



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 01:39 AM EDT

PDB ID : 8E3T / pdb_00008e3t
Title : Gallium-reconstituted nitrogenase MoFeP mutant S188A from *Azotobacter vinelandii* after IDS oxidation
Authors : Rutledge, H.L.; Tezcan, F.A.
Deposited on : 2022-08-17
Resolution : 2.20 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	:	9.0.015 (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

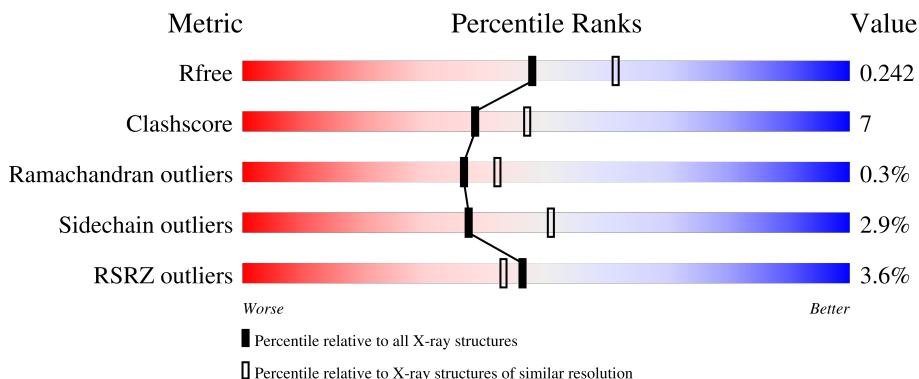
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	492	5% 76% 18% • •
1	C	492	6% 78% 15% • •
2	B	523	0% 89% 10% •
2	D	523	2% 87% 12% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32075 atoms, of which 15165 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C	H	N	O	S	0	0	0
			7281	2365	3563	634	695	24			
1	C	476	Total	C	H	N	O	S	0	0	0
			7266	2371	3536	637	698	24			

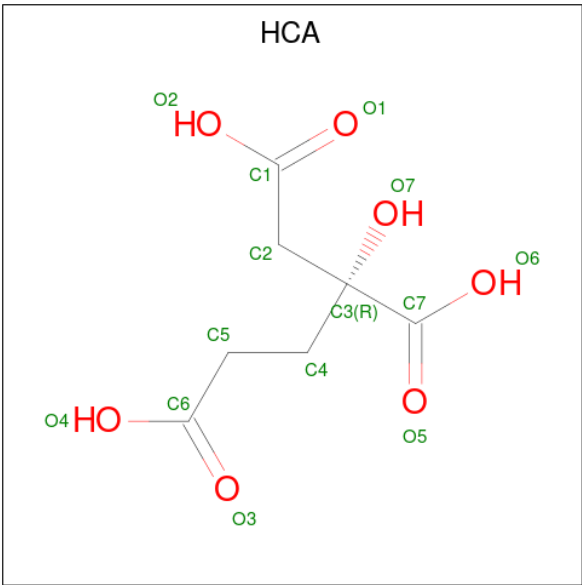
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	522	Total	C	H	N	O	S	0	0	0
			8162	2646	4017	697	774	28			
2	D	522	Total	C	H	N	O	S	0	0	0
			8186	2650	4037	701	770	28			

There are 2 discrepancies between the modelled and reference sequences:

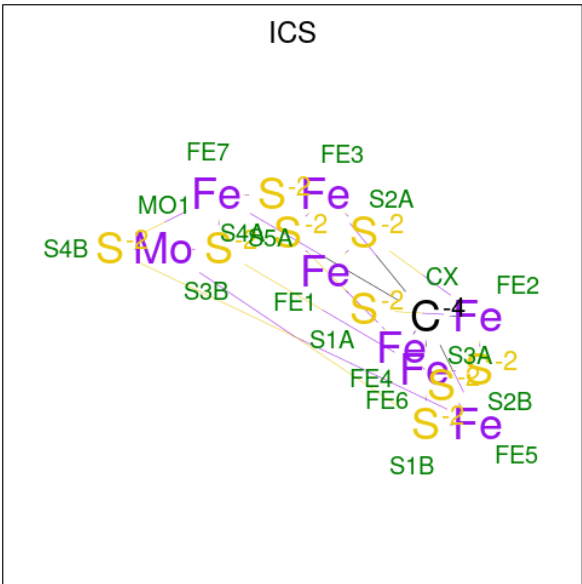
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	ALA	SER	engineered mutation	UNP C1DGZ8
D	188	ALA	SER	engineered mutation	UNP C1DGZ8

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	7	6	7		
3	C	1	Total	C	H	O	0	0
			20	7	6	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe₇MoS₉).



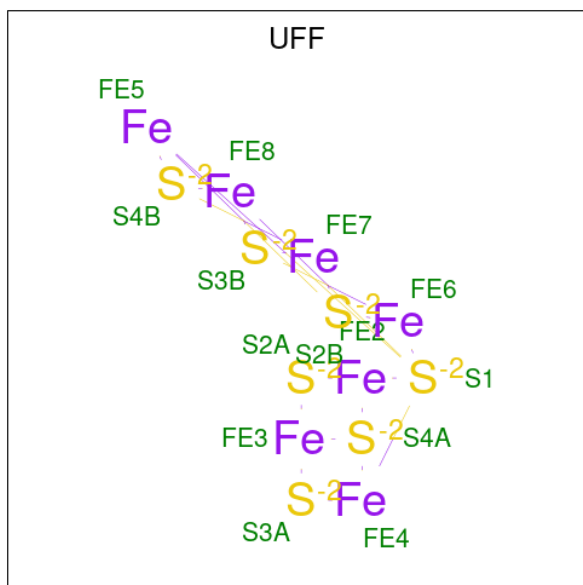
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	
							0	0

- Molecule 5 is FE(7)-S(7) CLUSTER (CCD ID: UFF) (formula: Fe_7S_7) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S		
			14	7	7	0	0
5	D	1	Total	Fe	S		
			14	7	7	0	0

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe		
			1	1	0	0
6	D	1	Total	Fe		
			1	1	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na		
			1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Na 1	0	0

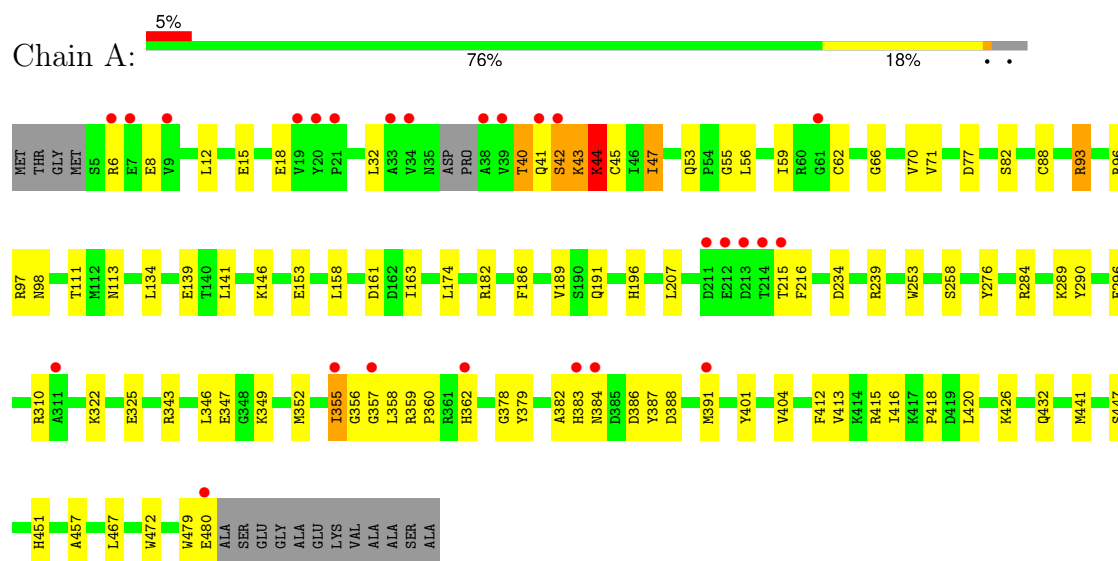
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	220	Total 220	O 220	0	0
8	B	343	Total 343	O 343	0	0
8	C	197	Total 197	O 197	0	0
8	D	312	Total 312	O 312	0	0

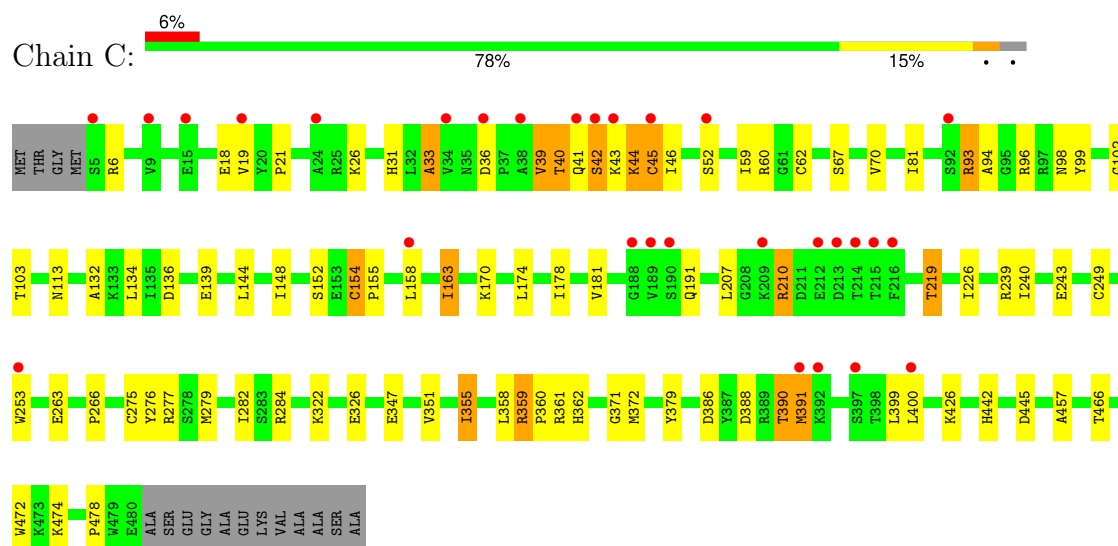
3 Residue-property plots

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

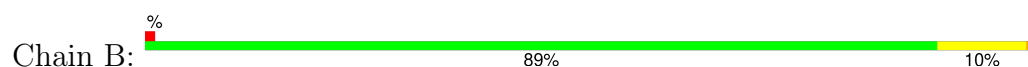
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

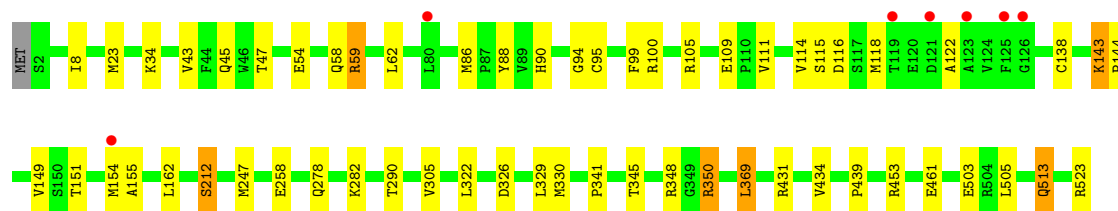


- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

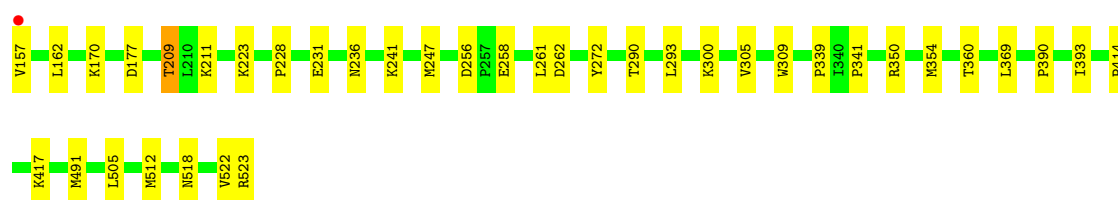
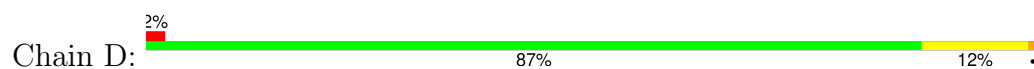


- Molecule 2: Nitrogenase molybdenum-iron protein beta chain





● Molecule 2: Nitrogenase molybdenum-iron protein beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.61Å 127.97Å 107.27Å 90.00° 108.85° 90.00°	Depositor
Resolution (Å)	54.13 – 2.20 54.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.9 (54.13-2.20) 87.9 (54.13-2.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.1-4122	Depositor
R, R_{free}	0.223 , 0.243 0.223 , 0.242	Depositor DCC
R_{free} test set	8684 reflections (8.76%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32075	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, UFF, ICS, NA, HCA

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	0.44	1/3804 (0.0%)	0.69	8/5137 (0.2%)
1	C	0.51	3/3818 (0.1%)	0.73	4/5161 (0.1%)
2	B	0.41	2/4251 (0.0%)	0.59	0/5755
2	D	0.38	3/4255 (0.1%)	0.53	0/5759
All	All	0.43	9/16128 (0.1%)	0.64	12/21812 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	ILE	C-O	-7.74	1.14	1.24
2	D	223	LYS	C-O	-7.33	1.14	1.23
2	D	108	ARG	C-O	-6.80	1.15	1.23
2	D	109	GLU	C-O	-6.19	1.17	1.24
1	C	33	ALA	C-O	-6.03	1.16	1.23
1	C	21	PRO	C-O	-5.54	1.17	1.23
2	B	109	GLU	C-O	-5.32	1.18	1.24
1	A	384	ASN	C-O	-5.22	1.17	1.24
2	B	143	LYS	C-O	-5.13	1.21	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	TRP	CA-C-N	6.61	133.59	121.70
1	A	253	TRP	C-N-CA	6.61	133.59	121.70
1	C	21	PRO	CA-C-O	-6.08	114.30	122.08
1	A	189	VAL	N-CA-C	-5.85	107.42	113.10
1	C	253	TRP	CA-C-N	5.79	132.12	121.70
1	C	253	TRP	C-N-CA	5.79	132.12	121.70
1	A	12	LEU	N-CA-C	-5.61	105.25	111.36
1	C	59	ILE	N-CA-C	-5.60	106.36	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	N-CA-C	-5.40	105.96	112.54
1	A	43	LYS	N-CA-C	-5.37	99.37	110.80
1	A	44	LYS	CA-C-N	-5.17	111.66	121.54
1	A	44	LYS	C-N-CA	-5.17	111.66	121.54

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	3718	3563	3605	78	0
1	C	3730	3536	3609	71	0
2	B	4145	4017	4015	38	0
2	D	4149	4037	4037	52	0
3	A	14	6	6	0	0
3	C	14	6	6	1	0
4	A	18	0	0	3	0
4	C	18	0	0	0	0
5	B	14	0	0	0	0
5	D	14	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	A	220	0	0	14	0
8	B	343	0	0	6	0
8	C	197	0	0	8	0
8	D	312	0	0	9	0
All	All	16910	15165	15278	213	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 (213) 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:A:41:GLN:HB2	1:A:44:LYS:HE2	1.30	1.12
1:C:42:SER:HB3	1:C:388:ASP:OD1	1.59	1.02
1:A:41:GLN:HB2	1:A:44:LYS:CE	1.94	0.97
4:A:502:ICS:S1A	8:A:615:HOH:O	2.33	0.85
1:C:41:GLN:NE2	1:C:44:LYS:HB2	1.91	0.83
2:B:122:ALA:HB2	8:B:717:HOH:O	1.79	0.83
2:D:84:LYS:HG2	8:D:957:HOH:O	1.77	0.83
1:C:144:LEU:HD11	2:D:43:VAL:HG21	1.61	0.82
1:A:43:LYS:O	1:A:44:LYS:HB2	1.78	0.82
1:A:41:GLN:CB	1:A:44:LYS:HE2	2.10	0.81
1:A:146:LYS:CE	8:A:608:HOH:O	2.30	0.80
1:C:154:CYS:SG	8:D:735:HOH:O	2.41	0.78
1:A:146:LYS:HE2	8:A:608:HOH:O	1.86	0.75
1:A:42:SER:HB3	1:A:388:ASP:OD1	1.88	0.74
1:A:357:GLY:C	8:A:615:HOH:O	2.30	0.74
1:A:96:ARG:NH2	4:A:502:ICS:S5A	2.61	0.74
1:C:347:GLU:OE1	1:C:371:GLY:HA3	1.89	0.73
1:A:196:HIS:HE1	8:A:729:HOH:O	1.70	0.73
2:D:84:LYS:CG	8:D:957:HOH:O	2.36	0.72
1:A:401:TYR:HB2	1:A:404:VAL:HG22	1.74	0.68
8:C:613:HOH:O	2:D:26:LYS:HD3	1.93	0.67
1:C:361:ARG:HB3	1:C:390:THR:HG23	1.78	0.66
2:D:247:MET:HG2	2:D:341:PRO:HD3	1.78	0.66
1:A:47:ILE:HD11	8:A:621:HOH:O	1.97	0.65
1:A:43:LYS:O	1:A:44:LYS:CB	2.45	0.64
2:B:322:LEU:HD23	1:C:474:LYS:HD3	1.78	0.64
2:D:272:TYR:HB2	8:D:957:HOH:O	2.00	0.61
1:A:276:TYR:OH	1:A:284:ARG:NH2	2.32	0.61
1:C:442:HIS:HB2	8:C:706:HOH:O	2.01	0.61
1:A:479:TRP:O	1:A:480:GLU:HB2	2.00	0.60
1:A:70:VAL:HG23	1:A:71:VAL:HG23	1.83	0.60
1:C:219:THR:HA	8:C:695:HOH:O	2.01	0.60
1:A:93:ARG:HD3	1:A:113:ASN:HB2	1.82	0.59
2:D:209:THR:HG21	2:D:309:TRP:HE1	1.68	0.59
1:C:40:THR:HA	1:C:391:MET:HE3	1.84	0.59
1:A:97:ARG:NH2	1:A:447:SER:O	2.36	0.58
1:A:355:ILE:HD12	1:A:441:MET:HB2	1.85	0.58
2:D:241:LYS:NZ	2:D:258:GLU:OE2	2.37	0.58
1:C:276:TYR:OH	1:C:284:ARG:NH2	2.37	0.57
1:A:420:LEU:HB2	1:A:467:LEU:HD13	1.85	0.57
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.87	0.57
1:A:457:ALA:HB1	2:B:8:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ARG:NH2	1:C:474:LYS:O	2.39	0.55
1:A:349:LYS:HG3	1:A:467:LEU:HD21	1.88	0.55
2:D:170:LYS:HD3	2:D:177:ASP:HA	1.87	0.55
2:B:45:GLN:HG3	8:B:768:HOH:O	2.07	0.55
8:A:783:HOH:O	2:D:360:THR:HB	2.07	0.55
2:D:124:VAL:HG13	8:D:704:HOH:O	2.07	0.55
1:C:36:ASP:OD2	1:C:39:VAL:HG12	2.07	0.55
1:C:277:ARG:NE	1:C:386:ASP:OD2	2.37	0.54
1:C:158:LEU:HD13	2:D:157:VAL:CG2	2.38	0.54
1:C:70:VAL:O	1:C:96:ARG:NH2	2.40	0.54
2:D:209:THR:HG21	2:D:309:TRP:NE1	2.22	0.54
1:C:158:LEU:HD13	2:D:157:VAL:HG21	1.90	0.53
2:B:154:MET:HG3	2:B:155:ALA:N	2.24	0.53
1:C:351:VAL:CG2	1:C:372:MET:HE2	2.38	0.53
1:C:457:ALA:HB1	2:D:8:ILE:HD12	1.88	0.53
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.91	0.52
2:B:90:HIS:ND1	2:B:116:ASP:OD2	2.42	0.52
1:C:243:GLU:OE1	2:D:26:LYS:HE2	2.10	0.52
3:C:501:HCA:O7	3:C:501:HCA:O1	2.23	0.52
2:B:118:MET:HE3	2:B:122:ALA:HB1	1.91	0.52
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.92	0.52
1:A:82:SER:HB3	1:A:153:GLU:OE2	2.11	0.51
1:A:412:PHE:O	1:A:416:ILE:HD12	2.10	0.51
1:C:42:SER:C	1:C:44:LYS:H	2.19	0.51
1:A:358:LEU:N	8:A:615:HOH:O	2.44	0.51
2:D:523:ARG:NH1	8:D:718:HOH:O	2.44	0.51
1:C:239:ARG:NH2	1:C:249:CYS:O	2.43	0.51
2:B:212:SER:O	2:B:212:SER:OG	2.20	0.51
2:D:88:TYR:O	2:D:149:VAL:HA	2.11	0.50
1:A:387:TYR:O	1:A:391:MET:HG2	2.11	0.50
1:C:359:ARG:NH2	1:C:442:HIS:O	2.45	0.50
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.93	0.50
1:C:207:LEU:HD23	1:C:207:LEU:O	2.11	0.50
1:C:240:ILE:N	2:D:23:MET:CE	2.75	0.50
2:B:326:ASP:OD2	2:B:348:ARG:NH1	2.45	0.50
2:D:261:LEU:HD23	8:D:817:HOH:O	2.11	0.50
1:A:310:ARG:HD3	1:A:325:GLU:OE2	2.12	0.49
2:B:100:ARG:HD2	2:B:111:VAL:O	2.12	0.49
2:B:88:TYR:O	2:B:149:VAL:HA	2.13	0.49
2:B:86:MET:HG2	2:B:138:CYS:SG	2.53	0.49
1:C:360:PRO:HG2	1:C:379:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:518:ASN:O	2:D:523:ARG:NH2	2.42	0.49
1:A:45:CYS:SG	1:A:391:MET:HE1	2.53	0.48
1:C:277:ARG:HD3	8:C:606:HOH:O	2.14	0.48
1:C:399:LEU:C	1:C:400:LEU:HD23	2.38	0.48
2:D:339:PRO:O	8:D:701:HOH:O	2.20	0.48
1:A:401:TYR:CD1	1:A:404:VAL:HG21	2.49	0.48
1:A:355:ILE:HG12	1:A:360:PRO:HG3	1.96	0.48
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.95	0.48
1:C:210:ARG:NH1	1:C:263:GLU:OE1	2.45	0.48
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.96	0.47
2:D:390:PRO:HB2	2:D:393:ILE:HD11	1.96	0.47
1:C:42:SER:CB	1:C:388:ASP:OD1	2.49	0.47
2:D:354:MET:SD	2:D:491:MET:HE2	2.53	0.47
1:A:15:GLU:HA	1:A:18:GLU:OE1	2.15	0.47
2:B:34:LYS:N	8:B:712:HOH:O	2.43	0.47
1:C:158:LEU:HD11	2:D:154:MET:HG2	1.97	0.47
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.95	0.47
1:A:383:HIS:N	1:A:383:HIS:ND1	2.62	0.47
1:C:139:GLU:HG3	1:C:174:LEU:HD13	1.95	0.47
1:A:141:LEU:HD11	2:B:59:ARG:HD3	1.96	0.47
1:C:60:ARG:HG2	8:C:625:HOH:O	2.14	0.47
1:C:322:LYS:O	1:C:326:GLU:HG3	2.15	0.47
1:A:161:ASP:OD2	8:A:601:HOH:O	2.20	0.46
1:C:240:ILE:CA	2:D:23:MET:CE	2.93	0.46
1:A:352:MET:HE3	1:A:418:PRO:HG3	1.96	0.46
8:B:941:HOH:O	1:C:94:ALA:HB1	2.15	0.46
1:C:158:LEU:CD1	2:D:157:VAL:HG21	2.45	0.46
2:B:513:GLN:HG3	1:C:103:THR:OG1	2.15	0.46
1:C:42:SER:HA	1:C:45:CYS:SG	2.55	0.46
1:A:41:GLN:CB	1:A:44:LYS:CE	2.80	0.46
1:A:289:LYS:HD3	1:A:290:TYR:CZ	2.51	0.46
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.98	0.46
1:C:210:ARG:HD3	1:C:263:GLU:HB3	1.97	0.46
1:A:42:SER:O	1:A:43:LYS:C	2.54	0.46
2:B:105:ARG:HD2	2:D:522:VAL:HG11	1.96	0.45
1:A:41:GLN:NE2	1:A:41:GLN:HA	2.29	0.45
1:A:352:MET:HE1	1:A:413:VAL:HA	1.97	0.45
1:A:356:GLY:HA3	4:A:502:ICS:S1B	2.57	0.45
1:A:158:LEU:HG	1:A:186:PHE:CE2	2.52	0.45
2:D:92:SER:CB	8:D:735:HOH:O	2.64	0.45
1:C:152:SER:OG	1:C:163:ILE:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TYR:CG	1:A:382:ALA:HB2	2.52	0.45
1:A:88:CYS:HB2	1:A:153:GLU:OE2	2.17	0.45
1:A:343:ARG:NH1	1:A:347:GLU:OE1	2.50	0.45
2:B:278:GLN:O	2:B:282:LYS:HG3	2.17	0.45
2:B:461:GLU:HG3	8:B:730:HOH:O	2.17	0.45
1:C:67:SER:OG	1:C:181:VAL:HG11	2.17	0.45
1:A:134:LEU:HG	2:B:62:LEU:HB2	1.99	0.45
1:C:136:ASP:OD1	8:C:601:HOH:O	2.21	0.44
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.99	0.44
1:C:62:CYS:O	1:C:191:GLN:HA	2.18	0.44
1:A:358:LEU:HB2	8:A:615:HOH:O	2.17	0.44
1:A:42:SER:CB	1:A:388:ASP:OD1	2.64	0.44
2:D:54:GLU:O	2:D:58:GLN:HG2	2.18	0.44
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.53	0.44
1:A:59:ILE:O	1:A:59:ILE:HG22	2.18	0.43
2:B:453:ARG:HD3	2:D:512:MET:SD	2.58	0.43
1:A:44:LYS:HB2	1:A:44:LYS:HE3	1.75	0.43
1:A:66:GLY:O	1:A:70:VAL:HG22	2.18	0.43
2:D:86:MET:HG2	2:D:138:CYS:SG	2.59	0.43
2:B:369:LEU:C	2:B:369:LEU:HD22	2.43	0.43
1:C:466:THR:O	1:C:472:TRP:NE1	2.46	0.43
1:A:139:GLU:HG3	1:A:174:LEU:HD23	1.99	0.43
1:A:163:ILE:HG12	1:A:182:ARG:HH11	1.84	0.43
2:B:54:GLU:O	2:B:58:GLN:HG2	2.18	0.43
8:B:929:HOH:O	1:C:99:TYR:HA	2.18	0.43
1:C:207:LEU:CD2	1:C:266:PRO:HG3	2.49	0.43
2:B:513:GLN:HG2	1:C:102:GLY:C	2.43	0.43
1:C:81:ILE:HD12	1:C:134:LEU:HD21	2.00	0.43
1:C:347:GLU:OE1	1:C:371:GLY:CA	2.63	0.43
2:D:118:MET:HB3	2:D:154:MET:HE1	2.01	0.43
1:A:139:GLU:HG3	1:A:174:LEU:CD2	2.48	0.43
1:A:432:GLN:HG2	1:A:472:TRP:HH2	1.83	0.43
1:C:132:ALA:HB1	1:C:170:LYS:HE2	2.00	0.43
1:C:226:ILE:HG22	1:C:279:MET:HB3	2.00	0.42
1:C:351:VAL:HG23	1:C:372:MET:HE2	2.00	0.42
1:C:207:LEU:HD21	1:C:266:PRO:HG3	2.00	0.42
2:D:241:LYS:NZ	2:D:256:ASP:OD2	2.51	0.42
1:A:77:ASP:OD2	1:A:258:SER:HB2	2.20	0.42
1:A:93:ARG:HD2	1:A:111:THR:O	2.20	0.42
2:B:434:VAL:HA	2:B:439:PRO:HD3	2.01	0.42
1:A:239:ARG:HG3	2:B:23:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:MET:SD	1:C:478:PRO:HB2	2.59	0.42
1:C:33:ALA:O	1:C:399:LEU:HD12	2.20	0.42
1:A:358:LEU:CB	8:A:615:HOH:O	2.67	0.42
1:C:359:ARG:N	1:C:360:PRO:CD	2.83	0.42
1:A:386:ASP:OD1	8:A:602:HOH:O	2.22	0.42
2:D:143:LYS:N	2:D:144:PRO:HD3	2.34	0.42
1:A:42:SER:N	1:A:388:ASP:OD1	2.40	0.42
1:C:243:GLU:OE1	2:D:26:LYS:CE	2.68	0.42
2:D:26:LYS:HE3	2:D:26:LYS:HB3	1.70	0.42
1:C:144:LEU:CD1	2:D:43:VAL:HG21	2.40	0.41
2:D:414:PRO:HA	2:D:417:LYS:HD3	2.02	0.41
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.89	0.41
2:B:345:THR:HG21	8:C:639:HOH:O	2.20	0.41
1:C:148:ILE:O	1:C:178:ILE:HA	2.20	0.41
2:D:369:LEU:HD11	2:D:393:ILE:HG23	2.01	0.41
1:A:55:GLY:HA2	2:B:114:VAL:HG21	2.01	0.41
1:A:62:CYS:O	1:A:191:GLN:HA	2.21	0.41
1:C:42:SER:C	1:C:44:LYS:N	2.78	0.41
2:D:121:ASP:HB3	2:D:125:PHE:CE2	2.56	0.41
1:A:401:TYR:HB2	1:A:404:VAL:CG2	2.45	0.41
2:B:43:VAL:O	2:B:47:THR:HG23	2.20	0.41
2:D:231:GLU:CD	2:D:236:ASN:HD22	2.29	0.41
2:D:290:THR:HB	2:D:305:VAL:HG11	2.03	0.41
1:A:296:GLU:HB3	8:A:695:HOH:O	2.21	0.41
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.56	0.41
2:B:143:LYS:N	2:B:144:PRO:CD	2.83	0.41
1:C:41:GLN:NE2	1:C:44:LYS:CB	2.75	0.41
1:A:32:LEU:HD13	1:A:412:PHE:HZ	1.85	0.41
2:D:131:MET:HE3	2:D:135:LEU:HD21	2.03	0.41
1:A:382:ALA:HB1	1:A:386:ASP:HB2	2.03	0.41
2:B:290:THR:HB	2:B:305:VAL:HG11	2.03	0.41
1:C:93:ARG:HG3	1:C:113:ASN:HB2	2.03	0.41
2:B:350:ARG:HD3	2:D:262:ASP:O	2.22	0.40
1:C:31:HIS:O	1:C:46:ILE:HD11	2.20	0.40
2:D:84:LYS:HD3	2:D:145:ASP:OD2	2.21	0.40
2:D:211:LYS:HE2	2:D:211:LYS:HB3	1.90	0.40
1:A:426:LYS:HE3	8:A:660:HOH:O	2.21	0.40
1:C:243:GLU:OE1	2:D:26:LYS:NZ	2.54	0.40
1:A:378:GLY:HA3	1:A:401:TYR:CD1	2.56	0.40
1:A:215:THR:O	1:A:216:PHE:C	2.64	0.40
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD23	1:A:467:LEU:HD23	2.02	0.40
1:C:239:ARG:NH1	2:D:27:LYS:HD2	2.37	0.40
1:C:426:LYS:HD3	8:C:636:HOH:O	2.21	0.40
1:A:55:GLY:C	2:B:114:VAL:HG21	2.46	0.40
1:A:355:ILE:HD12	1:A:441:MET:CB	2.51	0.40
1:C:207:LEU:HD12	1:C:282:ILE:HD11	2.03	0.40
2:D:228:PRO:HA	2:D:293:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/492 (96%)	438 (93%)	30 (6%)	2 (0%)	30	34
1	C	474/492 (96%)	446 (94%)	25 (5%)	3 (1%)	21	23
2	B	520/523 (99%)	503 (97%)	17 (3%)	0	100	100
2	D	520/523 (99%)	508 (98%)	12 (2%)	0	100	100
All	All	1984/2030 (98%)	1895 (96%)	84 (4%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	C	43	LYS
1	A	6	ARG
1	C	154	CYS
1	C	355	ILE

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	391/415 (94%)	380 (97%)	11 (3%)	38	52
1	C	392/415 (94%)	373 (95%)	19 (5%)	23	30
2	B	446/454 (98%)	434 (97%)	12 (3%)	39	53
2	D	447/454 (98%)	440 (98%)	7 (2%)	55	71
All	All	1676/1738 (96%)	1627 (97%)	49 (3%)	37	51

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	40	THR
1	A	42	SER
1	A	47	ILE
1	A	93	ARG
1	A	98	ASN
1	A	322	LYS
1	A	355	ILE
1	A	359	ARG
1	A	362	HIS
1	A	415	ARG
2	B	59	ARG
2	B	115	SER
2	B	212	SER
2	B	258	GLU
2	B	329	LEU
2	B	350	ARG
2	B	369	LEU
2	B	431	ARG
2	B	503	GLU
2	B	505	LEU
2	B	513	GLN
2	B	523	ARG
1	C	6	ARG

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Mol	Chain	Res	Type
1	C	18	GLU
1	C	19	VAL
1	C	26	LYS
1	C	39	VAL
1	C	40	THR
1	C	42	SER
1	C	44	LYS
1	C	45	CYS
1	C	52	SER
1	C	93	ARG
1	C	98	ASN
1	C	210	ARG
1	C	219	THR
1	C	359	ARG
1	C	362	HIS
1	C	390	THR
1	C	391	MET
1	C	445	ASP
2	D	23	MET
2	D	26	LYS
2	D	154	MET
2	D	209	THR
2	D	300	LYS
2	D	350	ARG
2	D	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	98	ASN
1	A	196	HIS
1	A	285	HIS
1	A	383	HIS
1	A	451	HIS
2	B	128	GLN
2	B	363	HIS
1	C	252	GLN
1	C	432	GLN
2	D	45	GLN
2	D	93	GLN
2	D	163	ASN

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Mol	Chain	Res	Type
2	D	185	HIS
2	D	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	HCA	C	501	4	13,13,13	1.04	0	15,18,18	1.18	1 (6%)
4	ICS	A	502	3,1	6,30,30	1.59	1 (16%)	-		
5	UFF	B	601	2,1	0,21,21	-	-	-		
4	ICS	C	502	3,1	6,30,30	1.62	1 (16%)	-		
5	UFF	D	601	2,1	0,21,21	-	-	-		
3	HCA	A	501	4	13,13,13	1.13	1 (7%)	15,18,18	2.20	7 (46%)

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	HCA	A	501	4	-	11/17/17/17	-
5	UFF	D	601	2,1	-	-	0/9/8/8
5	UFF	B	601	2,1	-	-	0/9/8/8
3	HCA	C	501	4	-	5/17/17/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S2B-FE6	-2.94	2.18	2.24
4	C	502	ICS	S2B-FE6	-2.93	2.18	2.24
3	A	501	HCA	O4-C6	-2.20	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	O6-C7-C3	4.37	121.52	113.14
3	A	501	HCA	O7-C3-C7	3.58	114.04	108.96
3	A	501	HCA	O3-C6-C5	-2.77	114.32	123.09
3	A	501	HCA	O4-C6-C5	2.63	122.30	114.00
3	C	501	HCA	O6-C7-C3	2.62	118.17	113.14
3	A	501	HCA	O2-C1-C2	2.54	122.38	114.35
3	A	501	HCA	O7-C3-C4	-2.22	105.33	108.88
3	A	501	HCA	O1-C1-C2	-2.19	116.74	122.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	A	501	HCA	O7-C3-C4-C5
3	C	501	HCA	C2-C3-C4-C5
3	C	501	HCA	O7-C3-C4-C5
3	A	501	HCA	O7-C3-C7-O5
3	A	501	HCA	O7-C3-C7-O6
3	C	501	HCA	C7-C3-C4-C5
3	A	501	HCA	C2-C3-C7-O5
3	A	501	HCA	C2-C3-C7-O6
3	A	501	HCA	C4-C3-C7-O6
3	A	501	HCA	C4-C3-C7-O5
3	A	501	HCA	O2-C1-C2-C3
3	C	501	HCA	C1-C2-C3-C7
3	A	501	HCA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C7-C3-C4-C5
3	C	501	HCA	C1-C2-C3-C4

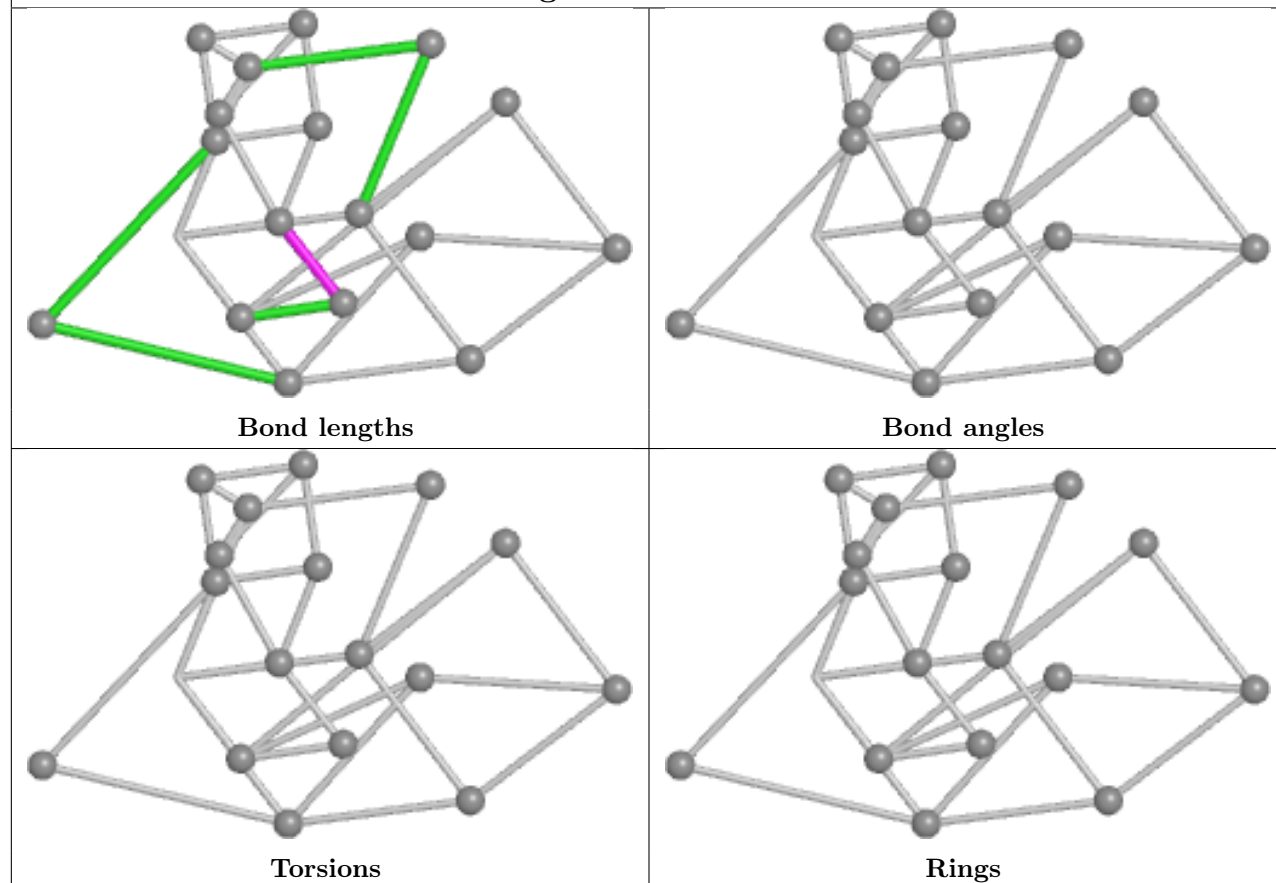
There are no ring outliers.

2 monomers are involved in 4 short contacts:

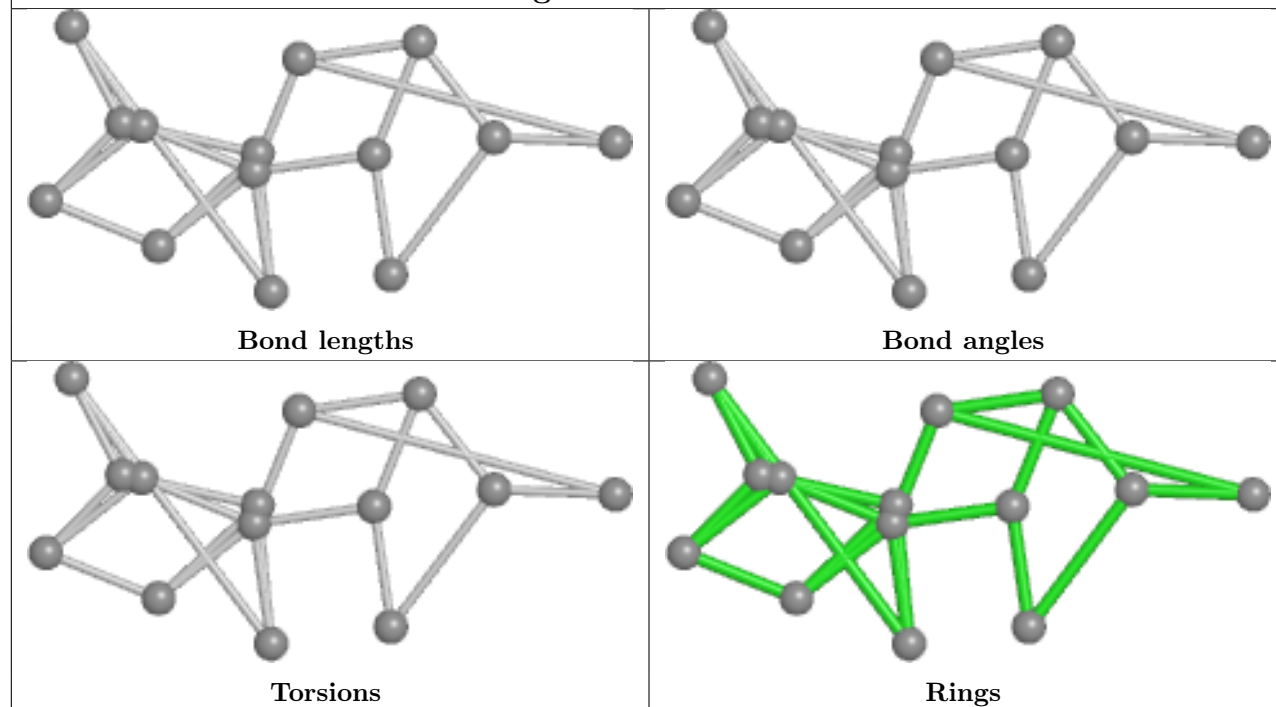
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	HCA	1	0
4	A	502	ICS	3	0

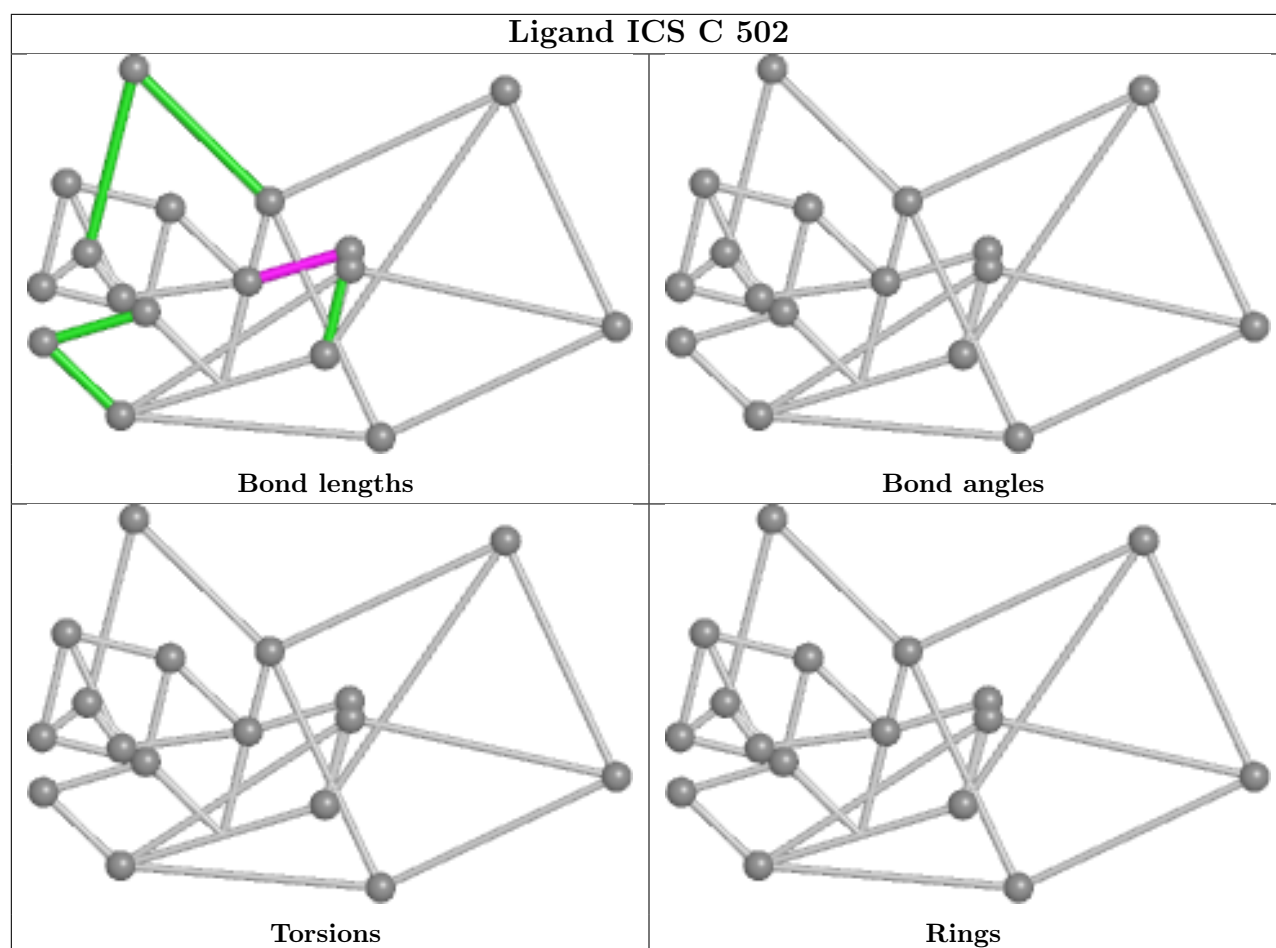
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

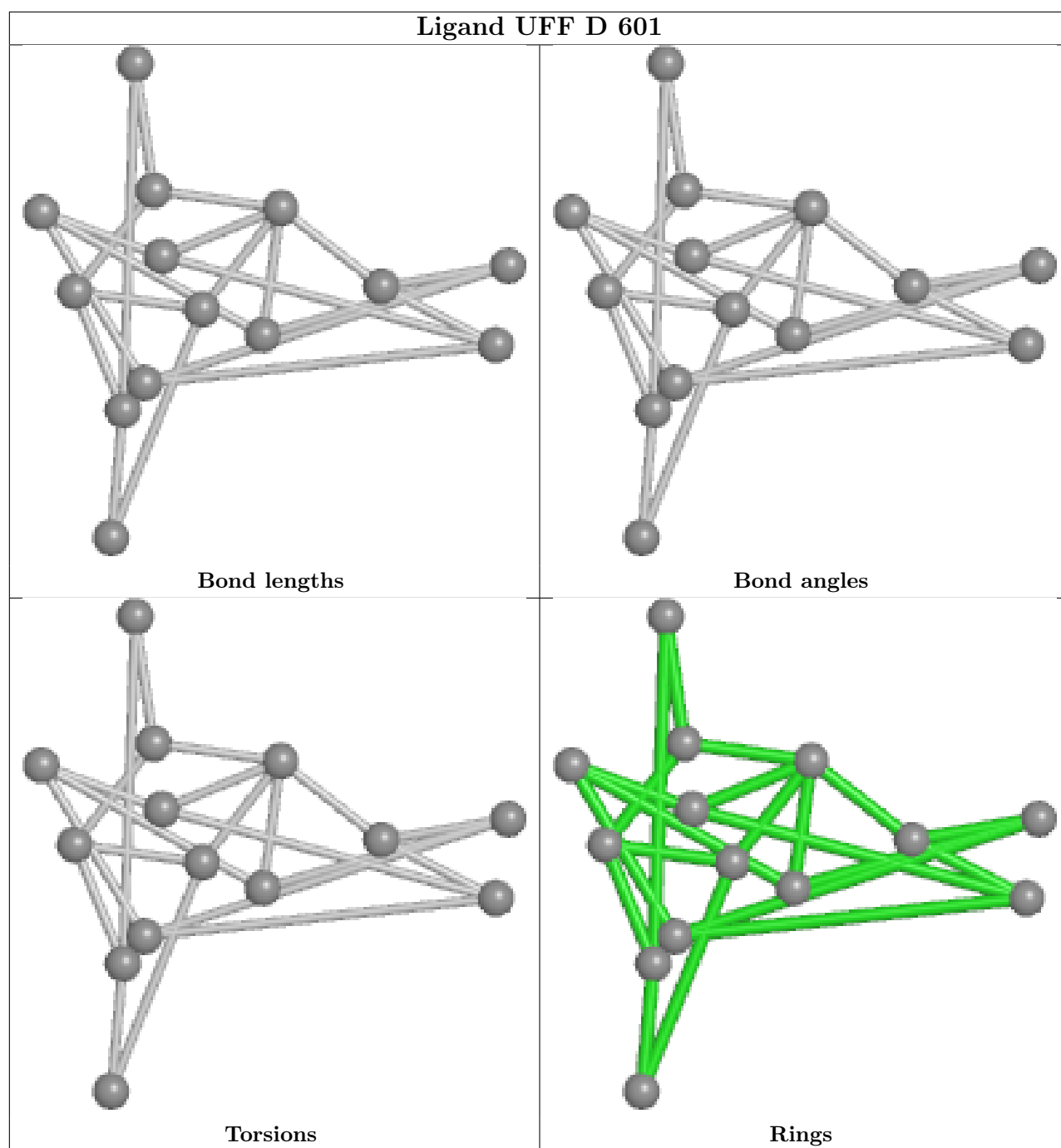
Ligand ICS A 502



Ligand UFF 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 ⓘ

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	474/492 (96%)	0.70	26 (5%)	30 27	21, 32, 48, 65	0
1	C	476/492 (96%)	0.71	29 (6%)	27 24	22, 33, 48, 59	0
2	B	522/523 (99%)	0.28	7 (1%)	75 73	18, 27, 38, 51	0
2	D	522/523 (99%)	0.31	10 (1%)	66 63	19, 27, 39, 53	0
All	All	1994/2030 (98%)	0.49	72 (3%)	46 43	18, 30, 45, 65	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	4.9
1	C	42	SER	3.8
1	A	215	THR	3.6
1	C	216	PHE	3.6
1	C	38	ALA	3.6
1	A	214	THR	3.5
2	D	123	ALA	3.5
1	A	39	VAL	3.5
2	B	123	ALA	3.5
1	C	24	ALA	3.3
1	C	213	ASP	3.2
1	C	45	CYS	3.1
1	A	33	ALA	3.1
1	C	5	SER	3.0
1	A	384	ASN	3.0
2	D	125	PHE	3.0
1	A	42	SER	2.9
2	B	125	PHE	2.8
1	A	20	TYR	2.8
1	C	253	TRP	2.8
1	C	392	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	60	GLU	2.7
2	D	157	VAL	2.7
1	C	52	SER	2.7
1	A	41	GLN	2.7
1	C	92	SER	2.7
2	D	124	VAL	2.6
1	C	189	VAL	2.6
1	C	391	MET	2.6
1	A	6	ARG	2.6
2	D	122	ALA	2.6
1	A	211	ASP	2.6
2	D	155	ALA	2.5
1	C	36	ASP	2.5
1	C	188	GLY	2.5
1	A	7	GLU	2.4
1	C	19	VAL	2.4
1	A	9	VAL	2.4
1	A	213	ASP	2.4
1	C	209	LYS	2.4
1	C	158	LEU	2.4
1	C	400	LEU	2.4
1	C	212	GLU	2.4
1	A	391	MET	2.3
1	A	480	GLU	2.3
1	A	357	GLY	2.3
1	A	362	HIS	2.3
1	C	214	THR	2.3
1	A	383	HIS	2.3
1	A	19	VAL	2.3
1	C	34	VAL	2.3
2	B	126	GLY	2.2
1	C	41	GLN	2.2
1	A	355	ILE	2.2
1	C	190	SER	2.2
1	C	397	SER	2.2
2	D	121	ASP	2.2
1	A	212	GLU	2.2
2	B	121	ASP	2.1
1	C	215	THR	2.1
2	D	154	MET	2.1
2	B	119	THR	2.1
1	A	311	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	43	LYS	2.1
1	C	9	VAL	2.1
1	A	61	GLY	2.1
2	B	154	MET	2.0
2	D	38	ASP	2.0
1	A	34	VAL	2.0
1	C	15	GLU	2.0
2	B	80	LEU	2.0
1	A	21	PRO	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](#)

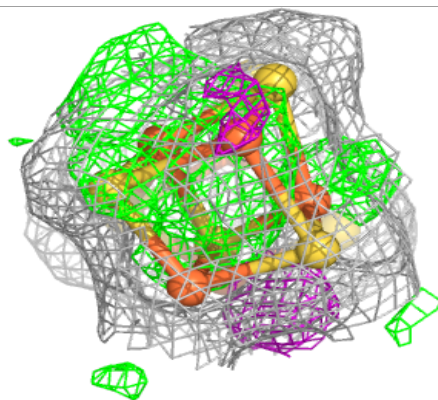
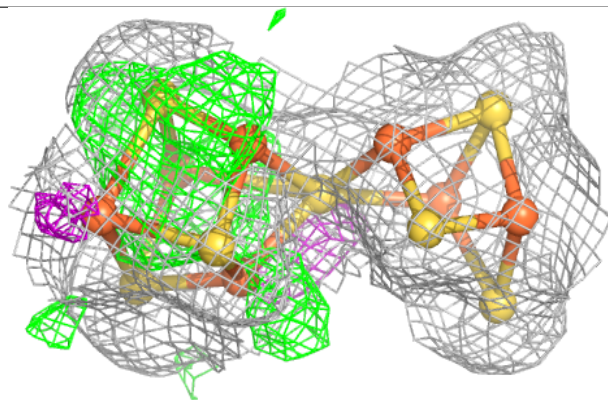
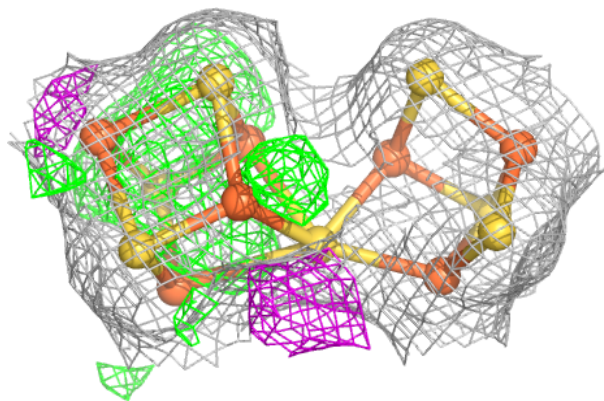
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NA	D	603	1/1	0.64	0.17	29,29,29,29	0
7	NA	B	603	1/1	0.69	0.14	28,28,28,28	0
3	HCA	A	501	14/14	0.84	0.13	26,29,36,36	0
6	FE	B	602	1/1	0.89	0.09	23,23,23,23	1
3	HCA	C	501	14/14	0.90	0.09	25,32,38,38	0
5	UFF	B	601	14/14	0.91	0.08	23,28,30,30	1
4	ICS	C	502	18/18	0.92	0.07	24,26,36,52	0
5	UFF	D	601	14/14	0.95	0.06	22,27,28,30	3
4	ICS	A	502	18/18	0.98	0.04	22,27,30,30	0
6	FE	D	602	1/1	0.98	0.07	22,22,22,22	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

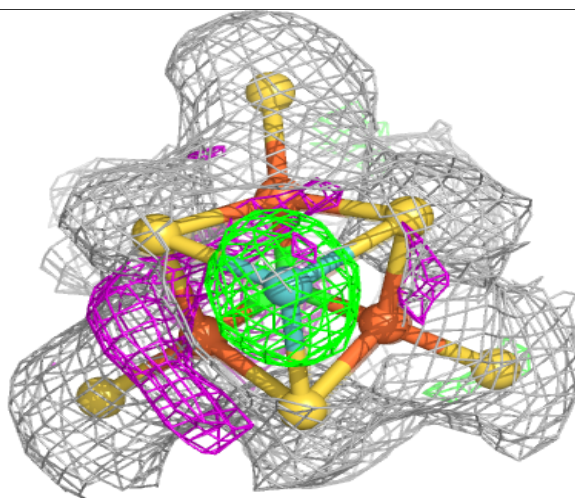
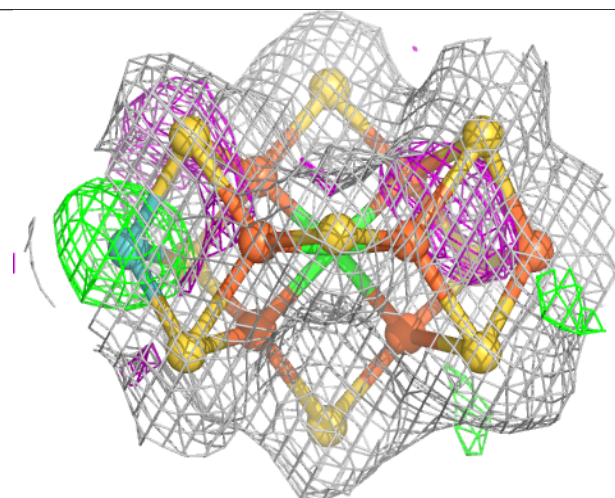
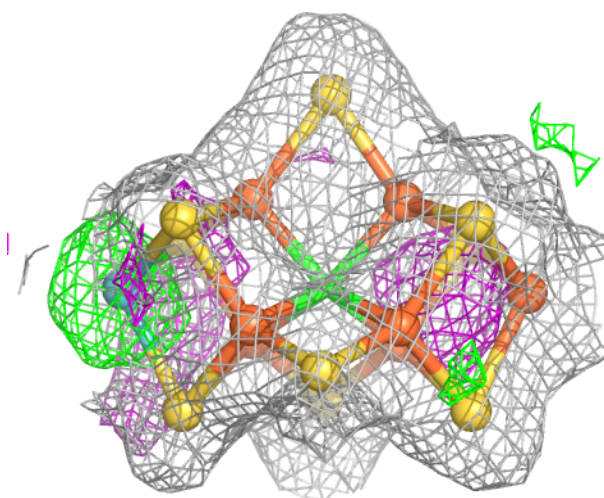
Electron density around UFF B 601:

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



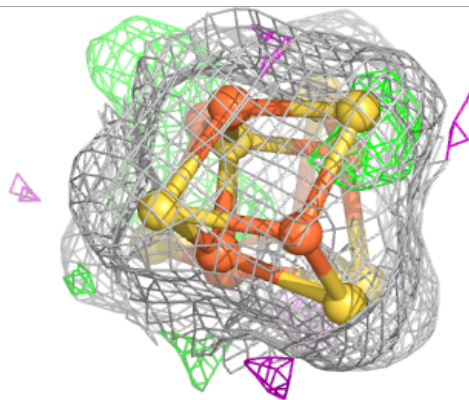
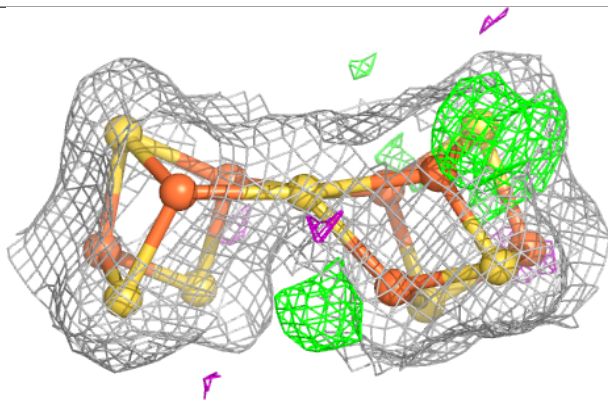
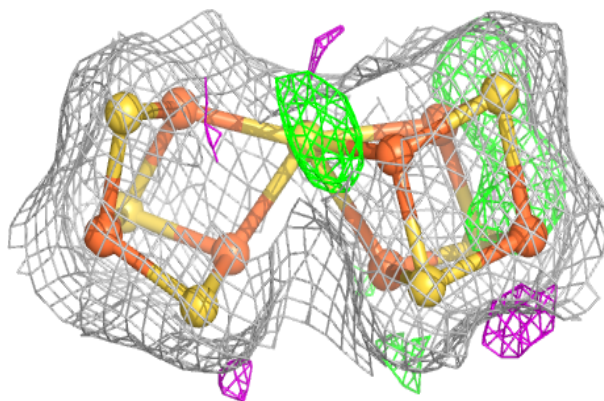
Electron density around ICS C 502:

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



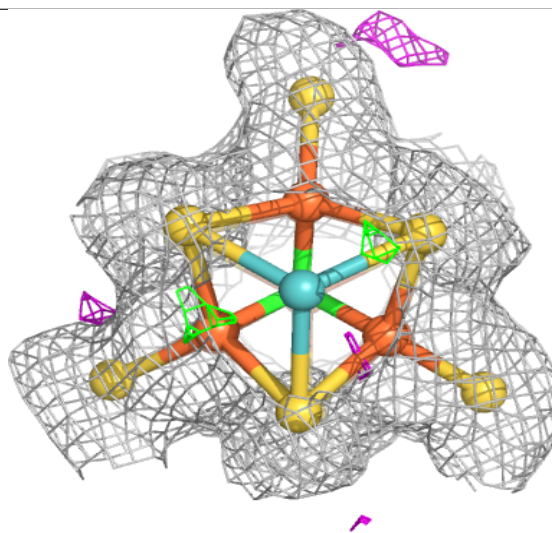
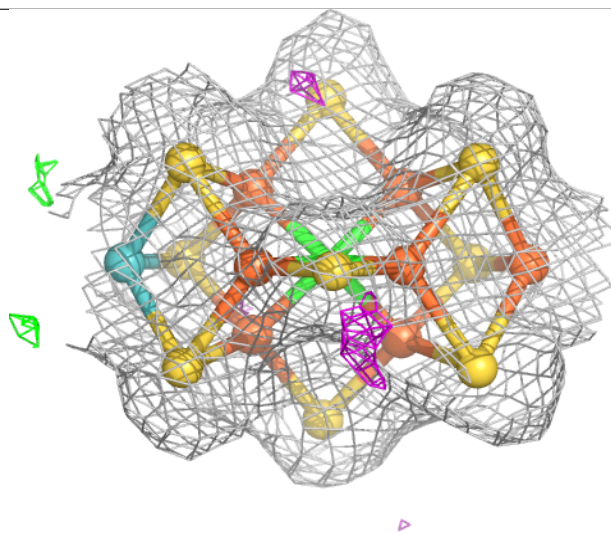
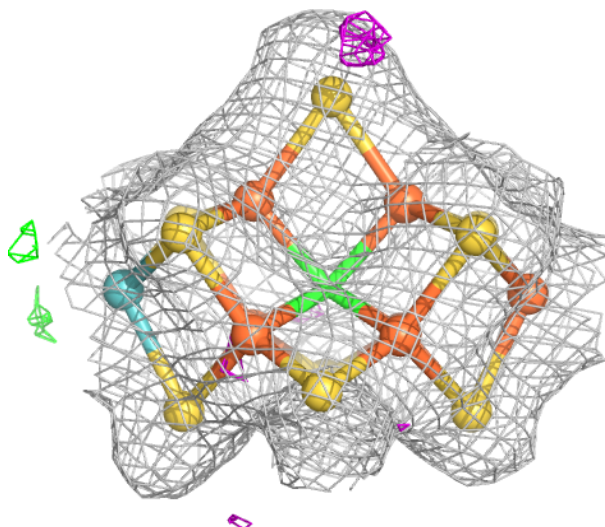
Electron density around UFF D 601:

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



Electron density around ICS 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.