



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:12 PM UTC

PDB ID : 8S1T / pdb_00008s1t
Title : BzdNO-cyclohexa-1,5-diene-1-carboxy-CoA complex
Authors : Ermler, U.; Boll, M.; Fuchs, J.; Demmer, U.
Deposited on : 2024-02-16
Resolution : 1.45 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

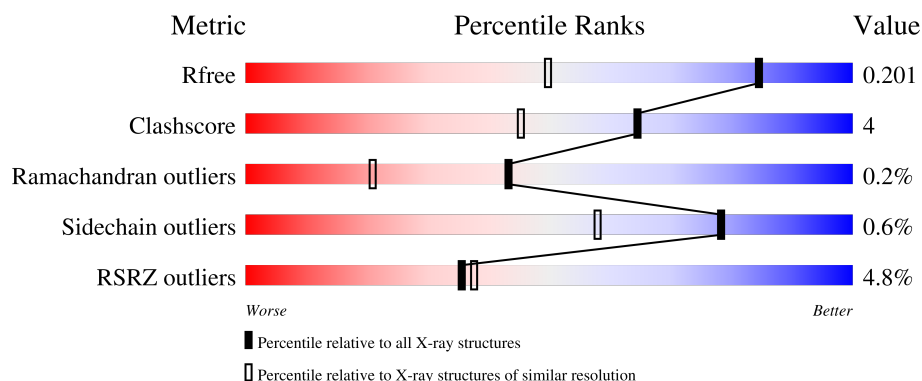
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	447	5% 89% 8% ..
1	C	447	4% 90% 6% .
2	B	379	4% 92% 7% .
2	D	379	5% 88% 11% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 27387 atoms, of which 12995 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 BzdO.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	S	0	14	0
			7090	2303	3480	617	664	26			
1	C	431	Total	C	H	N	O	S	0	6	0
			6936	2247	3415	599	650	25			

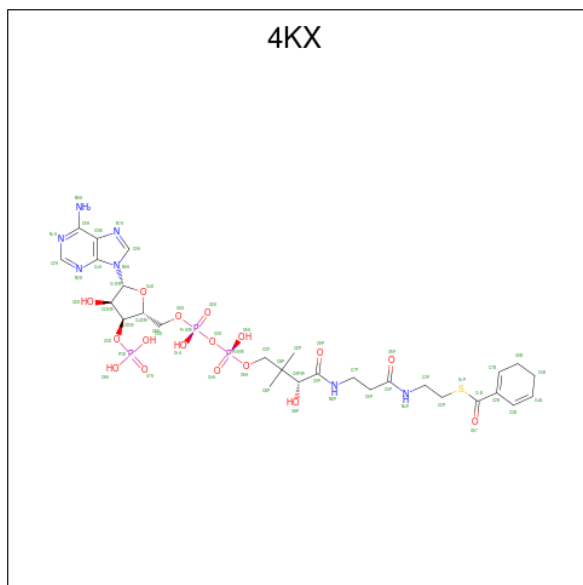
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP Q68VL9
A	439	ALA	-	expression tag	UNP Q68VL9
A	440	TRP	-	expression tag	UNP Q68VL9
A	441	SER	-	expression tag	UNP Q68VL9
A	442	HIS	-	expression tag	UNP Q68VL9
A	443	PRO	-	expression tag	UNP Q68VL9
A	444	GLN	-	expression tag	UNP Q68VL9
A	445	PHE	-	expression tag	UNP Q68VL9
A	446	GLU	-	expression tag	UNP Q68VL9
A	447	LYS	-	expression tag	UNP Q68VL9
C	438	SER	-	expression tag	UNP Q68VL9
C	439	ALA	-	expression tag	UNP Q68VL9
C	440	TRP	-	expression tag	UNP Q68VL9
C	441	SER	-	expression tag	UNP Q68VL9
C	442	HIS	-	expression tag	UNP Q68VL9
C	443	PRO	-	expression tag	UNP Q68VL9
C	444	GLN	-	expression tag	UNP Q68VL9
C	445	PHE	-	expression tag	UNP Q68VL9
C	446	GLU	-	expression tag	UNP Q68VL9
C	447	LYS	-	expression tag	UNP Q68VL9

- Molecule 2 is a protein called BzdN.

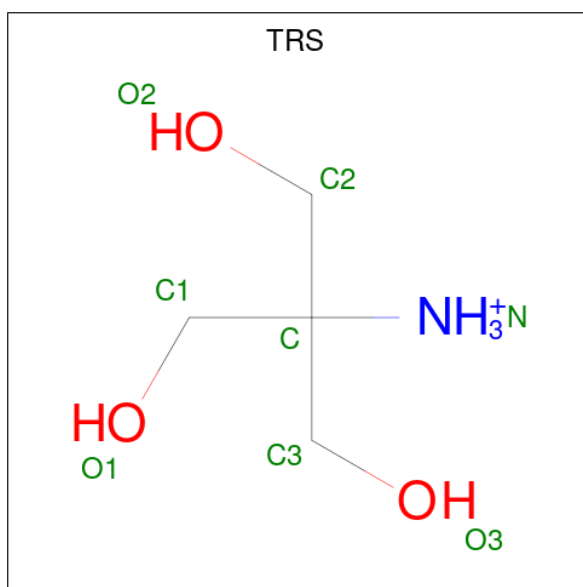
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	375	Total	C	H	N	O	S	0	7	0
			6011	1935	2961	527	568	20			
2	D	375	Total	C	H	N	O	S	0	13	0
			6082	1959	2995	532	576	20			

- Molecule 3 is 1,5 Dienoyl-CoA (CCD ID: 4KX) (formula: $C_{28}H_{42}N_7O_{17}P_3S$).



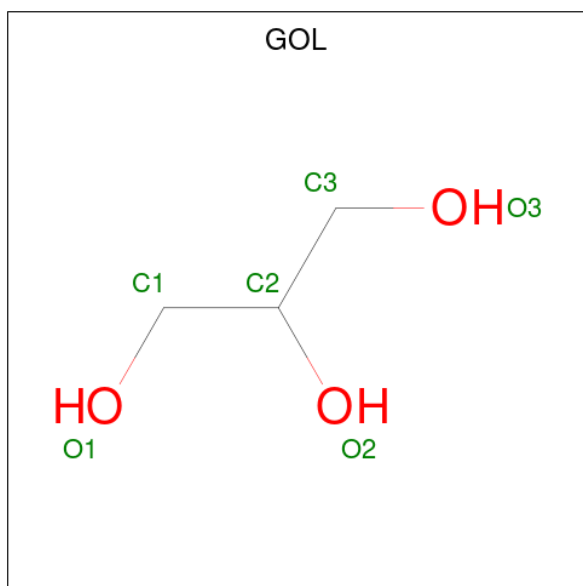
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			94	28	38	7	17	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			94	28	38	7	17	3	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



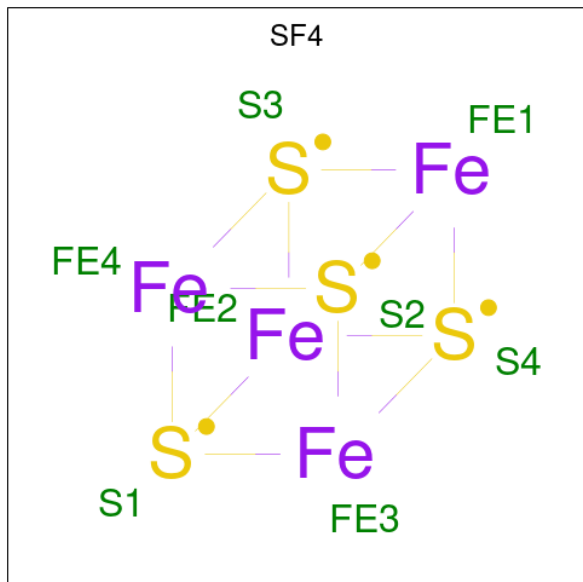
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	1
			38	8	22	2	6		
4	D	1	Total	C	H	N	O	0	1
			38	8	22	2	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



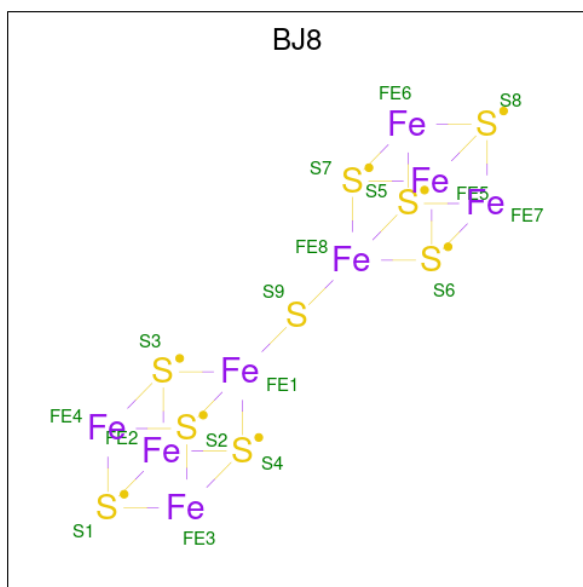
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			13	3	7	3		
5	C	1	Total	C	H	O	0	1
			25	6	13	6		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is Double cubane cluster (CCD ID: BJ8) (formula: Fe_8S_9).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			17	8	9		
7	D	1	Total	Fe	S	0	0
			17	8	9		

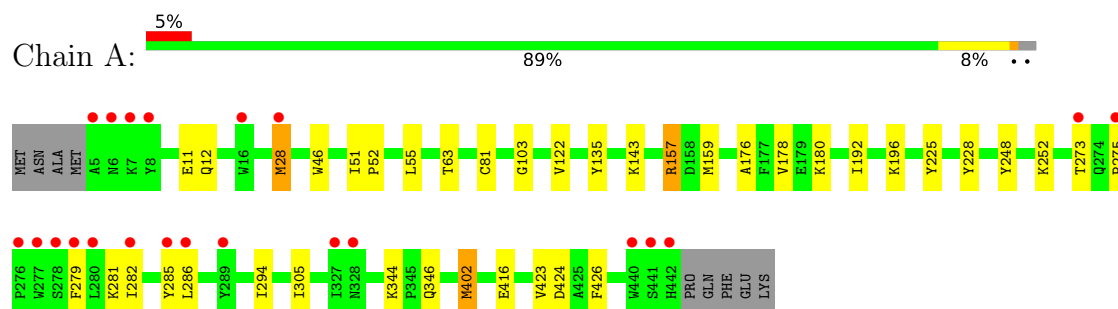
- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	272	Total	H	O	0	3
			277	2	275		
8	B	194	Total	O		0	1
			195	195			
8	C	261	Total	H	O	0	2
			265	2	263		
8	D	178	Total	O		0	1
			179	179			

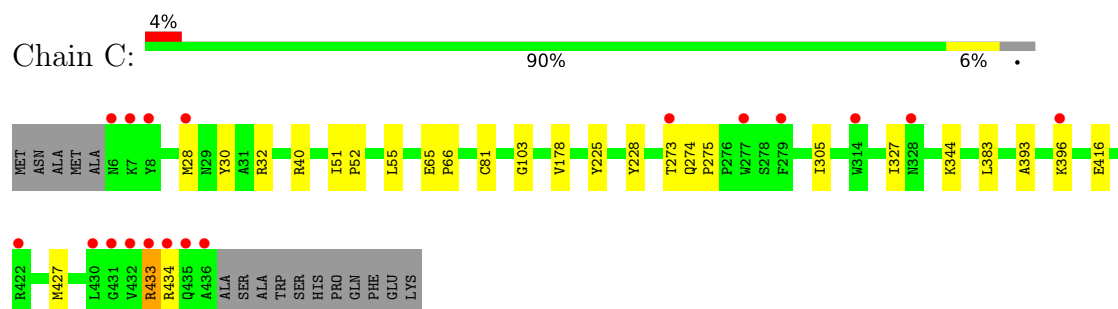
3 Residue-property plots [i](#)

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.

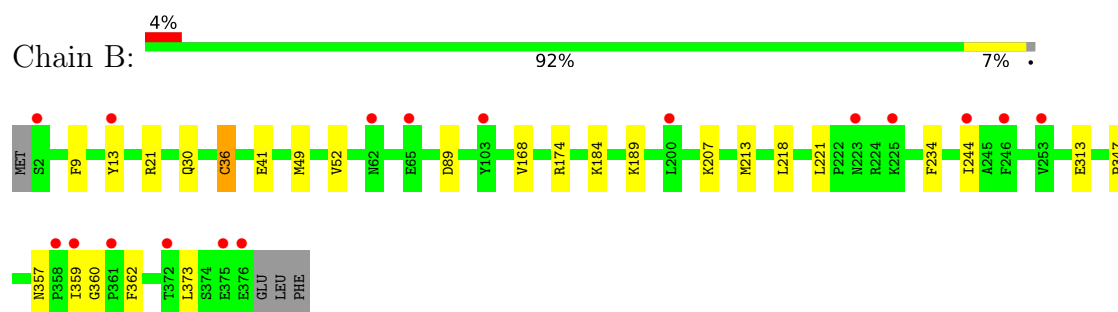
- Molecule 1: BzdO



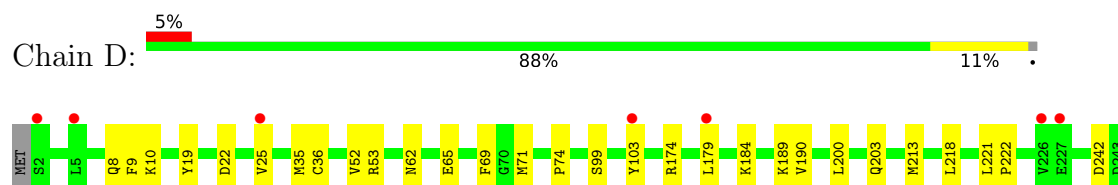
- Molecule 1: BzdO

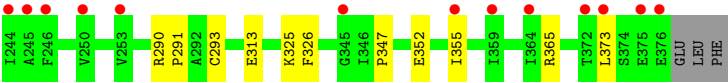


- Molecule 2: BzdN



- Molecule 2: BzdN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.21Å 102.75Å 86.82Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	43.60 – 1.45 43.60 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.60-1.45) 98.5 (43.60-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.182 , 0.200 0.182 , 0.201	Depositor DCC
R_{free} test set	15614 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27387	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.39% 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: 4KX, TRS, GOL, BJ8, SF4

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	0.46	1/3737 (0.0%)	0.63	0/5050
1	C	0.44	0/3620	0.63	0/4891
2	B	0.41	0/3149	0.60	0/4264
2	D	0.41	0/3201	0.60	0/4336
All	All	0.43	1/13707 (0.0%)	0.62	0/18541

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	MET	SD-CE	-5.16	1.66	1.79

There are no bond angle outliers.

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	3610	3480	3464	33	0
1	C	3521	3415	3405	20	0
2	B	3050	2961	2940	19	0
2	D	3087	2995	2945	29	0
3	A	56	38	38	0	0
3	C	56	38	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	22	24	0	0
4	D	16	22	24	0	0
5	A	6	7	8	1	0
5	C	12	13	15	3	0
6	A	8	0	0	0	0
6	C	8	0	0	0	0
7	B	17	0	0	0	0
7	D	17	0	0	1	0
8	A	275	2	0	6	0
8	B	195	0	0	2	0
8	C	263	2	0	5	0
8	D	179	0	0	1	0
All	All	14392	12995	12901	104	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 4.

All (104) 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:28[A]:MET:SD	8:A:787:HOH:O	2.39	0.79
1:A:344[B]:LYS:HG3	8:A:606:HOH:O	1.88	0.73
1:A:305:ILE:HD11	1:A:344[A]:LYS:HG2	1.74	0.70
2:D:179[B]:LEU:CD1	2:D:190:VAL:HG21	2.25	0.67
1:A:180:LYS:N	1:A:180:LYS:HD3	2.12	0.65
1:A:225:TYR:CZ	1:A:275:PRO:HG3	2.32	0.64
1:A:424[A]:ASP:OD2	8:A:601:HOH:O	2.14	0.64
1:C:396:LYS:NZ	8:C:602:HOH:O	2.26	0.64
2:B:359:ILE:HD12	2:B:360:GLY:N	2.12	0.63
1:C:305:ILE:HD11	1:C:344[A]:LYS:HG2	1.80	0.62
2:D:179[B]:LEU:HD11	2:D:190:VAL:HG21	1.81	0.62
5:C:502[A]:GOL:H11	8:C:635:HOH:O	2.02	0.59
1:A:273:THR:HG22	8:A:603:HOH:O	2.02	0.59
1:A:279[B]:PHE:CE1	1:A:416:GLU:OE1	2.56	0.58
1:A:279[B]:PHE:CE2	1:A:282:ILE:HB	2.37	0.58
1:A:46:TRP:CD1	1:A:344[B]:LYS:HZ3	2.23	0.56
2:D:62[A]:ASN:ND2	2:D:65:GLU:OE2	2.39	0.56
1:A:305:ILE:HD11	1:A:344[A]:LYS:CG	2.35	0.55
1:C:305:ILE:HD11	1:C:344[A]:LYS:CG	2.37	0.54
1:A:344[B]:LYS:HE3	8:A:644:HOH:O	2.08	0.53
2:B:13:TYR:CZ	2:B:244:ILE:HD12	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLN:HG2	2:D:213[B]:MET:HE3	1.91	0.53
2:D:22:ASP:O	2:D:25:VAL:HG22	2.09	0.52
2:D:9:PHE:CZ	2:D:213[B]:MET:HG3	2.45	0.52
1:A:28[A]:MET:HE3	1:A:28[A]:MET:HA	1.92	0.52
1:A:279[B]:PHE:CD1	1:A:416:GLU:OE1	2.62	0.52
1:A:279[B]:PHE:CD1	1:A:281:LYS:NZ	2.78	0.52
1:C:327[B]:ILE:HG23	1:C:327[B]:ILE:O	2.09	0.52
2:D:347:PRO:HG2	2:D:373:LEU:CD2	2.40	0.52
1:A:402[A]:MET:HG2	1:A:426:PHE:CG	2.46	0.51
1:C:225:TYR:CZ	1:C:275:PRO:HG3	2.45	0.51
1:A:294:ILE:HD12	1:A:294:ILE:C	2.35	0.51
2:D:35:MET:HB3	2:D:103[B]:TYR:CE2	2.46	0.51
2:B:218:LEU:HD23	2:B:221:LEU:HD12	1.93	0.51
2:D:69:PHE:CD2	2:D:71:MET:HG2	2.47	0.50
1:A:143:LYS:HG3	5:A:503:GOL:H31	1.94	0.49
2:D:325:LYS:HG2	2:D:326:PHE:CD2	2.47	0.49
2:D:325:LYS:HE2	2:D:352:GLU:OE1	2.11	0.49
2:B:184:LYS:HE2	2:B:313:GLU:OE2	2.12	0.49
2:B:184:LYS:HE3	2:B:313:GLU:HG3	1.94	0.49
1:A:279[B]:PHE:CE1	1:A:281:LYS:NZ	2.81	0.48
2:B:189:LYS:HD2	2:B:221:LEU:O	2.13	0.48
2:D:35:MET:HB3	2:D:103[B]:TYR:HE2	1.78	0.48
2:D:200:LEU:HD11	2:D:242:ASP:HB2	1.96	0.48
2:D:325:LYS:HG2	2:D:326:PHE:CE2	2.48	0.47
1:A:286:LEU:HD21	1:A:423:VAL:CG1	2.43	0.47
2:D:347:PRO:HG2	2:D:373:LEU:HD21	1.96	0.47
1:C:28[B]:MET:HE3	1:C:32:ARG:HH11	1.79	0.47
1:A:281:LYS:NZ	1:A:416:GLU:OE1	2.48	0.47
2:D:52:VAL:HG23	2:D:52:VAL:O	2.15	0.46
2:D:365:ARG:HG3	2:D:365:ARG:NH1	2.31	0.46
1:A:248:TYR:CE2	1:A:252:LYS:HE2	2.50	0.46
2:B:234:PHE:HE1	2:B:373:LEU:HD11	1.80	0.46
2:B:9:PHE:CZ	2:B:213[B]:MET:HG3	2.51	0.46
2:B:36:CYS:HB3	8:B:526:HOH:O	2.15	0.45
1:A:81:CYS:O	1:A:103:GLY:HA3	2.15	0.45
1:C:81:CYS:O	1:C:103:GLY:HA3	2.16	0.45
2:D:174:ARG:NH2	8:D:509:HOH:O	2.49	0.45
2:B:9:PHE:CZ	2:B:213[A]:MET:HG3	2.52	0.45
2:B:168:VAL:HG12	2:B:207:LYS:HB3	1.99	0.45
2:D:365:ARG:HG3	2:D:365:ARG:HH11	1.82	0.44
1:C:65:GLU:HB2	1:C:66:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ILE:HB	1:C:52:PRO:HD3	1.99	0.44
2:D:218:LEU:HD23	2:D:221:LEU:HD12	2.00	0.44
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.99	0.43
1:C:433:ARG:HA	1:C:433:ARG:NE	2.34	0.43
1:A:285:TYR:HE2	1:A:424[A]:ASP:OD1	2.01	0.43
1:A:55:LEU:HD11	1:A:178:VAL:HB	1.99	0.42
2:B:52:VAL:O	2:B:52:VAL:HG23	2.19	0.42
2:B:41:GLU:OE1	2:B:207:LYS:NZ	2.50	0.42
1:C:344[B]:LYS:HG3	8:C:630:HOH:O	2.18	0.42
5:C:502[A]:GOL:O2	8:C:601:HOH:O	2.20	0.42
2:D:179[B]:LEU:HD12	2:D:190:VAL:HG21	1.98	0.42
2:D:293:CYS:HB2	7:D:401:BJ8:S8	2.58	0.42
1:C:396:LYS:HE3	1:C:396:LYS:HB3	1.94	0.42
1:A:279[A]:PHE:CD2	1:A:416:GLU:HG2	2.54	0.42
2:D:10:LYS:NZ	2:D:10:LYS:HB3	2.35	0.42
2:D:189:LYS:NZ	2:D:222:PRO:O	2.53	0.42
2:B:347:PRO:HG2	2:B:373:LEU:CD2	2.50	0.42
1:C:427:MET:HA	1:C:427:MET:HE2	2.00	0.42
1:C:55:LEU:HD11	1:C:178:VAL:HB	2.02	0.41
8:A:708:HOH:O	5:C:502[A]:GOL:H2	2.19	0.41
2:B:30:GLN:HB2	2:B:49:MET:HG2	2.03	0.41
2:B:174:ARG:NH2	8:B:509:HOH:O	2.53	0.41
1:C:273:THR:HG21	1:C:383:LEU:HB3	2.03	0.41
1:A:11:GLU:HG2	1:A:12:GLN:O	2.21	0.41
1:A:122:VAL:HG11	1:A:135:TYR:HB3	2.02	0.41
2:D:290:ARG:HG2	2:D:291:PRO:HD2	2.03	0.41
2:B:168:VAL:CG1	2:B:207:LYS:HB3	2.51	0.41
2:B:357:ASN:HB3	2:B:362:PHE:HE1	1.86	0.41
1:C:433:ARG:HA	1:C:433:ARG:CZ	2.49	0.41
1:A:176:ALA:O	1:A:180:LYS:HD3	2.20	0.41
1:C:393:ALA:HA	1:C:396:LYS:HE3	2.03	0.41
2:D:53:ARG:HD3	2:D:203:GLN:OE1	2.20	0.41
2:D:184:LYS:HE2	2:D:313:GLU:HG3	2.02	0.41
2:D:19:TYR:CD1	2:D:19:TYR:C	2.99	0.41
1:A:192:ILE:O	1:A:196:LYS:HG3	2.22	0.40
2:D:74:PRO:HB3	2:D:355:ILE:HG13	2.04	0.40
1:C:30:TYR:O	1:C:40:ARG:HD3	2.21	0.40
1:C:393:ALA:O	1:C:396:LYS:HE3	2.20	0.40
2:B:21[A]:ARG:NH2	2:B:89:ASP:OD1	2.54	0.40
1:C:416:GLU:HG2	8:C:832:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/447 (101%)	441 (98%)	9 (2%)	0	100	100
1	C	435/447 (97%)	426 (98%)	8 (2%)	1 (0%)	43	21
2	B	380/379 (100%)	369 (97%)	10 (3%)	1 (0%)	36	16
2	D	386/379 (102%)	374 (97%)	9 (2%)	3 (1%)	16	3
All	All	1651/1652 (100%)	1610 (98%)	36 (2%)	5 (0%)	43	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	CYS
2	D	36	CYS
2	D	99[A]	SER
2	D	99[B]	SER
1	C	274	GLN

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	375/371 (101%)	367 (98%)	8 (2%)	47	14
1	C	365/371 (98%)	362 (99%)	3 (1%)	73	50
2	B	328/325 (101%)	328 (100%)	0	100	100
2	D	334/325 (103%)	334 (100%)	0	100	100
All	All	1402/1392 (101%)	1391 (99%)	11 (1%)	78	50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28[A]	MET
1	A	28[B]	MET
1	A	157[A]	ARG
1	A	157[B]	ARG
1	A	228	TYR
1	A	346	GLN
1	A	402[A]	MET
1	A	402[B]	MET
1	C	228	TYR
1	C	433	ARG
1	C	434	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	442	HIS
2	B	8	GLN
2	B	98	GLN
2	B	172	ASN
2	D	8	GLN
2	D	30	GLN
2	D	98	GLN
2	D	133	HIS
2	D	172	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

13 ligands 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$
6	SF4	C	503	8,1	0,12,12	-	-	-		
4	TRS	D	402[A]	-	7,7,7	0.47	0	9,9,9	0.58	0
6	SF4	A	504	8,1	0,12,12	-	-	-		
3	4KX	A	501	-	53,59,59	1.86	10 (18%)	77,87,87	1.77	16 (20%)
4	TRS	D	402[B]	-	7,7,7	0.61	0	9,9,9	0.67	0
3	4KX	C	501	-	53,59,59	1.85	12 (22%)	77,87,87	1.81	16 (20%)
5	GOL	A	503	-	5,5,5	0.76	0	5,5,5	1.15	1 (20%)
7	BJ8	B	401	2	6,26,26	2.68	4 (66%)	-		
4	TRS	A	502[A]	-	7,7,7	0.43	0	9,9,9	0.49	0
5	GOL	C	502[A]	-	5,5,5	1.33	1 (20%)	5,5,5	0.93	0
7	BJ8	D	401	2	6,26,26	1.79	3 (50%)	-		
4	TRS	A	502[B]	-	7,7,7	0.53	0	9,9,9	0.64	0
5	GOL	C	502[B]	-	5,5,5	1.04	0	5,5,5	1.12	1 (20%)

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
6	SF4	C	503	8,1	-	-	0/6/5/5
4	TRS	D	402[A]	-	-	4/9/9/9	-
6	SF4	A	504	8,1	-	-	0/6/5/5
3	4KX	A	501	-	-	3/53/79/79	0/4/4/4
4	TRS	D	402[B]	-	-	1/9/9/9	-
3	4KX	C	501	-	-	3/53/79/79	0/4/4/4
5	GOL	A	503	-	-	0/4/4/4	-
7	BJ8	B	401	2	-	-	0/12/10/10
4	TRS	A	502[A]	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	502[A]	-	-	4/4/4/4	-
7	BJ8	D	401	2	-	-	0/12/10/10
4	TRS	A	502[B]	-	-	2/9/9/9	-
5	GOL	C	502[B]	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	4KX	C6B-C7B	-5.52	1.35	1.50
3	A	501	4KX	C6B-C7B	-5.29	1.36	1.50
3	C	501	4KX	C3B-C4B	4.82	1.45	1.33
3	A	501	4KX	C3B-C2B	-4.79	1.33	1.43
3	C	501	4KX	C9P-N8P	4.73	1.44	1.33
3	A	501	4KX	C3B-C4B	4.70	1.45	1.33
3	A	501	4KX	C5P-N4P	4.50	1.44	1.33
3	A	501	4KX	C9P-N8P	4.39	1.43	1.33
7	B	401	BJ8	S5-FE8	4.16	2.34	2.28
3	A	501	4KX	C6A-N6A	4.07	1.44	1.34
3	C	501	4KX	C3B-C2B	-3.91	1.35	1.43
3	C	501	4KX	C5P-N4P	3.87	1.42	1.33
3	C	501	4KX	C6A-N6A	3.78	1.43	1.34
7	B	401	BJ8	S3-FE1	3.62	2.33	2.28
3	A	501	4KX	P3D-O3D	3.24	1.65	1.59
3	C	501	4KX	P3D-O3D	3.01	1.64	1.59
3	A	501	4KX	O2D-C2D	2.91	1.50	1.43
7	B	401	BJ8	S4-FE1	2.65	2.32	2.28
3	C	501	4KX	P2A-O3A	2.45	1.62	1.59
7	D	401	BJ8	S6-FE8	2.44	2.31	2.28
7	D	401	BJ8	S3-FE1	2.33	2.31	2.28
3	C	501	4KX	O3D-C3D	-2.31	1.36	1.44
3	A	501	4KX	P2A-O3A	2.30	1.62	1.59
3	A	501	4KX	O3D-C3D	-2.30	1.36	1.44
5	C	502[A]	GOL	O2-C2	-2.28	1.36	1.43
3	C	501	4KX	O57-C1B	2.27	1.27	1.22
7	D	401	BJ8	S2-FE1	2.23	2.31	2.28
3	C	501	4KX	C8A-N7A	2.21	1.35	1.31
3	C	501	4KX	O2D-C2D	2.17	1.48	1.43
7	B	401	BJ8	S6-FE8	2.01	2.31	2.28

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	4KX	C5M-C4A-N3A	-5.43	119.23	126.72
3	C	501	4KX	N3A-C2A-N1A	-5.34	120.50	128.58
3	C	501	4KX	C2P-S1P-C1B	4.99	105.73	99.85
3	C	501	4KX	C5M-C4A-N3A	-4.87	120.01	126.72
3	A	501	4KX	N3A-C2A-N1A	-4.64	121.56	128.58
3	A	501	4KX	N9A-C8A-N7A	-4.21	107.96	113.94
3	A	501	4KX	N3A-C4A-N9A	4.18	134.28	127.17
3	A	501	4KX	C5B-C4B-C3B	-4.02	115.04	122.95
3	C	501	4KX	C5B-C4B-C3B	-3.84	115.39	122.95
3	C	501	4KX	N9A-C8A-N7A	-3.78	108.57	113.94
3	A	501	4KX	C2P-S1P-C1B	3.77	104.29	99.85
3	A	501	4KX	C4A-N9A-C8A	3.75	109.67	105.74
3	C	501	4KX	O6A-CCP-CBP	-3.59	104.78	110.55
3	A	501	4KX	C2A-N3A-C4A	3.51	120.41	111.83
3	C	501	4KX	N3A-C4A-N9A	3.45	133.04	127.17
3	C	501	4KX	C2A-N3A-C4A	3.36	120.03	111.83
3	C	501	4KX	C4A-N9A-C8A	3.26	109.16	105.74
3	C	501	4KX	C7P-C6P-C5P	-3.04	107.32	112.39
3	A	501	4KX	C5M-N7A-C8A	2.96	108.11	103.45
3	C	501	4KX	C2A-N1A-C6A	2.86	123.42	118.73
3	C	501	4KX	CEP-CBP-CCP	2.78	112.81	108.22
3	C	501	4KX	C5M-N7A-C8A	2.73	107.74	103.45
3	C	501	4KX	C4A-C5M-N7A	-2.65	107.56	110.58
3	A	501	4KX	C7P-C6P-C5P	-2.64	108.00	112.39
3	A	501	4KX	C4A-C5M-N7A	-2.46	107.77	110.58
3	A	501	4KX	C2P-C3P-N4P	-2.29	107.62	112.41
3	A	501	4KX	O6A-CCP-CBP	-2.27	106.91	110.55
5	C	502[B]	GOL	C3-C2-C1	-2.25	103.54	111.80
5	A	503	GOL	C3-C2-C1	-2.23	103.62	111.80
3	A	501	4KX	CEP-CBP-CCP	2.17	111.81	108.22
3	A	501	4KX	CDP-CBP-CAP	2.14	112.41	108.77
3	C	501	4KX	C6P-C7P-N8P	-2.10	107.53	112.00
3	C	501	4KX	O3A-P1A-O2A	2.09	116.99	110.70
3	A	501	4KX	O5A-P2A-O6A	2.02	116.72	107.57

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	4KX	C3P-C2P-S1P-C1B
3	C	501	4KX	C3P-C2P-S1P-C1B
4	A	502[A]	TRS	N-C-C3-O3
4	D	402[A]	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	502[A]	GOL	O1-C1-C2-C3
5	C	502[A]	GOL	C1-C2-C3-O3
5	C	502[B]	GOL	O1-C1-C2-C3
5	C	502[A]	GOL	O1-C1-C2-O2
5	C	502[A]	GOL	O2-C2-C3-O3
4	D	402[A]	TRS	C1-C-C3-O3
4	A	502[A]	TRS	C1-C-C3-O3
5	C	502[B]	GOL	O1-C1-C2-O2
3	C	501	4KX	O5P-C5P-C6P-C7P
3	A	501	4KX	N4P-C5P-C6P-C7P
3	C	501	4KX	N4P-C5P-C6P-C7P
3	A	501	4KX	O5P-C5P-C6P-C7P
4	A	502[A]	TRS	C3-C-C2-O2
4	A	502[B]	TRS	C3-C-C2-O2
4	D	402[A]	TRS	C3-C-C2-O2
4	A	502[A]	TRS	N-C-C2-O2
4	A	502[B]	TRS	N-C-C2-O2
4	D	402[A]	TRS	N-C-C2-O2
4	D	402[B]	TRS	C2-C-C3-O3

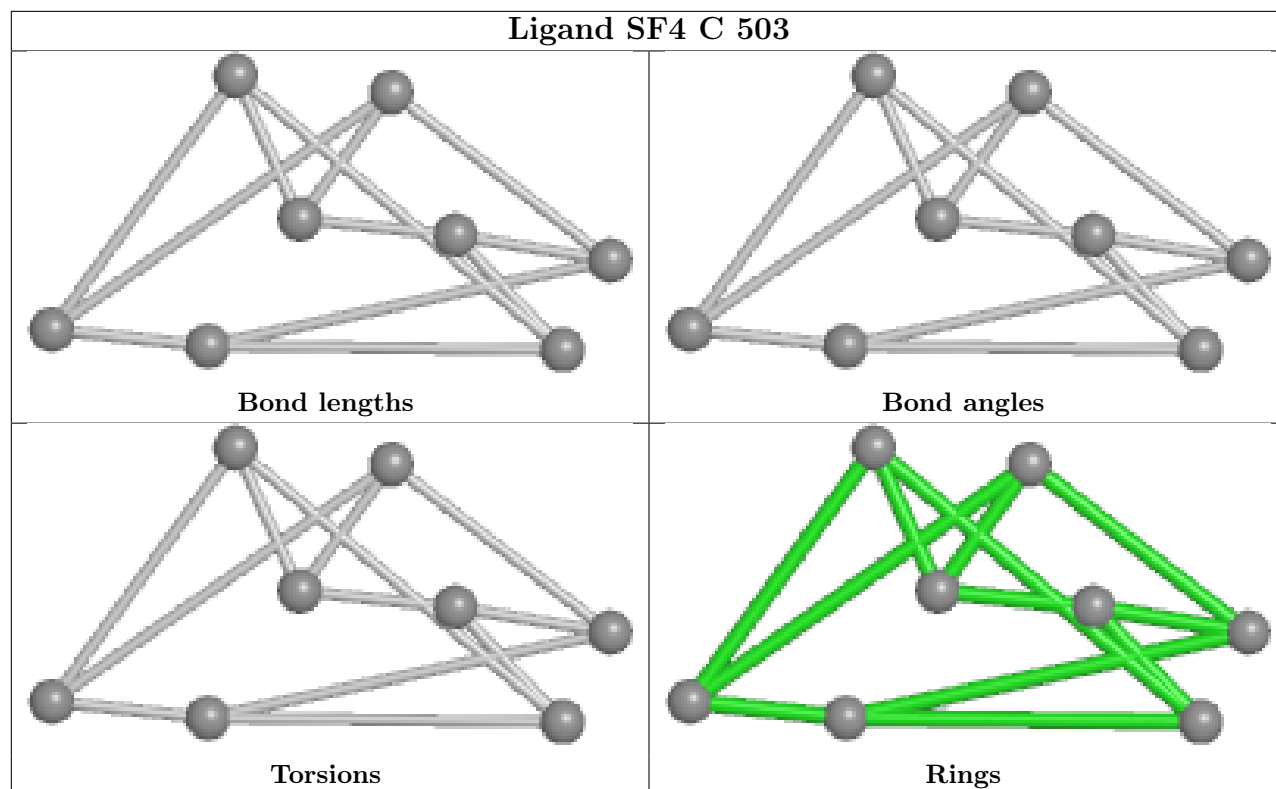
There are no ring outliers.

3 monomers are involved in 5 short contacts:

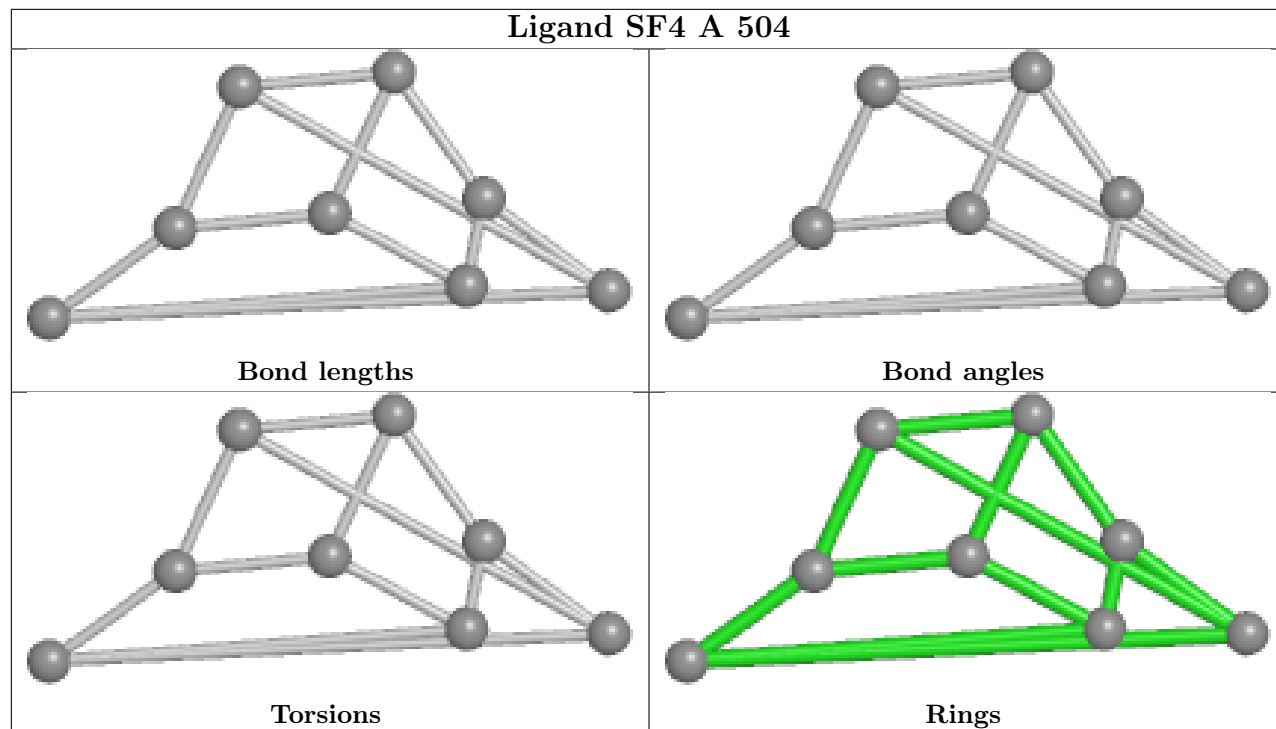
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	GOL	1	0
5	C	502[A]	GOL	3	0
7	D	401	BJ8	1	0

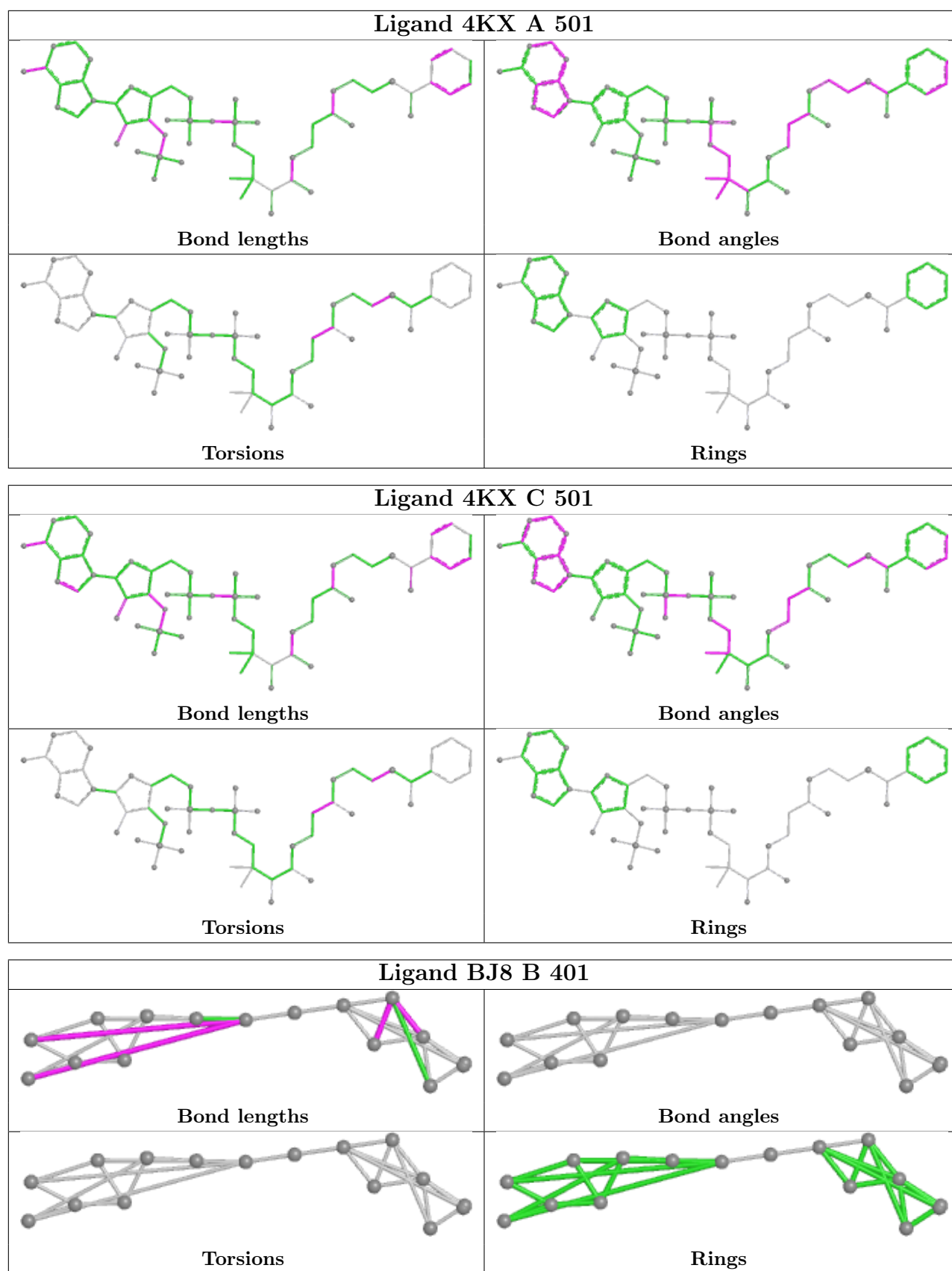
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

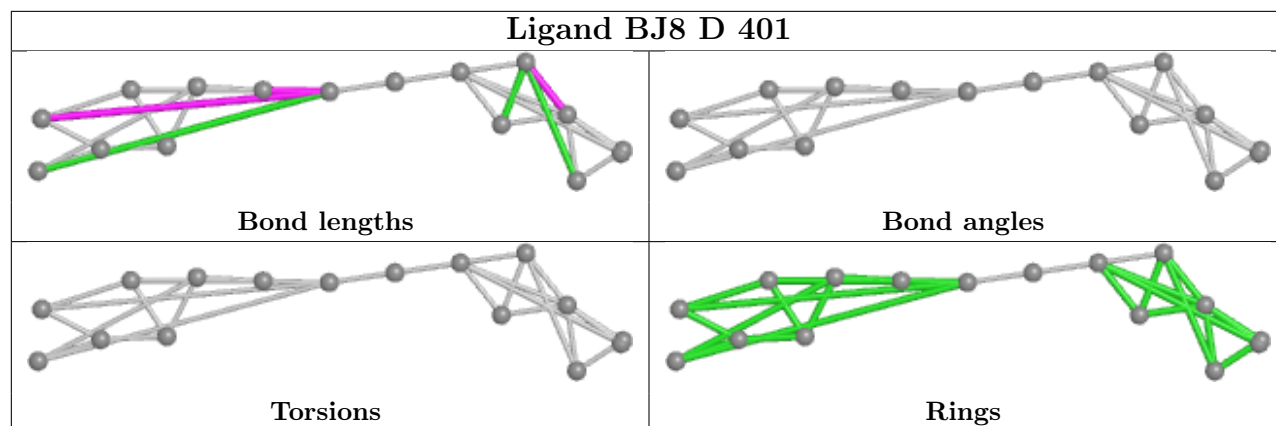
Ligand SF4 C 503



Ligand SF4 A 504







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	438/447 (97%)	0.19	22 (5%) 34 35	10, 23, 39, 74	9 (2%)
1	C	431/447 (96%)	0.27	18 (4%) 40 43	11, 24, 44, 89	5 (1%)
2	B	375/379 (98%)	0.35	17 (4%) 38 41	10, 27, 48, 70	4 (1%)
2	D	375/379 (98%)	0.50	20 (5%) 32 32	10, 27, 51, 69	8 (2%)
All	All	1619/1652 (98%)	0.32	77 (4%) 35 37	10, 25, 45, 89	26 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279[A]	PHE	7.5
1	A	440	TRP	7.3
1	A	5	ALA	6.8
1	C	436	ALA	6.7
2	D	244	ILE	5.1
2	B	244	ILE	5.1
1	C	434	ARG	4.8
1	A	277	TRP	4.7
2	B	2	SER	4.6
2	D	359	ILE	4.5
1	A	442	HIS	4.4
1	C	433	ARG	4.3
2	D	2	SER	4.1
1	C	432	VAL	4.1
2	D	226	VAL	4.0
1	A	6	ASN	3.7
1	C	431	GLY	3.6
1	C	435	GLN	3.5
2	B	359	ILE	3.4
1	A	328	ASN	3.3
1	C	273	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	6	ASN	3.2
2	D	245	ALA	3.1
1	C	328	ASN	3.0
2	D	376	GLU	3.0
1	C	314	TRP	3.0
1	A	273	THR	3.0
2	B	103	TYR	3.0
2	D	25	VAL	3.0
2	D	373	LEU	2.9
1	A	441	SER	2.9
2	B	376	GLU	2.9
2	D	355	ILE	2.8
1	C	7	LYS	2.8
2	B	62	ASN	2.8
2	D	364	ILE	2.7
1	A	327	ILE	2.7
1	C	422	ARG	2.7
1	A	275	PRO	2.6
1	C	396	LYS	2.6
1	A	276	PRO	2.6
2	B	372	THR	2.6
2	B	223	ASN	2.5
1	A	285	TYR	2.5
2	B	375	GLU	2.5
2	D	227	GLU	2.5
2	D	375	GLU	2.5
1	C	277	TRP	2.5
2	B	246	PHE	2.5
2	D	372	THR	2.4
2	B	65	GLU	2.4
1	A	8	TYR	2.4
1	A	278	SER	2.3
2	D	250	VAL	2.3
2	B	253	VAL	2.3
1	A	282	ILE	2.2
1	A	289	TYR	2.2
2	D	103[A]	TYR	2.2
1	A	7	LYS	2.2
2	D	253	VAL	2.2
1	A	16	TRP	2.2
2	B	225	LYS	2.2
1	C	279	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	286	LEU	2.1
2	D	179[A]	LEU	2.1
2	B	358	PRO	2.1
1	C	28[A]	MET	2.1
2	D	246	PHE	2.1
2	D	345	GLY	2.1
2	B	200	LEU	2.1
2	D	5	LEU	2.1
1	A	28[A]	MET	2.1
1	C	430	LEU	2.0
2	B	361	PRO	2.0
1	A	280	LEU	2.0
1	C	8	TYR	2.0
2	B	13	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRS	A	502[A]	8/8	0.79	0.10	23,28,31,31	19
4	TRS	A	502[B]	8/8	0.79	0.10	21,26,31,31	19
5	GOL	A	503	6/6	0.79	0.12	33,40,48,48	0
4	TRS	D	402[B]	8/8	0.86	0.10	17,26,31,31	19
4	TRS	D	402[A]	8/8	0.86	0.10	22,27,31,31	19
5	GOL	C	502[A]	6/6	0.86	0.12	23,27,34,34	13
5	GOL	C	502[B]	6/6	0.86	0.12	22,31,34,41	12
3	4KX	C	501	56/56	0.96	0.07	14,24,32,38	0
3	4KX	A	501	56/56	0.96	0.07	16,24,32,40	0

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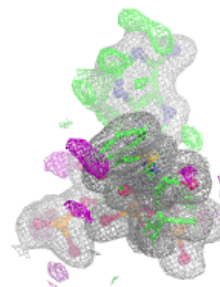
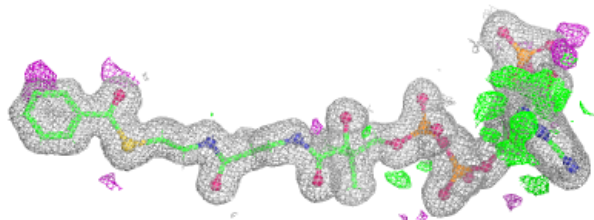
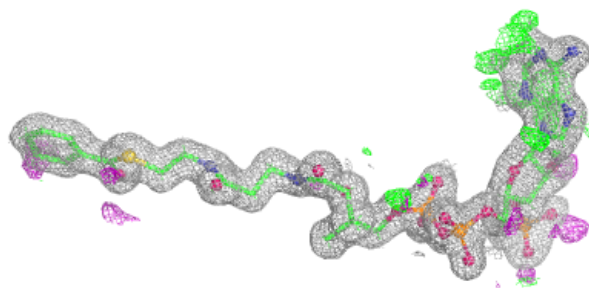
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BJ8	B	401	17/17	0.99	0.03	16,17,19,20	0
7	BJ8	D	401	17/17	0.99	0.03	17,18,19,20	0
6	SF4	A	504	8/8	1.00	0.02	15,16,16,16	0
6	SF4	C	503	8/8	1.00	0.02	15,16,17,17	0

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.

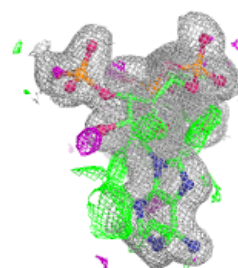
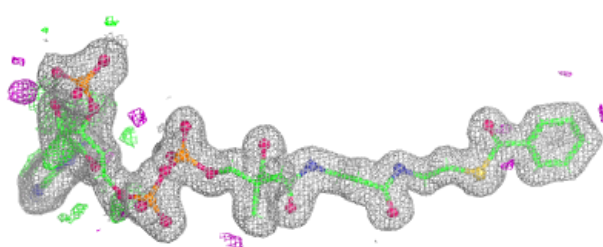
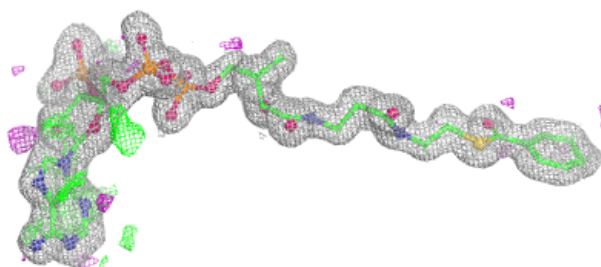
Electron density around 4KX C 501:

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

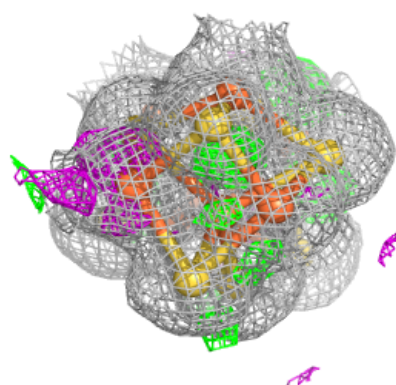
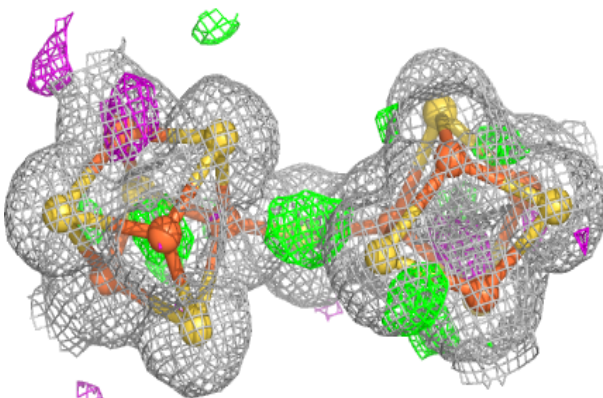
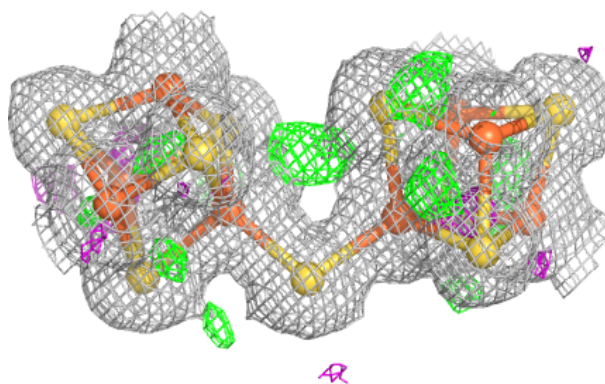


Electron density around 4KX A 501:

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

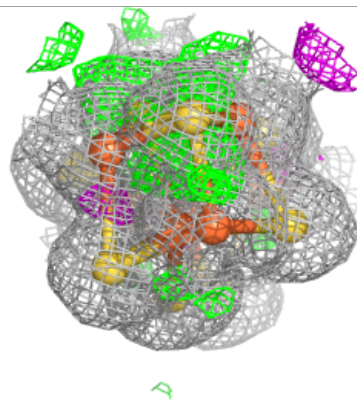
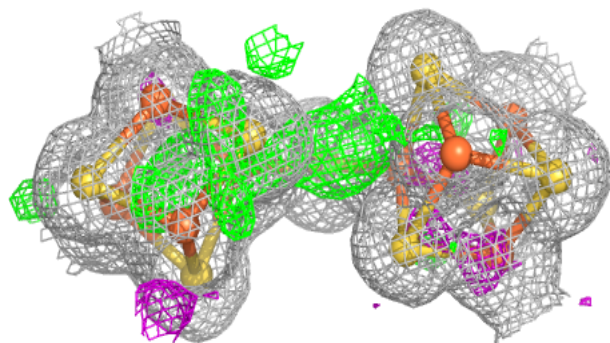
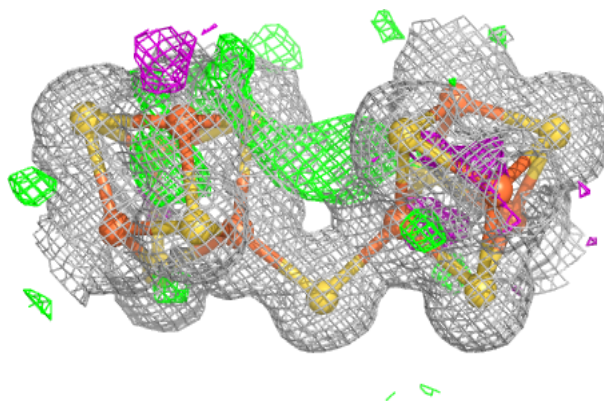
**Electron density around BJ8 B 401:**

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



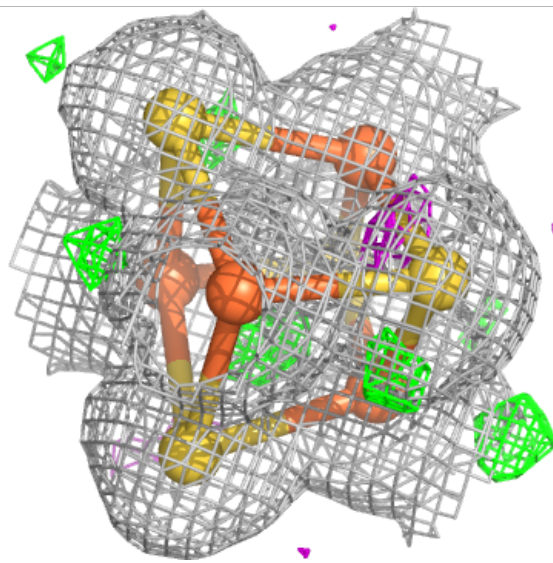
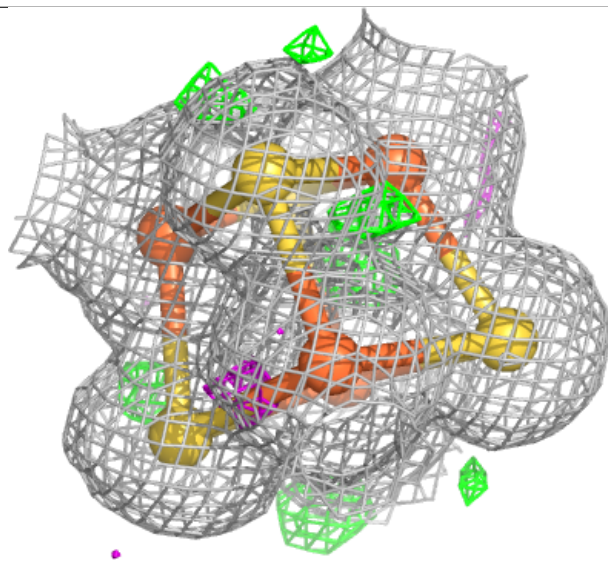
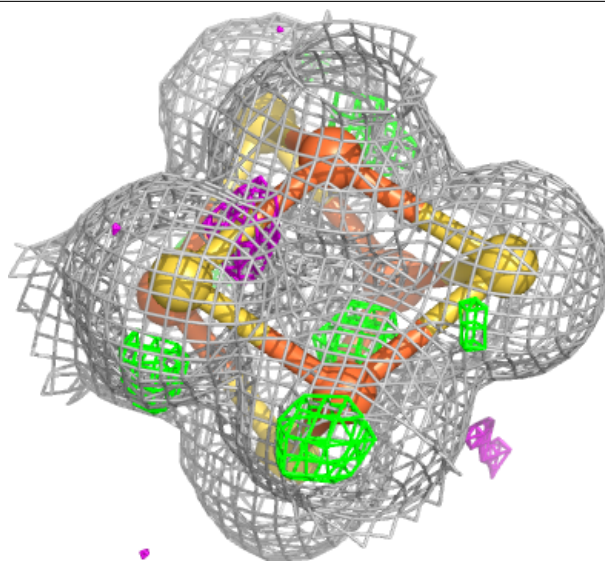
Electron density around BJ8 D 401:

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



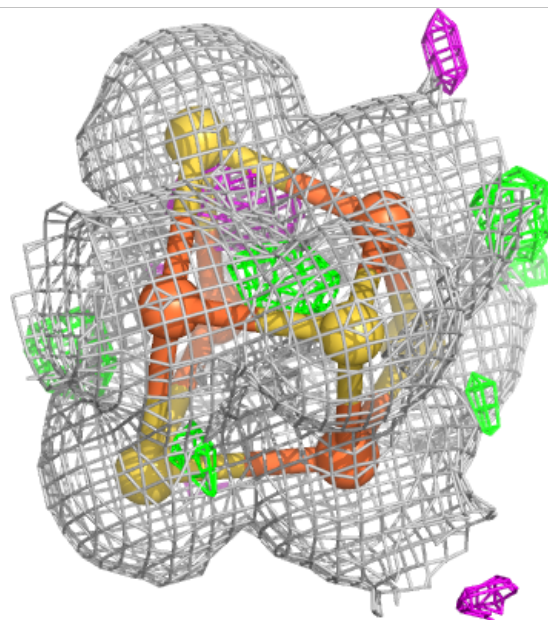
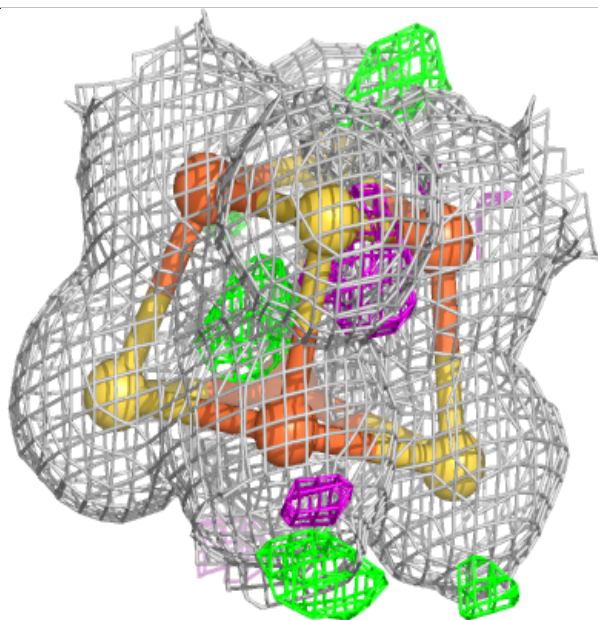
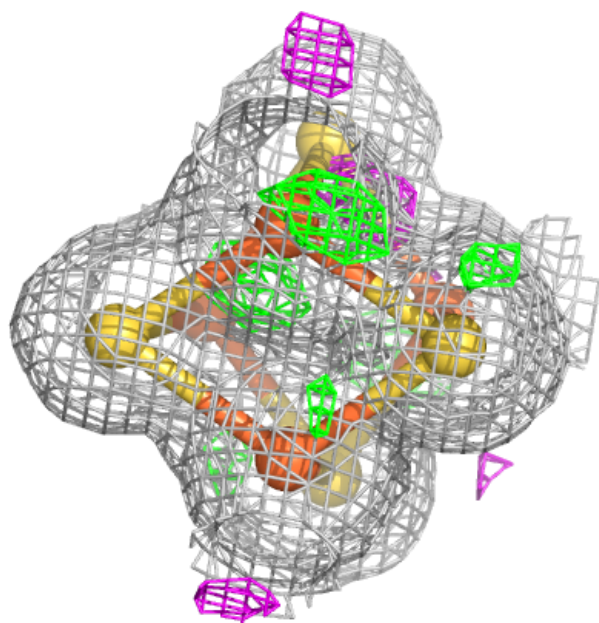
Electron density around SF4 A 504:

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



Electron density around SF4 C 503:

$2mF_o-DF_c$ (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.