



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:00 PM UTC

PDB ID : 8EPZ / pdb_00008epz
Title : Crystal structure of Fe-S cluster-dependent dehydratase from *Paralcaligenes ureilyticus* in complex with Mn
Authors : Bayaraa, T.; Lonhienne, T.; Guddat, L.W.
Deposited on : 2022-10-07
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

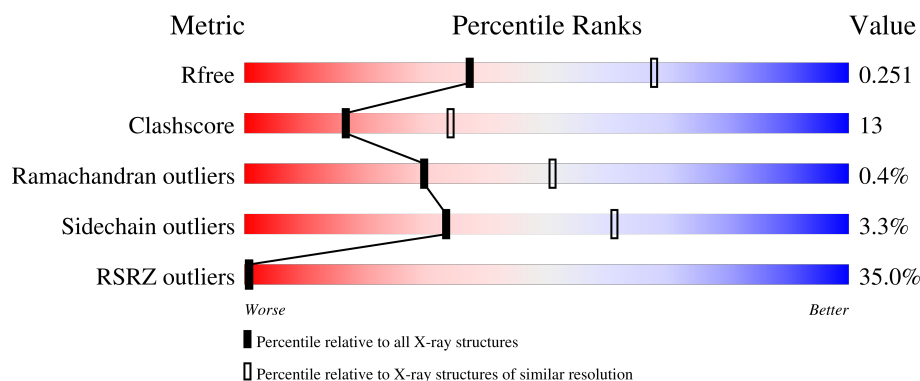
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	575	
1	B	575	

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
1	KCX	A	127	-	-	X	-
1	KCX	B	127	-	-	X	-
4	CO2	B	704	-	-	X	-

2 Entry composition [i](#)

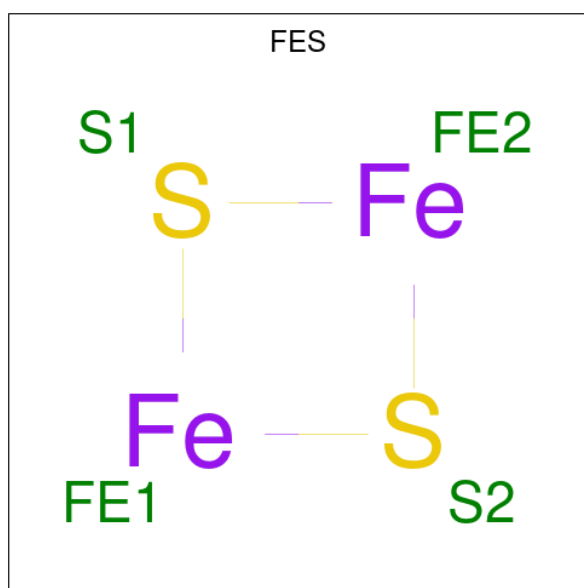
There are 6 unique types of molecules in this entry. The entry contains 8706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydroxyacid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	1	0
			4309	2691	781	799	38			
1	B	568	Total	C	N	O	S	0	0	0
			4304	2688	781	797	38			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

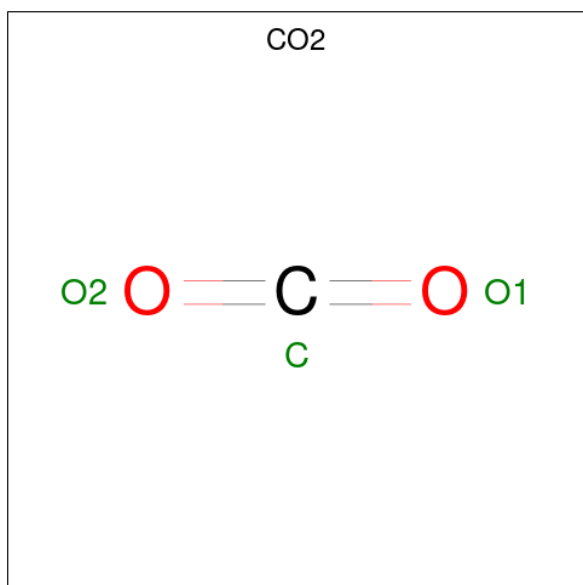


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	1	3		

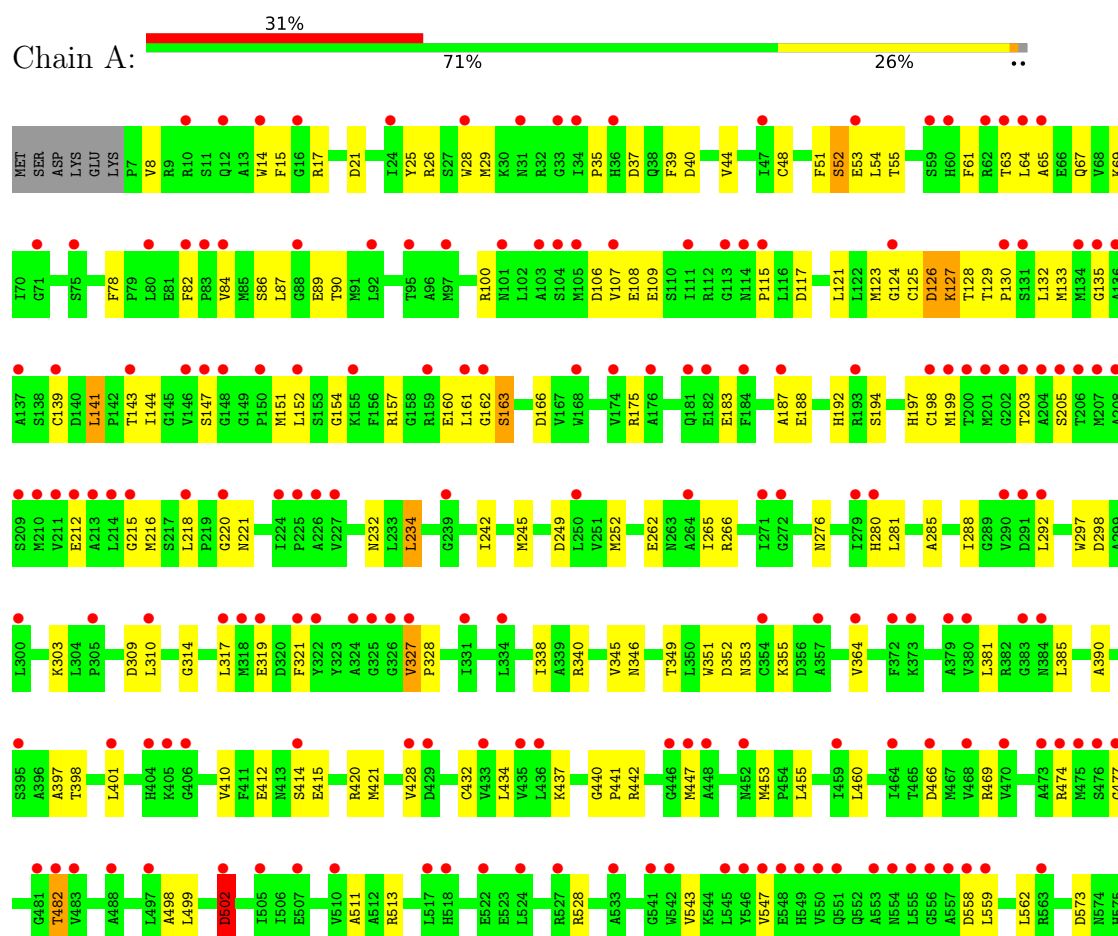
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	34	Total	O	0	0
			34	34		

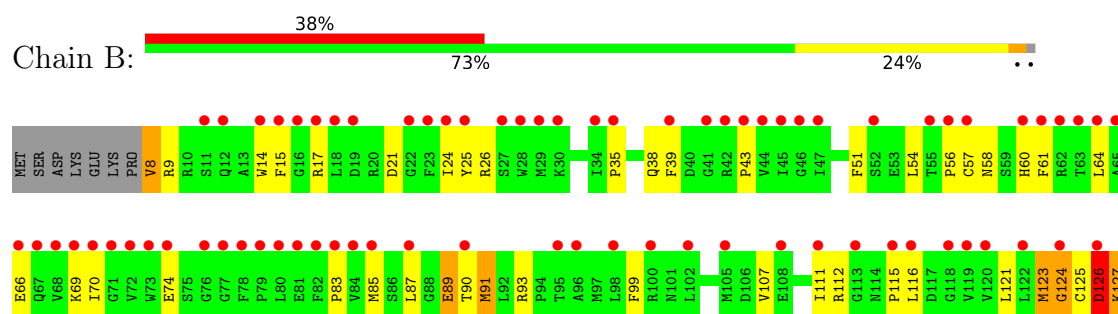
3 Residue-property plots [i](#)

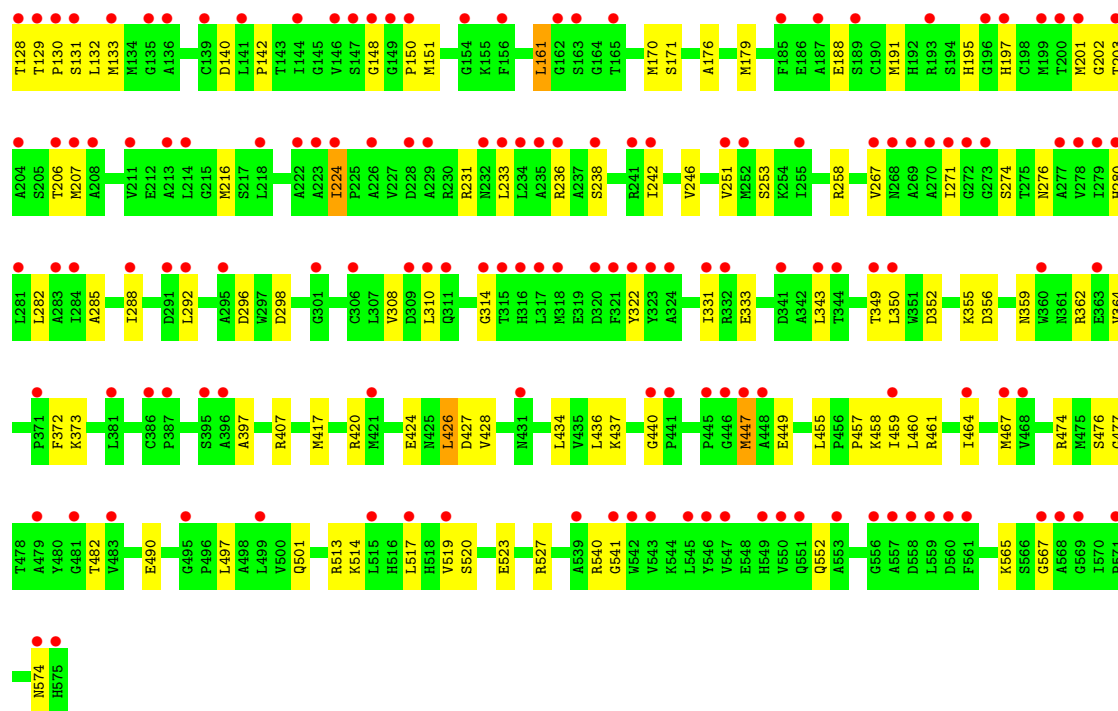
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dihydroxyacid dehydratase



• Molecule 1: Dihydroxyacid dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.64Å 113.14Å 182.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.60 48.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.11-2.60) 99.3 (48.11-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.210 , 0.251 0.212 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: BCT, FES, KCX, CO2, MN

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	0.23	0/4388	0.40	0/5946
1	B	0.30	0/4379	0.45	1/5931 (0.0%)
All	All	0.27	0/8767	0.43	1/11877 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ASP	CA-CB-CG	5.75	118.35	112.60

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	4309	0	4253	128	0
1	B	4304	0	4256	116	0
2	A	4	0	0	0	0
2	B	4	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	6	0	0	1	0
4	B	3	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	0	0
6	A	36	0	0	4	0
6	B	34	0	0	1	0
All	All	8706	0	8509	220	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 (220) 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:449:GLU:OE2	1:B:476:SER:HB3	1.58	1.01
1:B:449:GLU:OE2	1:B:476:SER:CB	2.19	0.89
1:A:108:GLU:OE2	1:B:540:ARG:NH2	2.07	0.87
1:A:52:SER:HB2	1:B:83:PRO:HD3	1.56	0.85
1:B:206:THR:HG21	1:B:274:SER:H	1.43	0.83
1:A:447:MET:O	1:A:474:ARG:NH1	2.12	0.81
1:A:139:CYS:SG	6:A:714:HOH:O	2.44	0.76
1:A:144:ILE:HD13	1:A:345:VAL:HG11	1.69	0.74
1:B:58:ASN:HD21	1:B:128:THR:HG21	1.51	0.74
1:B:127:KCX:OQ2	1:B:276:ASN:HB3	1.89	0.72
1:A:65:ALA:O	1:A:69:LYS:HG3	1.91	0.71
1:A:28:TRP:CD2	1:B:90:THR:HG21	2.26	0.70
1:B:449:GLU:OE2	1:B:476:SER:CA	2.39	0.70
1:B:17:ARG:O	1:B:26:ARG:NH2	2.26	0.68
1:A:398:THR:H	1:A:482:THR:HG22	1.58	0.68
1:A:573:ASP:OD2	1:B:93:ARG:NH2	2.27	0.68
1:A:89:GLU:OE2	1:A:126:ASP:CG	2.37	0.67
1:B:397:ALA:HB1	1:B:482:THR:HG22	1.77	0.65
1:A:562:LEU:HD23	1:B:541:GLY:HA2	1.78	0.65
1:B:125:CYS:O	1:B:128:THR:HG22	1.97	0.65
1:A:152:LEU:HD22	1:A:319:GLU:OE2	1.97	0.64
1:B:133:MET:HE1	1:B:216:MET:HG3	1.79	0.64
1:A:499:LEU:HD11	1:A:528:ARG:HG3	1.80	0.64
1:B:434:LEU:HD11	1:B:467:MET:HE3	1.80	0.64
1:A:28:TRP:CG	1:B:90:THR:HG21	2.34	0.62
1:A:199:MET:HG3	1:A:317:LEU:HD22	1.82	0.62
1:A:310:LEU:HD11	1:A:321:PHE:HB2	1.81	0.61
1:B:126:ASP:OD1	3:B:703:MN:MN	1.56	0.60
1:A:90:THR:HG22	1:B:24:ILE:HG23	1.84	0.59
1:A:121:LEU:HD22	1:A:132:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HD12	1:B:127:KCX:HB2	1.85	0.59
1:B:203:THR:HB	4:B:704:CO2:O1	2.03	0.59
1:A:133:MET:HE1	1:A:216:MET:HG3	1.83	0.59
1:A:310:LEU:O	1:A:314:GLY:N	2.31	0.59
1:A:558:ASP:OD2	1:A:559:LEU:N	2.36	0.58
1:B:161:LEU:HD23	1:B:191:MET:HB2	1.85	0.58
1:A:100:ARG:HH11	1:A:280:HIS:HD2	1.50	0.58
1:A:44:VAL:HA	1:A:78:PHE:HB3	1.85	0.58
1:A:129:THR:OG1	1:A:130:PRO:HD3	2.03	0.58
1:A:440:GLY:HA2	1:A:447:MET:HG3	1.85	0.58
1:A:15:PHE:HB3	1:A:39:PHE:HB3	1.85	0.57
1:B:89:GLU:CD	1:B:126:ASP:OD1	2.47	0.57
1:B:124:GLY:H	1:B:128:THR:CG2	2.17	0.57
1:A:54:LEU:HD11	1:B:116:LEU:HD21	1.86	0.57
1:A:466:ASP:OD2	1:A:482:THR:HG23	2.05	0.57
1:B:14:TRP:CD2	1:B:115:PRO:HB3	2.39	0.57
1:A:420:ARG:NH2	1:A:502:ASP:OD1	2.26	0.56
1:A:14:TRP:CE2	1:B:93:ARG:HD2	2.41	0.56
1:B:21:ASP:HB3	1:B:25:TYR:CE2	2.40	0.56
1:A:53:GLU:OE1	1:B:69:LYS:HE2	2.06	0.56
1:B:417:MET:HE2	1:B:436:LEU:HD11	1.87	0.55
1:A:127:KCX:HZ	1:A:474:ARG:NH2	2.04	0.55
1:A:61:PHE:HA	1:A:64:LEU:HB2	1.88	0.55
1:B:519:VAL:HG21	1:B:527:ARG:NH1	2.22	0.55
1:B:428:VAL:HG13	1:B:459:ILE:HD11	1.89	0.55
1:B:15:PHE:HB3	1:B:39:PHE:HB3	1.88	0.55
1:A:84:VAL:HG11	1:A:107:VAL:HG12	1.88	0.54
1:B:420:ARG:HE	1:B:426:LEU:HD11	1.70	0.54
1:B:519:VAL:HG21	1:B:527:ARG:HH12	1.71	0.54
1:A:437:LYS:HD3	1:A:498:ALA:HA	1.88	0.54
1:B:121:LEU:HD22	1:B:132:LEU:HB3	1.88	0.54
1:A:44:VAL:HG12	1:A:117:ASP:OD2	2.07	0.54
1:B:176:ALA:HB2	1:B:460:LEU:HB3	1.90	0.54
1:B:127:KCX:O	1:B:130:PRO:HD2	2.08	0.54
1:A:48:CYS:SG	1:A:132:LEU:HD21	2.48	0.53
1:A:397:ALA:HB1	1:A:482:THR:HG22	1.90	0.53
1:A:28:TRP:NE1	2:B:702:FES:S2	2.81	0.53
1:B:35:PRO:HG2	1:B:38:GLN:HG2	1.90	0.53
1:A:188:GLU:OE1	1:B:26:ARG:NH1	2.42	0.53
1:B:224:ILE:HG22	1:B:322:TYR:CE2	2.42	0.53
1:A:455:LEU:HB2	1:A:460:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:N	1:A:390:ALA:O	2.39	0.53
1:A:221:ASN:HA	1:A:234:LEU:HD21	1.91	0.53
1:A:15:PHE:O	1:A:26:ARG:NH1	2.40	0.52
1:A:25:TYR:O	1:B:91:MET:HE1	2.09	0.52
1:A:441:PRO:HG3	1:A:447:MET:HE2	1.92	0.52
1:B:126:ASP:OD1	4:B:704:CO2:C	2.57	0.52
1:B:74:GLU:OE2	1:B:236:ARG:NH2	2.35	0.52
1:B:310:LEU:O	1:B:314:GLY:N	2.42	0.52
1:A:100:ARG:HH11	1:A:280:HIS:CD2	2.26	0.51
1:B:202:GLY:O	1:B:206:THR:HG23	2.10	0.51
1:A:51:PHE:HB2	1:A:61:PHE:HB2	1.92	0.51
1:A:453:MET:HE3	1:A:469:ARG:HB3	1.92	0.51
1:B:14:TRP:CG	1:B:115:PRO:HB3	2.46	0.51
1:B:282:LEU:HD23	1:B:292:LEU:HD23	1.93	0.51
1:B:449:GLU:OE2	1:B:476:SER:HA	2.11	0.51
1:A:29:MET:HG2	1:B:91:MET:HE3	1.92	0.50
1:B:127:KCX:OQ2	1:B:276:ASN:CB	2.59	0.50
1:A:126:ASP:OD2	1:A:203:THR:HB	2.12	0.50
1:B:447:MET:HG2	1:B:474:ARG:HG3	1.93	0.50
1:B:87:LEU:CD1	1:B:127:KCX:HB2	2.40	0.50
1:B:298:ASP:OD1	1:B:513:ARG:NE	2.34	0.50
1:B:437:LYS:HD3	1:B:497:LEU:O	2.12	0.50
1:B:343:LEU:HA	1:B:349:THR:HA	1.93	0.50
1:B:43:PRO:HB3	1:B:246:VAL:HG11	1.93	0.50
1:B:288:ILE:O	1:B:565:LYS:NZ	2.45	0.49
1:A:29:MET:HG2	1:B:91:MET:CE	2.42	0.49
1:B:333:GLU:OE2	1:B:362:ARG:NH1	2.40	0.49
1:A:215:GLY:O	1:A:345:VAL:HG23	2.12	0.49
1:A:151:MET:HG2	1:A:197:HIS:O	2.13	0.49
1:A:37:ASP:O	1:A:40:ASP:HB2	2.13	0.48
1:A:309:ASP:OD2	6:A:701:HOH:O	2.20	0.48
1:A:428:VAL:HG23	1:A:432:CYS:HB2	1.95	0.48
1:A:125:CYS:O	1:A:128:THR:OG1	2.26	0.48
1:A:17:ARG:NH2	1:A:573:ASP:OD2	2.45	0.47
1:A:349:THR:HG22	1:A:352:ASP:OD2	2.15	0.47
1:A:434:LEU:HB2	1:A:469:ARG:HG2	1.97	0.47
1:B:258:ARG:HH22	1:B:296:ASP:CG	2.23	0.47
1:A:82:PHE:HB3	1:B:54:LEU:HD12	1.97	0.47
1:A:298:ASP:O	1:A:303:LYS:NZ	2.44	0.47
1:A:346:ASN:HD21	1:A:353:ASN:CG	2.23	0.46
1:B:57:CYS:SG	1:B:197:HIS:HA	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:O	1:B:70:ILE:HG13	2.14	0.46
1:B:127:KCX:C	1:B:130:PRO:HD2	2.46	0.46
1:B:203:THR:CB	4:B:704:CO2:O1	2.62	0.46
1:B:331:ILE:HD13	1:B:350:LEU:HD21	1.98	0.46
1:A:162:GLY:N	1:A:166:ASP:OD1	2.41	0.46
1:A:109:GLU:HB3	1:B:99:PHE:CE2	2.51	0.46
1:A:144:ILE:HG22	1:A:242:ILE:HD13	1.98	0.46
1:A:197:HIS:NE2	1:A:205:SER:OG	2.41	0.46
1:A:89:GLU:OE2	1:A:126:ASP:CB	2.62	0.46
1:A:127:KCX:HD3	1:A:127:KCX:N	2.30	0.46
1:A:17:ARG:NH1	1:B:93:ARG:HH22	2.14	0.46
1:A:161:LEU:HD11	1:A:187:ALA:HB1	1.97	0.46
1:B:140:ASP:OD1	1:B:253:SER:OG	2.27	0.46
1:B:285:ALA:HA	1:B:288:ILE:HG22	1.98	0.45
1:B:455:LEU:HG	1:B:467:MET:HE2	1.97	0.45
1:A:477:GLY:H	4:A:603:CO2:C	2.30	0.45
1:B:501:GLN:HB2	1:B:527:ARG:HH21	1.81	0.45
1:B:112:ARG:NH1	1:B:567:GLY:O	2.49	0.45
1:A:90:THR:HG22	1:B:24:ILE:CG2	2.46	0.45
1:A:123:MET:O	1:A:147:SER:HA	2.17	0.45
1:A:127:KCX:OQ2	1:A:276:ASN:ND2	2.49	0.45
1:A:327:VAL:HG22	1:A:328:PRO:HD3	1.98	0.45
1:A:151:MET:HG3	1:A:199:MET:HE2	1.98	0.45
1:A:26:ARG:NH2	1:B:188:GLU:OE1	2.45	0.45
1:A:163:SER:HB3	1:A:198:CYS:SG	2.56	0.45
1:B:224:ILE:HG12	1:B:231:ARG:NH2	2.32	0.45
1:B:440:GLY:HA2	1:B:447:MET:HG3	1.97	0.45
1:A:55:THR:HG21	1:A:86:SER:OG	2.17	0.45
1:B:476:SER:HA	4:B:704:CO2:O2	2.17	0.44
1:A:340:ARG:O	1:A:349:THR:OG1	2.28	0.44
1:B:308:VAL:HA	1:B:364:VAL:O	2.17	0.44
1:A:67:GLN:HG3	1:A:232:ASN:HB3	1.98	0.44
1:A:35:PRO:HB2	1:A:37:ASP:OD1	2.17	0.44
1:A:123:MET:SD	1:A:129:THR:HG22	2.57	0.44
1:A:265:ILE:HD11	1:A:292:LEU:HD11	2.00	0.44
1:A:285:ALA:HA	1:A:288:ILE:HG22	2.00	0.43
1:A:106:ASP:HA	1:B:85:MET:HE3	2.00	0.43
1:B:477:GLY:H	4:B:704:CO2:C	2.32	0.43
1:A:14:TRP:CD2	1:A:115:PRO:HB3	2.53	0.43
1:A:52:SER:CB	1:B:83:PRO:HD3	2.39	0.43
1:A:351:TRP:O	1:A:355:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:OD1	6:A:702:HOH:O	2.21	0.43
1:A:152:LEU:H	1:A:194:SER:HG	1.66	0.43
1:A:442:ARG:HD3	1:A:547:VAL:O	2.18	0.43
1:A:21:ASP:HB3	1:A:25:TYR:CE1	2.53	0.43
1:A:123:MET:HB2	1:A:129:THR:HG22	2.00	0.43
1:B:201:MET:HE2	1:B:271:ILE:HD12	2.01	0.43
1:B:520:SER:OG	1:B:523:GLU:N	2.43	0.43
1:A:511:ALA:O	1:A:513:ARG:NH1	2.52	0.43
1:B:123:MET:HB3	1:B:129:THR:HA	2.01	0.43
1:B:356:ASP:OD2	1:B:356:ASP:N	2.48	0.43
1:B:517:LEU:HG	1:B:519:VAL:HG12	2.00	0.43
1:A:29:MET:SD	1:B:56:PRO:HG3	2.59	0.43
1:A:212:GLU:OE2	1:A:220:GLY:N	2.41	0.43
1:A:15:PHE:CG	1:A:39:PHE:HD1	2.37	0.43
1:A:415:GLU:OE2	1:A:415:GLU:N	2.35	0.43
1:A:421:MET:HE1	1:A:434:LEU:HD23	2.01	0.43
1:B:206:THR:HG21	1:B:274:SER:N	2.22	0.43
1:B:574:ASN:OD1	1:B:574:ASN:N	2.40	0.43
1:A:127:KCX:HG2	6:A:718:HOH:O	2.19	0.42
1:A:154:GLY:O	1:A:160:GLU:HA	2.19	0.42
1:B:8:VAL:HG23	1:B:9:ARG:H	1.83	0.42
1:B:352:ASP:HA	1:B:355:LYS:HD3	2.01	0.42
1:B:148:GLY:O	1:B:231:ARG:HD3	2.19	0.42
1:A:127:KCX:C	1:A:130:PRO:HD2	2.49	0.42
1:A:410:VAL:O	1:A:420:ARG:NH1	2.52	0.42
1:A:87:LEU:HD13	1:A:127:KCX:HB2	2.02	0.42
1:A:121:LEU:HB3	1:A:123:MET:HE3	2.02	0.42
1:B:129:THR:HG21	1:B:207:MET:HB3	2.02	0.42
1:A:44:VAL:HG13	1:A:117:ASP:H	1.85	0.42
1:B:51:PHE:HB2	1:B:61:PHE:HB2	2.02	0.42
1:B:130:PRO:HB3	1:B:280:HIS:HB3	2.02	0.42
1:A:218:LEU:HB2	1:A:234:LEU:HD11	2.00	0.42
1:A:281:LEU:HB2	1:A:297:TRP:HZ2	1.85	0.41
1:A:434:LEU:HD22	1:A:469:ARG:HG2	2.01	0.41
1:B:142:PRO:HD3	1:B:251:VAL:HG12	2.01	0.41
1:B:407:ARG:NH2	1:B:427:ASP:O	2.38	0.41
1:B:238:SER:O	1:B:242:ILE:HG22	2.20	0.41
1:A:303:LYS:HB2	1:A:303:LYS:HE2	1.80	0.41
1:B:514:LYS:NZ	6:B:803:HOH:O	2.35	0.41
1:A:63:THR:O	1:A:67:GLN:HG2	2.20	0.41
1:A:415:GLU:H	1:A:415:GLU:CD	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:PRO:HD2	1:B:224:ILE:O	2.20	0.41
1:A:157:ARG:HH12	1:A:183:GLU:HG3	1.85	0.41
1:B:107:VAL:HG21	1:B:132:LEU:HA	2.02	0.41
1:A:51:PHE:O	1:B:83:PRO:HG3	2.21	0.41
1:B:151:MET:HG3	1:B:197:HIS:O	2.20	0.41
1:A:123:MET:HB2	1:A:129:THR:CG2	2.51	0.41
1:B:424:GLU:CD	1:B:461:ARG:HH12	2.28	0.41
1:A:107:VAL:HG23	1:A:135:GLY:HA3	2.03	0.41
1:B:420:ARG:HE	1:B:426:LEU:CD1	2.33	0.41
1:A:14:TRP:NE1	1:B:93:ARG:HD2	2.36	0.41
1:B:60:HIS:HB3	1:B:195:HIS:CG	2.56	0.41
1:A:151:MET:SD	1:A:192:HIS:HD2	2.44	0.40
1:B:111:ILE:HA	1:B:116:LEU:HD12	2.03	0.40
1:B:89:GLU:OE2	1:B:126:ASP:OD1	2.38	0.40
1:B:490:GLU:HG2	1:B:552:GLN:HE22	1.87	0.40
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.93	0.40
1:A:143:THR:HB	1:A:252:MET:HG2	2.03	0.40
1:A:543:VAL:O	1:A:547:VAL:HG23	2.20	0.40
1:B:359:ASN:ND2	1:B:362:ARG:HG2	2.36	0.40
1:B:457:PRO:O	1:B:461:ARG:HG3	2.21	0.40
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.89	0.40
1:B:372:PHE:CZ	1:B:373:LYS:HE2	2.56	0.40
1:A:87:LEU:CD1	1:A:127:KCX:HB2	2.51	0.40
1:A:245:MET:O	1:A:249:ASP:N	2.54	0.40
1:A:262:GLU:O	1:A:266:ARG:HG3	2.21	0.40
1:B:170:MET:HG2	1:B:179:MET:HE1	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	567/575 (99%)	530 (94%)	34 (6%)	3 (0%)	24	46
1	B	565/575 (98%)	535 (95%)	28 (5%)	2 (0%)	30	51
All	All	1132/1150 (98%)	1065 (94%)	62 (6%)	5 (0%)	30	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	ASP
1	B	126	ASP
1	A	126	ASP
1	B	124	GLY
1	A	124	GLY

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	450/461 (98%)	435 (97%)	15 (3%)	33	61
1	B	450/461 (98%)	435 (97%)	15 (3%)	33	61
All	All	900/922 (98%)	870 (97%)	30 (3%)	33	61

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

Mol	Chain	Res	Type
1	A	8	VAL
1	A	52	SER
1	A	141	LEU
1	A	163	SER
1	A	175	ARG
1	A	234	LEU
1	A	327	VAL
1	A	338	ILE
1	A	364	VAL
1	A	385	LEU
1	A	401	LEU

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Mol	Chain	Res	Type
1	A	412	GLU
1	A	414	SER
1	A	482	THR
1	A	502	ASP
1	B	8	VAL
1	B	64	LEU
1	B	89	GLU
1	B	91	MET
1	B	123	MET
1	B	131	SER
1	B	161	LEU
1	B	171	SER
1	B	224	ILE
1	B	233	LEU
1	B	267	VAL
1	B	426	LEU
1	B	447	MET
1	B	458	LYS
1	B	464	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	HIS
1	A	366	HIS
1	B	12	GLN
1	B	38	GLN
1	B	348	GLN
1	B	438	ASN
1	B	551	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	KCX	B	127	3,1	10,11,12	1.98	1 (10%)	6,12,14	4.66	1 (16%)
1	KCX	A	127	3,1	10,11,12	1.79	1 (10%)	6,12,14	2.89	1 (16%)

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
1	KCX	B	127	3,1	-	5/9/10/12	-
1	KCX	A	127	3,1	-	6/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	KCX	OQ1-CX	5.67	1.32	1.21
1	A	127	KCX	OQ1-CX	5.19	1.31	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	KCX	OQ1-CX-NZ	-11.40	107.60	124.92
1	A	127	KCX	OQ1-CX-NZ	-6.98	114.32	124.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	127	KCX	OQ1-CX-NZ-CE
1	A	127	KCX	OQ2-CX-NZ-CE
1	B	127	KCX	C-CA-CB-CG
1	B	127	KCX	OQ1-CX-NZ-CE
1	B	127	KCX	OQ2-CX-NZ-CE
1	B	127	KCX	CE-CD-CG-CB
1	A	127	KCX	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	A	127	KCX	CE-CD-CG-CB
1	A	127	KCX	C-CA-CB-CG
1	A	127	KCX	CG-CD-CE-NZ
1	B	127	KCX	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	127	KCX	6	0
1	A	127	KCX	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 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	$\# Z > 2$
4	CO2	A	604	-	2,2,2	1.08	0	1,1,1	0.51	0
2	FES	A	601	-	0,4,4	-	-	-	-	-
5	BCT	B	701	-	3,3,3	2.25	1 (33%)	2,3,3	0.12	0
4	CO2	A	603	3	2,2,2	1.08	0	1,1,1	0.49	0
4	CO2	B	704	3	2,2,2	0.87	0	1,1,1	0.51	0
2	FES	B	702	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
2	FES	B	702	1	-	-	0/1/1/1
2	FES	A	601	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	BCT	O1-C	3.64	1.38	1.25

There are no bond angle outliers.

There are no chirality outliers.

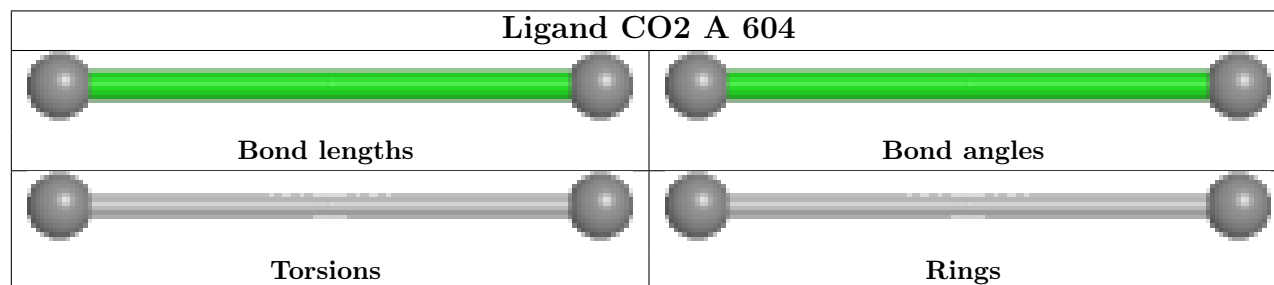
There are no torsion outliers.

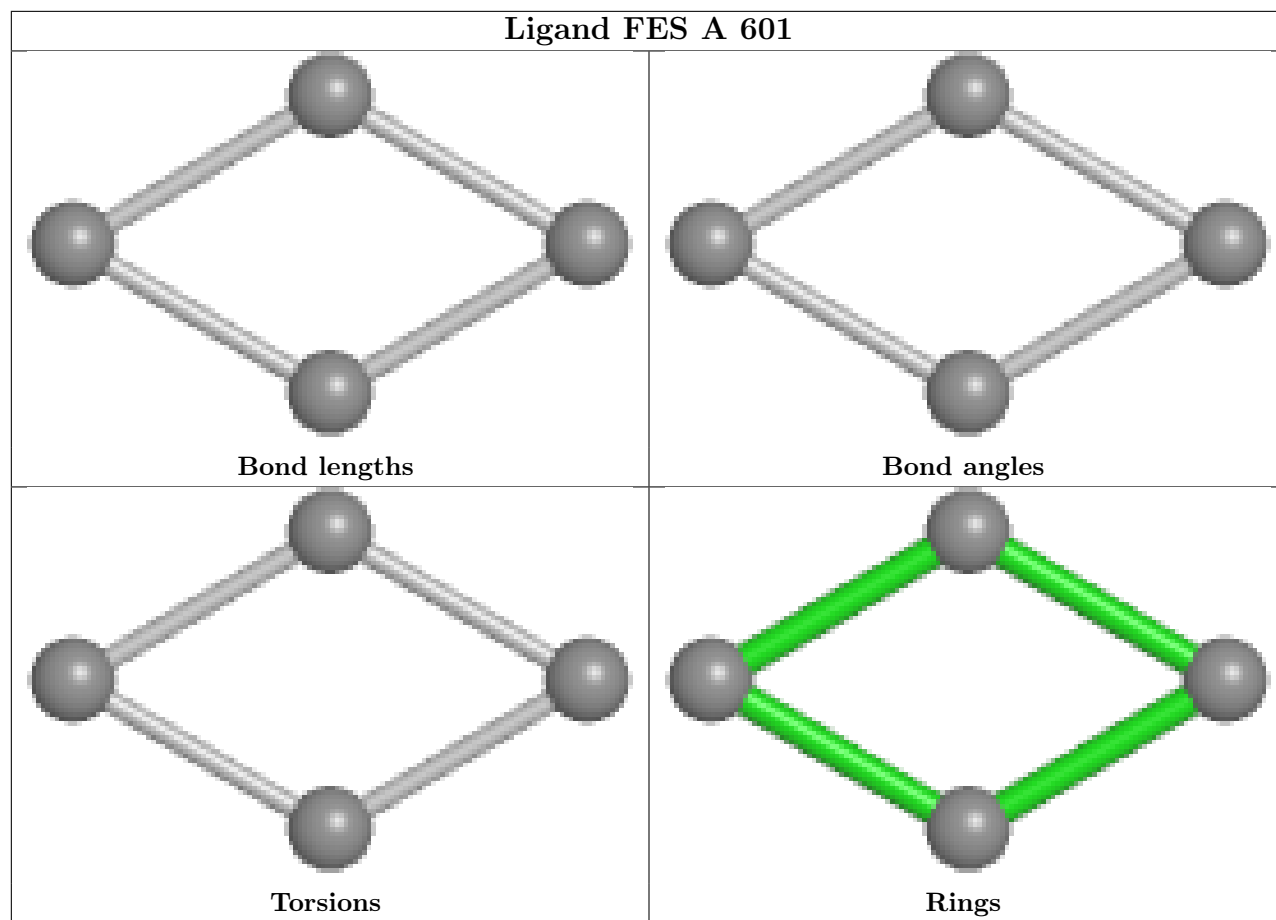
There are no ring outliers.

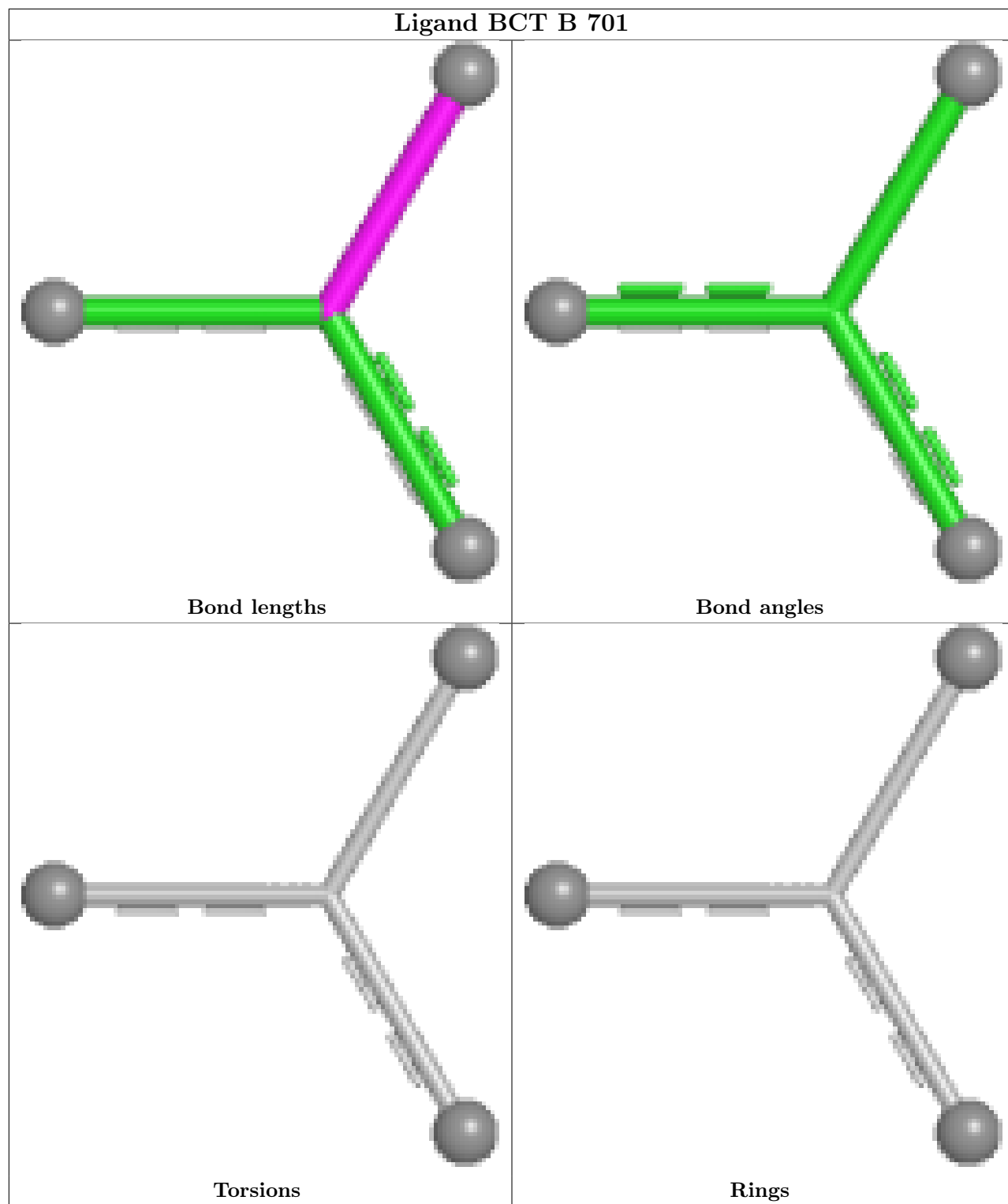
3 monomers are involved in 7 short contacts:

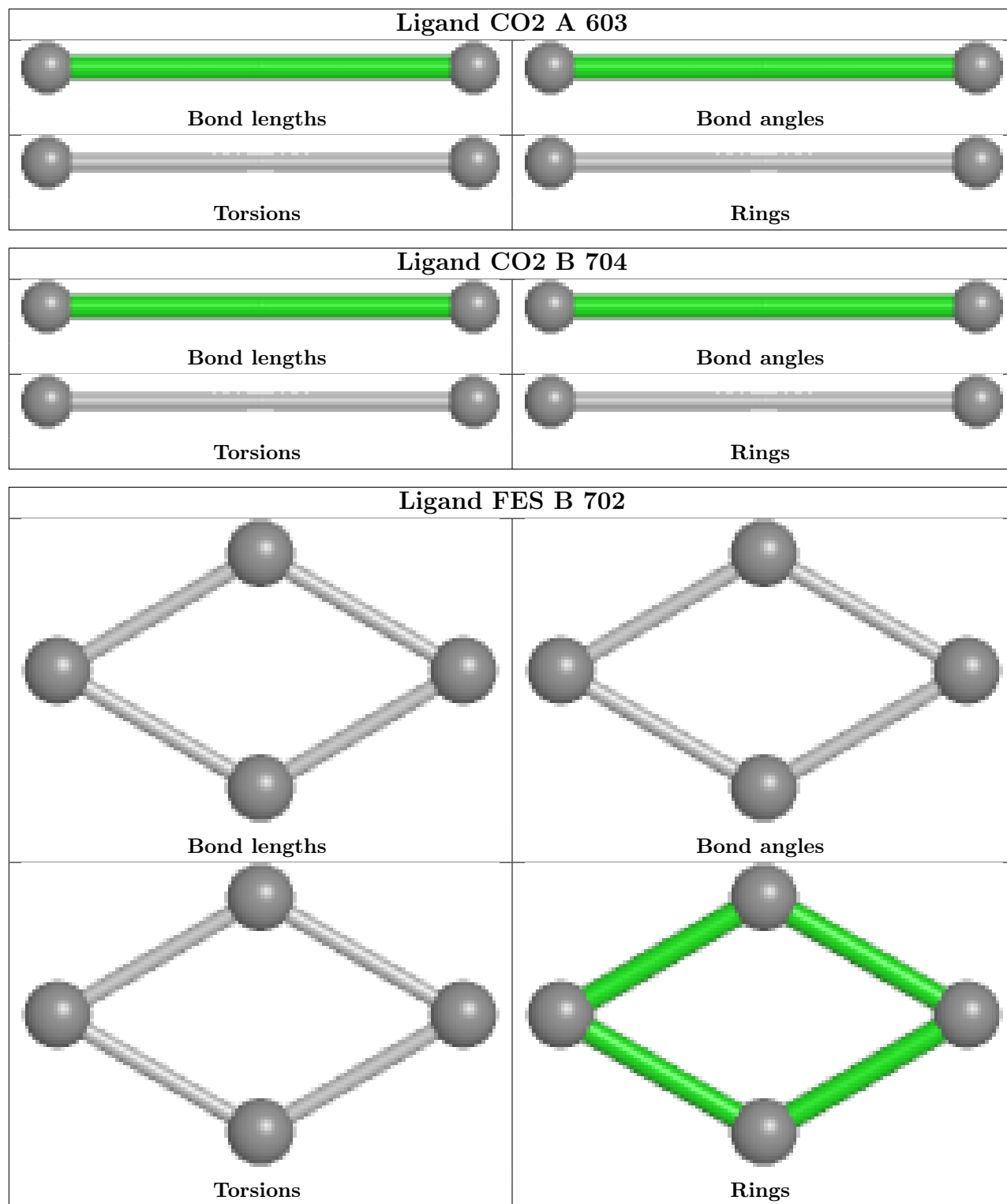
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	CO2	1	0
4	B	704	CO2	5	0
2	B	702	FES	1	0

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 ⓘ

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	568/575 (98%)	1.65	177 (31%)	1 1	41, 62, 83, 95	1 (0%)
1	B	567/575 (98%)	1.84	220 (38%)	1 0	37, 57, 75, 94	0
All	All	1135/1150 (98%)	1.75	397 (34%)	1 1	37, 59, 80, 95	1 (0%)

All (397) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	557	ALA	6.6
1	A	317	LEU	6.4
1	B	556	GLY	5.9
1	B	148	GLY	5.9
1	B	204	ALA	5.9
1	B	73	TRP	5.7
1	B	550	VAL	5.4
1	B	70	ILE	5.2
1	A	137	ALA	5.1
1	B	44	VAL	5.1
1	B	67	GLN	5.0
1	B	66	GLU	5.0
1	A	557	ALA	4.9
1	B	553	ALA	4.9
1	B	232	ASN	4.9
1	B	27	SER	4.8
1	B	129	THR	4.8
1	A	279	ILE	4.7
1	B	128	THR	4.7
1	A	174	VAL	4.6
1	B	446	GLY	4.6
1	B	79	PRO	4.6
1	B	315	THR	4.5
1	A	225	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	4.4
1	B	149	GLY	4.4
1	B	80	LEU	4.4
1	A	448	ALA	4.4
1	B	568	ALA	4.3
1	B	196	GLY	4.3
1	B	139	CYS	4.2
1	B	136	ALA	4.2
1	B	76	GLY	4.2
1	B	69	LYS	4.2
1	B	549	HIS	4.2
1	A	53	GLU	4.1
1	B	46	GLY	4.1
1	B	14	TRP	4.1
1	A	97	MET	4.1
1	B	447	MET	4.1
1	B	269	ALA	4.1
1	B	270	ALA	4.1
1	B	84	VAL	4.0
1	A	131	SER	4.0
1	A	476	SER	4.0
1	B	81	GLU	4.0
1	B	211	VAL	3.9
1	B	150	PRO	3.9
1	B	311	GLN	3.9
1	B	343	LEU	3.9
1	A	135	GLY	3.9
1	A	318	MET	3.9
1	B	233	LEU	3.9
1	B	314	GLY	3.8
1	B	131	SER	3.8
1	B	441	PRO	3.8
1	B	226	ALA	3.8
1	B	268	ASN	3.7
1	A	555	LEU	3.7
1	B	71	GLY	3.7
1	B	229	ALA	3.7
1	B	78	PHE	3.7
1	B	344	THR	3.7
1	A	483	VAL	3.7
1	B	24	ILE	3.6
1	B	63	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	349	THR	3.6
1	B	65	ALA	3.6
1	B	130	PRO	3.6
1	A	104	SER	3.6
1	B	206	THR	3.6
1	B	45	ILE	3.6
1	B	558	ASP	3.6
1	B	542	TRP	3.6
1	A	473	ALA	3.5
1	B	519	VAL	3.5
1	B	208	ALA	3.5
1	B	30	LYS	3.5
1	B	56	PRO	3.5
1	B	546	TYR	3.5
1	B	320	ASP	3.5
1	B	559	LEU	3.5
1	A	111	ILE	3.5
1	A	321	PHE	3.5
1	B	116	LEU	3.5
1	B	322	TYR	3.4
1	A	75	SER	3.4
1	B	98	LEU	3.4
1	A	208	ALA	3.4
1	A	481	GLY	3.4
1	A	227	VAL	3.4
1	A	475	MET	3.4
1	A	80	LEU	3.4
1	B	72	VAL	3.4
1	A	292	LEU	3.3
1	B	74	GLU	3.3
1	B	236	ARG	3.3
1	B	197	HIS	3.3
1	B	272	GLY	3.3
1	A	213	ALA	3.3
1	B	34	ILE	3.3
1	A	322	TYR	3.3
1	A	28	TRP	3.3
1	A	205	SER	3.3
1	A	305	PRO	3.3
1	B	60	HIS	3.3
1	A	550	VAL	3.3
1	A	64	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	64	LEU	3.2
1	B	310	LEU	3.2
1	A	549	HIS	3.2
1	B	135	GLY	3.2
1	A	184	PHE	3.2
1	A	510	VAL	3.2
1	B	47	ILE	3.2
1	A	62	ARG	3.2
1	B	574	ASN	3.2
1	A	181	GLN	3.2
1	A	136	ALA	3.2
1	B	147	SER	3.2
1	B	25	TYR	3.2
1	A	505	ILE	3.2
1	B	515	LEU	3.2
1	B	213	ALA	3.2
1	B	279	ILE	3.2
1	B	120	VAL	3.2
1	B	156	PHE	3.2
1	B	363	GLU	3.1
1	B	222	ALA	3.1
1	A	405	LYS	3.1
1	A	16	GLY	3.1
1	A	33	GLY	3.1
1	A	220	GLY	3.1
1	A	556	GLY	3.1
1	B	223	ALA	3.1
1	B	295	ALA	3.1
1	B	575	HIS	3.1
1	B	567	GLY	3.1
1	A	364	VAL	3.1
1	A	447	MET	3.1
1	B	350	LEU	3.0
1	A	88	GLY	3.0
1	B	111	ILE	3.0
1	B	144	ILE	3.0
1	B	18	LEU	3.0
1	B	551	GLN	3.0
1	A	477	GLY	3.0
1	A	527	ARG	3.0
1	B	118	GLY	3.0
1	B	241	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	23	PHE	3.0
1	B	321	PHE	3.0
1	A	545	LEU	3.0
1	A	203	THR	3.0
1	A	325	GLY	3.0
1	B	203	THR	3.0
1	B	187	ALA	3.0
1	A	459	ILE	3.0
1	A	176	ALA	3.0
1	B	316	HIS	2.9
1	A	24	ILE	2.9
1	A	162	GLY	2.9
1	B	146	VAL	2.9
1	B	468	VAL	2.9
1	B	381	LEU	2.9
1	A	198	CYS	2.9
1	B	273	GLY	2.9
1	B	569	GLY	2.9
1	A	533	ALA	2.9
1	B	324	ALA	2.9
1	B	11	SER	2.9
1	B	52	SER	2.9
1	A	331	ILE	2.9
1	B	271	ILE	2.9
1	B	16	GLY	2.9
1	A	497	LEU	2.9
1	A	210	MET	2.9
1	B	29	MET	2.9
1	A	406	GLY	2.9
1	B	165	THR	2.9
1	A	518	HIS	2.9
1	A	542	TRP	2.8
1	A	553	ALA	2.8
1	B	55	THR	2.8
1	B	141	LEU	2.8
1	B	396	ALA	2.8
1	A	327	VAL	2.8
1	B	185	PHE	2.8
1	A	250	LEU	2.8
1	B	200	THR	2.8
1	B	283	ALA	2.8
1	A	215	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	517	LEU	2.8
1	B	317	LEU	2.8
1	B	113	GLY	2.8
1	A	182	GLU	2.8
1	B	39	PHE	2.8
1	B	62	ARG	2.8
1	A	239	GLY	2.7
1	B	77	GLY	2.7
1	A	201	MET	2.7
1	A	101	ASN	2.7
1	A	272	GLY	2.7
1	A	63	THR	2.7
1	A	193	ARG	2.7
1	A	547	VAL	2.7
1	B	100	ARG	2.7
1	B	561	PHE	2.7
1	A	436	LEU	2.7
1	B	102	LEU	2.7
1	B	440	GLY	2.7
1	A	435	VAL	2.7
1	B	96	ALA	2.7
1	A	502	ASP	2.7
1	A	546	TYR	2.7
1	A	134	MET	2.7
1	A	71	GLY	2.7
1	B	323	TYR	2.6
1	A	218	LEU	2.6
1	B	292	LEU	2.6
1	A	488	ALA	2.6
1	A	206	THR	2.6
1	B	255	ILE	2.6
1	A	143	THR	2.6
1	B	61	PHE	2.6
1	B	207	MET	2.6
1	A	541	GLY	2.6
1	B	57	CYS	2.6
1	A	264	ALA	2.6
1	B	267	VAL	2.6
1	A	429	ASP	2.6
1	A	474	ARG	2.6
1	A	103	ALA	2.6
1	A	130	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	452	ASN	2.6
1	A	563	ARG	2.5
1	A	36	HIS	2.5
1	A	380	VAL	2.5
1	B	371	PRO	2.5
1	A	204	ALA	2.5
1	B	95	THR	2.5
1	B	331	ILE	2.5
1	A	290	VAL	2.5
1	A	59	SER	2.5
1	A	291	ASP	2.5
1	A	65	ALA	2.5
1	A	105	MET	2.5
1	B	277	ALA	2.5
1	A	168	TRP	2.5
1	A	558	ASP	2.5
1	B	162	GLY	2.5
1	B	479	ALA	2.5
1	A	124	GLY	2.4
1	A	207	MET	2.4
1	B	22	GLY	2.4
1	B	541	GLY	2.4
1	B	242	ILE	2.4
1	A	209	SER	2.4
1	B	291	ASP	2.4
1	B	481	GLY	2.4
1	B	82	PHE	2.4
1	A	152	LEU	2.4
1	A	310	LEU	2.4
1	B	464	ILE	2.4
1	B	28	TRP	2.4
1	B	108	GLU	2.4
1	B	228	ASP	2.4
1	B	115	PRO	2.4
1	A	107	VAL	2.4
1	B	547	VAL	2.4
1	A	324	ALA	2.4
1	B	42	ARG	2.4
1	A	334	LEU	2.4
1	A	524	LEU	2.4
1	B	218	LEU	2.4
1	A	200	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	280	HIS	2.4
1	A	466	ASP	2.4
1	A	139	CYS	2.4
1	A	113	GLY	2.4
1	A	383	GLY	2.4
1	A	428	VAL	2.4
1	B	448	ALA	2.4
1	A	214	LEU	2.3
1	B	133	MET	2.3
1	B	445	PRO	2.3
1	B	571	PRO	2.3
1	A	326	GLY	2.3
1	B	68	VAL	2.3
1	A	401	LEU	2.3
1	A	31	ASN	2.3
1	B	201	MET	2.3
1	A	155	LYS	2.3
1	B	395	SER	2.3
1	A	551	GLN	2.3
1	B	154	GLY	2.3
1	B	193	ARG	2.3
1	B	288	ILE	2.3
1	B	318	MET	2.3
1	A	14	TRP	2.3
1	B	12	GLN	2.3
1	A	161	LEU	2.3
1	A	559	LEU	2.3
1	A	379	ALA	2.3
1	A	95	THR	2.3
1	A	414	SER	2.3
1	B	41	GLY	2.3
1	B	495	GLY	2.3
1	B	543	VAL	2.3
1	A	187	ALA	2.2
1	B	284	ILE	2.2
1	B	252	MET	2.2
1	A	507	GLU	2.2
1	B	43	PRO	2.2
1	B	189	SER	2.2
1	A	433	VAL	2.2
1	A	271	ILE	2.2
1	A	464	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	10	ARG	2.2
1	A	147	SER	2.2
1	A	148	GLY	2.2
1	A	202	GLY	2.2
1	B	214	LEU	2.2
1	A	84	VAL	2.2
1	A	82	PHE	2.2
1	B	85	MET	2.2
1	A	354	CYS	2.2
1	B	17	ARG	2.2
1	A	150	PRO	2.2
1	A	372	PHE	2.2
1	A	357	ALA	2.2
1	A	522	GLU	2.2
1	B	387	PRO	2.2
1	B	301	GLY	2.2
1	B	467	MET	2.2
1	A	47	ILE	2.2
1	A	146	VAL	2.2
1	A	280	HIS	2.2
1	A	404	HIS	2.2
1	A	470	VAL	2.2
1	B	278	VAL	2.2
1	B	15	PHE	2.2
1	A	212	GLU	2.1
1	A	159	ARG	2.1
1	B	386	CYS	2.1
1	A	114	ASN	2.1
1	B	87	LEU	2.1
1	B	517	LEU	2.1
1	A	224	ILE	2.1
1	A	319	GLU	2.1
1	B	360	TRP	2.1
1	A	482	THR	2.1
1	B	90	THR	2.1
1	A	373	LYS	2.1
1	B	83	PRO	2.1
1	A	199	MET	2.1
1	B	105	MET	2.1
1	B	199	MET	2.1
1	B	281	LEU	2.1
1	B	309	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	163	SER	2.1
1	A	226	ALA	2.1
1	B	539	ALA	2.1
1	B	251	VAL	2.1
1	B	459	ILE	2.1
1	B	19	ASP	2.1
1	B	126	ASP	2.1
1	B	560	ASP	2.1
1	B	235	ALA	2.1
1	A	83	PRO	2.1
1	B	35	PRO	2.1
1	A	12	GLN	2.1
1	A	300	LEU	2.1
1	B	545	LEU	2.1
1	A	554	ASN	2.1
1	A	60	HIS	2.1
1	B	306	CYS	2.1
1	A	34	ILE	2.1
1	A	395	SER	2.0
1	B	238	SER	2.0
1	A	115	PRO	2.0
1	B	234	LEU	2.0
1	B	499	LEU	2.0
1	A	446	GLY	2.0
1	B	124	GLY	2.0
1	A	468	VAL	2.0
1	B	483	VAL	2.0
1	A	548	GLU	2.0
1	B	341	ASP	2.0
1	B	421	MET	2.0
1	A	92	LEU	2.0
1	B	122	LEU	2.0
1	A	384	ASN	2.0
1	B	224	ILE	2.0
1	B	431	ASN	2.0
1	B	119	VAL	2.0
1	B	332	ARG	2.0

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

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
1	KCX	B	127	12/13	0.72	0.22	49,56,66,72	0
1	KCX	A	127	12/13	0.77	0.14	54,58,66,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

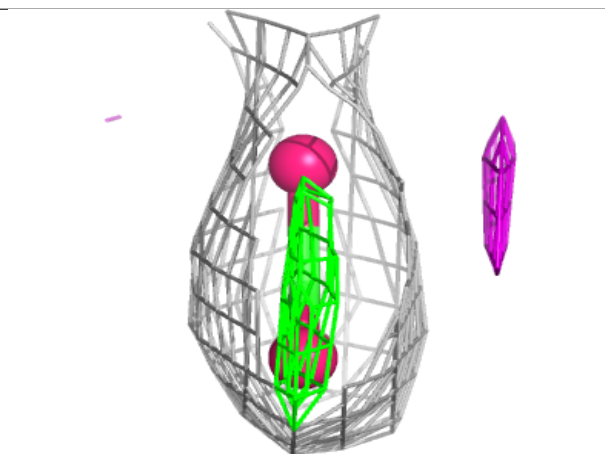
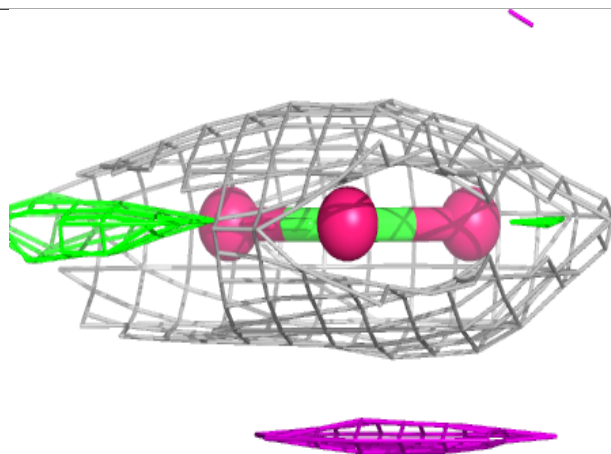
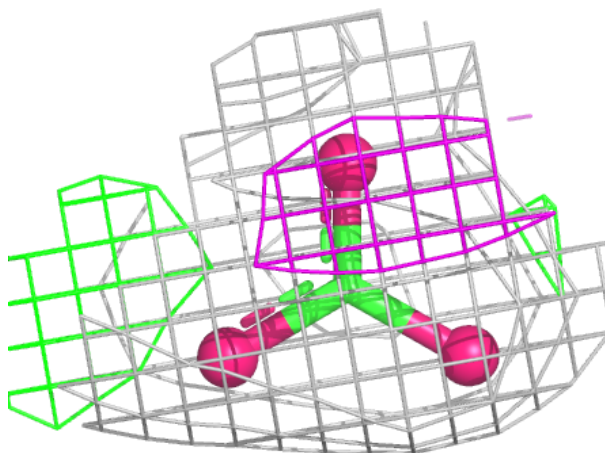
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BCT	B	701	4/4	0.66	0.29	56,66,67,71	0
4	CO2	A	603	3/3	0.70	0.22	56,56,64,65	0
4	CO2	A	604	3/3	0.75	0.21	58,58,64,65	0
4	CO2	B	704	3/3	0.81	0.11	66,66,66,70	0
2	FES	B	702	4/4	0.89	0.11	59,62,65,72	4
3	MN	A	602	1/1	0.89	0.09	71,71,71,71	0
2	FES	A	601	4/4	0.94	0.07	63,67,76,77	0
3	MN	B	703	1/1	0.98	0.08	73,73,73,73	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.

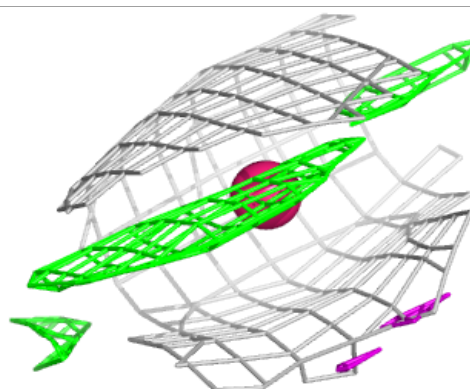
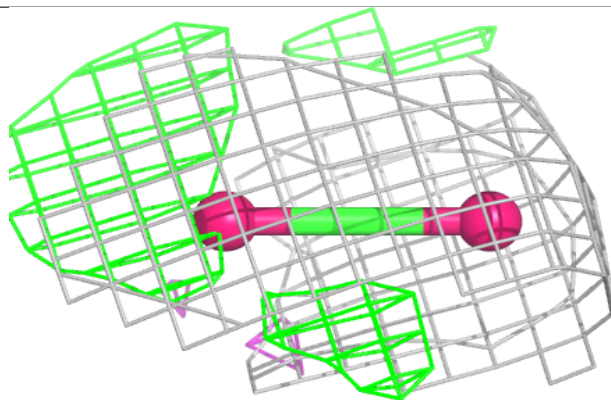
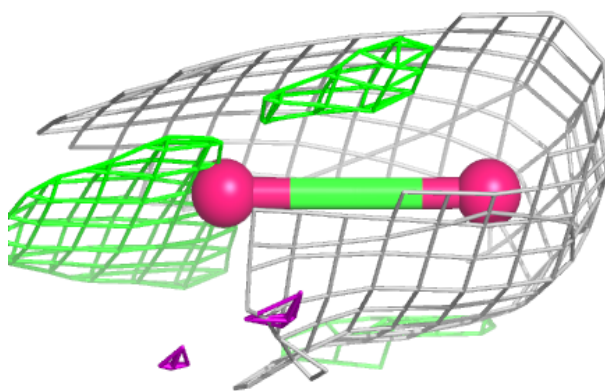
Electron density around BCT B 701:

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

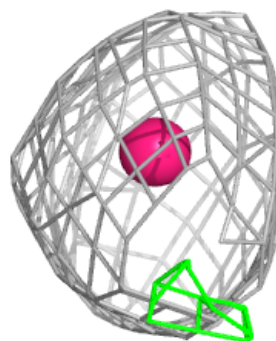
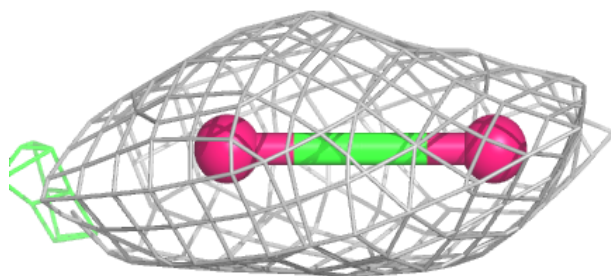
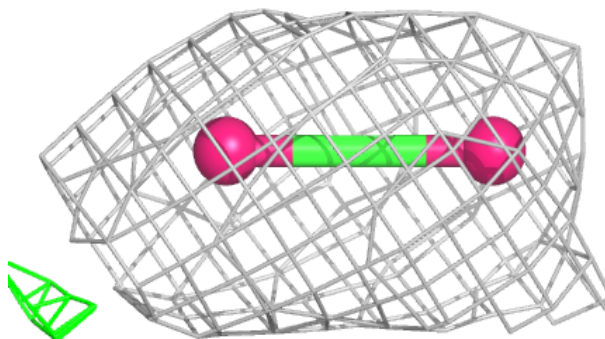


Electron density around CO2 A 603:

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

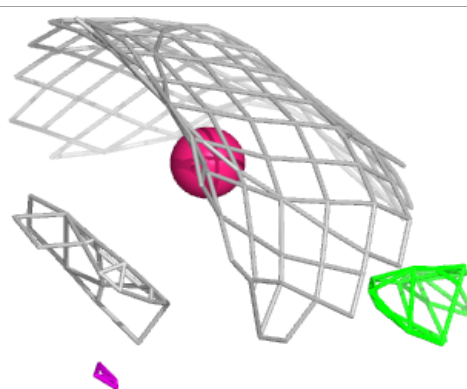
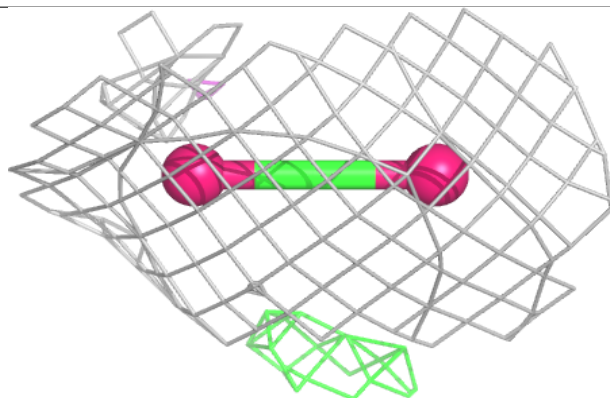
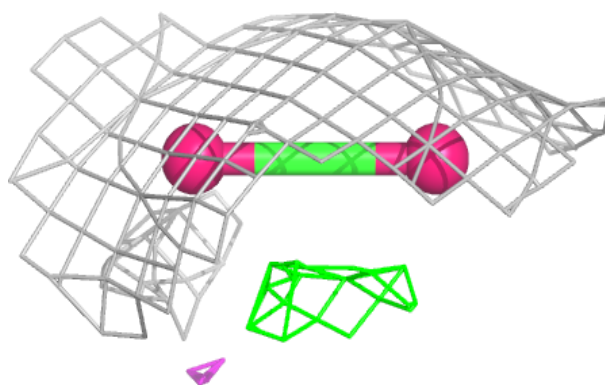
**Electron density around CO2 A 604:**

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



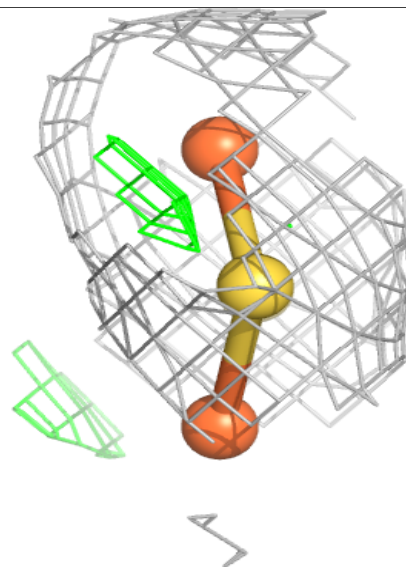
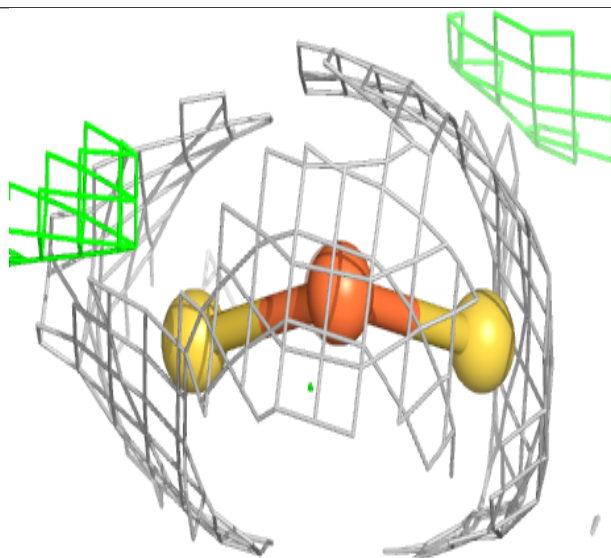
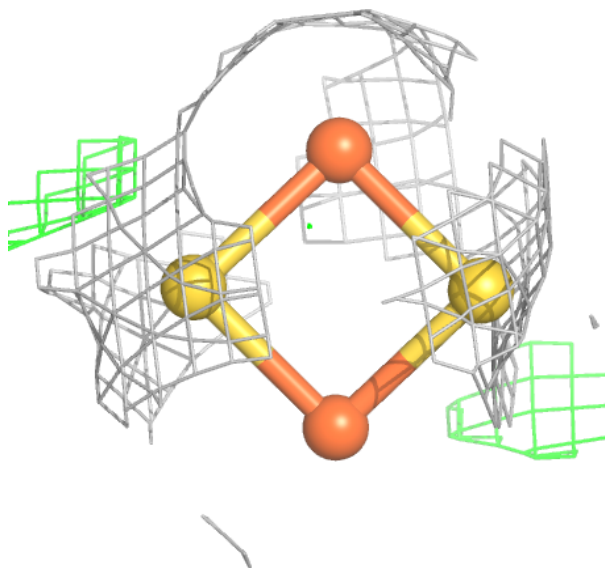
Electron density around CO2 B 704:

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



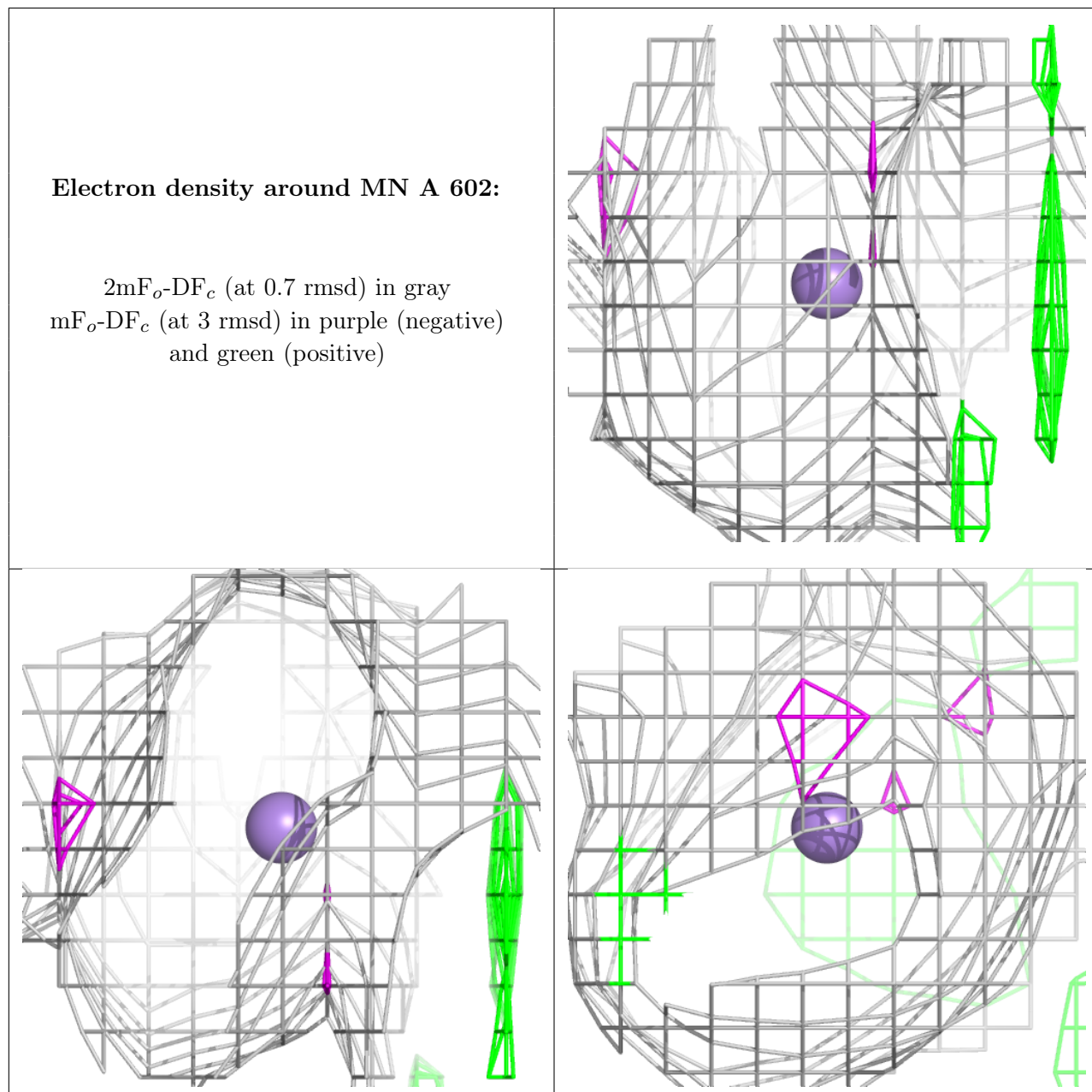
Electron density around FES B 702:

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



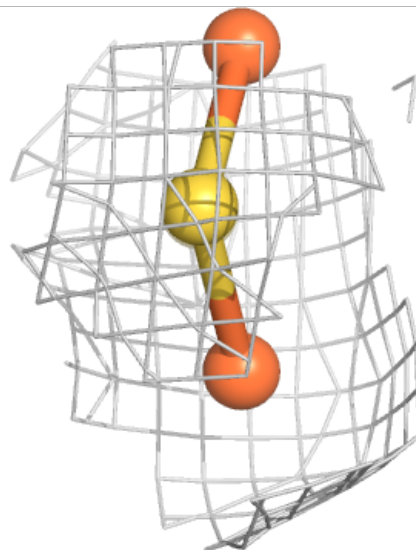
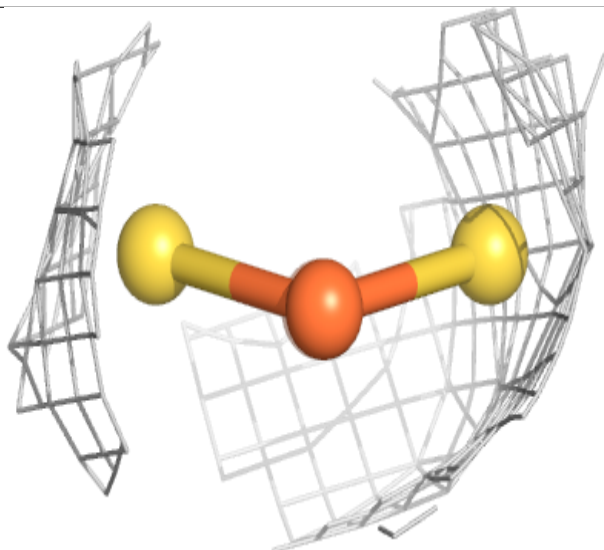
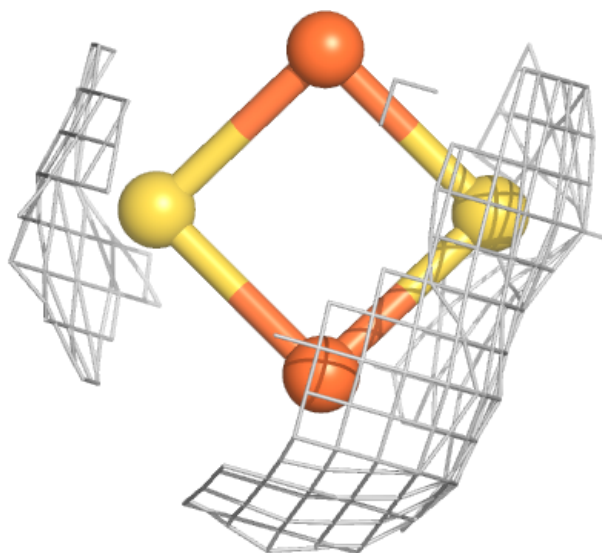
Electron density around MN A 602:

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



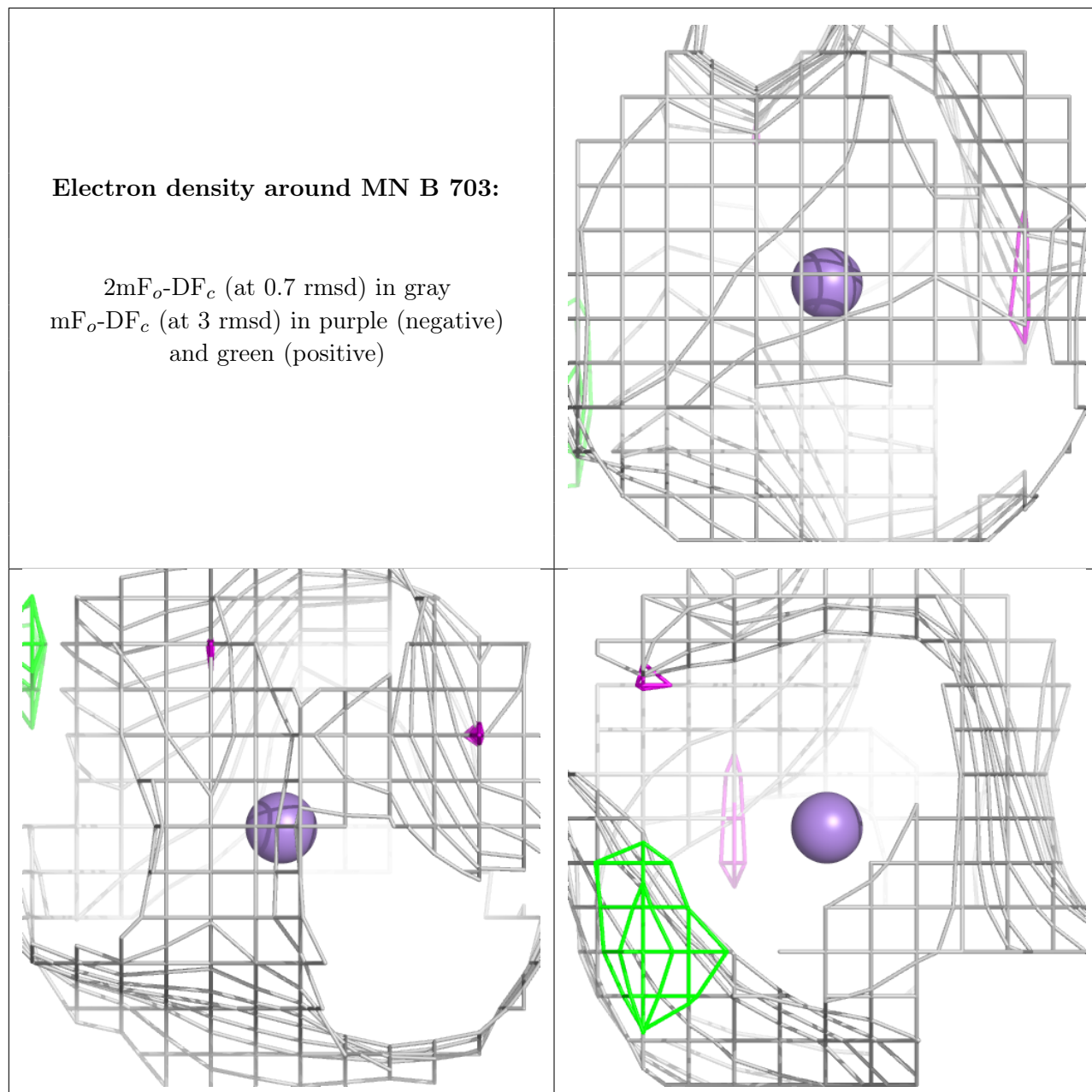
Electron density around FES A 601:

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



Electron density around MN B 703:

$2mF_o-DF_c$ (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.