



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:13 PM UTC

PDB ID : 8A90 / pdb_00008a90
Title : Crystal structure of FrsH
Authors : Schneberger, N.; Wirtz, D.A.; Cruesemann, M.; Hagelueken, G.
Deposited on : 2022-06-27
Resolution : 2.57 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

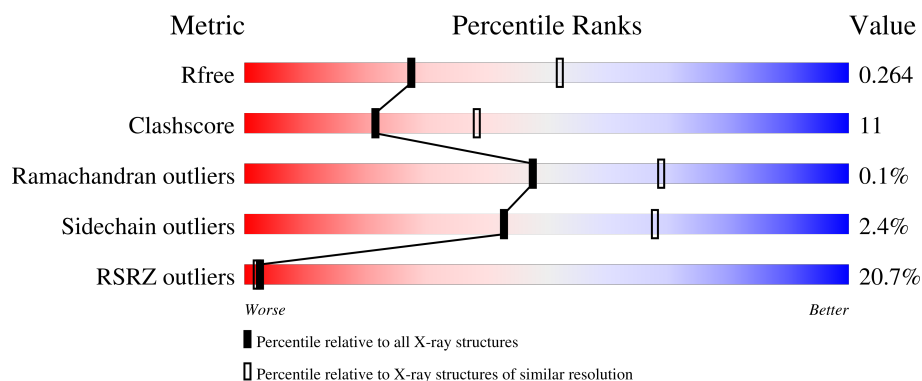
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	531	20% 76% 23% ..
1	B	531	21% 73% 25% .

2 Entry composition [i](#)

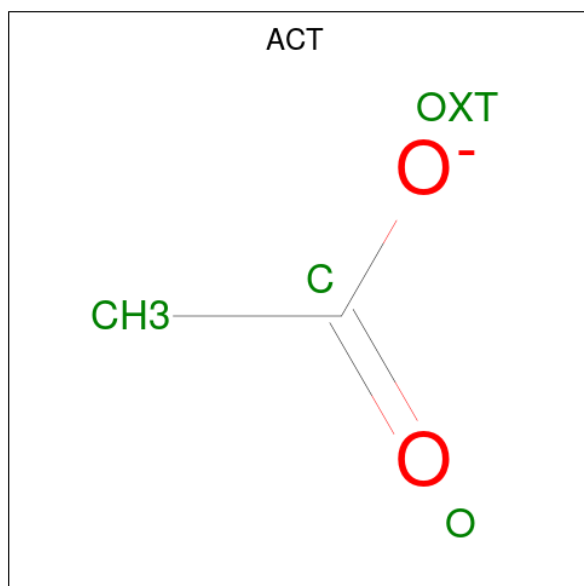
There are 6 unique types of molecules in this entry. The entry contains 8535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Non-heme diiron monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4218	2674	739	784	21			
1	B	530	Total	C	N	O	S	0	0	0
			4230	2682	741	786	21			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Fe 2 2	0	0
5	B	2	Total Fe 2 2	0	0

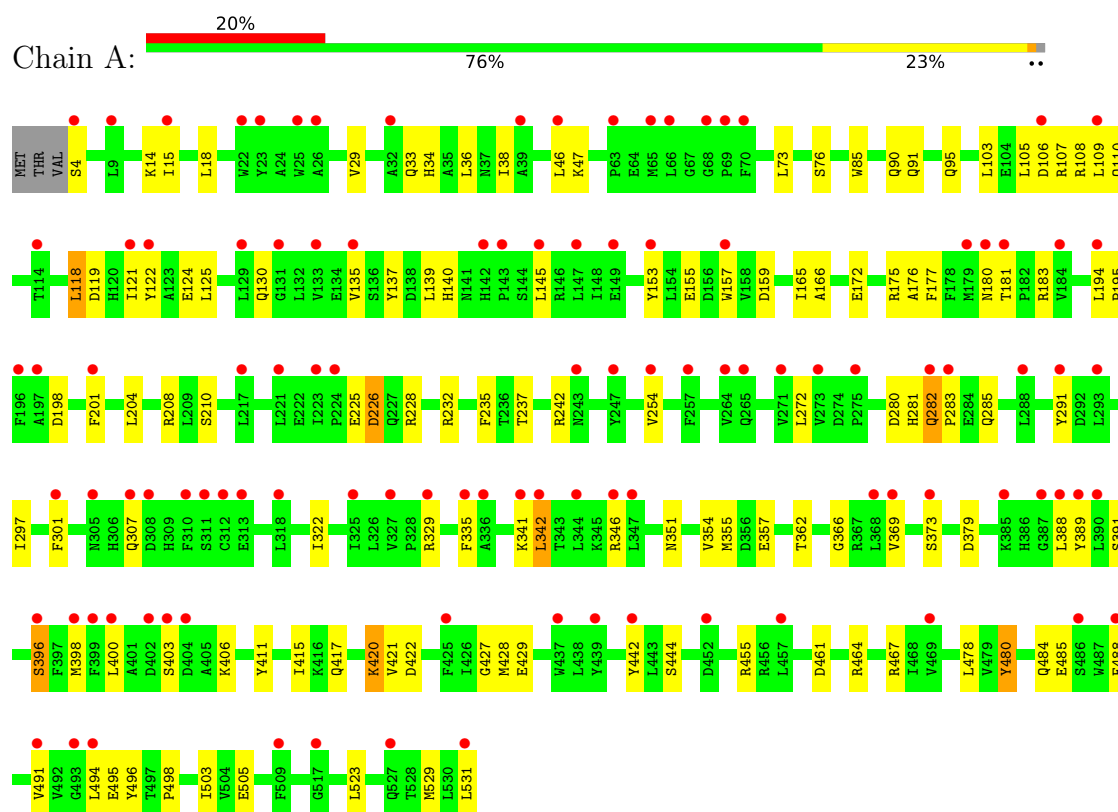
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total 36	O 36	0	0
6	B	19	Total 19	O 19	0	0

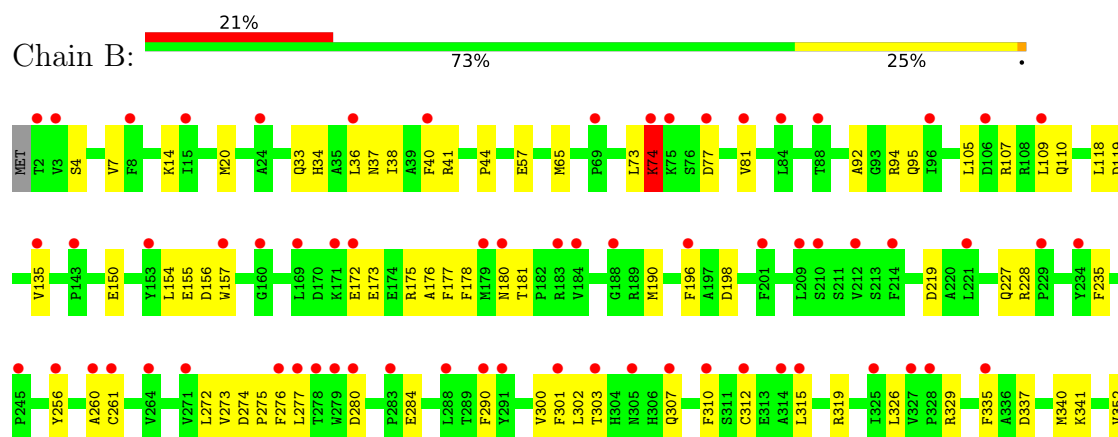
3 Residue-property plots

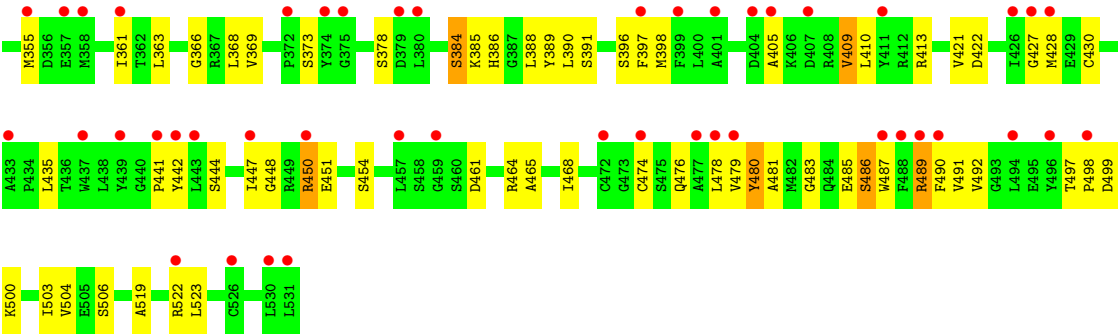
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Non-heme diiron monooxygenase



• Molecule 1: Non-heme diiron monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.72Å 117.72Å 234.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.57 48.02 – 2.57	Depositor EDS
% Data completeness (in resolution range)	87.5 (48.02-2.57) 81.5 (48.02-2.57)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.37 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20_4444	Depositor
R, R_{free}	0.217 , 0.264 0.217 , 0.264	Depositor DCC
R_{free} test set	1991 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.7	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	0.90	EDS
Total number of atoms	8535	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: GOL, O, FE, ACT

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	0.16	0/4321	0.41	2/5859 (0.0%)
1	B	0.20	1/4333 (0.0%)	0.53	8/5876 (0.1%)
All	All	0.18	1/8654 (0.0%)	0.48	10/11735 (0.1%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	489	ARG	CB-CG	-5.58	1.35	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ARG	CA-CB-CG	13.75	141.61	114.10
1	B	489	ARG	CB-CG-CD	-13.57	80.08	111.30
1	B	489	ARG	CB-CA-C	-12.70	89.75	110.84
1	A	282	GLN	CA-CB-CG	11.38	136.86	114.10
1	B	489	ARG	N-CA-C	6.96	122.79	111.37
1	B	489	ARG	CG-CD-NE	-6.90	96.82	112.00
1	A	282	GLN	CB-CA-C	6.28	122.55	110.17
1	B	489	ARG	CD-NE-CZ	-6.21	115.70	124.40
1	B	450	ARG	CB-CG-CD	-5.21	99.31	111.30
1	B	74	LYS	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	74	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4218	0	4113	86	0
1	B	4230	0	4125	103	0
2	A	8	0	6	0	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	36	0	0	2	0
6	B	19	0	0	1	0
All	All	8535	0	8268	180	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 11.

All (180) 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:B:173:GLU:HA	1:B:489:ARG:HH12	1.01	1.11
1:B:173:GLU:CA	1:B:489:ARG:HH12	1.70	1.02
1:B:173:GLU:HA	1:B:489:ARG:NH1	1.82	0.93
1:A:130:GLN:HB3	1:B:409:VAL:HG11	1.54	0.89
1:A:329:ARG:HD2	1:B:329:ARG:HD3	1.62	0.80
1:B:177:PHE:HB3	1:B:180:ASN:HB2	1.62	0.80
1:A:177:PHE:HB3	1:A:180:ASN:HB2	1.65	0.78
1:B:326:LEU:HB3	1:B:355:MET:HE2	1.72	0.72
1:B:173:GLU:C	1:B:489:ARG:HH12	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ARG:NH2	6:B:701:HOH:O	2.22	0.70
1:B:307:GLN:HG2	1:B:491:VAL:HG13	1.71	0.70
1:A:341:LYS:O	1:A:342:LEU:HB2	1.89	0.70
1:B:20:MET:HE1	1:B:92:ALA:HB2	1.74	0.69
1:A:155:GLU:OE1	1:B:413:ARG:NH1	2.27	0.68
1:B:489:ARG:HD2	1:B:490:PHE:HB3	1.76	0.67
1:B:483:GLY:HA3	1:B:492:VAL:HG11	1.74	0.67
1:B:57:GLU:OE2	1:B:74:LYS:HB2	1.95	0.67
1:B:105:LEU:HG	1:B:109:LEU:HD11	1.77	0.67
1:B:118:LEU:HD13	1:B:135:VAL:HG12	1.76	0.67
1:B:476:GLN:HG3	1:B:519:ALA:HB3	1.77	0.67
1:A:195:PRO:HG2	1:A:198:ASP:HB2	1.79	0.64
1:B:284:GLU:N	1:B:284:GLU:OE2	2.27	0.64
1:A:357:GLU:HB2	1:B:150:GLU:HG3	1.80	0.64
1:A:118:LEU:HD13	1:A:135:VAL:HG12	1.80	0.63
1:A:307:GLN:HG2	1:A:491:VAL:HG13	1.80	0.63
1:A:225:GLU:HA	1:A:228:ARG:HG3	1.80	0.63
1:A:398:MET:HE3	1:A:400:LEU:HD21	1.79	0.63
1:B:428:MET:HE2	1:B:506:SER:HA	1.80	0.63
1:B:487:TRP:HA	1:B:489:ARG:HH21	1.63	0.63
1:B:487:TRP:HA	1:B:489:ARG:NH2	2.13	0.62
1:B:497:THR:OG1	1:B:499:ASP:OD1	2.18	0.62
1:A:122:TYR:HA	1:A:125:LEU:HG	1.83	0.61
1:B:173:GLU:N	1:B:173:GLU:OE1	2.34	0.61
1:B:398:MET:HB2	1:B:421:VAL:HG11	1.82	0.61
1:B:405:ALA:HB2	1:B:468:ILE:HD11	1.80	0.61
1:A:226:ASP:N	1:A:226:ASP:OD1	2.35	0.59
1:A:29:VAL:O	1:A:346:ARG:NH1	2.36	0.59
1:A:254:VAL:HG13	1:A:531:LEU:HD21	1.84	0.58
1:B:173:GLU:C	1:B:489:ARG:NH1	2.61	0.58
1:A:398:MET:HB2	1:A:421:VAL:HG11	1.84	0.57
1:B:476:GLN:HG2	1:B:478:LEU:CD1	2.34	0.57
1:A:103:LEU:HD13	1:A:444:SER:HA	1.87	0.57
1:B:373:SER:O	1:B:385:LYS:NZ	2.37	0.57
1:B:94:ARG:HD2	1:B:157:TRP:HB3	1.86	0.57
1:A:341:LYS:HD3	1:A:354:VAL:HG21	1.87	0.57
1:A:341:LYS:HD3	1:A:354:VAL:CG2	2.35	0.56
1:B:173:GLU:CA	1:B:489:ARG:NH1	2.54	0.56
1:B:465:ALA:HA	1:B:468:ILE:HD12	1.87	0.55
1:A:33:GLN:NE2	1:A:335:PHE:O	2.29	0.55
1:B:14:LYS:HG2	1:B:175:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:GLN:HG2	1:B:478:LEU:HD11	1.89	0.54
1:A:34:HIS:CE1	1:A:38:ILE:HD11	2.41	0.54
1:B:107:ARG:NH1	1:B:444:SER:O	2.37	0.54
1:B:107:ARG:HG3	1:B:444:SER:HB2	1.91	0.53
1:A:242:ARG:HD2	1:A:291:TYR:O	2.09	0.53
1:B:34:HIS:CE1	1:B:38:ILE:HD11	2.43	0.53
1:A:406:LYS:NZ	1:B:119:ASP:OD1	2.34	0.53
1:A:379:ASP:HB2	1:A:455:ARG:HG2	1.90	0.53
1:A:108:ARG:HH22	1:A:124:GLU:HG3	1.74	0.52
1:A:464:ARG:HA	1:A:467:ARG:HD2	1.91	0.52
1:A:428:MET:HE1	1:A:505:GLU:HB3	1.91	0.52
1:B:33:GLN:O	1:B:37:ASN:ND2	2.42	0.52
1:A:498:PRO:HA	1:A:503:ILE:HG21	1.92	0.51
1:A:282:GLN:OE1	1:A:285:GLN:OE1	2.29	0.51
1:B:363:LEU:HD11	1:B:368:LEU:HD23	1.93	0.51
1:A:411:TYR:O	1:A:415:ILE:HG12	2.11	0.50
1:B:219:ASP:OD1	1:B:228:ARG:NH2	2.44	0.50
1:A:14:LYS:NZ	1:A:280:ASP:OD1	2.43	0.50
1:A:90:GLN:NE2	1:A:91:GLN:HG3	2.26	0.50
1:A:118:LEU:HD21	1:A:137:TYR:CZ	2.47	0.50
1:B:14:LYS:NZ	1:B:280:ASP:OD1	2.40	0.50
1:A:121:ILE:HG21	1:A:135:VAL:HG21	1.94	0.50
1:A:73:LEU:HG	1:A:181:THR:HG23	1.93	0.50
1:B:341:LYS:HA	1:B:352:VAL:HG11	1.93	0.50
1:A:107:ARG:NH2	6:A:702:HOH:O	2.42	0.49
1:B:14:LYS:HE2	1:B:172:GLU:HG3	1.95	0.49
1:B:172:GLU:O	1:B:489:ARG:CZ	2.60	0.49
1:B:256:TYR:CE2	1:B:523:LEU:HB3	2.49	0.48
1:A:18:LEU:HD11	1:A:166:ALA:HB2	1.96	0.48
1:A:398:MET:SD	1:A:421:VAL:HG21	2.54	0.48
1:B:92:ALA:HB1	1:B:95:GLN:HB2	1.96	0.47
1:B:378:SER:HB3	1:B:435:LEU:HD12	1.96	0.47
1:A:90:GLN:HE21	1:A:91:GLN:HG3	1.80	0.47
1:A:46:LEU:HB3	1:A:85:TRP:HB2	1.96	0.47
1:A:282:GLN:HA	1:A:283:PRO:HD3	1.62	0.47
1:A:14:LYS:HG2	1:A:175:ARG:HH21	1.79	0.47
1:B:40:PHE:HB2	1:B:441:PRO:HB3	1.97	0.47
1:B:479:VAL:HB	1:B:522:ARG:HA	1.97	0.47
1:A:165:ILE:HD11	1:A:201:PHE:CE2	2.50	0.47
1:B:173:GLU:OE2	1:B:486:SER:HB2	2.15	0.47
1:B:65:MET:HE2	1:B:65:MET:HB3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:O	1:A:110:GLN:HG2	2.16	0.46
1:A:366:GLY:HA3	1:A:391:SER:O	2.15	0.46
1:A:485:GLU:HB2	1:A:488:PHE:CE2	2.50	0.46
1:A:494:LEU:HD22	1:A:495:GLU:O	2.14	0.46
1:B:173:GLU:O	1:B:489:ARG:NH1	2.48	0.46
1:B:41:ARG:HB2	1:B:441:PRO:HG3	1.97	0.46
1:B:485:GLU:N	1:B:485:GLU:OE1	2.48	0.46
1:B:421:VAL:O	1:B:474:CYS:HA	2.15	0.46
1:B:451:GLU:OE2	1:B:451:GLU:N	2.33	0.46
1:A:103:LEU:O	1:A:107:ARG:HG3	2.16	0.46
1:B:390:LEU:HB3	1:B:397:PHE:HB2	1.96	0.46
1:B:41:ARG:C	1:B:44:PRO:HD2	2.41	0.46
1:B:198:ASP:O	1:B:319:ARG:NH2	2.46	0.45
1:A:95:GLN:HG3	1:A:157:TRP:CZ3	2.51	0.45
1:A:281:HIS:O	1:A:282:GLN:HB2	2.17	0.45
1:A:429:GLU:OE2	1:A:496:TYR:OH	2.32	0.45
1:B:105:LEU:O	1:B:109:LEU:HD12	2.17	0.45
1:A:165:ILE:HD12	1:A:194:LEU:HB3	1.97	0.45
1:B:260:ALA:HB2	1:B:481:ALA:HB2	1.98	0.45
1:A:396:SER:HB2	1:A:422:ASP:H	1.82	0.45
1:A:428:MET:HE2	1:A:428:MET:HB3	1.71	0.45
1:A:478:LEU:HB3	1:A:523:LEU:HD21	1.97	0.45
1:A:232:ARG:NH1	1:A:235:PHE:O	2.50	0.45
1:A:105:LEU:O	1:A:109:LEU:HG	2.17	0.44
1:A:272:LEU:HB2	1:A:297:ILE:HG21	1.99	0.44
1:A:176:ALA:O	1:A:183:ARG:NH2	2.50	0.44
1:A:417:GLN:CD	1:B:154:LEU:HD13	2.43	0.44
1:A:172:GLU:HG2	1:A:175:ARG:HE	1.83	0.44
1:B:155:GLU:HG3	1:B:156:ASP:N	2.33	0.44
1:B:337:ASP:OD1	1:B:384:SER:HB2	2.18	0.44
1:A:47:LYS:HG3	1:A:85:TRP:CZ2	2.53	0.44
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.74	0.44
1:A:153:TYR:CE1	1:A:342:LEU:HD23	2.53	0.44
1:B:366:GLY:HA3	1:B:391:SER:O	2.18	0.44
1:B:500:LYS:O	1:B:504:VAL:HG23	2.17	0.44
1:B:489:ARG:NH1	1:B:489:ARG:CG	2.78	0.43
1:B:190:MET:HE1	1:B:227:GLN:O	2.18	0.43
1:B:196:PHE:O	1:B:319:ARG:NH1	2.48	0.43
1:B:261:CYS:HA	1:B:273:VAL:O	2.18	0.43
1:B:361:ILE:HG13	1:B:368:LEU:HG	1.99	0.43
1:A:194:LEU:HD12	1:A:195:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HB3	1:B:300:VAL:HG22	2.00	0.43
1:B:77:ASP:O	1:B:81:VAL:HG23	2.18	0.43
1:B:274:ASP:OD1	1:B:303:THR:HG23	2.19	0.43
1:A:322:ILE:O	1:A:351:ASN:ND2	2.51	0.43
1:A:140:HIS:CD2	1:B:110:GLN:HG3	2.53	0.43
1:B:284:GLU:H	1:B:284:GLU:CD	2.25	0.43
1:B:489:ARG:CD	1:B:490:PHE:HB3	2.46	0.43
1:B:277:LEU:HD13	1:B:290:PHE:HD1	1.83	0.43
1:B:310:PHE:CD2	1:B:340:MET:HE3	2.54	0.43
1:A:254:VAL:HG22	1:A:529:MET:HB2	2.01	0.42
1:B:396:SER:OG	1:B:422:ASP:N	2.51	0.42
1:A:119:ASP:OD1	1:A:119:ASP:N	2.52	0.42
1:B:7:VAL:CG2	1:B:235:PHE:HB3	2.48	0.42
1:B:272:LEU:HG	1:B:275:PRO:HG3	2.01	0.42
1:B:310:PHE:HD2	1:B:340:MET:HE3	1.85	0.42
1:A:428:MET:HE3	1:A:461:ASP:HA	2.02	0.42
1:A:329:ARG:CD	1:B:329:ARG:HD3	2.43	0.42
1:A:15:ILE:HG23	1:A:165:ILE:CG2	2.50	0.42
1:B:301:PHE:CE1	1:B:388:LEU:HB2	2.55	0.42
1:A:15:ILE:HG23	1:A:165:ILE:HG23	2.02	0.42
1:A:420:LYS:HG2	1:A:421:VAL:N	2.35	0.42
1:A:301:PHE:CE2	1:A:388:LEU:HB2	2.55	0.41
1:B:178:PHE:CZ	1:B:307:GLN:HG3	2.54	0.41
1:A:139:LEU:HD11	1:B:335:PHE:HB2	2.02	0.41
1:B:36:LEU:HD23	1:B:442:TYR:HA	2.01	0.41
1:B:276:PHE:CZ	1:B:491:VAL:HG21	2.55	0.41
1:A:36:LEU:HD13	1:A:442:TYR:HD1	1.85	0.41
1:A:484:GLN:OE1	1:A:496:TYR:N	2.38	0.41
1:B:176:ALA:O	1:B:490:PHE:HB2	2.20	0.41
1:B:302:LEU:O	1:B:386:HIS:NE2	2.49	0.41
1:B:427:GLY:HA2	1:B:480:TYR:O	2.20	0.41
1:A:15:ILE:HD13	1:A:208:ARG:NH2	2.36	0.41
1:B:73:LEU:HG	1:B:181:THR:HG23	2.01	0.41
1:A:369:VAL:HB	1:A:389:TYR:HB3	2.03	0.41
1:B:315:LEU:HD23	1:B:315:LEU:HA	1.86	0.41
1:B:498:PRO:HA	1:B:503:ILE:HG21	2.02	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.87	0.41
1:A:159:ASP:N	1:A:159:ASP:OD1	2.54	0.41
1:A:427:GLY:O	6:A:701:HOH:O	2.22	0.41
1:B:447:ILE:HD12	1:B:448:GLY:H	1.85	0.41
1:B:489:ARG:HD2	1:B:490:PHE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLY:HA2	1:A:480:TYR:O	2.21	0.41
1:B:369:VAL:HB	1:B:389:TYR:HB3	2.03	0.40
1:B:461:ASP:OD1	1:B:464:ARG:HG3	2.22	0.40
1:A:400:LEU:HB3	1:A:403:SER:OG	2.21	0.40
1:B:326:LEU:HB3	1:B:355:MET:CE	2.46	0.40
1:B:276:PHE:HZ	1:B:491:VAL:HG21	1.86	0.40
1:A:355:MET:HE2	1:A:355:MET:HB3	1.82	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	526/531 (99%)	508 (97%)	17 (3%)	1 (0%)	43	63
1	B	528/531 (99%)	509 (96%)	19 (4%)	0	100	100
All	All	1054/1062 (99%)	1017 (96%)	36 (3%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	LEU

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	454/457 (99%)	442 (97%)	12 (3%)	40	66
1	B	455/457 (100%)	445 (98%)	10 (2%)	45	70
All	All	909/914 (100%)	887 (98%)	22 (2%)	43	68

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	76	SER
1	A	118	LEU
1	A	204	LEU
1	A	210	SER
1	A	226	ASP
1	A	237	THR
1	A	362	THR
1	A	373	SER
1	A	396	SER
1	A	420	LYS
1	A	480	TYR
1	B	4	SER
1	B	312	CYS
1	B	384	SER
1	B	409	VAL
1	B	410	LEU
1	B	430	CYS
1	B	450	ARG
1	B	454	SER
1	B	480	TYR
1	B	486	SER

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

Mol	Chain	Res	Type
1	A	90	GLN
1	A	281	HIS
1	A	309	HIS
1	A	476	GLN
1	A	527	GLN
1	B	110	GLN
1	B	241	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	601	-	3,3,3	1.22	0	3,3,3	1.49	0
3	GOL	A	603	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	B	601	-	5,5,5	0.94	0	5,5,5	1.06	0
3	GOL	A	602	-	5,5,5	0.94	0	5,5,5	1.08	0
2	ACT	A	604	-	3,3,3	1.38	0	3,3,3	1.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-
3	GOL	B	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	GOL	C1-C2-C3-O3
3	B	601	GOL	O2-C2-C3-O3

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	528/531 (99%)	1.39	108 (20%) 2 2	40, 55, 76, 96	0
1	B	530/531 (99%)	1.44	111 (20%) 2 2	39, 59, 83, 113	0
All	All	1058/1062 (99%)	1.41	219 (20%) 2 2	39, 56, 80, 113	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	ARG	5.7
1	A	341	LYS	5.1
1	B	399	PHE	4.4
1	B	531	LEU	4.3
1	B	442	TYR	4.1
1	B	135	VAL	4.1
1	B	443	LEU	4.1
1	B	276	PHE	4.0
1	B	143	PRO	4.0
1	A	147	LEU	3.9
1	A	387	GLY	3.8
1	B	3	VAL	3.7
1	B	404	ASP	3.7
1	A	149	GLU	3.6
1	B	335	PHE	3.6
1	A	531	LEU	3.6
1	B	490	PHE	3.6
1	B	288	LEU	3.5
1	B	307	GLN	3.4
1	A	335	PHE	3.4
1	B	401	ALA	3.3
1	A	369	VAL	3.3
1	A	494	LEU	3.2
1	A	398	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	VAL	3.2
1	A	221	LEU	3.2
1	B	447	ILE	3.2
1	A	282	GLN	3.1
1	B	428	MET	3.1
1	B	427	GLY	3.1
1	B	2	THR	3.1
1	B	361	ILE	3.1
1	B	188	GLY	3.1
1	A	399	PHE	3.1
1	B	277	LEU	3.1
1	A	312	CYS	3.1
1	B	441	PRO	3.1
1	B	426	ILE	3.1
1	B	283	PRO	3.0
1	B	172	GLU	3.0
1	A	109	LEU	3.0
1	A	145	LEU	3.0
1	A	194	LEU	2.9
1	A	404	ASP	2.9
1	A	65	MET	2.9
1	A	329	ARG	2.9
1	B	450	ARG	2.9
1	B	372	PRO	2.9
1	A	293	LEU	2.9
1	A	201	PHE	2.9
1	A	243	ASN	2.9
1	A	26	ALA	2.8
1	A	389	TYR	2.8
1	B	479	VAL	2.8
1	B	411	TYR	2.8
1	A	342	LEU	2.8
1	A	131	GLY	2.8
1	B	496	TYR	2.8
1	A	4	SER	2.7
1	A	224	PRO	2.7
1	B	234	TYR	2.7
1	B	315	LEU	2.7
1	A	325	ILE	2.7
1	A	39	ALA	2.7
1	A	437	TRP	2.7
1	B	256	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	374	TYR	2.7
1	A	181	THR	2.7
1	B	24	ALA	2.7
1	B	160	GLY	2.7
1	B	439	TYR	2.7
1	B	437	TRP	2.7
1	A	265	GLN	2.7
1	B	77	ASP	2.6
1	A	106	ASP	2.6
1	A	275	PRO	2.6
1	B	328	PRO	2.6
1	B	312	CYS	2.6
1	B	209	LEU	2.6
1	B	488	PHE	2.6
1	A	491	VAL	2.6
1	A	396	SER	2.6
1	A	63	PRO	2.6
1	A	68	GLY	2.6
1	A	179	MET	2.6
1	A	310	PHE	2.6
1	A	70	PHE	2.5
1	A	217	LEU	2.5
1	A	385	LYS	2.5
1	A	388	LEU	2.5
1	B	477	ALA	2.5
1	A	403	SER	2.5
1	A	346	ARG	2.5
1	A	517	GLY	2.5
1	B	357	GLU	2.5
1	A	157	TRP	2.5
1	A	9	LEU	2.5
1	B	290	PHE	2.5
1	A	133	VAL	2.5
1	B	327	VAL	2.5
1	B	36	LEU	2.5
1	A	254	VAL	2.5
1	A	273	VAL	2.5
1	B	355	MET	2.5
1	B	498	PRO	2.4
1	B	169	LEU	2.4
1	B	397	PHE	2.4
1	B	74	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	526	CYS	2.4
1	A	15	ILE	2.4
1	A	344	LEU	2.4
1	B	15	ILE	2.4
1	B	325	ILE	2.4
1	A	307	GLN	2.4
1	A	439	TYR	2.4
1	B	301	PHE	2.4
1	B	405	ALA	2.4
1	B	487	TRP	2.4
1	A	143	PRO	2.4
1	B	109	LEU	2.4
1	B	201	PHE	2.4
1	B	433	ALA	2.4
1	B	303	THR	2.3
1	B	375	GLY	2.3
1	A	66	LEU	2.3
1	A	129	LEU	2.3
1	A	196	PHE	2.3
1	A	264	VAL	2.3
1	B	407	ASP	2.3
1	B	472	CYS	2.3
1	B	69	PRO	2.3
1	B	210	SER	2.3
1	A	347	LEU	2.3
1	A	400	LEU	2.3
1	B	75	LYS	2.3
1	B	459	GLY	2.3
1	A	288	LEU	2.3
1	B	380	LEU	2.3
1	B	478	LEU	2.3
1	B	379	ASP	2.3
1	B	184	VAL	2.3
1	A	442	TYR	2.3
1	B	180	ASN	2.2
1	B	474	CYS	2.3
1	A	46	LEU	2.2
1	B	457	LEU	2.2
1	B	157	TRP	2.2
1	A	425	PHE	2.2
1	A	509	PHE	2.2
1	A	271	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	522	ARG	2.2
1	A	197	ALA	2.2
1	B	314	ALA	2.2
1	A	247	TYR	2.2
1	B	171	LYS	2.2
1	A	121	ILE	2.2
1	A	488	PHE	2.2
1	B	310	PHE	2.2
1	B	305	ASN	2.2
1	A	23	TYR	2.2
1	B	291	TYR	2.2
1	A	318	LEU	2.2
1	B	96	ILE	2.2
1	B	214	PHE	2.2
1	B	229	PRO	2.2
1	B	212	VAL	2.2
1	A	142	HIS	2.2
1	A	368	LEU	2.2
1	A	457	LEU	2.2
1	B	84	LEU	2.2
1	A	486	SER	2.2
1	A	308	ASP	2.2
1	A	327	VAL	2.1
1	B	81	VAL	2.1
1	A	114	THR	2.1
1	A	390	LEU	2.1
1	A	153	TYR	2.1
1	A	402	ASP	2.1
1	B	264	VAL	2.1
1	B	260	ALA	2.1
1	A	305	ASN	2.1
1	A	313	GLU	2.1
1	A	301	PHE	2.1
1	A	32	ALA	2.1
1	A	257	PHE	2.1
1	A	527	GLN	2.1
1	B	40	PHE	2.1
1	B	271	VAL	2.1
1	A	336	ALA	2.1
1	B	183	ARG	2.1
1	A	122	TYR	2.1
1	A	291	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	452	ASP	2.1
1	A	373	SER	2.1
1	A	69	PRO	2.1
1	B	261	CYS	2.1
1	B	358	MET	2.1
1	A	184	VAL	2.0
1	B	8	PHE	2.0
1	B	221	LEU	2.0
1	B	494	LEU	2.0
1	B	530	LEU	2.0
1	A	22	TRP	2.0
1	A	25	TRP	2.0
1	B	88	THR	2.0
1	B	106	ASP	2.0
1	A	283	PRO	2.0
1	B	153	TYR	2.0
1	B	179	MET	2.0
1	A	469	VAL	2.0
1	B	196	PHE	2.0
1	A	180	ASN	2.0
1	A	493	GLY	2.0
1	A	223	ILE	2.0
1	B	278	THR	2.0
1	B	279	TRP	2.0
1	B	245	PRO	2.0
1	B	280	ASP	2.0
1	A	311	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 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,

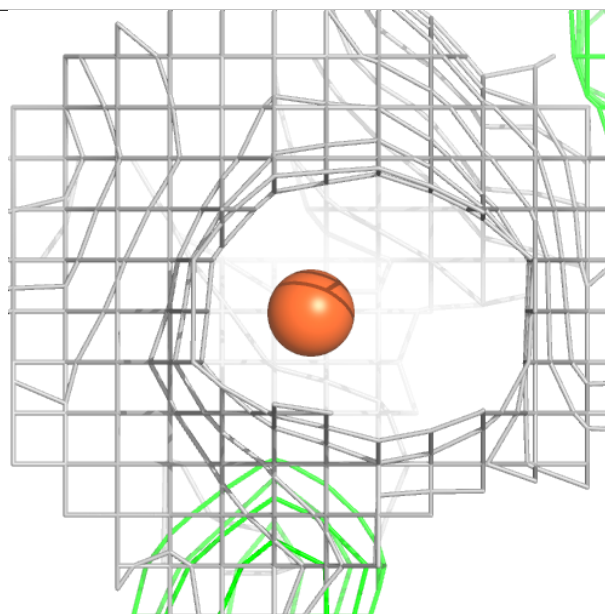
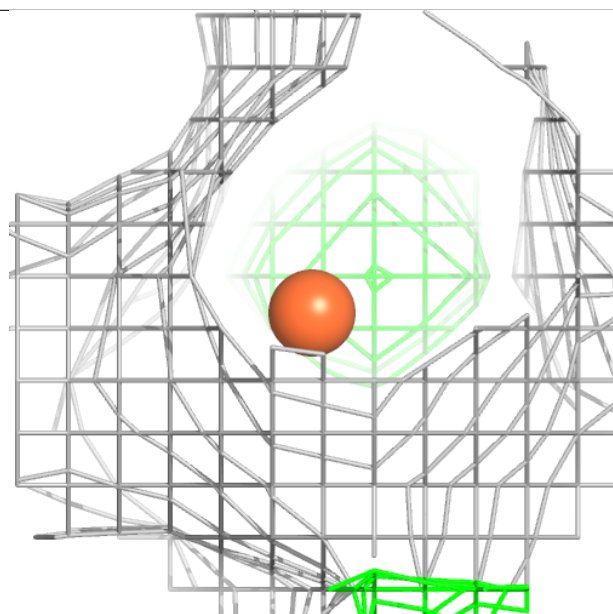
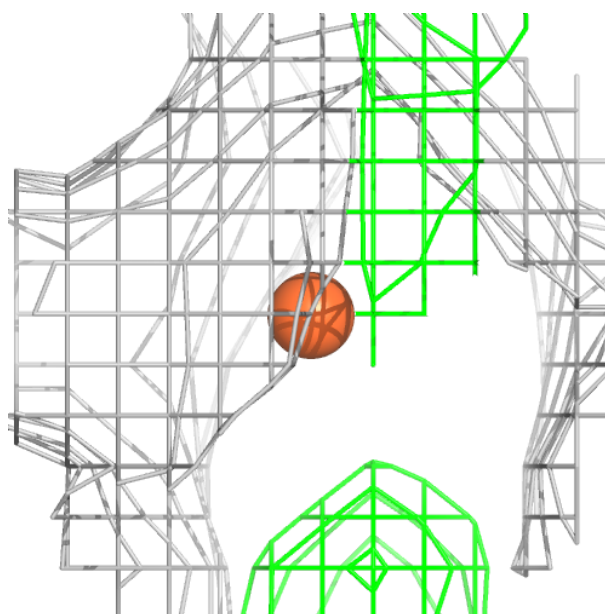
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	O	B	602	1/1	0.43	0.38	69,69,69,69	0
3	GOL	B	601	6/6	0.54	0.29	76,78,84,98	0
3	GOL	A	602	6/6	0.70	0.24	66,79,84,93	0
2	ACT	A	604	4/4	0.85	0.12	53,61,87,88	0
3	GOL	A	603	6/6	0.85	0.18	57,69,78,88	0
2	ACT	A	601	4/4	0.86	0.18	69,71,74,88	0
4	O	A	605	1/1	0.90	0.20	54,54,54,54	0
5	FE	B	603	1/1	0.98	0.03	46,46,46,46	0
5	FE	A	607	1/1	0.99	0.05	38,38,38,38	0
5	FE	A	606	1/1	0.99	0.11	43,43,43,43	0
5	FE	B	604	1/1	0.99	0.03	51,51,51,51	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.

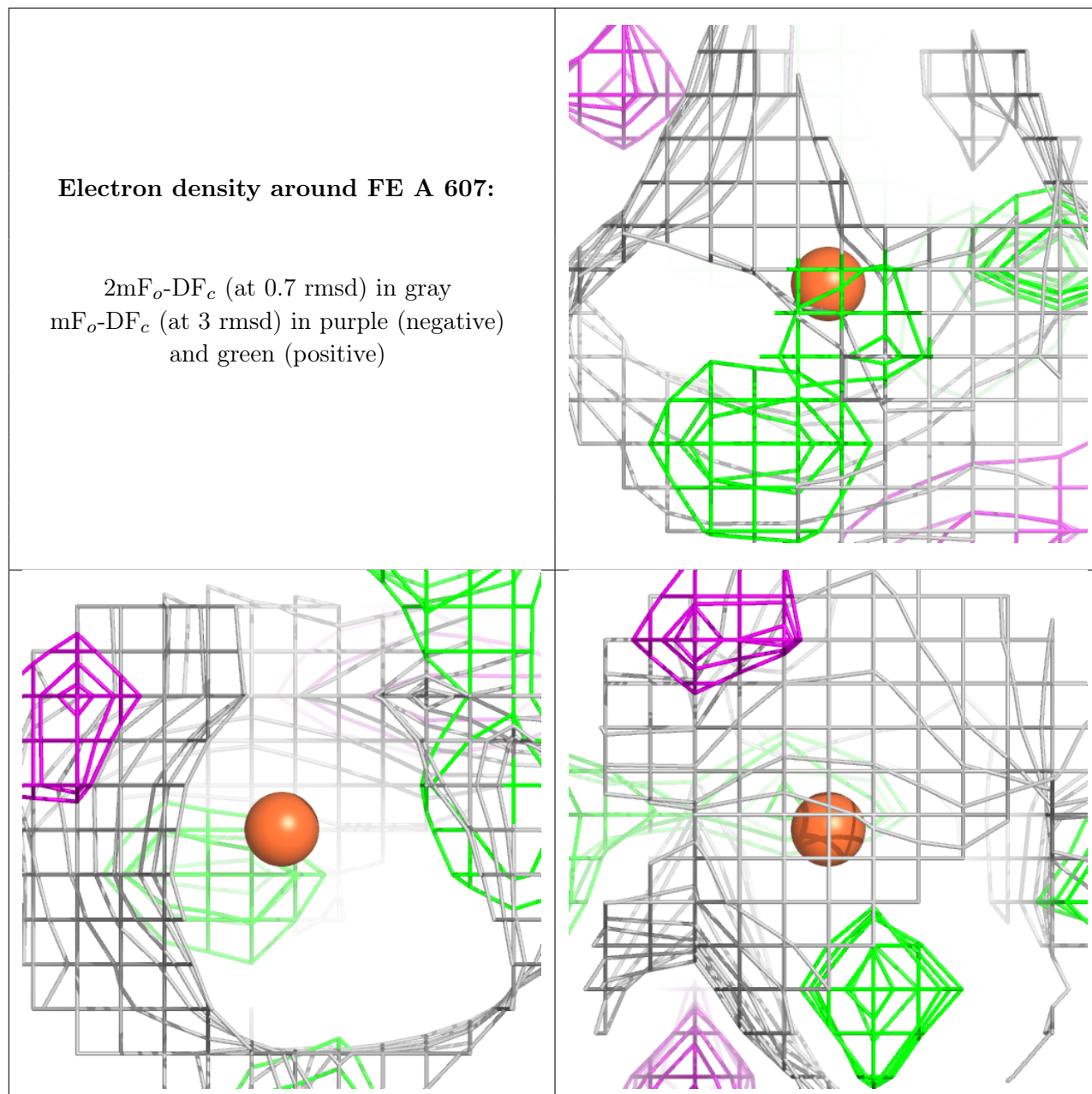
Electron density around FE B 603:

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



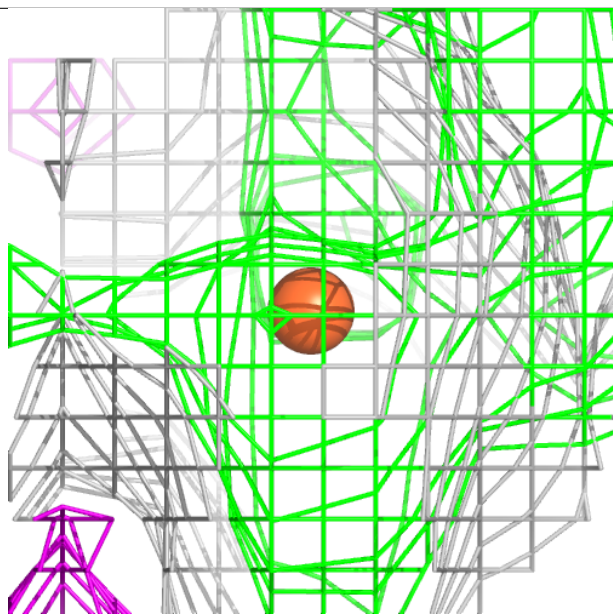
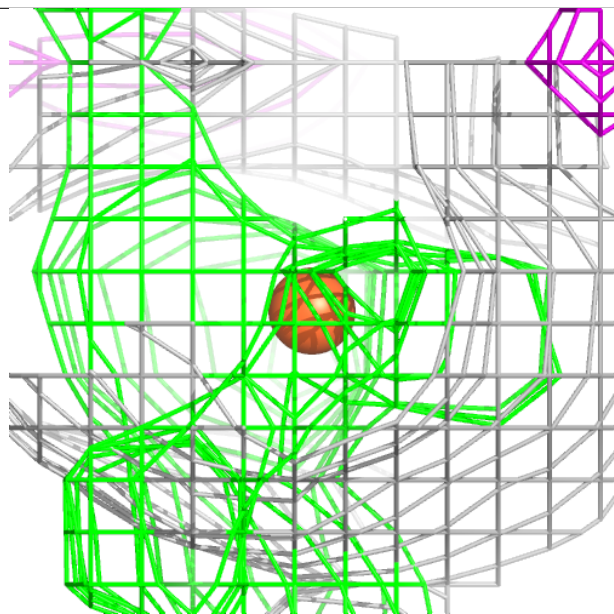
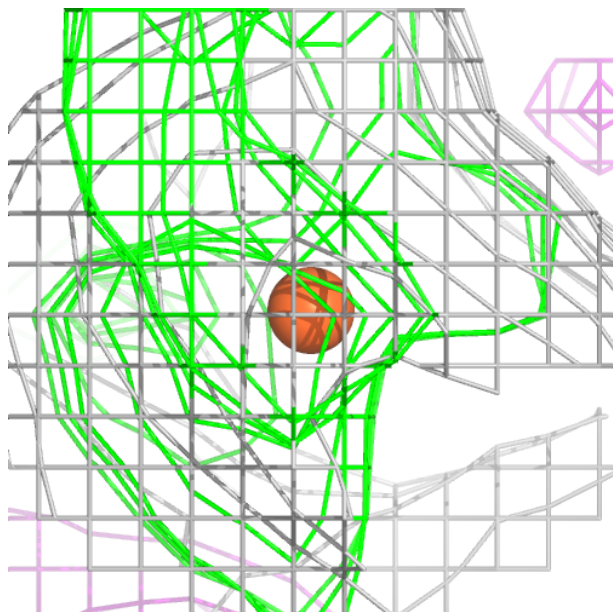
Electron density around FE A 607:

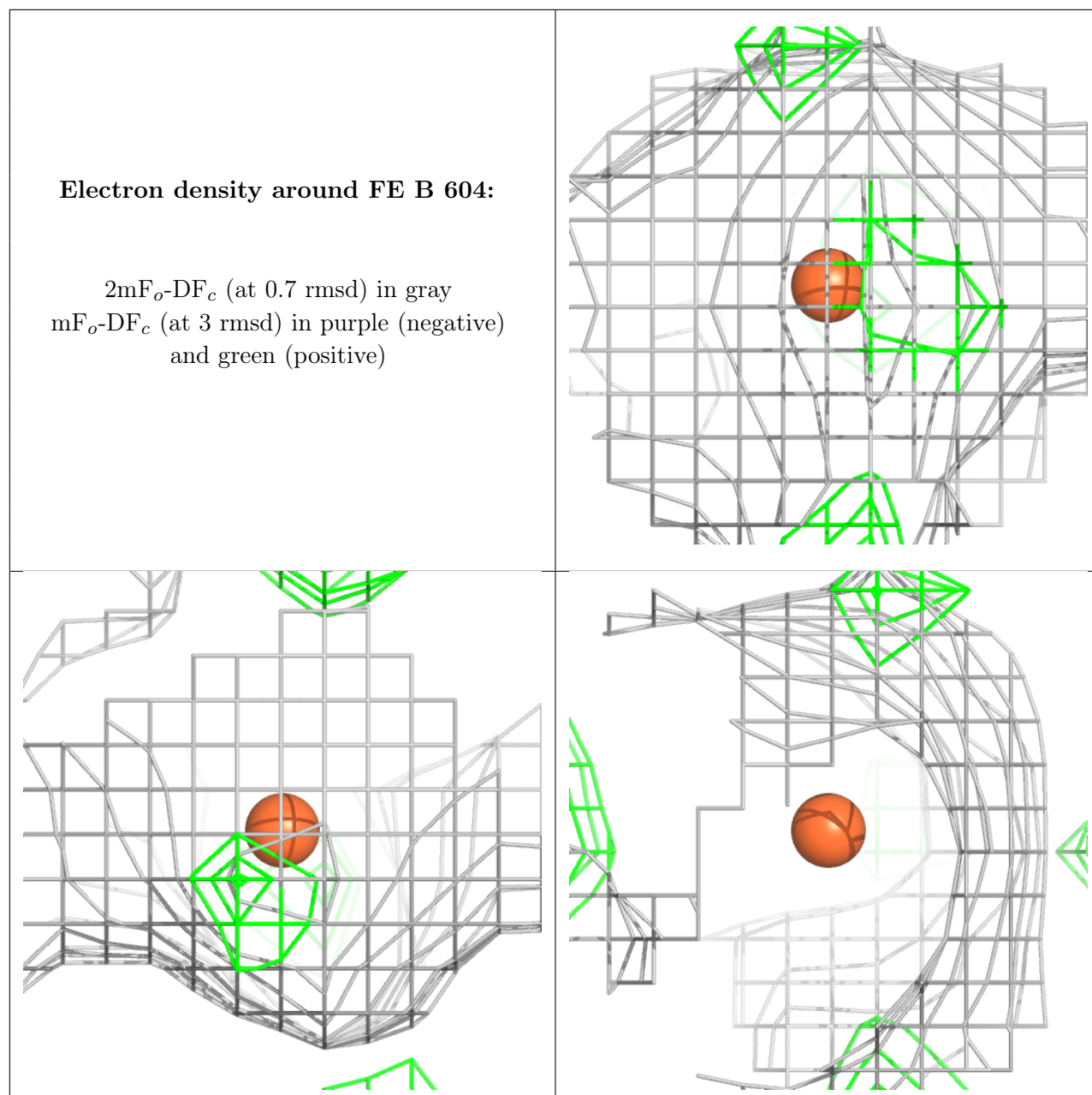
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 606:

$2mF_o-DF_c$ (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.