



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 7V25 / pdb_00007v25
Title : Crystal Structure of phthalate dioxygenase in complex with phthalate
Authors : Mahto, J.K.; Kumar, P.
Deposited on : 2021-08-07
Resolution : 2.74 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:

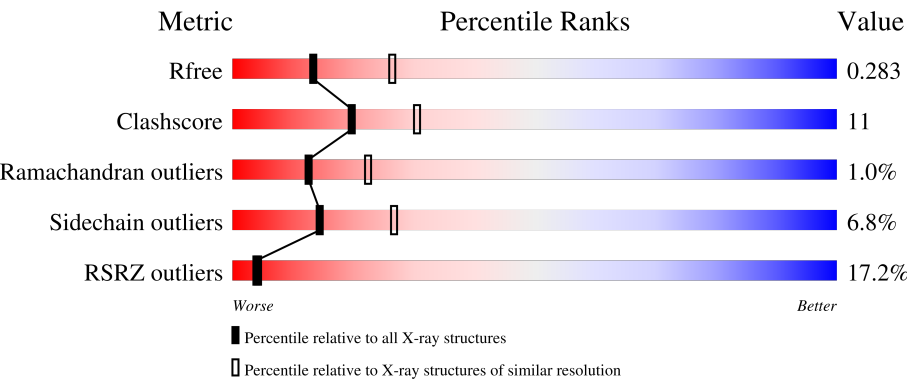
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	439	9% 72% 18% • 7%
1	B	439	17% 70% 23% • •
1	C	439	13% 70% 21% • 7%
1	D	439	14% 64% 26% • 8%
1	E	439	20% 67% 20% • 10%

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Mol	Chain	Length	Quality of chain
1	F	439	24% 64% 27% • 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20542 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 Rieske (2Fe-2S) domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	423	Total	C	N	O	S	0	0	0
			3323	2094	588	617	24			
1	A	407	Total	C	N	O	S	0	0	0
			3213	2029	567	594	23			
1	C	407	Total	C	N	O	S	0	0	0
			3212	2029	567	593	23			
1	D	405	Total	C	N	O	S	0	0	0
			3203	2023	565	592	23			
1	E	395	Total	C	N	O	S	0	0	0
			3095	1952	545	574	24			
1	F	409	Total	C	N	O	S	0	0	0
			3228	2038	569	597	24			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

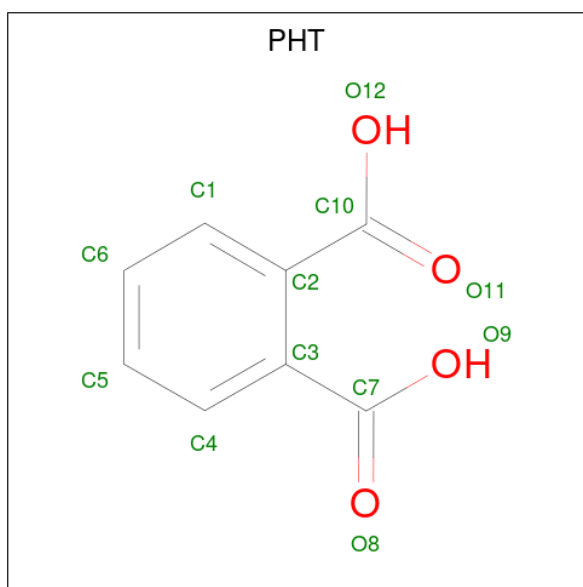
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is PHTHALIC ACID (CCD ID: PHT) (formula: $C_8H_6O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	8	4		

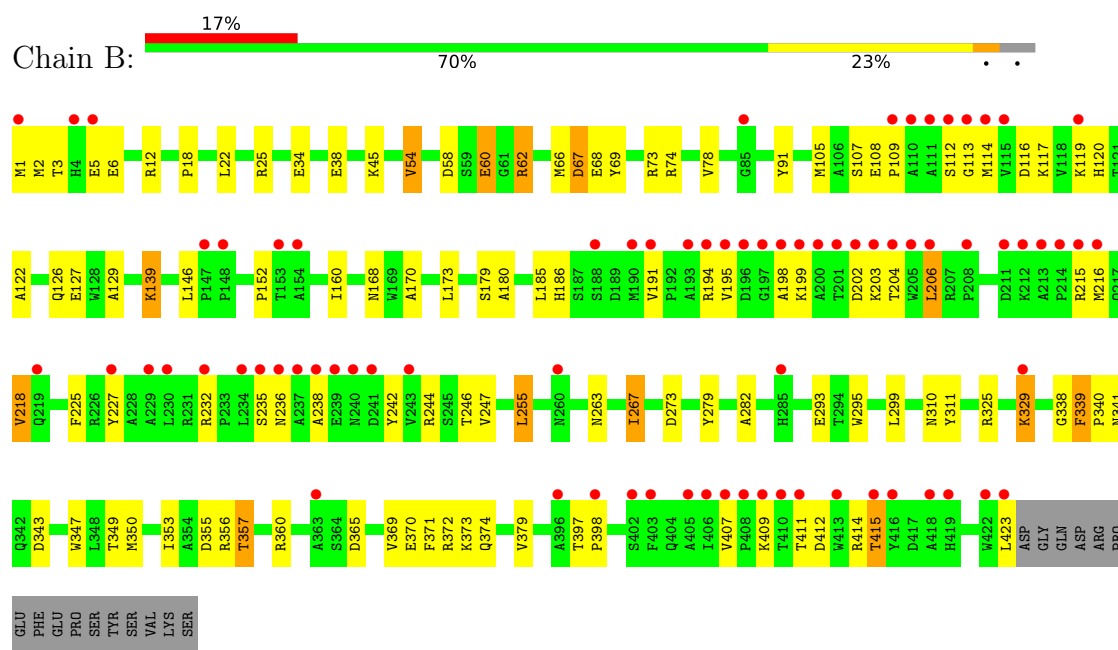
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	208	Total	O	0	0
			208	208		
5	A	204	Total	O	0	0
			204	204		
5	C	208	Total	O	0	0
			208	208		
5	D	198	Total	O	0	0
			198	198		
5	E	200	Total	O	0	0
			200	200		
5	F	208	Total	O	0	0
			208	208		

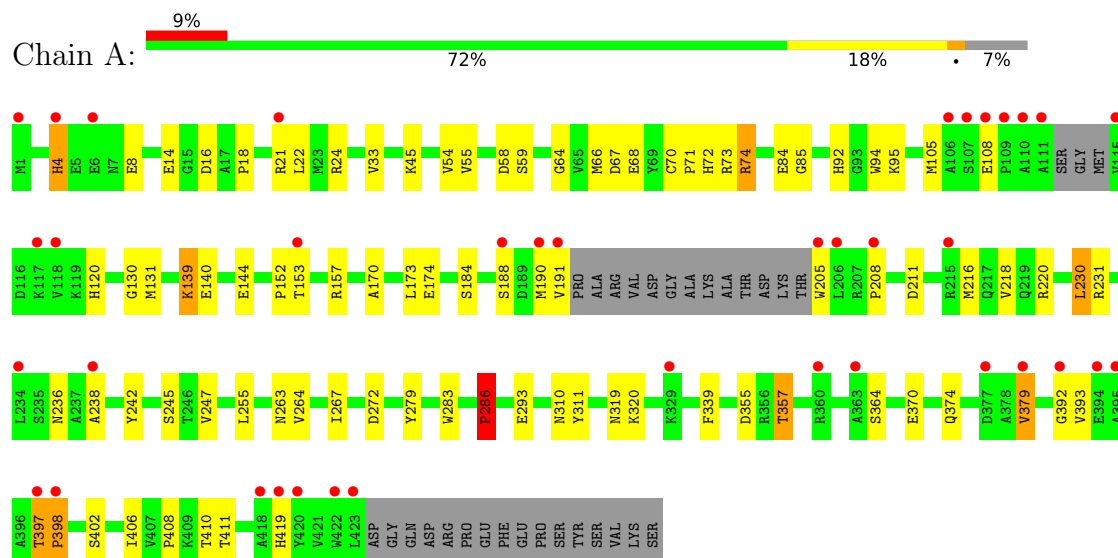
3 Residue-property plots [i](#)

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.

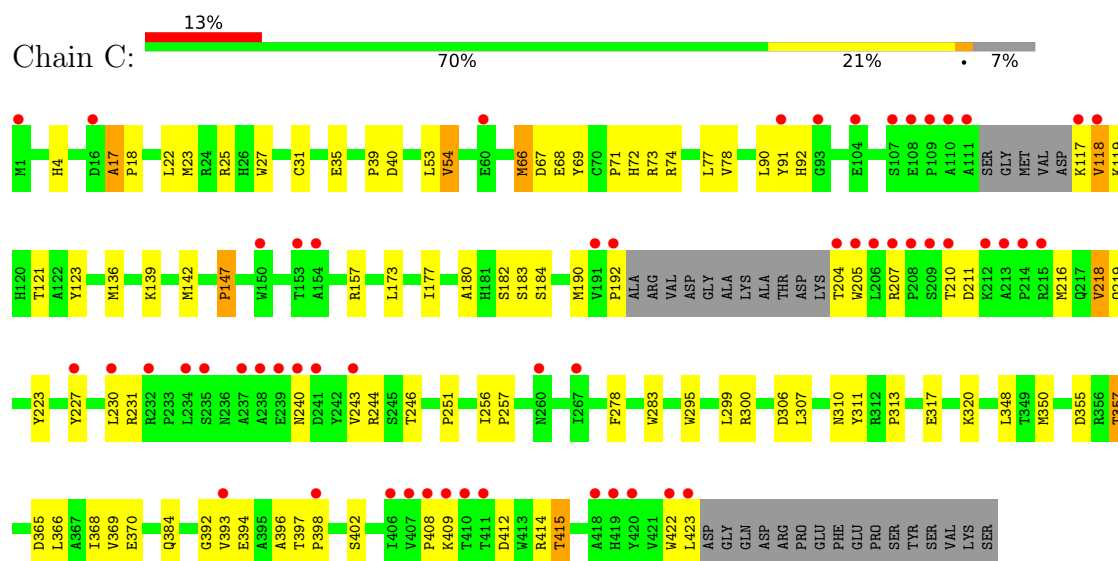
• Molecule 1: Rieske (2Fe-2S) domain protein



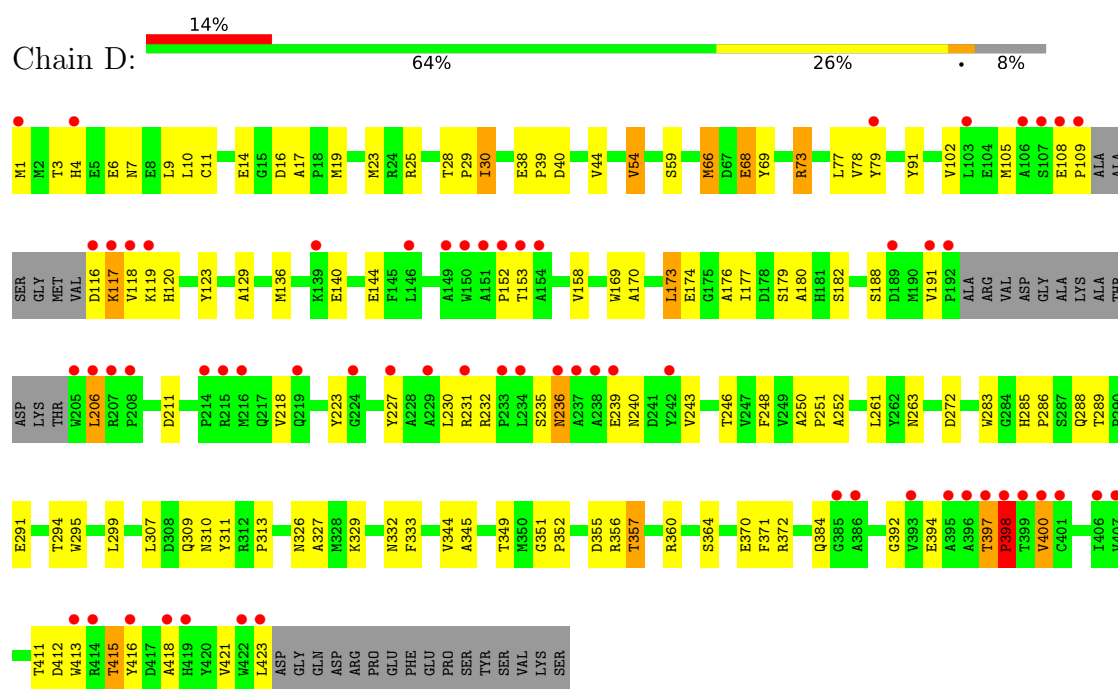
• Molecule 1: Rieske (2Fe-2S) domain protein



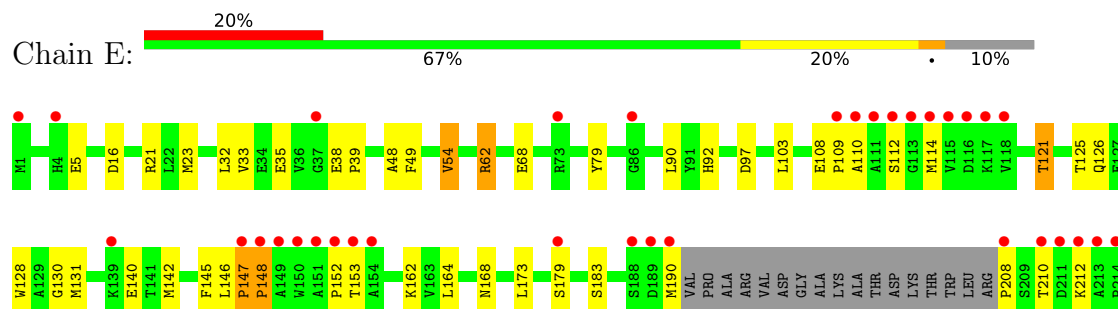
• Molecule 1: Rieske (2Fe-2S) domain protein

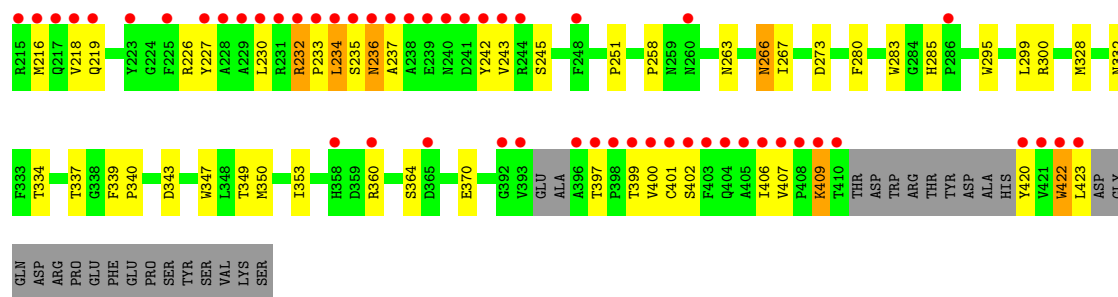


• Molecule 1: Rieske (2Fe-2S) domain protein

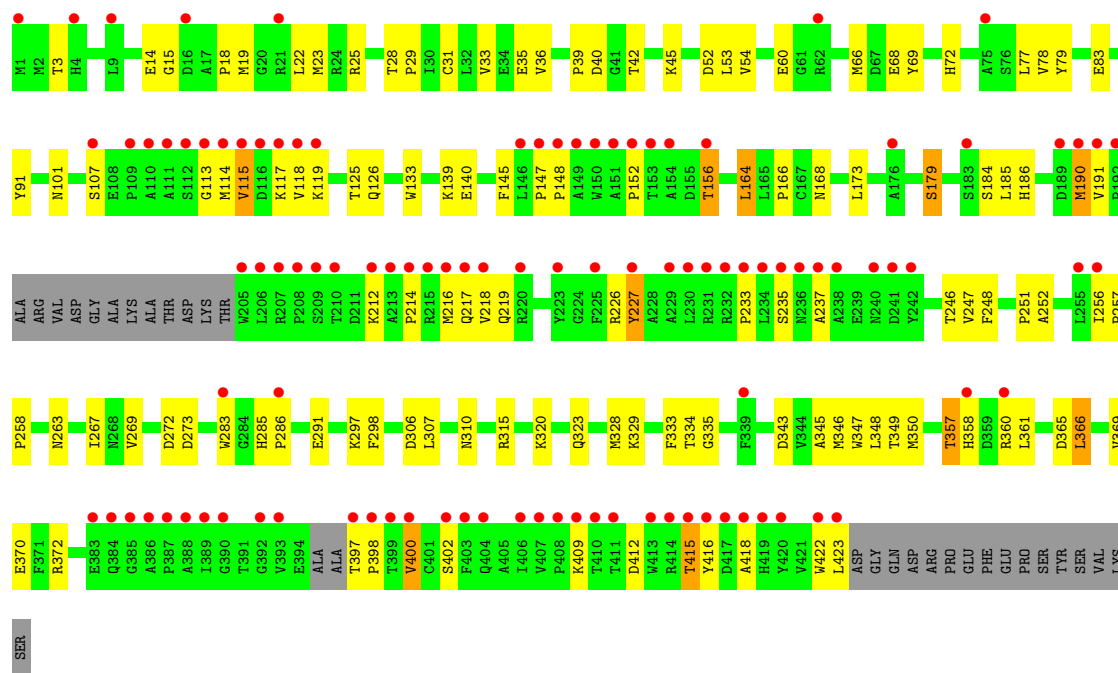


• Molecule 1: Rieske (2Fe-2S) domain protein





• Molecule 1: Rieske (2Fe-2S) domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.03Å 122.18Å 162.94Å 90.00° 101.13° 90.00°	Depositor
Resolution (Å)	159.88 – 2.74 159.88 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.0 (159.88-2.74) 98.0 (159.88-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.283 0.207 , 0.283	Depositor DCC
R_{free} test set	4388 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	20542	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: PHT, FES, FE2

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	0.53	0/3301	1.07	0/4497
1	B	0.52	0/3414	1.09	6/4652 (0.1%)
1	C	0.52	0/3301	1.06	5/4498 (0.1%)
1	D	0.53	0/3292	1.04	3/4485 (0.1%)
1	E	0.53	0/3176	1.07	4/4320 (0.1%)
1	F	0.51	0/3317	1.05	2/4518 (0.0%)
All	All	0.52	0/19801	1.06	20/26970 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	121	THR	CB-CA-C	6.27	122.90	110.42
1	B	329	LYS	CB-CA-C	6.20	121.40	110.85
1	B	67	ASP	CB-CA-C	6.07	119.79	109.72
1	E	397	THR	CB-CA-C	5.99	118.12	110.22
1	B	62	ARG	CB-CA-C	5.88	119.56	109.51
1	D	294	THR	CA-CB-OG1	-5.54	101.29	109.60
1	D	68	GLU	CB-CG-CD	5.46	121.89	112.60
1	B	194	ARG	CB-CA-C	5.46	117.88	109.03
1	C	415	THR	CB-CA-C	5.43	118.15	109.02
1	F	69	TYR	CB-CA-C	5.40	118.93	110.19
1	C	147	PRO	N-CA-C	5.36	117.24	110.70
1	B	69	TYR	CB-CA-C	5.30	118.49	109.80
1	F	42	THR	CA-CB-OG1	-5.27	101.69	109.60
1	C	177	ILE	CA-C-N	-5.19	115.24	123.23
1	C	177	ILE	C-N-CA	-5.19	115.24	123.23
1	C	69	TYR	CB-CA-C	5.16	118.25	109.53
1	B	58	ASP	CA-CB-CG	5.15	117.75	112.60
1	E	125	THR	CA-CB-OG1	-5.14	101.89	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	273	ASP	CB-CA-C	5.09	119.25	110.79
1	D	289	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3213	0	3096	56	0
1	B	3323	0	3210	79	0
1	C	3212	0	3097	65	0
1	D	3203	0	3084	86	0
1	E	3095	0	2993	67	0
1	F	3228	0	3110	105	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
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
3	E	4	0	0	1	0
3	F	4	0	0	0	0
4	B	12	0	4	0	0
5	A	204	0	0	9	0
5	B	208	0	0	6	0
5	C	208	0	0	8	0
5	D	198	0	0	9	0
5	E	200	0	0	8	0
5	F	208	0	0	15	0
All	All	20542	0	18594	434	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 (434) 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:2:MET:HE1	1:B:372:ARG:HD3	1.27	1.13
1:F:23:MET:HE2	1:F:251:PRO:HB2	1.21	1.13
1:F:397:THR:HB	1:F:398:PRO:HD3	1.31	1.08
1:B:66:MET:CE	1:B:120:HIS:HD2	1.70	1.03
1:C:216:MET:HE2	1:C:227:TYR:HE2	1.23	1.02
1:E:54:VAL:HG22	1:E:68:GLU:HA	1.45	0.98
1:E:218:VAL:HG11	1:E:370:GLU:HG2	1.46	0.97
1:B:66:MET:HE3	1:B:120:HIS:HD2	1.29	0.96
1:F:397:THR:CB	1:F:398:PRO:HD3	1.97	0.93
1:C:216:MET:HE2	1:C:227:TYR:CE2	2.04	0.92
1:E:420:TYR:HE1	1:E:422:TRP:HE3	1.23	0.85
1:B:66:MET:CE	1:B:120:HIS:CD2	2.59	0.84
1:B:397:THR:HB	1:B:398:PRO:HD2	1.59	0.84
1:D:230:LEU:CD2	1:D:243:VAL:HG22	2.08	0.83
1:C:218:VAL:HG11	1:C:370:GLU:HG2	1.59	0.83
1:A:211:ASP:HB3	1:A:231:ARG:HB3	1.61	0.82
1:F:23:MET:HE2	1:F:251:PRO:CB	2.08	0.81
1:D:397:THR:HB	1:D:398:PRO:HD2	1.62	0.81
1:B:218:VAL:HG11	1:B:370:GLU:HG2	1.62	0.81
1:D:230:LEU:HD23	1:D:243:VAL:HG22	1.62	0.80
1:B:91:TYR:HE2	1:C:350:MET:HE1	1.48	0.79
1:C:4:HIS:HB3	5:C:672:HOH:O	1.82	0.79
1:B:360:ARG:NH2	1:F:118:VAL:HG13	1.98	0.78
1:F:173:LEU:HD21	1:F:248:PHE:HE1	1.48	0.78
1:D:118:VAL:HG13	1:E:360:ARG:NH2	1.98	0.78
1:B:360:ARG:HH22	1:F:118:VAL:HG13	1.50	0.76
1:D:307:LEU:HD23	1:D:313:PRO:HA	1.68	0.76
1:B:66:MET:HE3	1:B:120:HIS:CD2	2.19	0.75
1:C:216:MET:CE	1:C:227:TYR:HE2	1.99	0.75
1:F:212:LYS:O	1:F:214:PRO:HD3	1.87	0.75
1:E:54:VAL:CG2	1:E:68:GLU:HA	2.17	0.74
1:E:420:TYR:HE1	1:E:422:TRP:CE3	2.05	0.74
1:B:235:SER:HB2	5:B:754:HOH:O	1.89	0.73
1:D:356:ARG:HG2	1:D:372:ARG:NH2	2.03	0.72
1:E:334:THR:HG23	5:E:643:HOH:O	1.89	0.72
1:F:397:THR:CB	1:F:398:PRO:CD	2.67	0.72
1:F:54:VAL:HG23	1:F:68:GLU:HA	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HG22	1:B:68:GLU:HA	1.72	0.72
1:B:2:MET:CE	1:B:372:ARG:HD3	2.14	0.71
1:C:412:ASP:HB3	1:C:415:THR:HG22	1.73	0.71
1:D:4:HIS:HB3	5:D:735:HOH:O	1.91	0.71
1:B:412:ASP:O	1:B:415:THR:HG22	1.90	0.70
1:C:310:ASN:O	1:C:311:TYR:HB2	1.90	0.70
1:F:218:VAL:HG12	1:F:219:GLN:N	2.07	0.70
1:F:117:LYS:HA	5:F:684:HOH:O	1.91	0.70
1:C:91:TYR:HE2	1:F:350:MET:HE1	1.55	0.70
1:E:263:ASN:HB2	1:E:283:TRP:CE2	2.27	0.69
1:F:173:LEU:HD21	1:F:248:PHE:CE1	2.27	0.69
1:F:412:ASP:O	1:F:415:THR:HG22	1.92	0.69
1:F:263:ASN:HB2	1:F:283:TRP:CE2	2.28	0.68
1:D:7:ASN:OD1	1:D:356:ARG:HD2	1.93	0.68
1:E:328:MET:HA	1:E:332:ASN:O	1.95	0.67
1:F:416:TYR:CE2	1:F:418:ALA:HB2	2.30	0.66
1:B:247:VAL:HB	1:B:255:LEU:HB2	1.77	0.66
1:A:16:ASP:HB3	5:A:705:HOH:O	1.94	0.66
1:D:416:TYR:CE2	1:D:418:ALA:HB2	2.31	0.66
1:F:101:ASN:HD22	1:F:119:LYS:HD2	1.60	0.65
1:A:393:VAL:HG12	5:A:723:HOH:O	1.97	0.65
1:F:101:ASN:ND2	1:F:119:LYS:HD2	2.11	0.65
1:C:54:VAL:CG2	1:C:68:GLU:HA	2.27	0.64
1:E:285:HIS:HD2	1:E:423:LEU:HB2	1.62	0.64
1:B:350:MET:HE1	1:F:91:TYR:HE2	1.60	0.64
1:A:397:THR:HB	1:A:398:PRO:HD2	1.79	0.64
1:D:295:TRP:CE2	1:D:299:LEU:HD11	2.33	0.64
1:D:23:MET:CE	1:D:251:PRO:HB2	2.27	0.64
1:F:306:ASP:HB3	1:F:315:ARG:HH12	1.63	0.63
1:D:412:ASP:O	1:D:415:THR:HG22	1.99	0.63
1:D:416:TYR:HE2	1:D:418:ALA:HB2	1.63	0.63
1:A:66:MET:HE3	1:A:120:HIS:HD2	1.64	0.63
1:E:233:PRO:HG3	1:E:242:TYR:HB2	1.81	0.63
1:F:179:SER:HB2	1:F:227:TYR:OH	1.99	0.63
1:F:54:VAL:CG2	1:F:68:GLU:HA	2.29	0.62
1:E:128:TRP:HH2	1:E:153:THR:HA	1.64	0.62
1:E:232:ARG:HD2	1:E:237:ALA:HB1	1.79	0.62
1:A:263:ASN:HB2	1:A:283:TRP:CE2	2.33	0.62
1:E:401:CYS:SG	1:E:420:TYR:HB3	2.40	0.62
1:E:230:LEU:HD23	1:E:243:VAL:HG22	1.82	0.62
1:D:310:ASN:O	1:D:311:TYR:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD23	1:B:186:HIS:CE1	2.34	0.62
1:E:218:VAL:CG1	1:E:370:GLU:HG2	2.26	0.61
1:F:343:ASP:HB3	1:F:347:TRP:CZ2	2.36	0.61
1:C:190:MET:HE2	1:C:205:TRP:CE3	2.36	0.61
1:A:16:ASP:HB2	5:A:626:HOH:O	2.00	0.60
1:D:285:HIS:CD2	1:D:286:PRO:HD2	2.36	0.60
1:B:139:LYS:HG3	5:B:767:HOH:O	2.01	0.60
1:E:97:ASP:HB3	1:E:103:LEU:HD21	1.83	0.60
1:B:107:SER:HB2	1:C:180:ALA:HB1	1.82	0.60
1:F:19:MET:O	1:F:23:MET:HG3	2.02	0.60
1:F:166:PRO:HD2	1:F:348:LEU:HD21	1.84	0.60
1:B:236:ASN:C	1:B:238:ALA:H	2.09	0.59
1:C:118:VAL:HG12	1:F:360:ARG:HH21	1.68	0.59
1:C:216:MET:CE	1:C:227:TYR:CE2	2.79	0.59
1:F:416:TYR:HE2	1:F:418:ALA:HB2	1.68	0.59
1:A:14:GLU:OE2	1:A:272:ASP:HB2	2.02	0.59
1:C:219:GLN:HE21	1:C:414:ARG:HD3	1.67	0.59
1:C:240:ASN:OD1	1:C:408:PRO:HA	2.01	0.59
1:F:218:VAL:HG11	1:F:370:GLU:HG2	1.83	0.59
1:F:218:VAL:CG1	1:F:219:GLN:N	2.64	0.59
1:D:397:THR:HB	1:D:398:PRO:CD	2.33	0.58
1:F:45:LYS:HE2	1:F:68:GLU:OE1	2.02	0.58
1:B:329:LYS:HG3	5:F:744:HOH:O	2.03	0.58
1:E:183:SER:HB3	1:E:212:LYS:HA	1.85	0.58
1:B:5:GLU:HG2	5:B:680:HOH:O	2.04	0.58
1:C:54:VAL:HG22	1:C:68:GLU:HA	1.86	0.58
1:C:365:ASP:O	1:C:369:VAL:HG23	2.04	0.57
1:B:397:THR:HB	1:B:398:PRO:CD	2.33	0.57
1:A:144:GLU:HB3	5:A:758:HOH:O	2.05	0.57
1:F:173:LEU:HD22	1:F:252:ALA:HA	1.86	0.57
1:A:66:MET:HE3	1:A:120:HIS:CD2	2.39	0.57
1:D:1:MET:CG	5:D:746:HOH:O	2.52	0.57
1:F:33:VAL:O	1:F:36:VAL:HG22	2.04	0.57
1:B:355:ASP:OD1	1:B:357:THR:HB	2.03	0.57
1:C:54:VAL:HG21	1:C:77:LEU:HB2	1.87	0.57
1:D:230:LEU:HD22	1:D:243:VAL:HG22	1.87	0.57
1:D:140:GLU:HB2	5:D:737:HOH:O	2.04	0.57
1:D:355:ASP:OD1	1:D:357:THR:HB	2.05	0.56
1:C:211:ASP:HB3	1:C:231:ARG:HG2	1.85	0.56
1:F:258:PRO:HB3	1:F:263:ASN:HA	1.88	0.56
1:D:39:PRO:O	1:D:40:ASP:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:LYS:HG3	5:F:774:HOH:O	2.04	0.56
1:A:131:MET:HE2	1:A:279:TYR:CD1	2.41	0.56
1:D:23:MET:HE3	1:D:251:PRO:HB2	1.87	0.56
1:F:156:THR:HG23	1:F:422:TRP:HZ3	1.71	0.56
1:D:384:GLN:HA	1:D:384:GLN:NE2	2.20	0.56
1:E:235:SER:O	1:E:236:ASN:HB2	2.05	0.56
1:F:115:VAL:HG11	5:F:786:HOH:O	2.06	0.56
1:B:114:MET:HA	1:B:117:LYS:HG2	1.88	0.55
1:B:60:GLU:HG3	1:B:62:ARG:NH1	2.21	0.55
1:C:397:THR:HB	1:C:398:PRO:HD2	1.88	0.55
5:B:710:HOH:O	1:C:317:GLU:HG2	2.07	0.55
1:D:1:MET:HG2	5:D:746:HOH:O	2.07	0.55
1:E:232:ARG:HD2	1:E:237:ALA:CB	2.36	0.55
1:E:263:ASN:HB2	1:E:283:TRP:NE1	2.22	0.55
1:F:54:VAL:HG21	1:F:77:LEU:HB2	1.88	0.55
1:F:218:VAL:CG1	1:F:219:GLN:H	2.20	0.55
1:F:237:ALA:HB3	5:F:751:HOH:O	2.05	0.55
1:A:18:PRO:HB2	1:A:379:VAL:HG22	1.89	0.55
1:D:356:ARG:HG2	1:D:372:ARG:CZ	2.36	0.55
1:F:218:VAL:HG23	1:F:366:LEU:HD23	1.89	0.55
1:F:216:MET:O	1:F:217:GLN:HG2	2.07	0.54
1:D:102:VAL:HG11	1:D:105:MET:HE2	1.89	0.54
1:A:230:LEU:HD23	1:A:230:LEU:N	2.22	0.54
1:A:218:VAL:HG11	1:A:370:GLU:HG2	1.90	0.54
1:F:125:THR:HA	1:F:133:TRP:O	2.07	0.54
1:F:397:THR:HB	1:F:398:PRO:CD	2.19	0.54
1:B:152:PRO:HB3	1:B:398:PRO:HB3	1.89	0.54
1:A:211:ASP:CB	1:A:231:ARG:HB3	2.34	0.54
1:F:29:PRO:O	1:F:269:VAL:HG21	2.08	0.54
1:B:170:ALA:HB3	1:B:356:ARG:NH2	2.22	0.54
1:D:261:LEU:HA	1:D:288:GLN:HE21	1.72	0.54
1:E:295:TRP:CE2	1:E:299:LEU:HD11	2.43	0.54
1:A:22:LEU:C	1:A:22:LEU:HD23	2.32	0.54
1:D:173:LEU:HD13	1:D:252:ALA:HA	1.90	0.54
1:C:91:TYR:HE2	1:F:350:MET:CE	2.21	0.54
1:D:23:MET:HE2	1:D:251:PRO:HB2	1.89	0.54
1:F:226:ARG:HG2	1:F:247:VAL:HG22	1.90	0.54
1:E:285:HIS:CD2	1:E:423:LEU:HB2	2.43	0.54
1:A:70:CYS:SG	1:A:71:PRO:HD2	2.47	0.53
1:E:235:SER:O	1:E:236:ASN:CB	2.56	0.53
1:E:216:MET:HE2	1:E:364:SER:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:HB2	1:B:108:GLU:HB3	1.91	0.53
1:D:73:ARG:HH11	1:D:73:ARG:HG3	1.72	0.53
1:B:109:PRO:O	1:B:112:SER:HB2	2.09	0.53
1:B:116:ASP:O	1:B:119:LYS:NZ	2.41	0.53
1:F:400:VAL:HG21	5:F:617:HOH:O	2.09	0.53
1:A:73:ARG:O	1:A:74:ARG:HB2	2.09	0.52
1:B:66:MET:HE2	1:B:120:HIS:CD2	2.45	0.52
1:A:45:LYS:HE2	1:A:68:GLU:OE1	2.09	0.52
1:C:39:PRO:O	1:C:40:ASP:HB2	2.09	0.52
1:D:177:ILE:HG13	1:D:177:ILE:O	2.10	0.52
1:C:92:HIS:HB2	3:C:502:FES:S1	2.50	0.52
1:D:129:ALA:HB1	1:D:158:VAL:HG11	1.91	0.52
1:D:263:ASN:HB2	1:D:283:TRP:CE2	2.44	0.52
1:B:199:LYS:HD2	1:B:202:ASP:OD2	2.10	0.52
1:A:92:HIS:HB2	3:A:502:FES:S2	2.50	0.52
1:C:355:ASP:OD1	1:C:357:THR:HB	2.09	0.52
1:D:69:TYR:O	1:D:120:HIS:HE1	1.92	0.52
1:B:227:TYR:CE1	1:B:246:THR:HB	2.45	0.52
1:F:345:ALA:O	1:F:349:THR:HG23	2.10	0.52
1:A:247:VAL:HB	1:A:255:LEU:HD12	1.91	0.51
1:E:62:ARG:HG3	1:E:62:ARG:HH11	1.75	0.51
1:B:54:VAL:HG13	1:B:78:VAL:HG22	1.92	0.51
1:B:202:ASP:HB2	1:B:206:LEU:HD22	1.91	0.51
1:E:16:ASP:O	1:E:21:ARG:HD3	2.10	0.51
1:B:216:MET:HE3	1:B:227:TYR:CE2	2.45	0.51
1:A:16:ASP:O	1:A:21:ARG:NH1	2.44	0.51
1:E:179:SER:HB2	1:E:227:TYR:OH	2.11	0.51
1:C:227:TYR:CE1	1:C:246:THR:HB	2.46	0.50
1:B:113:GLY:O	1:B:117:LYS:HE3	2.11	0.50
1:D:345:ALA:O	1:D:349:THR:HG23	2.12	0.50
1:F:113:GLY:N	5:F:604:HOH:O	2.45	0.50
1:B:238:ALA:O	1:B:409:LYS:HE3	2.12	0.50
1:A:208:PRO:HD2	1:A:242:TYR:CZ	2.46	0.50
1:D:179:SER:OG	1:D:231:ARG:NH2	2.45	0.50
1:D:397:THR:CB	1:D:398:PRO:HD2	2.38	0.50
1:F:184:SER:O	1:F:333:PHE:CD2	2.65	0.50
1:A:24:ARG:HD2	5:A:628:HOH:O	2.12	0.50
1:C:90:LEU:HD13	1:F:334:THR:HG22	1.93	0.50
1:A:392:GLY:HA2	5:A:753:HOH:O	2.11	0.50
1:E:210:THR:HB	5:E:682:HOH:O	2.12	0.50
1:A:4:HIS:O	1:A:8:GLU:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LYS:HE3	5:F:772:HOH:O	2.11	0.49
1:F:256:ILE:HD13	1:F:256:ILE:N	2.27	0.49
1:C:397:THR:HB	1:C:398:PRO:CD	2.41	0.49
1:F:60:GLU:HG3	5:F:674:HOH:O	2.12	0.49
1:B:350:MET:CE	1:F:91:TYR:HE2	2.24	0.49
1:A:157:ARG:NH1	1:A:286:PRO:O	2.45	0.49
1:E:360:ARG:HG3	1:E:360:ARG:NH1	2.27	0.49
1:C:54:VAL:HG23	1:C:68:GLU:HA	1.95	0.49
1:D:38:GLU:HB2	5:D:742:HOH:O	2.13	0.49
1:F:152:PRO:HA	1:F:398:PRO:CG	2.43	0.49
1:F:400:VAL:HB	5:F:671:HOH:O	2.12	0.49
1:B:12:ARG:HD3	1:B:273:ASP:OD2	2.12	0.49
1:A:408:PRO:C	1:A:410:THR:H	2.21	0.49
1:C:190:MET:HE2	1:C:205:TRP:CZ3	2.48	0.49
1:D:360:ARG:NH2	5:D:606:HOH:O	2.46	0.49
1:D:66:MET:HE3	1:D:120:HIS:CD2	2.48	0.48
1:E:162:LYS:HE3	1:E:164:LEU:CD1	2.43	0.48
1:C:412:ASP:HB3	1:C:415:THR:CG2	2.43	0.48
1:F:323:GLN:NE2	1:F:328:MET:SD	2.87	0.48
1:B:60:GLU:HG3	1:B:62:ARG:HH11	1.78	0.48
1:B:365:ASP:O	1:B:369:VAL:HG23	2.14	0.48
1:B:38:GLU:HB2	5:B:678:HOH:O	2.14	0.48
1:B:369:VAL:HG12	1:B:373:LYS:HE3	1.95	0.48
1:C:23:MET:C	1:C:25:ARG:H	2.20	0.48
1:C:23:MET:HG2	1:C:251:PRO:HG3	1.95	0.48
1:D:227:TYR:CE1	1:D:246:THR:HB	2.49	0.48
1:E:162:LYS:HE3	1:E:164:LEU:HD11	1.96	0.48
1:C:192:PRO:HG3	1:C:210:THR:HG22	1.95	0.48
1:C:256:ILE:CG2	1:C:257:PRO:HD2	2.44	0.48
1:F:227:TYR:CE2	1:F:246:THR:HB	2.49	0.48
1:F:18:PRO:HD2	5:F:612:HOH:O	2.13	0.47
1:F:328:MET:HG3	1:F:335:GLY:HA3	1.95	0.47
1:B:126:GLN:HG3	1:B:127:GLU:N	2.28	0.47
1:A:55:VAL:HA	1:A:64:GLY:O	2.13	0.47
1:A:94:TRP:CZ2	1:A:105:MET:HE2	2.50	0.47
1:A:374:GLN:NE2	5:A:608:HOH:O	2.47	0.47
1:D:261:LEU:HB3	1:D:288:GLN:HG2	1.96	0.47
1:F:365:ASP:O	1:F:369:VAL:HG23	2.14	0.47
1:B:339:PHE:N	1:B:340:PRO:CD	2.78	0.47
1:C:22:LEU:C	1:C:22:LEU:HD23	2.40	0.47
1:E:168:ASN:HB2	1:E:353:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:VAL:HG11	1:E:370:GLU:CG	2.31	0.47
1:D:117:LYS:HB2	1:D:117:LYS:NZ	2.30	0.47
1:D:392:GLY:C	1:D:394:GLU:H	2.22	0.47
1:E:360:ARG:HG3	1:E:360:ARG:HH11	1.79	0.47
1:F:258:PRO:HD3	1:F:402:SER:OG	2.15	0.47
1:A:355:ASP:OD1	1:A:357:THR:HB	2.14	0.47
1:A:397:THR:CB	1:A:398:PRO:HD2	2.44	0.47
1:E:140:GLU:C	1:E:142:MET:H	2.23	0.47
1:E:343:ASP:HB3	1:E:347:TRP:CZ2	2.50	0.47
1:D:291:GLU:OE1	1:F:291:GLU:HG3	2.14	0.47
1:E:126:GLN:HG2	1:E:145:PHE:CG	2.49	0.47
1:F:343:ASP:HB3	1:F:347:TRP:CE2	2.50	0.47
1:B:3:THR:HG23	1:B:6:GLU:OE2	2.15	0.47
1:D:69:TYR:O	1:D:120:HIS:CE1	2.68	0.47
1:D:123:TYR:CE2	1:D:136:MET:HE3	2.50	0.47
1:D:173:LEU:HD22	1:D:371:PHE:CE1	2.50	0.47
1:F:101:ASN:HD22	1:F:119:LYS:CD	2.26	0.47
1:F:156:THR:HG23	1:F:422:TRP:CZ3	2.50	0.47
1:B:202:ASP:O	1:B:204:THR:N	2.45	0.47
1:D:170:ALA:O	1:D:174:GLU:HG3	2.15	0.47
1:E:400:VAL:HG13	5:E:694:HOH:O	2.15	0.47
1:F:22:LEU:C	1:F:22:LEU:HD23	2.39	0.47
1:F:233:PRO:C	1:F:235:SER:H	2.23	0.46
1:D:191:VAL:O	1:D:206:LEU:HA	2.15	0.46
1:A:139:LYS:HG2	1:A:140:GLU:N	2.31	0.46
1:E:242:TYR:HD1	1:E:406:ILE:HG12	1.80	0.46
1:B:236:ASN:C	1:B:238:ALA:N	2.73	0.46
1:C:295:TRP:CE2	1:C:299:LEU:HD11	2.51	0.46
1:C:31:CYS:HB2	1:C:35:GLU:OE2	2.15	0.46
1:F:346:MET:HE2	1:F:346:MET:HA	1.98	0.46
1:B:91:TYR:CE2	1:C:350:MET:HE1	2.39	0.46
1:A:84:GLU:HB2	1:A:95:LYS:NZ	2.30	0.46
1:C:118:VAL:CG1	1:F:360:ARG:NH2	2.79	0.46
1:A:94:TRP:CD1	1:A:105:MET:HG2	2.51	0.46
1:E:233:PRO:O	1:E:234:LEU:C	2.59	0.46
1:A:157:ARG:O	1:A:283:TRP:HA	2.15	0.45
1:C:123:TYR:CD1	1:C:136:MET:HA	2.50	0.45
1:B:180:ALA:HB1	1:F:107:SER:OG	2.16	0.45
1:D:11:CYS:SG	1:D:356:ARG:NH1	2.89	0.45
1:D:14:GLU:OE2	1:D:272:ASP:HB2	2.16	0.45
1:D:236:ASN:HB3	1:D:240:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:ASP:HB3	1:F:68:GLU:OE1	2.17	0.45
1:F:263:ASN:HB2	1:F:283:TRP:NE1	2.31	0.45
1:B:25:ARG:HA	1:B:25:ARG:HD3	1.69	0.45
1:D:116:ASP:HA	1:D:119:LYS:NZ	2.32	0.45
1:E:110:ALA:C	1:E:112:SER:H	2.23	0.45
1:F:256:ILE:CG2	1:F:257:PRO:HD2	2.47	0.45
1:D:23:MET:C	1:D:25:ARG:H	2.24	0.45
1:D:79:TYR:HE2	1:E:349:THR:HG21	1.81	0.45
1:D:291:GLU:HG3	1:F:291:GLU:OE1	2.16	0.45
1:E:300:ARG:HD2	5:E:604:HOH:O	2.16	0.45
1:E:62:ARG:HG3	1:E:62:ARG:NH1	2.32	0.45
1:F:168:ASN:HB2	1:F:273:ASP:O	2.17	0.45
1:D:332:ASN:OD1	1:D:333:PHE:N	2.49	0.45
1:B:170:ALA:HB3	1:B:356:ARG:HH22	1.80	0.45
1:A:33:VAL:HG23	1:A:130:GLY:C	2.42	0.45
1:A:319:ASN:O	1:A:320:LYS:HB2	2.16	0.45
1:C:300:ARG:HD2	5:C:629:HOH:O	2.15	0.45
1:D:309:GLN:HB2	5:D:780:HOH:O	2.16	0.45
1:E:32:LEU:HB2	1:E:35:GLU:HG3	1.99	0.45
1:B:295:TRP:CE2	1:B:299:LEU:HD11	2.52	0.45
1:A:170:ALA:O	1:A:174:GLU:HG3	2.17	0.45
1:F:39:PRO:O	1:F:40:ASP:HB2	2.16	0.45
1:D:54:VAL:HG13	1:D:78:VAL:HG22	1.98	0.44
1:D:91:TYR:HE2	1:E:350:MET:CE	2.31	0.44
1:D:413:TRP:C	1:D:415:THR:H	2.25	0.44
1:B:225:PHE:HD2	1:B:374:GLN:OE1	1.99	0.44
1:E:128:TRP:NE1	1:E:148:PRO:HD2	2.32	0.44
1:A:216:MET:HE2	1:A:364:SER:O	2.18	0.44
1:C:25:ARG:NH1	5:C:603:HOH:O	2.37	0.44
1:D:169:TRP:N	5:D:609:HOH:O	2.51	0.44
1:F:357:THR:HG22	1:F:358:HIS:CD2	2.52	0.44
1:A:58:ASP:HB2	1:A:85:GLY:HA2	1.99	0.44
1:A:220:ARG:HD3	1:A:370:GLU:OE2	2.17	0.44
1:A:310:ASN:O	1:A:311:TYR:HB2	2.17	0.44
1:D:117:LYS:NZ	1:D:117:LYS:CB	2.81	0.44
1:A:74:ARG:HA	1:A:74:ARG:HD2	1.68	0.44
1:D:248:PHE:CZ	1:D:250:ALA:HA	2.53	0.44
1:D:349:THR:C	1:D:351:GLY:N	2.75	0.44
1:F:25:ARG:HA	1:F:25:ARG:HD3	1.72	0.44
1:B:66:MET:HG2	1:B:122:ALA:HB2	2.00	0.43
1:C:25:ARG:HD3	1:C:25:ARG:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASP:HB3	1:D:231:ARG:HB3	1.99	0.43
1:E:92:HIS:HB2	3:E:502:FES:S2	2.58	0.43
1:B:329:LYS:HD2	5:F:744:HOH:O	2.18	0.43
1:C:53:LEU:HA	1:C:66:MET:O	2.18	0.43
1:D:54:VAL:CG2	1:D:68:GLU:HA	2.48	0.43
1:E:108:GLU:O	1:E:110:ALA:N	2.52	0.43
1:F:256:ILE:HG22	1:F:257:PRO:HD2	2.00	0.43
1:C:230:LEU:HD22	1:C:243:VAL:HG22	2.00	0.43
1:F:164:LEU:HD22	1:F:310:ASN:O	2.18	0.43
1:F:218:VAL:HG12	1:F:219:GLN:H	1.79	0.43
1:F:297:LYS:O	1:F:298:PHE:C	2.59	0.43
1:D:413:TRP:C	1:D:415:THR:N	2.75	0.43
1:E:266:ASN:HB2	1:E:280:PHE:HD1	1.83	0.43
1:C:118:VAL:HG12	1:F:360:ARG:NH2	2.31	0.43
1:D:73:ARG:HG3	1:D:73:ARG:NH1	2.33	0.43
1:E:146:LEU:HD13	5:E:785:HOH:O	2.18	0.43
1:F:400:VAL:HG12	5:F:622:HOH:O	2.18	0.43
1:A:72:HIS:CD2	1:A:94:TRP:CZ2	3.06	0.43
1:A:236:ASN:C	1:A:238:ALA:H	2.26	0.43
1:B:173:LEU:CD2	1:B:371:PHE:CE1	3.01	0.43
1:B:267:ILE:HG23	1:B:279:TYR:HB2	2.00	0.43
1:E:23:MET:HG2	1:E:251:PRO:HG3	1.99	0.43
1:F:14:GLU:OE2	1:F:272:ASP:HB2	2.19	0.43
1:B:129:ALA:O	1:B:160:ILE:HD11	2.19	0.43
1:B:242:TYR:CE2	1:B:244:ARG:HD2	2.54	0.43
1:C:23:MET:HG2	1:C:251:PRO:CG	2.48	0.43
1:C:190:MET:HB2	5:C:601:HOH:O	2.18	0.43
1:F:53:LEU:HA	1:F:66:MET:O	2.19	0.43
1:F:147:PRO:O	1:F:397:THR:CG2	2.67	0.43
1:B:168:ASN:HB2	1:B:353:ILE:HG12	2.01	0.43
1:D:3:THR:N	1:D:6:GLU:OE2	2.48	0.43
1:D:349:THR:C	1:D:351:GLY:H	2.27	0.43
1:A:16:ASP:CB	5:A:705:HOH:O	2.60	0.43
1:C:67:ASP:HB2	5:C:651:HOH:O	2.18	0.43
1:C:223:TYR:CG	1:C:396:ALA:HB2	2.53	0.43
1:F:68:GLU:HG3	1:F:78:VAL:HG23	2.01	0.43
1:B:18:PRO:HB2	1:B:379:VAL:CG2	2.49	0.42
1:B:282:ALA:HB2	1:B:295:TRP:CZ2	2.54	0.42
1:B:310:ASN:O	1:B:311:TYR:HB2	2.18	0.42
1:B:343:ASP:HB3	1:B:347:TRP:CZ2	2.54	0.42
1:A:419:HIS:HB3	5:A:677:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:PHE:CD1	1:B:339:PHE:C	2.97	0.42
1:C:68:GLU:HG3	1:C:78:VAL:HG23	2.00	0.42
1:C:91:TYR:CE2	1:F:350:MET:CE	3.02	0.42
1:D:180:ALA:HB2	1:D:364:SER:HB2	2.01	0.42
1:A:67:ASP:HB3	1:A:120:HIS:CE1	2.54	0.42
1:D:54:VAL:HG21	1:D:77:LEU:HB2	2.01	0.42
1:F:22:LEU:HD23	1:F:22:LEU:O	2.18	0.42
1:A:245:SER:O	1:A:402:SER:HB2	2.19	0.42
1:F:166:PRO:HD2	1:F:348:LEU:CD2	2.48	0.42
1:B:293:GLU:HB3	1:A:293:GLU:HB3	2.01	0.42
1:B:225:PHE:CD1	1:B:225:PHE:C	2.98	0.42
1:E:337:THR:HG21	5:E:669:HOH:O	2.19	0.42
1:C:4:HIS:CE1	5:C:633:HOH:O	2.73	0.42
1:C:139:LYS:HE2	5:C:731:HOH:O	2.20	0.42
1:B:173:LEU:HD23	1:B:371:PHE:CE1	2.55	0.42
1:C:392:GLY:C	1:C:394:GLU:H	2.28	0.42
1:D:352:PRO:HD2	5:D:674:HOH:O	2.19	0.42
1:E:48:ALA:O	1:E:49:PHE:C	2.62	0.41
1:B:22:LEU:C	1:B:22:LEU:HD23	2.45	0.41
1:A:72:HIS:HB2	1:A:94:TRP:CD2	2.54	0.41
1:E:339:PHE:CG	1:E:340:PRO:HD3	2.55	0.41
1:F:3:THR:HB	5:F:685:HOH:O	2.19	0.41
1:C:25:ARG:HD2	5:C:603:HOH:O	2.18	0.41
1:C:73:ARG:O	1:C:74:ARG:HB2	2.20	0.41
1:D:29:PRO:C	1:D:30:ILE:HD13	2.45	0.41
1:D:326:ASN:O	1:D:327:ALA:C	2.63	0.41
1:B:45:LYS:HE3	1:B:68:GLU:OE1	2.20	0.41
1:A:236:ASN:C	1:A:238:ALA:N	2.78	0.41
1:C:157:ARG:O	1:C:283:TRP:HA	2.21	0.41
1:A:263:ASN:C	1:A:264:VAL:HG23	2.46	0.41
1:B:338:GLY:O	1:B:341:ASN:HB2	2.20	0.41
1:D:16:ASP:O	1:D:17:ALA:C	2.64	0.41
1:C:17:ALA:HA	1:C:18:PRO:HD3	1.95	0.41
1:E:79:TYR:O	1:E:90:LEU:HD11	2.20	0.41
1:F:397:THR:OG1	1:F:398:PRO:CD	2.69	0.41
1:C:71:PRO:O	1:F:360:ARG:HD3	2.21	0.41
1:D:108:GLU:HG3	1:D:109:PRO:HD2	2.02	0.41
1:E:128:TRP:CH2	1:E:153:THR:HA	2.51	0.41
1:B:325:ARG:HD3	1:B:325:ARG:HA	1.77	0.41
1:B:349:THR:HG21	1:F:79:TYR:CE2	2.55	0.41
1:D:10:LEU:HD12	1:D:19:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:VAL:HG11	1:D:370:GLU:HG2	2.03	0.41
1:D:232:ARG:HB3	1:D:232:ARG:CZ	2.51	0.41
1:E:23:MET:HG2	1:E:251:PRO:CG	2.51	0.41
1:E:232:ARG:NH1	5:E:609:HOH:O	2.54	0.41
1:F:31:CYS:HB2	1:F:35:GLU:OE2	2.21	0.41
1:F:185:LEU:HD23	1:F:186:HIS:CE1	2.56	0.41
1:F:190:MET:HE1	5:F:760:HOH:O	2.20	0.41
1:F:361:LEU:HD11	1:F:372:ARG:NH1	2.36	0.41
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.86	0.41
1:A:94:TRP:CH2	1:A:105:MET:HE2	2.56	0.41
1:B:199:LYS:HG3	5:B:747:HOH:O	2.21	0.40
1:D:25:ARG:HA	1:D:25:ARG:HD3	1.70	0.40
1:D:91:TYR:HE2	1:E:350:MET:HE1	1.86	0.40
1:D:173:LEU:O	1:D:176:ALA:N	2.47	0.40
1:E:332:ASN:HB2	5:E:739:HOH:O	2.21	0.40
1:F:126:GLN:HG2	1:F:145:PHE:CD2	2.56	0.40
1:F:416:TYR:CD2	1:F:418:ALA:HB2	2.57	0.40
1:E:258:PRO:HD3	1:E:402:SER:OG	2.21	0.40
1:C:27:TRP:HZ2	1:C:142:MET:HE3	1.87	0.40
1:C:207:ARG:NH1	1:C:244:ARG:HH12	2.19	0.40
1:C:307:LEU:HD23	1:C:313:PRO:HA	2.04	0.40
1:D:223:TYR:CE2	1:D:400:VAL:HG21	2.57	0.40
1:B:108:GLU:O	1:B:109:PRO:C	2.64	0.40
1:E:420:TYR:CE1	1:E:422:TRP:HE3	2.16	0.40
1:E:33:VAL:HG23	1:E:130:GLY:C	2.46	0.40
1:E:38:GLU:HB3	1:E:39:PRO:HD2	2.03	0.40
1:E:227:TYR:O	1:E:245:SER:HA	2.22	0.40
1:F:285:HIS:CE1	1:F:423:LEU:HD11	2.57	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	401/439 (91%)	368 (92%)	29 (7%)	4 (1%)	12	22
1	B	421/439 (96%)	386 (92%)	33 (8%)	2 (0%)	24	40
1	C	401/439 (91%)	369 (92%)	29 (7%)	3 (1%)	18	32
1	D	399/439 (91%)	367 (92%)	29 (7%)	3 (1%)	16	29
1	E	387/439 (88%)	350 (90%)	30 (8%)	7 (2%)	6	11
1	F	403/439 (92%)	368 (91%)	31 (8%)	4 (1%)	12	22
All	All	2412/2634 (92%)	2208 (92%)	181 (8%)	23 (1%)	12	22

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	236	ASN
1	F	15	GLY
1	A	74	ARG
1	E	409	LYS
1	B	198	ALA
1	C	72	HIS
1	D	236	ASN
1	E	109	PRO
1	E	422	TRP
1	F	72	HIS
1	B	74	ARG
1	A	286	PRO
1	C	17	ALA
1	C	422	TRP
1	D	152	PRO
1	D	398	PRO
1	F	148	PRO
1	E	147	PRO
1	E	152	PRO
1	A	152	PRO
1	F	286	PRO
1	A	398	PRO
1	E	148	PRO

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	337/363 (93%)	316 (94%)	21 (6%)	16	30
1	B	348/363 (96%)	323 (93%)	25 (7%)	13	24
1	C	337/363 (93%)	312 (93%)	25 (7%)	13	23
1	D	337/363 (93%)	310 (92%)	27 (8%)	11	20
1	E	326/363 (90%)	307 (94%)	19 (6%)	18	33
1	F	340/363 (94%)	320 (94%)	20 (6%)	18	32
All	All	2025/2178 (93%)	1888 (93%)	137 (7%)	14	27

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	34	GLU
1	B	54	VAL
1	B	60	GLU
1	B	67	ASP
1	B	73	ARG
1	B	139	LYS
1	B	146	LEU
1	B	179	SER
1	B	191	VAL
1	B	195	VAL
1	B	203	LYS
1	B	206	LEU
1	B	218	VAL
1	B	232	ARG
1	B	255	LEU
1	B	263	ASN
1	B	267	ILE
1	B	339	PHE
1	B	357	THR
1	B	407	VAL
1	B	411	THR
1	B	414	ARG
1	B	415	THR
1	B	423	LEU
1	A	4	HIS
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	59	SER
1	A	108	GLU
1	A	139	LYS
1	A	153	THR
1	A	173	LEU
1	A	184	SER
1	A	188	SER
1	A	190	MET
1	A	191	VAL
1	A	205	TRP
1	A	230	LEU
1	A	267	ILE
1	A	286	PRO
1	A	339	PHE
1	A	357	THR
1	A	379	VAL
1	A	397	THR
1	A	406	ILE
1	A	411	THR
1	C	54	VAL
1	C	66	MET
1	C	117	LYS
1	C	118	VAL
1	C	119	LYS
1	C	121	THR
1	C	147	PRO
1	C	173	LEU
1	C	182	SER
1	C	183	SER
1	C	184	SER
1	C	204	THR
1	C	218	VAL
1	C	278	PHE
1	C	306	ASP
1	C	320	LYS
1	C	348	LEU
1	C	357	THR
1	C	366	LEU
1	C	368	ILE
1	C	384	GLN
1	C	393	VAL
1	C	402	SER

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Mol	Chain	Res	Type
1	C	409	LYS
1	C	423	LEU
1	D	9	LEU
1	D	28	THR
1	D	30	ILE
1	D	44	VAL
1	D	54	VAL
1	D	59	SER
1	D	66	MET
1	D	73	ARG
1	D	117	LYS
1	D	144	GLU
1	D	153	THR
1	D	173	LEU
1	D	182	SER
1	D	188	SER
1	D	206	LEU
1	D	235	SER
1	D	239	GLU
1	D	329	LYS
1	D	344	VAL
1	D	357	THR
1	D	397	THR
1	D	398	PRO
1	D	400	VAL
1	D	411	THR
1	D	415	THR
1	D	421	VAL
1	D	423	LEU
1	E	5	GLU
1	E	54	VAL
1	E	62	ARG
1	E	114	MET
1	E	121	THR
1	E	131	MET
1	E	147	PRO
1	E	173	LEU
1	E	190	MET
1	E	208	PRO
1	E	219	GLN
1	E	226	ARG
1	E	232	ARG

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Mol	Chain	Res	Type
1	E	234	LEU
1	E	266	ASN
1	E	267	ILE
1	E	399	THR
1	E	407	VAL
1	E	409	LYS
1	F	28	THR
1	F	83	GLU
1	F	114	MET
1	F	115	VAL
1	F	140	GLU
1	F	156	THR
1	F	164	LEU
1	F	179	SER
1	F	190	MET
1	F	191	VAL
1	F	227	TYR
1	F	267	ILE
1	F	307	LEU
1	F	320	LYS
1	F	329	LYS
1	F	357	THR
1	F	366	LEU
1	F	400	VAL
1	F	409	LYS
1	F	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	HIS
1	B	120	HIS
1	B	288	GLN
1	B	332	ASN
1	A	101	ASN
1	A	171	GLN
1	A	275	ASN
1	A	288	GLN
1	C	92	HIS
1	C	168	ASN
1	C	219	GLN
1	C	236	ASN

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Mol	Chain	Res	Type
1	C	266	ASN
1	C	268	ASN
1	C	404	GLN
1	D	120	HIS
1	D	240	ASN
1	D	263	ASN
1	D	266	ASN
1	D	268	ASN
1	D	288	GLN
1	D	384	GLN
1	D	404	GLN
1	E	219	GLN
1	E	275	ASN
1	F	101	ASN
1	F	259	ASN
1	F	260	ASN
1	F	288	GLN
1	F	358	HIS

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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	FES	B	502	1	0,4,4	-	-	-		
3	FES	E	502	1	0,4,4	-	-	-		
4	PHT	B	503	-	12,12,12	1.11	1 (8%)	16,16,16	1.04	0
3	FES	C	502	1	0,4,4	-	-	-		
3	FES	D	502	1	0,4,4	-	-	-		
3	FES	F	502	1	0,4,4	-	-	-		
3	FES	A	502	1	0,4,4	-	-	-		

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	FES	B	502	1	-	-	0/1/1/1
3	FES	E	502	1	-	-	0/1/1/1
4	PHT	B	503	-	-	2/8/8/8	0/1/1/1
3	FES	C	502	1	-	-	0/1/1/1
3	FES	D	502	1	-	-	0/1/1/1
3	FES	F	502	1	-	-	0/1/1/1
3	FES	A	502	1	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	PHT	O9-C7	-2.07	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

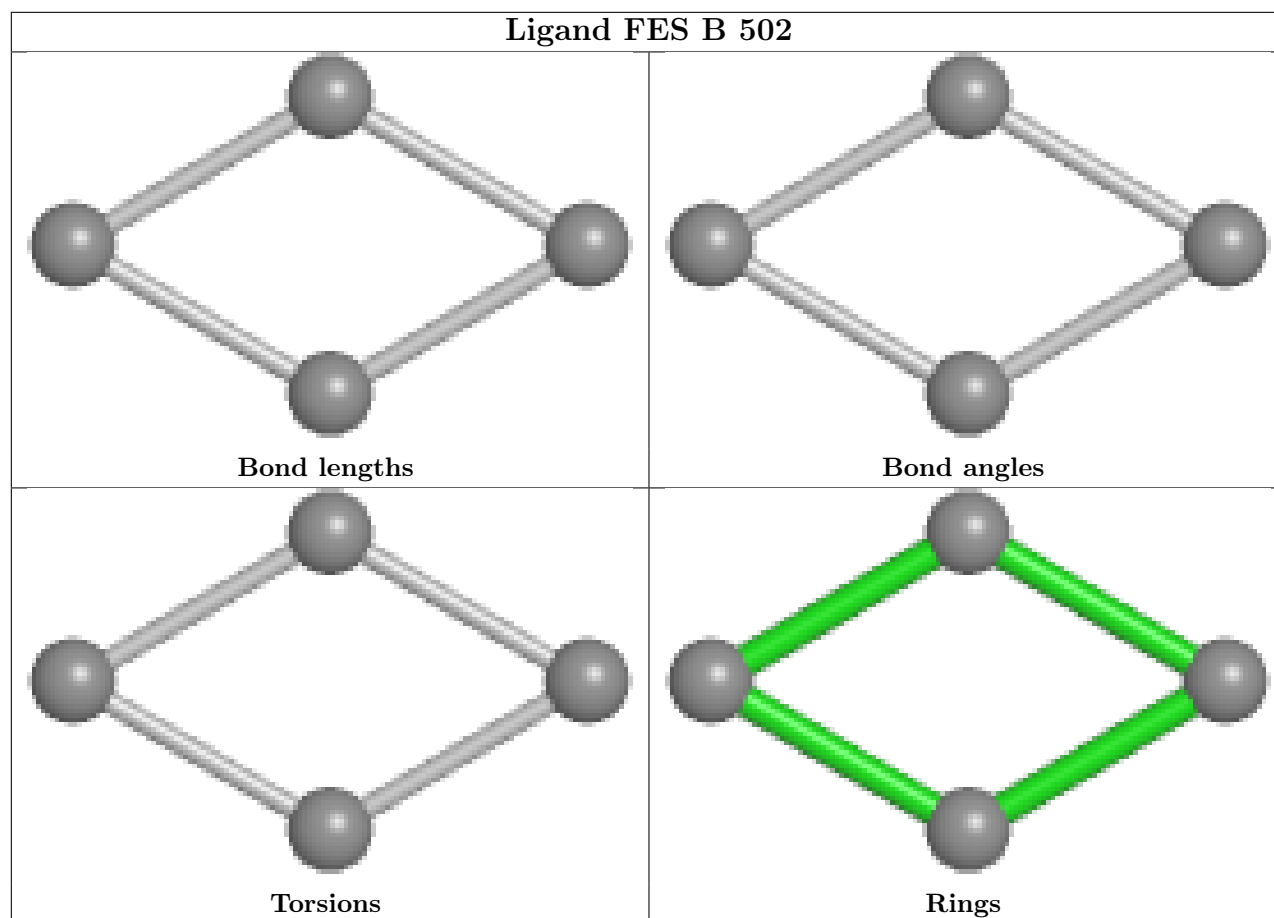
Mol	Chain	Res	Type	Atoms
4	B	503	PHT	C4-C3-C7-O9
4	B	503	PHT	C4-C3-C7-O8

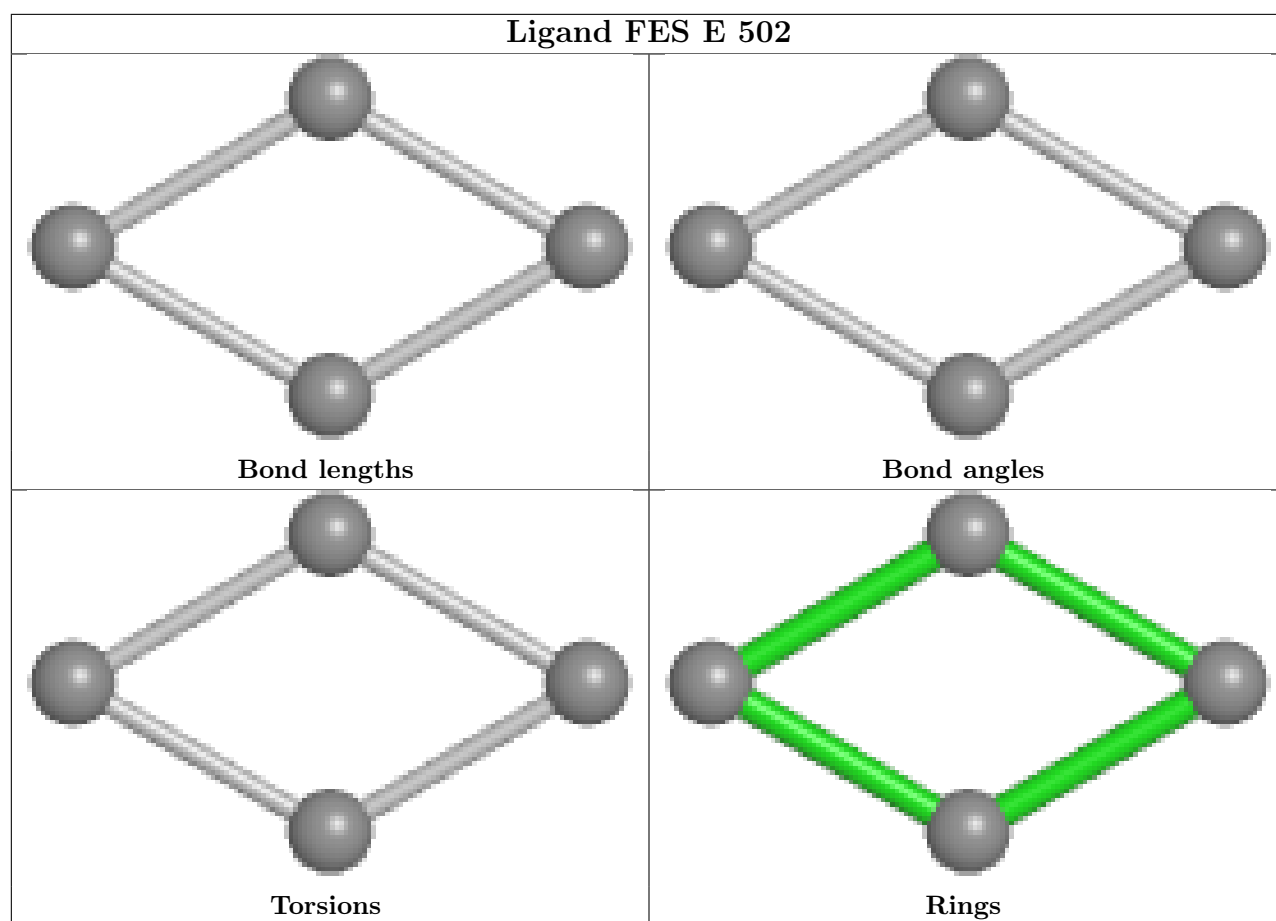
There are no ring outliers.

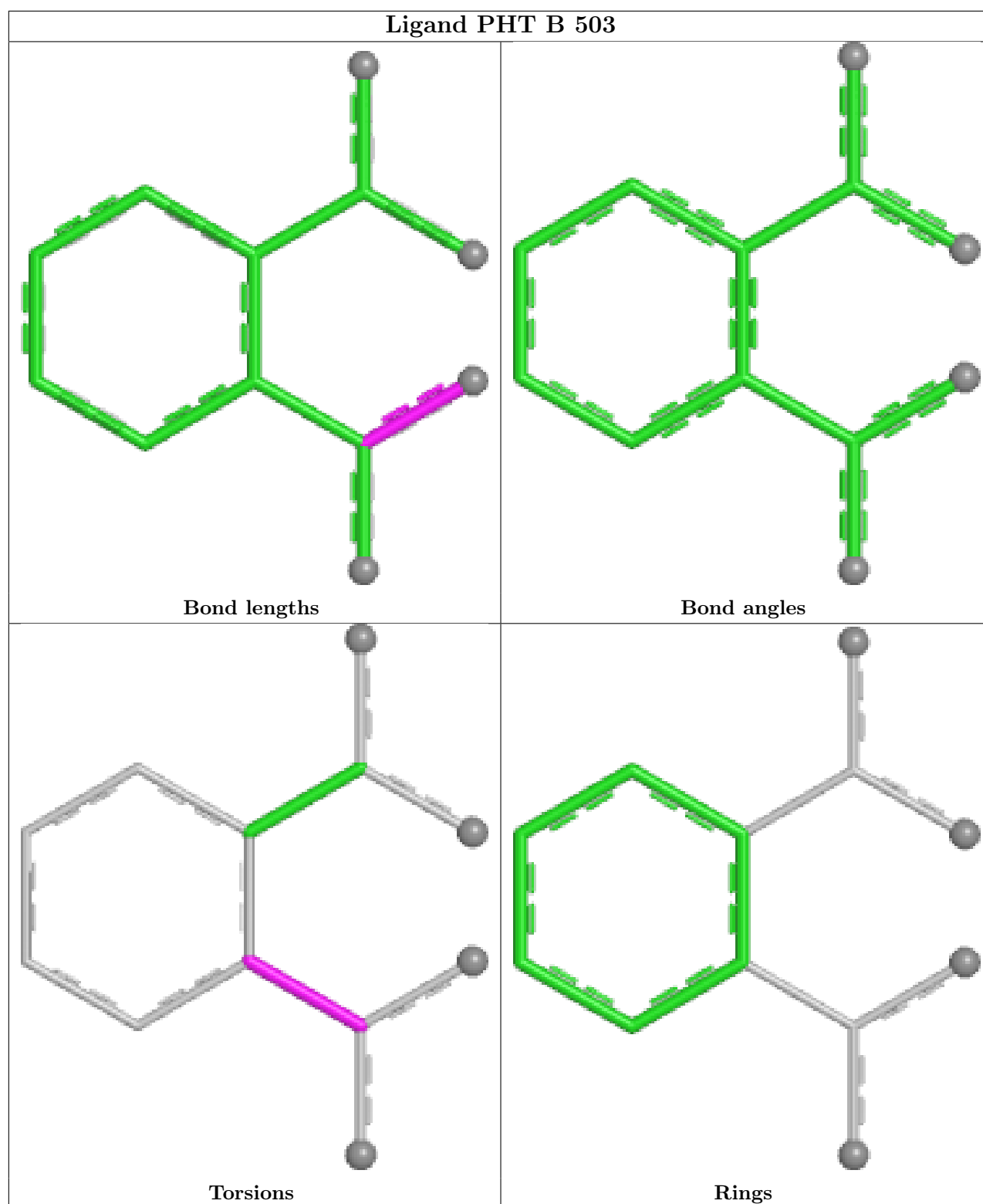
3 monomers are involved in 3 short contacts:

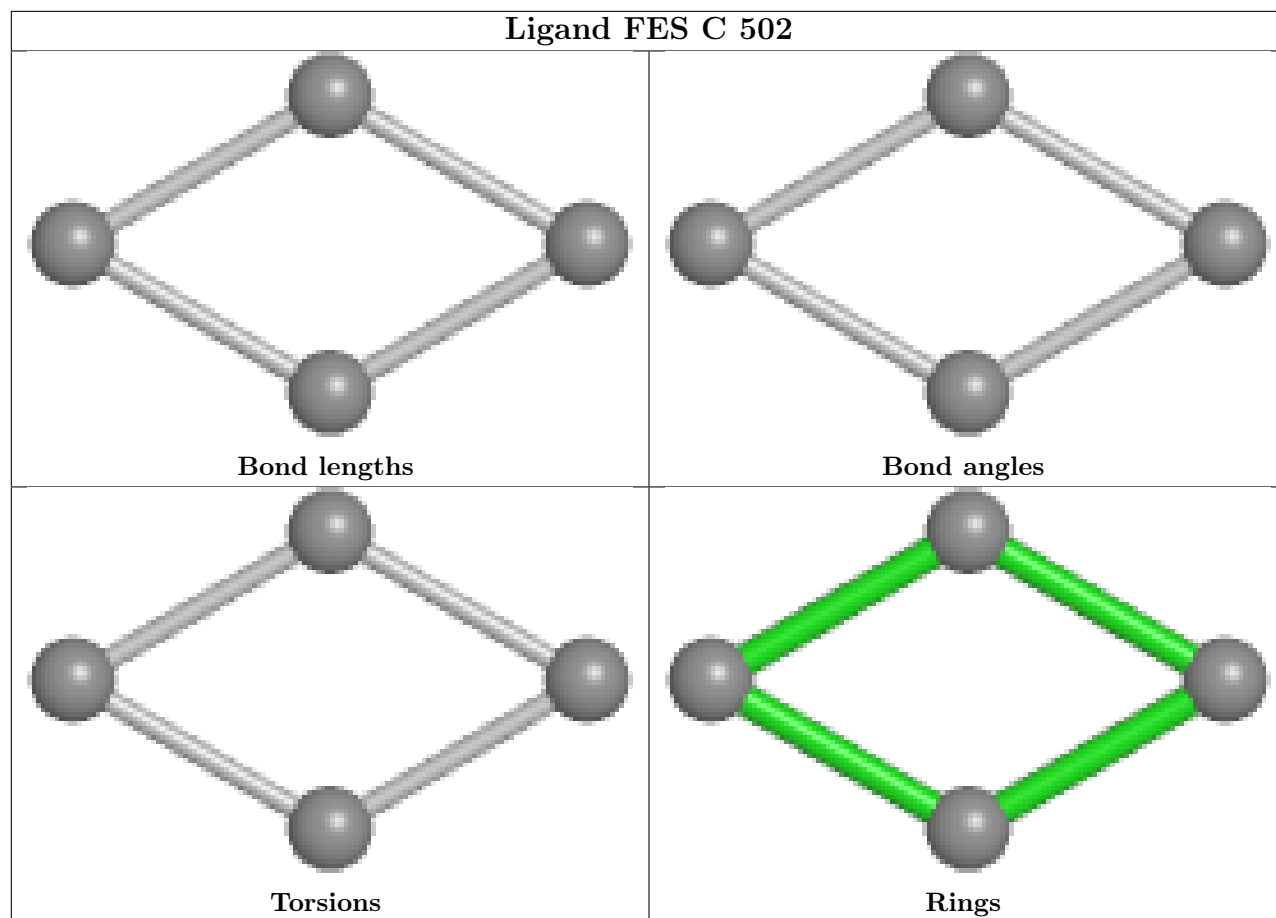
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	FES	1	0
3	C	502	FES	1	0
3	A	502	FES	1	0

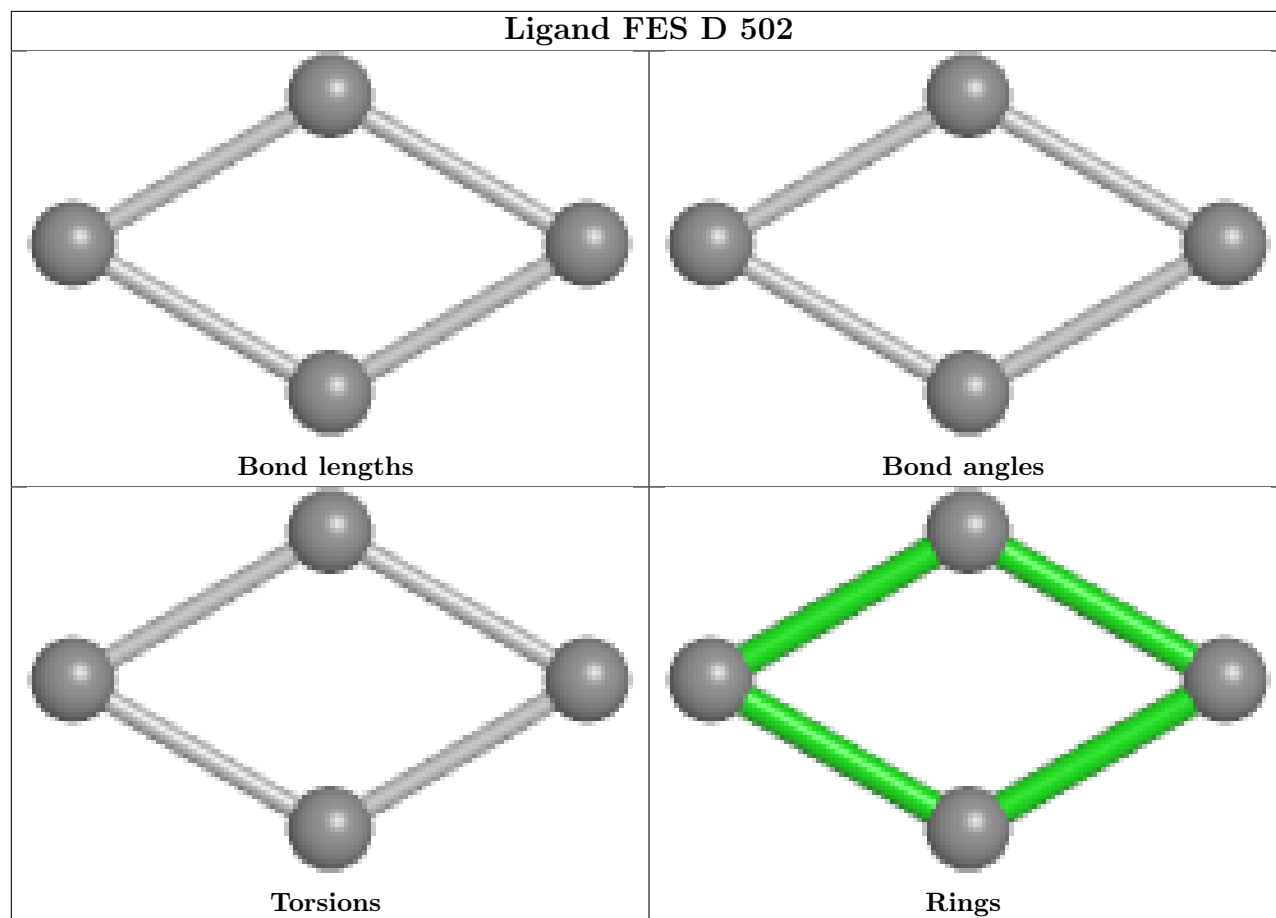
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

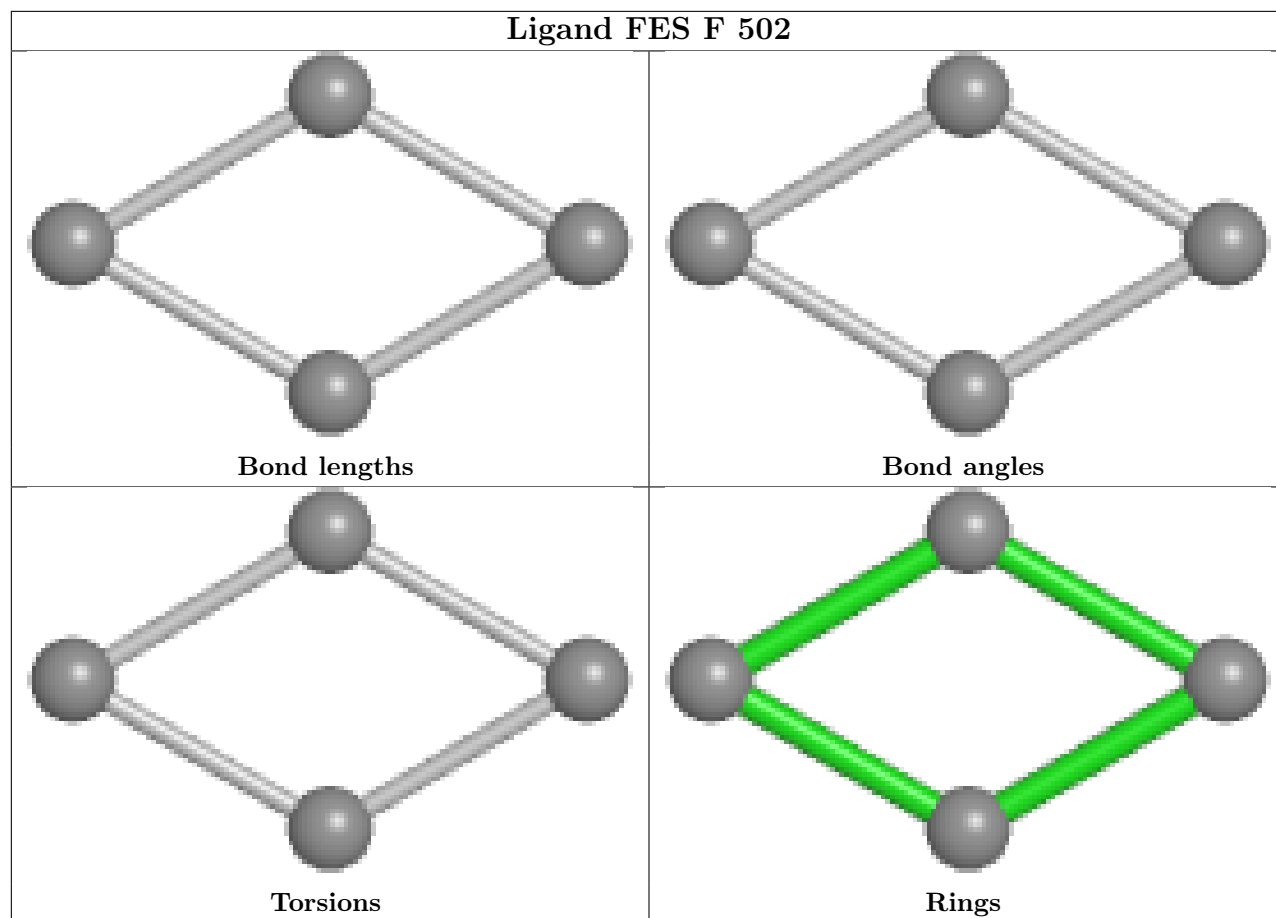


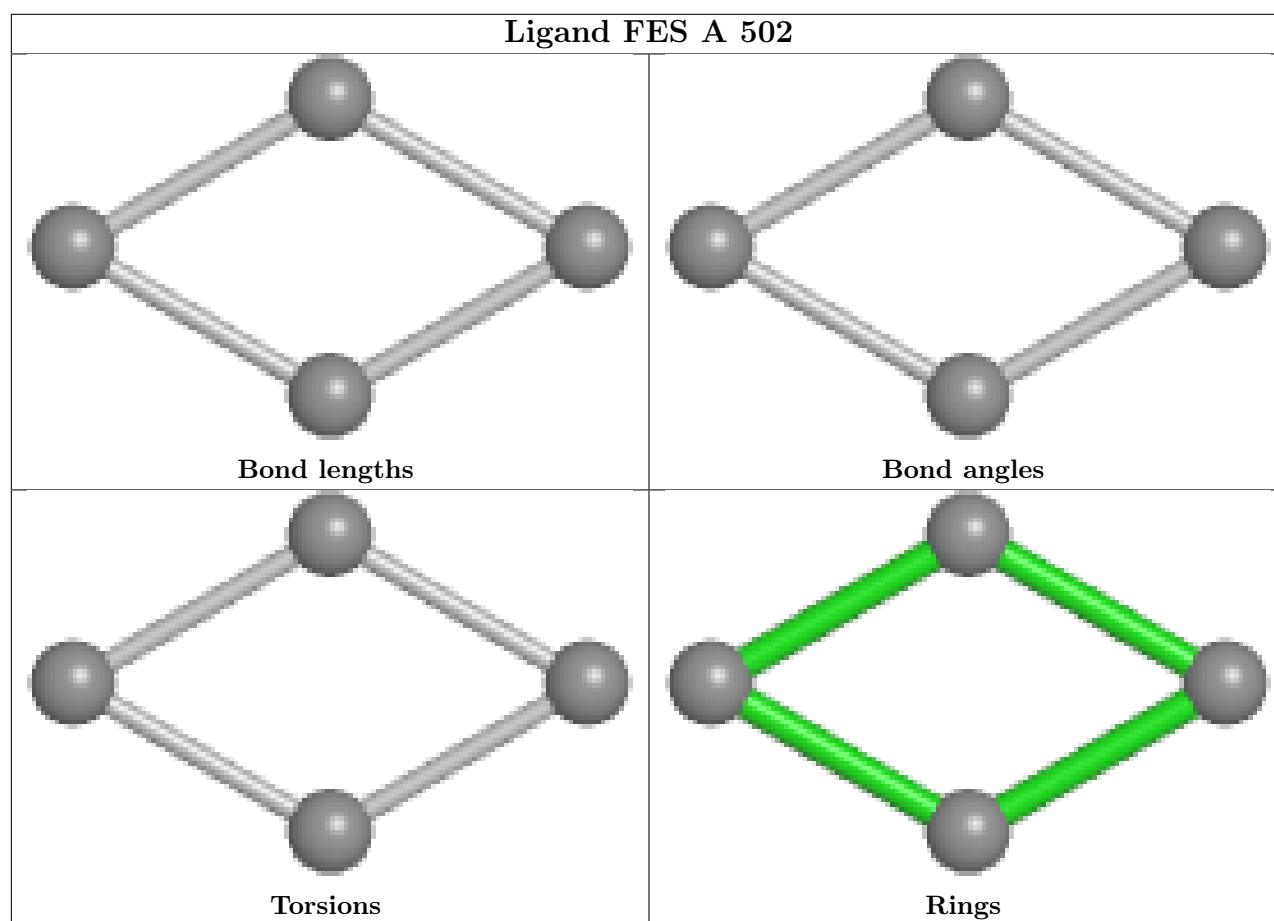












5.7 Other polymers [i](#)

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	407/439 (92%)	0.68	38 (9%)	14 14	22, 40, 75, 116	0
1	B	423/439 (96%)	0.93	76 (17%)	3 4	21, 40, 104, 159	0
1	C	407/439 (92%)	0.80	55 (13%)	7 6	23, 40, 98, 136	0
1	D	405/439 (92%)	0.94	61 (15%)	5 5	25, 44, 91, 128	0
1	E	395/439 (89%)	1.18	86 (21%)	2 2	24, 43, 132, 187	0
1	F	409/439 (93%)	1.33	105 (25%)	1 1	28, 49, 114, 132	0
All	All	2446/2634 (92%)	0.97	421 (17%)	4 4	21, 43, 107, 187	0

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	7.4
1	A	398	PRO	7.3
1	E	234	LEU	7.2
1	C	111	ALA	6.7
1	E	405	ALA	6.7
1	B	198	ALA	6.7
1	B	195	VAL	6.7
1	E	400	VAL	6.1
1	F	191	VAL	6.0
1	A	110	ALA	6.0
1	E	423	LEU	5.9
1	E	110	ALA	5.9
1	E	148	PRO	5.8
1	F	192	PRO	5.8
1	A	205	TRP	5.8
1	F	208	PRO	5.8
1	E	214	PRO	5.7
1	B	110	ALA	5.6
1	C	423	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	190	MET	5.4
1	C	109	PRO	5.3
1	F	153	THR	5.3
1	B	201	THR	5.3
1	E	393	VAL	5.2
1	B	197	GLY	5.1
1	D	206	LEU	5.0
1	C	208	PRO	4.9
1	A	111	ALA	4.9
1	F	406	ILE	4.9
1	E	399	THR	4.9
1	E	216	MET	4.9
1	C	205	TRP	4.8
1	D	423	LEU	4.8
1	F	393	VAL	4.8
1	D	109	PRO	4.7
1	E	208	PRO	4.7
1	D	398	PRO	4.7
1	C	238	ALA	4.7
1	E	229	ALA	4.7
1	E	235	SER	4.7
1	E	401	CYS	4.7
1	F	387	PRO	4.7
1	E	236	ASN	4.6
1	F	151	ALA	4.6
1	E	407	VAL	4.6
1	C	237	ALA	4.6
1	C	204	THR	4.5
1	B	203	LYS	4.4
1	A	115	VAL	4.4
1	D	154	ALA	4.4
1	C	107	SER	4.4
1	E	240	ASN	4.4
1	C	215	ARG	4.4
1	E	111	ALA	4.4
1	E	227	TYR	4.4
1	F	148	PRO	4.3
1	F	152	PRO	4.3
1	E	230	LEU	4.3
1	B	205	TRP	4.3
1	F	386	ALA	4.3
1	E	422	TRP	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	205	TRP	4.3
1	B	196	ASP	4.3
1	E	408	PRO	4.3
1	B	1	MET	4.3
1	F	230	LEU	4.2
1	D	191	VAL	4.2
1	B	202	ASP	4.2
1	F	415	THR	4.2
1	C	234	LEU	4.2
1	E	239	GLU	4.1
1	B	204	THR	4.1
1	D	399	THR	4.1
1	F	410	THR	4.1
1	F	189	ASP	4.1
1	C	210	THR	4.1
1	A	109	PRO	4.1
1	E	242	TYR	4.1
1	E	420	TYR	4.1
1	E	237	ALA	4.1
1	E	115	VAL	4.1
1	E	243	VAL	4.0
1	F	111	ALA	4.0
1	E	403	PHE	4.0
1	E	109	PRO	3.9
1	A	153	THR	3.9
1	B	115	VAL	3.9
1	F	209	SER	3.9
1	B	111	ALA	3.9
1	A	423	LEU	3.9
1	E	238	ALA	3.9
1	C	419	HIS	3.9
1	C	192	PRO	3.8
1	D	397	THR	3.8
1	F	422	TRP	3.8
1	D	107	SER	3.8
1	E	210	THR	3.8
1	F	408	PRO	3.8
1	B	406	ILE	3.8
1	F	206	LEU	3.7
1	F	237	ALA	3.7
1	C	191	VAL	3.7
1	C	411	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	117	LYS	3.7
1	E	215	ARG	3.7
1	F	115	VAL	3.7
1	F	398	PRO	3.7
1	E	397	THR	3.7
1	D	192	PRO	3.7
1	B	423	LEU	3.7
1	F	150	TRP	3.7
1	F	416	TYR	3.7
1	E	398	PRO	3.7
1	B	199	LYS	3.6
1	B	200	ALA	3.6
1	F	213	ALA	3.6
1	B	109	PRO	3.6
1	F	218	VAL	3.6
1	B	329	LYS	3.6
1	D	106	ALA	3.6
1	E	212	LYS	3.6
1	F	109	PRO	3.6
1	F	238	ALA	3.6
1	E	410	THR	3.5
1	F	190	MET	3.5
1	F	384	GLN	3.5
1	A	191	VAL	3.5
1	E	213	ALA	3.5
1	D	233	PRO	3.5
1	F	234	LEU	3.5
1	B	241	ASP	3.5
1	C	110	ALA	3.5
1	D	419	HIS	3.5
1	F	399	THR	3.4
1	B	213	ALA	3.4
1	D	214	PRO	3.4
1	E	152	PRO	3.4
1	E	4	HIS	3.4
1	F	4	HIS	3.4
1	C	117	LYS	3.4
1	F	411	THR	3.4
1	F	241	ASP	3.4
1	F	403	PHE	3.4
1	C	410	THR	3.4
1	B	238	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	240	ASN	3.4
1	A	420	TYR	3.4
1	E	260	ASN	3.4
1	E	406	ILE	3.3
1	D	416	TYR	3.3
1	A	108	GLU	3.3
1	E	151	ALA	3.3
1	C	407	VAL	3.3
1	C	207	ARG	3.3
1	C	239	GLU	3.3
1	E	421	VAL	3.3
1	B	422	TRP	3.3
1	D	236	ASN	3.3
1	C	241	ASP	3.3
1	E	73	ARG	3.3
1	A	419	HIS	3.3
1	F	223	TYR	3.3
1	B	418	ALA	3.3
1	F	118	VAL	3.3
1	B	114	MET	3.2
1	B	398	PRO	3.2
1	B	411	THR	3.2
1	E	404	GLN	3.2
1	B	227	TYR	3.2
1	D	385	GLY	3.2
1	D	396	ALA	3.2
1	F	154	ALA	3.2
1	C	118	VAL	3.2
1	F	212	LYS	3.2
1	E	113	GLY	3.2
1	B	237	ALA	3.2
1	C	409	LYS	3.2
1	B	408	PRO	3.2
1	D	152	PRO	3.2
1	F	400	VAL	3.2
1	F	1	MET	3.1
1	B	113	GLY	3.1
1	B	229	ALA	3.1
1	E	228	ALA	3.1
1	A	21	ARG	3.1
1	D	207	ARG	3.1
1	F	147	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	406	ILE	3.1
1	E	117	LYS	3.1
1	E	154	ALA	3.1
1	F	229	ALA	3.1
1	B	243	VAL	3.1
1	A	107	SER	3.1
1	F	207	ARG	3.1
1	B	153	THR	3.1
1	D	1	MET	3.1
1	D	205	TRP	3.1
1	C	408	PRO	3.0
1	B	234	LEU	3.0
1	B	410	THR	3.0
1	D	149	ALA	3.0
1	E	149	ALA	3.0
1	C	153	THR	3.0
1	C	406	ILE	3.0
1	A	6	GLU	3.0
1	F	116	ASP	3.0
1	F	385	GLY	3.0
1	F	110	ALA	3.0
1	E	233	PRO	2.9
1	F	119	LYS	2.9
1	B	236	ASN	2.9
1	A	190	MET	2.9
1	F	227	TYR	2.9
1	A	238	ALA	2.9
1	B	206	LEU	2.9
1	F	117	LYS	2.9
1	C	422	TRP	2.9
1	D	116	ASP	2.9
1	D	227	TYR	2.9
1	D	153	THR	2.9
1	F	397	THR	2.9
1	F	383	GLU	2.9
1	E	114	MET	2.9
1	F	235	SER	2.9
1	E	211	ASP	2.9
1	E	37	GLY	2.9
1	D	151	ALA	2.9
1	E	396	ALA	2.9
1	F	149	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	117	LYS	2.9
1	F	114	MET	2.9
1	E	112	SER	2.9
1	D	400	VAL	2.9
1	C	398	PRO	2.8
1	F	413	TRP	2.8
1	B	416	TYR	2.8
1	B	396	ALA	2.8
1	E	153	THR	2.8
1	F	388	ALA	2.8
1	B	194	ARG	2.8
1	C	16	ASP	2.8
1	C	206	LEU	2.8
1	F	214	PRO	2.8
1	C	420	TYR	2.8
1	E	223	TYR	2.8
1	F	418	ALA	2.8
1	B	413	TRP	2.8
1	B	405	ALA	2.8
1	D	237	ALA	2.8
1	F	210	THR	2.8
1	C	393	VAL	2.7
1	E	232	ARG	2.7
1	D	242	TYR	2.7
1	D	108	GLU	2.7
1	A	363	ALA	2.7
1	F	176	ALA	2.7
1	C	154	ALA	2.7
1	E	139	LYS	2.7
1	E	150	TRP	2.7
1	E	188	SER	2.7
1	B	112	SER	2.6
1	C	235	SER	2.6
1	D	150	TRP	2.6
1	D	238	ALA	2.6
1	D	422	TRP	2.6
1	B	211	ASP	2.6
1	E	241	ASP	2.6
1	F	9	LEU	2.6
1	A	397	THR	2.6
1	F	217	GLN	2.6
1	E	1	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	232	ARG	2.6
1	B	419	HIS	2.6
1	A	360	ARG	2.6
1	E	244	ARG	2.6
1	E	392	GLY	2.6
1	D	393	VAL	2.6
1	C	60	GLU	2.6
1	E	118	VAL	2.6
1	B	215	ARG	2.5
1	C	108	GLU	2.5
1	B	154	ALA	2.5
1	F	404	GLN	2.5
1	D	189	ASP	2.5
1	F	242	TYR	2.5
1	B	407	VAL	2.5
1	B	363	ALA	2.5
1	B	235	SER	2.5
1	B	212	LYS	2.5
1	C	150	TRP	2.5
1	E	189	ASP	2.5
1	B	193	ALA	2.5
1	C	209	SER	2.5
1	D	146	LEU	2.5
1	F	62	ARG	2.5
1	F	231	ARG	2.5
1	B	214	PRO	2.5
1	B	191	VAL	2.5
1	B	403	PHE	2.5
1	F	21	ARG	2.4
1	D	234	LEU	2.4
1	E	402	SER	2.4
1	E	116	ASP	2.4
1	B	147	PRO	2.4
1	C	1	MET	2.4
1	D	208	PRO	2.4
1	F	423	LEU	2.4
1	F	402	SER	2.4
1	F	417	ASP	2.4
1	C	214	PRO	2.4
1	D	118	VAL	2.4
1	F	407	VAL	2.4
1	D	418	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	146	LEU	2.4
1	F	236	ASN	2.4
1	E	358	HIS	2.4
1	A	394	GLU	2.4
1	F	409	LYS	2.4
1	C	243	VAL	2.4
1	D	407	VAL	2.4
1	A	395	ALA	2.4
1	C	418	ALA	2.4
1	F	225	PHE	2.4
1	B	230	LEU	2.4
1	F	255	LEU	2.4
1	F	256	ILE	2.4
1	E	365	ASP	2.4
1	B	216	MET	2.4
1	E	86	GLY	2.4
1	B	119	LYS	2.3
1	B	409	LYS	2.3
1	F	220	ARG	2.3
1	F	75	ALA	2.3
1	D	4	HIS	2.3
1	C	240	ASN	2.3
1	F	232	ARG	2.3
1	B	85	GLY	2.3
1	C	93	GLY	2.3
1	A	118	VAL	2.3
1	A	106	ALA	2.3
1	B	239	GLU	2.3
1	B	188	SER	2.3
1	A	188	SER	2.3
1	E	231	ARG	2.3
1	E	286	PRO	2.3
1	A	379	VAL	2.3
1	D	401	CYS	2.2
1	B	4	HIS	2.2
1	F	358	HIS	2.2
1	F	420	TYR	2.2
1	B	240	ASN	2.2
1	F	215	ARG	2.2
1	F	233	PRO	2.2
1	B	219	GLN	2.2
1	D	224	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	413	TRP	2.2
1	D	395	ALA	2.2
1	D	239	GLU	2.2
1	A	215	ARG	2.2
1	D	231	ARG	2.2
1	B	148	PRO	2.2
1	E	217	GLN	2.2
1	A	377	ASP	2.2
1	A	422	TRP	2.2
1	B	5	GLU	2.2
1	C	104	GLU	2.2
1	F	156	THR	2.2
1	D	215	ARG	2.2
1	F	360	ARG	2.2
1	A	329	LYS	2.2
1	F	113	GLY	2.2
1	A	4	HIS	2.2
1	E	225	PHE	2.2
1	F	419	HIS	2.2
1	B	415	THR	2.2
1	B	260	ASN	2.2
1	E	147	PRO	2.2
1	D	219	GLN	2.2
1	B	190	MET	2.2
1	A	1	MET	2.2
1	F	112	SER	2.2
1	F	183	SER	2.2
1	F	389	ILE	2.2
1	A	418	ALA	2.1
1	D	229	ALA	2.1
1	C	232	ARG	2.1
1	C	91	TYR	2.1
1	C	227	TYR	2.1
1	E	409	LYS	2.1
1	A	234	LEU	2.1
1	F	283	TRP	2.1
1	D	414	ARG	2.1
1	D	119	LYS	2.1
1	C	260	ASN	2.1
1	F	216	MET	2.1
1	F	16	ASP	2.1
1	B	402	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	179	SER	2.1
1	E	248	PHE	2.1
1	C	213	ALA	2.1
1	F	414	ARG	2.1
1	F	390	GLY	2.1
1	D	386	ALA	2.1
1	B	208	PRO	2.1
1	C	230	LEU	2.1
1	D	103	LEU	2.1
1	B	285	HIS	2.1
1	E	218	VAL	2.1
1	E	219	GLN	2.0
1	A	392	GLY	2.0
1	E	360	ARG	2.0
1	F	339	PHE	2.0
1	C	212	LYS	2.0
1	D	139	LYS	2.0
1	F	107	SER	2.0
1	D	216	MET	2.0
1	A	208	PRO	2.0
1	F	286	PRO	2.0
1	C	267	ILE	2.0
1	F	392	GLY	2.0
1	D	79	TYR	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](#)

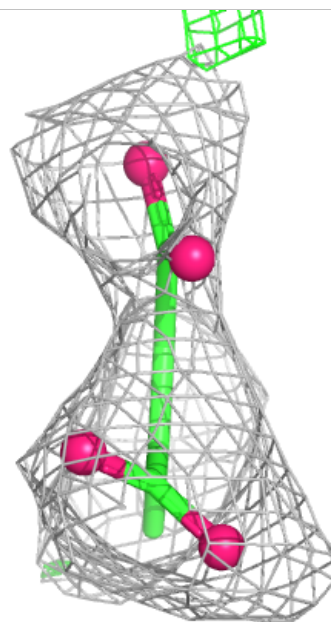
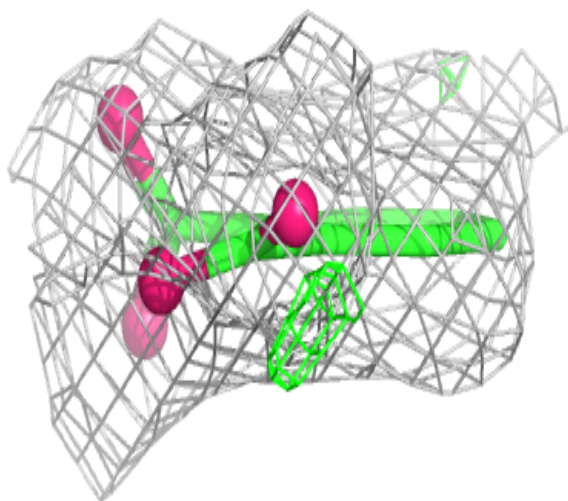
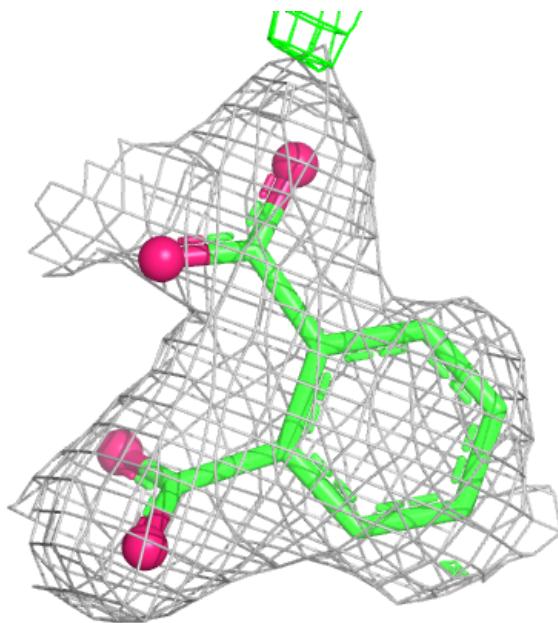
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PHT	B	503	12/12	0.83	0.20	62,75,84,88	0
2	FE2	E	501	1/1	0.97	0.07	40,40,40,40	0
3	FES	C	502	4/4	0.98	0.05	39,41,41,50	0
3	FES	F	502	4/4	0.98	0.04	33,35,36,45	0
2	FE2	F	501	1/1	0.98	0.04	45,45,45,45	0
3	FES	A	502	4/4	0.99	0.03	30,33,36,40	0
2	FE2	C	501	1/1	0.99	0.02	30,30,30,30	0
3	FES	D	502	4/4	0.99	0.03	35,38,40,44	0
3	FES	E	502	4/4	0.99	0.02	25,27,30,32	0
2	FE2	D	501	1/1	0.99	0.03	34,34,34,34	0
3	FES	B	502	4/4	0.99	0.04	29,29,33,35	0
2	FE2	A	501	1/1	1.00	0.02	27,27,27,27	0
2	FE2	B	501	1/1	1.00	0.02	36,36,36,36	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.

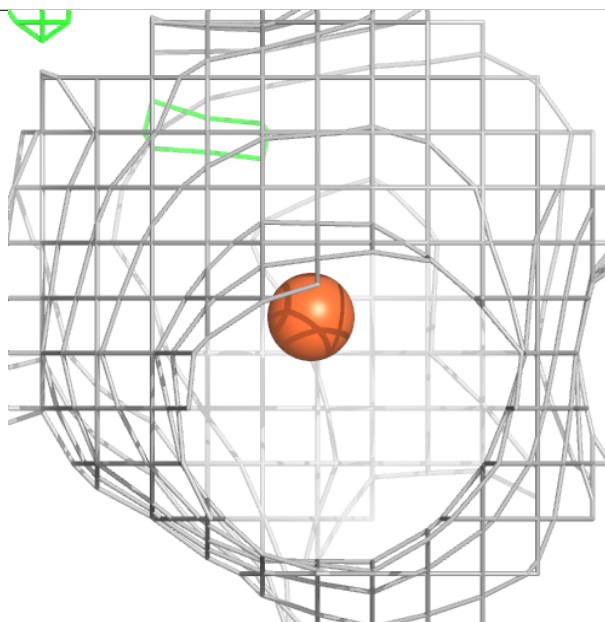
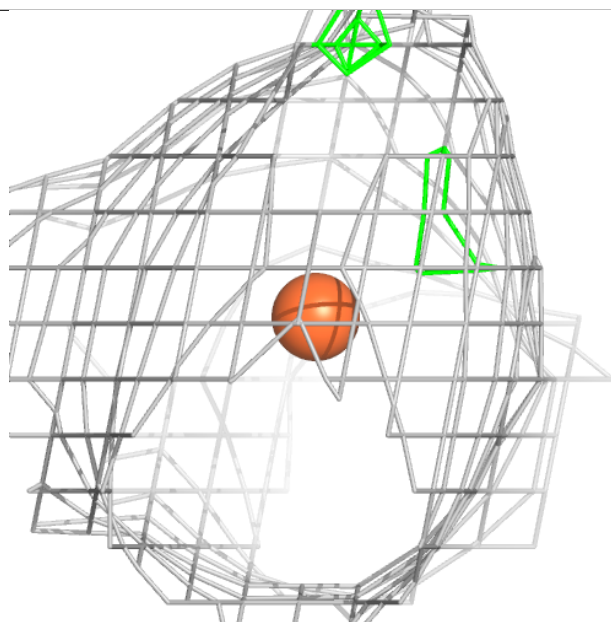
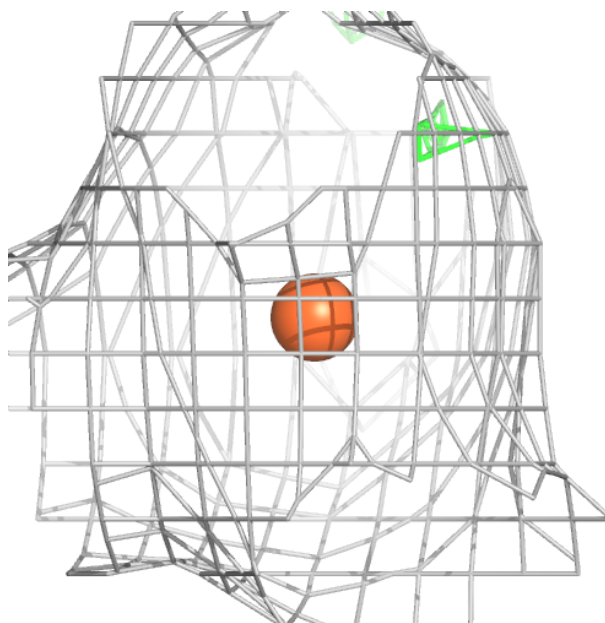
Electron density around PHT B 503:

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



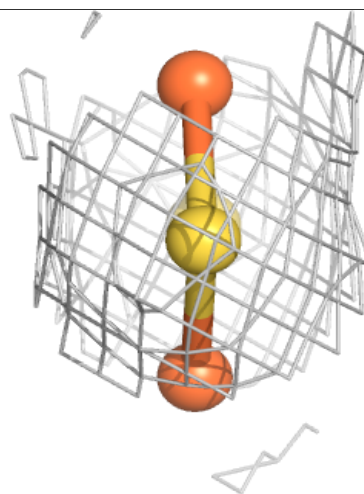
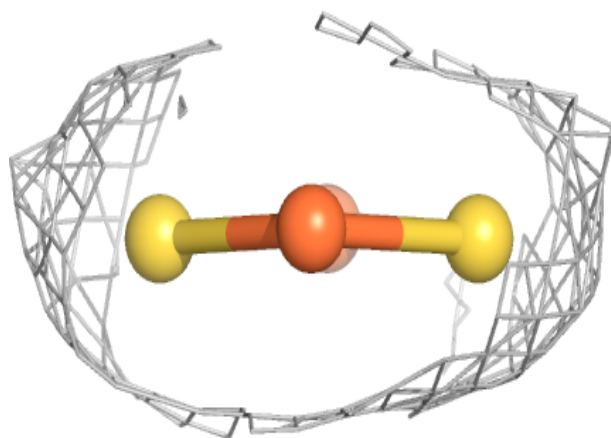
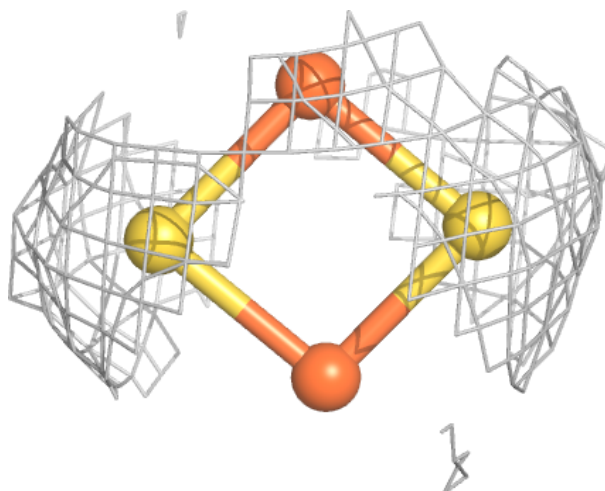
Electron density around FE2 E 501:

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



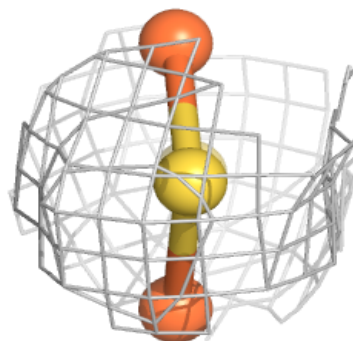
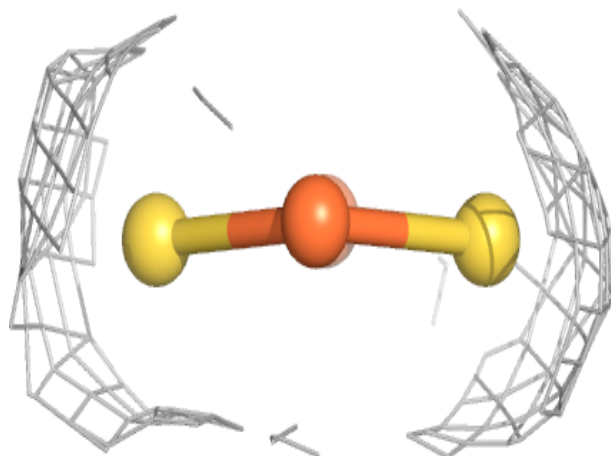
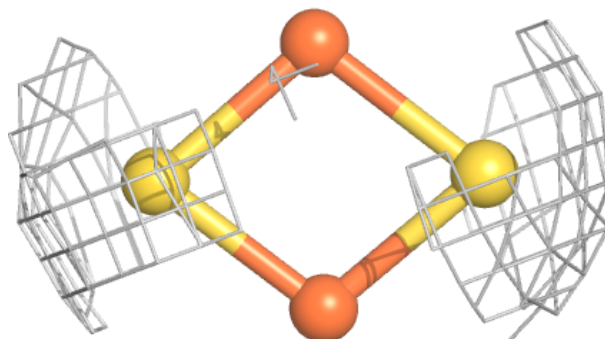
Electron density around FES C 502:

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



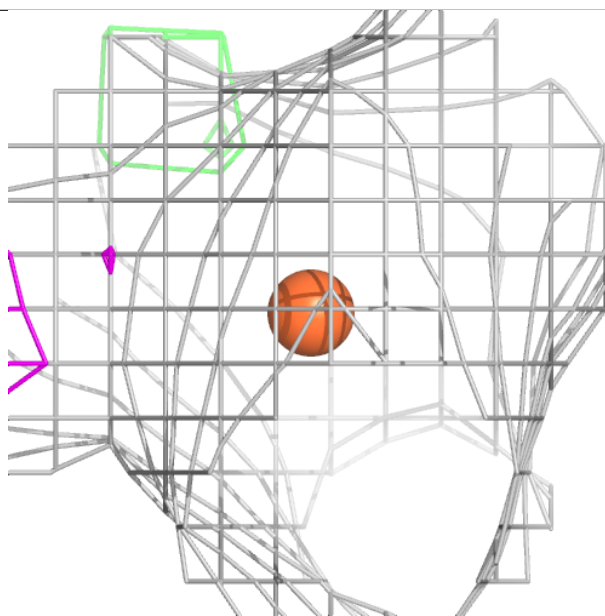
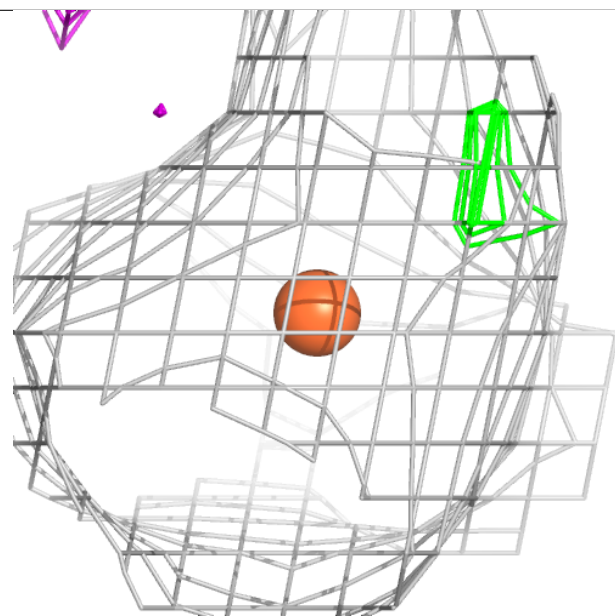
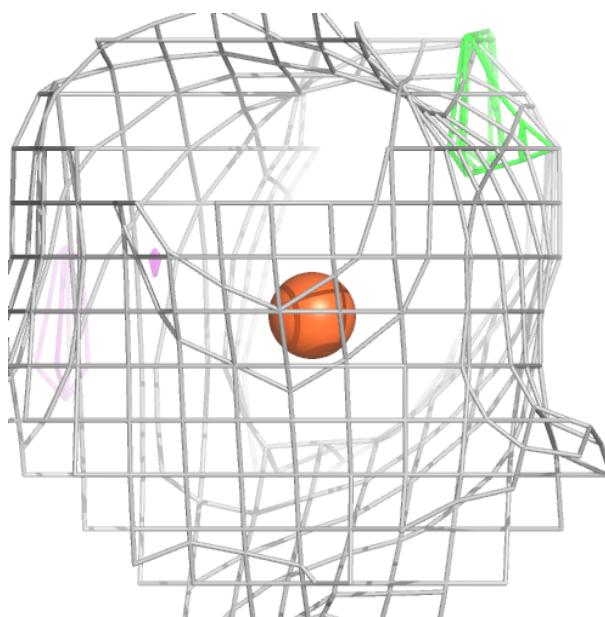
Electron density around FES F 502:

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



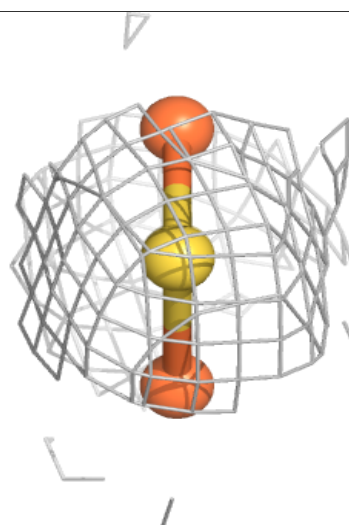
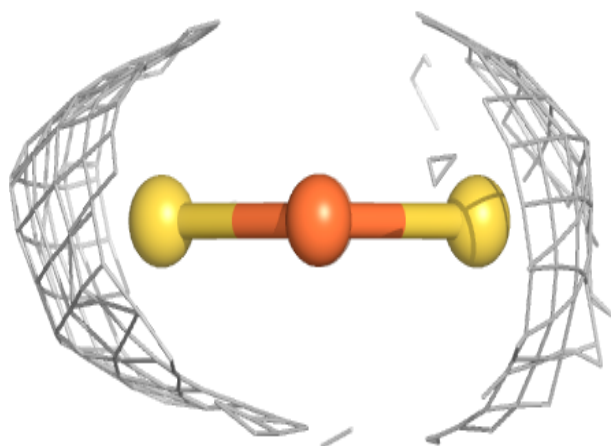
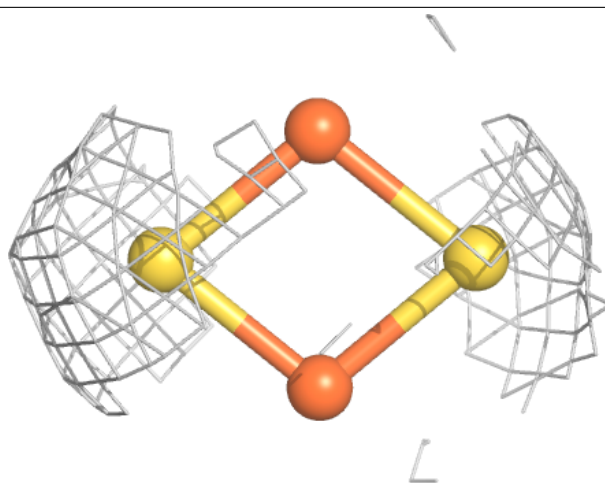
Electron density around FE2 F 501:

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



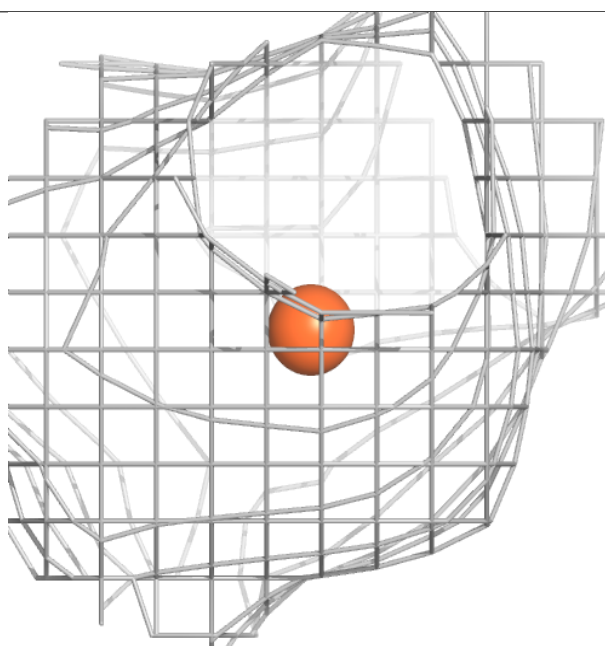
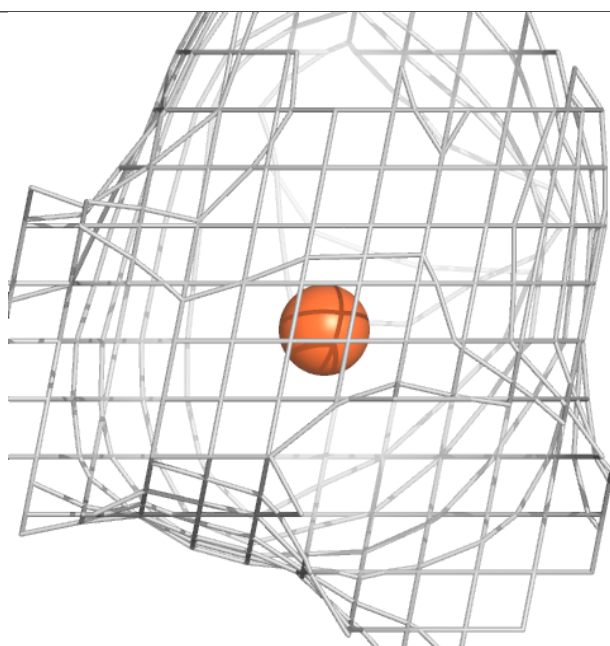
Electron density around FES A 502:

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



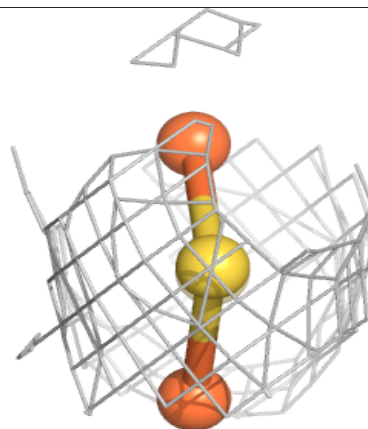
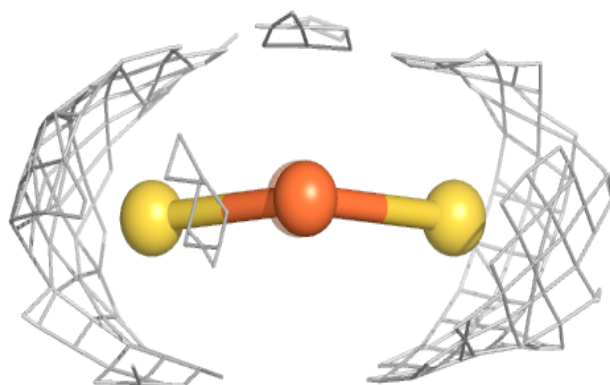
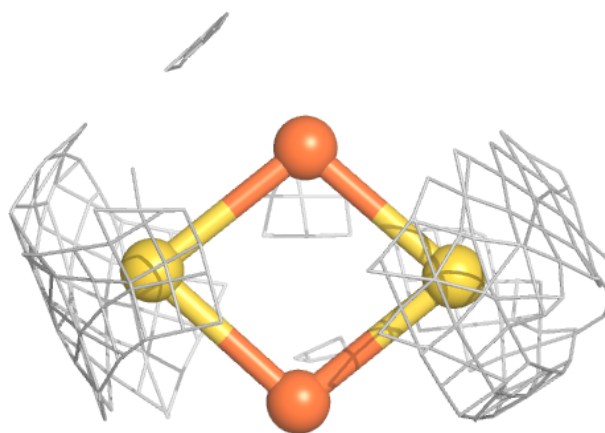
Electron density around FE2 C 501:

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



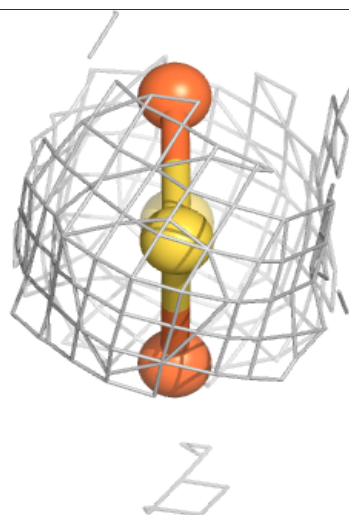
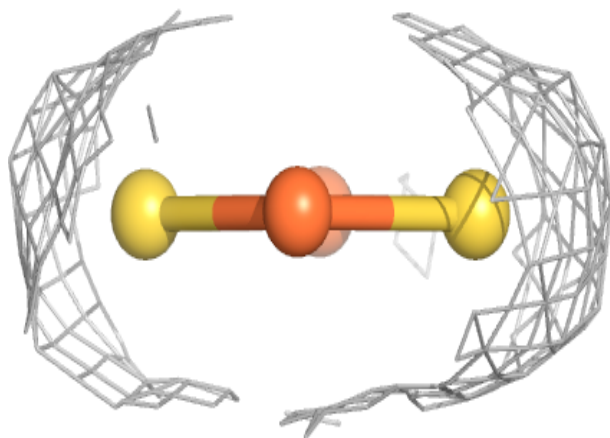
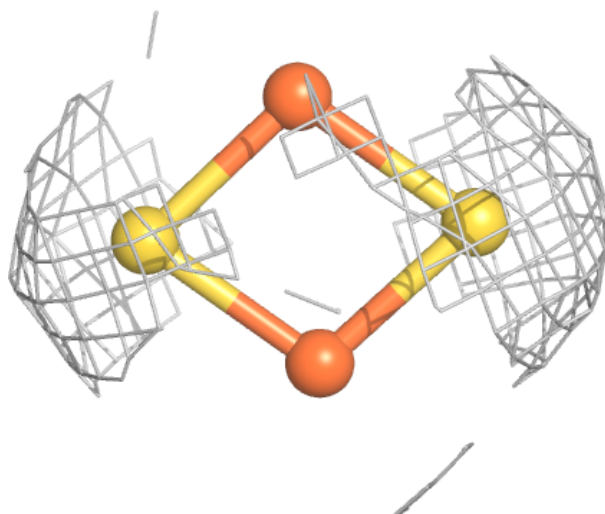
Electron density around FES D 502:

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



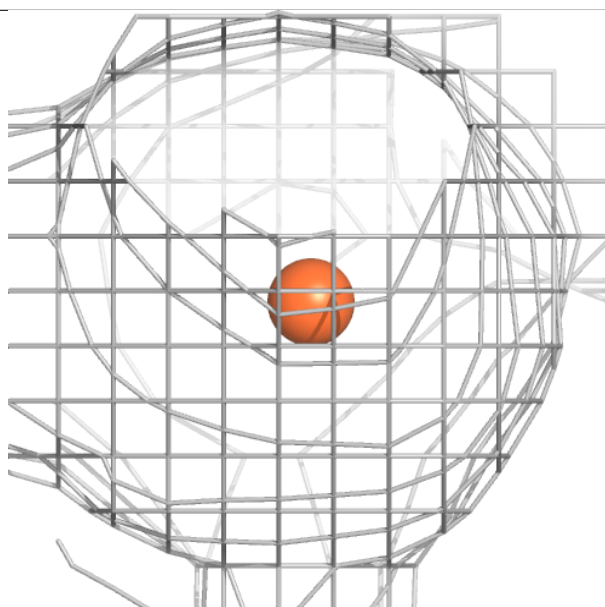
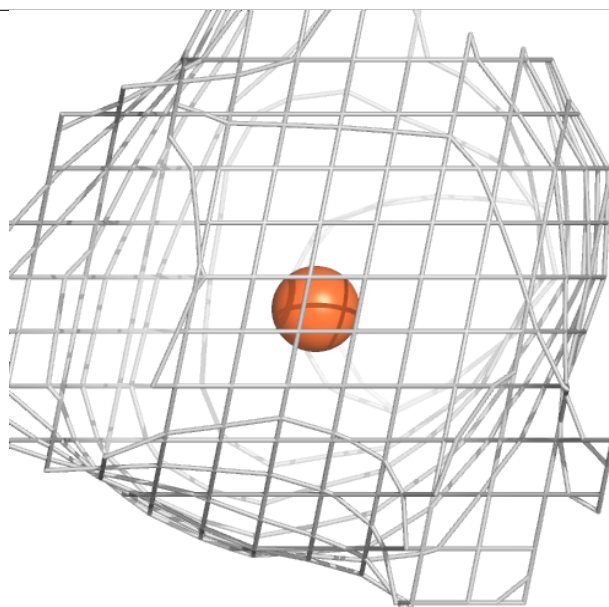
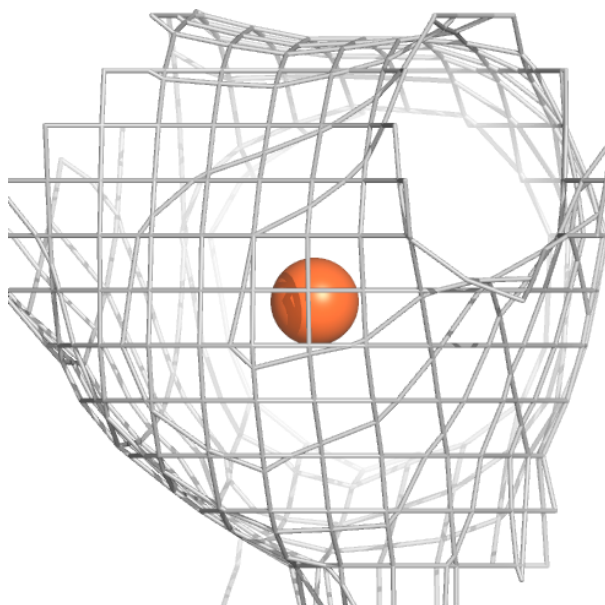
Electron density around FES E 502:

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



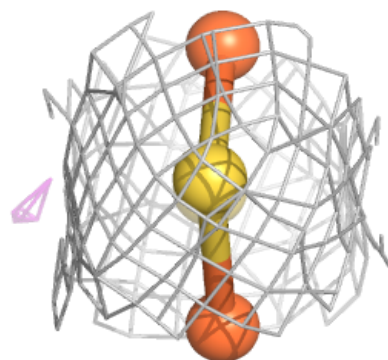
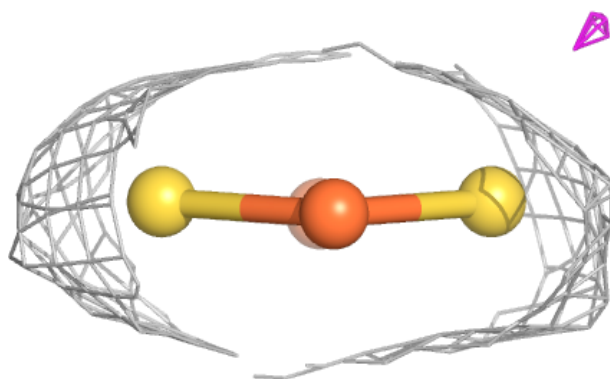
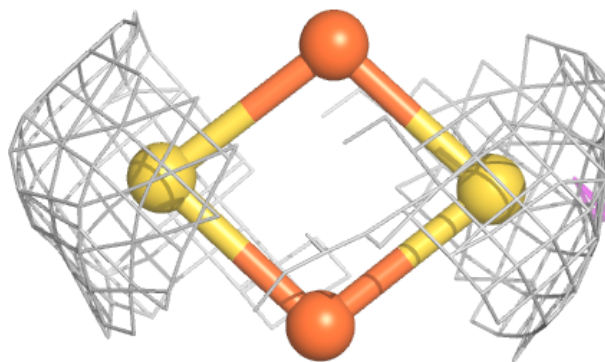
Electron density around FE2 D 501:

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



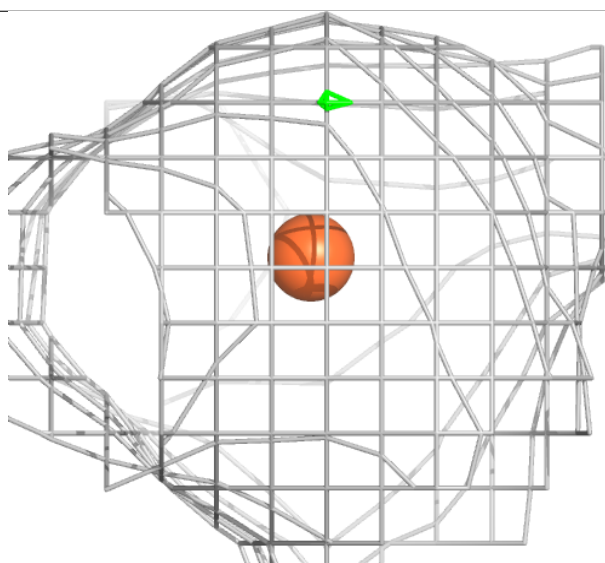
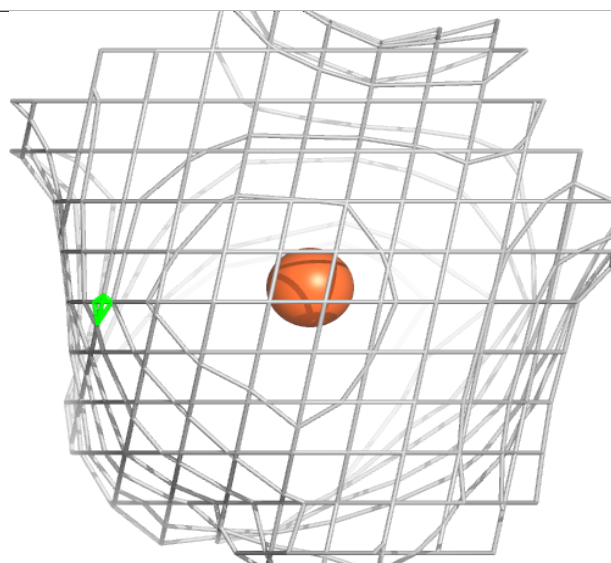
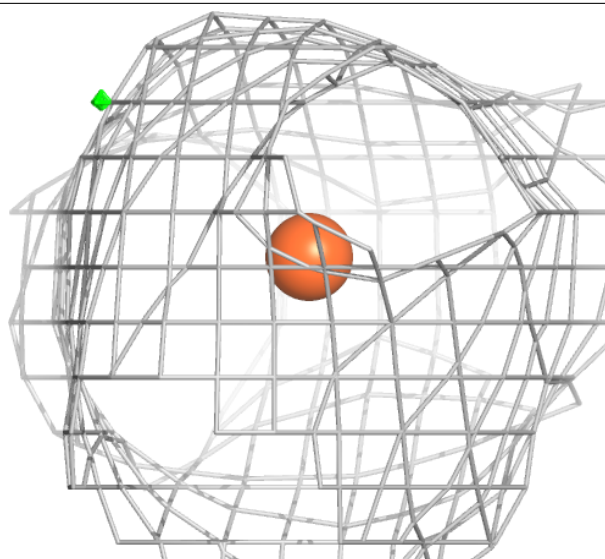
Electron density around FES B 502:

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



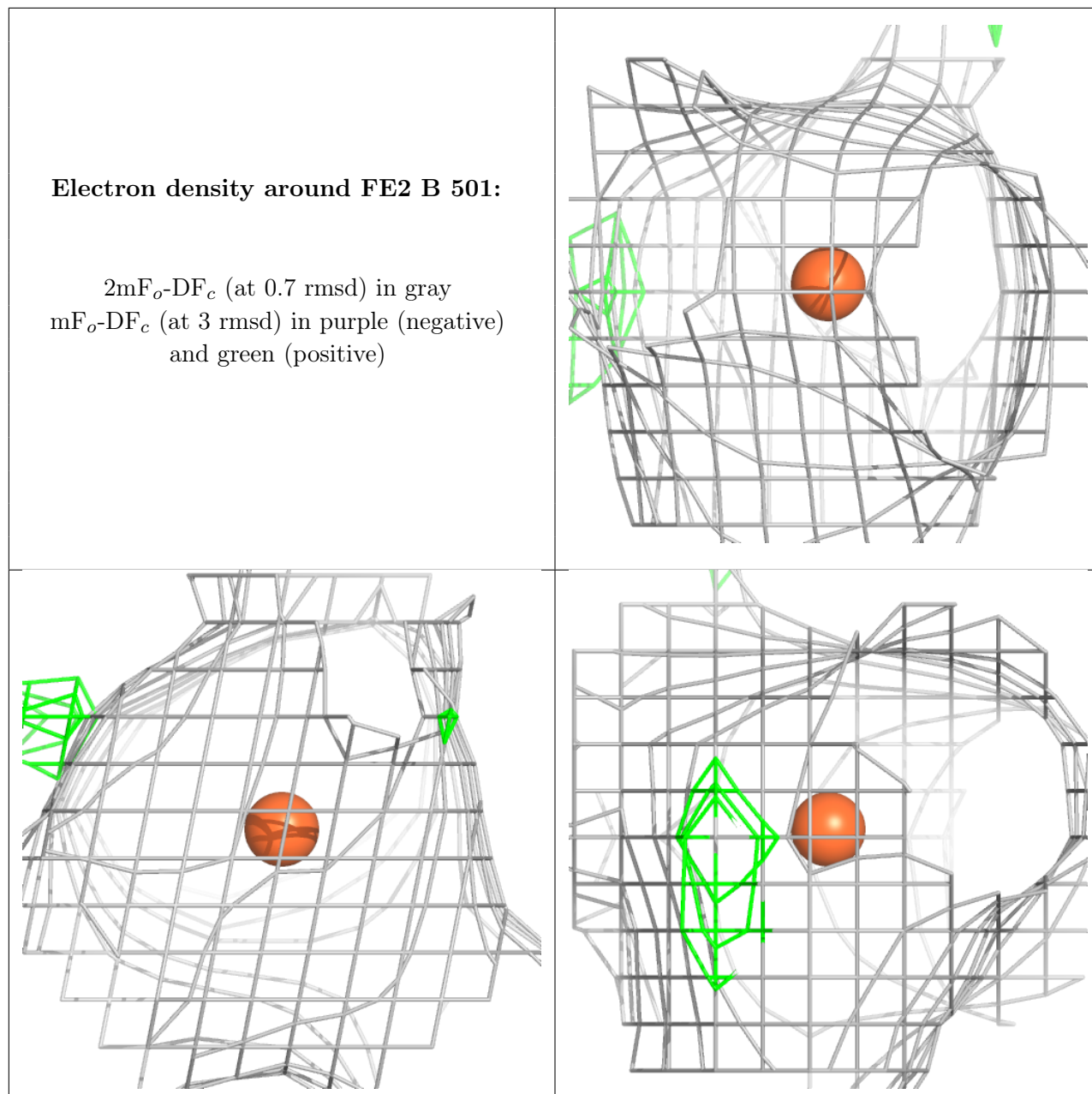
Electron density around FE2 A 501:

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



Electron density around FE2 B 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.