Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2026 – 09:30 pm BST

PDB ID	:	6GM2 / pdb_00006gm2
Title	:	[FeFe]-hydrogenase CpI from Clostridium pasteurianum, variant E282D
Authors	:	Duan, J.; Esselborn, J.; Hofmann, E.; Winkler, M.; Happe, T.
Deposited on	:	2018-05-24
Resolution	:	2.76 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 (i) 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 (i)) were used in the production of this report:

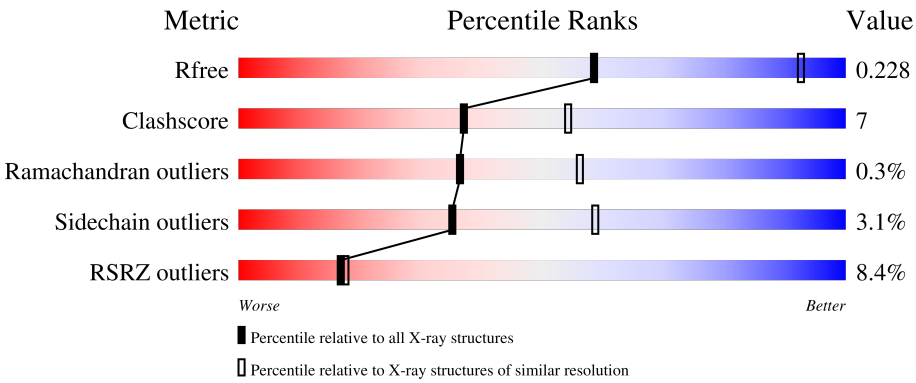
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 <=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	584	9% 80% 18% ••
1	B	584	7% 80% 16% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9117 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.

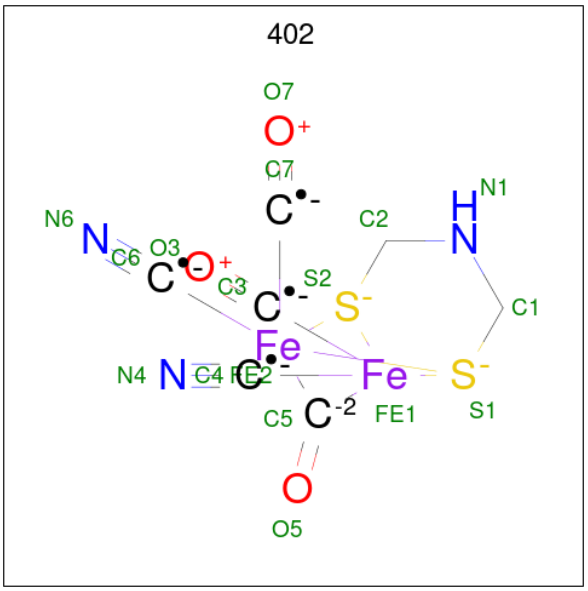
- Molecule 1 is a protein called Iron hydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	4492	2815	774	864	39	0	0	0
1	B	572	4442	2783	764	856	39	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

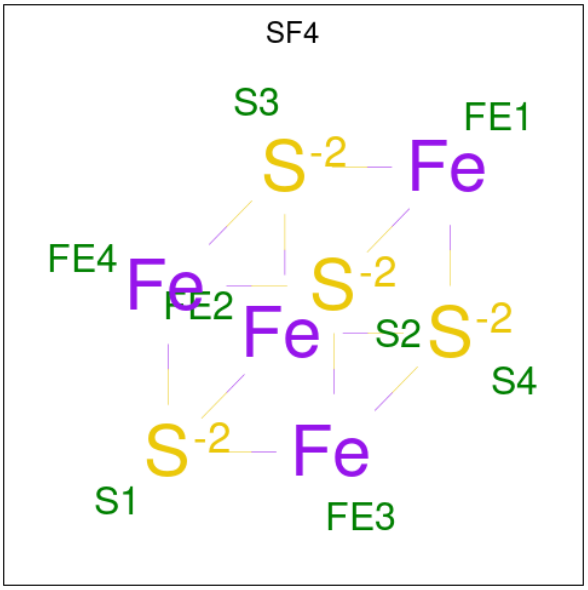
Chain	Residue	Modelled	Actual	Comment	Reference
A	282	ASP	GLU	engineered mutation	UNP P29166
A	575	SER	-	expression tag	UNP P29166
A	576	ALA	-	expression tag	UNP P29166
A	577	TRP	-	expression tag	UNP P29166
A	578	SER	-	expression tag	UNP P29166
A	579	HIS	-	expression tag	UNP P29166
A	580	PRO	-	expression tag	UNP P29166
A	581	GLN	-	expression tag	UNP P29166
A	582	PHE	-	expression tag	UNP P29166
A	583	GLU	-	expression tag	UNP P29166
A	584	LYS	-	expression tag	UNP P29166
B	282	ASP	GLU	engineered mutation	UNP P29166
B	575	SER	-	expression tag	UNP P29166
B	576	ALA	-	expression tag	UNP P29166
B	577	TRP	-	expression tag	UNP P29166
B	578	SER	-	expression tag	UNP P29166
B	579	HIS	-	expression tag	UNP P29166
B	580	PRO	-	expression tag	UNP P29166
B	581	GLN	-	expression tag	UNP P29166
B	582	PHE	-	expression tag	UNP P29166
B	583	GLU	-	expression tag	UNP P29166
B	584	LYS	-	expression tag	UNP P29166

- Molecule 2 is dicarbonyl[bis(cyanide-kappaC)]-mu-(iminodimethanethiolatato-1kappaS:2kappaS)-mu-(oxomethylidene)diiron(2+) (CCD ID: 402) (formula: $C_7H_5Fe_2N_3O_3S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	N	O	S		
2	A	1	17	7	2	3	3	2	0	0
2	B	1	17	7	2	3	3	2	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



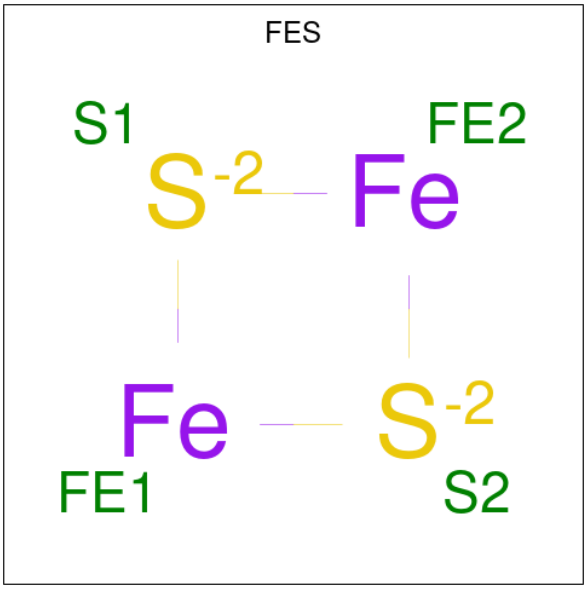
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0
3	A	1	8	4	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	B	1	Total Fe S 4 2 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is water.

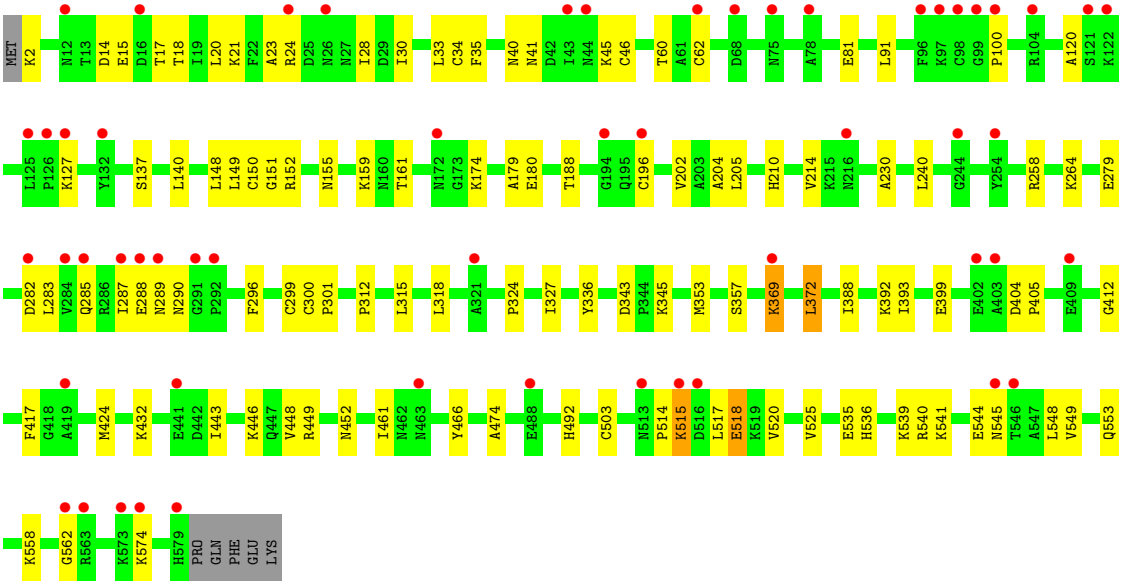
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	38	38	38	0	0
			Total	O		
6	B	38	38	38	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

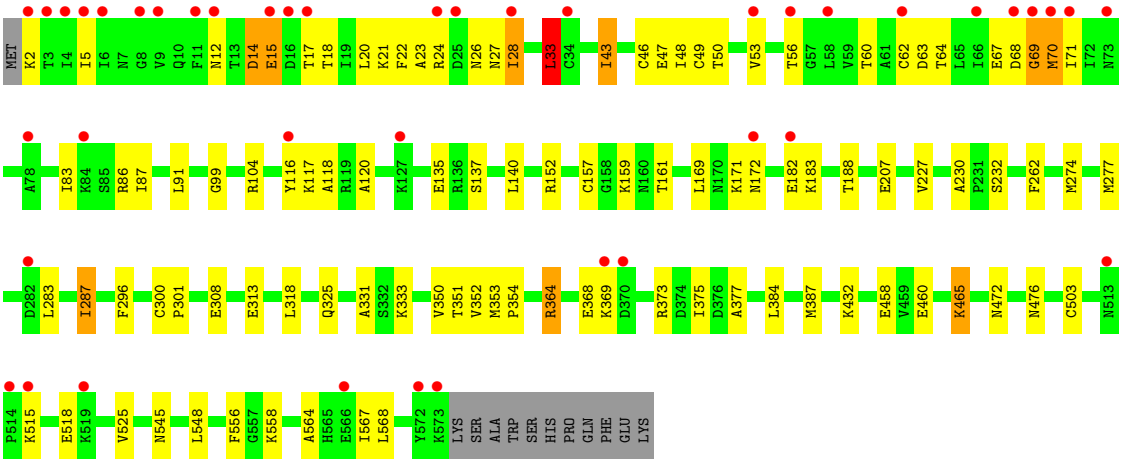
• Molecule 1: Iron hydrogenase 1

Chain A:



• Molecule 1: Iron hydrogenase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.87Å 72.82Å 102.91Å 90.00° 96.86° 90.00°	Depositor
Resolution (Å)	47.88 – 2.76 47.88 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.88-2.76) 99.9 (47.88-2.76)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.276 0.229 , 0.228	Depositor DCC
R_{free} test set	1704 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9117	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 402, SF4, FES, MG

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	0.31	0/4568	0.76	3/6153 (0.0%)
1	B	0.32	0/4515	0.77	3/6081 (0.0%)
All	All	0.32	0/9083	0.76	6/12234 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	GLY	N-CA-C	-10.26	102.48	114.69
1	A	289	ASN	N-CA-C	-8.30	103.28	113.41
1	B	364	ARG	CA-C-N	5.24	124.69	119.24
1	B	364	ARG	C-N-CA	5.24	124.69	119.24
1	A	558	LYS	CA-C-N	5.23	125.21	120.03
1	A	558	LYS	C-N-CA	5.23	125.21	120.03

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	4492	0	4449	68	0
1	B	4442	0	4402	60	0
2	A	17	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	17	0	5	1	0
3	A	32	0	0	2	0
3	B	32	0	0	0	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
5	B	1	0	0	0	0
6	A	38	0	0	1	0
6	B	38	0	0	0	0
All	All	9117	0	8861	127	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 7.

All (127) 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:47:GLU:HA	4:B:606:FES:S1	2.22	0.80
1:A:518:GLU:H	1:A:518:GLU:CD	1.90	0.79
1:A:312:PRO:HB2	1:A:574:LYS:HG3	1.65	0.79
1:B:432:LYS:NZ	1:B:460:GLU:O	2.16	0.78
1:A:20:LEU:HD11	1:A:24:ARG:CZ	2.22	0.70
1:B:2:LYS:HE3	1:B:12:ASN:HD21	1.58	0.68
1:A:24:ARG:NH2	1:A:30:ILE:O	2.27	0.67
1:B:67:GLU:HB2	1:B:70:MET:HG3	1.77	0.65
1:A:40:ASN:OD1	6:A:701:HOH:O	2.15	0.63
1:B:33:LEU:O	1:B:152:ARG:HD2	1.98	0.63
1:A:287:ILE:O	1:A:290:ASN:N	2.30	0.63
1:B:15:GLU:OE1	1:B:17:THR:OG1	2.17	0.62
1:B:47:GLU:O	1:B:50:THR:OG1	2.16	0.61
1:A:345:LYS:HA	1:A:372:LEU:HD11	1.84	0.58
1:A:24:ARG:CZ	1:A:515:LYS:HE2	2.33	0.57
1:A:279:GLU:HA	1:A:282:ASP:OD1	2.04	0.57
1:B:60:THR:OG1	1:B:63:ASP:OD1	2.23	0.56
1:B:556:PHE:HE1	1:B:567:ILE:HD11	1.70	0.56
1:A:539:LYS:HD2	1:A:544:GLU:HB3	1.87	0.55
1:B:67:GLU:H	1:B:70:MET:HE2	1.72	0.55
1:B:53:VAL:HG23	1:B:56:THR:HB	1.89	0.55
1:A:503:CYS:CB	2:A:600:402:C4	2.86	0.54
1:B:183:LYS:HE3	1:B:188:THR:HG22	1.89	0.53
1:B:99:GLY:O	1:B:104:ARG:NH1	2.42	0.53
1:A:343:ASP:OD1	1:A:345:LYS:HG3	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:HG22	1:B:377:ALA:HB3	1.92	0.52
1:A:515:LYS:HA	1:A:518:GLU:OE2	2.11	0.51
1:B:169:LEU:HD13	1:B:182:GLU:HG2	1.93	0.51
1:B:20:LEU:O	1:B:24:ARG:HG3	2.11	0.51
1:B:503:CYS:CB	2:B:601:402:C4	2.89	0.51
1:B:17:THR:HG22	1:B:18:THR:O	2.10	0.51
1:A:2:LYS:NZ	1:A:15:GLU:O	2.44	0.51
1:B:91:LEU:HB3	1:B:120:ALA:HB2	1.92	0.51
1:A:196:CYS:HB3	1:A:205:LEU:HD13	1.93	0.51
1:A:91:LEU:HB3	1:A:120:ALA:HB2	1.92	0.51
1:B:2:LYS:HD2	1:B:14:ASP:OD1	2.11	0.50
1:A:282:ASP:HA	1:A:285:GLN:CG	2.41	0.50
1:A:150:CYS:N	3:A:603:SF4:S1	2.83	0.50
1:A:443:ILE:HG21	1:A:541:LYS:HE2	1.93	0.50
1:A:34:CYS:SG	1:A:41:ASN:N	2.77	0.50
1:B:352:VAL:HG21	1:B:384:LEU:HD22	1.92	0.50
1:A:23:ALA:HB1	1:A:28:ILE:HB	1.93	0.50
1:A:432:LYS:HA	1:A:461:ILE:HG23	1.94	0.50
1:A:151:GLY:O	1:A:155:ASN:ND2	2.44	0.49
1:A:33:LEU:HD21	1:A:148:LEU:HD13	1.93	0.49
1:B:325:GLN:HG2	1:B:375:ILE:HG13	1.95	0.49
1:B:5:ILE:HB	1:B:71:ILE:HG23	1.94	0.49
1:A:520:VAL:HG13	1:A:525:VAL:HG21	1.95	0.48
1:A:535:GLU:HG3	1:A:536:HIS:CD2	2.48	0.48
1:B:515:LYS:O	1:B:518:GLU:HG2	2.13	0.48
1:A:258:ARG:NH2	1:A:404:ASP:OD1	2.45	0.48
1:A:301:PRO:HG2	1:A:357:SER:HB3	1.96	0.48
1:B:230:ALA:HB2	1:B:353:MET:SD	2.53	0.48
1:B:283:LEU:O	1:B:287:ILE:HG23	2.12	0.48
1:A:230:ALA:HB2	1:A:353:MET:SD	2.54	0.48
1:B:116:TYR:O	1:B:118:ALA:N	2.47	0.48
1:A:549:VAL:O	1:A:553:GLN:HG3	2.15	0.47
1:A:517:LEU:N	1:A:518:GLU:OE2	2.48	0.47
1:B:325:GLN:HG3	1:B:351:THR:HG21	1.96	0.47
1:A:34:CYS:HB2	1:A:46:CYS:SG	2.52	0.47
1:B:277:MET:HG3	1:B:548:LEU:HD21	1.97	0.47
1:A:369:LYS:HD2	1:A:369:LYS:HA	1.55	0.47
1:A:17:THR:OG1	1:A:18:THR:N	2.46	0.47
1:A:518:GLU:CD	1:A:518:GLU:N	2.67	0.47
1:B:17:THR:HG23	1:B:21:LYS:HB3	1.96	0.46
1:B:68:ASP:OD1	1:B:69:GLY:N	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLU:OE1	1:B:373:ARG:NH1	2.44	0.46
1:A:264:LYS:HG3	1:A:336:TYR:OH	2.16	0.46
1:B:22:PHE:O	1:B:26:ASN:ND2	2.47	0.46
1:B:83:ILE:O	1:B:87:ILE:HG13	2.15	0.46
1:B:23:ALA:HB1	1:B:28:ILE:HG22	1.97	0.46
1:B:545:ASN:HB3	1:B:548:LEU:HB3	1.98	0.46
1:B:68:ASP:C	1:B:70:MET:H	2.23	0.45
1:A:545:ASN:HB3	1:A:548:LEU:HB3	1.98	0.45
1:B:333:LYS:NZ	1:B:373:ARG:O	2.43	0.45
1:A:210:HIS:O	1:A:214:VAL:HG23	2.17	0.44
1:B:308:GLU:OE2	1:B:364:ARG:NH2	2.48	0.44
1:A:388:ILE:HG23	1:A:393:ILE:HB	1.99	0.44
1:B:232:SER:HB2	1:B:354:PRO:HG3	1.99	0.44
1:B:171:LYS:O	1:B:172:ASN:HB3	2.18	0.44
1:A:424:MET:HG2	1:A:448:VAL:HG11	1.99	0.43
1:A:466:TYR:HD2	1:A:492:HIS:ND1	2.15	0.43
1:B:49:CYS:SG	1:B:62:CYS:N	2.88	0.43
1:A:45:LYS:HE2	1:A:60:THR:HG21	2.01	0.43
1:A:127:LYS:HE2	1:A:127:LYS:HB2	1.86	0.43
1:A:515:LYS:HA	1:A:518:GLU:CD	2.44	0.43
1:B:43:ILE:H	1:B:43:ILE:HG12	1.57	0.43
1:B:86:ARG:HD3	1:B:86:ARG:HA	1.74	0.43
1:B:227:VAL:HB	1:B:262:PHE:CD1	2.54	0.43
1:A:137:SER:HB3	1:A:140:LEU:O	2.18	0.43
1:B:83:ILE:O	1:B:86:ARG:HB2	2.19	0.43
1:A:35:PHE:HB2	1:A:62:CYS:SG	2.59	0.43
1:A:324:PRO:HA	1:A:327:ILE:HG22	2.01	0.42
1:B:207:GLU:OE1	1:B:207:GLU:N	2.49	0.42
1:A:404:ASP:HA	1:A:405:PRO:HD3	1.76	0.42
1:A:296:PHE:HB2	1:A:318:LEU:HD23	2.00	0.42
1:A:283:LEU:O	1:A:287:ILE:HG13	2.19	0.42
1:A:417:PHE:HB3	2:A:600:402:S1	2.60	0.42
1:A:14:ASP:OD1	1:A:14:ASP:N	2.53	0.42
1:A:34:CYS:SG	1:A:40:ASN:HB2	2.59	0.42
1:A:301:PRO:HD2	3:A:601:SF4:S2	2.60	0.42
1:A:202:VAL:HG23	1:A:204:ALA:H	1.84	0.42
1:A:503:CYS:HB2	2:A:600:402:C4	2.48	0.42
1:A:150:CYS:SG	1:A:152:ARG:HD3	2.60	0.41
1:A:514:PRO:HA	1:A:517:LEU:HD12	2.01	0.41
1:B:387:MET:HE3	1:B:387:MET:HB2	1.93	0.41
1:B:564:ALA:O	1:B:568:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PRO:HA	1:A:315:LEU:HG	2.01	0.41
1:A:412:GLY:H	1:A:540:ARG:HA	1.86	0.41
1:B:157:CYS:O	1:B:161:THR:OG1	2.34	0.41
1:A:179:ALA:HB1	1:A:188:THR:HG21	2.02	0.41
1:B:458:GLU:HG2	1:B:465:LYS:HG2	2.02	0.41
1:A:299:CYS:C	2:A:600:402:H8	2.46	0.41
1:B:296:PHE:HB2	1:B:318:LEU:HD12	2.03	0.41
1:A:446:LYS:HG3	1:A:449:ARG:HD2	2.02	0.41
1:A:161:THR:HA	1:A:474:ALA:HB3	2.03	0.41
1:B:33:LEU:HD13	1:B:46:CYS:SG	2.61	0.41
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.89	0.40
1:B:137:SER:HB3	1:B:140:LEU:O	2.22	0.40
1:B:472:ASN:O	1:B:476:ASN:ND2	2.47	0.40
1:B:300:CYS:HA	1:B:301:PRO:HD2	1.89	0.40
1:B:274:MET:HE1	1:B:331:ALA:HB2	2.04	0.40
1:A:45:LYS:HB3	4:A:605:FES:S1	2.62	0.40
1:A:300:CYS:HA	1:A:301:PRO:HD2	1.92	0.40
1:A:452:ASN:ND2	1:B:63:ASP:OD2	2.54	0.40
1:B:230:ALA:HB3	1:B:354:PRO:HD3	2.03	0.40
1:B:277:MET:HE3	1:B:277:MET:HB3	2.00	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	576/584 (99%)	541 (94%)	33 (6%)	2 (0%)	36	56
1	B	570/584 (98%)	536 (94%)	32 (6%)	2 (0%)	30	50
All	All	1146/1168 (98%)	1077 (94%)	65 (6%)	4 (0%)	36	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	562	GLY
1	B	117	LYS
1	B	33	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/499 (99%)	480 (97%)	13 (3%)	40	63
1	B	488/499 (98%)	471 (96%)	17 (4%)	32	56
All	All	981/998 (98%)	951 (97%)	30 (3%)	35	59

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	81	GLU
1	A	159	LYS
1	A	174	LYS
1	A	180	GLU
1	A	240	LEU
1	A	288	GLU
1	A	369	LYS
1	A	372	LEU
1	A	392	LYS
1	A	399	GLU
1	A	515	LYS
1	A	518	GLU
1	B	14	ASP
1	B	15	GLU
1	B	27	ASN
1	B	28	ILE
1	B	33	LEU
1	B	43	ILE
1	B	48	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	64	THR
1	B	70	MET
1	B	135	GLU
1	B	159	LYS
1	B	287	ILE
1	B	313	GLU
1	B	369	LYS
1	B	465	LYS
1	B	525	VAL
1	B	558	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	41	ASN
1	A	155	ASN
1	A	316	ASN
1	A	317	ASN
1	A	490	GLN
1	A	532	ASN
1	A	536	HIS
1	B	12	ASN
1	B	464	ASN
1	B	545	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	SF4	A	601	1	0,12,12	-	-	-		
3	SF4	B	604	1	0,12,12	-	-	-		
3	SF4	A	603	1	0,12,12	-	-	-		
4	FES	B	606	1	0,4,4	-	-	-		
2	402	A	600	1	13,19,19	2.48	7 (53%)	2,36,36	5.64	1 (50%)
4	FES	A	605	1	0,4,4	-	-	-		
3	SF4	B	605	1	0,12,12	-	-	-		
2	402	B	601	1	13,19,19	2.45	7 (53%)	2,36,36	6.25	1 (50%)
3	SF4	B	603	1	0,12,12	-	-	-		
3	SF4	A	602	1	0,12,12	-	-	-		
3	SF4	B	602	6,1	0,12,12	-	-	-		
3	SF4	A	604	1	0,12,12	-	-	-		

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	SF4	A	601	1	-	-	0/6/5/5
3	SF4	B	604	1	-	-	0/6/5/5
3	SF4	A	603	1	-	-	0/6/5/5
4	FES	B	606	1	-	-	0/1/1/1
2	402	A	600	1	-	-	0/5/3/3
4	FES	A	605	1	-	-	0/1/1/1
3	SF4	B	605	1	-	-	0/6/5/5
2	402	B	601	1	-	-	0/5/3/3
3	SF4	B	603	1	-	-	0/6/5/5
3	SF4	A	602	1	-	-	0/6/5/5
3	SF4	B	602	6,1	-	-	0/6/5/5
3	SF4	A	604	1	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	402	S1-FE2	4.61	2.32	2.26
2	A	600	402	S1-FE2	4.49	2.32	2.26
2	A	600	402	C4-N4	4.02	1.22	1.15
2	B	601	402	C4-N4	3.92	1.22	1.15
2	A	600	402	O3-C3	3.09	1.23	1.15
2	B	601	402	O3-C3	3.07	1.23	1.15
2	A	600	402	S2-FE1	3.03	2.30	2.26
2	B	601	402	S2-FE1	2.91	2.30	2.26
2	A	600	402	C2-S2	2.56	1.89	1.85
2	B	601	402	S2-FE2	2.53	2.29	2.26
2	A	600	402	S2-FE2	2.53	2.29	2.26
2	B	601	402	C2-S2	2.47	1.89	1.85
2	A	600	402	S1-FE1	2.19	2.29	2.26
2	B	601	402	S1-FE1	2.02	2.29	2.26

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	402	S2-C2-N1	-8.84	92.85	117.18
2	A	600	402	S2-C2-N1	-7.95	95.28	117.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

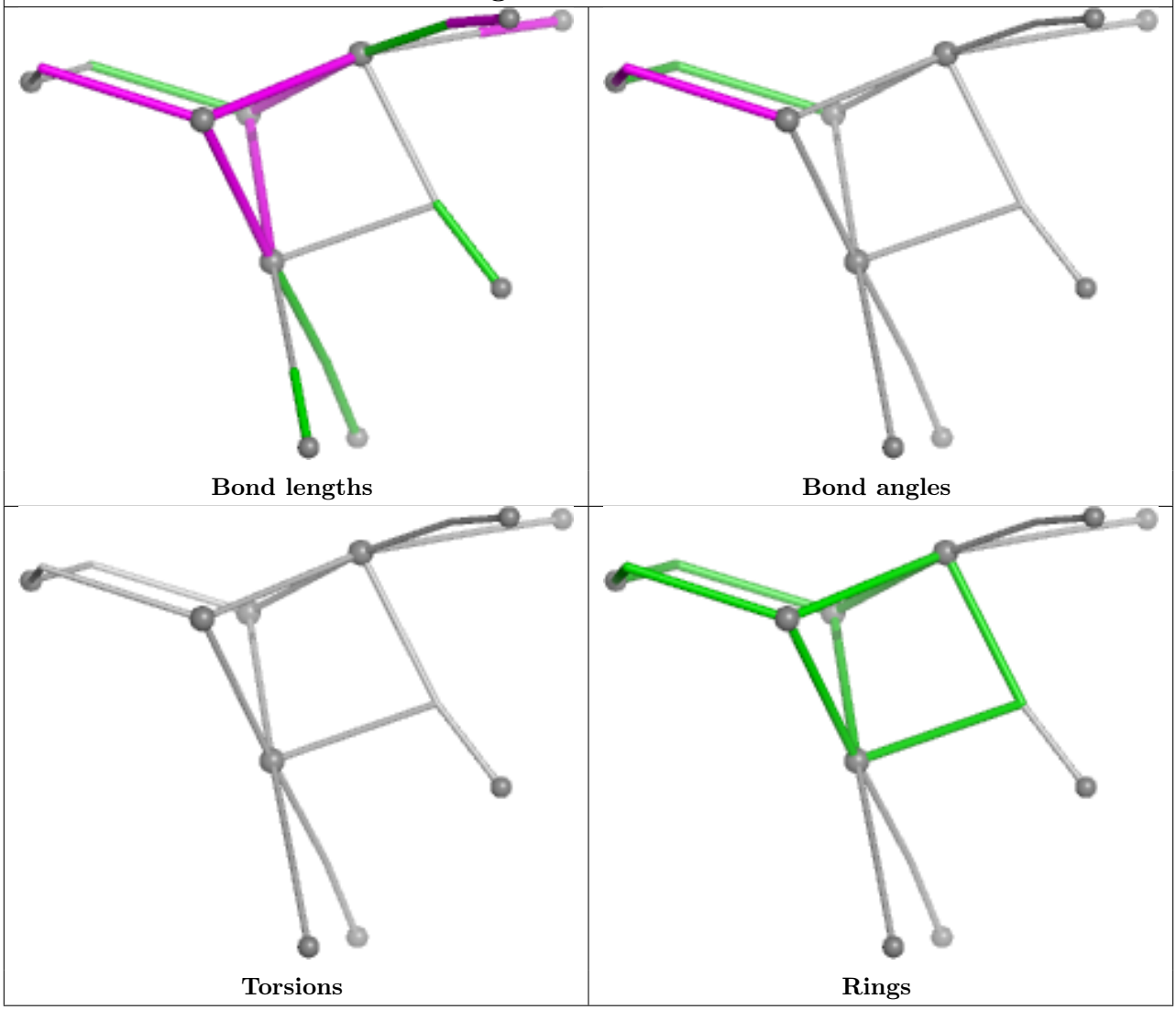
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SF4	1	0
3	A	603	SF4	1	0
4	B	606	FES	1	0
2	A	600	402	4	0
4	A	605	FES	1	0
2	B	601	402	1	0

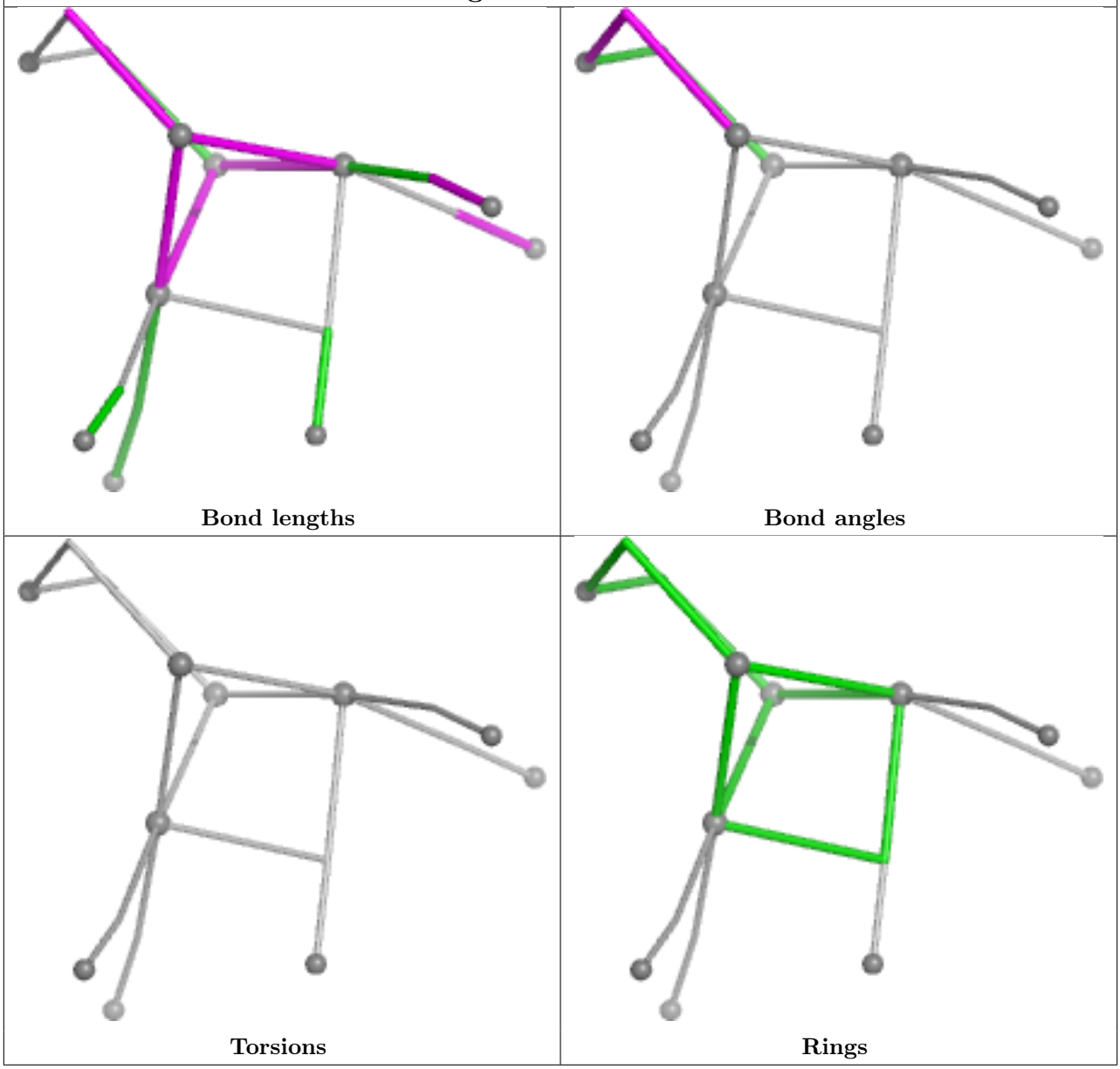
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 402 A 600



Ligand 402 B 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	578/584 (98%)	0.84	55 (9%)	14	13	20, 33, 53, 66	0
1	B	572/584 (97%)	0.51	42 (7%)	21	21	17, 29, 61, 83	0
All	All	1150/1168 (98%)	0.67	97 (8%)	17	17	17, 32, 55, 83	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	9.9
1	A	96	PHE	5.3
1	B	3	THR	4.6
1	A	100	PRO	4.0
1	A	403	ALA	3.9
1	B	2	LYS	3.8
1	B	8	GLY	3.7
1	B	172	ASN	3.6
1	A	488	GLU	3.5
1	A	44	ASN	3.4
1	B	16	ASP	3.4
1	A	126	PRO	3.3
1	A	409	GLU	3.3
1	B	6	ILE	3.2
1	B	572	TYR	3.2
1	B	11	PHE	3.1
1	A	574	LYS	3.1
1	B	71	ILE	3.1
1	B	9	VAL	3.0
1	A	402	GLU	3.0
1	A	573	LYS	3.0
1	A	285	GLN	2.9
1	A	62	CYS	2.9
1	B	514	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	127	LYS	2.8
1	B	15	GLU	2.8
1	B	116	TYR	2.8
1	A	98	CYS	2.8
1	B	127	LYS	2.8
1	A	172	ASN	2.7
1	A	244	GLY	2.7
1	B	513	ASN	2.7
1	A	515	LYS	2.7
1	A	441	GLU	2.7
1	A	196	CYS	2.7
1	B	69	GLY	2.7
1	A	288	GLU	2.6
1	A	369	LYS	2.6
1	B	73	ASN	2.6
1	A	287	ILE	2.6
1	B	182	GLU	2.6
1	B	12	ASN	2.6
1	A	97	LYS	2.5
1	B	369	LYS	2.5
1	A	291	GLY	2.5
1	A	12	ASN	2.5
1	A	545	ASN	2.5
1	B	4	ILE	2.5
1	A	122	LYS	2.5
1	B	58	LEU	2.5
1	A	419	ALA	2.5
1	B	515	LYS	2.4
1	A	104	ARG	2.4
1	B	5	ILE	2.4
1	A	43	ILE	2.4
1	B	62	CYS	2.4
1	B	70	MET	2.4
1	A	16	ASP	2.4
1	A	516	ASP	2.4
1	B	34	CYS	2.4
1	B	519	LYS	2.4
1	A	321	ALA	2.4
1	B	66	ILE	2.3
1	A	463	ASN	2.3
1	A	24	ARG	2.3
1	A	132	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	292	PRO	2.3
1	B	28	ILE	2.3
1	A	546	THR	2.3
1	B	84	LYS	2.3
1	A	289	ASN	2.3
1	A	78	ALA	2.2
1	B	566	GLU	2.2
1	B	17	THR	2.2
1	B	68	ASP	2.2
1	B	56	THR	2.2
1	B	24	ARG	2.2
1	A	282	ASP	2.2
1	A	75	ASN	2.2
1	B	573	LYS	2.2
1	B	370	ASP	2.2
1	A	121	SER	2.2
1	A	194	GLY	2.1
1	A	562	GLY	2.1
1	A	125	LEU	2.1
1	A	216	ASN	2.1
1	A	579	HIS	2.1
1	A	284	VAL	2.1
1	B	53	VAL	2.1
1	A	26	ASN	2.1
1	A	563	ARG	2.1
1	B	78	ALA	2.1
1	B	25	ASP	2.0
1	A	254	TYR	2.0
1	A	68	ASP	2.0
1	B	282	ASP	2.0
1	A	513	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

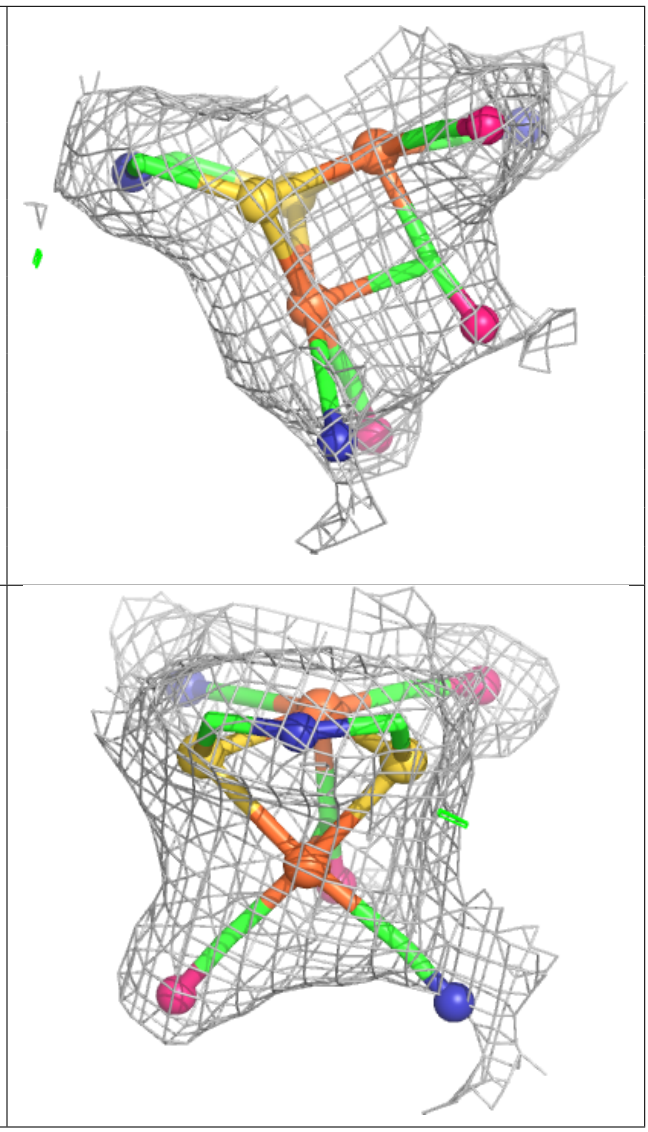
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FES	B	606	4/4	0.86	0.22	36,39,71,99	0
5	MG	B	607	1/1	0.95	0.07	26,26,26,26	0
3	SF4	A	603	8/8	0.98	0.04	20,22,25,26	0
3	SF4	A	604	8/8	0.98	0.05	28,37,41,42	0
3	SF4	B	602	8/8	0.98	0.04	14,17,20,21	0
2	402	A	600	17/17	0.98	0.07	20,26,31,32	0
2	402	B	601	17/17	0.98	0.07	21,23,26,27	0
3	SF4	B	603	8/8	0.99	0.02	13,17,19,20	0
3	SF4	B	604	8/8	0.99	0.04	16,20,22,22	0
3	SF4	B	605	8/8	0.99	0.04	25,28,32,32	0
4	FES	A	605	4/4	0.99	0.04	22,23,25,29	0
3	SF4	A	602	8/8	0.99	0.04	16,18,22,23	0
3	SF4	A	601	8/8	0.99	0.04	17,20,23,23	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.

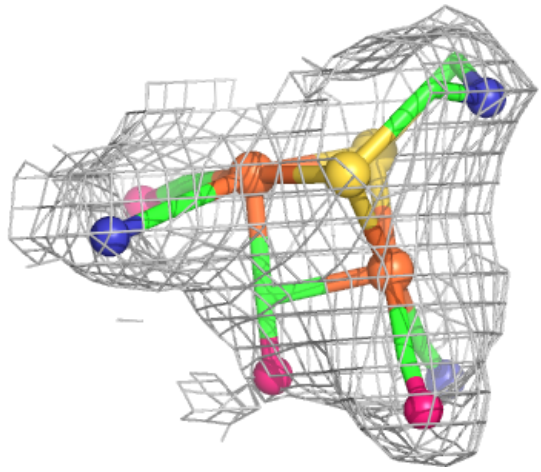
Electron density around 402 A 600:

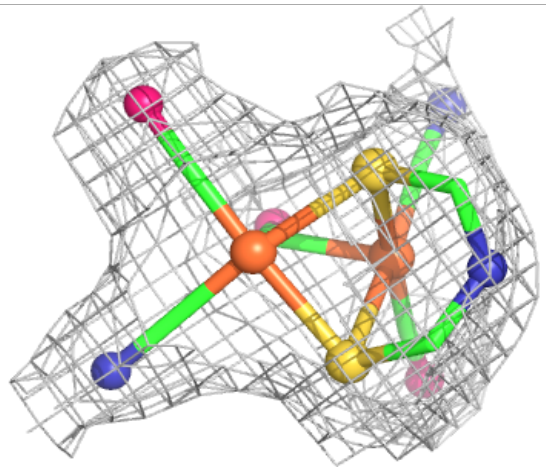
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

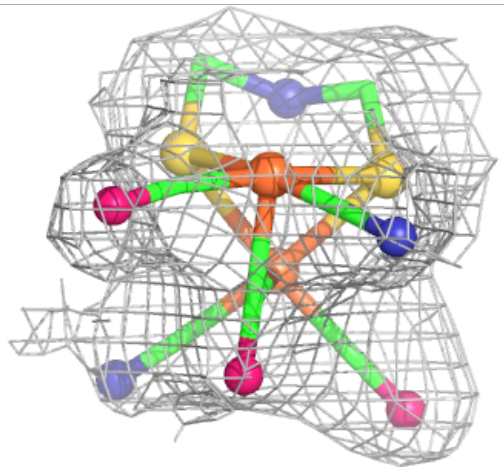


Electron density around 402 B 601:

$2mF_o$-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 (i)

There are no such residues in this entry.