



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:51 AM UTC

PDB ID : 8S2R / pdb_00008s2r
Title : BzdNO in partially coenzyme A - free state
Authors : Ermler, U.; Boll, M.; Fuchs, J.; Demmer, U.
Deposited on : 2024-02-19
Resolution : 1.60 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

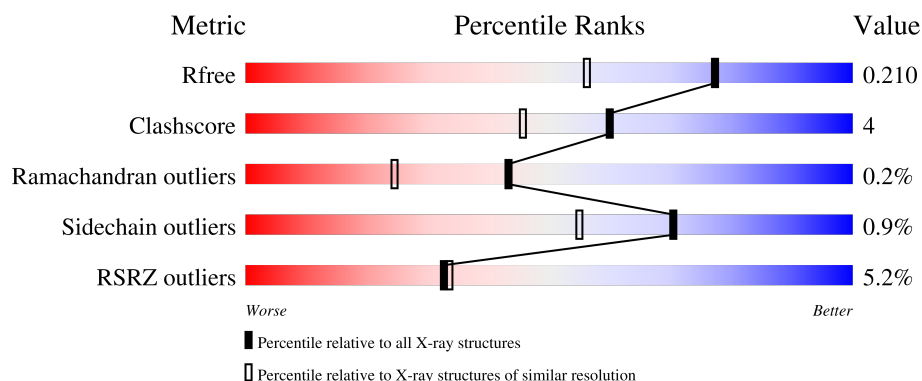
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

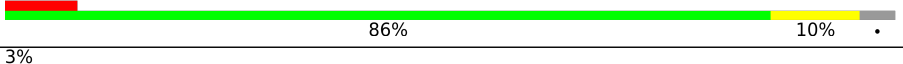
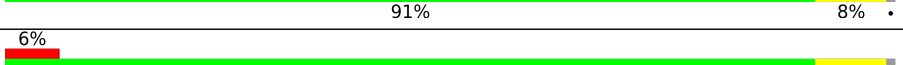
The reported resolution of this entry is 1.60 Å.

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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	447	
1	C	447	
2	B	379	
2	D	379	

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
4	GOL	A	502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14200 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 BzdO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	8	0
			3603	2296	619	662	26			
1	C	429	Total	C	N	O	S	0	1	0
			3472	2216	590	641	25			

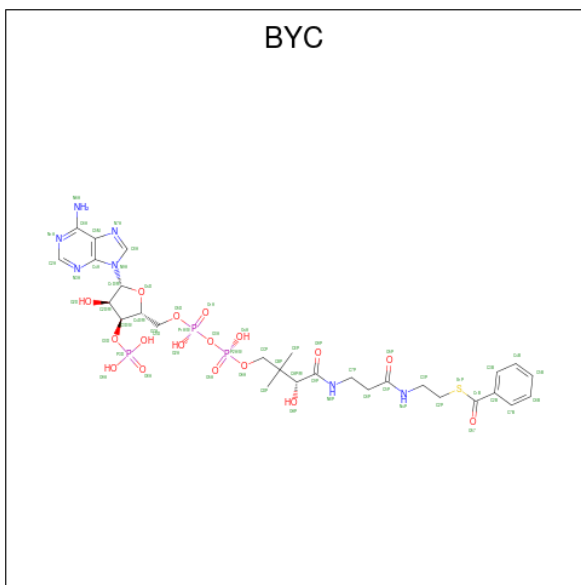
There are 20 discrepancies between the modelled and reference sequences:

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 3064	C 1943	N 532	O 569	S 20	0	5	0
2	D	375	Total 3061	C 1940	N 531	O 571	S 19	0	5	0

- Molecule 3 is benzoyl coenzyme A (CCD ID: BYC) (formula: $\text{C}_{28}\text{H}_{40}\text{N}_7\text{O}_{17}\text{P}_3\text{S}$).



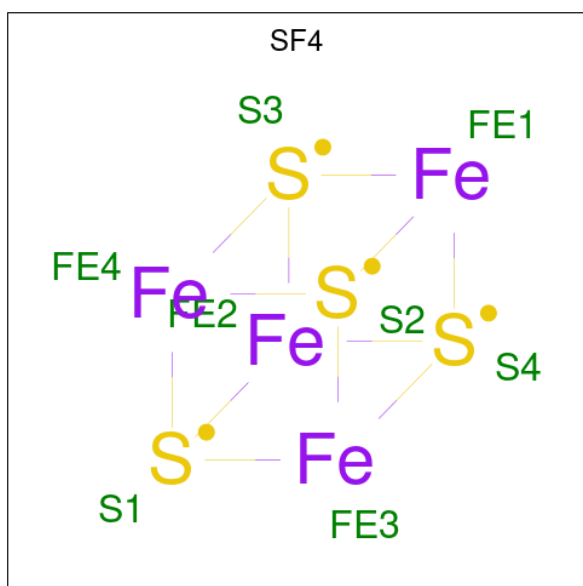
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 56	C 28	N 7	O 17	P 3	S 1	0	0
3	C	1	Total 56	C 28	N 7	O 17	P 3	S 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



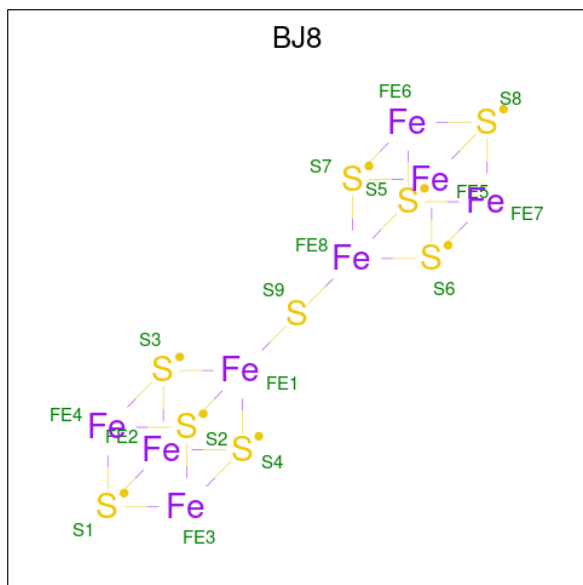
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



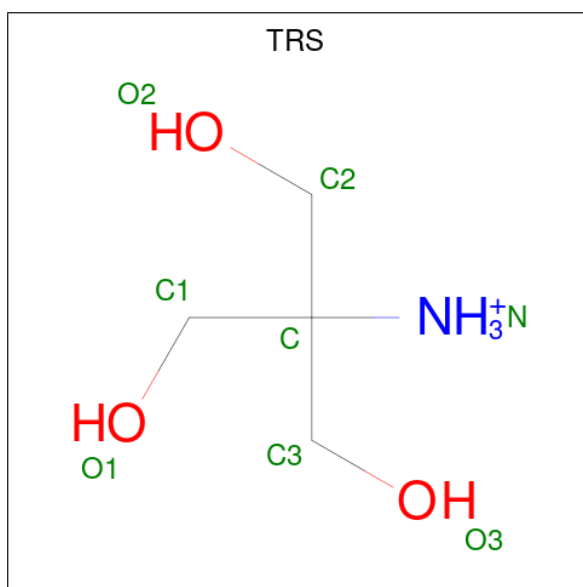
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is Double cubane cluster (CCD ID: BJ8) (formula: Fe_8S_9).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $\text{C}_4\text{H}_{12}\text{NO}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		

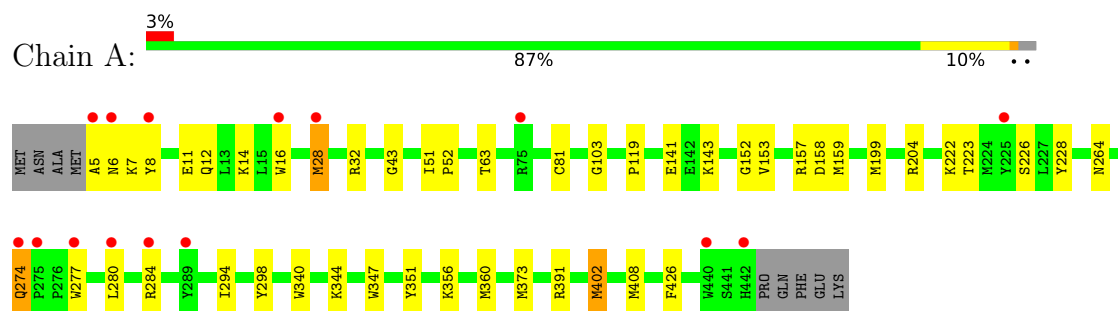
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	257	Total	O	0	1
			258	258		
8	B	161	Total	O	0	1
			162	162		
8	C	219	Total	O	0	2
			221	221		
8	D	156	Total	O	0	1
			157	157		

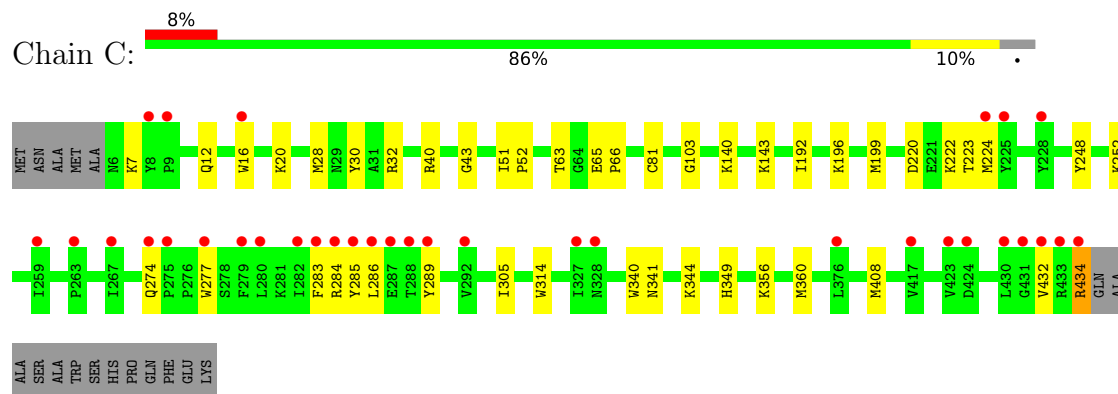
3 Residue-property plots [i](#)

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.

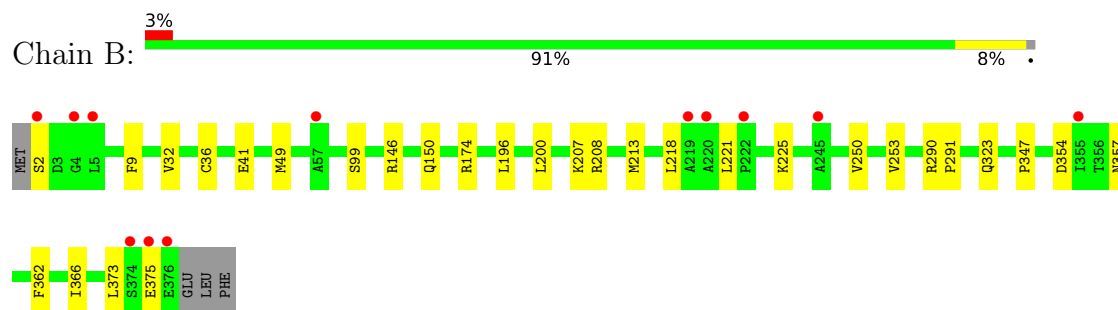
• Molecule 1: BzdO



• Molecule 1: BzdO

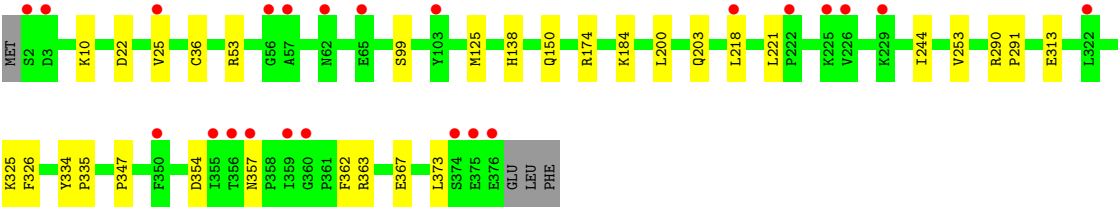


• Molecule 2: BzdN



• 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	208.17Å 102.71Å 86.90Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	48.45 – 1.60 48.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.1 (48.45-1.60) 86.1 (48.45-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.183 , 0.211 0.183 , 0.210	Depositor DCC
R_{free} test set	10124 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14200	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 11.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOD, BYC, BJ8, TRS, SF4, GOL

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	0.78	1/3697 (0.0%)	0.82	4/4992 (0.1%)
1	C	0.71	0/3563	0.78	0/4815
2	B	0.67	0/3140	0.77	0/4251
2	D	0.65	0/3137	0.77	0/4249
All	All	0.71	1/13537 (0.0%)	0.79	4/18307 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	GLN	C-N	13.16	1.48	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLN	CA-C-N	8.49	129.13	120.38
1	A	274	GLN	C-N-CA	8.49	129.13	120.38
1	A	274	GLN	O-C-N	-7.92	112.21	121.32
1	A	274	GLN	CB-CG-CD	5.02	121.13	112.60

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	3603	0	3485	46	0
1	C	3472	0	3357	35	0
2	B	3064	0	2969	15	0
2	D	3061	0	2959	17	0
3	A	56	0	36	3	0
3	C	56	0	36	4	0
4	A	6	0	8	9	0
4	C	18	0	24	3	0
5	A	8	0	0	0	0
5	C	8	0	0	0	0
6	B	17	0	0	0	0
6	D	17	0	0	0	0
7	B	8	0	12	1	0
7	D	8	0	12	0	0
8	A	258	0	0	5	0
8	B	162	0	0	1	0
8	C	221	0	0	0	0
8	D	157	0	0	1	0
All	All	14200	0	12898	113	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 (113) 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:344:LYS:HG3	8:A:631:HOH:O	1.74	0.88
1:A:274:GLN:HB2	8:A:609:HOH:O	1.73	0.87
1:A:28[B]:MET:HE3	1:A:32:ARG:HH11	1.43	0.81
1:C:434:ARG:O	1:C:434:ARG:HG2	1.85	0.76
1:A:274:GLN:O	1:A:274:GLN:HG2	1.87	0.75
1:A:12:GLN:HB3	3:A:501:BYC:N6A	2.03	0.74
1:A:277:TRP:CH2	3:A:501:BYC:HDP A	2.26	0.71
1:C:222:LYS:HD2	1:C:284:ARG:CZ	2.20	0.71
1:C:222:LYS:HD2	1:C:284:ARG:NH1	2.08	0.69
2:B:290:ARG:HG2	2:B:291:PRO:HD2	1.74	0.69
1:C:220:ASP:O	1:C:224:MET:HG3	1.92	0.69
1:C:222:LYS:HE3	1:C:283:PHE:HB3	1.74	0.68
2:B:218:LEU:HD23	2:B:221:LEU:HD12	1.74	0.68
1:A:143[A]:LYS:HG3	4:A:502:GOL:H31	1.76	0.66
2:D:363:ARG:O	2:D:367:GLU:HG3	1.95	0.66
2:D:125:MET:HG3	2:D:138:HIS:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:LEU:HD23	2:D:221:LEU:HD12	1.81	0.62
1:C:305:ILE:HD11	1:C:344:LYS:HG2	1.81	0.62
1:A:284:ARG:NE	3:A:501:BYC:O8A	2.33	0.61
1:C:28[B]:MET:HE3	1:C:32:ARG:HH11	1.64	0.61
1:C:434:ARG:O	1:C:434:ARG:CG	2.47	0.61
1:A:157[B]:ARG:NH1	1:A:158:ASP:OD1	2.34	0.60
1:A:402[A]:MET:HG2	1:A:426:PHE:CG	2.38	0.59
1:C:220:ASP:OD2	1:C:222:LYS:HG2	2.03	0.59
1:A:391[B]:ARG:HD2	8:A:791:HOH:O	2.04	0.57
1:A:356:LYS:O	1:A:360:MET:HG3	2.05	0.57
1:A:7:LYS:HG3	1:A:8:TYR:CE2	2.40	0.56
2:D:325:LYS:HG2	2:D:326:PHE:CD2	2.39	0.56
2:D:325:LYS:HG2	2:D:326:PHE:CE2	2.40	0.56
1:A:5:ALA:HB3	1:A:264:ASN:HB3	1.88	0.55
1:A:28[B]:MET:HE3	1:A:32:ARG:HD3	1.88	0.55
1:C:20:LYS:NZ	3:C:501:BYC:HEPB	2.23	0.54
1:A:222:LYS:HE2	1:A:280:LEU:HB3	1.91	0.53
1:C:356:LYS:O	1:C:360:MET:HG3	2.09	0.53
1:C:222:LYS:CE	1:C:283:PHE:HB3	2.37	0.53
1:A:28[B]:MET:CE	1:A:32:ARG:HH11	2.18	0.53
2:D:22:ASP:O	2:D:25:VAL:HG22	2.10	0.52
2:D:174:ARG:NH2	8:D:504:HOH:O	2.40	0.52
1:A:43:GLY:O	1:A:63:THR:HA	2.10	0.52
1:A:143[B]:LYS:HE2	4:A:502:GOL:H2	1.91	0.51
1:A:16:TRP:CH2	1:A:226:SER:HB2	2.45	0.51
1:A:143[B]:LYS:CE	4:A:502:GOL:H2	2.41	0.51
1:C:143:LYS:HE2	4:C:502:GOL:H2	1.93	0.51
1:C:20:LYS:HZ1	3:C:501:BYC:HEPB	1.76	0.51
2:D:357:ASN:HB3	2:D:362:PHE:HE2	1.76	0.51
1:A:143[B]:LYS:HG3	4:A:502:GOL:H31	1.92	0.50
2:B:362:PHE:O	2:B:366:ILE:HG13	2.11	0.50
1:A:16:TRP:CZ3	1:A:223:THR:HG23	2.46	0.50
1:C:12:GLN:HB3	3:C:501:BYC:N6A	2.27	0.50
1:A:28[A]:MET:HE3	1:A:28[A]:MET:HA	1.94	0.50
1:A:402[A]:MET:HG2	1:A:426:PHE:CD1	2.47	0.50
1:A:274:GLN:HG3	1:A:408:MET:HG3	1.94	0.49
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.94	0.49
1:A:157[A]:ARG:NH2	8:A:606:HOH:O	2.46	0.49
2:B:9:PHE:CZ	2:B:213[B]:MET:HG3	2.48	0.49
1:C:341:ASN:O	1:C:344:LYS:HG3	2.13	0.48
1:A:143[A]:LYS:HD2	4:A:502:GOL:C3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ARG:NH2	8:B:507:HOH:O	2.46	0.47
1:A:204:ARG:HA	1:A:204:ARG:HD3	1.74	0.47
1:A:81:CYS:O	1:A:103:GLY:HA3	2.14	0.47
1:A:153:VAL:HG23	1:A:159:MET:HE1	1.97	0.47
1:C:65:GLU:HB2	1:C:66:PRO:HD3	1.97	0.47
1:C:81:CYS:O	1:C:103:GLY:HA3	2.14	0.47
1:A:119:PRO:HG3	8:A:614:HOH:O	2.15	0.46
1:A:274:GLN:HB3	1:A:298:TYR:CZ	2.50	0.46
1:A:294:ILE:HD12	1:A:294:ILE:C	2.41	0.45
1:A:141:GLU:O	4:A:502:GOL:H12	2.17	0.45
1:C:143:LYS:HE2	4:C:502:GOL:C2	2.46	0.45
1:A:143[A]:LYS:CG	4:A:502:GOL:H31	2.44	0.45
1:A:199:MET:HG2	1:A:340:TRP:CD2	2.51	0.45
2:B:250:VAL:O	2:B:253:VAL:HG22	2.16	0.45
1:A:11:GLU:OE2	1:A:14:LYS:HE2	2.16	0.45
2:B:290:ARG:HG2	2:B:291:PRO:CD	2.45	0.45
1:A:373:MET:HB3	1:A:402[A]:MET:HE2	1.99	0.45
1:C:274:GLN:HG3	1:C:408:MET:HG3	1.98	0.44
2:D:334:TYR:HB3	2:D:335:PRO:HD3	1.99	0.44
1:C:7:LYS:HA	1:C:7:LYS:HE2	1.98	0.44
1:A:143[A]:LYS:HD2	4:A:502:GOL:H31	1.99	0.44
1:C:143:LYS:HE2	4:C:502:GOL:C3	2.48	0.44
2:D:184:LYS:HE2	2:D:313:GLU:HG2	2.00	0.44
2:B:41:GLU:OE2	2:B:207:LYS:NZ	2.51	0.44
1:C:192:ILE:O	1:C:196:LYS:HG3	2.18	0.44
1:C:199:MET:HG2	1:C:340:TRP:CD2	2.53	0.44
1:C:285:TYR:CE2	1:C:289:TYR:HE2	2.35	0.44
2:D:10:LYS:NZ	2:D:10:LYS:HB3	2.33	0.44
1:C:16:TRP:CZ3	1:C:223:THR:HG23	2.53	0.43
2:B:225:LYS:O	2:B:225:LYS:HG3	2.18	0.43
2:B:347:PRO:HG2	2:B:373:LEU:CD2	2.48	0.43
1:C:30:TYR:O	1:C:40:ARG:HD3	2.19	0.43
1:C:248:TYR:OH	1:C:252:LYS:HE3	2.18	0.43
1:A:152:GLY:HA2	1:A:351:TYR:OH	2.18	0.43
1:C:43:GLY:O	1:C:63:THR:HA	2.17	0.43
2:B:196:LEU:O	2:B:200:LEU:HB2	2.19	0.43
2:B:354:ASP:H	2:B:357:ASN:HD21	1.65	0.43
1:C:51:ILE:HB	1:C:52:PRO:HD3	1.99	0.43
2:D:347:PRO:HG2	2:D:373:LEU:CD2	2.49	0.43
1:C:277:TRP:CH2	3:C:501:BYC:HDPA	2.55	0.42
2:B:208[B]:ARG:NH1	2:B:208[B]:ARG:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:ASP:H	2:D:357:ASN:HD21	1.68	0.42
2:D:200:LEU:HD23	2:D:244:ILE:HD11	2.01	0.42
1:A:158:ASP:OD2	7:B:402:TRS:H32	2.19	0.42
1:C:305:ILE:HD11	1:C:344:LYS:CG	2.47	0.42
2:D:290:ARG:HG2	2:D:291:PRO:HD2	2.01	0.42
1:C:286:LEU:HD23	1:C:286:LEU:HA	1.66	0.42
1:A:344:LYS:HD2	1:A:347:TRP:CD1	2.55	0.41
2:B:146:ARG:O	2:B:150:GLN:HG3	2.20	0.41
2:B:32:VAL:HG21	2:B:49:MET:SD	2.60	0.41
1:C:140:LYS:HE3	1:C:140:LYS:HB3	1.93	0.41
1:A:274:GLN:HB3	1:A:298:TYR:CE2	2.56	0.40
1:C:349:HIS:HB3	1:C:356:LYS:HB2	2.03	0.40
2:D:53:ARG:HD3	2:D:203:GLN:OE1	2.21	0.40
2:D:357:ASN:HB3	2:D:362:PHE:CE2	2.55	0.40
1:A:143[A]:LYS:HG3	4:A:502:GOL:H11	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	444/447 (99%)	432 (97%)	12 (3%)	0	100	100
1	C	428/447 (96%)	419 (98%)	9 (2%)	0	100	100
2	B	378/379 (100%)	368 (97%)	7 (2%)	3 (1%)	16	5
2	D	378/379 (100%)	367 (97%)	8 (2%)	3 (1%)	16	5
All	All	1628/1652 (98%)	1586 (97%)	36 (2%)	6 (0%)	43	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	36	CYS
2	D	99[A]	SER
2	D	99[B]	SER
2	B	36	CYS
2	B	99[A]	SER
2	B	99[B]	SER

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	371/371 (100%)	365 (98%)	6 (2%)	55	33
1	C	359/371 (97%)	356 (99%)	3 (1%)	73	59
2	B	326/325 (100%)	322 (99%)	4 (1%)	63	43
2	D	326/325 (100%)	324 (99%)	2 (1%)	78	66
All	All	1382/1392 (99%)	1367 (99%)	15 (1%)	70	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	28[A]	MET
1	A	28[B]	MET
1	A	228	TYR
1	A	402[A]	MET
1	A	402[B]	MET
2	B	2	SER
2	B	323[A]	GLN
2	B	323[B]	GLN
2	B	375	GLU
1	C	314	TRP
1	C	432	VAL
1	C	434	ARG
2	D	150	GLN
2	D	253	VAL

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

Mol	Chain	Res	Type
1	A	328	ASN
1	A	390	ASN
1	A	442	HIS
2	B	8	GLN
2	B	62	ASN
2	B	98	GLN
2	B	324	GLN
1	C	6	ASN
1	C	346	GLN
2	D	98	GLN
2	D	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
4	GOL	C	503[A]	-	5,5,5	0.08	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TRS	B	402	-	7,7,7	0.21	0	9,9,9	0.79	0
6	BJ8	D	401	2	6,26,26	3.35	4 (66%)	-		
4	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.32	0
3	BYC	A	501	-	57,59,59	1.73	9 (15%)	81,87,87	2.84	30 (37%)
5	SF4	A	503	1,8	0,12,12	-	-	-		
6	BJ8	B	401	2	6,26,26	4.73	5 (83%)	-		
5	SF4	C	504	1,8	0,12,12	-	-	-		
4	GOL	C	502	-	5,5,5	1.97	2 (40%)	5,5,5	0.81	0
4	GOL	C	503[B]	-	5,5,5	1.53	2 (40%)	5,5,5	0.75	0
7	TRS	D	402	-	7,7,7	0.69	0	9,9,9	1.15	1 (11%)
3	BYC	C	501	-	57,59,59	1.76	9 (15%)	81,87,87	2.59	24 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	503[A]	-	-	4/4/4/4	-
7	TRS	B	402	-	-	2/9/9/9	-
6	BJ8	D	401	2	-	-	0/12/10/10
4	GOL	A	502	-	-	0/4/4/4	-
3	BYC	A	501	-	-	19/55/71/71	0/4/4/4
5	SF4	A	503	1,8	-	-	0/6/5/5
6	BJ8	B	401	2	-	-	0/12/10/10
5	SF4	C	504	1,8	-	-	0/6/5/5
4	GOL	C	502	-	-	2/4/4/4	-
4	GOL	C	503[B]	-	-	2/4/4/4	-
7	TRS	D	402	-	-	2/9/9/9	-
3	BYC	C	501	-	-	17/55/71/71	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	BJ8	S5-FE8	6.21	2.37	2.28
3	A	501	BYC	C5P-N4P	6.07	1.47	1.33
6	B	401	BJ8	S3-FE1	5.99	2.37	2.28
3	C	501	BYC	C9P-N8P	5.75	1.47	1.33
3	A	501	BYC	C9P-N8P	5.26	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	401	BJ8	S6-FE8	5.25	2.36	2.28
3	C	501	BYC	C5P-N4P	5.16	1.45	1.33
6	B	401	BJ8	S6-FE8	4.96	2.35	2.28
6	D	401	BJ8	S2-FE1	4.91	2.35	2.28
3	C	501	BYC	C6A-N6A	4.63	1.46	1.34
3	A	501	BYC	C6A-N6A	4.47	1.45	1.34
6	B	401	BJ8	S4-FE1	4.36	2.34	2.28
3	C	501	BYC	P1A-O3A	4.34	1.64	1.59
3	C	501	BYC	P2A-O3A	4.30	1.64	1.59
6	B	401	BJ8	S2-FE1	3.99	2.34	2.28
3	A	501	BYC	C2B-C1B	-3.73	1.42	1.49
3	C	501	BYC	C2B-C1B	-3.52	1.42	1.49
3	A	501	BYC	P2A-O3A	3.37	1.63	1.59
4	C	502	GOL	C3-C2	3.02	1.63	1.51
6	D	401	BJ8	S3-FE1	2.76	2.32	2.28
4	C	502	GOL	C1-C2	2.73	1.62	1.51
3	A	501	BYC	P1A-O3A	2.73	1.62	1.59
3	A	501	BYC	C4B-C3B	2.51	1.43	1.38
4	C	503[B]	GOL	C1-C2	2.49	1.61	1.51
3	C	501	BYC	C8A-N7A	2.34	1.36	1.31
4	C	503[B]	GOL	C3-C2	2.27	1.60	1.51
3	A	501	BYC	C8A-N7A	2.23	1.36	1.31
3	A	501	BYC	C8A-N9A	-2.23	1.33	1.37
3	C	501	BYC	C8A-N9A	-2.15	1.33	1.37
6	D	401	BJ8	S7-FE8	2.07	2.31	2.28
3	C	501	BYC	OAP-CAP	2.01	1.45	1.42

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	BYC	C4A-N9A-C8A	13.51	119.92	105.74
3	C	501	BYC	C4A-N9A-C8A	12.18	118.53	105.74
3	A	501	BYC	N9A-C8A-N7A	-9.02	101.14	113.94
3	C	501	BYC	N9A-C8A-N7A	-8.25	102.23	113.94
3	C	501	BYC	N3A-C2A-N1A	-6.80	118.29	128.58
3	A	501	BYC	N3A-C2A-N1A	-6.64	118.54	128.58
3	A	501	BYC	N3A-C4A-N9A	6.03	137.42	127.17
3	C	501	BYC	N3A-C4A-N9A	5.86	137.14	127.17
3	A	501	BYC	C2P-S1P-C1B	4.42	105.06	99.85
3	A	501	BYC	C3P-N4P-C5P	4.36	130.95	122.82
3	A	501	BYC	C5M-C4A-N9A	-4.21	101.22	105.81
3	A	501	BYC	C5M-N7A-C8A	4.21	110.06	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	BYC	CEP-CBP-CDP	-4.16	100.91	109.20
3	C	501	BYC	C5M-C4A-N3A	-4.13	121.02	126.72
3	C	501	BYC	C7P-C6P-C5P	-4.13	105.52	112.39
3	C	501	BYC	C5M-N7A-C8A	4.03	109.78	103.45
3	A	501	BYC	CDP-CBP-CAP	4.00	115.59	108.77
3	A	501	BYC	C5M-C4A-N3A	-3.89	121.36	126.72
3	A	501	BYC	C2A-N3A-C4A	3.88	121.31	111.83
3	C	501	BYC	C2A-N3A-C4A	3.83	121.19	111.83
3	C	501	BYC	C5M-C4A-N9A	-3.65	101.84	105.81
3	A	501	BYC	O5P-C5P-N4P	3.52	129.93	123.03
3	C	501	BYC	C2A-N1A-C6A	3.47	124.43	118.73
3	A	501	BYC	C4A-N9A-C1D	-3.32	118.86	126.63
3	C	501	BYC	CDP-CBP-CAP	3.22	114.26	108.77
3	C	501	BYC	C2P-S1P-C1B	3.22	103.64	99.85
3	A	501	BYC	C6B-C7B-C2B	-3.06	117.36	120.36
3	C	501	BYC	C4A-N9A-C1D	-2.98	119.66	126.63
3	A	501	BYC	C7P-C6P-C5P	-2.92	107.54	112.39
3	A	501	BYC	C2A-N1A-C6A	2.84	123.39	118.73
3	C	501	BYC	O2A-P1A-O1A	-2.69	99.94	112.44
3	A	501	BYC	C1D-N9A-C8A	-2.67	121.17	127.09
3	C	501	BYC	CEP-CBP-CDP	-2.67	103.89	109.20
3	A	501	BYC	C4D-O4D-C1D	-2.61	103.71	109.47
3	C	501	BYC	C4A-C5M-N7A	-2.60	107.61	110.58
3	A	501	BYC	C4A-C5M-N7A	-2.56	107.66	110.58
3	A	501	BYC	O7A-P3D-O3D	2.51	115.62	105.85
3	A	501	BYC	C2B-C1B-S1P	2.50	119.57	114.97
3	A	501	BYC	C6P-C5P-N4P	-2.46	111.87	116.34
3	C	501	BYC	O4A-P2A-O5A	-2.40	101.27	112.44
3	C	501	BYC	C1D-N9A-C8A	-2.39	121.79	127.09
3	A	501	BYC	O4A-P2A-O3A	2.35	113.64	107.27
3	A	501	BYC	O9A-P3D-O3D	2.31	114.84	105.85
3	C	501	BYC	O9A-P3D-O3D	2.27	114.69	105.85
3	C	501	BYC	C6P-C7P-N8P	-2.26	107.18	112.00
3	C	501	BYC	C7P-N8P-C9P	-2.19	118.61	122.55
3	A	501	BYC	C7B-C2B-C3B	2.17	121.33	118.57
3	A	501	BYC	O4A-P2A-O5A	-2.15	102.45	112.44
3	A	501	BYC	O5P-C5P-C6P	-2.11	118.19	122.02
7	D	402	TRS	C3-C-N	2.08	113.48	108.17
3	A	501	BYC	C6P-C7P-N8P	-2.08	107.57	112.00
3	C	501	BYC	OAP-CAP-CBP	2.06	114.94	110.18
3	C	501	BYC	C4D-O4D-C1D	-2.03	104.99	109.47
3	A	501	BYC	CDP-CBP-CCP	2.02	111.55	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	BYC	O2A-P1A-O3A	2.01	112.69	107.27

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	BYC	C3P-C2P-S1P-C1B
3	A	501	BYC	CCP-O6A-P2A-O3A
3	A	501	BYC	CCP-O6A-P2A-O5A
3	A	501	BYC	C9P-CAP-CBP-CCP
3	A	501	BYC	C9P-CAP-CBP-CDP
3	A	501	BYC	OAP-CAP-CBP-CCP
3	A	501	BYC	OAP-CAP-CBP-CDP
3	A	501	BYC	CAP-CBP-CCP-O6A
3	A	501	BYC	CDP-CBP-CCP-O6A
3	A	501	BYC	CEP-CBP-CCP-O6A
3	C	501	BYC	C3P-C2P-S1P-C1B
3	C	501	BYC	CCP-O6A-P2A-O5A
3	C	501	BYC	C9P-CAP-CBP-CCP
3	C	501	BYC	C9P-CAP-CBP-CDP
3	C	501	BYC	OAP-CAP-CBP-CCP
3	C	501	BYC	OAP-CAP-CBP-CDP
3	C	501	BYC	CAP-CBP-CCP-O6A
3	C	501	BYC	CDP-CBP-CCP-O6A
3	C	501	BYC	CEP-CBP-CCP-O6A
4	C	502	GOL	O1-C1-C2-C3
4	C	503[A]	GOL	O1-C1-C2-C3
4	C	503[B]	GOL	C1-C2-C3-O3
7	B	402	TRS	N-C-C2-O2
4	C	503[A]	GOL	C1-C2-C3-O3
4	C	503[A]	GOL	O1-C1-C2-O2
4	C	503[B]	GOL	O2-C2-C3-O3
3	A	501	BYC	C2D-C3D-O3D-P3D
3	A	501	BYC	OAP-CAP-CBP-CEP
3	C	501	BYC	OAP-CAP-CBP-CEP
3	A	501	BYC	P1A-O3A-P2A-O5A
4	C	502	GOL	O1-C1-C2-O2
4	C	503[A]	GOL	O2-C2-C3-O3
7	B	402	TRS	C3-C-C2-O2
7	D	402	TRS	C1-C-C2-O2
7	D	402	TRS	N-C-C2-O2
3	A	501	BYC	P2A-O3A-P1A-O5D

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Mol	Chain	Res	Type	Atoms
3	A	501	BYC	CCP-O6A-P2A-O4A
3	C	501	BYC	CCP-O6A-P2A-O3A
3	C	501	BYC	CCP-O6A-P2A-O4A
3	A	501	BYC	C4D-C3D-O3D-P3D
3	A	501	BYC	C5P-C6P-C7P-N8P
3	C	501	BYC	C3D-O3D-P3D-O9A
3	C	501	BYC	O5P-C5P-C6P-C7P
3	C	501	BYC	C4D-C5D-O5D-P1A
3	A	501	BYC	C9P-CAP-CBP-CEP
3	C	501	BYC	C9P-CAP-CBP-CEP
3	A	501	BYC	C3D-O3D-P3D-O7A
3	C	501	BYC	N4P-C5P-C6P-C7P

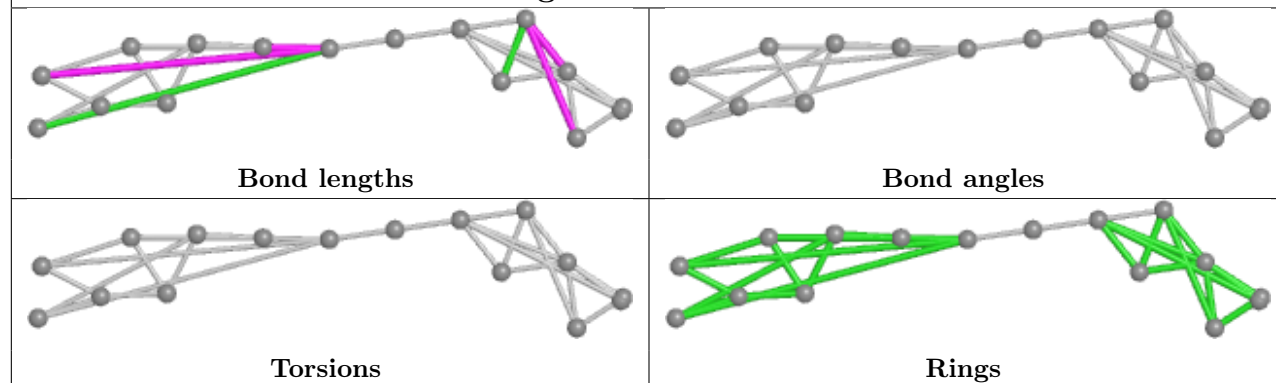
There are no ring outliers.

5 monomers are involved in 20 short contacts:

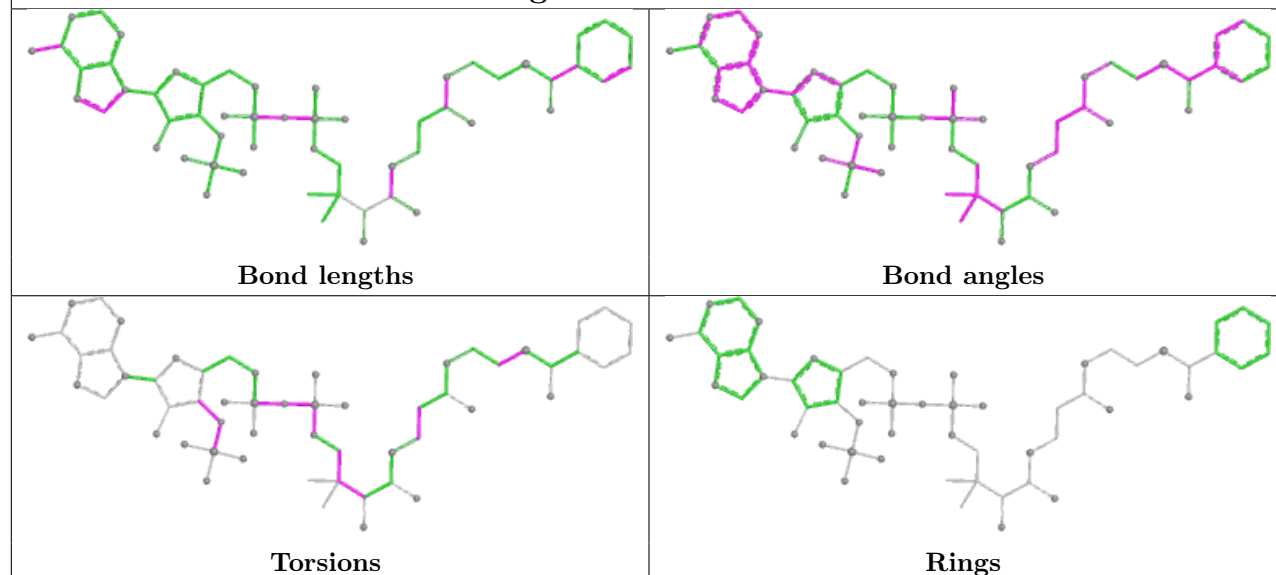
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	402	TRS	1	0
4	A	502	GOL	9	0
3	A	501	BYC	3	0
4	C	502	GOL	3	0
3	C	501	BYC	4	0

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.

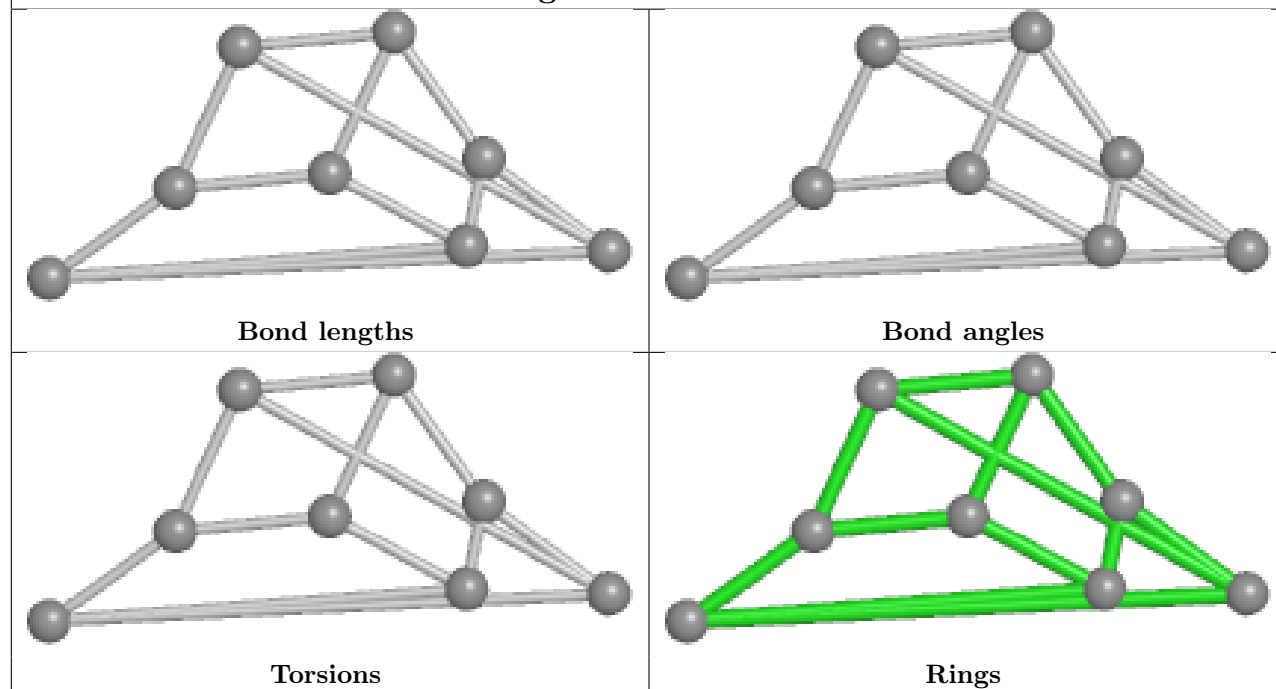
Ligand BJ8 D 401

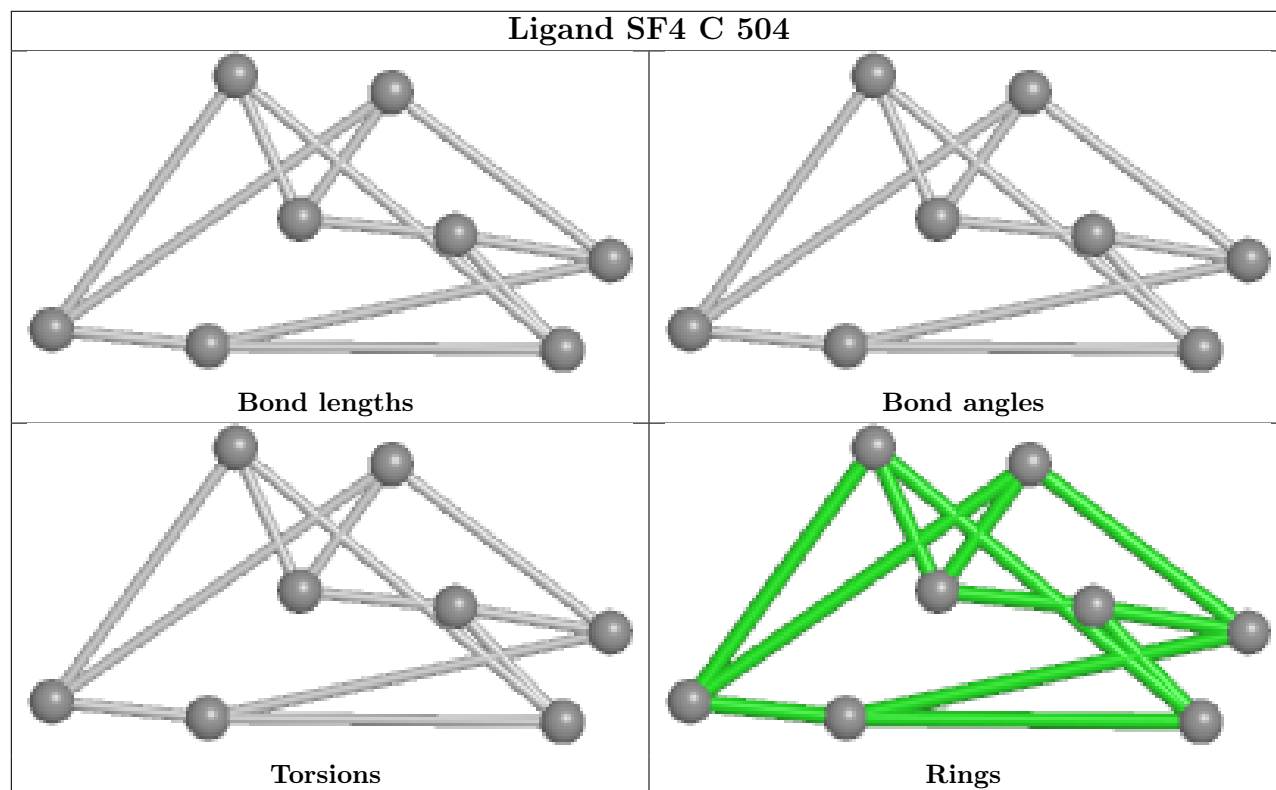
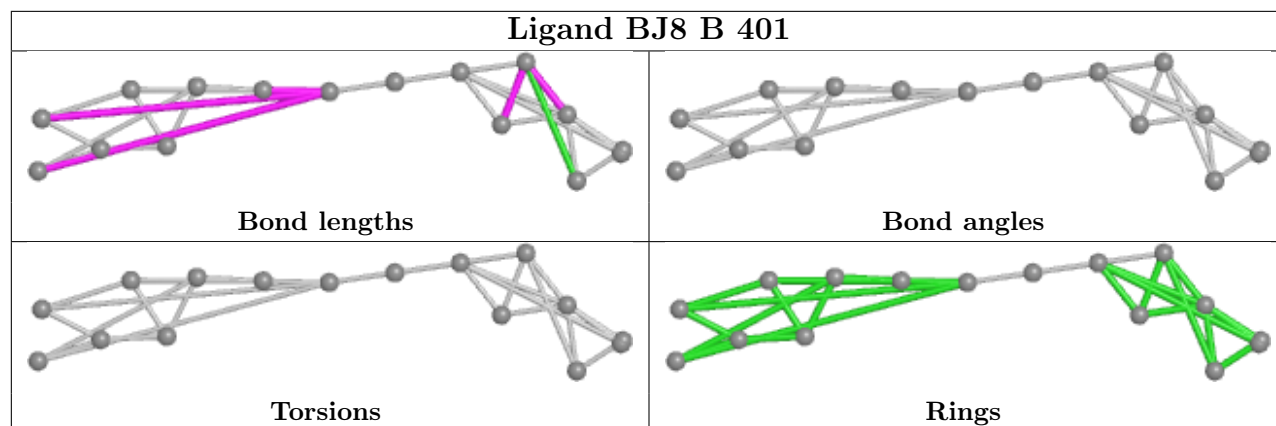


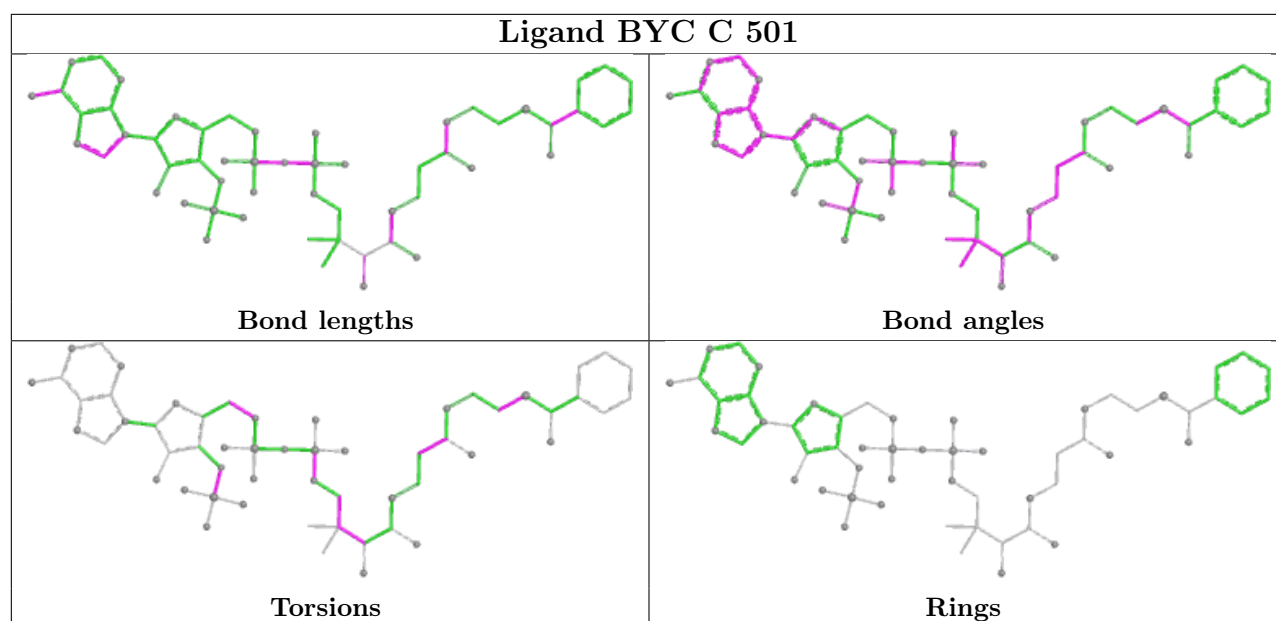
Ligand BYC A 501



Ligand SF4 A 503







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%)	0.33	15 (3%) 48 50	12, 25, 40, 90	8 (1%)
1	C	429/447 (95%)	0.56	34 (7%) 18 19	16, 28, 54, 107	1 (0%)
2	B	375/379 (98%)	0.50	12 (3%) 50 53	11, 29, 46, 94	5 (1%)
2	D	375/379 (98%)	0.61	23 (6%) 27 27	11, 30, 50, 92	5 (1%)
All	All	1617/1652 (97%)	0.49	84 (5%) 33 33	11, 28, 48, 107	19 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	TRP	5.2
1	C	280	LEU	5.0
1	A	274	GLN	4.4
1	C	283	PHE	4.4
1	C	431	GLY	4.4
1	C	277	TRP	4.2
1	C	289	TYR	4.1
1	A	5	ALA	4.0
1	C	432	VAL	4.0
2	D	56	GLY	3.9
1	A	16	TRP	3.8
2	D	359	ILE	3.7
1	A	277	TRP	3.7
1	A	6	ASN	3.6
1	A	280	LEU	3.5
1	C	288	THR	3.2
2	D	229	LYS	3.2
1	C	417	VAL	3.2
2	D	2	SER	3.1
2	D	374	SER	3.1
2	D	355	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	284	ARG	3.0
1	C	434	ARG	3.0
1	C	282	ILE	2.9
1	C	285	TYR	2.9
1	C	267	ILE	2.9
2	D	62[A]	ASN	2.9
2	B	4	GLY	2.8
1	C	16	TRP	2.8
1	C	430	LEU	2.8
2	D	25	VAL	2.7
2	D	225	LYS	2.7
1	C	286	LEU	2.7
2	D	103	TYR	2.7
2	B	219	ALA	2.7
1	C	8	TYR	2.6
2	B	2	SER	2.6
1	C	274	GLN	2.6
2	D	226	VAL	2.6
2	B	376	GLU	2.6
1	A	442	HIS	2.5
1	C	279	PHE	2.5
1	C	287	GLU	2.5
1	C	423	VAL	2.5
1	C	433	ARG	2.5
2	B	375	GLU	2.5
2	D	218	LEU	2.5
1	C	292	VAL	2.4
2	D	3	ASP	2.4
2	D	65	GLU	2.3
2	D	375	GLU	2.3
1	A	289	TYR	2.3
1	C	225	TYR	2.3
2	D	322	LEU	2.3
1	A	75	ARG	2.3
1	A	225	TYR	2.3
1	C	224	MET	2.3
2	D	350	PHE	2.2
1	A	275	PRO	2.2
2	D	356	THR	2.2
1	C	259	ILE	2.2
1	C	9	PRO	2.2
2	B	222	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	376	GLU	2.2
2	B	220	ALA	2.1
1	A	284	ARG	2.1
1	C	376	LEU	2.1
2	D	357	ASN	2.1
1	C	275	PRO	2.1
2	D	222	PRO	2.1
1	C	327	ILE	2.1
2	B	245	ALA	2.1
1	C	328	ASN	2.1
1	C	263	PRO	2.1
2	B	355	ILE	2.1
2	B	57	ALA	2.1
2	B	374	SER	2.1
2	B	5	LEU	2.1
1	A	8	TYR	2.1
1	C	228	TYR	2.1
2	D	57	ALA	2.0
1	A	28[A]	MET	2.0
1	C	424	ASP	2.0
2	D	360	GLY	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.

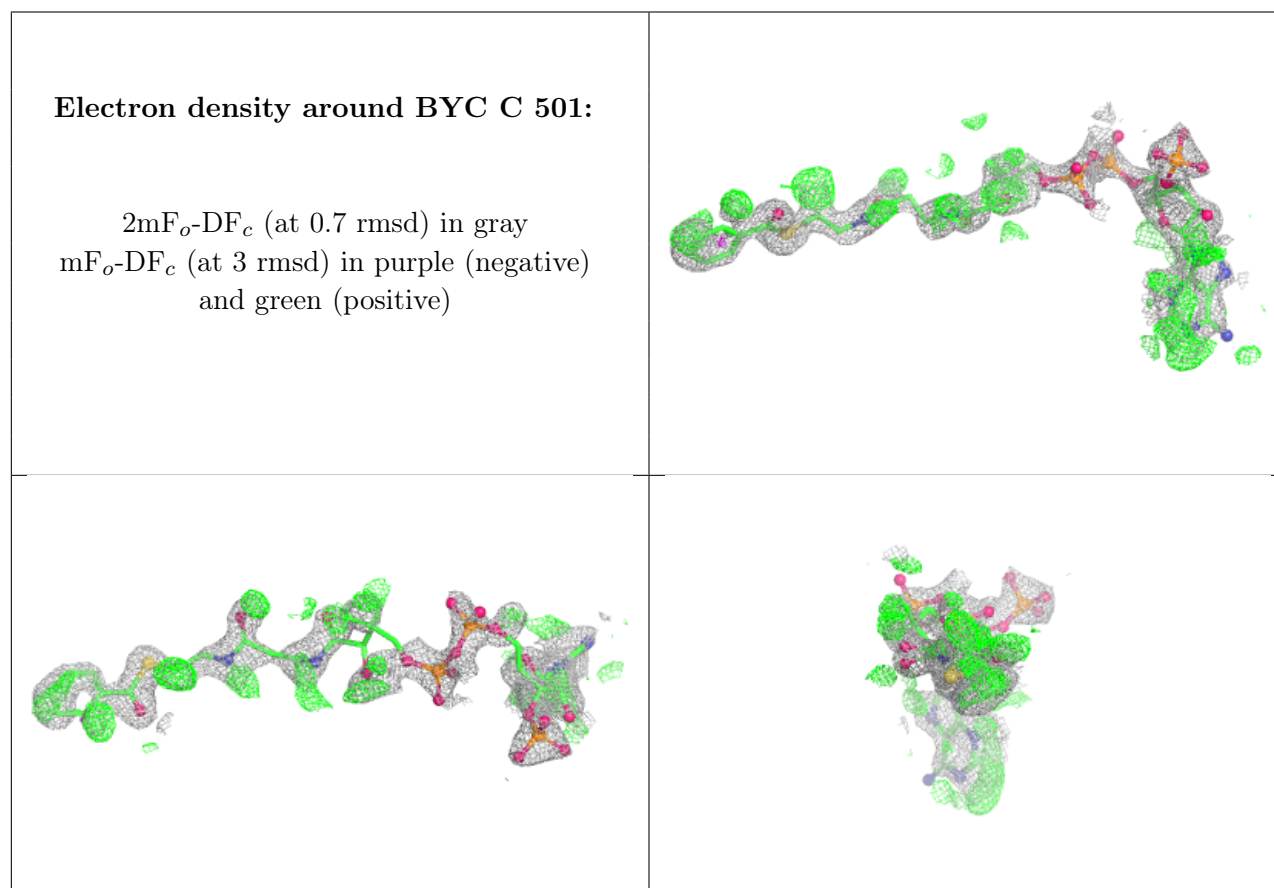
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BYC	C	501	56/56	0.68	0.27	17,43,52,61	56
3	BYC	A	501	56/56	0.69	0.28	15,40,50,56	56

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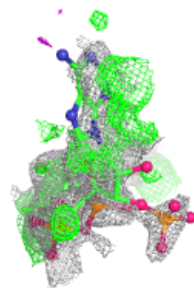
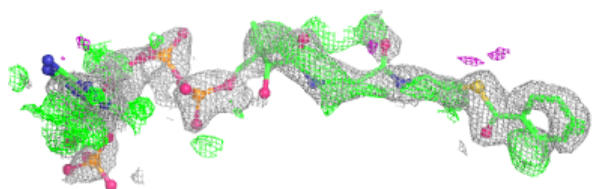
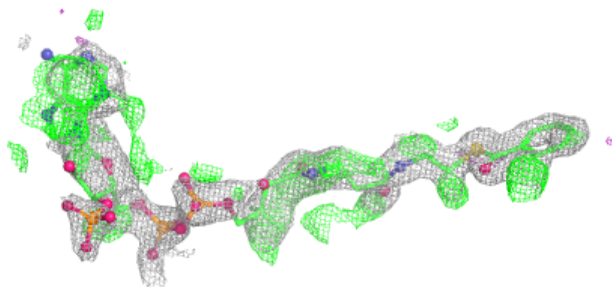
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	502	6/6	0.82	0.13	41,44,45,51	0
4	GOL	A	502	6/6	0.83	0.12	36,37,40,44	0
4	GOL	C	503[A]	6/6	0.87	0.12	27,28,31,34	6
4	GOL	C	503[B]	6/6	0.87	0.12	25,31,34,34	6
7	TRS	D	402	8/8	0.88	0.11	27,28,29,31	0
7	TRS	B	402	8/8	0.90	0.09	26,27,31,42	0
6	BJ8	B	401	17/17	0.99	0.04	21,24,26,27	0
6	BJ8	D	401	17/17	0.99	0.03	23,24,27,28	0
5	SF4	A	503	8/8	0.99	0.03	19,20,21,23	0
5	SF4	C	504	8/8	0.99	0.03	21,21,23,25	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.

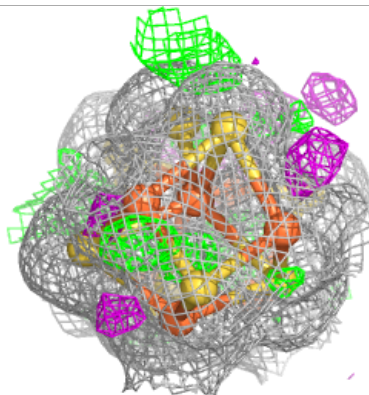
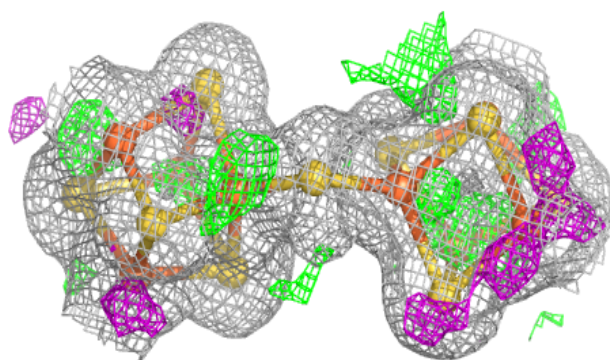
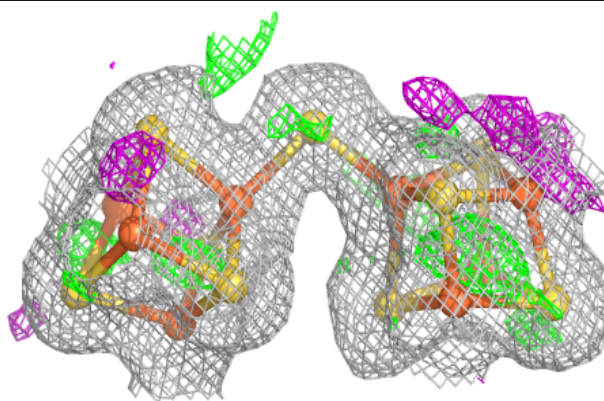


Electron density around BYC A 501:

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

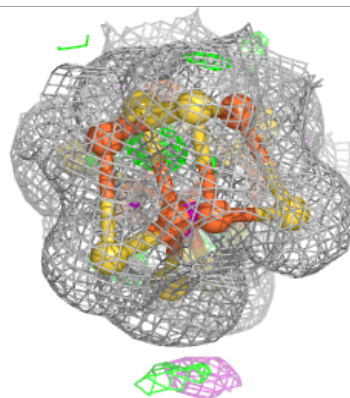
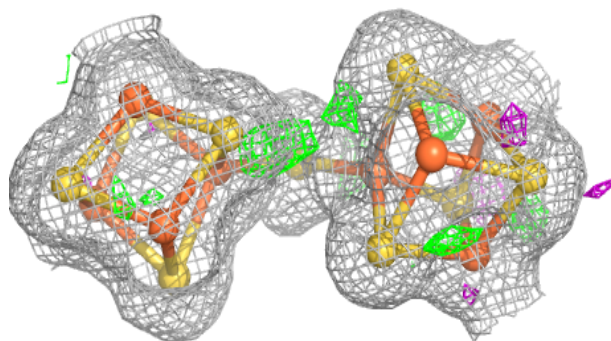
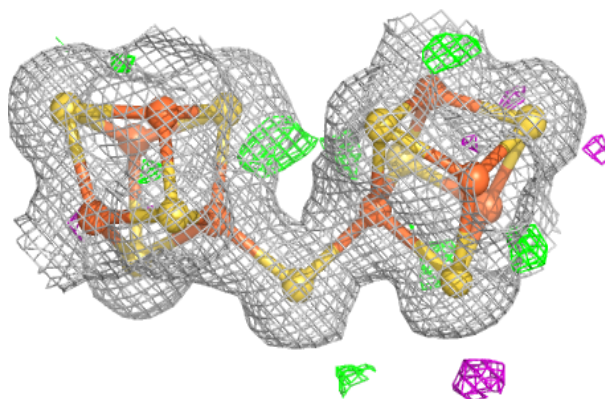
**Electron density around BJ8 B 401:**

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



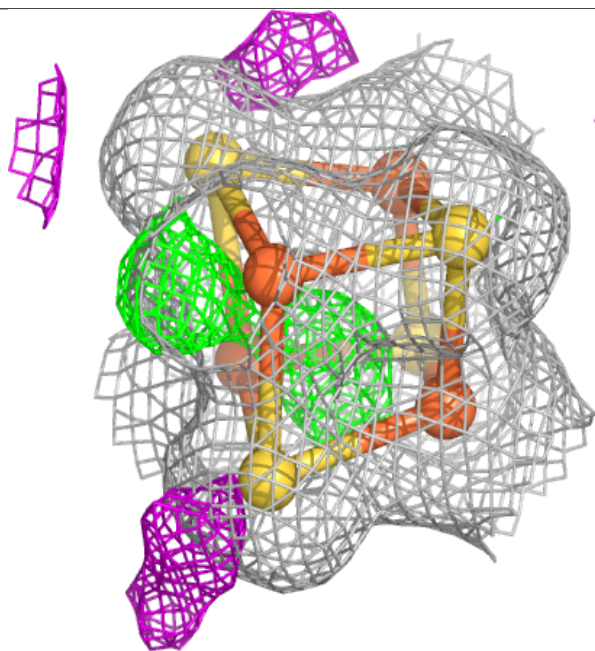
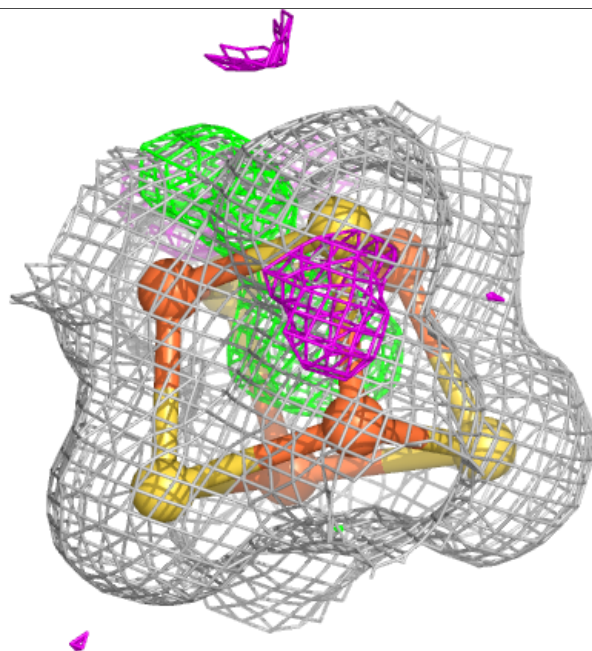
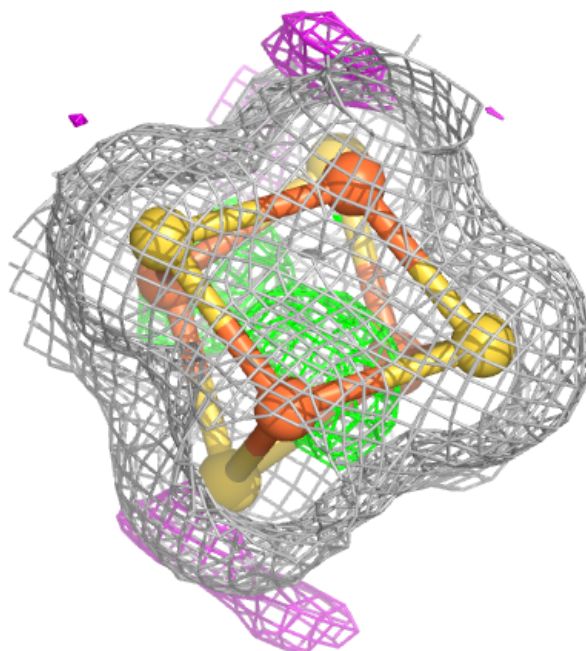
Electron density around BJ8 D 401:

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



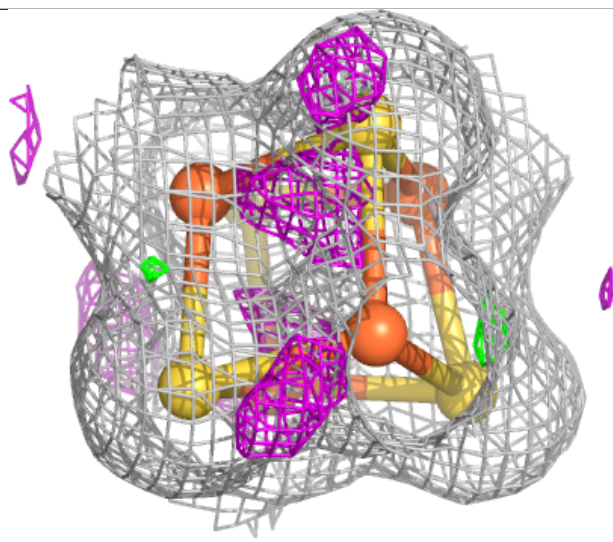
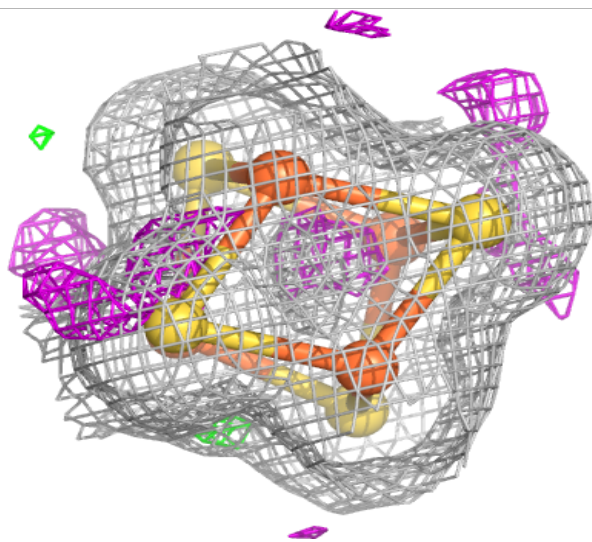
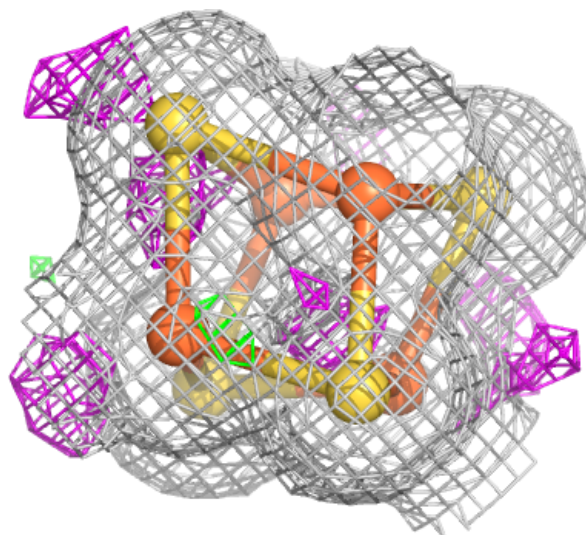
Electron density around SF4 A 503:

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



Electron density around SF4 C 504:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.