



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:09 AM EDT

PDB ID : 7QR6 / pdb_00007qr6
Title : Stilbene dioxygenase (NOV1) from *Novosphingobium aromaticivorans*:
Ser283Phe mutant
Authors : Alvigini, L.; Mattevi, A.
Deposited on : 2022-01-10
Resolution : 2.90 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

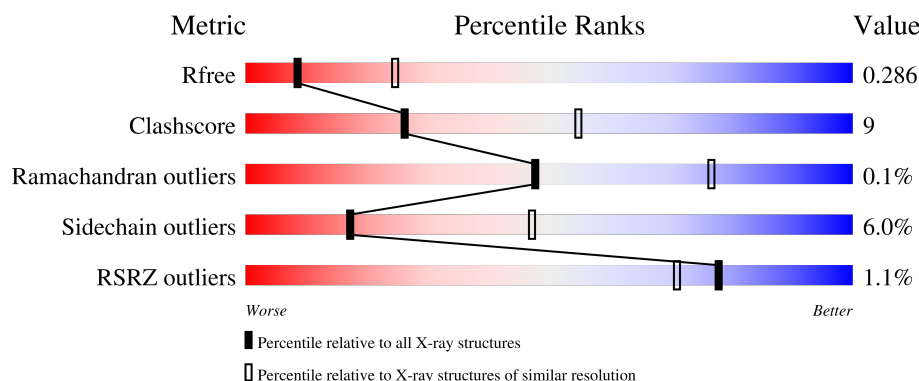
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	494	
1	B	494	
1	C	494	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11370 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 Dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	1	0
			3760	2397	648	690	25			
1	B	476	Total	C	N	O	S	0	1	0
			3795	2418	654	698	25			
1	C	475	Total	C	N	O	S	0	1	0
			3791	2418	654	694	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	PHE	SER	conflict	UNP Q2GA76
B	283	PHE	SER	conflict	UNP Q2GA76
C	283	PHE	SER	conflict	UNP Q2GA76

- 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	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		

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

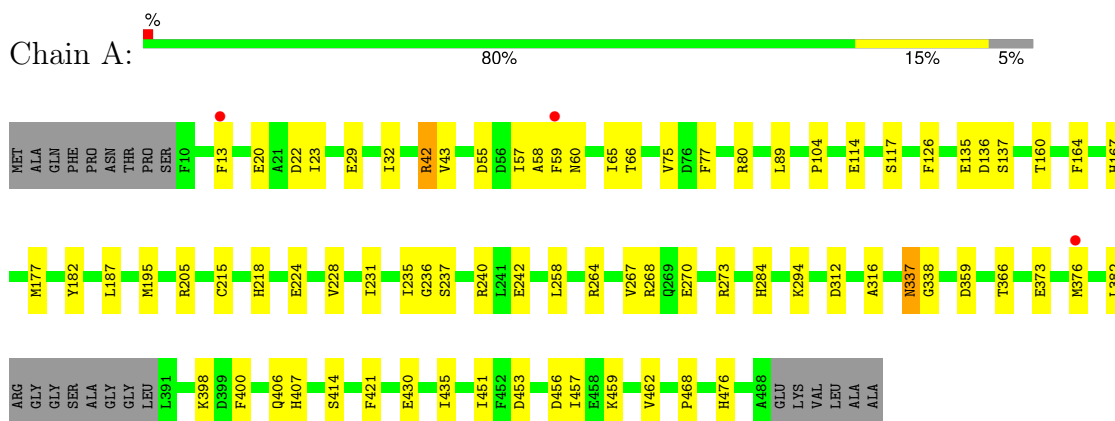
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	6	Total O 6 6	0	0
4	C	2	Total O 2 2	0	0

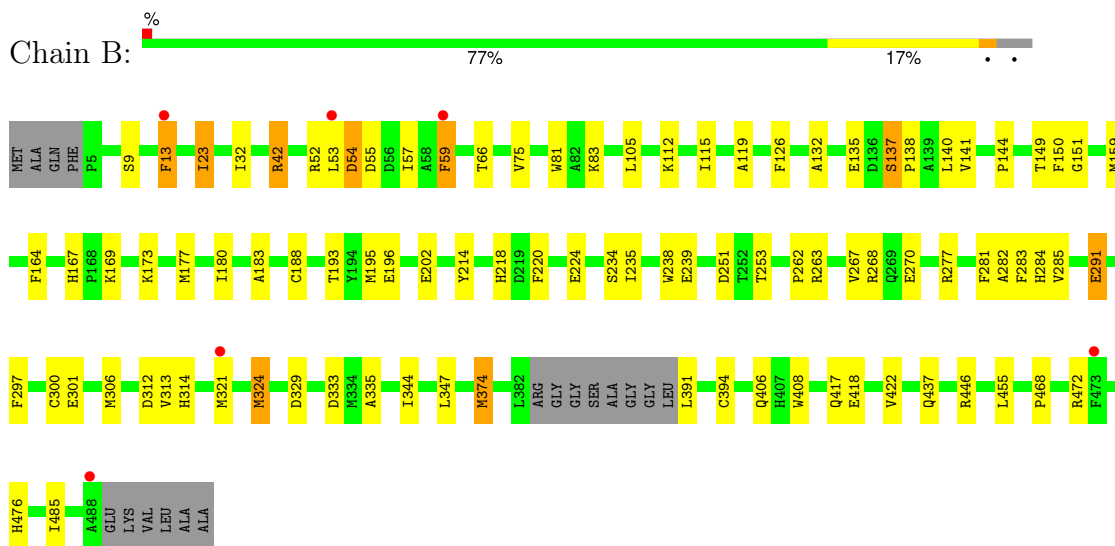
3 Residue-property plots [i](#)

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.

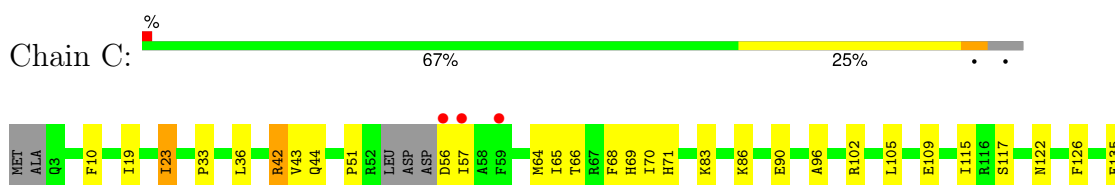
• Molecule 1: Dioxygenase

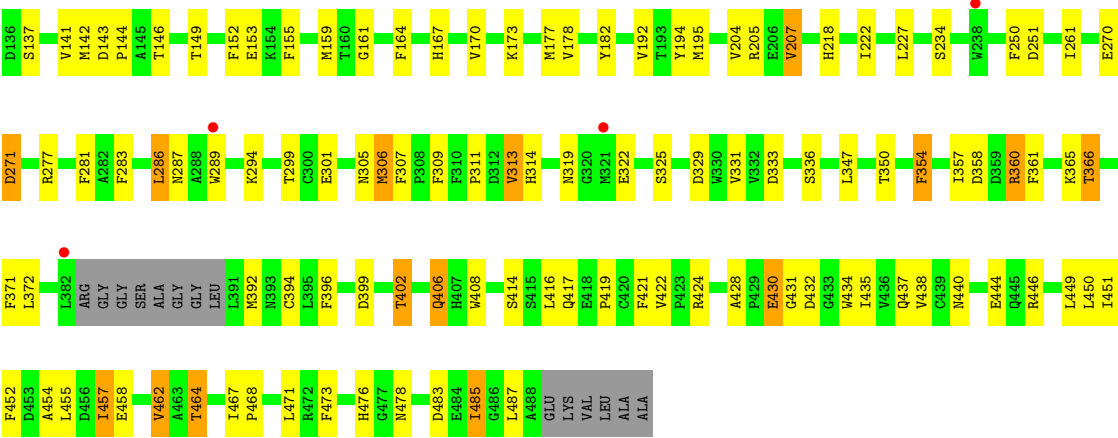


• Molecule 1: Dioxygenase



• Molecule 1: Dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	178.47Å 187.98Å 105.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.90 49.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.04-2.90) 91.2 (49.04-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.291 0.218 , 0.286	Depositor DCC
R_{free} test set	1698 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11370	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: OXY, 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	0.99	0/3874	1.31	5/5255 (0.1%)
1	B	1.00	1/3911 (0.0%)	1.27	1/5307 (0.0%)
1	C	0.99	1/3907 (0.0%)	1.30	1/5300 (0.0%)
All	All	0.99	2/11692 (0.0%)	1.29	7/15862 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	VAL	N-CA	5.10	1.49	1.45
1	C	422	VAL	N-CA	5.00	1.49	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ASP	CB-CA-C	-6.75	96.99	110.42
1	B	13	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	13	PHE	CA-CB-CG	5.36	119.16	113.80
1	C	354	PHE	CB-CA-C	5.34	115.00	111.20
1	A	160	THR	CA-C-N	5.30	125.01	119.92
1	A	160	THR	C-N-CA	5.30	125.01	119.92
1	A	55	ASP	CA-C-O	-5.18	116.42	122.37

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	3760	0	3575	38	0
1	B	3795	0	3608	57	0
1	C	3791	0	3604	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
4	C	2	0	0	0	0
All	All	11370	0	10787	209	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (209) 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:53:LEU:HD23	1:B:54:ASP:H	1.04	1.09
1:C:144:PRO:CB	1:C:485:ILE:HG22	1.82	1.09
1:C:144:PRO:HB2	1:C:485:ILE:HG22	1.40	1.02
1:B:53:LEU:HD23	1:B:54:ASP:N	1.76	1.00
1:B:53:LEU:CD2	1:B:55:ASP:H	1.88	0.87
1:C:358:ASP:OD1	1:C:360:ARG:HG2	1.75	0.87
1:B:53:LEU:CD2	1:B:54:ASP:H	1.88	0.84
1:C:144:PRO:HB2	1:C:485:ILE:CG2	2.08	0.83
1:B:53:LEU:HD23	1:B:55:ASP:H	1.45	0.81
1:C:86:LYS:O	1:C:90:GLU:HG3	1.81	0.80
1:C:144:PRO:HB3	1:C:485:ILE:HG22	1.64	0.80
1:C:122:ASN:HD21	1:C:478:ASN:HD21	1.27	0.79
1:C:360:ARG:NH2	1:C:428:ALA:O	2.17	0.78
1:C:399:ASP:OD2	1:C:402:THR:CG2	2.33	0.76
1:C:159:MET:HE3	1:C:161:GLY:O	1.86	0.76
1:C:361:PHE:CD2	1:C:430:GLU:HG3	2.22	0.75
1:C:69:HIS:HE1	1:C:71:HIS:ND1	1.87	0.72
1:C:33:PRO:HB2	1:C:36:LEU:HD12	1.71	0.72
1:A:312:ASP:OD2	1:A:316:ALA:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLU:OE2	1:C:155:PHE:N	2.21	0.69
1:A:337:ASN:N	1:A:337:ASN:HD22	1.92	0.67
1:C:319:ASN:ND2	1:C:322:GLU:CD	2.53	0.66
1:C:286:LEU:CD1	1:C:357:ILE:CG2	2.72	0.66
1:A:42:ARG:HD3	1:A:66:THR:HB	1.77	0.66
1:C:281:PHE:CD2	1:C:305:ASN:HA	2.31	0.65
1:B:196:GLU:OE2	1:B:263:ARG:NH2	2.29	0.65
1:C:361:PHE:HE2	1:C:430:GLU:HA	1.62	0.64
1:C:277:ARG:NH1	1:C:301:GLU:OE1	2.29	0.64
1:C:286:LEU:HD12	1:C:357:ILE:CG2	2.28	0.64
1:A:23:ILE:HD13	1:A:468:PRO:HG2	1.80	0.63
1:B:291:GLU:HG2	1:B:291:GLU:O	1.98	0.63
1:A:23:ILE:HD13	1:A:468:PRO:CG	2.29	0.63
1:C:289:TRP:CE3	1:C:365:LYS:HA	2.33	0.63
1:C:286:LEU:HD12	1:C:357:ILE:HG23	1.81	0.63
1:B:53:LEU:HD23	1:B:55:ASP:N	2.12	0.62
1:A:22:ASP:C	1:A:23:ILE:HG13	2.24	0.62
1:C:399:ASP:OD2	1:C:402:THR:HG23	1.99	0.62
1:C:431:GLY:O	1:C:455:LEU:HD21	2.00	0.62
1:A:20:GLU:HG2	1:A:80:ARG:HA	1.82	0.62
1:A:273:ARG:NH2	1:A:338:GLY:O	2.34	0.61
1:C:117:SER:HB2	1:C:137:SER:HB2	1.83	0.61
1:B:53:LEU:CD2	1:B:55:ASP:N	2.61	0.60
1:B:262:PRO:O	1:B:267:VAL:HG21	2.00	0.60
1:C:319:ASN:ND2	1:C:322:GLU:CG	2.65	0.59
1:C:250:PHE:O	1:C:313:VAL:HG22	2.03	0.59
1:C:286:LEU:HD11	1:C:357:ILE:HG22	1.82	0.59
1:C:358:ASP:OD1	1:C:360:ARG:CG	2.49	0.59
1:C:286:LEU:CD1	1:C:357:ILE:HG23	2.34	0.58
1:C:167:HIS:CD2	1:C:218:HIS:CE1	2.92	0.58
1:C:361:PHE:CE2	1:C:430:GLU:HA	2.39	0.57
1:A:22:ASP:O	1:A:23:ILE:HG13	2.05	0.57
1:C:454:ALA:O	1:C:457:ILE:HG23	2.05	0.57
1:B:251:ASP:OD1	1:B:253:THR:HB	2.05	0.56
1:B:406:GLN:NE2	1:B:455:LEU:O	2.38	0.56
1:C:69:HIS:HE1	1:C:71:HIS:CG	2.23	0.56
1:C:42:ARG:HD2	1:C:66:THR:HB	1.87	0.56
1:C:286:LEU:HD11	1:C:357:ILE:CG2	2.35	0.56
1:A:228:VAL:HG12	1:A:258:LEU:HD11	1.87	0.55
1:B:235:ILE:HD12	1:B:235:ILE:C	2.32	0.55
1:B:140:LEU:HD12	1:B:151:GLY:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ILE:O	1:A:462:VAL:HG22	2.06	0.55
1:C:126:PHE:CD2	1:C:177:MET:HE3	2.42	0.54
1:C:450:LEU:HD22	1:C:464:THR:HG23	1.87	0.54
1:C:69:HIS:HE1	1:C:71:HIS:CE1	2.25	0.54
1:A:32:ILE:HD13	1:A:75:VAL:HG23	1.90	0.54
1:C:167:HIS:CE1	1:C:476:HIS:CD2	2.91	0.54
1:C:366:THR:HG22	1:C:430:GLU:CD	2.32	0.54
1:C:182:TYR:HA	1:C:192:VAL:HG22	1.90	0.54
1:C:281:PHE:CE2	1:C:305:ASN:OD1	2.61	0.54
1:B:268:ARG:NE	1:B:270:GLU:OE2	2.41	0.54
1:C:319:ASN:HD21	1:C:322:GLU:HG3	1.73	0.53
1:C:23:ILE:CD1	1:C:468:PRO:HG2	2.39	0.53
1:B:42:ARG:HD2	1:B:66:THR:HB	1.90	0.53
1:C:83:LYS:HB2	1:C:149:THR:HG21	1.91	0.53
1:B:23:ILE:HD13	1:B:468:PRO:CG	2.38	0.53
1:C:178:VAL:HG11	1:C:222:ILE:HG21	1.91	0.53
1:B:83:LYS:HB2	1:B:149:THR:HG21	1.91	0.52
1:B:126:PHE:CD2	1:B:177:MET:HE3	2.44	0.52
1:B:42:ARG:CD	1:B:66:THR:HB	2.41	0.51
1:C:434:TRP:HB3	1:C:452:PHE:O	2.10	0.51
1:C:329:ASP:HB2	1:C:347:LEU:HD21	1.93	0.51
1:B:188:CYS:HA	1:B:214:TYR:CE2	2.46	0.51
1:C:90:GLU:OE2	1:C:96:ALA:HA	2.10	0.50
1:A:456:ASP:O	1:A:459:LYS:HG2	2.11	0.50
1:A:421:PHE:HA	1:A:435:ILE:HD13	1.94	0.50
1:B:218:HIS:CD2	1:B:283:PHE:CZ	2.99	0.50
1:C:33:PRO:HB2	1:C:36:LEU:CD1	2.40	0.50
1:C:361:PHE:CE2	1:C:430:GLU:HB2	2.47	0.49
1:C:431:GLY:O	1:C:455:LEU:CD2	2.60	0.49
1:B:277:ARG:NH1	1:B:301:GLU:OE1	2.38	0.49
1:C:361:PHE:CE2	1:C:430:GLU:CB	2.95	0.49
1:B:32:ILE:HD13	1:B:75:VAL:HG23	1.94	0.49
1:C:69:HIS:CE1	1:C:71:HIS:CG	3.00	0.49
1:C:142:MET:HG2	1:C:149:THR:HA	1.94	0.49
1:B:183:ALA:HB2	1:B:214:TYR:HE2	1.78	0.49
1:C:417:GLN:HG3	1:C:438:VAL:O	2.12	0.49
1:A:373:GLU:OE1	1:A:407:HIS:ND1	2.45	0.48
1:A:89:LEU:HD11	1:A:114:GLU:OE1	2.14	0.48
1:C:287:ASN:ND2	1:C:366:THR:OG1	2.46	0.48
1:A:235:ILE:C	1:A:235:ILE:HD12	2.38	0.48
1:C:218:HIS:CD2	1:C:283:PHE:CZ	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:PHE:CE2	1:C:430:GLU:CA	2.96	0.48
1:A:167:HIS:CD2	1:A:218:HIS:CE1	3.02	0.48
1:C:227:LEU:HD23	1:C:261:ILE:HD13	1.95	0.48
1:C:143:ASP:HB3	1:C:146:THR:OG1	2.13	0.48
1:C:350:THR:HG21	1:C:396:PHE:CE2	2.49	0.47
1:C:309:PHE:O	1:C:311:PRO:HD3	2.14	0.47
1:B:119:ALA:HB1	1:B:132:ALA:HB1	1.96	0.47
1:B:169:LYS:HE2	1:B:220:PHE:O	2.15	0.47
1:B:374:MET:HG3	1:B:391:LEU:O	2.14	0.47
1:A:237:SER:OG	1:A:240:ARG:HG3	2.15	0.47
1:C:406:GLN:NE2	1:C:455:LEU:O	2.41	0.47
1:A:117:SER:HB2	1:A:137:SER:CB	2.45	0.47
1:A:236:GLY:HA2	1:A:240:ARG:HD3	1.97	0.47
1:C:42:ARG:NH1	1:C:44:GLN:HB3	2.29	0.47
1:C:68:PHE:O	1:C:70:ILE:HG13	2.14	0.47
1:B:141:VAL:HG23	1:B:150:PHE:HB2	1.96	0.47
1:C:135:GLU:HA	1:C:164:PHE:O	2.15	0.47
1:C:406:GLN:HG2	1:C:458:GLU:HB3	1.96	0.47
1:C:251:ASP:OD1	1:C:314:HIS:HE1	1.98	0.47
1:C:358:ASP:OD1	1:C:360:ARG:CD	2.64	0.46
1:C:399:ASP:OD2	1:C:402:THR:HG22	2.14	0.46
1:B:417:GLN:O	1:B:437:GLN:NE2	2.48	0.46
1:A:398:LYS:HG2	1:A:400:PHE:CE1	2.50	0.46
1:A:136:ASP:OD1	1:A:137:SER:OG	2.31	0.46
1:C:167:HIS:HD2	1:C:218:HIS:CE1	2.34	0.46
1:C:361:PHE:CD2	1:C:430:GLU:CG	2.96	0.46
1:C:416:LEU:HD22	1:C:437:GLN:OE1	2.16	0.46
1:A:136:ASP:OD1	1:A:136:ASP:C	2.58	0.46
1:B:188:CYS:HA	1:B:214:TYR:CD2	2.51	0.46
1:C:319:ASN:ND2	1:C:322:GLU:HG3	2.28	0.46
1:A:366:THR:HB	1:A:430:GLU:OE2	2.16	0.46
1:B:23:ILE:HD13	1:B:468:PRO:HG3	1.96	0.46
1:B:282:ALA:HA	1:B:300:CYS:O	2.15	0.46
1:C:350:THR:HG21	1:C:396:PHE:CD2	2.51	0.46
1:B:81:TRP:HB2	1:B:83:LYS:HE2	1.97	0.45
1:B:115:ILE:HG23	1:B:137:SER:HB3	1.98	0.45
1:C:319:ASN:HD21	1:C:322:GLU:CG	2.28	0.45
1:C:218:HIS:CD2	1:C:283:PHE:CE1	3.05	0.45
1:B:312:ASP:OD1	1:B:314:HIS:N	2.46	0.45
1:B:281:PHE:CD1	1:B:306:MET:HG3	2.52	0.45
1:B:313:VAL:HG23	1:B:314:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG23	1:A:65:ILE:HD13	1.99	0.45
1:B:23:ILE:CD1	1:B:468:PRO:HG2	2.47	0.45
1:B:291:GLU:O	1:B:291:GLU:CG	2.65	0.45
1:C:19:ILE:O	1:C:64:MET:HE3	2.16	0.45
1:C:227:LEU:CD2	1:C:261:ILE:HD13	2.47	0.45
1:B:138:PRO:HG3	1:B:159:MET:HE1	1.98	0.45
1:C:117:SER:HB2	1:C:137:SER:CB	2.46	0.45
1:C:195:MET:HA	1:C:205:ARG:O	2.17	0.45
1:C:83:LYS:HB2	1:C:149:THR:CB	2.47	0.44
1:B:105:LEU:N	1:B:105:LEU:HD23	2.32	0.44
1:A:195:MET:HA	1:A:205:ARG:O	2.18	0.44
1:C:451:ILE:O	1:C:462:VAL:HG22	2.17	0.44
1:C:68:PHE:CD2	1:C:449:LEU:HD22	2.52	0.44
1:B:53:LEU:CD2	1:B:54:ASP:N	2.62	0.43
1:B:144:PRO:HB2	1:B:485:ILE:HG22	2.00	0.43
1:B:329:ASP:HB2	1:B:347:LEU:HD21	2.00	0.43
1:C:294:LYS:HE3	1:C:333:ASP:OD2	2.17	0.43
1:A:167:HIS:CE1	1:A:284:HIS:CD2	3.07	0.43
1:B:126:PHE:CD2	1:B:177:MET:CE	3.00	0.43
1:A:406:GLN:OE1	1:A:457:ILE:N	2.52	0.43
1:A:58:ALA:C	1:A:60:ASN:H	2.26	0.43
1:C:42:ARG:HH12	1:C:44:GLN:HB3	1.84	0.43
1:C:358:ASP:OD1	1:C:358:ASP:C	2.60	0.43
1:A:135:GLU:HA	1:A:164:PHE:O	2.18	0.43
1:C:421:PHE:HA	1:C:435:ILE:HD13	2.00	0.43
1:C:115:ILE:HG21	1:C:152:PHE:CE2	2.54	0.42
1:C:286:LEU:HD12	1:C:286:LEU:C	2.44	0.42
1:A:104:PRO:HG2	1:A:187:LEU:HD22	2.00	0.42
1:C:43:VAL:HG23	1:C:65:ILE:HD13	2.01	0.42
1:C:467:ILE:HD13	1:C:471:LEU:HD11	2.01	0.42
1:B:23:ILE:HD13	1:B:468:PRO:HG2	2.00	0.42
1:B:253:THR:HG22	1:B:253:THR:O	2.19	0.42
1:B:167:HIS:CE1	1:B:284:HIS:CD2	3.08	0.42
1:B:418:GLU:OE2	1:B:476:HIS:ND1	2.47	0.42
1:C:10:PHE:CZ	1:C:51:PRO:HG3	2.54	0.42
1:B:135:GLU:HA	1:B:164:PHE:O	2.19	0.42
1:C:126:PHE:CD2	1:C:177:MET:CE	3.03	0.42
1:B:333:ASP:OD1	1:B:335:ALA:HB3	2.20	0.42
1:C:43:VAL:HG23	1:C:65:ILE:CD1	2.50	0.41
1:C:23:ILE:CD1	1:C:468:PRO:CG	2.98	0.41
1:C:33:PRO:O	1:C:36:LEU:HD12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASP:OD2	1:A:459:LYS:NZ	2.50	0.41
1:B:285:VAL:HG22	1:B:297:PHE:CZ	2.56	0.41
1:C:218:HIS:HD2	1:C:283:PHE:CE1	2.38	0.41
1:C:414:SER:HA	1:C:440:ASN:O	2.19	0.41
1:C:283:PHE:CZ	1:C:307:PHE:HZ	2.38	0.41
1:C:419:PRO:HA	1:C:437:GLN:HB3	2.02	0.41
1:B:173:LYS:NZ	1:B:224:GLU:OE2	2.43	0.41
1:A:126:PHE:CD2	1:A:177:MET:HE3	2.55	0.41
1:A:312:ASP:OD2	1:A:316:ALA:CB	2.66	0.41
1:A:23:ILE:HD12	1:A:77:PHE:CD1	2.55	0.41
1:C:319:ASN:HD21	1:C:322:GLU:CD	2.25	0.41
1:C:394:CYS:HA	1:C:408:TRP:O	2.21	0.41
1:A:215:CYS:SG	1:A:231:ILE:HG23	2.61	0.41
1:C:424[B]:ARG:NE	1:C:432:ASP:OD2	2.54	0.41
1:B:180:ILE:HA	1:B:193:THR:O	2.21	0.41
1:C:173:LYS:HD3	1:C:173:LYS:HA	1.88	0.41
1:C:144:PRO:CB	1:C:485:ILE:CG2	2.71	0.40
1:C:354:PHE:CD2	1:C:372:LEU:HD12	2.56	0.40
1:C:69:HIS:CD2	1:C:487:LEU:HD13	2.56	0.40
1:C:286:LEU:HD22	1:C:371:PHE:CE2	2.56	0.40
1:A:167:HIS:CE1	1:A:476:HIS:CD2	3.07	0.40
1:B:394:CYS:HA	1:B:408:TRP:O	2.21	0.40
1:C:271:ASP:OD1	1:C:271:ASP:N	2.53	0.40
1:C:194:TYR:CD2	1:C:207:VAL:CG2	3.05	0.40
1:C:281:PHE:CD1	1:C:306:MET:HG3	2.56	0.40
1:B:324:MET:HE2	1:B:324:MET:HA	2.03	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	468/494 (95%)	445 (95%)	22 (5%)	1 (0%)	43	72
1	B	473/494 (96%)	445 (94%)	27 (6%)	1 (0%)	43	72
1	C	470/494 (95%)	442 (94%)	28 (6%)	0	100	100
All	All	1411/1482 (95%)	1332 (94%)	77 (6%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	PHE
1	A	59	PHE

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	395/409 (97%)	380 (96%)	15 (4%)	29	64
1	B	400/409 (98%)	378 (94%)	22 (6%)	19	50
1	C	399/409 (98%)	364 (91%)	35 (9%)	9	29
All	All	1194/1227 (97%)	1122 (94%)	72 (6%)	17	47

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	42	ARG
1	A	57	ILE
1	A	182	TYR
1	A	224	GLU
1	A	242	GLU
1	A	264	ARG
1	A	267	VAL
1	A	268	ARG
1	A	270	GLU
1	A	294	LYS

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	376	MET
1	A	382	LEU
1	A	414	SER
1	B	9	SER
1	B	13	PHE
1	B	23	ILE
1	B	42	ARG
1	B	52	ARG
1	B	54	ASP
1	B	57	ILE
1	B	59	PHE
1	B	112	LYS
1	B	137	SER
1	B	195	MET
1	B	202	GLU
1	B	234	SER
1	B	238	TRP
1	B	239	GLU
1	B	291	GLU
1	B	321	MET
1	B	324	MET
1	B	344	ILE
1	B	374	MET
1	B	446	ARG
1	B	472	ARG
1	C	23	ILE
1	C	42	ARG
1	C	56	ASP
1	C	57	ILE
1	C	102	ARG
1	C	105	LEU
1	C	109	GLU
1	C	141	VAL
1	C	170	VAL
1	C	204	VAL
1	C	207	VAL
1	C	234	SER
1	C	270	GLU
1	C	271	ASP
1	C	286	LEU
1	C	299	THR

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Mol	Chain	Res	Type
1	C	306	MET
1	C	313	VAL
1	C	325	SER
1	C	331	VAL
1	C	336	SER
1	C	360	ARG
1	C	366	THR
1	C	392	MET
1	C	402	THR
1	C	406	GLN
1	C	430	GLU
1	C	444	GLU
1	C	446	ARG
1	C	457	ILE
1	C	462	VAL
1	C	464	THR
1	C	473	PHE
1	C	483	ASP
1	C	485	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	69	HIS
1	A	91	ASN
1	A	305	ASN
1	A	337	ASN
1	A	437	GLN
1	B	48	GLN
1	B	69	HIS
1	B	91	ASN
1	B	437	GLN
1	C	48	GLN
1	C	69	HIS
1	C	74	GLN
1	C	79	GLN
1	C	287	ASN
1	C	314	HIS
1	C	319	ASN
1	C	337	ASN
1	C	407	HIS

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Mol	Chain	Res	Type
1	C	466	ASN
1	C	478	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
3	OXY	A	502	2	1,1,1	0.19	0	-		
3	OXY	B	502	2	1,1,1	0.14	0	-		
3	OXY	C	502	2	1,1,1	0.20	0	-		

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	471/494 (95%)	-0.16	3 (0%) 85 81	33, 60, 90, 142	1 (0%)
1	B	476/494 (96%)	-0.06	6 (1%) 75 67	36, 63, 98, 153	1 (0%)
1	C	475/494 (96%)	0.31	7 (1%) 72 64	52, 87, 112, 152	1 (0%)
All	All	1422/1482 (95%)	0.03	16 (1%) 78 71	33, 68, 108, 153	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	PHE	4.3
1	C	321	MET	4.1
1	B	473	PHE	3.8
1	A	13	PHE	3.5
1	B	59	PHE	3.2
1	C	59	PHE	3.0
1	B	13	PHE	2.3
1	B	53	LEU	2.3
1	C	57	ILE	2.2
1	C	56	ASP	2.2
1	B	488	ALA	2.1
1	B	321	MET	2.1
1	C	238	TRP	2.1
1	A	376	MET	2.1
1	C	289	TRP	2.1
1	C	382	LEU	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

There are no oligosaccharides in this entry.

6.4 Ligands

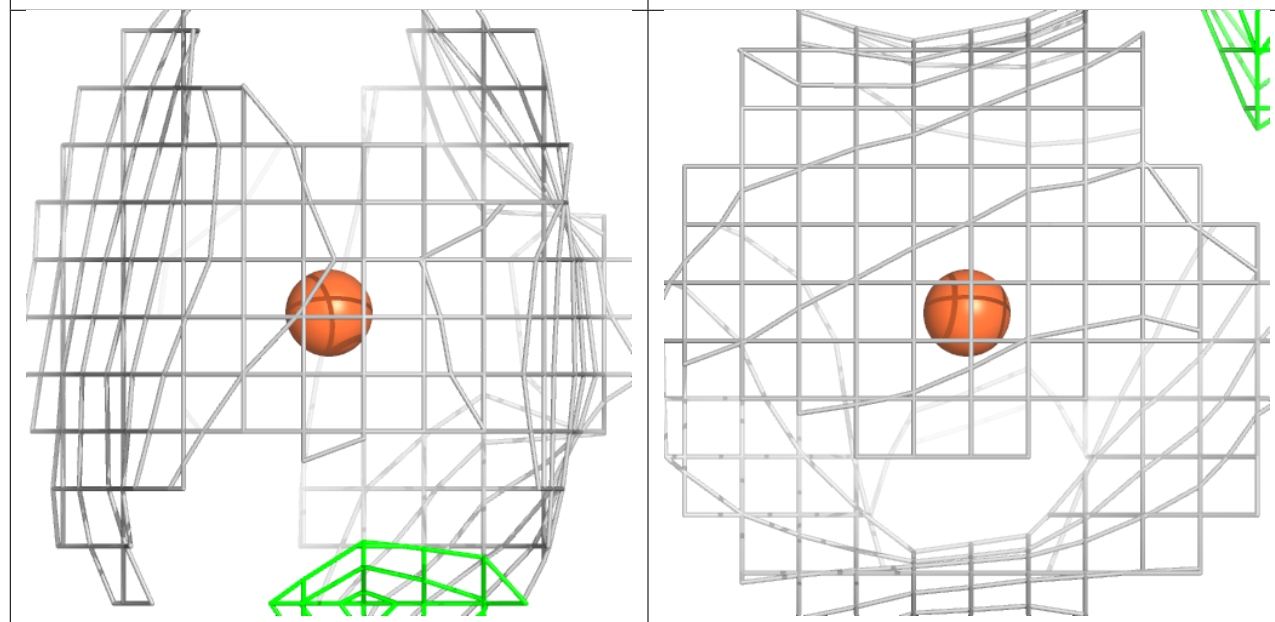
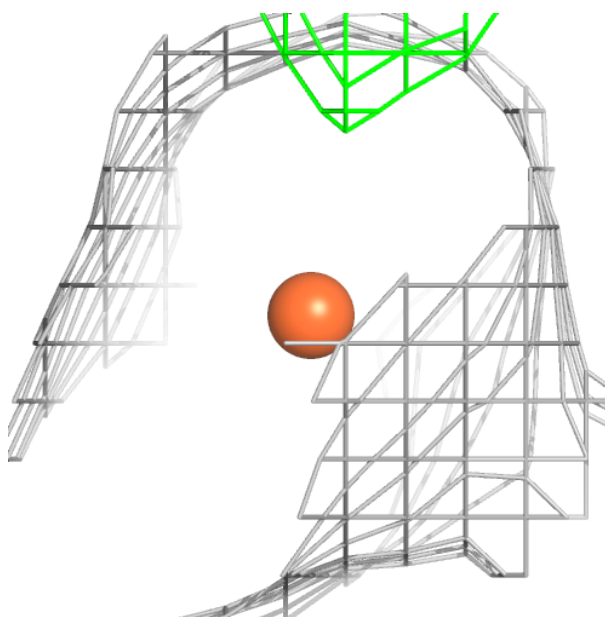
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXY	B	502	2/2	0.84	0.24	68,68,68,70	2
3	OXY	C	502	2/2	0.93	0.10	59,59,59,67	2
3	OXY	A	502	2/2	0.94	0.15	35,35,35,43	2
2	FE	C	501	1/1	0.99	0.02	60,60,60,60	1
2	FE	A	501	1/1	1.00	0.02	41,41,41,41	1
2	FE	B	501	1/1	1.00	0.02	51,51,51,51	1

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.

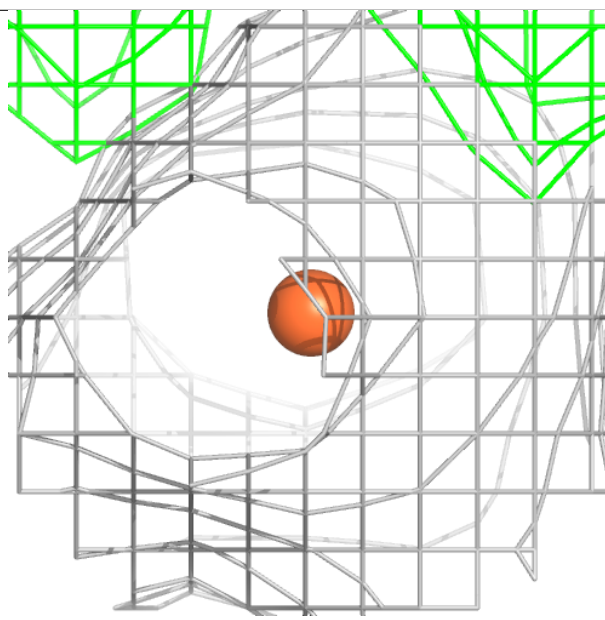
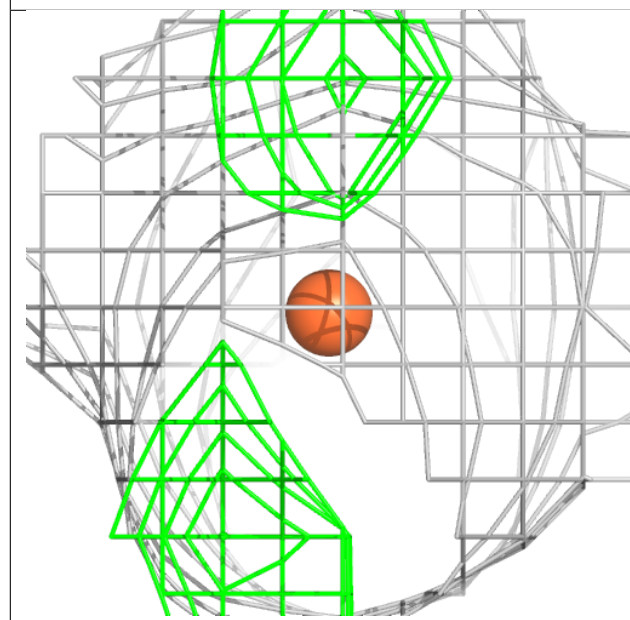
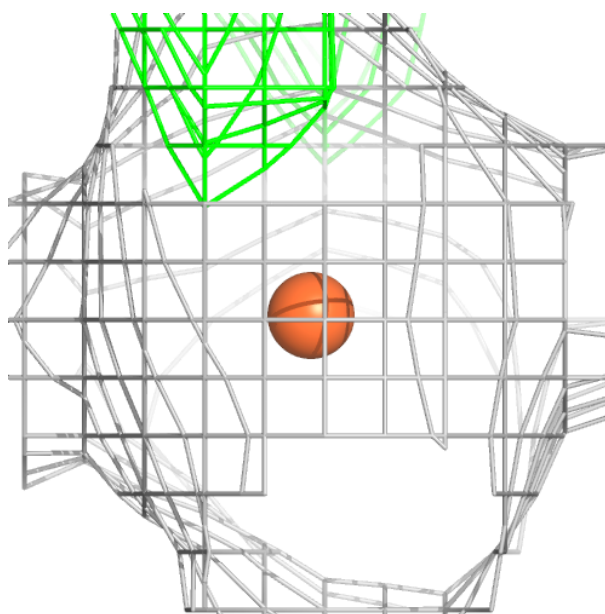
Electron density around FE C 501:

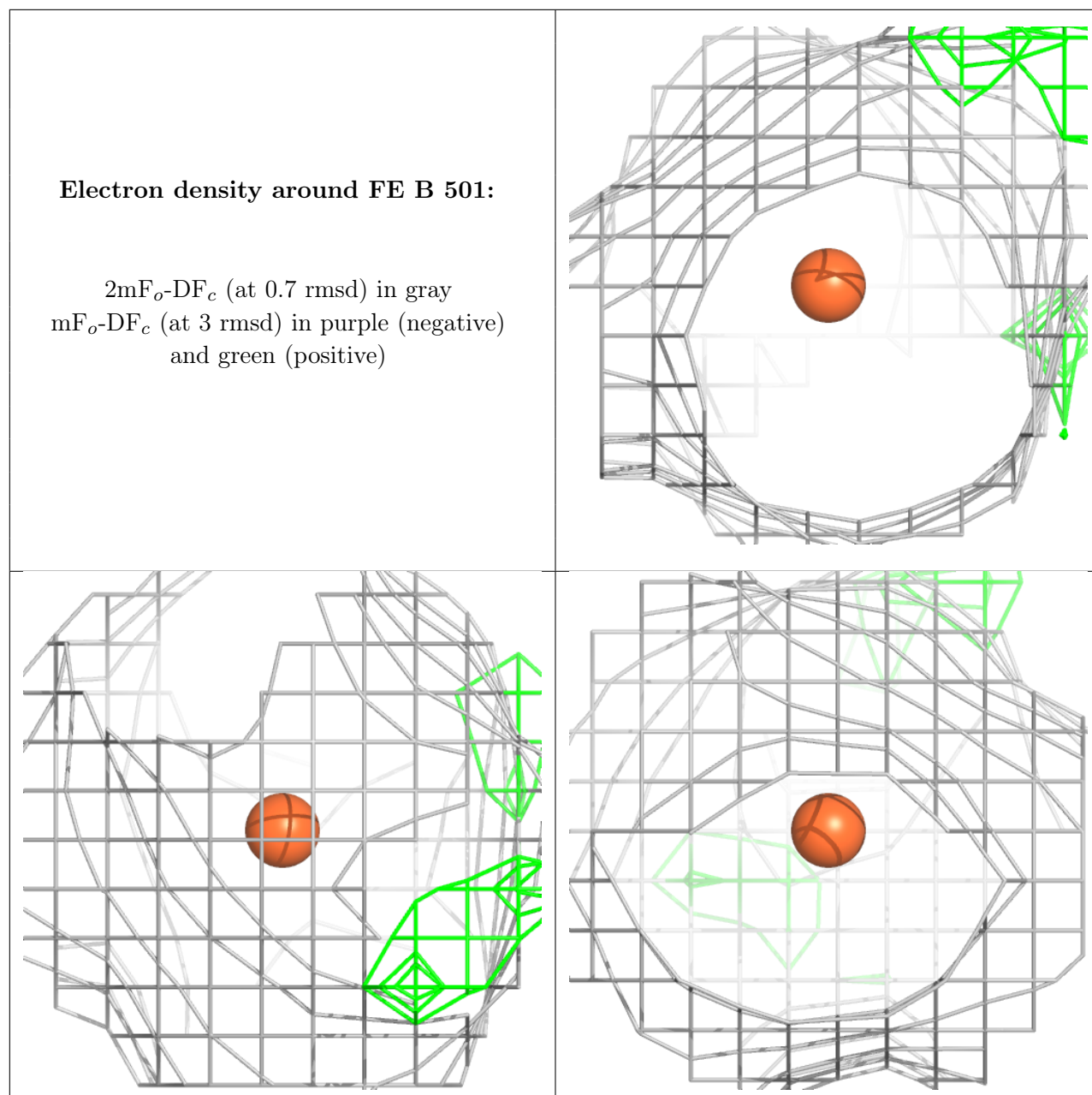
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE A 501:

$2mF_o-DF_c$ (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.