



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:17 PM UTC

PDB ID : 8ZYB / pdb_00008zyb
Title : a-KG dependent oxygenase
Authors : Fan, A.; Fan, S.; Wu, M.; Sun, Z.
Deposited on : 2024-06-17
Resolution : 2.58 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:

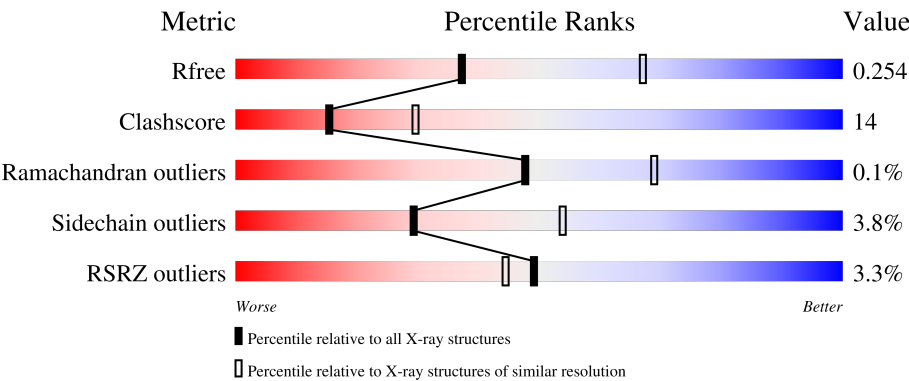
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	282	% 70% 24% ..
1	B	282	2% 71% 22% 5%
1	C	282	4% 71% 24% ..
1	D	282	% 64% 29% 5%
1	E	282	2% 75% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	282	3% 72% 25% ..
1	G	282	5% 67% 27% • •
1	H	282	6% 64% 27% • 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17100 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 DhiD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	276	Total	C	N	O	S	0	0	0
			2159	1367	379	404	9			
1	A	270	Total	C	N	O	S	0	0	0
			2106	1333	372	392	9			
1	B	269	Total	C	N	O	S	0	0	0
			2101	1331	369	392	9			
1	C	278	Total	C	N	O	S	0	0	0
			2169	1374	380	406	9			
1	D	269	Total	C	N	O	S	0	0	0
			2105	1335	371	390	9			
1	F	278	Total	C	N	O	S	0	0	0
			2169	1374	380	406	9			
1	G	270	Total	C	N	O	S	0	0	0
			2120	1345	372	394	9			
1	H	259	Total	C	N	O	S	0	0	0
			2026	1283	357	377	9			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Fe 1	0	0
2	H	1	Total 1	Fe 1	0	0

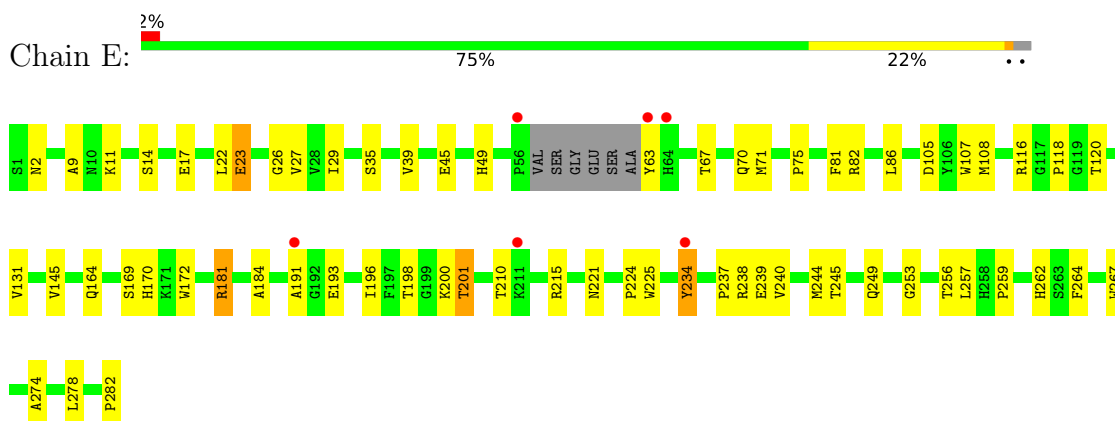
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	29	Total 29	O 29	0	0
3	A	27	Total 27	O 27	0	0
3	B	24	Total 24	O 24	0	0
3	C	11	Total 11	O 11	0	0
3	D	15	Total 15	O 15	0	0
3	F	14	Total 14	O 14	0	0
3	G	14	Total 14	O 14	0	0
3	H	3	Total 3	O 3	0	0

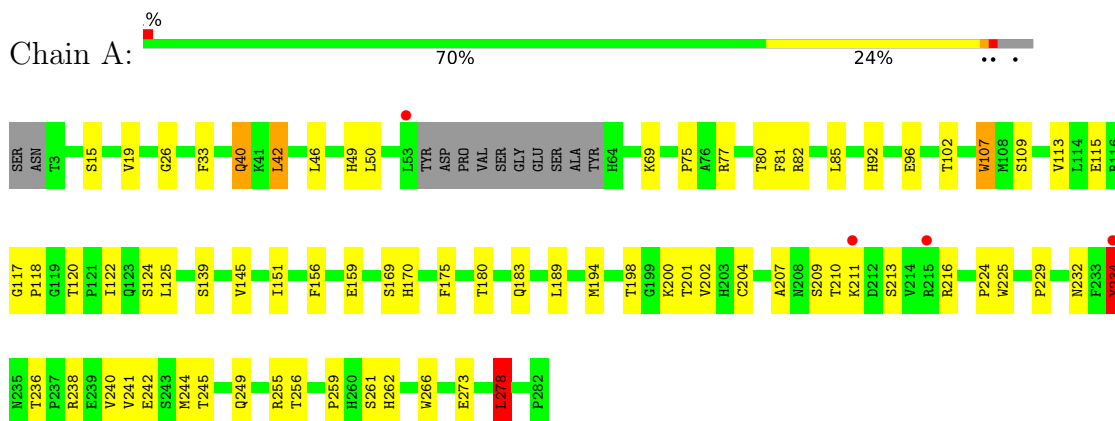
3 Residue-property plots [i](#)

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.

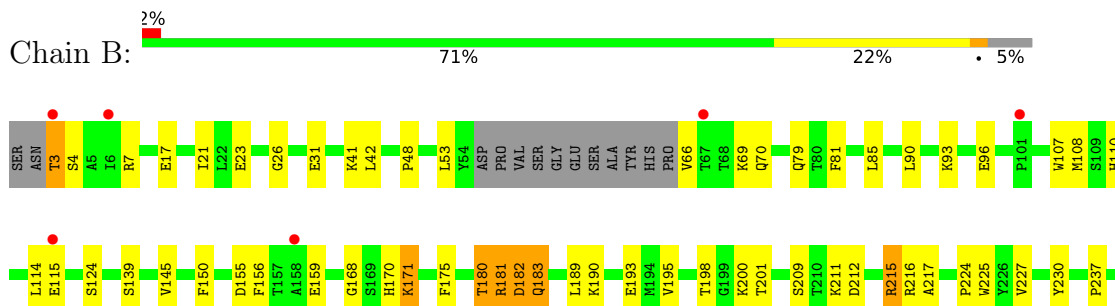
• Molecule 1: DhiD



• Molecule 1: DhiD

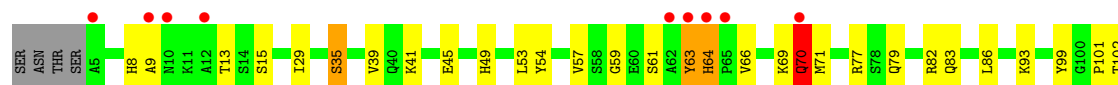


• Molecule 1: DhiD

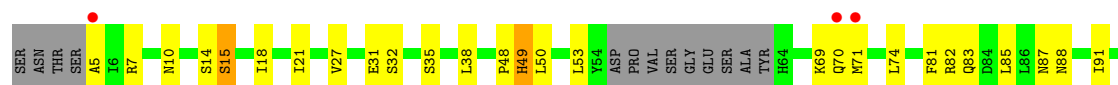




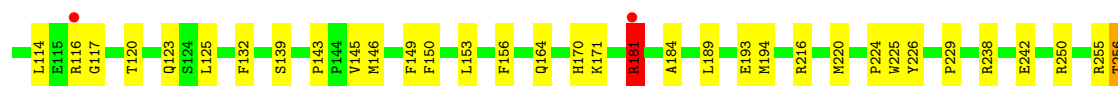
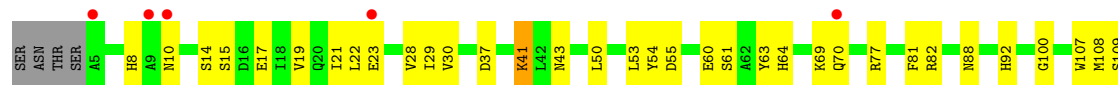
• Molecule 1: DhiD



• Molecule 1: DhiD

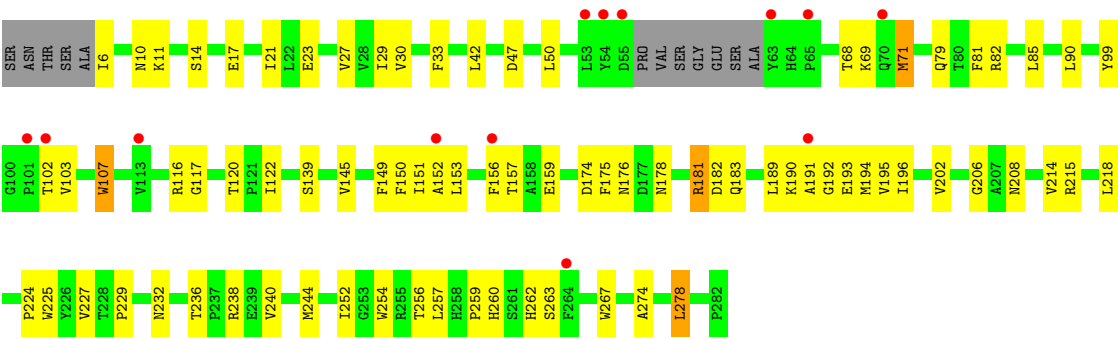


• Molecule 1: DhiD

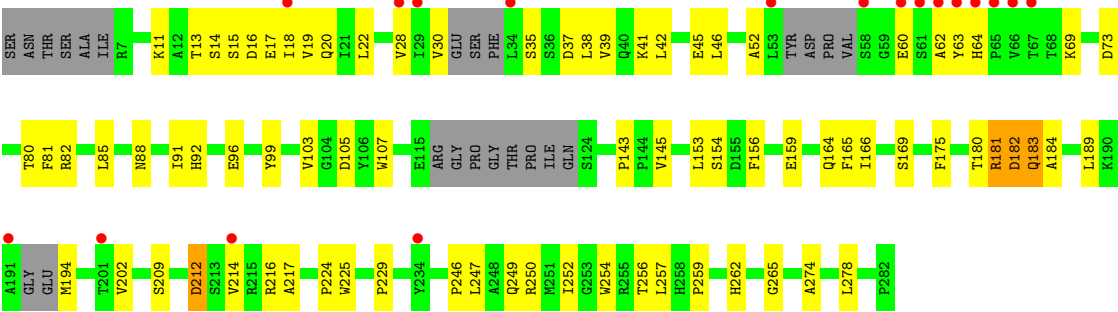


• Molecule 1: DhiD





• Molecule 1: DhiD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	368.94Å 78.25Å 81.91Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	30.57 – 2.58 30.57 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.57-2.58) 97.5 (30.57-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.257 0.203 , 0.254	Depositor DCC
R_{free} test set	2017 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17100	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: FE

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	0.29	0/2164	0.64	6/2945 (0.2%)
1	B	0.28	0/2158	0.61	4/2936 (0.1%)
1	C	0.40	2/2231 (0.1%)	0.75	12/3039 (0.4%)
1	D	0.31	0/2164	0.61	5/2945 (0.2%)
1	E	0.25	0/2220	0.63	4/3023 (0.1%)
1	F	0.31	1/2231 (0.0%)	0.61	7/3039 (0.2%)
1	G	0.33	0/2180	0.60	0/2967
1	H	0.51	1/2079 (0.0%)	0.74	5/2824 (0.2%)
All	All	0.35	4/17427 (0.0%)	0.65	43/23718 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	C	0	2
1	D	0	1
1	E	0	1
1	G	0	2
1	H	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	143	PRO	CA-C	-12.74	1.43	1.52
1	F	143	PRO	CA-C	-6.87	1.47	1.52
1	C	215	ARG	CD-NE	6.43	1.55	1.46
1	C	181	ARG	CB-CG	-5.02	1.37	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	GLN	CB-CG-CD	12.48	133.82	112.60
1	E	22	LEU	CA-C-N	-12.28	103.45	122.60
1	E	22	LEU	C-N-CA	-12.28	103.45	122.60
1	H	143	PRO	O-C-N	-10.99	115.98	121.15
1	A	216	ARG	CB-CG-CD	-10.39	87.40	111.30
1	D	69	LYS	CB-CG-CD	-9.13	90.31	111.30
1	A	234	TYR	CA-CB-CG	8.72	129.60	113.90
1	C	181	ARG	N-CA-CB	-7.85	98.13	110.22
1	E	23	GLU	CA-CB-CG	7.80	129.71	114.10
1	B	41	LYS	CA-CB-CG	7.80	129.69	114.10
1	B	41	LYS	CB-CA-C	-7.66	98.86	110.88
1	C	215	ARG	CA-CB-CG	-7.58	98.94	114.10
1	F	143	PRO	O-C-N	-7.28	117.73	121.15
1	C	180	THR	CA-C-N	7.21	130.66	120.28
1	C	180	THR	C-N-CA	7.21	130.66	120.28
1	F	41	LYS	CB-CG-CD	-6.80	95.66	111.30
1	C	69	LYS	CA-C-N	-6.65	110.96	121.87
1	C	69	LYS	C-N-CA	-6.65	110.96	121.87
1	F	41	LYS	CG-CD-CE	6.35	125.90	111.30
1	F	22	LEU	CA-C-N	-5.99	112.29	120.44
1	F	22	LEU	C-N-CA	-5.99	112.29	120.44
1	B	23	GLU	CB-CG-CD	5.73	122.33	112.60
1	B	171	LYS	CA-CB-CG	5.72	125.54	114.10
1	E	234	TYR	CA-CB-CG	5.70	124.17	113.90
1	H	175	PHE	CA-C-N	-5.63	110.59	121.58
1	H	175	PHE	C-N-CA	-5.63	110.59	121.58
1	F	139	SER	CB-CA-C	-5.59	110.11	116.54
1	C	215	ARG	CB-CG-CD	5.51	123.97	111.30
1	D	48	PRO	CA-C-N	-5.44	111.62	121.14
1	D	48	PRO	C-N-CA	-5.44	111.62	121.14
1	A	278	LEU	CB-CG-CD1	5.41	126.93	110.70
1	A	234	TYR	N-CA-CB	5.40	119.36	110.39
1	C	215	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	A	216	ARG	CG-CD-NE	5.29	123.65	112.00
1	D	69	LYS	N-CA-CB	-5.26	101.61	111.13
1	F	181	ARG	CB-CG-CD	5.24	123.35	111.30
1	A	234	TYR	CB-CA-C	-5.18	99.49	110.31
1	C	63	TYR	N-CA-C	5.18	116.39	108.52
1	D	278	LEU	CA-CB-CG	5.17	134.41	116.30
1	H	13	THR	CA-C-N	5.16	129.04	120.94
1	H	13	THR	C-N-CA	5.16	129.04	120.94
1	C	276	GLN	CA-CB-CG	5.12	124.34	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	GLN	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	ARG	Sidechain
1	B	215	ARG	Sidechain
1	B	216	ARG	Sidechain
1	C	181	ARG	Sidechain
1	C	215	ARG	Sidechain
1	D	49	HIS	Sidechain
1	E	181	ARG	Sidechain
1	G	181	ARG	Sidechain
1	G	215	ARG	Sidechain
1	H	181	ARG	Sidechain

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	2106	0	2031	58	1
1	B	2101	0	2026	48	1
1	C	2169	0	2082	61	0
1	D	2105	0	2028	60	1
1	E	2159	0	2074	57	1
1	F	2169	0	2082	64	0
1	G	2120	0	2036	65	0
1	H	2026	0	1945	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	3	0
3	B	24	0	0	1	0
3	C	11	0	0	0	0
3	D	15	0	0	1	0
3	E	29	0	0	6	0
3	F	14	0	0	7	0
3	G	14	0	0	2	0
3	H	3	0	0	1	0
All	All	17100	0	16304	449	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (449) 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:G:189:LEU:HD23	1:G:193:GLU:CB	1.74	1.18
1:G:189:LEU:HD23	1:G:193:GLU:HB2	1.32	1.08
1:A:118:PRO:HB3	1:A:211:LYS:HA	1.40	1.03
1:C:163:THR:H	1:C:215:ARG:HH22	1.00	0.98
1:F:123:GLN:O	1:F:181:ARG:NH2	1.98	0.96
1:B:70:GLN:HG3	1:H:62:ALA:HB2	1.47	0.95
1:E:198:THR:HG22	1:E:200:LYS:H	1.28	0.95
1:G:189:LEU:HD23	1:G:193:GLU:HB3	1.48	0.93
1:D:198:THR:HG22	1:D:200:LYS:H	1.35	0.92
1:G:189:LEU:CD2	1:G:193:GLU:HB2	2.00	0.91
1:A:198:THR:HG22	1:A:200:LYS:H	1.35	0.90
1:G:42:LEU:HD23	1:G:153:LEU:HD21	1.52	0.89
1:G:190:LYS:N	1:G:193:GLU:OE2	2.05	0.88
1:H:14:SER:HB3	1:H:17:GLU:HG3	1.57	0.85
1:F:50:LEU:O	1:F:69:LYS:NZ	2.09	0.84
1:F:37:ASP:HB3	1:F:41:LYS:NZ	1.93	0.84
1:C:161:GLY:O	1:C:215:ARG:NH1	2.13	0.81
1:H:96:GLU:OE2	3:H:401:HOH:O	1.99	0.81
1:F:10:ASN:ND2	1:F:29:ILE:O	2.16	0.79
1:D:239:GLU:OE2	1:D:239:GLU:N	2.15	0.79
1:F:261:SER:OG	3:F:402:HOH:O	2.00	0.79
1:A:210:THR:HG21	1:A:213:SER:HB3	1.64	0.78
1:F:82:ARG:NH1	3:F:403:HOH:O	2.08	0.77
1:D:122:ILE:HG12	1:D:181:ARG:HH21	1.49	0.77
1:C:163:THR:N	1:C:215:ARG:HH22	1.81	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ALA:O	3:D:401:HOH:O	2.03	0.77
1:H:88:ASN:HB3	1:H:91:ILE:HD12	1.67	0.77
1:D:156:PHE:HZ	1:D:217:ALA:HB2	1.49	0.76
1:B:256:THR:HG23	1:B:274:ALA:H	1.51	0.76
1:G:156:PHE:HD2	1:G:189:LEU:HB2	1.50	0.75
1:E:170:HIS:HB3	1:E:201:THR:HG22	1.68	0.75
1:G:116:ARG:HB3	1:G:120:THR:HG21	1.67	0.74
1:F:125:LEU:HG	1:F:181:ARG:HH11	1.53	0.74
1:F:37:ASP:O	1:F:41:LYS:HD2	1.88	0.74
1:E:70:GLN:HE22	1:F:60:GLU:HA	1.53	0.73
1:E:256:THR:HG23	1:E:274:ALA:H	1.53	0.73
1:E:234:TYR:HB2	1:A:278:LEU:HD21	1.71	0.73
1:F:55:ASP:HB3	1:F:60:GLU:HG2	1.69	0.72
1:F:23:GLU:O	1:F:170:HIS:NE2	2.23	0.72
1:G:159:GLU:OE2	1:G:159:GLU:N	2.19	0.72
1:A:170:HIS:HB3	1:A:201:THR:HG22	1.73	0.71
1:C:122:ILE:CD1	1:C:181:ARG:HH22	2.04	0.70
1:F:17:GLU:O	1:F:21:ILE:HD12	1.90	0.70
1:F:37:ASP:HB3	1:F:41:LYS:HZ1	1.56	0.70
1:E:81:PHE:CZ	1:E:108:MET:HE1	2.27	0.70
1:C:70:GLN:HG2	1:C:113:VAL:O	1.92	0.69
1:F:10:ASN:HD22	1:F:30:VAL:HA	1.56	0.69
1:H:164:GLN:HB3	1:H:184:ALA:HB1	1.75	0.69
1:A:236:THR:O	3:A:401:HOH:O	2.11	0.69
1:C:122:ILE:HD11	1:C:181:ARG:HH22	1.57	0.68
1:E:131:VAL:HG11	1:F:63:TYR:HB2	1.74	0.68
1:F:100:GLY:O	3:F:404:HOH:O	2.11	0.68
1:A:238:ARG:O	1:A:242:GLU:HG3	1.94	0.68
1:G:30:VAL:HG21	1:G:194:MET:HE3	1.77	0.67
1:C:79:GLN:HE21	1:C:83:GLN:HG3	1.59	0.67
1:G:156:PHE:CD2	1:G:189:LEU:HB2	2.30	0.67
1:B:156:PHE:HZ	1:B:217:ALA:HB2	1.60	0.66
1:E:81:PHE:HZ	1:E:108:MET:HE1	1.61	0.66
1:F:125:LEU:N	1:F:181:ARG:HH12	1.92	0.66
1:B:31:GLU:HA	1:B:193:GLU:HG2	1.77	0.66
1:H:182:ASP:C	1:H:184:ALA:H	2.04	0.66
1:D:153:LEU:HB2	1:D:216:ARG:HG2	1.76	0.66
1:C:41:LYS:O	1:C:45:GLU:HG3	1.95	0.66
1:F:256:THR:HG22	1:F:274:ALA:H	1.60	0.65
1:A:69:LYS:HB2	1:A:115:GLU:HB2	1.78	0.65
1:H:156:PHE:HB2	1:H:189:LEU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:H	1:C:215:ARG:NH2	1.84	0.65
1:D:256:THR:HG23	1:D:274:ALA:H	1.62	0.65
1:G:174:ASP:OD1	1:G:176:ASN:ND2	2.18	0.65
1:H:156:PHE:HD2	1:H:189:LEU:HD12	1.61	0.65
1:F:23:GLU:OE1	1:F:171:LYS:HE3	1.95	0.65
1:C:108:MET:CE	1:C:220:MET:HG2	2.27	0.65
1:H:18:ILE:HG23	1:H:28:VAL:HG11	1.78	0.64
1:H:156:PHE:HZ	1:H:217:ALA:HB2	1.63	0.64
1:A:46:LEU:HD13	1:A:113:VAL:HG21	1.80	0.63
1:C:156:PHE:CD2	1:C:189:LEU:HD12	2.34	0.63
1:E:234:TYR:CB	1:A:278:LEU:HD21	2.29	0.63
1:F:250:ARG:NH1	3:F:401:HOH:O	1.92	0.63
1:D:10:ASN:ND2	1:D:31:GLU:O	2.31	0.63
1:B:170:HIS:HB3	1:B:201:THR:HG22	1.81	0.63
1:G:236:THR:O	3:G:401:HOH:O	2.14	0.63
1:F:37:ASP:HB3	1:F:41:LYS:HZ2	1.62	0.62
1:G:17:GLU:O	1:G:21:ILE:HD12	1.97	0.62
1:E:238:ARG:NH1	1:E:278:LEU:O	2.32	0.62
1:H:156:PHE:CD2	1:H:189:LEU:HD12	2.34	0.62
1:C:162:ALA:HB3	1:C:186:THR:CG2	2.29	0.62
1:G:256:THR:HG23	1:G:274:ALA:H	1.64	0.62
1:C:156:PHE:CZ	1:C:215:ARG:HD3	2.35	0.61
1:E:86:LEU:HD21	1:E:108:MET:HE3	1.80	0.61
1:B:42:LEU:HD11	1:B:85:LEU:HD11	1.82	0.61
1:C:215:ARG:HG2	1:C:216:ARG:N	2.14	0.61
1:G:117:GLY:HA2	1:G:214:VAL:HG12	1.82	0.61
1:D:31:GLU:HA	1:D:193:GLU:HG2	1.81	0.61
1:C:108:MET:HE1	1:C:220:MET:HG2	1.82	0.61
1:F:10:ASN:HD21	1:F:28:VAL:HG22	1.65	0.61
1:B:198:THR:HB	1:B:201:THR:HG23	1.82	0.60
1:G:152:ALA:HA	1:G:156:PHE:HZ	1.64	0.60
1:C:276:GLN:HE21	1:C:282:PRO:HA	1.66	0.60
1:A:118:PRO:HB3	1:A:211:LYS:CA	2.26	0.60
1:D:15:SER:HA	1:D:18:ILE:HD13	1.84	0.60
1:C:162:ALA:HA	1:C:215:ARG:NH2	2.16	0.60
1:B:150:PHE:HB3	1:B:195:VAL:HG13	1.84	0.59
1:C:70:GLN:HB2	1:C:114:LEU:HA	1.83	0.59
1:F:117:GLY:O	1:F:120:THR:OG1	2.20	0.59
1:H:14:SER:CB	1:H:17:GLU:HG3	2.31	0.59
1:E:234:TYR:HE1	1:A:234:TYR:CD1	2.20	0.59
1:D:164:GLN:HB3	1:D:184:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:ILE:HG13	1:H:254:TRP:HD1	1.66	0.59
1:H:42:LEU:O	1:H:46:LEU:HD23	2.03	0.59
1:E:75:PRO:O	1:E:82:ARG:HD3	2.02	0.59
1:D:238:ARG:NH1	1:D:278:LEU:O	2.35	0.58
1:E:253:GLY:O	1:A:234:TYR:OH	2.20	0.58
1:C:156:PHE:HZ	1:C:217:ALA:HB2	1.69	0.58
1:B:7:ARG:HG2	1:B:21:ILE:HD13	1.85	0.58
1:H:159:GLU:OE1	1:H:159:GLU:N	2.36	0.58
1:A:241:VAL:O	1:A:249:GLN:NE2	2.37	0.58
1:B:180:THR:HG23	1:B:182:ASP:H	1.69	0.58
1:G:225:TRP:CE2	1:G:259:PRO:HB3	2.39	0.58
1:E:116:ARG:HB3	1:E:120:THR:HG21	1.85	0.58
1:B:17:GLU:O	1:B:21:ILE:HG13	2.03	0.58
1:F:256:THR:HG21	1:F:273:GLU:HA	1.85	0.58
1:H:92:HIS:CE1	1:H:247:LEU:HD11	2.39	0.58
1:A:69:LYS:NZ	3:A:404:HOH:O	2.37	0.57
1:H:14:SER:HB3	1:H:17:GLU:H	1.68	0.57
1:B:26:GLY:O	1:B:201:THR:HG21	2.05	0.57
1:E:198:THR:HG23	3:E:407:HOH:O	2.05	0.57
1:A:75:PRO:O	1:A:82:ARG:HD3	2.05	0.56
1:B:110:HIS:CE1	1:H:63:TYR:HE2	2.23	0.56
1:B:282:PRO:O	3:B:401:HOH:O	2.18	0.56
1:H:166:ILE:O	1:H:169:SER:OG	2.23	0.56
1:C:122:ILE:HD13	1:C:181:ARG:NH2	2.21	0.56
1:C:156:PHE:CE1	1:C:215:ARG:HD3	2.40	0.56
1:E:239:GLU:N	1:E:239:GLU:OE2	2.38	0.56
1:A:151:ILE:HG12	1:A:194:MET:HG3	1.88	0.56
1:B:198:THR:HG22	1:B:200:LYS:H	1.71	0.56
1:C:162:ALA:HA	1:C:215:ARG:CZ	2.36	0.56
1:A:225:TRP:CE2	1:A:259:PRO:HB3	2.41	0.56
1:C:99:TYR:HB3	1:C:103:VAL:HB	1.87	0.56
1:F:108:MET:HE2	1:F:220:MET:HG2	1.87	0.55
1:F:153:LEU:HB2	1:F:216:ARG:HG2	1.88	0.55
1:G:190:LYS:HG3	1:G:191:ALA:H	1.70	0.55
1:H:17:GLU:HA	1:H:20:GLN:HG2	1.86	0.55
1:E:35:SER:O	1:E:39:VAL:HG23	2.06	0.55
1:A:256:THR:HG22	1:A:273:GLU:HG2	1.89	0.55
1:E:282:PRO:O	3:E:401:HOH:O	2.18	0.55
1:B:3:THR:HG22	1:B:4:SER:H	1.70	0.55
1:H:16:ASP:O	1:H:20:GLN:HG2	2.06	0.55
1:A:92:HIS:O	1:A:96:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:CD2	1:B:189:LEU:HD12	2.41	0.55
1:D:156:PHE:HD2	1:D:189:LEU:HD12	1.72	0.55
1:H:30:VAL:CG2	1:H:194:MET:HG2	2.37	0.55
1:H:166:ILE:HG23	1:H:183:GLN:HB3	1.89	0.55
1:B:70:GLN:HG2	1:B:114:LEU:HD12	1.87	0.55
1:D:237:PRO:O	1:D:241:VAL:HG23	2.06	0.55
1:H:182:ASP:C	1:H:184:ALA:N	2.65	0.54
1:A:240:VAL:O	1:A:244:MET:HG3	2.07	0.54
1:B:155:ASP:HA	1:B:190:LYS:O	2.07	0.54
1:D:240:VAL:O	1:D:244:MET:HG3	2.08	0.54
1:G:145:VAL:O	1:G:224:PRO:HD3	2.08	0.54
1:D:7:ARG:NH2	1:D:21:ILE:HD12	2.23	0.54
1:F:8:HIS:HA	1:F:29:ILE:HB	1.88	0.54
1:H:246:PRO:HA	1:H:249:GLN:OE1	2.08	0.54
1:H:169:SER:HB2	1:H:202:VAL:HG23	1.89	0.54
1:D:225:TRP:CE2	1:D:259:PRO:HB3	2.43	0.54
1:G:156:PHE:HB2	1:G:189:LEU:H	1.73	0.54
1:E:256:THR:HG22	1:E:267:TRP:O	2.08	0.53
1:E:11:LYS:CD	1:E:11:LYS:H	2.19	0.53
1:B:159:GLU:H	1:B:159:GLU:CD	2.15	0.53
1:D:256:THR:CG2	1:D:274:ALA:H	2.21	0.53
1:F:125:LEU:H	1:F:181:ARG:NH1	2.06	0.53
1:F:189:LEU:HB3	1:F:193:GLU:HB2	1.91	0.53
1:A:26:GLY:O	1:A:201:THR:HG21	2.08	0.53
1:A:117:GLY:O	1:A:120:THR:OG1	2.25	0.53
1:D:116:ARG:HD3	1:D:215:ARG:NH2	2.23	0.53
1:F:125:LEU:N	1:F:181:ARG:NH1	2.56	0.53
1:E:26:GLY:O	1:E:201:THR:HG21	2.08	0.53
1:C:237:PRO:HB2	1:C:240:VAL:HG23	1.91	0.53
1:E:191:ALA:C	1:E:193:GLU:H	2.17	0.52
1:G:79:GLN:HG3	1:G:82:ARG:NH2	2.24	0.52
1:E:245:THR:O	1:E:249:GLN:HG3	2.10	0.52
1:E:145:VAL:O	1:E:224:PRO:HD3	2.10	0.52
1:E:225:TRP:CE2	1:E:259:PRO:HB3	2.45	0.52
1:B:256:THR:HG22	1:B:267:TRP:O	2.08	0.52
1:F:164:GLN:HB3	1:F:184:ALA:HB1	1.91	0.52
1:D:32:SER:H	1:D:193:GLU:HG3	1.74	0.52
1:G:262:HIS:CE1	1:H:63:TYR:HA	2.44	0.52
1:H:156:PHE:CZ	1:H:217:ALA:HB2	2.45	0.52
1:H:225:TRP:CE2	1:H:259:PRO:HB3	2.45	0.52
1:E:63:TYR:N	3:E:403:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:PHE:HE1	1:D:215:ARG:HG2	1.75	0.52
1:H:256:THR:CG2	1:H:274:ALA:H	2.23	0.52
1:G:150:PHE:HB3	1:G:195:VAL:HG12	1.91	0.52
1:A:255:ARG:NH1	1:A:273:GLU:OE1	2.38	0.52
1:A:262:HIS:CD2	1:F:63:TYR:HA	2.44	0.52
1:B:168:GLY:O	1:B:171:LYS:HB2	2.10	0.52
1:B:269:ILE:HG13	1:G:232:ASN:HB3	1.90	0.52
1:C:122:ILE:CD1	1:C:181:ARG:NH2	2.72	0.52
1:G:152:ALA:HB3	1:G:192:GLY:HA2	1.91	0.52
1:H:30:VAL:HG21	1:H:194:MET:HE3	1.91	0.51
1:B:212:ASP:N	1:B:212:ASP:OD1	2.44	0.51
1:G:23:GLU:O	1:G:23:GLU:HG2	2.10	0.51
1:B:69:LYS:HB2	1:B:115:GLU:HB2	1.91	0.51
1:B:224:PRO:HG2	1:B:227:VAL:HG23	1.92	0.51
1:C:70:GLN:HG2	1:C:113:VAL:C	2.35	0.51
1:F:14:SER:HA	3:F:413:HOH:O	2.11	0.51
1:A:33:PHE:CD2	1:A:194:MET:HE2	2.45	0.51
1:D:14:SER:O	1:D:18:ILE:HD12	2.11	0.51
1:C:49:HIS:O	1:C:53:LEU:HG	2.10	0.51
1:H:274:ALA:O	1:H:278:LEU:HG	2.11	0.51
1:G:191:ALA:O	1:G:193:GLU:N	2.35	0.51
1:E:234:TYR:HE1	1:A:234:TYR:CE1	2.29	0.51
1:B:180:THR:HG22	1:B:183:GLN:HG3	1.93	0.51
1:F:145:VAL:O	1:F:224:PRO:HD3	2.11	0.51
1:E:234:TYR:CE1	1:A:234:TYR:CD1	2.99	0.50
1:F:116:ARG:HG3	1:F:116:ARG:HH11	1.76	0.50
1:E:105:ASP:OD2	3:E:402:HOH:O	2.19	0.50
1:F:8:HIS:CD2	1:F:29:ILE:HD12	2.47	0.50
1:H:256:THR:HG23	1:H:274:ALA:H	1.76	0.50
1:B:230:TYR:CZ	1:H:63:TYR:HB3	2.46	0.50
1:C:225:TRP:CE2	1:C:259:PRO:HB3	2.46	0.50
1:H:145:VAL:O	1:H:224:PRO:HD3	2.10	0.50
1:C:35:SER:O	1:C:39:VAL:HG23	2.12	0.50
1:F:274:ALA:O	1:F:278:LEU:HG	2.12	0.50
1:D:275:GLY:O	1:D:280:LEU:HB2	2.11	0.50
1:H:81:PHE:HA	1:H:85:LEU:HB2	1.93	0.50
1:G:6:ILE:HG23	1:G:27:VAL:HG13	1.93	0.49
1:H:41:LYS:O	1:H:45:GLU:HG3	2.12	0.49
1:D:83:GLN:O	1:D:87:ASN:ND2	2.41	0.49
1:H:182:ASP:O	1:H:184:ALA:N	2.45	0.49
1:C:9:ALA:O	1:C:13:THR:OG1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ILE:N	3:G:404:HOH:O	2.45	0.49
1:B:93:LYS:O	1:B:96:GLU:HG3	2.12	0.49
1:G:29:ILE:HG12	1:G:189:LEU:HD11	1.94	0.49
1:E:239:GLU:H	1:E:239:GLU:CD	2.18	0.49
1:A:210:THR:HG22	1:A:213:SER:H	1.77	0.49
1:G:224:PRO:HG2	1:G:227:VAL:HG23	1.94	0.49
1:B:274:ALA:O	1:B:278:LEU:HG	2.13	0.49
1:C:57:VAL:HG11	1:D:240:VAL:HA	1.95	0.49
1:D:50:LEU:HD23	1:D:53:LEU:HD11	1.94	0.49
1:G:81:PHE:HD1	1:G:85:LEU:HD12	1.78	0.49
1:A:232:ASN:OD1	1:A:234:TYR:CD1	2.66	0.49
1:F:225:TRP:CE2	1:F:259:PRO:HB3	2.47	0.49
1:C:107:TRP:CZ2	1:C:229:PRO:HD3	2.48	0.48
1:D:150:PHE:HB3	1:D:195:VAL:HG13	1.96	0.48
1:H:107:TRP:CZ2	1:H:229:PRO:HD3	2.48	0.48
1:G:190:LYS:HG3	1:G:191:ALA:N	2.28	0.48
1:F:15:SER:O	1:F:19:VAL:HG23	2.13	0.48
1:G:244:MET:HE1	1:G:252:ILE:HD13	1.94	0.48
1:D:275:GLY:HA2	1:D:278:LEU:HD12	1.96	0.48
1:G:30:VAL:CG2	1:G:194:MET:HB3	2.43	0.48
1:B:225:TRP:CE2	1:B:259:PRO:HB3	2.49	0.48
1:H:14:SER:HB3	1:H:17:GLU:CG	2.38	0.48
1:F:81:PHE:CZ	1:F:108:MET:HE1	2.49	0.48
1:A:82:ARG:HG2	1:A:244:MET:HG2	1.94	0.48
1:E:11:LYS:H	1:E:11:LYS:HD3	1.79	0.48
1:E:198:THR:HB	1:E:201:THR:HG23	1.95	0.48
1:E:11:LYS:H	1:E:11:LYS:CE	2.26	0.47
1:B:237:PRO:O	1:B:240:VAL:HG22	2.14	0.47
1:E:240:VAL:O	1:E:244:MET:HG3	2.13	0.47
1:C:156:PHE:HB2	1:C:189:LEU:HB2	1.96	0.47
1:D:159:GLU:HG3	1:D:210:THR:HG22	1.96	0.47
1:F:43:ASN:HD21	1:F:153:LEU:HB3	1.79	0.47
1:H:156:PHE:CD2	1:H:189:LEU:HB2	2.49	0.47
1:A:198:THR:HB	1:A:201:THR:HG23	1.96	0.47
1:A:209:SER:O	1:A:211:LYS:HG3	2.14	0.47
1:C:145:VAL:O	1:C:224:PRO:HD3	2.13	0.47
1:D:125:LEU:HB3	1:D:202:VAL:CG1	2.44	0.47
1:E:45:GLU:HA	1:B:48:PRO:HB3	1.96	0.47
1:A:156:PHE:HB2	1:A:189:LEU:HB2	1.96	0.47
1:C:8:HIS:HD2	1:C:29:ILE:HD12	1.80	0.47
1:C:149:PHE:HB3	1:C:194:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:SER:HA	1:D:175:PHE:CG	2.49	0.47
1:C:53:LEU:HD11	1:C:71:MET:SD	2.54	0.47
1:D:110:HIS:HA	1:D:231:GLU:HG3	1.96	0.47
1:G:152:ALA:HA	1:G:156:PHE:CZ	2.48	0.47
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.82	0.47
1:G:149:PHE:HB3	1:G:194:MET:SD	2.55	0.47
1:D:81:PHE:HA	1:D:85:LEU:HB2	1.96	0.47
1:D:118:PRO:HB3	1:D:210:THR:O	2.15	0.47
1:D:156:PHE:CD2	1:D:189:LEU:HD12	2.48	0.47
1:F:81:PHE:HZ	1:F:108:MET:HE1	1.79	0.47
1:A:102:THR:N	3:A:402:HOH:O	2.38	0.46
1:C:70:GLN:HB2	1:C:114:LEU:HD12	1.97	0.46
1:H:225:TRP:HB2	1:H:257:LEU:HD13	1.97	0.46
1:G:189:LEU:HB3	1:G:193:GLU:CD	2.40	0.46
1:E:198:THR:HB	1:E:201:THR:CG2	2.45	0.46
1:C:164:GLN:HB3	1:C:184:ALA:HB1	1.97	0.46
1:G:153:LEU:HD11	1:G:218:LEU:HB2	1.96	0.46
1:C:102:THR:HA	1:C:260:HIS:NE2	2.31	0.46
1:C:118:PRO:HB3	1:C:210:THR:O	2.16	0.46
1:G:256:THR:HG22	1:G:267:TRP:O	2.16	0.46
1:C:156:PHE:HD2	1:C:189:LEU:HD12	1.79	0.46
1:G:99:TYR:HB3	1:G:103:VAL:HB	1.97	0.46
1:G:256:THR:CG2	1:G:274:ALA:H	2.29	0.46
1:D:113:VAL:HG22	1:D:218:LEU:CD1	2.45	0.46
1:G:33:PHE:CE1	1:G:90:LEU:HD23	2.51	0.46
1:G:178:ASN:O	1:G:202:VAL:HG11	2.16	0.46
1:G:252:ILE:HG13	1:G:254:TRP:HD1	1.80	0.46
1:G:262:HIS:HE1	1:H:63:TYR:HA	1.80	0.46
1:E:2:ASN:ND2	3:E:405:HOH:O	2.49	0.46
1:A:245:THR:O	1:A:249:GLN:HG3	2.15	0.46
1:B:66:VAL:HG22	1:H:52:ALA:HA	1.98	0.46
1:D:237:PRO:O	1:D:240:VAL:HG13	2.16	0.46
1:E:274:ALA:O	1:E:278:LEU:HG	2.16	0.45
1:B:245:THR:O	1:B:249:GLN:HG3	2.16	0.45
1:C:15:SER:OG	1:C:93:LYS:HE2	2.16	0.45
1:D:123:GLN:O	1:D:181:ARG:NH2	2.49	0.45
1:G:122:ILE:HG21	1:G:181:ARG:HH22	1.81	0.45
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.66	0.45
1:F:256:THR:CG2	1:F:274:ALA:H	2.29	0.45
1:G:10:ASN:O	1:G:11:LYS:HB3	2.17	0.45
1:A:15:SER:O	1:A:19:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ARG:O	1:F:242:GLU:HG3	2.17	0.45
1:C:116:ARG:HE	1:C:116:ARG:HB2	1.17	0.45
1:D:128:ASP:C	1:D:130:ALA:H	2.25	0.45
1:G:33:PHE:CD2	1:G:194:MET:HE2	2.52	0.45
1:G:102:THR:HA	1:G:260:HIS:NE2	2.31	0.45
1:F:23:GLU:C	1:F:23:GLU:CD	2.84	0.45
1:F:77:ARG:NH2	3:F:406:HOH:O	2.40	0.45
1:D:35:SER:H	1:D:38:LEU:HD12	1.82	0.45
1:D:122:ILE:HG12	1:D:181:ARG:NH2	2.25	0.45
1:D:145:VAL:O	1:D:224:PRO:HD3	2.16	0.45
1:G:151:ILE:HG12	1:G:194:MET:HG3	1.99	0.45
1:H:15:SER:O	1:H:19:VAL:HG23	2.17	0.45
1:F:61:SER:O	1:F:64:HIS:HB2	2.18	0.44
1:H:62:ALA:O	1:H:63:TYR:CG	2.71	0.44
1:E:169:SER:HA	1:E:172:TRP:CD1	2.53	0.44
1:A:122:ILE:HB	1:A:207:ALA:HB2	1.99	0.44
1:A:125:LEU:HD23	1:A:204:CYS:HB3	1.99	0.44
1:D:49:HIS:HB2	1:D:71:MET:SD	2.57	0.44
1:H:99:TYR:HB3	1:H:103:VAL:HB	1.98	0.44
1:B:70:GLN:HG2	1:B:114:LEU:CD1	2.48	0.44
1:G:122:ILE:HD12	1:G:206:GLY:HA2	1.98	0.44
1:H:41:LYS:HG2	1:H:80:THR:HG21	1.99	0.44
1:C:101:PRO:O	1:C:260:HIS:NE2	2.50	0.44
1:A:107:TRP:CZ2	1:A:229:PRO:HD3	2.53	0.44
1:F:70:GLN:HG2	1:F:114:LEU:HD13	2.00	0.44
1:B:159:GLU:OE1	1:B:159:GLU:N	2.45	0.44
1:B:256:THR:CG2	1:B:274:ALA:H	2.27	0.44
1:G:107:TRP:CZ2	1:G:229:PRO:HD3	2.53	0.44
1:G:47:ASP:HA	1:G:50:LEU:HD12	2.00	0.43
1:E:221:ASN:ND2	1:F:63:TYR:OH	2.47	0.43
1:D:139:SER:HA	1:D:175:PHE:CD2	2.53	0.43
1:D:190:LYS:N	1:D:193:GLU:OE1	2.37	0.43
1:D:125:LEU:HD23	1:D:204:CYS:HB3	2.00	0.43
1:G:181:ARG:O	1:G:183:GLN:N	2.52	0.43
1:H:39:VAL:HG13	1:H:153:LEU:HD13	2.00	0.43
1:D:85:LEU:HA	1:D:85:LEU:HD23	1.71	0.43
1:D:117:GLY:O	1:D:120:THR:OG1	2.35	0.43
1:E:118:PRO:HB3	1:E:210:THR:O	2.18	0.43
1:E:215:ARG:NH1	3:E:406:HOH:O	2.52	0.43
1:E:262:HIS:CE1	1:E:264:PHE:HB3	2.54	0.43
1:D:194:MET:HE3	1:D:196:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ASN:ND2	1:F:29:ILE:C	2.76	0.43
1:G:238:ARG:NH1	1:G:278:LEU:O	2.51	0.43
1:E:70:GLN:NE2	1:F:60:GLU:HA	2.28	0.43
1:A:159:GLU:CD	1:A:159:GLU:H	2.27	0.43
1:G:117:GLY:O	1:G:208:ASN:ND2	2.51	0.43
1:H:105:ASP:OD1	1:H:250:ARG:NH1	2.51	0.43
1:C:189:LEU:C	1:C:190:LYS:HD3	2.43	0.43
1:E:27:VAL:HA	1:E:196:ILE:O	2.19	0.43
1:A:109:SER:HA	1:A:229:PRO:HB3	2.00	0.43
1:E:225:TRP:HB2	1:E:257:LEU:HD13	2.01	0.42
1:A:42:LEU:HD13	1:A:80:THR:HB	2.02	0.42
1:B:230:TYR:CE1	1:H:63:TYR:HB3	2.55	0.42
1:C:82:ARG:HD3	1:C:240:VAL:HG12	2.01	0.42
1:E:234:TYR:HB3	1:A:278:LEU:CD2	2.49	0.42
1:A:159:GLU:OE1	1:A:159:GLU:N	2.52	0.42
1:A:256:THR:CG2	1:A:273:GLU:HG2	2.49	0.42
1:C:101:PRO:O	1:C:260:HIS:CD2	2.72	0.42
1:C:238:ARG:NH1	1:C:278:LEU:O	2.52	0.42
1:C:244:MET:HE1	1:C:252:ILE:HD13	2.00	0.42
1:H:252:ILE:HG13	1:H:254:TRP:CD1	2.51	0.42
1:E:11:LYS:H	1:E:11:LYS:HE2	1.82	0.42
1:C:59:GLY:O	1:C:61:SER:N	2.52	0.42
1:C:166:ILE:HD12	1:C:202:VAL:HG11	2.00	0.42
1:F:37:ASP:CB	1:F:41:LYS:HZ1	2.30	0.42
1:E:49:HIS:HB2	1:E:71:MET:HE1	2.01	0.42
1:E:86:LEU:HD23	1:E:86:LEU:HA	1.76	0.42
1:E:164:GLN:HB3	1:E:184:ALA:HB1	2.00	0.42
1:A:232:ASN:OD1	1:A:234:TYR:HD1	2.03	0.42
1:C:64:HIS:O	1:C:66:VAL:HG23	2.20	0.42
1:F:53:LEU:HD23	1:F:54:TYR:CE2	2.55	0.42
1:F:156:PHE:CD2	1:F:189:LEU:HD12	2.54	0.42
1:B:139:SER:HA	1:B:175:PHE:CD2	2.55	0.42
1:C:53:LEU:HB2	1:C:54:TYR:CD1	2.54	0.42
1:E:9:ALA:N	1:E:29:ILE:O	2.51	0.42
1:H:88:ASN:CB	1:H:91:ILE:HD12	2.44	0.42
1:B:145:VAL:O	1:B:224:PRO:HD3	2.19	0.42
1:D:135:ILE:HG21	1:D:145:VAL:HG21	2.02	0.42
1:H:262:HIS:ND1	1:H:265:GLY:O	2.50	0.42
1:A:145:VAL:O	1:A:224:PRO:HD3	2.20	0.41
1:B:225:TRP:HB2	1:B:257:LEU:HD13	2.02	0.41
1:G:27:VAL:HA	1:G:196:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PHE:HZ	1:B:108:MET:HE1	1.85	0.41
1:A:169:SER:HB2	1:A:202:VAL:HG23	2.02	0.41
1:F:88:ASN:O	1:F:92:HIS:HD2	2.04	0.41
1:A:49:HIS:CE1	1:A:77:ARG:HG2	2.56	0.41
1:B:211:LYS:HB3	1:B:211:LYS:HE3	1.58	0.41
1:C:211:LYS:HB3	1:C:211:LYS:HE3	1.82	0.41
1:D:116:ARG:HD3	1:D:215:ARG:HH22	1.85	0.41
1:F:109:SER:HA	1:F:229:PRO:HB3	2.02	0.41
1:F:116:ARG:HG3	1:F:116:ARG:NH1	2.36	0.41
1:G:189:LEU:CD2	1:G:193:GLU:CB	2.64	0.41
1:E:191:ALA:C	1:E:193:GLU:N	2.78	0.41
1:E:234:TYR:CE1	1:A:234:TYR:CG	3.08	0.41
1:D:71:MET:HE2	1:D:71:MET:HB3	1.80	0.41
1:F:255:ARG:NH2	1:F:281:LYS:O	2.48	0.41
1:H:82:ARG:HE	1:H:82:ARG:HB2	1.64	0.41
1:B:150:PHE:HB3	1:B:195:VAL:CG1	2.48	0.41
1:D:49:HIS:N	1:D:49:HIS:CD2	2.89	0.41
1:G:71:MET:HB3	1:G:71:MET:HE2	1.58	0.41
1:C:189:LEU:HA	1:C:193:GLU:OE1	2.21	0.41
1:D:88:ASN:HB3	1:D:91:ILE:HD12	2.01	0.41
1:A:81:PHE:HA	1:A:85:LEU:HB2	2.03	0.41
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.92	0.41
1:D:74:LEU:HD21	1:D:113:VAL:HG23	2.03	0.41
1:D:169:SER:HB2	1:D:202:VAL:HG23	2.03	0.41
1:F:181:ARG:H	1:F:181:ARG:HG2	1.53	0.41
1:A:180:THR:H	1:A:183:GLN:HE21	1.69	0.41
1:D:82:ARG:HD2	1:D:240:VAL:HG23	2.03	0.41
1:F:132:PHE:CE2	1:F:146:MET:HE3	2.56	0.41
1:F:225:TRP:CD2	1:F:259:PRO:HB3	2.55	0.41
1:F:226:TYR:OH	3:F:405:HOH:O	2.21	0.41
1:G:149:PHE:HD2	1:G:194:MET:SD	2.43	0.41
1:G:157:THR:HB	1:G:159:GLU:OE2	2.20	0.41
1:H:11:LYS:HB2	1:H:11:LYS:HE3	1.71	0.41
1:H:154:SER:HG	1:H:216:ARG:H	1.66	0.41
1:E:14:SER:N	1:E:17:GLU:OE2	2.35	0.41
1:C:256:THR:CG2	1:C:274:ALA:H	2.34	0.41
1:D:156:PHE:CZ	1:D:217:ALA:HB2	2.41	0.41
1:F:53:LEU:HD21	1:F:70:GLN:O	2.21	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.97	0.40
1:A:49:HIS:ND1	1:A:77:ARG:HG2	2.36	0.40
1:A:256:THR:OG1	1:A:266:TRP:O	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASP:C	1:D:130:ALA:N	2.79	0.40
1:F:149:PHE:HB3	1:F:194:MET:SD	2.62	0.40
1:B:81:PHE:CZ	1:B:108:MET:HE1	2.56	0.40
1:C:53:LEU:HD21	1:C:77:ARG:HH21	1.87	0.40
1:D:27:VAL:HG23	1:D:197:PHE:HB3	2.03	0.40
1:H:62:ALA:C	1:H:64:HIS:N	2.78	0.40
1:A:139:SER:HA	1:A:175:PHE:CG	2.56	0.40
1:A:210:THR:CG2	1:A:213:SER:HB3	2.42	0.40
1:C:70:GLN:CB	1:C:114:LEU:HD12	2.52	0.40
1:C:256:THR:HG21	1:C:273:GLU:HA	2.04	0.40
1:E:237:PRO:O	1:E:240:VAL:HG22	2.21	0.40
1:G:107:TRP:CZ3	1:G:257:LEU:HD21	2.57	0.40
1:G:139:SER:HA	1:G:175:PHE:CD2	2.57	0.40
1:H:165:PHE:O	1:H:184:ALA:HA	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLN:OE1	1:B:79:GLN:NE2[1_545]	1.74	0.46
1:E:63:TYR:O	1:D:270:ARG:NH1[1_565]	2.18	0.02

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	266/282 (94%)	254 (96%)	12 (4%)	0	100	100
1	B	265/282 (94%)	246 (93%)	19 (7%)	0	100	100
1	C	276/282 (98%)	253 (92%)	23 (8%)	0	100	100
1	D	265/282 (94%)	248 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	272/282 (96%)	259 (95%)	13 (5%)	0	100	100
1	F	276/282 (98%)	260 (94%)	16 (6%)	0	100	100
1	G	266/282 (94%)	253 (95%)	13 (5%)	0	100	100
1	H	249/282 (88%)	228 (92%)	19 (8%)	2 (1%)	16	32
All	All	2135/2256 (95%)	2001 (94%)	132 (6%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	183	GLN
1	H	212	ASP

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	227/237 (96%)	220 (97%)	7 (3%)	35	60
1	B	226/237 (95%)	216 (96%)	10 (4%)	25	48
1	C	233/237 (98%)	226 (97%)	7 (3%)	36	62
1	D	226/237 (95%)	215 (95%)	11 (5%)	22	44
1	E	233/237 (98%)	228 (98%)	5 (2%)	47	71
1	F	233/237 (98%)	226 (97%)	7 (3%)	36	62
1	G	228/237 (96%)	219 (96%)	9 (4%)	28	53
1	H	218/237 (92%)	205 (94%)	13 (6%)	17	36
All	All	1824/1896 (96%)	1755 (96%)	69 (4%)	29	54

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	23	GLU
1	E	67	THR

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Mol	Chain	Res	Type
1	E	107	TRP
1	E	181	ARG
1	E	201	THR
1	A	40	GLN
1	A	42	LEU
1	A	107	TRP
1	A	124	SER
1	A	234	TYR
1	A	261	SER
1	A	278	LEU
1	B	3	THR
1	B	90	LEU
1	B	107	TRP
1	B	124	SER
1	B	180	THR
1	B	181	ARG
1	B	182	ASP
1	B	183	GLN
1	B	209	SER
1	B	215	ARG
1	C	35	SER
1	C	63	TYR
1	C	64	HIS
1	C	70	GLN
1	C	107	TRP
1	C	113	VAL
1	C	159	GLU
1	D	15	SER
1	D	70	GLN
1	D	107	TRP
1	D	124	SER
1	D	210	THR
1	D	212	ASP
1	D	214	VAL
1	D	240	VAL
1	D	257	LEU
1	D	261	SER
1	D	278	LEU
1	F	107	TRP
1	F	150	PHE
1	F	181	ARG
1	F	256	THR

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Mol	Chain	Res	Type
1	F	257	LEU
1	F	261	SER
1	F	278	LEU
1	G	14	SER
1	G	68	THR
1	G	69	LYS
1	G	71	MET
1	G	107	TRP
1	G	182	ASP
1	G	240	VAL
1	G	263	SER
1	G	278	LEU
1	H	22	LEU
1	H	35	SER
1	H	37	ASP
1	H	38	LEU
1	H	60	GLU
1	H	69	LYS
1	H	73	ASP
1	H	180	THR
1	H	181	ARG
1	H	182	ASP
1	H	209	SER
1	H	212	ASP
1	H	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	GLN
1	E	40	GLN
1	E	276	GLN
1	A	83	GLN
1	A	178	ASN
1	A	183	GLN
1	A	262	HIS
1	A	271	ASN
1	B	221	ASN
1	B	258	HIS
1	C	8	HIS
1	C	20	GLN
1	C	40	GLN

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Mol	Chain	Res	Type
1	C	70	GLN
1	C	79	GLN
1	C	271	ASN
1	C	276	GLN
1	D	20	GLN
1	D	136	HIS
1	F	8	HIS
1	F	10	ASN
1	F	43	ASN
1	F	87	ASN
1	F	176	ASN
1	G	70	GLN
1	G	110	HIS
1	H	79	GLN
1	H	208	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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	270/282 (95%)	-0.02	4 (1%) 72 69	31, 56, 86, 104	0
1	B	269/282 (95%)	0.03	7 (2%) 57 52	35, 59, 92, 120	0
1	C	278/282 (98%)	0.16	12 (4%) 40 35	41, 65, 95, 125	0
1	D	269/282 (95%)	0.18	4 (1%) 72 69	38, 69, 103, 125	0
1	E	276/282 (97%)	-0.17	6 (2%) 62 58	28, 47, 76, 118	0
1	F	278/282 (98%)	0.20	8 (2%) 53 49	37, 69, 99, 123	0
1	G	270/282 (95%)	0.37	13 (4%) 35 31	37, 77, 116, 139	0
1	H	259/282 (91%)	0.72	18 (6%) 23 19	30, 93, 139, 165	0
All	All	2169/2256 (96%)	0.18	72 (3%) 49 44	28, 65, 112, 165	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	63	TYR	6.5
1	E	234	TYR	4.8
1	D	70	GLN	4.5
1	H	62	ALA	4.4
1	A	234	TYR	4.3
1	C	9	ALA	4.2
1	H	191	ALA	4.0
1	H	66	VAL	4.0
1	G	102	THR	3.9
1	H	53	LEU	3.7
1	H	65	PRO	3.6
1	B	67	THR	3.6
1	C	62	ALA	3.6
1	H	64	HIS	3.5
1	G	63	TYR	3.4
1	G	55	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	10	ASN	3.4
1	C	70	GLN	3.4
1	F	10	ASN	3.3
1	E	63	TYR	3.3
1	G	156	PHE	3.2
1	C	5	ALA	3.0
1	F	23	GLU	3.0
1	H	58	SER	3.0
1	G	152	ALA	2.9
1	H	61	SER	2.9
1	H	67	THR	2.8
1	H	34	LEU	2.8
1	C	63	TYR	2.7
1	D	5	ALA	2.7
1	B	101	PRO	2.7
1	C	215	ARG	2.7
1	B	115	GLU	2.6
1	A	211	LYS	2.6
1	F	9	ALA	2.6
1	C	65	PRO	2.6
1	C	12	ALA	2.6
1	H	234	TYR	2.6
1	H	60	GLU	2.5
1	G	113	VAL	2.5
1	B	278	LEU	2.5
1	G	264	PHE	2.5
1	G	54	TYR	2.5
1	H	201	THR	2.5
1	G	53	LEU	2.4
1	H	28	VAL	2.4
1	D	71	MET	2.4
1	G	70	GLN	2.3
1	E	64	HIS	2.3
1	E	191	ALA	2.3
1	H	18	ILE	2.3
1	E	211	LYS	2.3
1	G	101	PRO	2.3
1	F	5	ALA	2.2
1	F	278	LEU	2.2
1	E	56	PRO	2.2
1	C	158	ALA	2.2
1	F	116	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	53	LEU	2.1
1	G	65	PRO	2.1
1	B	3	THR	2.1
1	F	70	GLN	2.1
1	G	191	ALA	2.1
1	B	158	ALA	2.1
1	A	215	ARG	2.0
1	B	6	ILE	2.0
1	D	101	PRO	2.0
1	C	64	HIS	2.0
1	F	181	ARG	2.0
1	H	214	VAL	2.0
1	C	191	ALA	2.0
1	H	29	ILE	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](#)

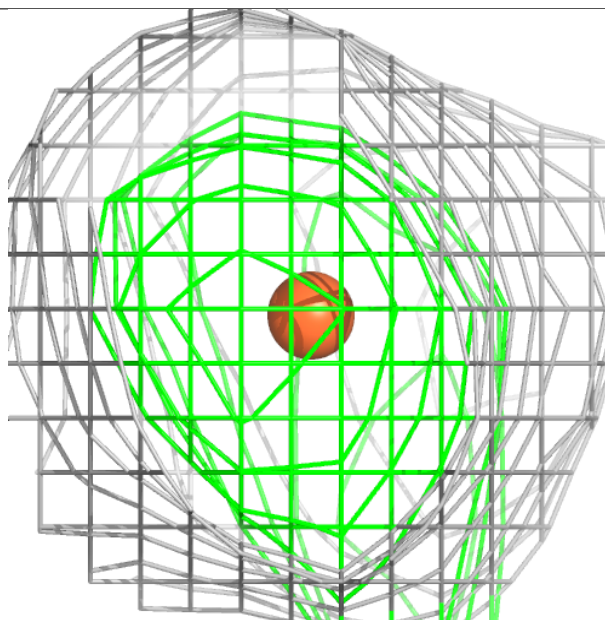
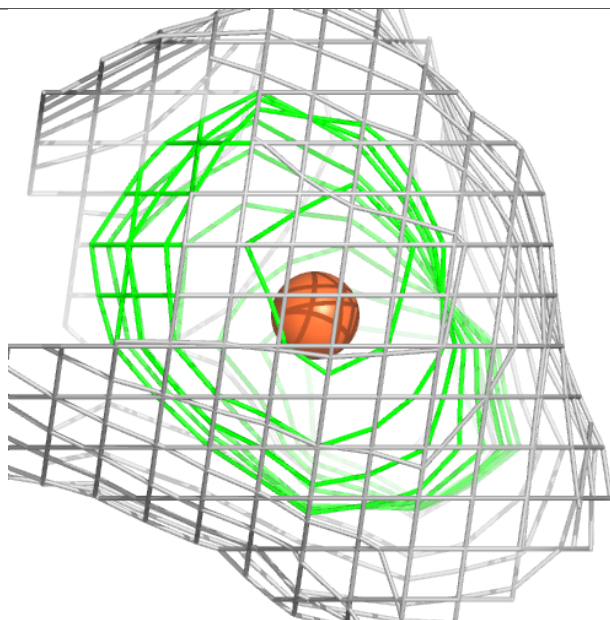
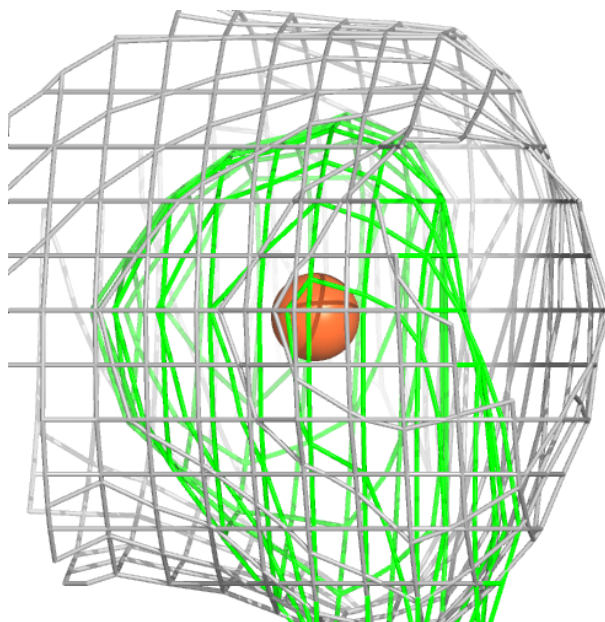
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	H	301	1/1	0.83	0.24	144,144,144,144	0
2	FE	G	301	1/1	0.95	0.15	66,66,66,66	0
2	FE	D	301	1/1	0.97	0.09	53,53,53,53	0
2	FE	F	301	1/1	0.98	0.11	55,55,55,55	0
2	FE	C	301	1/1	0.98	0.11	54,54,54,54	0
2	FE	A	301	1/1	0.98	0.11	49,49,49,49	0
2	FE	B	301	1/1	0.99	0.08	48,48,48,48	0
2	FE	E	301	1/1	0.99	0.12	44,44,44,44	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.

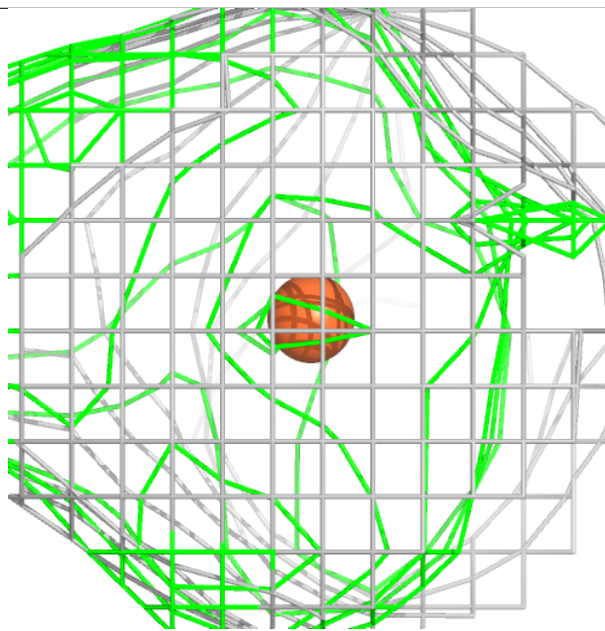
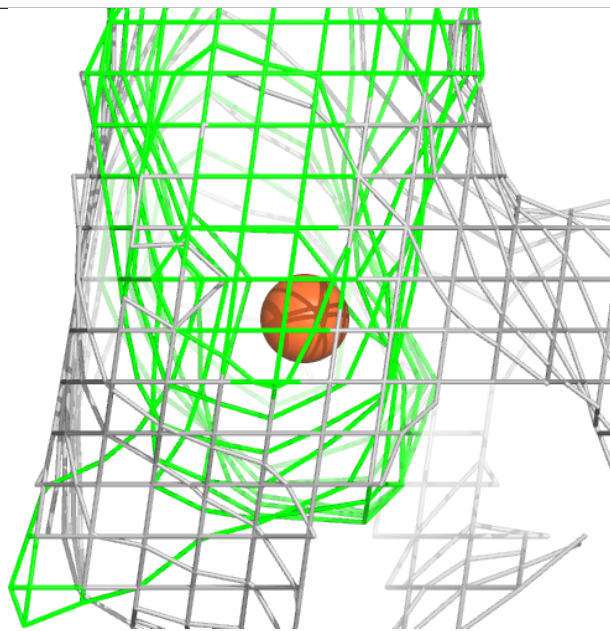
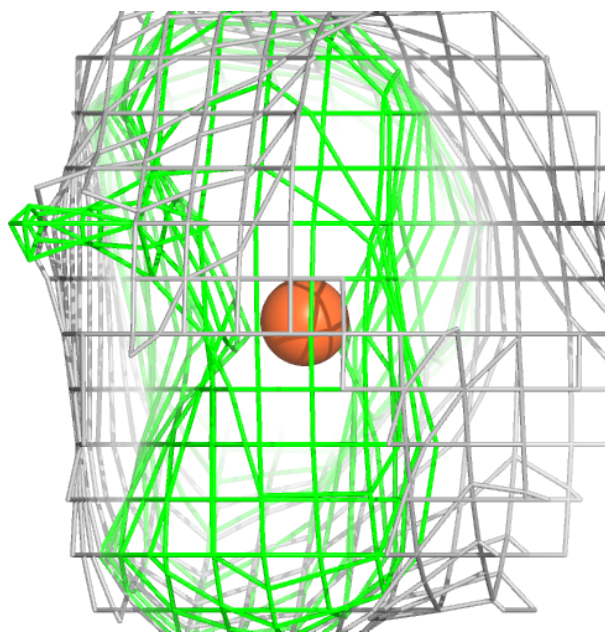
Electron density around FE H 301:

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



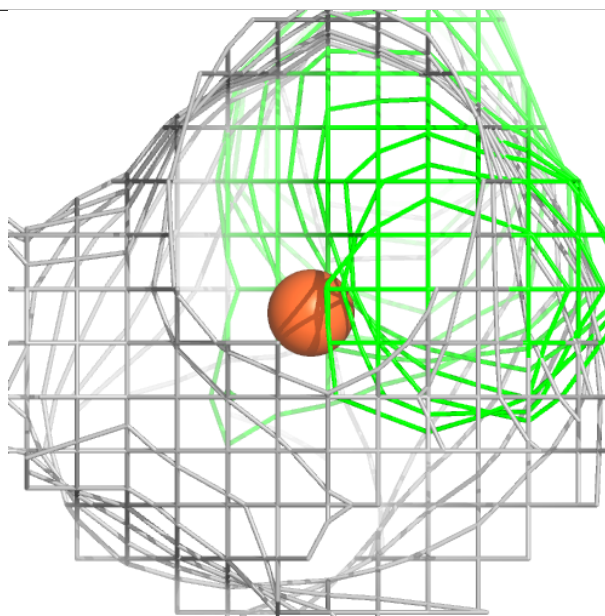
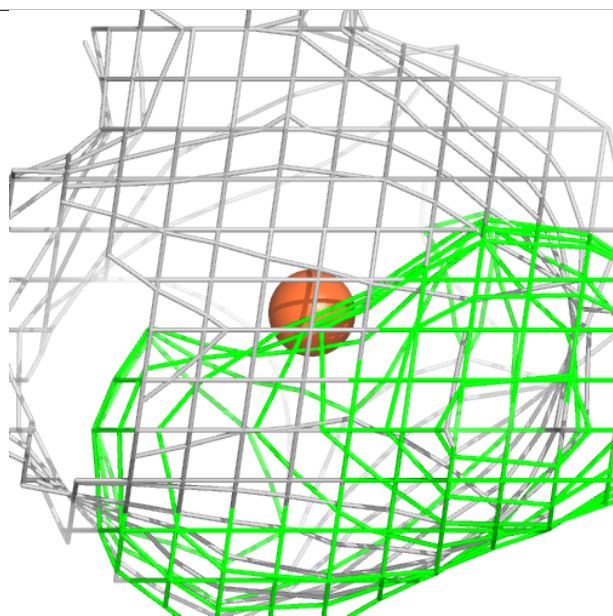
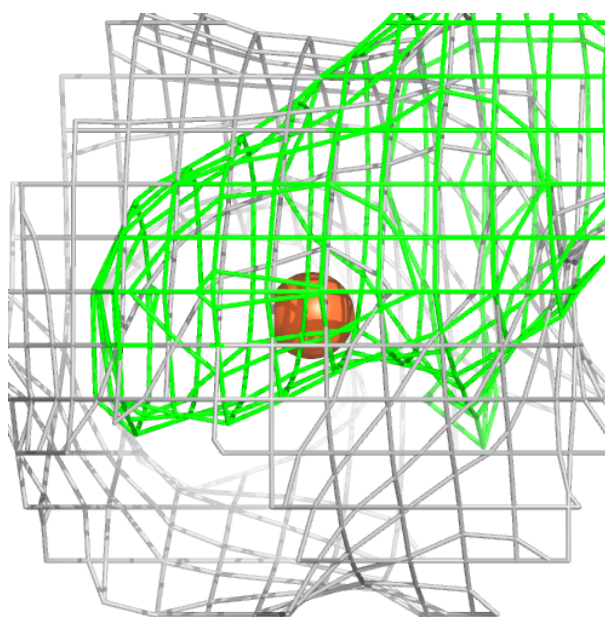
Electron density around FE G 301:

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



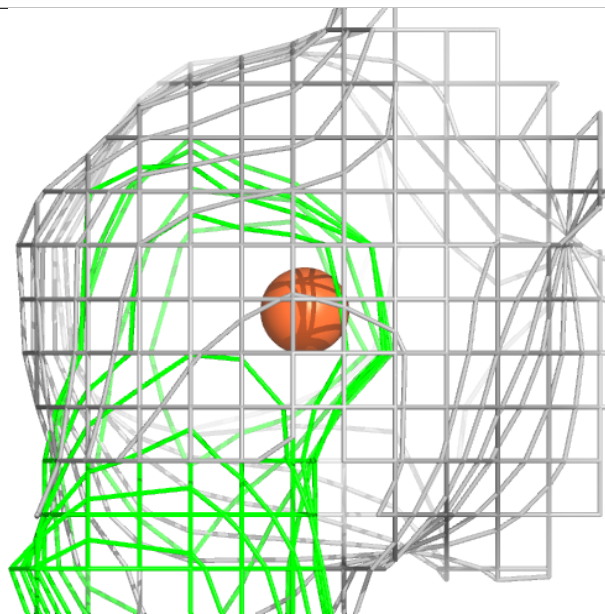
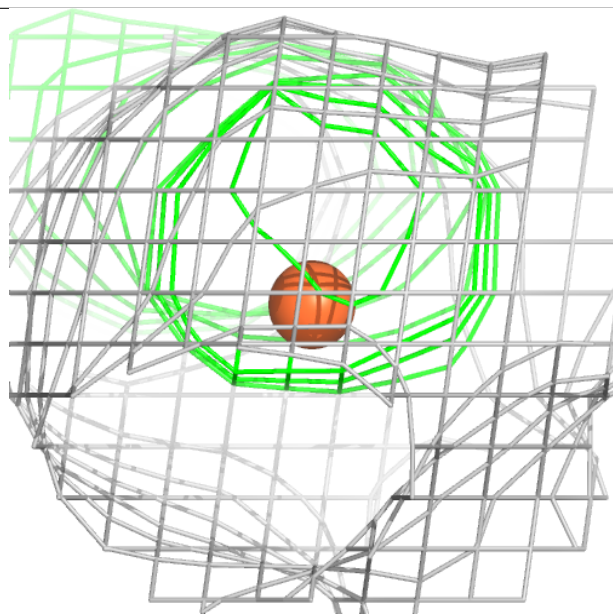
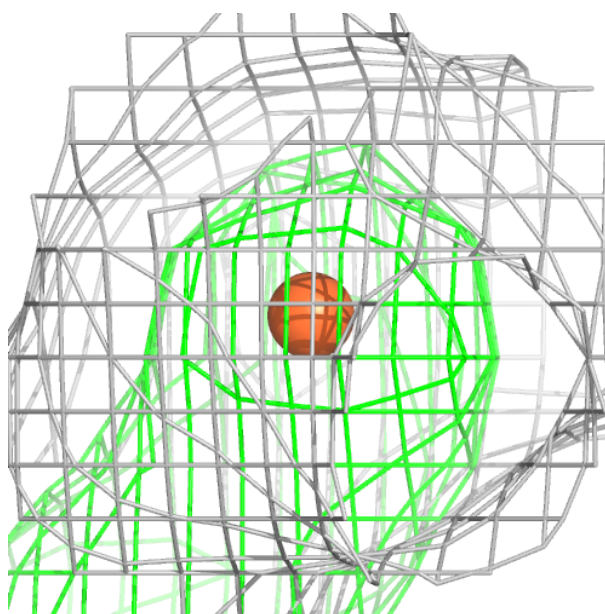
Electron density around FE D 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



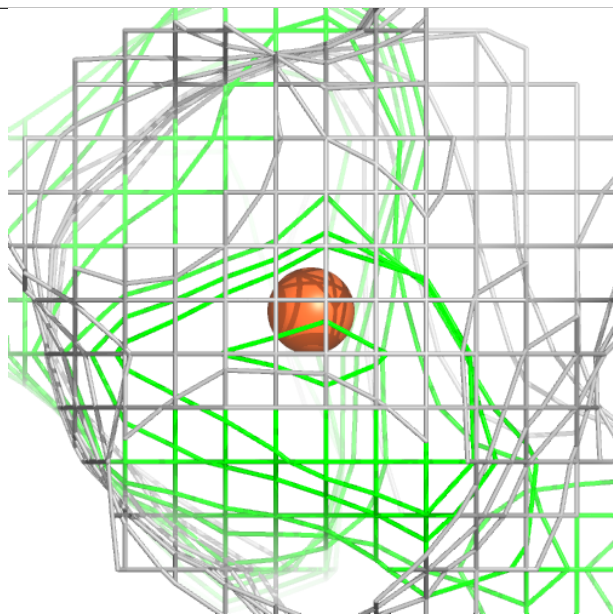
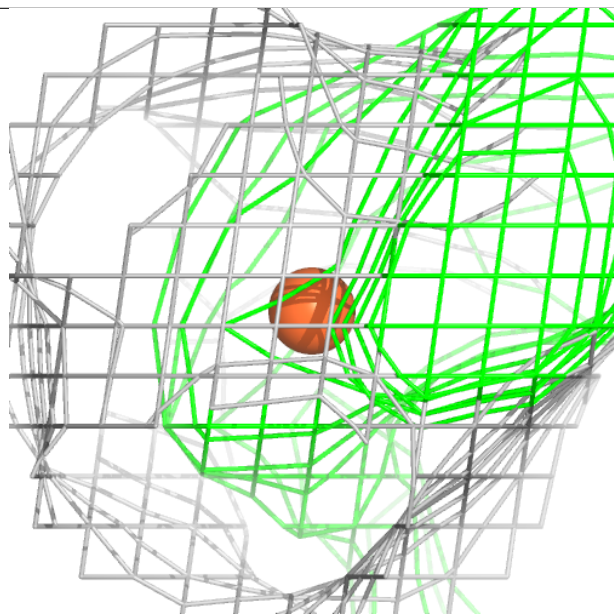
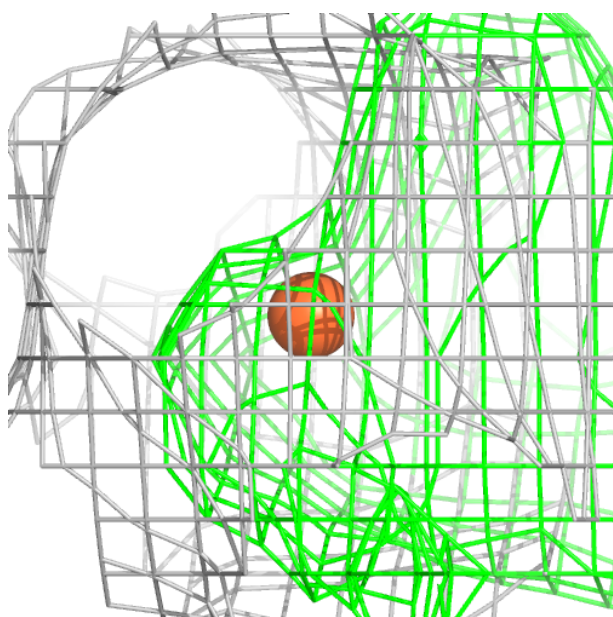
Electron density around FE F 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



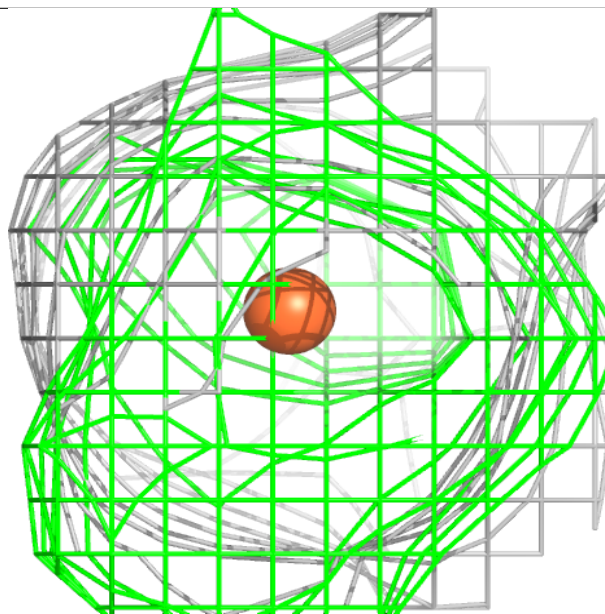
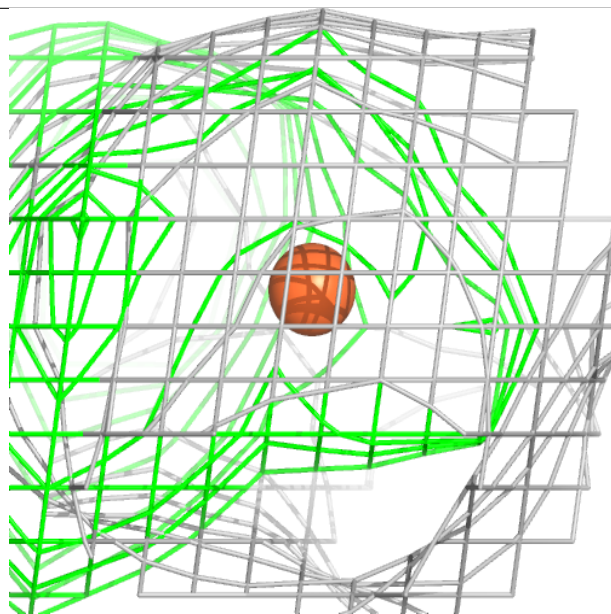
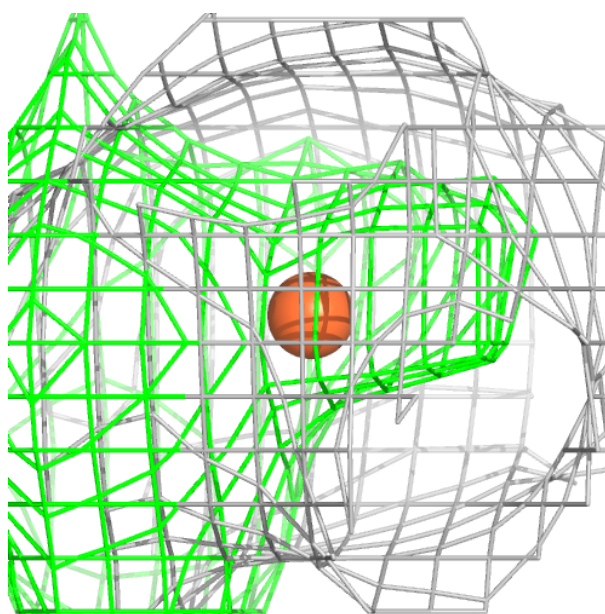
Electron density around FE C 301:

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



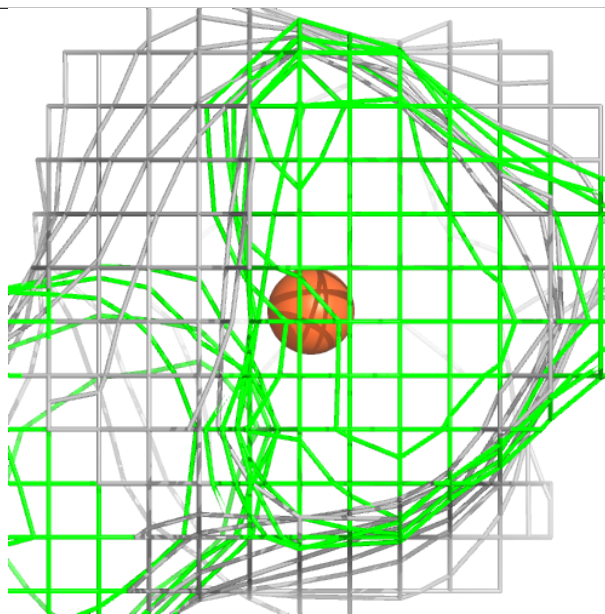
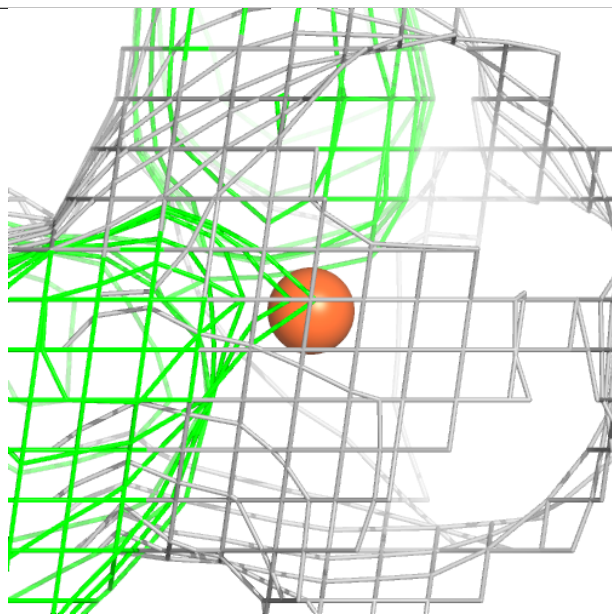
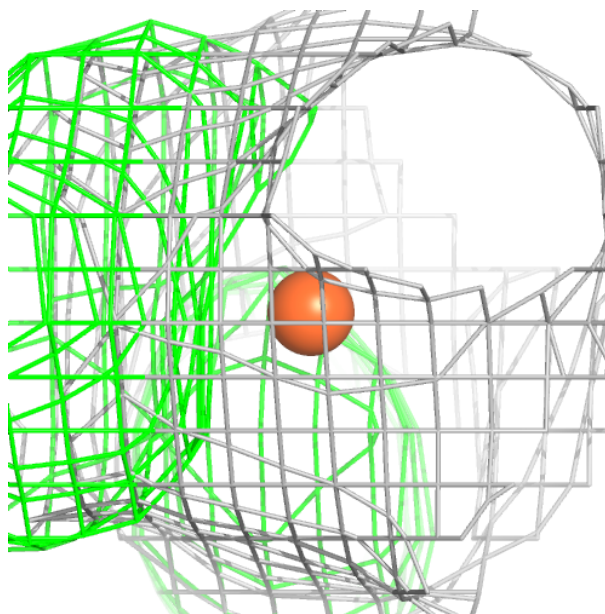
Electron density around FE A 301:

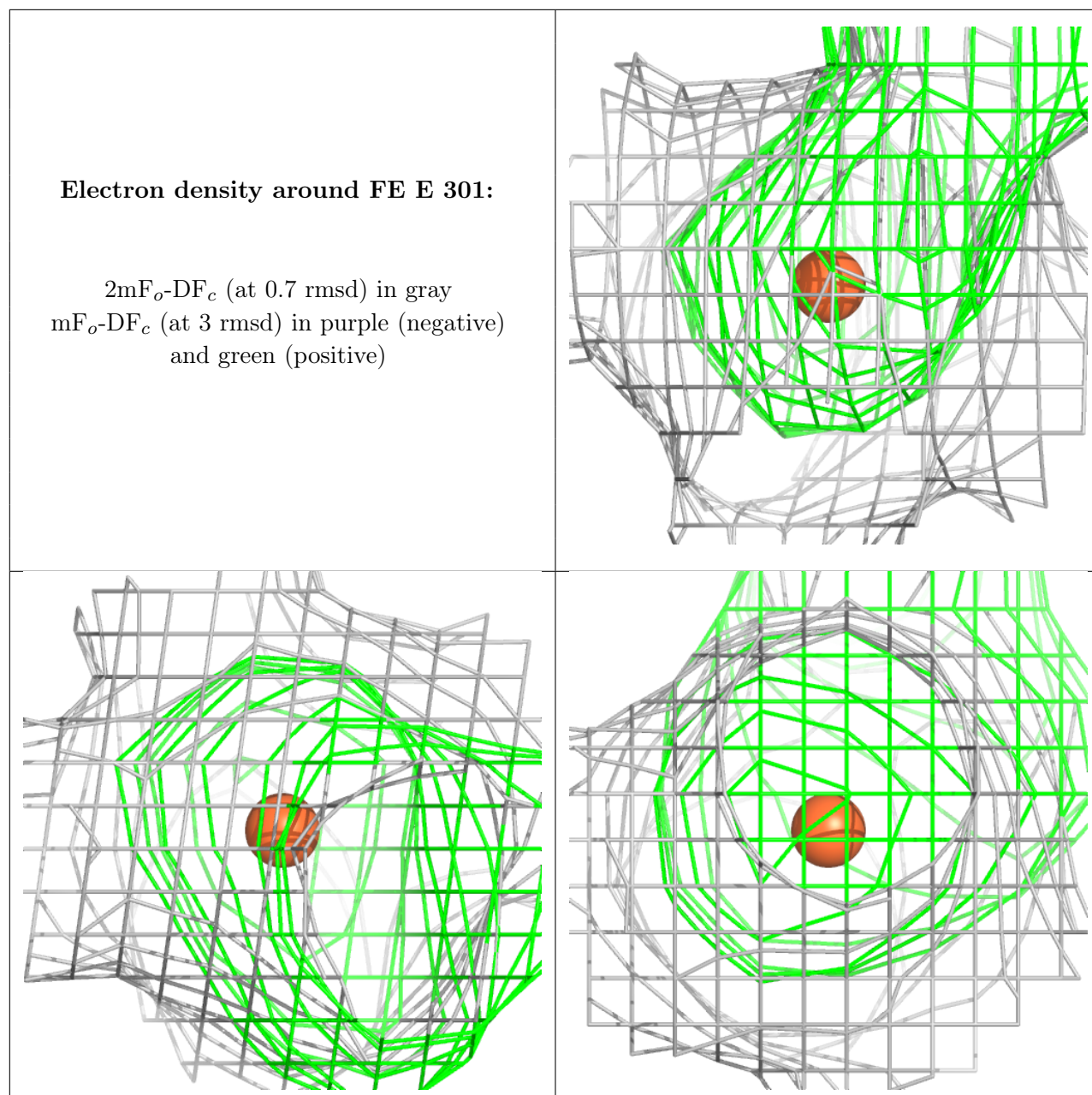
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.