2	1:F:71:ILE:HG12	2.30	0.47
1:C:217:ASN:ND2	1:H:71:ILE:HB	2.29	0.47
1:E:17:THR:HB	1:E:149:ALA:HB1	1.96	0.47
1:E:111:ARG:HB2	1:E:200:SER:HB2	1.97	0.47
1:G:78:ARG:O	1:G:82:THR:HG22	2.15	0.47
1:D:85:ALA:H	1:D:112:ARG:HH21	1.62	0.47
1:D:85:ALA:N	1:D:112:ARG:HH21	2.13	0.47
1:D:15:LYS:HB3	1:D:15:LYS:HE3	1.55	0.46
1:F:76:ALA:O	1:F:80:VAL:HG23	2.14	0.46
1:A:112:ARG:HD2	1:A:199:VAL:HG12	1.97	0.46
1:E:62:LEU:HD12	1:E:63:ASP:N	2.30	0.46
1:A:241:LEU:O	1:A:245:VAL:HG23	2.15	0.46
1:F:141:GLY:HA3	1:F:173:LYS:O	2.16	0.46
1:G:122:ASP:OD2	1:G:126:ARG:NH2	2.48	0.46
1:H:92:VAL:HG13	1:H:100:SER:HB3	1.97	0.46
1:B:51:PHE:HZ	1:B:163:HIS:HD1	1.64	0.46
1:F:23:THR:O	1:F:26:LYS:HG2	2.15	0.46
1:H:9:GLY:CA	1:H:103:MET:HE1	2.45	0.46
1:A:76:ALA:O	1:A:80:VAL:HG23	2.16	0.46
1:A:71:ILE:HG23	1:F:78:ARG:HH12	1.80	0.46
1:A:57:PRO:HD2	1:A:76:ALA:HB2	1.99	0.45
1:A:98:GLU:HB3	1:B:235:GLN:O	2.16	0.45
1:C:5:VAL:HG13	1:C:87:VAL:HG13	1.98	0.45
1:E:251:HIS:O	1:E:255:THR:HG23	2.16	0.45
1:H:190:LEU:HD13	1:H:227:VAL:HG22	1.98	0.45
1:G:87:VAL:HA	1:G:113:PRO:HB2	1.98	0.45
1:H:193:MET:HE3	1:H:219:LEU:HD22	1.97	0.45
1:D:109:GLU:O	1:D:203:ALA:HB2	2.17	0.45
1:E:213:ARG:O	1:E:217:ASN:ND2	2.49	0.45
1:A:235:GLN:O	1:B:98:GLU:HB3	2.16	0.45
1:H:121:MET:HG3	1:H:125:LYS:HZ3	1.82	0.45
1:B:263:LYS:HD3	1:B:263:LYS:HA	1.76	0.45
1:E:141:GLY:HA3	1:E:173:LYS:O	2.16	0.45
1:B:109:GLU:O	1:B:203:ALA:HB2	2.17	0.44
1:C:87:VAL:HA	1:C:113:PRO:HB2	1.99	0.44
1:C:96:CYS:SG	1:C:99:ARG:NH1	2.90	0.44
1:E:190:LEU:HD13	1:E:227:VAL:HG22	1.99	0.44
1:A:15:LYS:NZ	1:A:55:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASN:HB2	1:E:66:ASN:ND2	2.33	0.44
1:H:121:MET:SD	1:H:131:LEU:HD12	2.57	0.44
1:C:131:LEU:HD23	1:C:131:LEU:HA	1.82	0.44
1:E:8:VAL:C	1:E:15:LYS:HD3	2.43	0.44
1:A:38:GLU:HB2	1:A:57:PRO:HA	1.99	0.43
1:C:236:VAL:HG12	1:D:98:GLU:HG2	1.99	0.43
1:D:111:ARG:HB2	1:D:200:SER:HB2	2.00	0.43
1:E:78:ARG:O	1:E:82:THR:HG22	2.17	0.43
1:E:92:VAL:HG13	1:E:100:SER:HB2	2.00	0.43
1:H:64:SER:HB2	1:H:214:LEU:HD13	2.01	0.43
1:D:256:HIS:O	1:D:259:ARG:NH2	2.40	0.43
1:G:15:LYS:HA	1:G:91:VAL:HG21	2.00	0.43
1:D:121:MET:HE2	1:D:121:MET:HB3	1.89	0.43
1:H:131:LEU:HD23	1:H:131:LEU:HA	1.82	0.43
1:B:226:ASN:O	1:B:230:ARG:HG2	2.18	0.43
1:E:179:TYR:HA	1:E:245:VAL:HG21	2.01	0.43
1:B:56:LEU:HD13	1:B:76:ALA:HA	2.00	0.43
1:H:124:LEU:HD12	1:H:124:LEU:HA	1.80	0.43
1:B:69:ASN:HB3	1:B:70:SER:H	1.63	0.43
1:C:35:VAL:HG11	1:C:75:ILE:HD12	2.01	0.43
1:G:85:ALA:H	1:G:112:ARG:NH2	2.16	0.43
1:H:212:ASP:O	1:H:216:ILE:HG13	2.18	0.43
1:H:219:LEU:HB2	1:H:224:ARG:HG3	2.00	0.43
1:F:60:TYR:HE1	1:F:99:ARG:HH11	1.66	0.42
1:G:65:GLY:HA3	1:G:78:ARG:HH21	1.83	0.42
1:F:15:LYS:HB3	1:F:15:LYS:HE3	1.53	0.42
1:H:102:TYR:HE1	1:H:246:ARG:HD3	1.83	0.42
1:H:112:ARG:HD2	1:H:199:VAL:HG12	2.01	0.42
1:A:35:VAL:O	1:A:37:VAL:N	2.53	0.42
1:D:132:ASP:HB2	1:D:259:ARG:CZ	2.49	0.42
1:A:247:TYR:HB2	1:B:240:LEU:HG	2.01	0.42
1:C:111:ARG:HB2	1:C:200:SER:HB2	2.01	0.42
1:C:121:MET:SD	1:C:124:LEU:HD22	2.60	0.42
1:F:194:PHE:HB3	1:F:204:LEU:HD12	2.01	0.42
1:B:33:ALA:HA	1:G:197:GLN:HE22	1.85	0.42
1:F:131:LEU:HD23	1:F:131:LEU:HA	1.89	0.42
1:C:33:ALA:HB2	1:H:82:THR:CG2	2.48	0.42
1:B:84:PRO:HA	1:B:112:ARG:HH22	1.84	0.42
1:D:74:SER:O	1:D:78:ARG:HD2	2.20	0.42
1:F:220:LYS:HE3	1:F:223:GLU:OE2	2.19	0.42
1:F:187:ILE:O	1:F:191:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASP:HB2	1:B:163:HIS:HE1	1.85	0.41
1:F:81:LEU:HD23	1:F:81:LEU:HA	1.91	0.41
1:C:47:ALA:HB3	1:C:163:HIS:CD2	2.55	0.41
1:D:221:GLU:O	1:D:225:GLN:HG2	2.20	0.41
1:F:253:LEU:O	1:F:257:VAL:HG22	2.21	0.41
1:G:154:GLN:HA	1:G:157:ARG:HD2	2.01	0.41
1:A:68:SER:C	1:A:70:SER:H	2.28	0.41
1:B:74:SER:O	1:B:78:ARG:HB2	2.20	0.41
1:F:2:LYS:HE2	1:F:2:LYS:HB3	1.68	0.41
1:C:78:ARG:HG2	1:C:214:LEU:HD11	2.02	0.41
1:C:107:LEU:HB3	1:C:114:MET:SD	2.60	0.41
1:F:179:TYR:HE2	1:F:242:VAL:HG13	1.86	0.41
1:H:111:ARG:HB2	1:H:200:SER:HB2	2.03	0.41
1:C:183:PHE:CE1	1:C:238:ILE:HG23	2.56	0.41
1:E:88:ILE:HD11	1:E:112:ARG:HE	1.86	0.41
1:E:183:PHE:HE1	1:E:238:ILE:HG12	1.85	0.41
1:E:197:GLN:HG3	1:E:199:VAL:H	1.86	0.41
1:E:197:GLN:CG	1:E:198:ALA:H	2.33	0.41
1:F:111:ARG:NE	1:F:174:GLN:HE21	2.18	0.41
1:B:2:LYS:HE3	1:B:2:LYS:HB3	1.92	0.40
1:D:123:ALA:O	1:D:127:GLU:HG2	2.20	0.40
1:E:13:SER:O	1:E:119:ASN:ND2	2.43	0.40
1:A:6:LEU:HD23	1:A:54:THR:HB	2.03	0.40
1:B:124:LEU:HD21	1:B:131:LEU:HG	2.04	0.40
1:E:164:LYS:NZ	1:E:168:GLN:OE1	2.53	0.40
1:B:213:ARG:HA	1:B:213:ARG:HD2	1.75	0.40
1:D:139:PHE:O	1:D:175:ILE:HG12	2.21	0.40
1:E:136:LEU:HD12	1:E:136:LEU:HA	1.93	0.40
1:G:216:ILE:HG23	1:G:224:ARG:HG2	2.03	0.40
1:H:13:SER:HA	1:H:93:ASP:HB2	2.03	0.40
1:A:135:GLN:HB3	1:A:257:VAL:HG12	2.02	0.40
1:C:22:LEU:HD23	1:C:159:LYS:HE2	2.03	0.40
1:E:134:LYS:H	1:E:134:LYS:HG2	1.56	0.40
1:E:212:ASP:O	1:E:216:ILE:HG12	2.21	0.40
1:G:189:GLU:HB3	1:G:230:ARG:HH21	1.87	0.40
1:H:179:TYR:HE2	1:H:242:VAL:HG13	1.87	0.40
1:H:6:LEU:HD23	1:H:54:THR:HB	2.02	0.40
1:H:108:ARG:HD2	1:H:108:ARG:HA	1.99	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	250/285 (88%)	239 (96%)	11 (4%)	0	100	100
1	B	243/285 (85%)	234 (96%)	8 (3%)	1 (0%)	30	60
1	C	251/285 (88%)	237 (94%)	14 (6%)	0	100	100
1	D	242/285 (85%)	231 (96%)	10 (4%)	1 (0%)	30	60
1	E	241/285 (85%)	225 (93%)	16 (7%)	0	100	100
1	F	243/285 (85%)	232 (96%)	11 (4%)	0	100	100
1	G	247/285 (87%)	236 (96%)	10 (4%)	1 (0%)	30	60
1	H	220/285 (77%)	210 (96%)	9 (4%)	1 (0%)	24	56
All	All	1937/2280 (85%)	1844 (95%)	89 (5%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	37	VAL
1	H	175	ILE
1	G	68	SER
1	B	70	SER

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	219/244 (90%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/244 (88%)	215 (100%)	1 (0%)	81	80
1	C	220/244 (90%)	220 (100%)	0	100	100
1	D	215/244 (88%)	215 (100%)	0	100	100
1	E	214/244 (88%)	213 (100%)	1 (0%)	81	80
1	F	217/244 (89%)	216 (100%)	1 (0%)	81	80
1	G	217/244 (89%)	217 (100%)	0	100	100
1	H	206/244 (84%)	206 (100%)	0	100	100
All	All	1724/1952 (88%)	1721 (100%)	3 (0%)	87	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ILE
1	E	184	GLU
1	F	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	130	HIS
1	A	244	ASN
1	B	4	GLN
1	B	12	ASN
1	B	46	HIS
1	B	168	GLN
1	B	231	GLN
1	C	31	ASN
1	C	46	HIS
1	C	90	ASN
1	C	106	GLN
1	C	135	GLN
1	C	217	ASN
1	C	244	ASN
1	D	66	ASN
1	D	151	ASN
1	D	174	GLN
1	D	217	ASN

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Mol	Chain	Res	Type
1	D	231	GLN
1	D	232	HIS
1	E	66	ASN
1	E	154	GLN
1	E	226	ASN
1	E	232	HIS
1	E	244	ASN
1	F	4	GLN
1	F	10	ASN
1	F	46	HIS
1	F	163	HIS
1	F	174	GLN
1	F	244	ASN
1	G	4	GLN
1	G	130	HIS
1	G	150	ASN
1	G	168	GLN
1	G	178	HIS
1	H	90	ASN
1	H	235	GLN
1	H	244	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	254/285 (89%)	-0.74	0	100	100	87, 130, 179, 270	0
1	B	251/285 (88%)	-0.69	0	100	100	94, 131, 185, 306	0
1	C	255/285 (89%)	-0.69	1 (0%)	88	72	86, 131, 176, 233	0
1	D	248/285 (87%)	-0.71	0	100	100	101, 139, 197, 240	0
1	E	247/285 (86%)	-0.65	0	100	100	109, 159, 206, 270	0
1	F	251/285 (88%)	-0.66	0	100	100	105, 148, 205, 264	0
1	G	251/285 (88%)	-0.67	0	100	100	109, 150, 201, 236	0
1	H	234/285 (82%)	-0.64	0	100	100	110, 161, 211, 265	0
All	All	1991/2280 (87%)	-0.68	1 (0%)	92	87	86, 143, 200, 306	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	ALA	2.3

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,

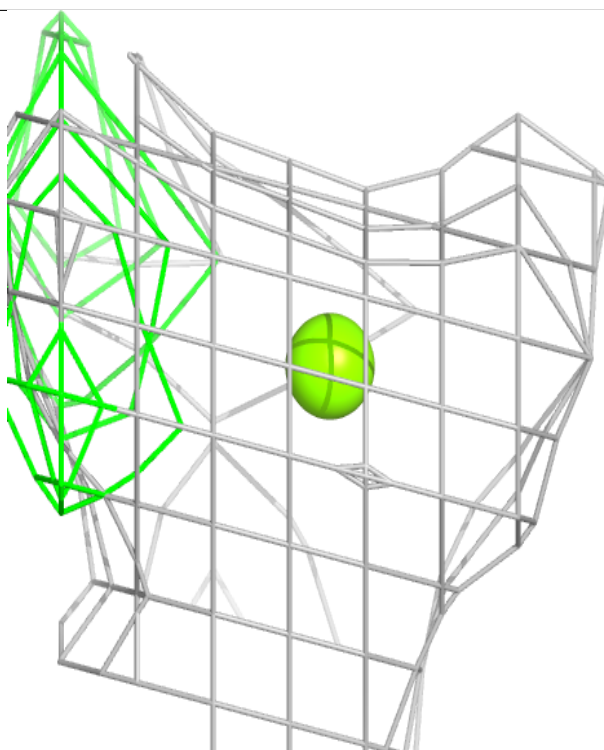
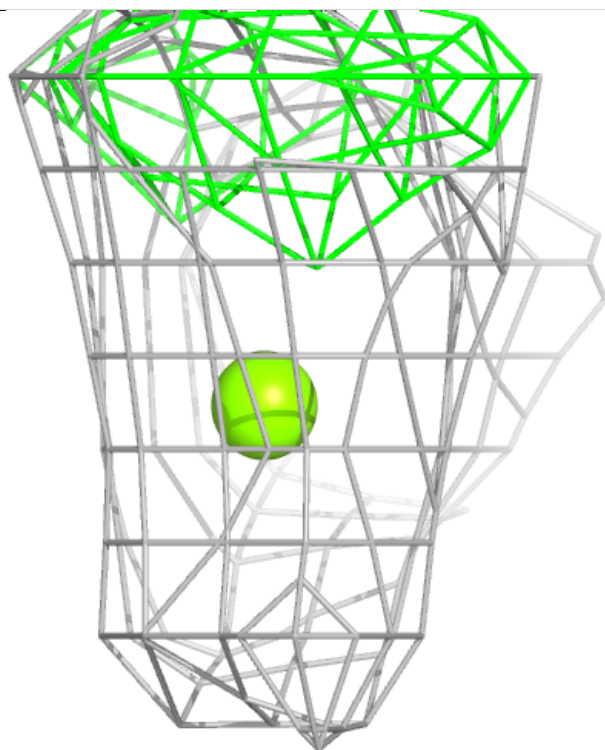
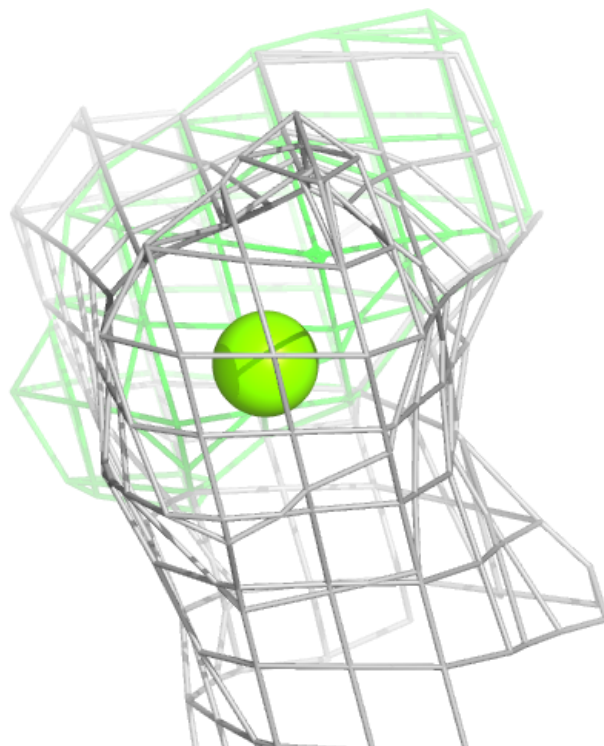
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	C	301	1/1	0.13	0.16	141,141,141,141	0
2	MG	A	302	1/1	0.66	0.07	118,118,118,118	0
2	MG	A	301	1/1	0.81	0.12	137,137,137,137	0
2	MG	B	301	1/1	0.84	0.09	111,111,111,111	0
2	MG	C	302	1/1	0.86	0.10	110,110,110,110	0
2	MG	D	301	1/1	0.88	0.05	135,135,135,135	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.

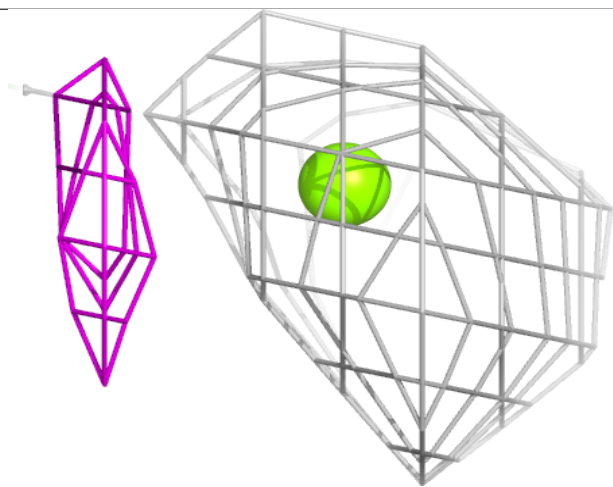
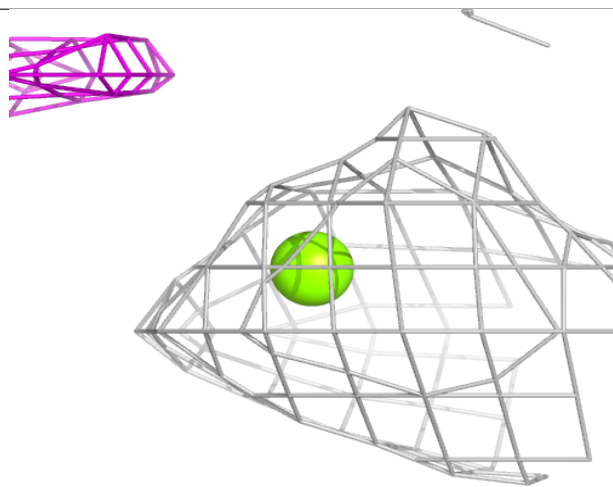
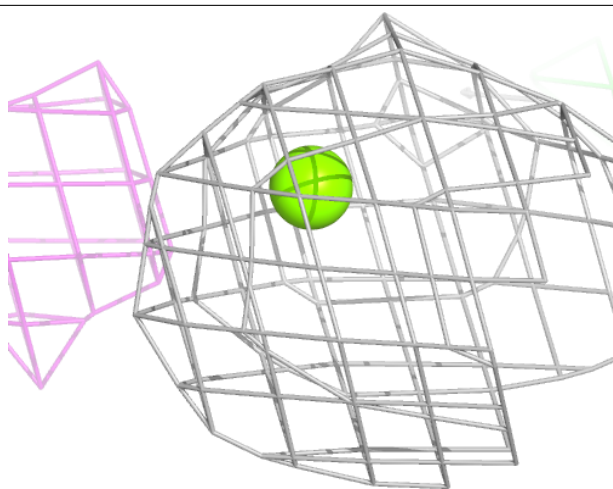
Electron density around MG C 301:

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



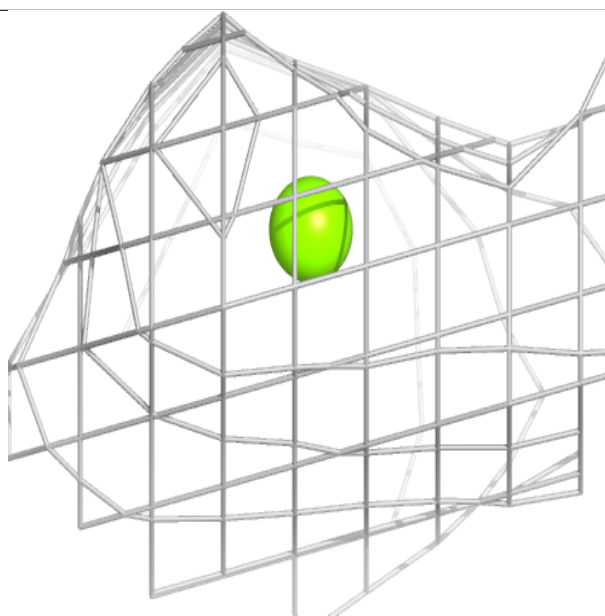
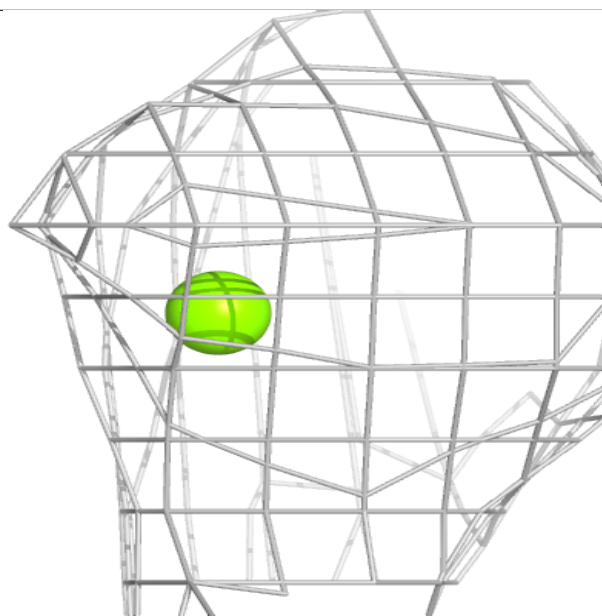
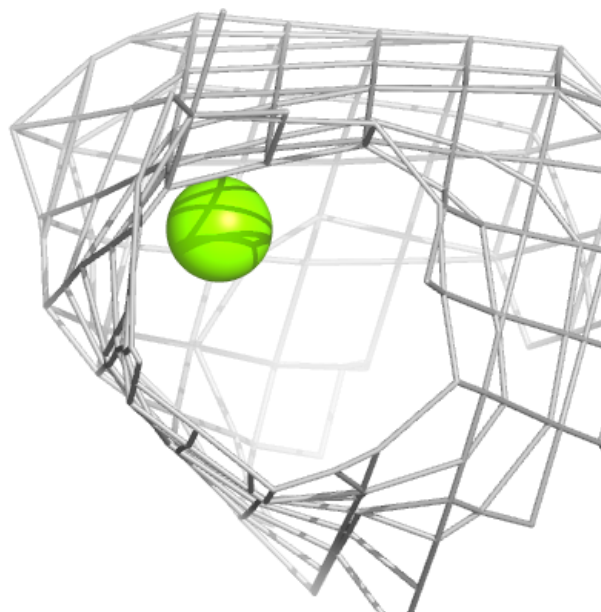
Electron density around MG A 302:

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



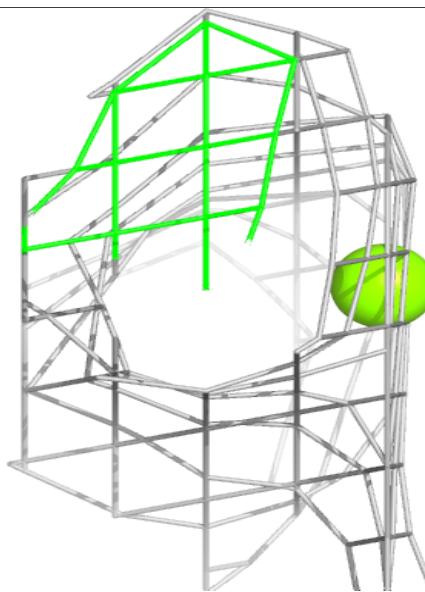
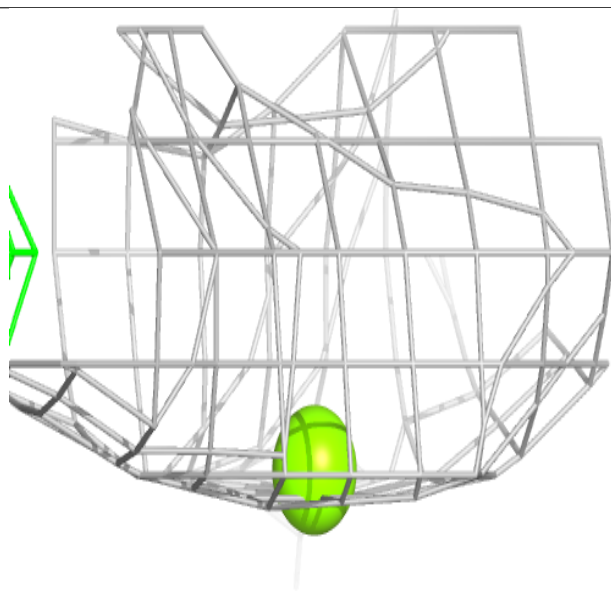
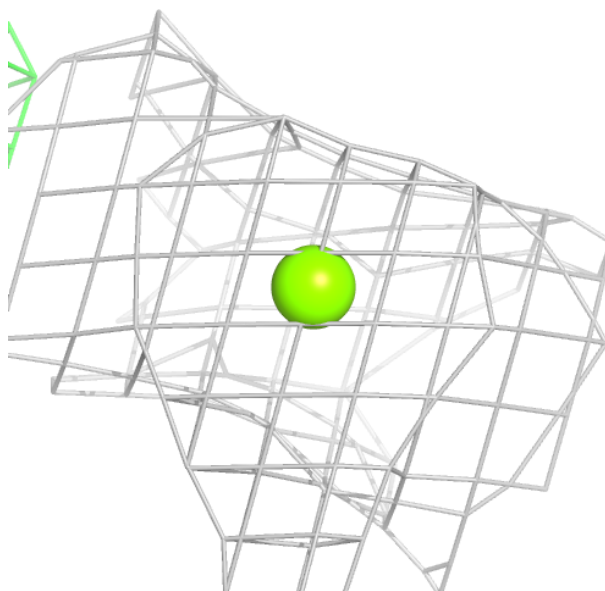
Electron density around MG A 301:

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



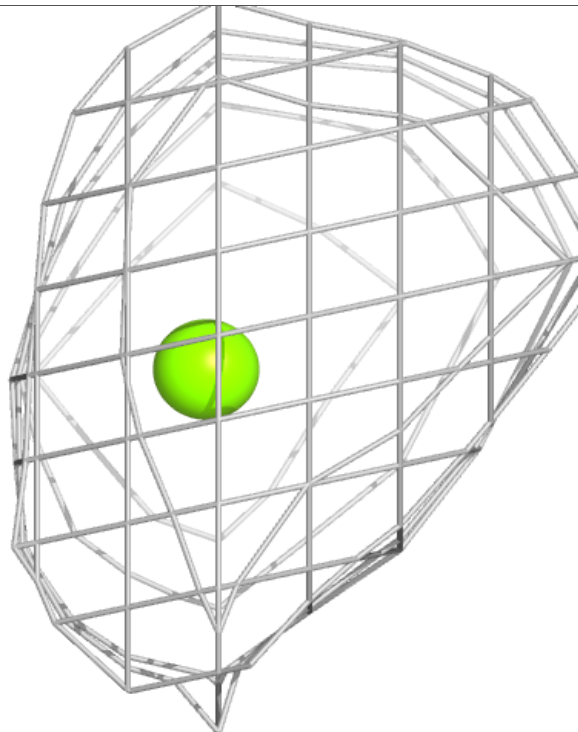
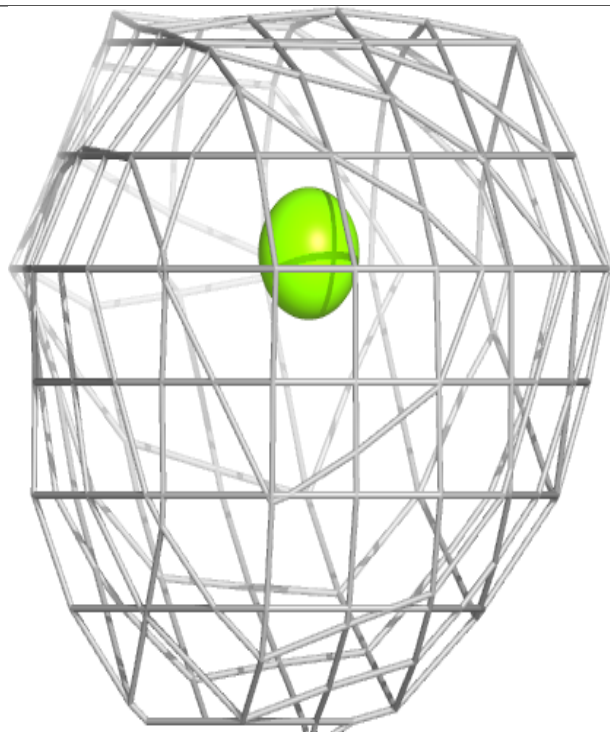
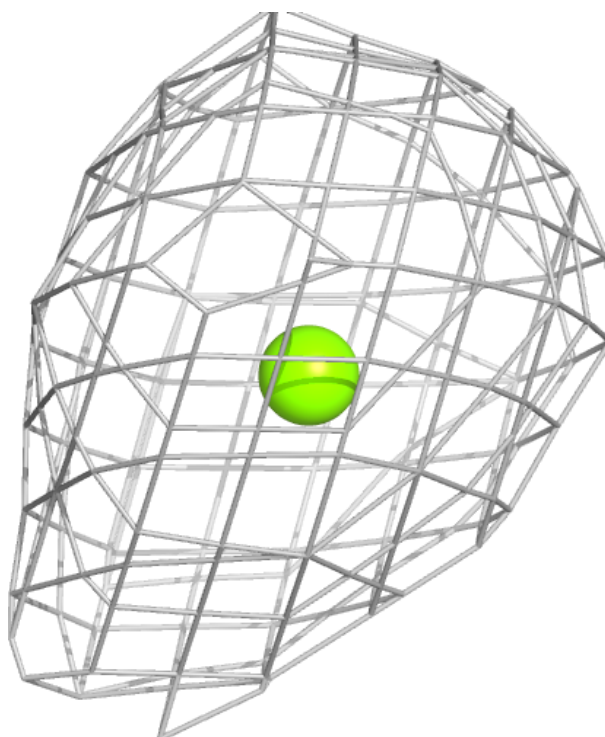
Electron density around MG B 301:

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



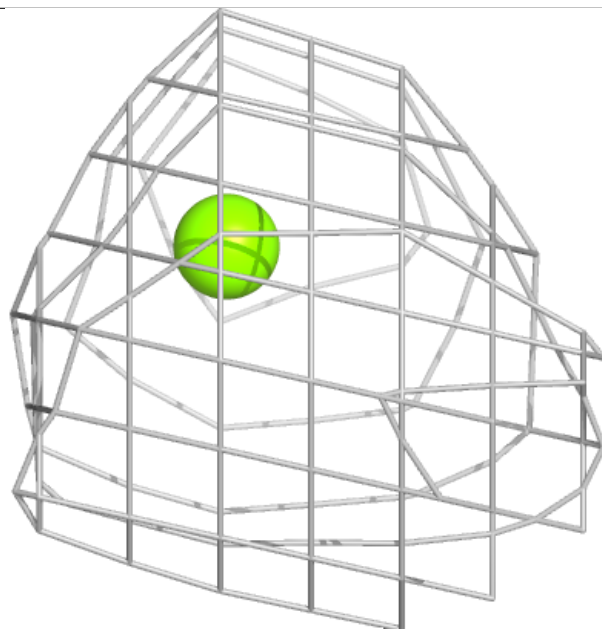
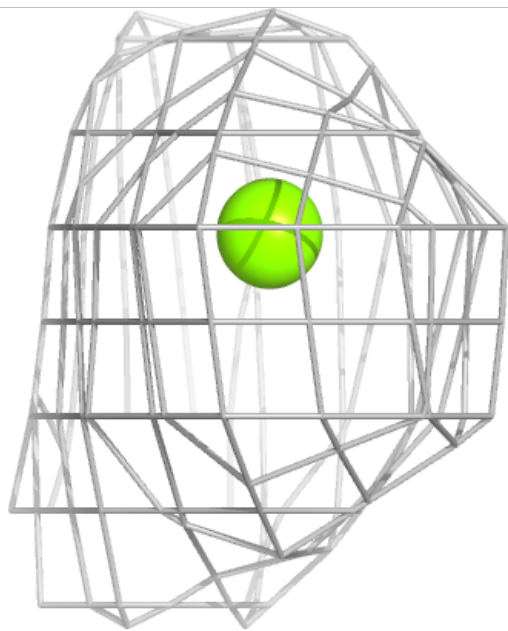
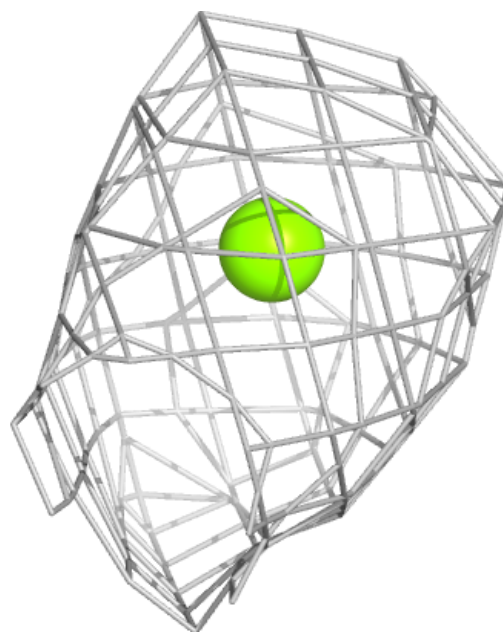
Electron density around MG C 302:

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



Electron density around MG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.