



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2021 – 12:17 PM JST

PDB ID : 7V28  
Title : Crystal Structure of phthalate dioxygenase in complex with terephthalate  
Authors : Mahto, J.K.; Kumar, P.  
Deposited on : 2021-08-07  
Resolution : 3.07 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

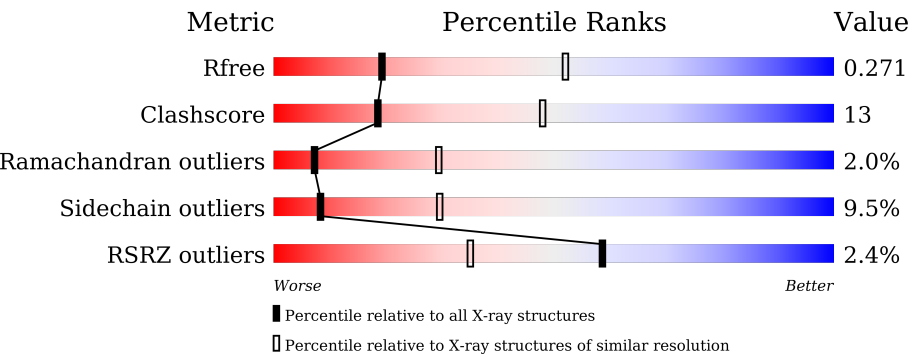
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.24  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.24

# 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 3.07 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))
$R_{free}$	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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  $\geq 3$ , 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	<div><div></div><div>63%24%6%8%</div></div>
1	B	439	<div><div>%</div><div>67%26%. .</div></div>
1	C	439	<div><div>2%</div><div>63%26%.7%</div></div>
1	D	439	<div><div></div><div>59%29%.8%</div></div>
1	E	439	<div><div>7%</div><div>61%28%.7%</div></div>
1	F	439	<div><div>3%</div><div>61%29%.8%</div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	D	502	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19601 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.

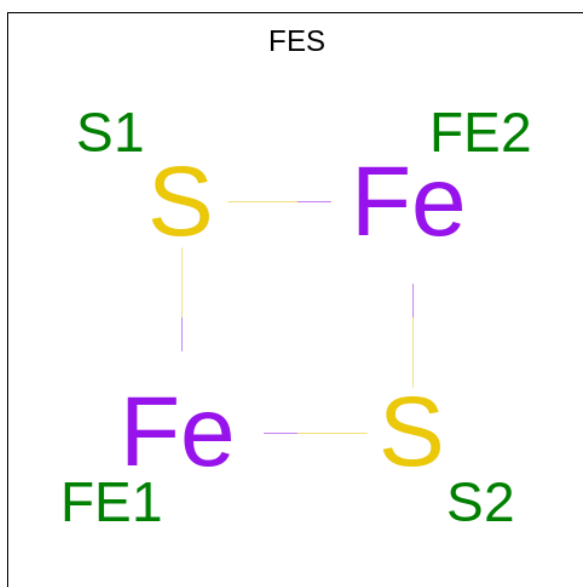
- Molecule 1 is a protein called Rieske (2Fe-2S) domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3192	2011	564	593	24			
1	B	425	Total	C	N	O	S	0	0	0
			3335	2100	590	621	24			
1	C	407	Total	C	N	O	S	0	0	0
			3202	2017	566	595	24			
1	D	404	Total	C	N	O	S	0	0	0
			3186	2008	563	591	24			
1	E	407	Total	C	N	O	S	0	0	0
			3202	2017	566	595	24			
1	F	406	Total	C	N	O	S	0	0	0
			3194	2012	565	594	23			

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

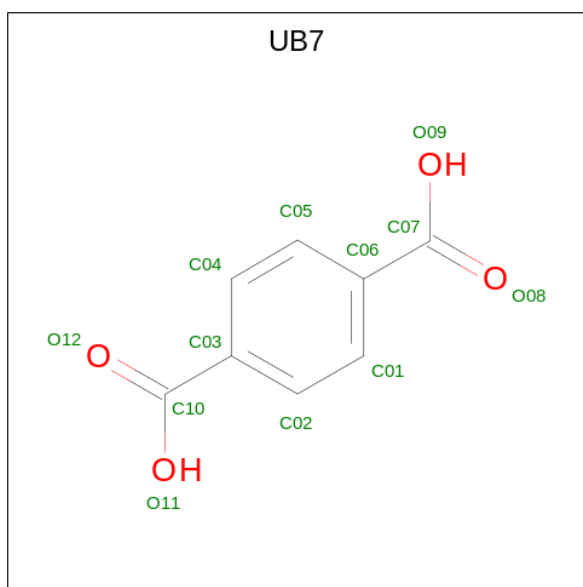
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	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 terephthalic acid (three-letter code: UB7) (formula: C<sub>8</sub>H<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

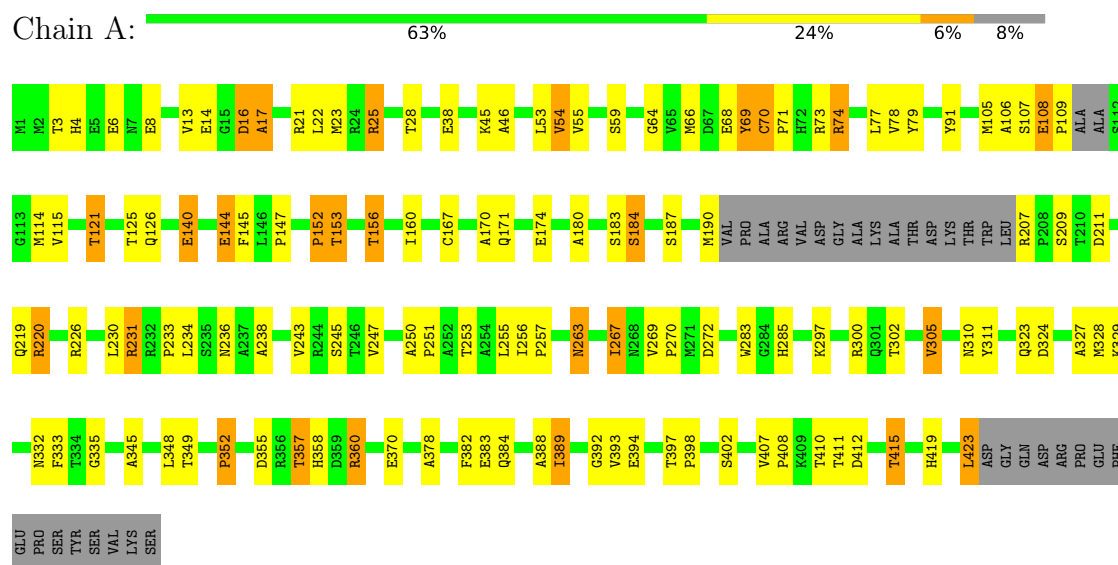
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	41	Total	O	0	0
			41	41		
5	C	41	Total	O	0	0
			41	41		
5	D	43	Total	O	0	0
			43	43		
5	E	40	Total	O	0	0
			40	40		
5	F	36	Total	O	0	0
			36	36		

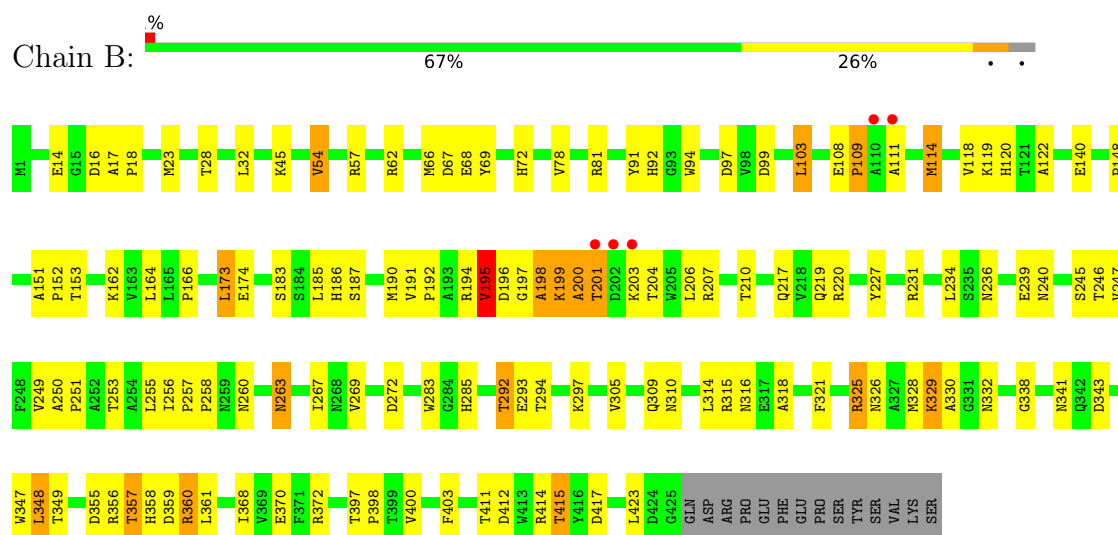
### 3 Residue-property plots

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.

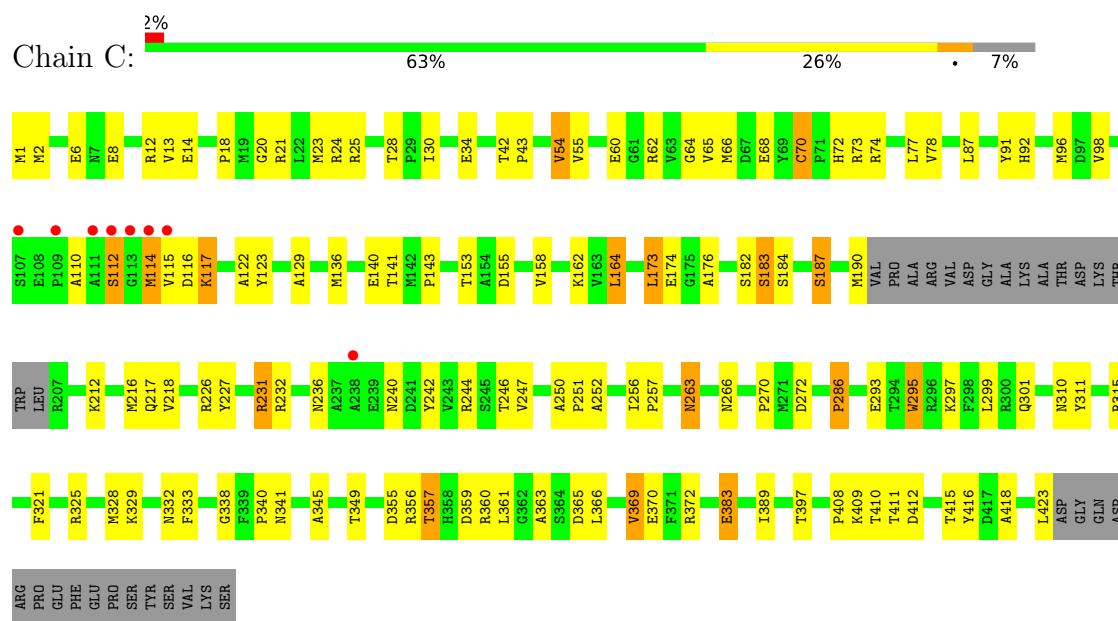
#### • Molecule 1: Rieske (2Fe-2S) domain protein



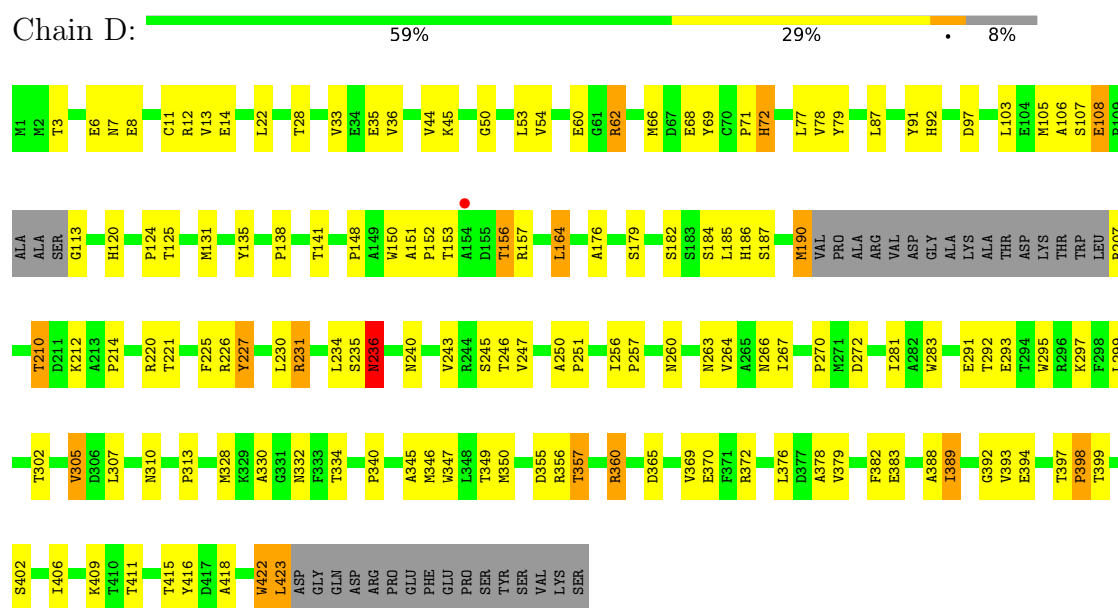
#### • Molecule 1: Rieske (2Fe-2S) domain protein



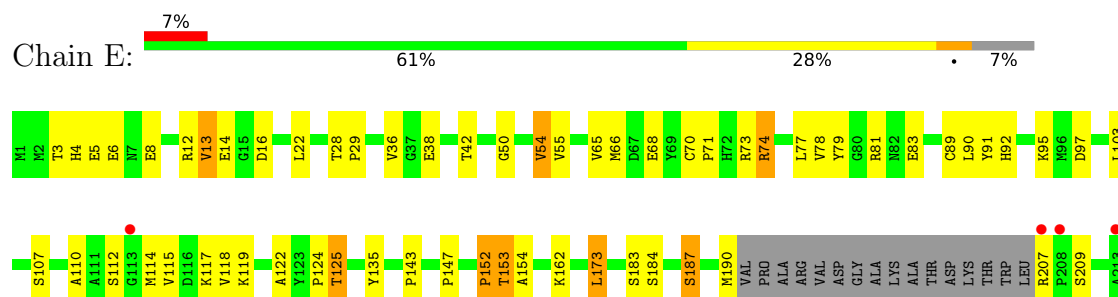
#### • Molecule 1: Rieske (2Fe-2S) domain protein



- 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, $\alpha$ , $\beta$ , $\gamma$	179.25Å 122.67Å 163.50Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	160.43 – 3.07 160.43 – 3.07	Depositor EDS
% Data completeness (in resolution range)	97.6 (160.43-3.07) 97.6 (160.43-3.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.212 , 0.266 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	3161 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	19601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FES, FE2, UB7

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	0.34	0/3278	0.76	1/4462 (0.0%)
1	B	0.34	0/3426	0.78	0/4668
1	C	0.35	0/3289	0.76	1/4479 (0.0%)
1	D	0.34	0/3272	0.76	0/4454
1	E	0.34	0/3289	0.74	0/4479
1	F	0.32	0/3281	0.75	0/4469
All	All	0.34	0/19835	0.76	2/27011 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	ARG	CG-CD-NE	-5.33	100.61	111.80
1	A	69	TYR	CB-CA-C	5.14	120.68	110.40

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	3192	0	3073	75	0
1	B	3335	0	3217	83	0
1	C	3202	0	3084	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3186	0	3068	99	0
1	E	3202	0	3084	87	0
1	F	3194	0	3075	90	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	0	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	2	0
3	E	4	0	0	1	0
3	F	4	0	0	1	0
4	B	12	0	0	0	0
5	A	47	0	0	2	0
5	B	41	0	0	0	0
5	C	41	0	0	3	0
5	D	43	0	0	5	0
5	E	40	0	0	6	0
5	F	36	0	0	0	0
All	All	19601	0	18601	502	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 13.

All (502) 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:E:360:ARG:HG3	1:E:360:ARG:HH11	1.00	1.17
1:D:60:GLU:HG3	1:D:62:ARG:NH1	1.66	1.11
1:D:360:ARG:HG3	1:D:360:ARG:HH11	1.17	1.07
1:C:218:VAL:HG11	1:C:370:GLU:HG2	1.39	1.00
1:D:230:LEU:HD23	1:D:243:VAL:HG22	1.42	0.98
1:C:231:ARG:HH11	1:C:231:ARG:CG	1.78	0.95
1:C:231:ARG:HH11	1:C:231:ARG:HG2	1.29	0.94
1:E:218:VAL:HG11	1:E:370:GLU:HG2	1.47	0.94
1:F:183:SER:HB3	1:F:212:LYS:HG2	1.50	0.94
1:B:360:ARG:HG3	1:B:360:ARG:HH11	1.35	0.92
1:F:173:LEU:HD13	1:F:252:ALA:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ALA:HB1	1:D:389:ILE:HG21	1.53	0.91
1:C:217:GLN:O	1:C:227:TYR:HB2	1.72	0.89
1:E:360:ARG:HG3	1:E:360:ARG:NH1	1.75	0.88
1:B:397:THR:HB	1:B:398:PRO:CD	2.04	0.86
1:C:54:VAL:HG22	1:C:68:GLU:HA	1.58	0.86
1:D:383:GLU:HG2	5:D:609:HOH:O	1.75	0.85
1:D:392:GLY:HA3	5:D:622:HOH:O	1.75	0.84
1:D:378:ALA:HB1	1:D:389:ILE:CG2	2.06	0.84
1:C:14:GLU:OE2	1:C:272:ASP:HB2	1.76	0.83
1:D:60:GLU:CG	1:D:62:ARG:NH1	2.41	0.83
1:F:355:ASP:OD1	1:F:357:THR:HB	1.77	0.83
1:B:66:MET:HE3	1:B:120:HIS:HD2	1.44	0.82
1:D:256:ILE:HB	1:D:264:VAL:HG12	1.61	0.82
1:F:227:TYR:CE1	1:F:246:THR:HB	2.15	0.82
1:D:220:ARG:HD3	1:D:370:GLU:OE2	1.79	0.81
1:E:397:THR:HB	1:E:398:PRO:CD	2.12	0.79
1:E:360:ARG:HH11	1:E:360:ARG:CG	1.88	0.78
1:E:407:VAL:HG21	1:E:416:TYR:HE1	1.48	0.78
1:F:261:LEU:HD23	1:F:288:GLN:HG2	1.66	0.78
1:D:378:ALA:CB	1:D:389:ILE:HG21	2.14	0.78
1:C:110:ALA:HB1	1:C:115:VAL:HG11	1.64	0.77
1:E:397:THR:HB	1:E:398:PRO:HD3	1.67	0.77
1:D:360:ARG:HH11	1:D:360:ARG:CG	1.98	0.77
1:D:356:ARG:HG2	1:D:372:ARG:NH2	2.00	0.76
1:B:315:ARG:HB3	1:B:321:PHE:HA	1.68	0.76
1:F:126:GLN:HG2	1:F:145:PHE:CD2	2.21	0.75
1:B:185:LEU:HD23	1:B:186:HIS:CE1	2.22	0.75
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.51	0.75
1:F:173:LEU:CD1	1:F:252:ALA:HA	2.16	0.75
1:C:112:SER:HB3	5:C:623:HOH:O	1.87	0.74
1:C:412:ASP:O	1:C:415:THR:HG22	1.88	0.74
1:D:295:TRP:CE2	1:D:299:LEU:HD11	2.22	0.74
1:A:397:THR:HB	1:A:398:PRO:CD	2.17	0.74
1:B:217:GLN:O	1:B:227:TYR:HB2	1.87	0.74
1:B:397:THR:HB	1:B:398:PRO:HD3	1.69	0.74
1:F:258:PRO:HB3	1:F:263:ASN:HA	1.69	0.73
1:C:20:GLY:O	1:C:24:ARG:HG3	1.89	0.72
1:B:54:VAL:HG22	1:B:68:GLU:HA	1.71	0.72
1:F:184:SER:O	1:F:333:PHE:CE2	2.43	0.71
1:F:226:ARG:HG2	1:F:247:VAL:HG22	1.71	0.71
1:D:302:THR:HB	1:D:305:VAL:HG13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:HG3	1:A:109:PRO:HD2	1.74	0.70
1:D:60:GLU:CG	1:D:62:ARG:HH11	2.04	0.70
1:E:184:SER:O	1:E:187:SER:HB2	1.91	0.70
1:F:124:PRO:HG2	1:F:135:TYR:HB3	1.74	0.70
1:E:407:VAL:HG21	1:E:416:TYR:CE1	2.27	0.69
1:A:231:ARG:HH11	1:A:231:ARG:HG2	1.58	0.69
1:D:60:GLU:HG3	1:D:62:ARG:HH11	1.55	0.69
1:D:156:THR:HG23	1:D:422:TRP:HZ3	1.57	0.69
1:C:256:ILE:HG23	1:C:257:PRO:HD2	1.74	0.69
1:F:153:THR:HG22	1:F:154:ALA:H	1.58	0.68
1:B:219:GLN:HE21	1:B:414:ARG:HD2	1.58	0.68
1:B:66:MET:CE	1:B:120:HIS:HD2	2.06	0.68
1:D:60:GLU:HG3	1:D:62:ARG:HH12	1.52	0.68
1:A:14:GLU:OE2	1:A:272:ASP:HB2	1.92	0.68
1:A:147:PRO:HB3	1:A:152:PRO:O	1.93	0.68
1:E:54:VAL:HG22	1:E:68:GLU:HA	1.74	0.68
1:A:4:HIS:O	1:A:8:GLU:HG2	1.93	0.67
1:C:416:TYR:CE2	1:C:418:ALA:HB2	2.29	0.67
1:C:60:GLU:HG2	1:C:62:ARG:HH11	1.59	0.67
1:C:226:ARG:HG2	1:C:247:VAL:HG22	1.76	0.67
1:D:92:HIS:HB2	3:D:502:FES:S1	2.35	0.67
1:E:220:ARG:HD3	1:E:370:GLU:OE2	1.94	0.67
1:F:285:HIS:CD2	1:F:423:LEU:HD12	2.30	0.67
1:D:355:ASP:OD1	1:D:357:THR:HB	1.94	0.66
1:B:219:GLN:NE2	1:B:414:ARG:HD2	2.11	0.66
1:D:299:LEU:HB3	1:D:340:PRO:HG2	1.78	0.66
1:C:263:ASN:HB3	5:C:601:HOH:O	1.96	0.66
1:C:173:LEU:HD13	1:C:252:ALA:HA	1.76	0.66
1:E:263:ASN:HB2	1:E:283:TRP:NE1	2.11	0.66
1:B:66:MET:HG2	1:B:122:ALA:HB2	1.77	0.65
1:E:73:ARG:O	1:E:74:ARG:HB2	1.96	0.65
1:E:359:ASP:HB3	1:E:361:LEU:HD21	1.78	0.65
1:C:231:ARG:CG	1:C:231:ARG:NH1	2.49	0.65
1:A:220:ARG:NH1	1:A:370:GLU:OE2	2.30	0.64
1:B:285:HIS:CD2	1:B:423:LEU:HD12	2.32	0.64
1:D:14:GLU:OE2	1:D:272:ASP:HB2	1.98	0.64
1:A:170:ALA:O	1:A:174:GLU:HG3	1.98	0.64
1:E:239:GLU:HG2	1:E:239:GLU:O	1.98	0.64
1:A:302:THR:HB	1:A:305:VAL:HG13	1.80	0.64
1:B:227:TYR:CE1	1:B:246:THR:HB	2.33	0.63
1:B:368:ILE:O	1:B:372:ARG:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PHE:C	1:A:384:GLN:H	2.02	0.63
1:D:7:ASN:O	1:D:11:CYS:HB2	1.98	0.63
1:F:343:ASP:HB3	1:F:347:TRP:CZ2	2.34	0.63
1:E:235:SER:O	1:E:236:ASN:HB2	1.98	0.63
1:B:236:ASN:O	1:B:240:ASN:HB2	1.99	0.62
1:E:242:TYR:OH	1:E:244:ARG:NH2	2.32	0.62
1:D:397:THR:HB	1:D:398:PRO:HD2	1.80	0.62
1:F:14:GLU:OE2	1:F:272:ASP:HB2	1.98	0.62
1:A:140:GLU:CD	1:A:140:GLU:H	2.03	0.62
1:D:179:SER:O	1:D:231:ARG:NH2	2.32	0.62
1:F:57:ARG:NH1	1:F:63:VAL:HG23	2.14	0.62
1:D:14:GLU:HG2	1:D:50:GLY:HA3	1.82	0.61
1:A:355:ASP:OD1	1:A:357:THR:HB	2.00	0.61
1:B:330:ALA:HB2	1:D:330:ALA:HB2	1.82	0.61
1:C:227:TYR:CE1	1:C:246:THR:HB	2.35	0.61
1:E:300:ARG:HD2	5:E:605:HOH:O	2.00	0.61
1:A:360:ARG:HB2	1:E:71:PRO:O	2.01	0.61
1:C:184:SER:O	1:C:187:SER:HB3	2.00	0.61
1:B:360:ARG:HG3	1:B:360:ARG:NH1	2.10	0.61
1:F:227:TYR:HE1	1:F:246:THR:HB	1.64	0.61
1:B:54:VAL:HG13	1:B:78:VAL:HG22	1.83	0.60
1:F:109:PRO:C	1:F:111:ALA:H	2.05	0.60
1:F:261:LEU:CD2	1:F:288:GLN:HG2	2.31	0.60
1:B:92:HIS:HB2	3:B:502:FES:S1	2.42	0.60
1:A:73:ARG:O	1:A:74:ARG:HB2	2.02	0.59
1:B:343:ASP:HB3	1:B:347:TRP:CZ2	2.37	0.59
1:C:114:MET:HA	1:C:117:LYS:HB2	1.83	0.59
1:F:57:ARG:HH11	1:F:57:ARG:HG3	1.67	0.59
1:F:285:HIS:HD2	1:F:423:LEU:HD12	1.67	0.59
1:D:156:THR:HG23	1:D:422:TRP:CZ3	2.37	0.59
1:A:70:CYS:HB2	1:A:77:LEU:HD21	1.83	0.59
1:C:2:MET:HE3	1:C:6:GLU:HB3	1.85	0.59
1:D:423:LEU:HA	5:D:636:HOH:O	2.03	0.58
1:C:55:VAL:HG13	1:C:65:VAL:HG22	1.85	0.58
1:C:54:VAL:HG13	1:C:78:VAL:HG22	1.86	0.58
1:D:105:MET:O	1:D:107:SER:N	2.35	0.58
1:C:176:ALA:HB2	1:C:266:ASN:HD22	1.68	0.58
1:E:124:PRO:HG2	1:E:135:TYR:HB3	1.86	0.58
1:E:14:GLU:HG2	1:E:50:GLY:HA3	1.86	0.58
1:C:231:ARG:HG2	1:C:231:ARG:NH1	2.08	0.58
1:F:359:ASP:HB3	1:F:361:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:CD2	1:D:243:VAL:HG22	2.24	0.57
1:C:60:GLU:CG	1:C:62:ARG:HH11	2.18	0.57
1:E:13:VAL:HG21	1:E:270:PRO:HB2	1.85	0.57
1:F:168:ASN:HB2	1:F:273:ASP:O	2.05	0.57
1:D:382:PHE:CD1	1:D:388:ALA:HB2	2.39	0.57
1:C:231:ARG:HE	1:C:244:ARG:HD3	1.68	0.57
1:D:345:ALA:O	1:D:349:THR:HG23	2.04	0.57
1:F:382:PHE:C	1:F:384:GLN:H	2.07	0.57
1:C:164:LEU:HD22	1:C:310:ASN:O	2.05	0.57
1:C:416:TYR:HE2	1:C:418:ALA:HB2	1.70	0.57
1:F:263:ASN:HB2	1:F:283:TRP:NE1	2.20	0.56
1:C:66:MET:HG2	1:C:122:ALA:HB2	1.85	0.56
1:B:66:MET:CE	1:B:120:HIS:CD2	2.87	0.56
1:B:166:PRO:HD2	1:B:348:LEU:HD21	1.86	0.56
1:A:126:GLN:HG2	1:A:145:PHE:CD1	2.41	0.56
1:F:123:TYR:CD1	1:F:136:MET:HA	2.40	0.56
1:C:244:ARG:NH1	1:C:257:PRO:HB2	2.19	0.56
1:B:397:THR:HB	1:B:398:PRO:HD2	1.86	0.56
1:D:226:ARG:HG2	1:D:247:VAL:HG22	1.87	0.56
1:F:328:MET:HG3	1:F:335:GLY:HA3	1.88	0.55
1:A:219:GLN:OE1	1:A:226:ARG:NH1	2.39	0.55
1:A:54:VAL:HG22	1:A:68:GLU:HA	1.89	0.55
1:D:97:ASP:HB3	1:D:103:LEU:HD11	1.87	0.55
1:B:355:ASP:OD1	1:B:357:THR:HB	2.06	0.55
1:F:239:GLU:O	1:F:239:GLU:HG2	2.06	0.55
1:B:174:GLU:HG2	1:B:368:ILE:HG23	1.88	0.55
1:E:407:VAL:HB	5:E:601:HOH:O	2.07	0.55
1:B:412:ASP:O	1:B:415:THR:HB	2.07	0.55
1:F:380:LYS:O	1:F:384:GLN:HG3	2.07	0.55
1:A:357:THR:HG22	1:A:358:HIS:ND1	2.22	0.55
1:D:360:ARG:HG3	1:D:360:ARG:NH1	1.98	0.55
1:F:396:ALA:O	1:F:397:THR:HG23	2.07	0.55
1:E:309:GLN:HG2	5:E:636:HOH:O	2.07	0.54
1:F:126:GLN:HG2	1:F:145:PHE:CE2	2.42	0.54
1:B:195:VAL:HG21	1:B:206:LEU:HB3	1.89	0.54
1:D:182:SER:HB3	1:D:190:MET:HG3	1.90	0.54
1:A:247:VAL:HB	1:A:255:LEU:HD12	1.89	0.54
1:E:8:GLU:OE2	1:E:12:ARG:NE	2.37	0.54
1:E:340:PRO:O	1:E:344:VAL:HG23	2.08	0.54
1:A:256:ILE:HG23	1:A:257:PRO:HD2	1.90	0.54
1:C:231:ARG:HH11	1:C:231:ARG:HG3	1.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:ARG:HG2	1:D:372:ARG:CZ	2.37	0.53
1:D:79:TYR:CE2	1:E:349:THR:HG21	2.44	0.53
1:B:99:ASP:O	1:B:122:ALA:HB3	2.09	0.53
1:E:65:VAL:HG23	1:E:125:THR:HG21	1.91	0.53
1:A:394:GLU:OE2	1:A:394:GLU:HA	2.08	0.53
1:A:407:VAL:HG12	1:A:408:PRO:HD2	1.91	0.53
1:B:66:MET:HE3	1:B:120:HIS:CD2	2.35	0.53
1:B:199:LYS:HG3	1:B:260:ASN:HD22	1.73	0.53
1:B:359:ASP:HB3	1:B:361:LEU:HD21	1.89	0.53
1:F:357:THR:HG22	1:F:358:HIS:ND1	2.23	0.53
1:A:211:ASP:HB3	1:A:231:ARG:HB3	1.90	0.53
1:B:108:GLU:OE2	1:C:363:ALA:N	2.42	0.53
1:D:393:VAL:HG13	1:D:394:GLU:HG2	1.91	0.53
1:E:110:ALA:C	1:E:112:SER:H	2.11	0.53
1:A:323:GLN:HA	1:A:335:GLY:O	2.08	0.53
1:B:201:THR:H	1:B:203:LYS:H	1.56	0.53
1:B:256:ILE:HG23	1:B:257:PRO:HD2	1.90	0.53
1:B:349:THR:HG21	1:F:79:TYR:HE2	1.73	0.52
1:A:230:LEU:CD2	1:A:243:VAL:HG22	2.39	0.52
1:A:412:ASP:O	1:A:415:THR:HG22	2.09	0.52
1:B:397:THR:CB	1:B:398:PRO:CD	2.81	0.52
1:B:349:THR:HG21	1:F:79:TYR:CE2	2.45	0.52
1:C:218:VAL:HG11	1:C:370:GLU:CG	2.26	0.52
1:F:109:PRO:O	1:F:111:ALA:N	2.42	0.52
1:E:219:GLN:NE2	1:E:414:ARG:HD3	2.24	0.52
1:A:231:ARG:HH11	1:A:231:ARG:CG	2.21	0.52
1:B:148:PRO:HG2	1:B:151:ALA:HB3	1.92	0.52
1:B:328:MET:HA	1:B:332:ASN:O	2.09	0.52
1:E:397:THR:CB	1:E:398:PRO:HD3	2.35	0.52
1:D:124:PRO:HG2	1:D:135:TYR:HB3	1.92	0.52
1:E:263:ASN:HB2	1:E:283:TRP:CE2	2.45	0.52
1:A:397:THR:HB	1:A:398:PRO:HD2	1.90	0.52
1:A:22:LEU:O	1:A:25:ARG:HB2	2.10	0.51
1:C:54:VAL:CG2	1:C:68:GLU:HA	2.37	0.51
1:C:218:VAL:HG23	1:C:366:LEU:CD2	2.40	0.51
1:D:236:ASN:O	1:D:240:ASN:HB2	2.10	0.51
1:E:328:MET:HA	1:E:332:ASN:O	2.10	0.51
1:A:230:LEU:HD23	1:A:243:VAL:HG22	1.92	0.51
1:A:382:PHE:CD1	1:A:388:ALA:HB2	2.46	0.51
1:B:197:GLY:O	1:B:198:ALA:HB2	2.11	0.51
1:C:2:MET:HE3	1:C:6:GLU:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:TYR:OH	1:C:244:ARG:NH2	2.43	0.51
1:C:345:ALA:O	1:C:349:THR:HG23	2.10	0.51
1:D:8:GLU:O	1:D:12:ARG:HG3	2.10	0.51
1:D:397:THR:HB	1:D:398:PRO:CD	2.40	0.51
1:E:118:VAL:C	1:E:119:LYS:HE2	2.30	0.51
1:D:235:SER:O	1:D:236:ASN:HB2	2.10	0.51
1:D:376:LEU:HA	1:D:379:VAL:HG12	1.93	0.51
1:F:382:PHE:CD1	1:F:388:ALA:HB2	2.46	0.51
1:A:54:VAL:HG13	1:A:78:VAL:HG22	1.91	0.51
1:C:218:VAL:CG1	1:C:370:GLU:HG2	2.28	0.51
1:D:150:TRP:CZ3	1:D:281:ILE:HD13	2.46	0.51
1:D:378:ALA:HB1	1:D:389:ILE:HG22	1.89	0.51
1:B:309:GLN:OE1	1:B:309:GLN:HA	2.10	0.51
1:E:339:PHE:CG	1:E:340:PRO:HD3	2.46	0.51
1:B:191:VAL:HG22	1:B:204:THR:OG1	2.11	0.50
1:A:153:THR:O	1:A:156:THR:OG1	2.28	0.50
1:A:53:LEU:HA	1:A:66:MET:O	2.11	0.50
1:B:32:LEU:HG	1:B:162:LYS:HD3	1.93	0.50
1:D:79:TYR:HE2	1:E:349:THR:HG21	1.76	0.50
1:A:16:ASP:O	1:A:21:ARG:NH1	2.45	0.50
1:E:401:CYS:SG	1:E:419:HIS:O	2.70	0.50
1:A:71:PRO:O	1:D:360:ARG:HB2	2.11	0.50
1:A:408:PRO:C	1:A:410:THR:H	2.15	0.50
1:F:356:ARG:HD3	1:F:372:ARG:NE	2.26	0.50
1:A:236:ASN:C	1:A:238:ALA:H	2.15	0.50
1:C:70:CYS:HB2	1:C:77:LEU:HD21	1.93	0.50
1:B:210:THR:HG23	1:B:234:LEU:HD21	1.93	0.50
1:F:129:ALA:O	1:F:158:VAL:HG11	2.12	0.50
1:A:328:MET:HA	1:A:332:ASN:O	2.11	0.50
1:D:164:LEU:HD22	1:D:310:ASN:O	2.12	0.50
1:F:263:ASN:HB2	1:F:283:TRP:CE2	2.47	0.50
1:C:299:LEU:HD22	1:C:340:PRO:CG	2.41	0.49
1:D:72:HIS:HB3	3:D:502:FES:S2	2.52	0.49
1:C:183:SER:HB2	1:C:212:LYS:HG2	1.93	0.49
1:B:245:SER:HB3	1:B:403:PHE:CE2	2.48	0.49
1:C:24:ARG:HH21	1:C:136:MET:HB3	1.77	0.49
1:C:162:LYS:HE3	1:C:311:TYR:CG	2.48	0.49
1:C:246:THR:OG1	1:C:257:PRO:HD3	2.13	0.49
1:F:218:VAL:CG1	1:F:219:GLN:N	2.76	0.49
1:F:295:TRP:CE2	1:F:299:LEU:HD11	2.47	0.49
1:E:226:ARG:HH21	1:E:403:PHE:HE2	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ARG:HB2	1:F:71:PRO:O	2.12	0.49
1:F:109:PRO:C	1:F:111:ALA:N	2.66	0.49
1:B:97:ASP:HB3	1:B:103:LEU:HD11	1.95	0.49
1:D:231:ARG:HG2	1:D:231:ARG:NH1	2.24	0.49
1:C:23:MET:SD	1:C:270:PRO:HG3	2.52	0.49
1:C:328:MET:HA	1:C:332:ASN:O	2.13	0.49
1:D:397:THR:O	1:D:399:THR:N	2.45	0.49
1:A:263:ASN:HB2	1:A:283:TRP:CE2	2.47	0.49
1:C:21:ARG:HH12	1:C:383:GLU:HG2	1.78	0.49
1:D:148:PRO:HG2	1:D:151:ALA:HB3	1.95	0.49
1:E:66:MET:HG2	1:E:122:ALA:HB2	1.95	0.49
1:F:22:LEU:C	1:F:22:LEU:HD23	2.33	0.49
1:F:157:ARG:O	1:F:283:TRP:HA	2.13	0.49
1:A:126:GLN:HG2	1:A:145:PHE:CG	2.48	0.48
1:E:3:THR:OG1	1:E:6:GLU:HG3	2.13	0.48
1:F:285:HIS:CD2	1:F:423:LEU:CD1	2.96	0.48
1:E:216:MET:HE1	1:E:229:ALA:HB2	1.95	0.48
1:E:295:TRP:CE2	1:E:299:LEU:HD11	2.48	0.48
1:D:33:VAL:O	1:D:36:VAL:HG22	2.12	0.48
1:B:343:ASP:HB3	1:B:347:TRP:CH2	2.47	0.48
1:F:95:LYS:O	1:F:103:LEU:N	2.41	0.48
1:F:368:ILE:O	1:F:372:ARG:HG3	2.13	0.48
1:E:42:THR:HB	5:E:610:HOH:O	2.14	0.48
1:E:227:TYR:CE1	1:E:246:THR:HB	2.49	0.48
1:E:307:LEU:HD23	1:E:313:PRO:HA	1.95	0.48
1:B:173:LEU:O	1:B:173:LEU:HG	2.13	0.48
1:D:231:ARG:HH11	1:D:231:ARG:CG	2.24	0.48
1:C:140:GLU:CD	1:C:140:GLU:H	2.17	0.48
1:B:195:VAL:HG11	1:B:206:LEU:HD13	1.95	0.48
1:C:236:ASN:HB2	5:C:637:HOH:O	2.13	0.48
1:C:293:GLU:OE1	1:C:293:GLU:HA	2.14	0.48
1:A:13:VAL:HG21	1:A:270:PRO:HB2	1.97	0.47
1:A:45:LYS:HG2	1:A:46:ALA:N	2.29	0.47
1:E:173:LEU:HD13	1:E:252:ALA:HA	1.96	0.47
1:E:184:SER:O	1:E:333:PHE:CE2	2.67	0.47
1:C:13:VAL:HG21	1:C:270:PRO:HB2	1.97	0.47
1:C:92:HIS:HB2	3:C:502:FES:S2	2.55	0.47
1:D:35:GLU:HB3	1:D:44:VAL:HG21	1.95	0.47
1:D:291:GLU:O	1:D:292:THR:C	2.53	0.47
1:F:365:ASP:O	1:F:369:VAL:HG23	2.15	0.47
1:D:210:THR:O	1:D:212:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:SER:O	1:D:402:SER:HB2	2.15	0.47
1:E:70:CYS:HB2	1:E:77:LEU:HD21	1.97	0.47
1:F:147:PRO:HA	1:F:148:PRO:HD2	1.86	0.47
1:B:94:TRP:HZ3	1:B:118:VAL:HG11	1.80	0.47
1:F:218:VAL:HG12	1:F:219:GLN:N	2.30	0.47
1:A:16:ASP:O	1:A:17:ALA:C	2.52	0.47
1:A:25:ARG:HA	1:A:25:ARG:HD3	1.55	0.47
1:E:54:VAL:HG13	1:E:78:VAL:HG22	1.97	0.47
1:E:95:LYS:HE2	1:E:103:LEU:HD12	1.97	0.47
1:B:109:PRO:C	1:B:111:ALA:H	2.17	0.46
1:D:176:ALA:HB2	1:D:266:ASN:HD22	1.81	0.46
1:F:173:LEU:HD22	1:F:371:PHE:CE1	2.50	0.46
1:A:333:PHE:O	1:E:81:ARG:NH1	2.48	0.46
1:A:382:PHE:C	1:A:384:GLN:N	2.69	0.46
1:C:173:LEU:O	1:C:174:GLU:C	2.54	0.46
1:D:372:ARG:O	1:D:376:LEU:HD12	2.16	0.46
1:C:256:ILE:CG2	1:C:257:PRO:HD2	2.44	0.46
1:E:92:HIS:HB2	3:E:502:FES:S2	2.55	0.46
1:E:207:ARG:NH2	5:E:603:HOH:O	2.48	0.46
1:E:236:ASN:O	1:E:240:ASN:HB2	2.16	0.46
1:A:16:ASP:HB2	5:A:706:HOH:O	2.16	0.46
1:E:16:ASP:HB2	5:E:627:HOH:O	2.16	0.46
1:E:77:LEU:CD2	1:E:89:CYS:HB2	2.45	0.46
1:B:14:GLU:OE2	1:B:272:ASP:HB2	2.16	0.46
1:B:17:ALA:HA	1:B:18:PRO:HD3	1.80	0.46
1:E:74:ARG:HD2	1:E:74:ARG:HA	1.62	0.46
1:A:105:MET:O	1:A:107:SER:N	2.49	0.46
1:C:240:ASN:OD1	1:C:408:PRO:HA	2.16	0.46
1:C:299:LEU:HB3	1:C:340:PRO:HG2	1.98	0.46
1:D:184:SER:O	1:D:187:SER:OG	2.29	0.46
1:F:256:ILE:HG23	1:F:257:PRO:HD2	1.97	0.46
1:A:397:THR:HB	1:A:398:PRO:HD3	1.96	0.46
1:C:28:THR:HG22	1:C:30:ILE:HD13	1.97	0.46
1:E:227:TYR:O	1:E:245:SER:HA	2.16	0.46
1:F:80:GLY:HA2	1:F:90:LEU:HG	1.98	0.46
1:A:184:SER:O	1:A:187:SER:OG	2.31	0.45
1:A:263:ASN:HB2	1:A:283:TRP:NE1	2.31	0.45
1:E:355:ASP:OD1	1:E:357:THR:HB	2.15	0.45
1:F:218:VAL:HG11	1:F:370:GLU:HG2	1.97	0.45
1:A:392:GLY:C	1:A:394:GLU:H	2.19	0.45
1:D:108:GLU:OE2	1:E:362:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:MET:SD	1:C:96:MET:N	2.89	0.45
1:C:129:ALA:HB1	1:C:158:VAL:HG11	1.98	0.45
1:A:297:LYS:O	1:A:300:ARG:HD3	2.16	0.45
1:C:355:ASP:OD1	1:C:357:THR:HB	2.17	0.45
1:E:236:ASN:C	1:E:238:ALA:H	2.19	0.45
1:D:256:ILE:HG23	1:D:257:PRO:HD2	1.97	0.45
1:E:256:ILE:O	1:E:257:PRO:C	2.55	0.45
1:F:57:ARG:NH1	1:F:63:VAL:CG2	2.80	0.45
1:F:126:GLN:HG2	1:F:145:PHE:CG	2.51	0.45
1:B:164:LEU:HD22	1:B:310:ASN:O	2.17	0.45
1:C:325:ARG:HA	1:C:325:ARG:HD3	1.79	0.45
1:E:248:PHE:CZ	1:E:250:ALA:HA	2.51	0.45
1:A:28:THR:CG2	1:A:269:VAL:HG13	2.47	0.45
1:B:357:THR:HG22	1:B:358:HIS:ND1	2.32	0.45
1:C:73:ARG:HH12	1:C:92:HIS:CE1	2.35	0.45
1:E:260:ASN:HB2	1:E:261:LEU:HG	1.99	0.45
1:B:28:THR:CG2	1:B:269:VAL:HG11	2.47	0.45
1:C:295:TRP:HA	1:C:295:TRP:CE3	2.52	0.45
1:A:285:HIS:CD2	1:A:423:LEU:HD12	2.51	0.45
1:E:153:THR:HG22	1:E:154:ALA:H	1.82	0.45
1:C:231:ARG:NH1	1:C:231:ARG:HG3	2.31	0.44
1:D:138:PRO:O	1:D:141:THR:OG1	2.31	0.44
1:D:307:LEU:HD23	1:D:313:PRO:HA	1.98	0.44
1:F:256:ILE:CD1	1:F:264:VAL:HG12	2.47	0.44
1:B:195:VAL:HG21	1:B:206:LEU:CB	2.47	0.44
1:A:209:SER:HB2	1:A:233:PRO:HA	1.98	0.44
1:D:416:TYR:CE2	1:D:418:ALA:HB2	2.52	0.44
1:B:247:VAL:HB	1:B:255:LEU:HB2	1.98	0.44
1:D:69:TYR:O	1:D:120:HIS:HE1	2.00	0.44
1:D:131:MET:CE	1:D:281:ILE:HD11	2.48	0.44
1:D:214:PRO:HB3	1:D:231:ARG:HG3	1.99	0.44
1:E:97:ASP:OD2	1:E:97:ASP:C	2.55	0.44
1:F:135:TYR:CE1	1:F:143:PRO:HD2	2.52	0.44
1:B:316:ASN:OD1	1:B:318:ALA:HB3	2.17	0.44
1:F:2:MET:HA	1:F:6:GLU:OE2	2.18	0.44
1:F:22:LEU:HG	1:F:388:ALA:HB1	2.00	0.44
1:F:173:LEU:CD1	1:F:252:ALA:CA	2.92	0.44
1:F:258:PRO:HD3	1:F:402:SER:OG	2.18	0.44
1:A:180:ALA:HB1	1:E:107:SER:HB2	2.00	0.44
1:B:69:TYR:O	1:B:120:HIS:CE1	2.71	0.44
1:A:253:THR:OG1	1:A:267:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:MET:CG	1:F:122:ALA:HB2	2.47	0.44
1:A:250:ALA:HB1	1:A:251:PRO:HA	2.00	0.44
1:A:345:ALA:O	1:A:349:THR:HG23	2.17	0.44
1:B:69:TYR:O	1:B:120:HIS:HE1	2.01	0.44
1:D:3:THR:OG1	1:D:6:GLU:HG3	2.18	0.44
1:E:36:VAL:HG11	1:E:55:VAL:HG12	1.99	0.44
1:E:173:LEU:HD12	1:E:268:ASN:ND2	2.32	0.44
1:E:216:MET:HB3	1:E:366:LEU:HB3	2.00	0.44
1:E:245:SER:O	1:E:402:SER:HB2	2.18	0.44
1:A:378:ALA:HB1	1:A:389:ILE:HB	2.00	0.43
1:C:23:MET:HG2	1:C:251:PRO:HG2	1.99	0.43
1:F:42:THR:HA	1:F:43:PRO:HD3	1.92	0.43
1:B:67:ASP:HB3	1:B:120:HIS:CE1	2.53	0.43
1:B:247:VAL:HG11	1:B:400:VAL:CG1	2.48	0.43
1:E:81:ARG:NE	1:E:83:GLU:OE1	2.46	0.43
1:A:167:CYS:HB3	1:A:348:LEU:HD23	1.99	0.43
1:D:53:LEU:HA	1:D:66:MET:O	2.19	0.43
1:F:13:VAL:HG21	1:F:270:PRO:HB2	1.99	0.43
1:B:257:PRO:HA	1:B:258:PRO:HD2	1.88	0.43
1:C:356:ARG:HD3	1:C:372:ARG:NE	2.34	0.43
1:D:221:THR:HG23	1:D:225:PHE:HA	2.01	0.43
1:C:359:ASP:HB3	1:C:361:LEU:HD21	2.00	0.43
1:B:250:ALA:HB1	1:B:251:PRO:HA	2.01	0.43
1:F:249:VAL:HB	1:F:253:THR:HB	1.99	0.43
1:B:203:LYS:O	1:B:204:THR:HB	2.19	0.43
1:E:28:THR:HG22	1:E:29:PRO:O	2.19	0.43
1:E:219:GLN:HE21	1:E:414:ARG:HD3	1.84	0.43
1:A:236:ASN:C	1:A:238:ALA:N	2.72	0.43
1:B:360:ARG:NH1	1:B:360:ARG:CG	2.78	0.43
1:C:8:GLU:OE2	1:C:12:ARG:NE	2.38	0.43
1:F:24:ARG:NH1	1:F:49:PHE:HB2	2.34	0.43
1:A:310:ASN:O	1:A:311:TYR:HB2	2.18	0.43
1:B:81:ARG:NH1	1:C:333:PHE:HA	2.34	0.43
1:C:365:ASP:O	1:C:369:VAL:HG23	2.19	0.43
1:D:176:ALA:HB2	1:D:266:ASN:ND2	2.34	0.43
1:D:360:ARG:CG	1:D:360:ARG:NH1	2.66	0.43
1:E:224:GLY:HA3	1:E:248:PHE:O	2.19	0.43
1:F:53:LEU:HA	1:F:66:MET:O	2.19	0.43
1:A:69:TYR:HB2	1:A:74:ARG:NH1	2.33	0.42
1:B:338:GLY:O	1:B:341:ASN:HB2	2.19	0.42
1:D:11:CYS:SG	1:D:356:ARG:NH1	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ALA:HB1	1:D:251:PRO:HA	2.01	0.42
1:E:215:ARG:HB2	1:E:230:LEU:HB2	2.00	0.42
1:D:292:THR:O	1:D:295:TRP:HB3	2.19	0.42
1:F:291:GLU:O	1:F:292:THR:C	2.58	0.42
1:E:79:TYR:O	1:E:90:LEU:HD11	2.20	0.42
1:F:156:THR:HG21	1:F:283:TRP:HE3	1.84	0.42
1:F:208:PRO:HD2	1:F:242:TYR:CZ	2.54	0.42
1:D:22:LEU:HG	1:D:388:ALA:HB1	2.01	0.42
1:A:55:VAL:HA	1:A:64:GLY:O	2.19	0.42
1:D:157:ARG:HA	5:D:602:HOH:O	2.18	0.42
1:E:147:PRO:O	1:E:397:THR:HG22	2.19	0.42
1:E:173:LEU:HD12	1:E:268:ASN:HD22	1.84	0.42
1:E:223:TYR:CG	1:E:396:ALA:HB2	2.54	0.42
1:F:226:ARG:HH21	1:F:403:PHE:HE2	1.68	0.42
1:A:79:TYR:CE2	1:D:349:THR:HG21	2.54	0.42
1:B:114:MET:O	1:B:118:VAL:HG23	2.18	0.42
1:B:357:THR:HG22	1:B:358:HIS:CE1	2.54	0.42
1:C:66:MET:CG	1:C:122:ALA:HB2	2.50	0.42
1:D:328:MET:HA	1:D:332:ASN:O	2.19	0.42
1:F:167:CYS:SG	1:F:172:ILE:HD11	2.60	0.42
1:F:260:ASN:OD1	1:F:260:ASN:N	2.52	0.42
1:B:192:PRO:CB	1:B:210:THR:HG22	2.50	0.42
1:D:77:LEU:HB3	1:D:87:LEU:HD21	2.01	0.42
1:F:72:HIS:HB3	3:F:502:FES:S2	2.60	0.42
1:F:293:GLU:OE1	1:F:293:GLU:HA	2.20	0.42
1:E:162:LYS:HD2	1:E:279:TYR:CE1	2.55	0.42
1:E:230:LEU:HD23	1:E:243:VAL:HG22	2.00	0.42
1:B:220:ARG:HD3	1:B:370:GLU:OE2	2.20	0.42
1:A:144:GLU:HG2	5:A:722:HOH:O	2.20	0.41
1:B:325:ARG:HD3	1:B:325:ARG:HA	1.59	0.41
1:C:315:ARG:HB3	1:C:321:PHE:HA	2.02	0.41
1:E:22:LEU:HD23	1:E:22:LEU:C	2.39	0.41
1:F:166:PRO:HD2	1:F:348:LEU:HD21	2.02	0.41
1:A:3:THR:N	1:A:6:GLU:OE2	2.50	0.41
1:D:346:MET:O	1:D:350:MET:HG3	2.20	0.41
1:F:382:PHE:C	1:F:384:GLN:N	2.73	0.41
1:B:263:ASN:HB2	1:B:283:TRP:CE2	2.55	0.41
1:B:292:THR:HG22	1:B:293:GLU:N	2.35	0.41
1:C:123:TYR:CD1	1:C:136:MET:HA	2.55	0.41
1:C:295:TRP:HA	1:C:295:TRP:HE3	1.86	0.41
1:B:249:VAL:HB	1:B:253:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ASP:O	1:D:369:VAL:HG23	2.20	0.41
1:F:103:LEU:HD23	1:F:103:LEU:HA	1.88	0.41
1:A:220:ARG:H	1:A:220:ARG:HG2	1.62	0.41
1:B:94:TRP:CZ3	1:B:118:VAL:HG11	2.55	0.41
1:D:150:TRP:HA	1:D:283:TRP:CZ2	2.56	0.41
1:D:185:LEU:HD23	1:D:186:HIS:CE1	2.55	0.41
1:F:209:SER:OG	1:F:211:ASP:HB3	2.21	0.41
1:C:173:LEU:HD13	1:C:252:ALA:CA	2.49	0.41
1:F:110:ALA:C	1:F:112:SER:H	2.23	0.41
1:C:42:THR:HA	1:C:43:PRO:HD3	1.93	0.41
1:C:77:LEU:HB3	1:C:87:LEU:HD21	2.02	0.41
1:C:301:GLN:HE22	1:C:341:ASN:CG	2.23	0.41
1:F:30:ILE:O	1:F:31:CYS:HB3	2.20	0.41
1:F:332:ASN:HD22	1:F:333:PHE:N	2.19	0.41
1:C:64:GLY:CA	1:C:98:VAL:HB	2.51	0.41
1:C:141:THR:O	1:C:143:PRO:HD3	2.20	0.41
1:C:250:ALA:HB1	1:C:251:PRO:HA	2.02	0.41
1:C:293:GLU:HB3	1:E:293:GLU:HB3	2.02	0.41
1:D:71:PRO:O	1:E:360:ARG:HB2	2.20	0.41
1:D:293:GLU:OE2	1:F:297:LYS:NZ	2.54	0.41
1:E:412:ASP:HB3	1:E:415:THR:HB	2.03	0.41
1:A:22:LEU:HD23	1:A:23:MET:N	2.36	0.41
1:D:347:TRP:HA	1:D:350:MET:CE	2.50	0.41
1:E:135:TYR:CE1	1:E:143:PRO:HD2	2.56	0.41
1:F:357:THR:HG22	1:F:358:HIS:CE1	2.56	0.41
1:B:200:ALA:HA	1:B:204:THR:O	2.21	0.40
1:A:245:SER:O	1:A:402:SER:HB2	2.21	0.40
1:A:324:ASP:O	1:A:327:ALA:HB3	2.22	0.40
1:B:57:ARG:HA	1:B:62:ARG:O	2.21	0.40
1:B:326:ASN:O	1:B:329:LYS:N	2.54	0.40
1:F:221:THR:HB	1:F:222:GLY:H	1.78	0.40
1:C:18:PRO:HB3	1:C:383:GLU:HG3	2.03	0.40
1:D:13:VAL:HG21	1:D:270:PRO:HB2	2.03	0.40
1:D:68:GLU:HG3	1:D:78:VAL:HG23	2.04	0.40
1:D:113:GLY:HA2	5:D:617:HOH:O	2.21	0.40
1:F:184:SER:O	1:F:333:PHE:CD2	2.73	0.40
1:D:227:TYR:CE1	1:D:246:THR:HB	2.56	0.40
1:D:45:LYS:HB2	1:D:78:VAL:HG21	2.04	0.40
1:F:157:ARG:HB2	1:F:286:PRO:HA	2.04	0.40
1:F:224:GLY:HA3	1:F:248:PHE:O	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/439 (91%)	350 (88%)	41 (10%)	8 (2%)	7	29
1	B	423/439 (96%)	368 (87%)	45 (11%)	10 (2%)	6	25
1	C	403/439 (92%)	354 (88%)	44 (11%)	5 (1%)	13	42
1	D	398/439 (91%)	362 (91%)	30 (8%)	6 (2%)	10	37
1	E	403/439 (92%)	354 (88%)	43 (11%)	6 (2%)	10	37
1	F	402/439 (92%)	358 (89%)	31 (8%)	13 (3%)	4	20
All	All	2428/2634 (92%)	2146 (88%)	234 (10%)	48 (2%)	7	29

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ALA
1	B	199	LYS
1	B	200	ALA
1	D	236	ASN
1	E	152	PRO
1	F	152	PRO
1	F	238	ALA
1	A	352	PRO
1	A	383	GLU
1	C	72	HIS
1	C	74	ARG
1	C	112	SER
1	D	106	ALA
1	E	209	SER
1	E	419	HIS
1	F	15	GLY
1	F	58	ASP
1	F	74	ARG
1	F	110	ALA
1	F	383	GLU

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Mol	Chain	Res	Type
1	B	196	ASP
1	D	72	HIS
1	D	152	PRO
1	D	422	TRP
1	F	72	HIS
1	A	121	THR
1	B	72	HIS
1	B	152	PRO
1	B	207	ARG
1	D	398	PRO
1	E	74	ARG
1	F	272	ASP
1	F	389	ILE
1	A	74	ARG
1	A	106	ALA
1	B	109	PRO
1	B	195	VAL
1	F	286	PRO
1	A	152	PRO
1	A	389	ILE
1	B	356	ARG
1	C	286	PRO
1	C	338	GLY
1	A	17	ALA
1	F	177	ILE
1	E	13	VAL
1	E	393	VAL
1	F	147	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	336/363 (93%)	299 (89%)	37 (11%)	6	23
1	B	349/363 (96%)	315 (90%)	34 (10%)	8	28
1	C	336/363 (93%)	302 (90%)	34 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	335/363 (92%)	305 (91%)	30 (9%)	9	32
1	E	336/363 (93%)	303 (90%)	33 (10%)	8	28
1	F	335/363 (92%)	311 (93%)	24 (7%)	14	42
All	All	2027/2178 (93%)	1835 (90%)	192 (10%)	8	29

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	25	ARG
1	A	38	GLU
1	A	54	VAL
1	A	59	SER
1	A	70	CYS
1	A	91	TYR
1	A	108	GLU
1	A	114	MET
1	A	115	VAL
1	A	121	THR
1	A	125	THR
1	A	140	GLU
1	A	144	GLU
1	A	153	THR
1	A	156	THR
1	A	160	ILE
1	A	171	GLN
1	A	183	SER
1	A	184	SER
1	A	190	MET
1	A	207	ARG
1	A	220	ARG
1	A	231	ARG
1	A	234	LEU
1	A	263	ASN
1	A	267	ILE
1	A	305	VAL
1	A	329	LYS
1	A	352	PRO
1	A	357	THR
1	A	360	ARG
1	A	393	VAL

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Mol	Chain	Res	Type
1	A	411	THR
1	A	415	THR
1	A	419	HIS
1	A	423	LEU
1	B	16	ASP
1	B	23	MET
1	B	45	LYS
1	B	54	VAL
1	B	91	TYR
1	B	103	LEU
1	B	114	MET
1	B	119	LYS
1	B	140	GLU
1	B	153	THR
1	B	173	LEU
1	B	183	SER
1	B	187	SER
1	B	190	MET
1	B	194	ARG
1	B	195	VAL
1	B	201	THR
1	B	231	ARG
1	B	239	GLU
1	B	263	ASN
1	B	267	ILE
1	B	292	THR
1	B	294	THR
1	B	297	LYS
1	B	305	VAL
1	B	314	LEU
1	B	325	ARG
1	B	329	LYS
1	B	348	LEU
1	B	357	THR
1	B	360	ARG
1	B	411	THR
1	B	415	THR
1	B	417	ASP
1	C	1	MET
1	C	34	GLU
1	C	54	VAL
1	C	70	CYS

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Mol	Chain	Res	Type
1	C	91	TYR
1	C	114	MET
1	C	116	ASP
1	C	117	LYS
1	C	153	THR
1	C	155	ASP
1	C	164	LEU
1	C	173	LEU
1	C	182	SER
1	C	183	SER
1	C	187	SER
1	C	190	MET
1	C	216	MET
1	C	231	ARG
1	C	232	ARG
1	C	263	ASN
1	C	286	PRO
1	C	295	TRP
1	C	297	LYS
1	C	329	LYS
1	C	357	THR
1	C	360	ARG
1	C	369	VAL
1	C	383	GLU
1	C	389	ILE
1	C	397	THR
1	C	409	LYS
1	C	410	THR
1	C	411	THR
1	C	423	LEU
1	D	28	THR
1	D	54	VAL
1	D	62	ARG
1	D	91	TYR
1	D	108	GLU
1	D	125	THR
1	D	153	THR
1	D	156	THR
1	D	164	LEU
1	D	190	MET
1	D	207	ARG
1	D	210	THR

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Mol	Chain	Res	Type
1	D	227	TYR
1	D	231	ARG
1	D	234	LEU
1	D	236	ASN
1	D	260	ASN
1	D	263	ASN
1	D	267	ILE
1	D	297	LYS
1	D	305	VAL
1	D	334	THR
1	D	357	THR
1	D	360	ARG
1	D	389	ILE
1	D	406	ILE
1	D	409	LYS
1	D	411	THR
1	D	415	THR
1	D	423	LEU
1	E	4	HIS
1	E	5	GLU
1	E	38	GLU
1	E	54	VAL
1	E	91	TYR
1	E	114	MET
1	E	115	VAL
1	E	117	LYS
1	E	125	THR
1	E	152	PRO
1	E	153	THR
1	E	173	LEU
1	E	183	SER
1	E	187	SER
1	E	190	MET
1	E	227	TYR
1	E	234	LEU
1	E	239	GLU
1	E	260	ASN
1	E	263	ASN
1	E	266	ASN
1	E	305	VAL
1	E	329	LYS
1	E	357	THR

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Mol	Chain	Res	Type
1	E	360	ARG
1	E	397	THR
1	E	399	THR
1	E	400	VAL
1	E	409	LYS
1	E	410	THR
1	E	411	THR
1	E	412	ASP
1	E	415	THR
1	F	16	ASP
1	F	54	VAL
1	F	91	TYR
1	F	114	MET
1	F	115	VAL
1	F	139	LYS
1	F	140	GLU
1	F	147	PRO
1	F	153	THR
1	F	168	ASN
1	F	179	SER
1	F	210	THR
1	F	232	ARG
1	F	260	ASN
1	F	263	ASN
1	F	267	ILE
1	F	302	THR
1	F	305	VAL
1	F	357	THR
1	F	360	ARG
1	F	389	ILE
1	F	409	LYS
1	F	415	THR
1	F	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	B	120	HIS
1	B	301	GLN
1	C	266	ASN
1	D	120	HIS

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Mol	Chain	Res	Type
1	D	266	ASN
1	D	332	ASN
1	E	219	GLN
1	F	332	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	E	502	1	0,4,4	-	-	-		
4	UB7	B	503	-	8,12,12	4.55	2 (25%)	10,16,16	0.43	0
3	FES	C	502	1	0,4,4	-	-	-		
3	FES	B	502	1	0,4,4	-	-	-		
3	FES	D	502	1	0,4,4	-	-	-		
3	FES	F	502	1	0,4,4	-	-	-		
3	FES	A	602	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
4	UB7	B	503	-	-	0/0/8/8	0/1/1/1
3	FES	E	502	1	-	-	0/1/1/1
3	FES	C	502	1	-	-	0/1/1/1
3	FES	B	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	602	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	UB7	C03-C10	10.50	1.57	1.47
4	B	503	UB7	C06-C07	7.37	1.54	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

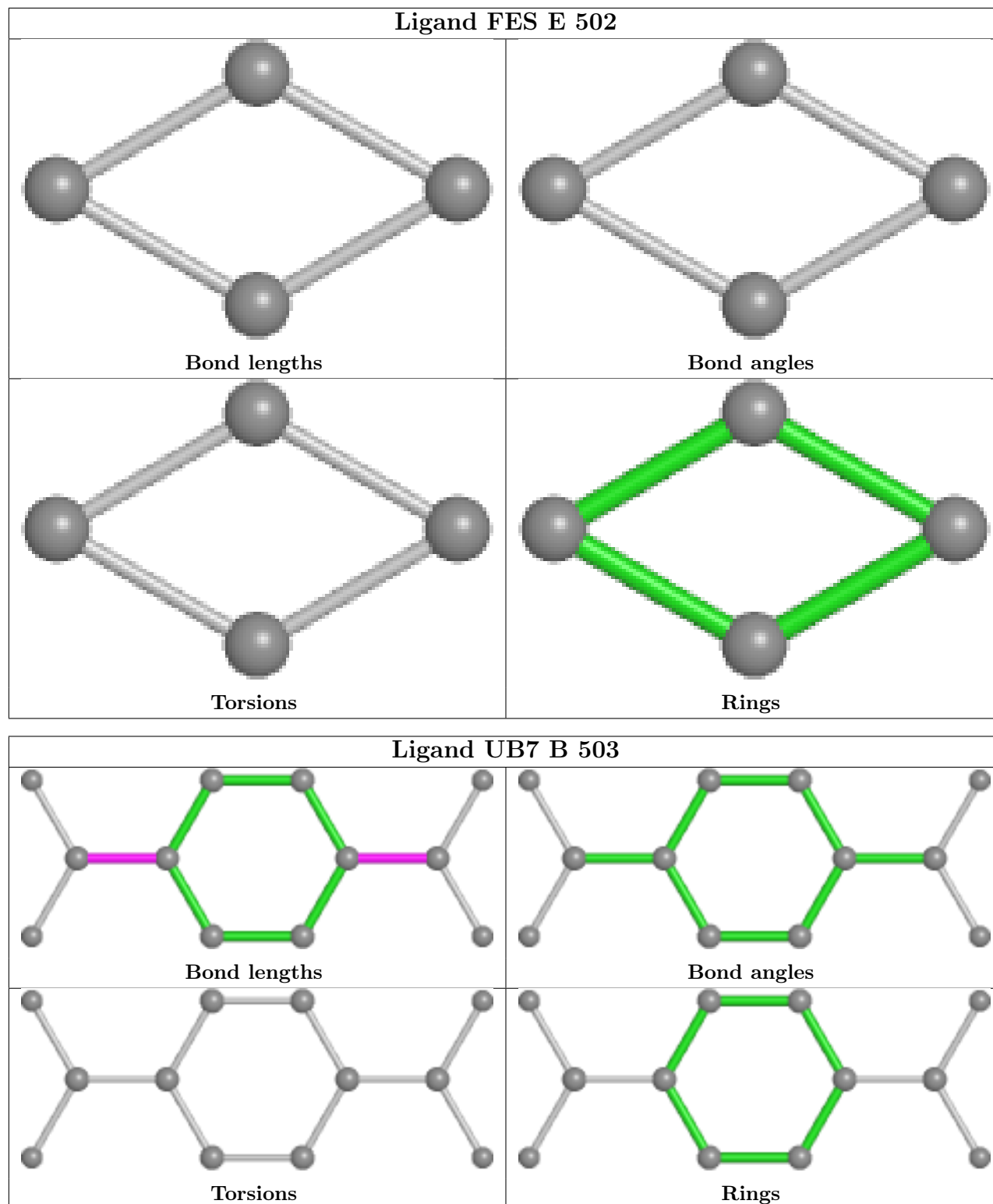
There are no ring outliers.

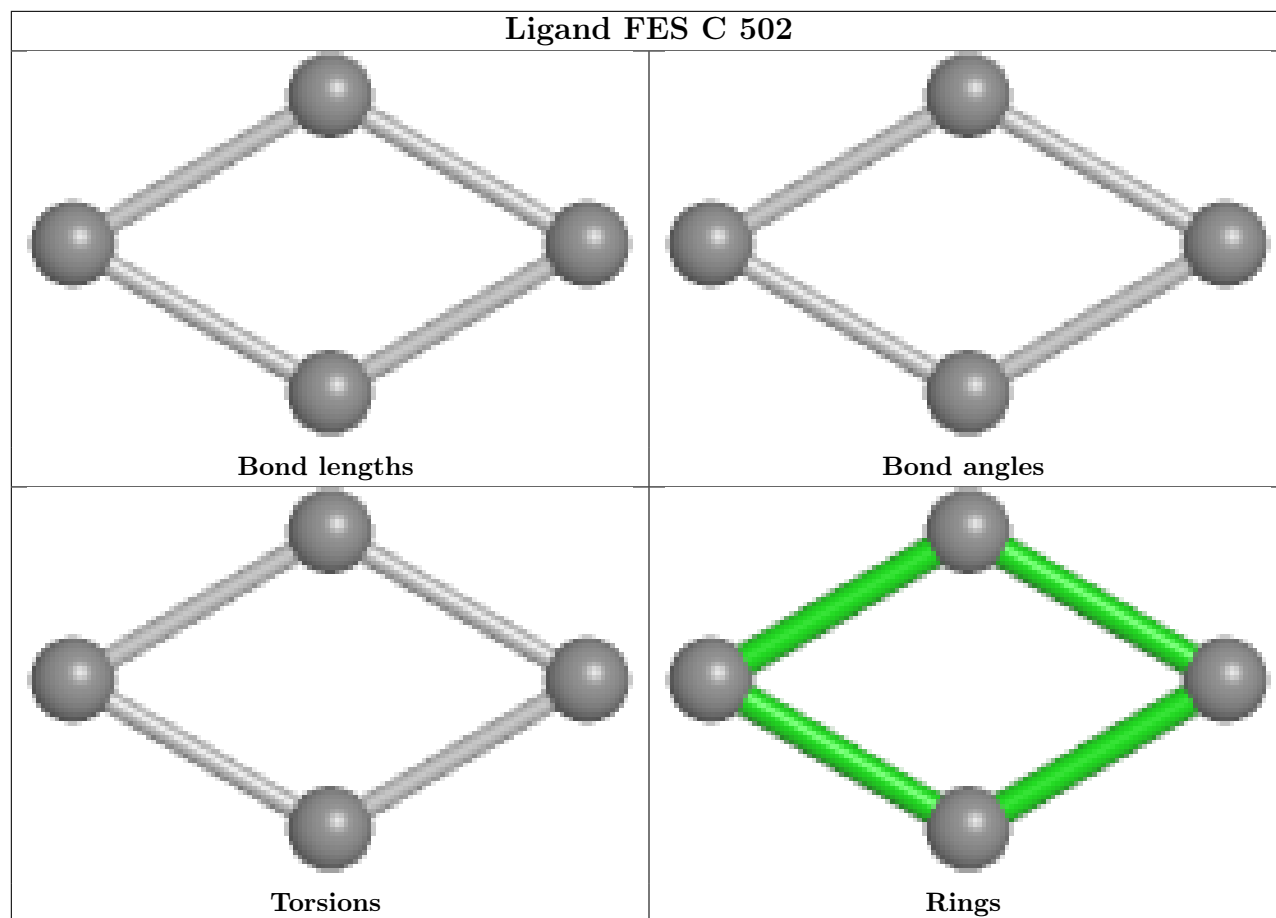
5 monomers are involved in 6 short contacts:

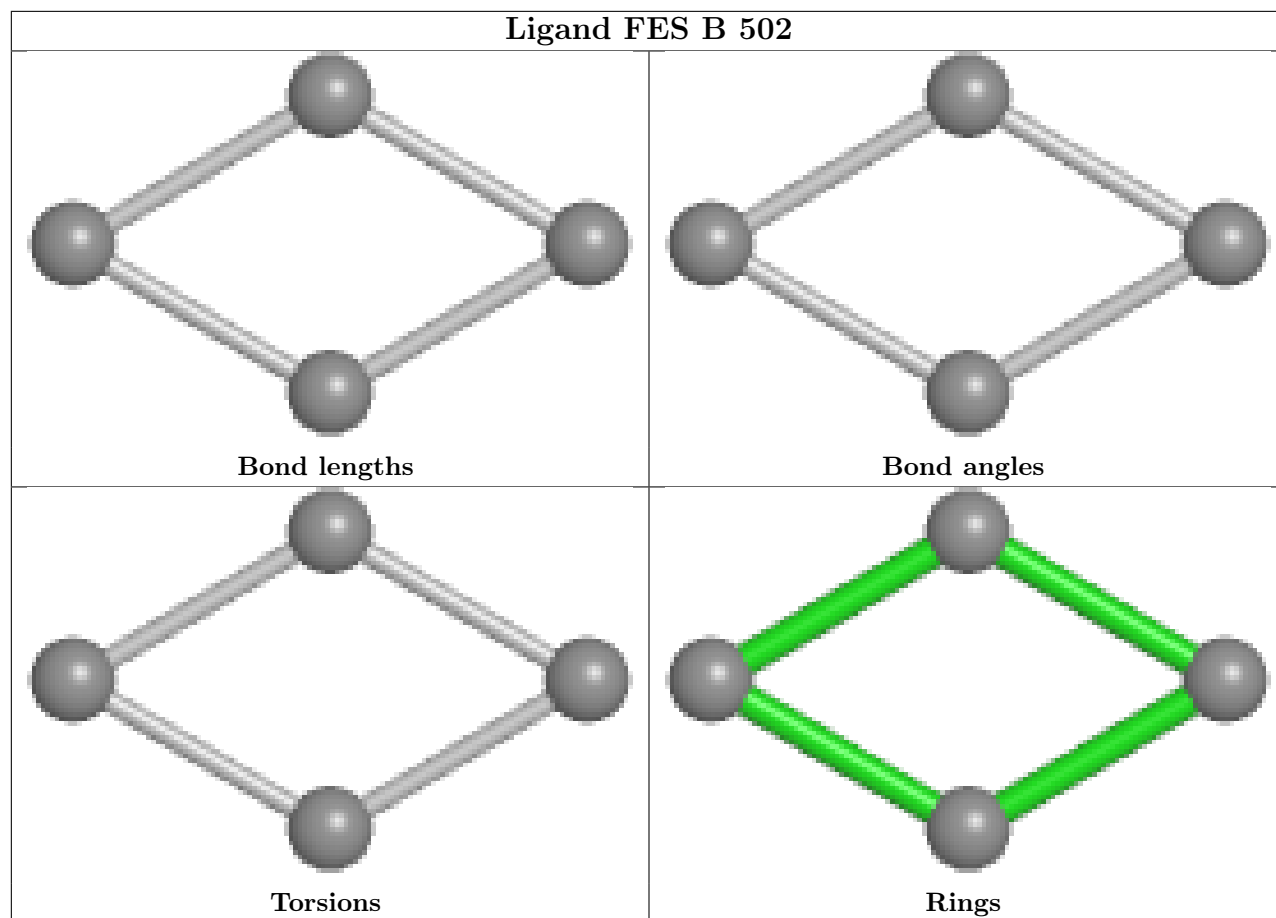
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	FES	1	0
3	C	502	FES	1	0
3	B	502	FES	1	0
3	D	502	FES	2	0
3	F	502	FES	1	0

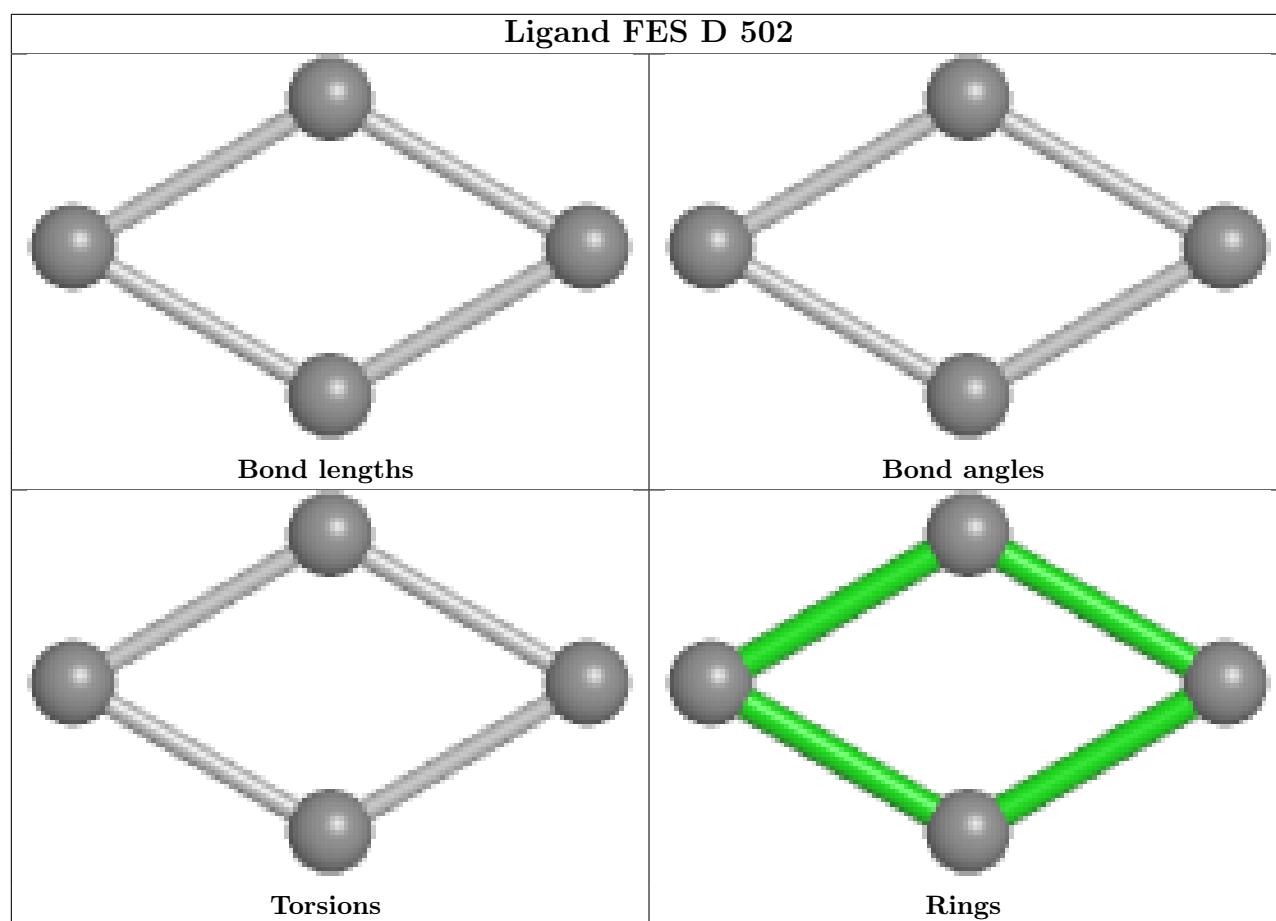
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

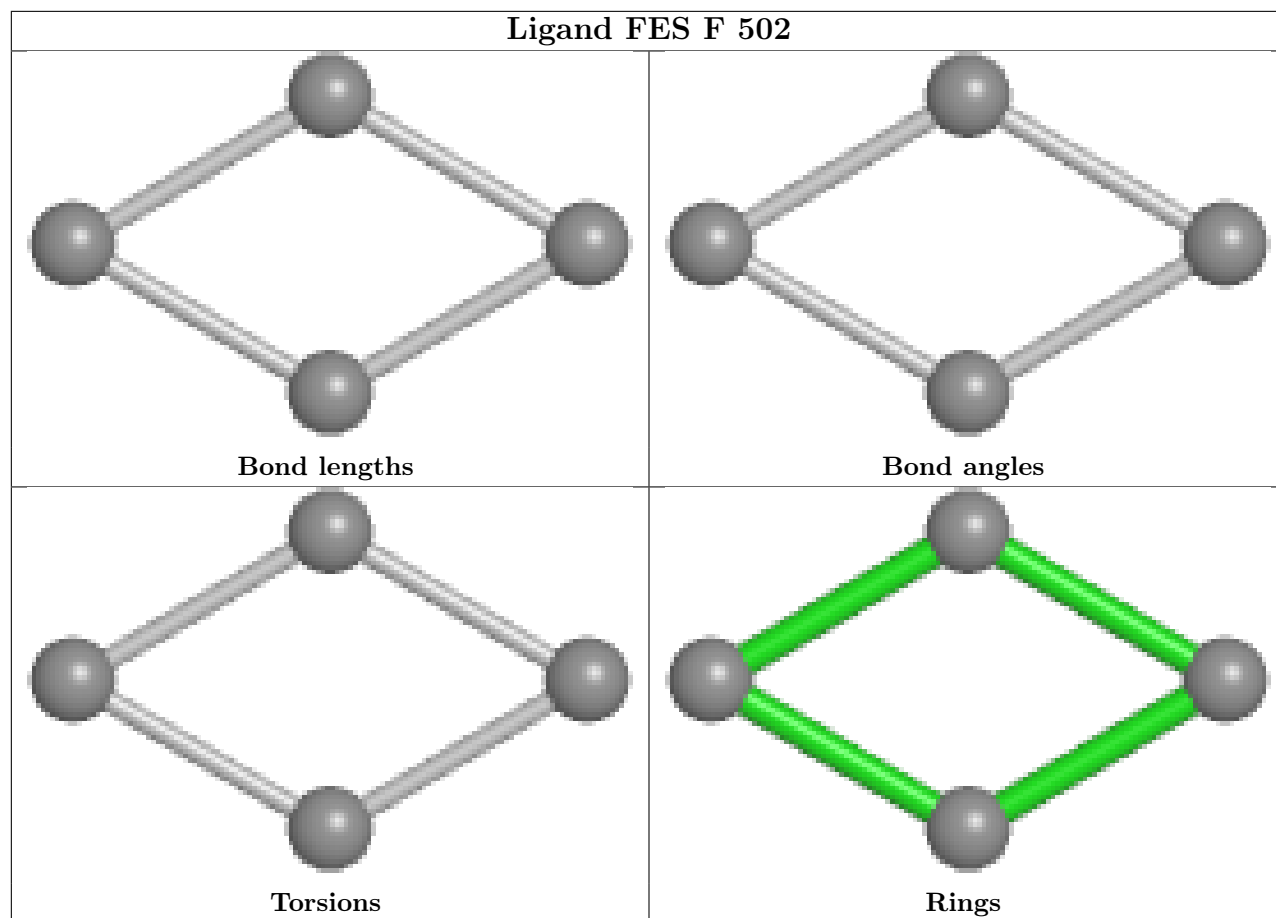
equivalents in the CSD to analyse the geometry.

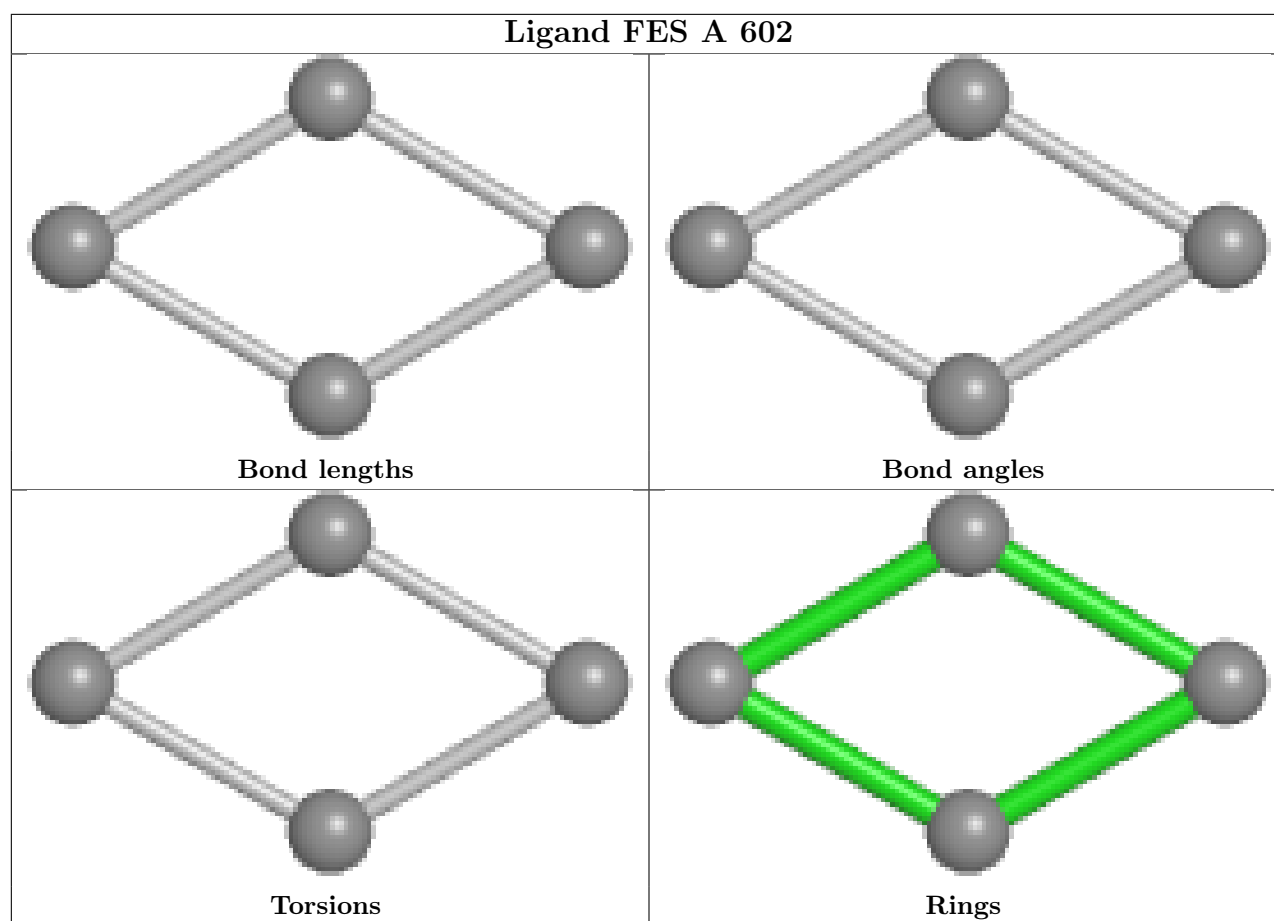












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/439 (92%)	-0.17	0 <span>100</span> <span>100</span>	18, 35, 66, 108	0
1	B	425/439 (96%)	-0.09	5 (1%) <span>79</span> <span>60</span>	17, 36, 85, 134	0
1	C	407/439 (92%)	-0.09	8 (1%) <span>65</span> <span>43</span>	20, 36, 91, 186	0
1	D	404/439 (92%)	-0.12	1 (0%) <span>95</span> <span>89</span>	19, 38, 75, 115	0
1	E	407/439 (92%)	0.17	32 (7%) <span>12</span> <span>4</span>	18, 39, 116, 142	0
1	F	406/439 (92%)	0.05	12 (2%) <span>50</span> <span>26</span>	22, 41, 95, 132	0
All	All	2454/2634 (93%)	-0.04	58 (2%) <span>59</span> <span>35</span>	17, 37, 93, 186	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	SER	6.0
1	C	114	MET	5.4
1	E	399	THR	5.3
1	B	202	ASP	5.3
1	E	401	CYS	4.3
1	E	395	ALA	4.2
1	E	400	VAL	3.9
1	E	416	TYR	3.5
1	E	415	THR	3.3
1	E	207	ARG	3.2
1	E	398	PRO	3.1
1	E	411	THR	3.1
1	F	234	LEU	3.1
1	F	208	PRO	3.1
1	F	230	LEU	3.0
1	E	413	TRP	2.9
1	E	234	LEU	2.9
1	E	412	ASP	2.9
1	E	237	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	154	ALA	2.9
1	C	113	GLY	2.9
1	F	385	GLY	2.9
1	B	110	ALA	2.9
1	E	406	ILE	2.8
1	E	417	ASP	2.8
1	F	396	ALA	2.7
1	C	111	ALA	2.7
1	E	236	ASN	2.6
1	B	201	THR	2.6
1	E	213	ALA	2.6
1	F	214	PRO	2.6
1	E	240	ASN	2.6
1	F	237	ALA	2.5
1	E	414	ARG	2.5
1	B	111	ALA	2.5
1	F	154	ALA	2.4
1	E	397	THR	2.4
1	E	235	SER	2.4
1	B	203	LYS	2.4
1	E	396	ALA	2.4
1	E	228	ALA	2.3
1	E	419	HIS	2.3
1	C	109	PRO	2.3
1	F	235	SER	2.3
1	E	230	LEU	2.3
1	E	407	VAL	2.3
1	C	238	ALA	2.2
1	E	229	ALA	2.2
1	C	115	VAL	2.2
1	E	208	PRO	2.2
1	E	215	ARG	2.2
1	E	238	ALA	2.1
1	E	113	GLY	2.1
1	C	107	SER	2.1
1	E	410	THR	2.0
1	F	209	SER	2.0
1	F	410	THR	2.0
1	F	212	LYS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

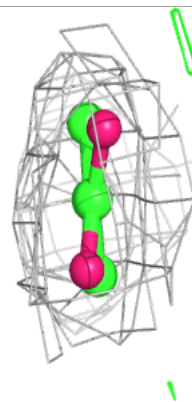
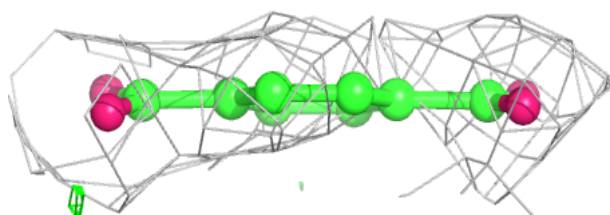
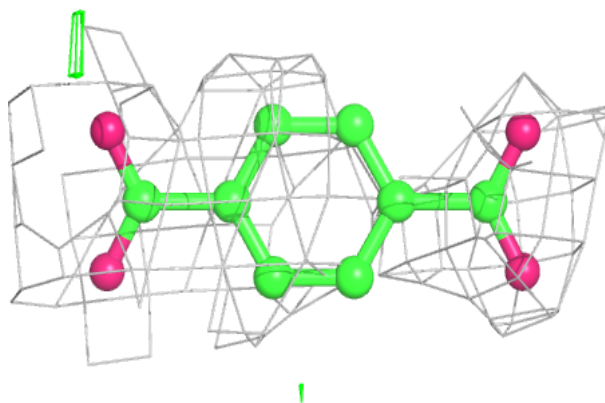
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	UB7	B	503	12/12	0.87	0.31	61,75,89,89	0
2	FE2	D	501	1/1	0.97	0.09	25,25,25,25	0
2	FE2	B	501	1/1	0.98	0.13	29,29,29,29	0
2	FE2	F	501	1/1	0.98	0.09	26,26,26,26	0
3	FES	E	502	4/4	0.98	0.14	20,21,24,25	0
2	FE2	C	501	1/1	0.98	0.12	24,24,24,24	0
3	FES	A	602	4/4	0.99	0.12	28,34,34,38	0
3	FES	B	502	4/4	0.99	0.12	26,28,30,32	0
3	FES	C	502	4/4	0.99	0.12	36,38,38,39	0
3	FES	D	502	4/4	0.99	0.13	32,34,37,37	0
2	FE2	E	501	1/1	0.99	0.13	23,23,23,23	0
3	FES	F	502	4/4	0.99	0.12	31,32,35,36	0
2	FE2	A	601	1/1	0.99	0.11	16,16,16,16	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.

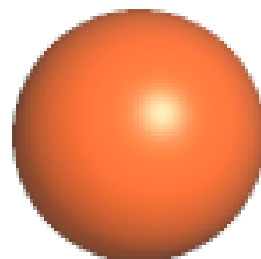
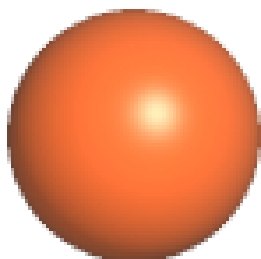
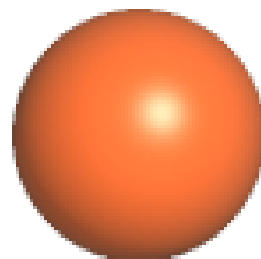
**Electron density around UB7 B 503:**

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



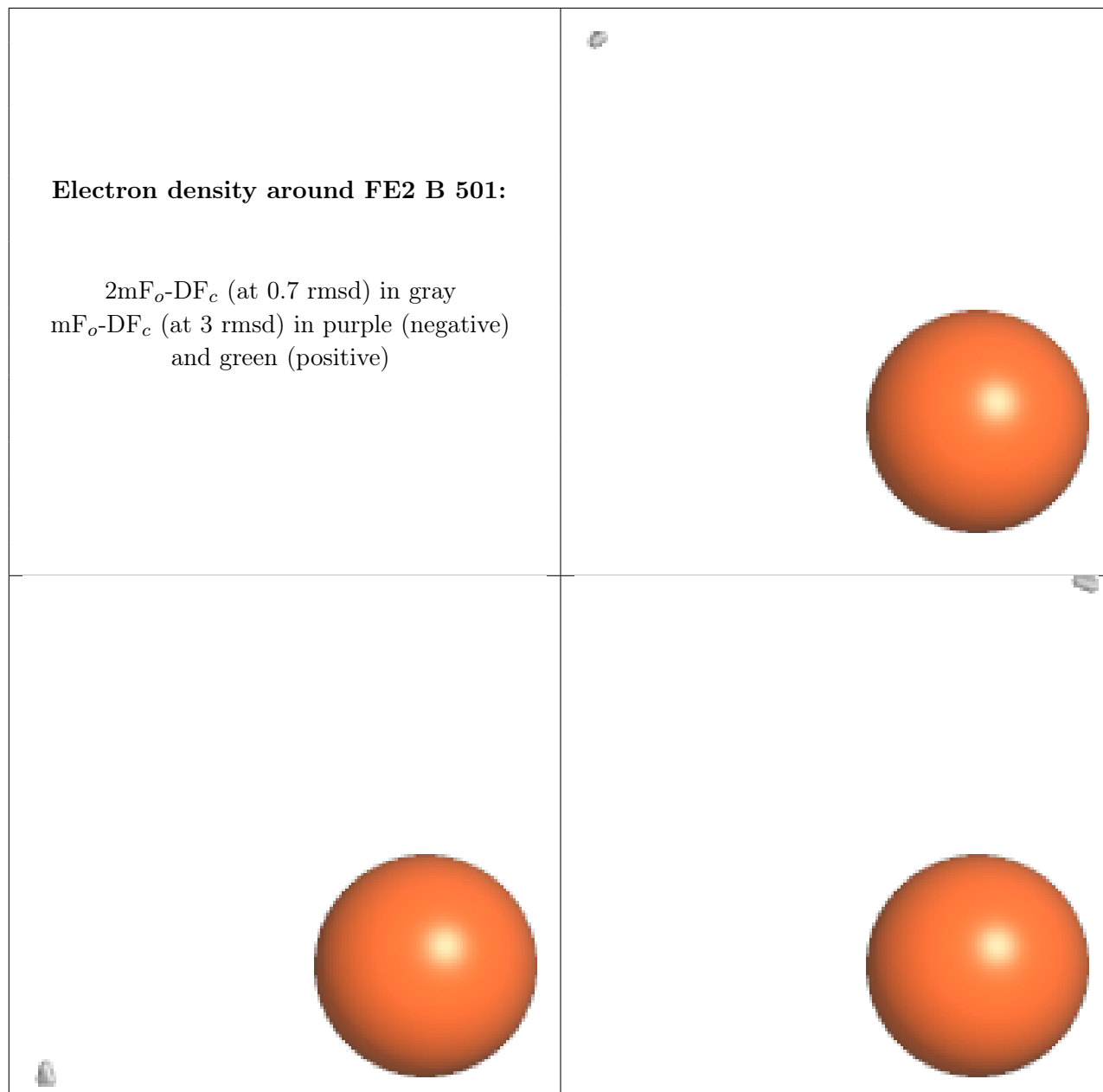
**Electron density around FE2 D 501:**

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



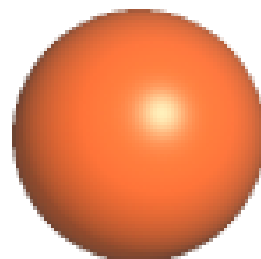
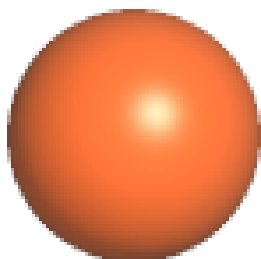
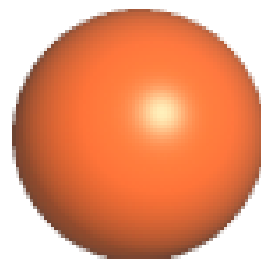
**Electron density around FE2 B 501:**

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



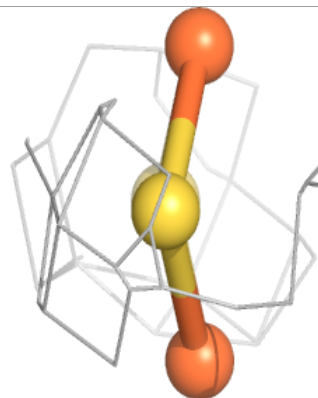
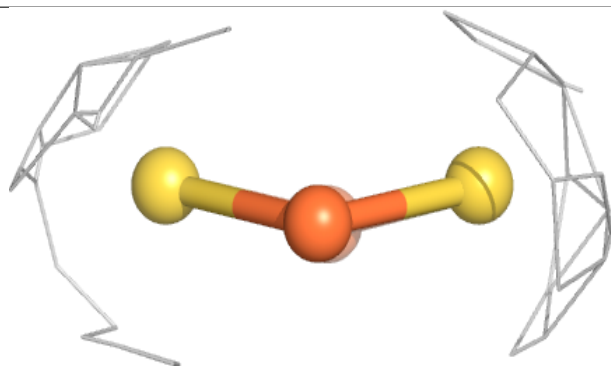
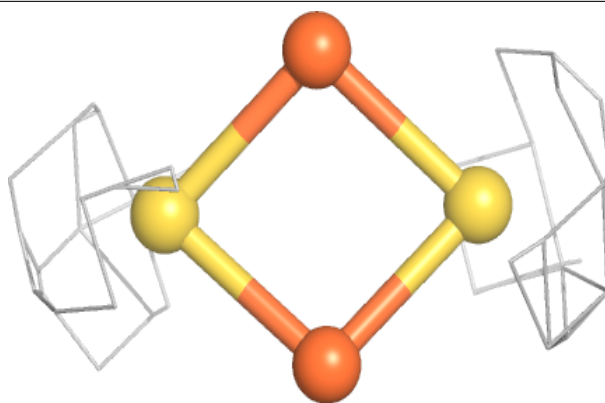
**Electron density around FE2 F 501:**

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



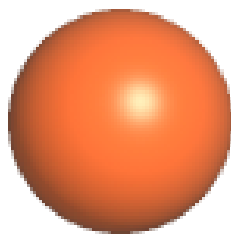
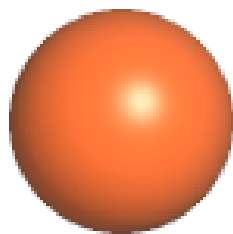
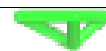
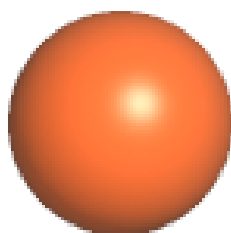
**Electron density around FES E 502:**

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



**Electron density around FE2 C 501:**

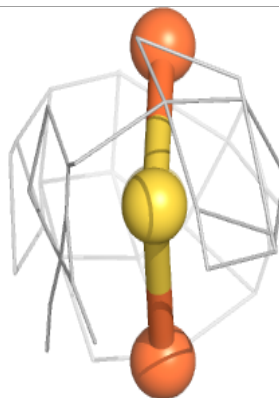
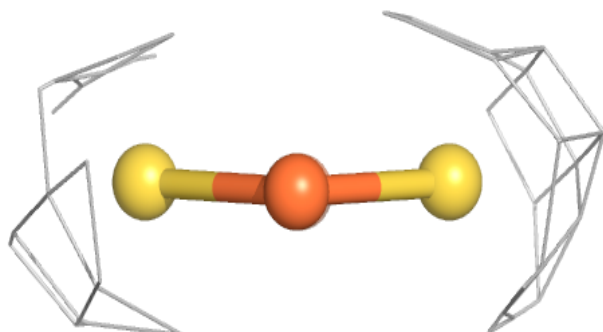
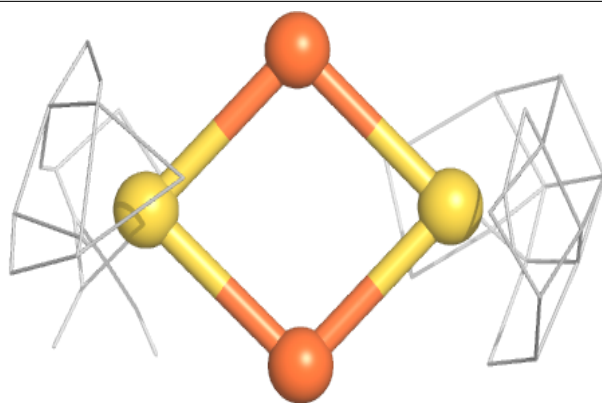
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



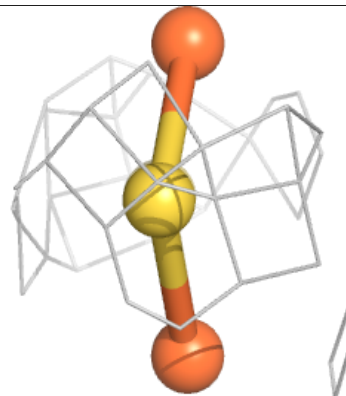
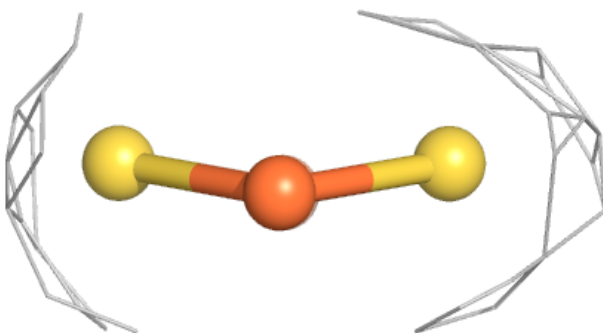
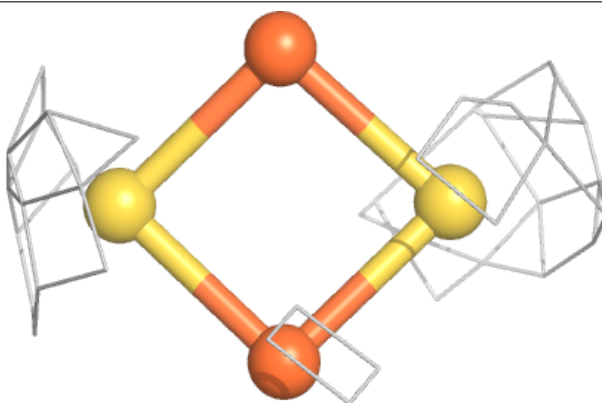


**Electron density around FES A 602:**

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and green (positive)

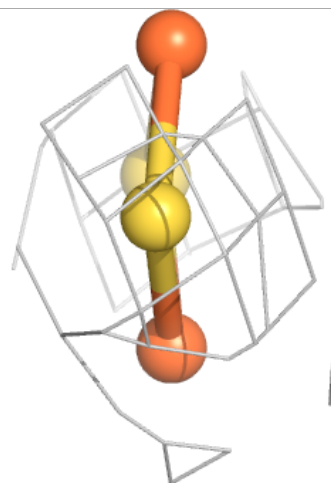
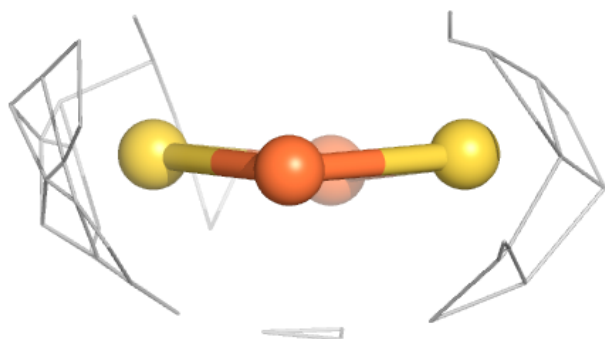
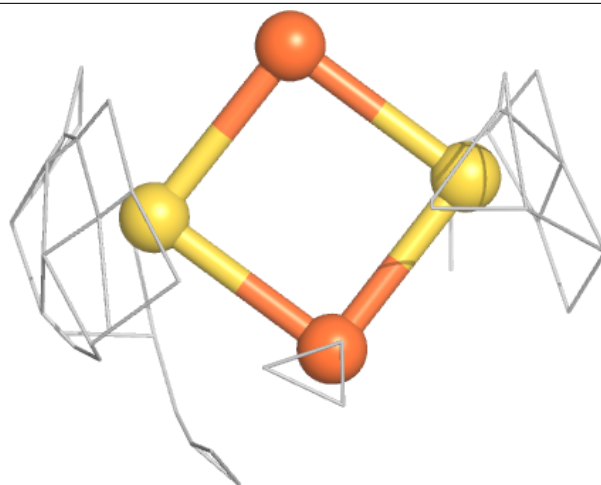
**Electron density around FES B 502:**

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



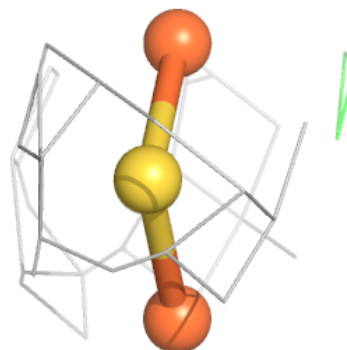
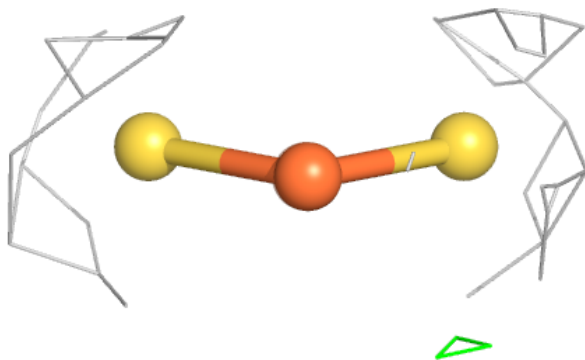
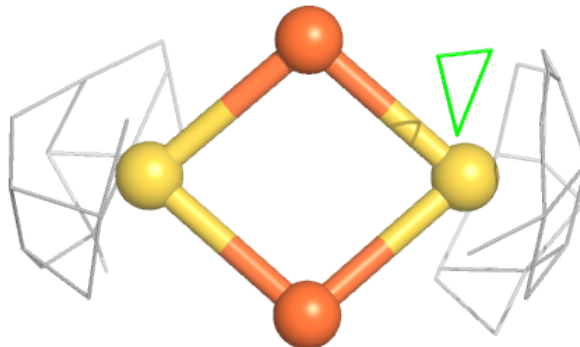
**Electron density around FES C 502:**

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and green (positive)



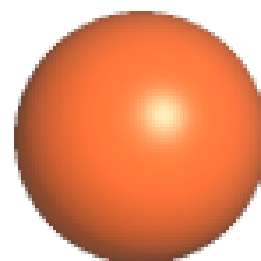
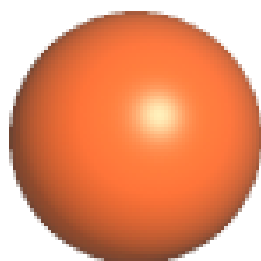
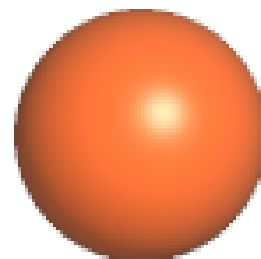
**Electron density around FES D 502:**

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



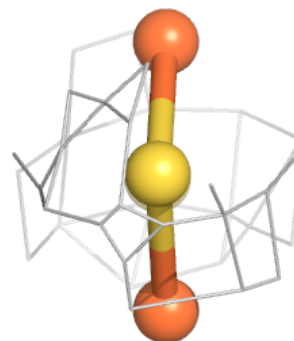
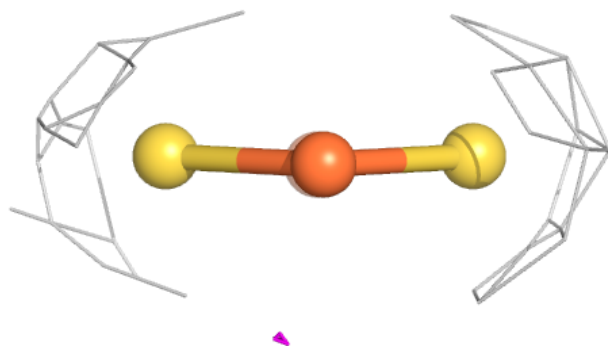
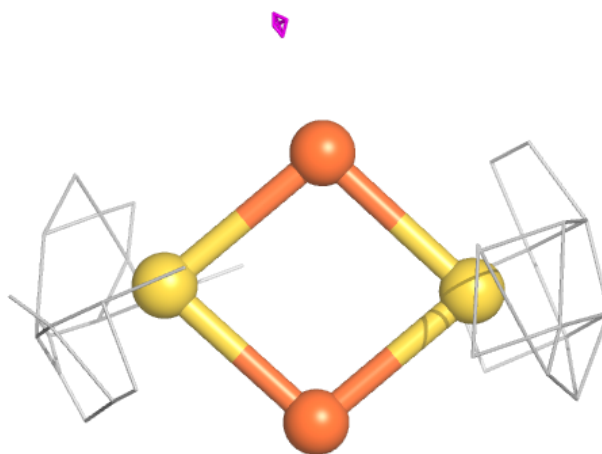
**Electron density around FE2 E 501:**

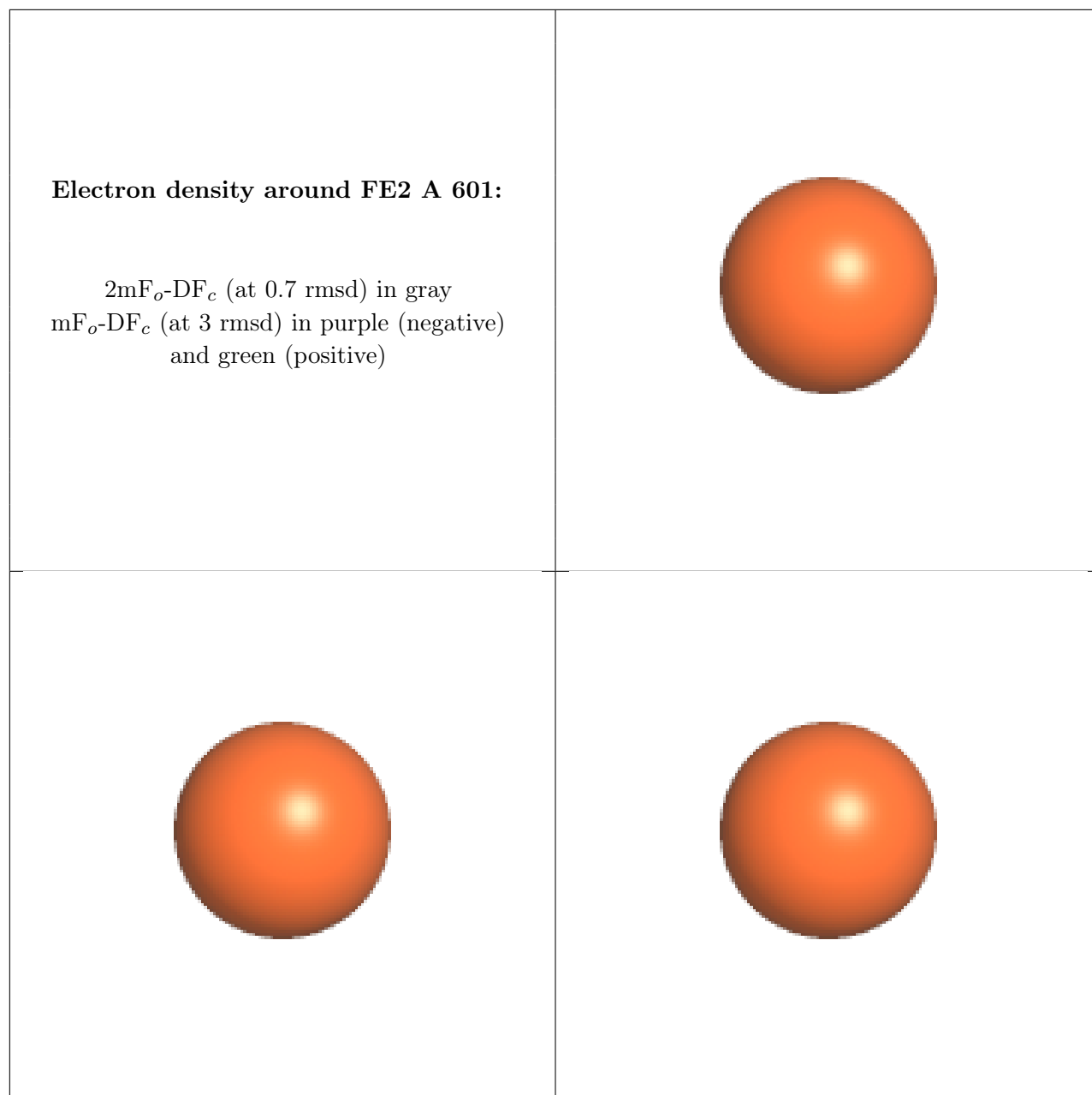
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FES 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.