



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:27 AM UTC

PDB ID : 8S02 / pdb_00008s02
Title : BzdNO-benzoyl-CoA complex
Authors : Ermler, U.; Boll, M.; Fuchs, J.; Demmer, U.
Deposited on : 2024-02-13
Resolution : 1.35 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

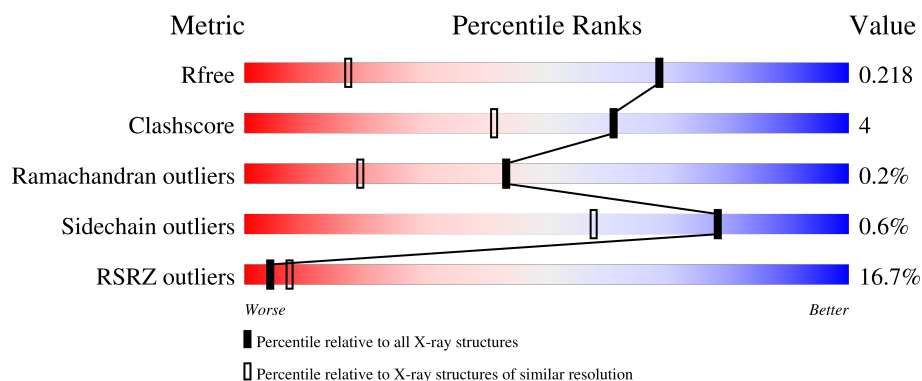
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	11% 90% 8% .
1	C	447	16% 88% 8% .
2	B	379	18% 91% 8% .
2	D	379	22% 87% 12% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14359 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
			3599	2294	615	664	26			
1	C	431	Total	C	N	O	S	0	3	0
			3512	2239	598	649	26			

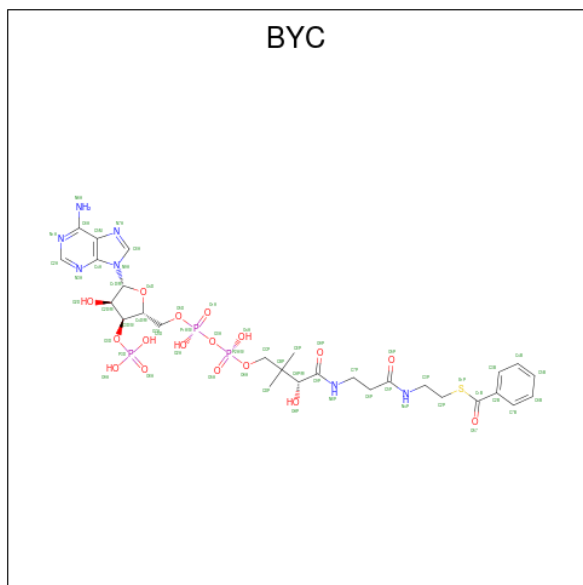
There are 20 discrepancies between the modelled and reference sequences:

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	N	O	S	0	7	0
			3080	1951	535	574	20			
2	D	375	Total	C	N	O	S	0	7	0
			3074	1949	530	575	20			

- Molecule 3 is benzoyl coenzyme A (CCD ID: BYC) (formula: $C_{28}H_{40}N_7O_{17}P_3S$).



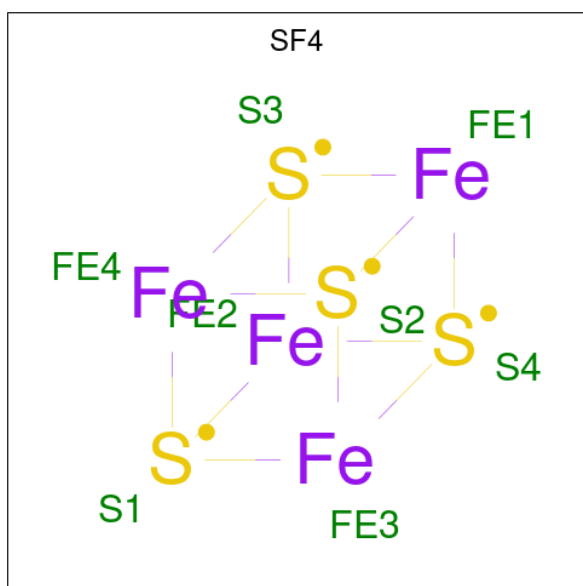
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



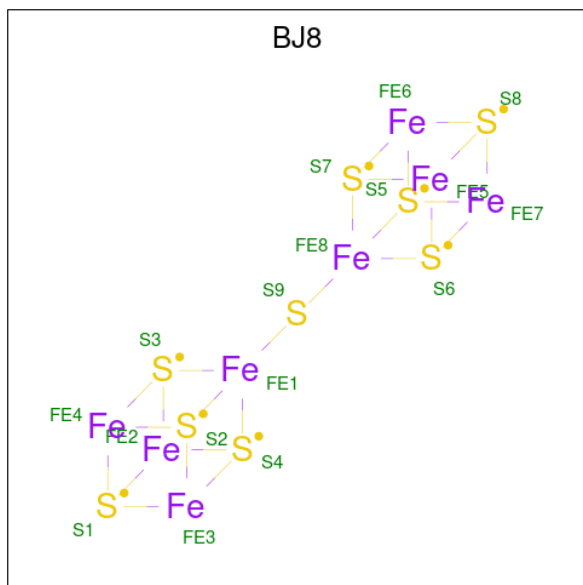
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	1
			12	6	6		

- 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	1
			16	8	2	6		
7	C	1	Total	C	N	O	0	1
			16	8	2	6		

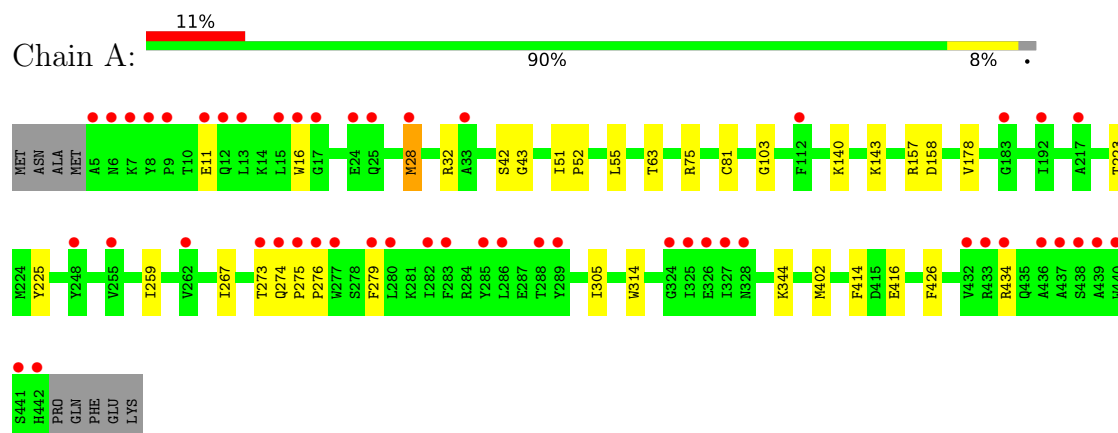
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	276	Total	O	0	0
			276	276		
8	B	182	Total	O	0	0
			182	182		
8	C	241	Total	O	0	1
			242	242		
8	D	176	Total	O	0	0
			176	176		

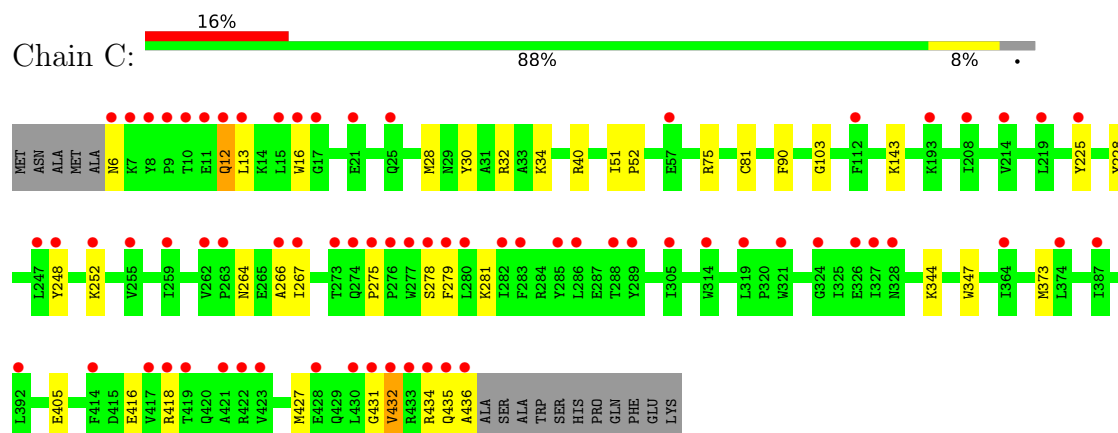
3 Residue-property plots [i](#)

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.

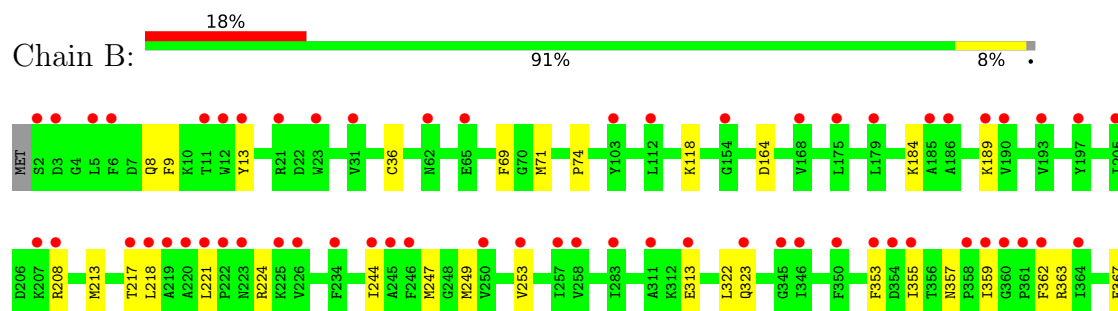
• Molecule 1: BzdO

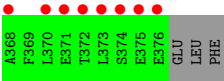


• Molecule 1: BzdO

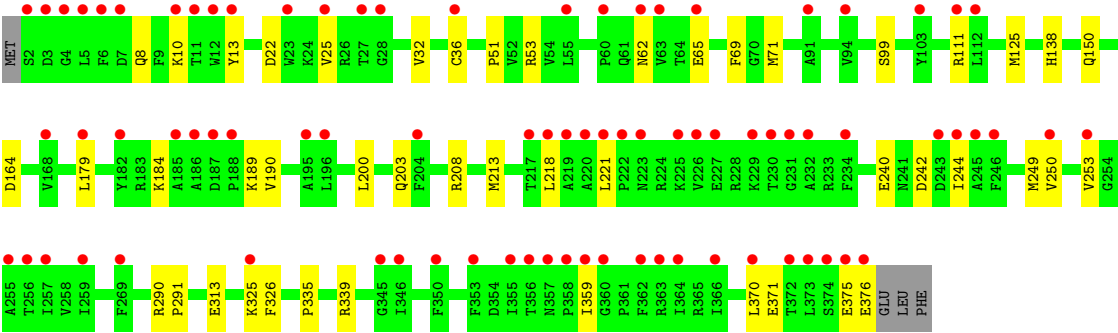
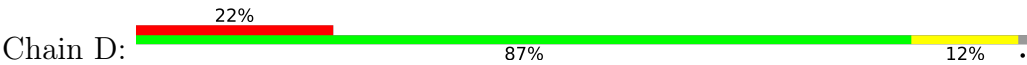


• Molecule 2: BzdN





● 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	208.85Å 102.79Å 86.82Å 90.00° 102.48° 90.00°	Depositor
Resolution (Å)	40.03 – 1.35 40.03 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.03-1.35) 99.4 (40.03-1.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.35Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.199 , 0.217 0.200 , 0.218	Depositor DCC
R_{free} test set	19358 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.4	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	14359	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.00% 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: TRS, BJ8, GOL, BYC, DOD, 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	0.36	0/3694	0.60	0/4992
1	C	0.36	0/3603	0.61	0/4868
2	B	0.34	0/3156	0.59	0/4273
2	D	0.32	0/3150	0.57	0/4267
All	All	0.35	0/13603	0.59	0/18400

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	434	ARG	Sidechain
2	D	111	ARG	Sidechain

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	3599	0	3467	26	0
1	C	3512	0	3393	35	0
2	B	3080	0	2977	18	0
2	D	3074	0	2968	32	0
3	A	56	0	36	0	0
3	C	56	0	36	2	0
4	A	6	0	8	1	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	16	0	24	0	0
7	C	16	0	24	0	0
8	A	276	0	0	3	0
8	B	182	0	0	3	0
8	C	242	0	0	7	0
8	D	176	0	0	1	0
All	All	14359	0	12957	111	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 (111) 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:42[A]:SER:OG	8:A:601:HOH:O	1.84	0.96
1:C:13:LEU:HB2	8:C:609:HOH:O	1.74	0.86
1:C:267:ILE:HD11	1:C:432:VAL:HG11	1.59	0.82
1:C:6:ASN:HD22	1:C:264:ASN:HB3	1.47	0.80
1:C:6:ASN:ND2	1:C:264:ASN:HB3	1.97	0.79
1:C:344:LYS:HG3	8:C:643:HOH:O	1.83	0.79
2:D:8:GLN:HG2	2:D:213[B]:MET:HE3	1.67	0.77
1:C:16:TRP:HB2	8:C:609:HOH:O	1.86	0.75
1:C:267:ILE:CD1	1:C:432:VAL:HG11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:HG2	2:B:213[A]:MET:HE3	1.73	0.71
2:D:179[B]:LEU:HD11	2:D:190:VAL:HG21	1.73	0.70
1:C:344:LYS:HD2	1:C:347:TRP:CD1	2.28	0.69
2:D:253:VAL:HG23	2:D:370:LEU:HD11	1.77	0.66
1:C:435:GLN:HG3	1:C:436:ALA:N	2.12	0.63
1:A:28[A]:MET:HE3	1:A:28[A]:MET:HA	1.82	0.62
2:B:218:LEU:HD23	2:B:221:LEU:HD12	1.82	0.62
2:B:247:MET:HE3	8:B:632:HOH:O	1.99	0.62
1:C:405:GLU:H	1:C:418:ARG:HH22	1.48	0.61
2:D:62[A]:ASN:ND2	2:D:65:GLU:OE1	2.33	0.61
4:C:504[A]:GOL:H11	8:C:625:HOH:O	1.99	0.61
1:A:28[B]:MET:HE3	1:A:32:ARG:HH11	1.68	0.59
2:D:218:LEU:HD23	2:D:221:LEU:HD12	1.85	0.59
1:A:157[B]:ARG:NH1	1:A:158:ASP:OD1	2.36	0.58
2:D:179[B]:LEU:CD1	2:D:190:VAL:HG21	2.33	0.58
2:D:325:LYS:HG2	2:D:326:PHE:CD2	2.39	0.57
2:B:164[A]:ASP:OD1	2:B:208[A]:ARG:NH2	2.38	0.57
2:B:217:THR:HG22	8:B:512:HOH:O	2.04	0.56
1:A:402[A]:MET:HG2	1:A:426:PHE:CG	2.41	0.56
1:A:11:GLU:HG3	1:A:259:ILE:HD12	1.89	0.55
1:A:225:TYR:CZ	1:A:275:PRO:HG3	2.41	0.55
1:C:12[B]:GLN:HG2	3:C:501:BYC:C6A	2.37	0.55
1:C:13:LEU:HD12	8:C:609:HOH:O	2.07	0.54
1:A:273:THR:HG22	8:A:608:HOH:O	2.08	0.53
2:D:150:GLN:OE1	8:D:501:HOH:O	2.19	0.53
1:C:28[B]:MET:HE3	1:C:32:ARG:HH11	1.72	0.52
1:A:279[B]:PHE:CD2	1:A:414:PHE:CE2	2.97	0.52
1:C:344:LYS:HD2	1:C:347:TRP:NE1	2.24	0.52
2:D:125:MET:HG3	2:D:138:HIS:CE1	2.44	0.52
2:B:208[A]:ARG:NH1	8:B:504:HOH:O	2.42	0.52
1:C:16:TRP:CE3	8:C:609:HOH:O	2.53	0.52
1:C:12[A]:GLN:HG3	3:C:501:BYC:C6A	2.41	0.51
2:B:9:PHE:CZ	2:B:213[A]:MET:HG3	2.46	0.51
2:D:179[B]:LEU:HD12	2:D:179[B]:LEU:O	2.11	0.50
2:B:74:PRO:HB3	2:B:355:ILE:HG13	1.93	0.50
2:D:325:LYS:HG2	2:D:326:PHE:CE2	2.48	0.48
1:C:431:GLY:C	1:C:432:VAL:HG12	2.39	0.48
1:C:427:MET:HA	1:C:427:MET:HE2	1.94	0.48
1:A:267:ILE:HD11	1:A:434:ARG:HH22	1.79	0.48
2:D:189:LYS:HD3	2:D:221:LEU:O	2.14	0.48
1:A:279[B]:PHE:CD2	1:A:414:PHE:HE2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:ARG:HD3	2:D:203:GLN:OE1	2.15	0.47
1:A:276:PRO:HB2	1:A:279[A]:PHE:HD1	1.81	0.46
2:D:249:MET:O	2:D:253:VAL:HG13	2.15	0.46
1:A:81:CYS:O	1:A:103:GLY:HA3	2.16	0.45
1:A:143:LYS:HD2	4:A:502:GOL:H31	1.98	0.45
1:C:143:LYS:HE2	4:C:503:GOL:C3	2.46	0.45
1:C:81:CYS:O	1:C:103:GLY:HA3	2.16	0.45
1:A:402[A]:MET:HG2	1:A:426:PHE:CD1	2.51	0.45
2:B:357:ASN:HB3	2:B:362:PHE:HE2	1.80	0.45
1:A:279[A]:PHE:CE2	1:A:416:GLU:HG3	2.52	0.45
1:A:276:PRO:HB2	1:A:279[A]:PHE:CD1	2.51	0.45
1:C:279:PHE:CE1	1:C:281:LYS:HE2	2.52	0.44
2:B:13:TYR:CZ	2:B:244:ILE:HD12	2.51	0.44
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.98	0.44
2:D:22:ASP:O	2:D:25:VAL:HG22	2.18	0.44
2:B:118:LYS:HA	2:B:118:LYS:HD3	1.86	0.44
1:C:435:GLN:HG3	1:C:436:ALA:H	1.79	0.44
2:D:184:LYS:HE2	2:D:313:GLU:HG2	1.99	0.44
1:C:416:GLU:HG2	8:C:812:HOH:O	2.17	0.44
1:C:51:ILE:HB	1:C:52:PRO:HD3	1.99	0.43
1:A:43:GLY:O	1:A:63:THR:HA	2.18	0.43
1:C:266:ALA:C	1:C:267:ILE:HG13	2.42	0.43
1:A:28[B]:MET:HE3	1:A:32:ARG:NH1	2.33	0.43
1:C:248:TYR:OH	1:C:252:LYS:HE3	2.18	0.43
2:D:32:VAL:HG13	2:D:51:PRO:HA	2.01	0.43
1:A:305:ILE:HD11	1:A:344[A]:LYS:CG	2.49	0.43
1:A:305:ILE:HD11	1:A:344[A]:LYS:HG3	2.00	0.43
2:D:240:GLU:OE2	2:D:242:ASP:HB3	2.19	0.42
2:D:249:MET:HG3	2:D:359:ILE:HG12	2.01	0.42
1:C:143:LYS:HE2	4:C:503:GOL:C2	2.49	0.42
2:D:164[B]:ASP:OD1	2:D:208:ARG:NH2	2.52	0.42
1:C:279:PHE:HE1	1:C:281:LYS:HE2	1.84	0.42
1:C:225:TYR:CZ	1:C:275:PRO:HG3	2.55	0.42
2:B:363:ARG:O	2:B:367:GLU:HG3	2.19	0.42
2:D:290:ARG:HG2	2:D:291:PRO:HD2	2.02	0.42
1:C:405:GLU:H	1:C:418:ARG:NH2	2.15	0.42
2:D:69:PHE:CD2	2:D:71:MET:HG2	2.55	0.42
2:D:179[B]:LEU:HD13	2:D:179[B]:LEU:HA	1.77	0.42
1:A:16:TRP:CZ3	1:A:223:THR:HG23	2.55	0.41
2:B:249:MET:O	2:B:253:VAL:HG13	2.20	0.41
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:371:GLU:O	2:D:375:GLU:HG3	2.20	0.41
2:D:250:VAL:O	2:D:253:VAL:HG22	2.20	0.41
1:A:55:LEU:HD11	1:A:178:VAL:HB	2.00	0.41
2:B:189:LYS:NZ	2:B:224:ARG:O	2.54	0.41
2:B:69:PHE:CD2	2:B:71:MET:HG2	2.55	0.41
2:B:184:LYS:NZ	2:B:313:GLU:OE1	2.53	0.41
2:B:322:LEU:HD22	2:B:353:PHE:CE1	2.56	0.41
1:C:75:ARG:HE	1:C:278:SER:HB2	1.86	0.41
2:D:10:LYS:HE3	2:D:10:LYS:HB3	1.73	0.41
2:D:13:TYR:CZ	2:D:244:ILE:HD13	2.56	0.41
1:C:373:MET:HE2	1:C:373:MET:HB3	1.90	0.40
2:D:200:LEU:HD11	2:D:242:ASP:HB2	2.03	0.40
1:A:75:ARG:NH2	1:A:279[A]:PHE:CE2	2.84	0.40
1:A:140:LYS:HE3	1:A:140:LYS:HB3	1.88	0.40
8:A:771:HOH:O	2:D:339:ARG:HD2	2.22	0.40
2:B:13:TYR:CE2	2:B:244:ILE:HD12	2.55	0.40
1:C:30:TYR:O	1:C:40:ARG:HD3	2.21	0.40
1:C:90:PHE:CD1	2:D:335:PRO:HG2	2.57	0.40
2:D:179[B]:LEU:HD12	2:D:179[B]:LEU:C	2.45	0.40
2:D:221:LEU:HD23	2:D:221:LEU:HA	1.92	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%)	434 (98%)	9 (2%)	1 (0%)	43	19
1	C	433/447 (97%)	424 (98%)	9 (2%)	0	100	100
2	B	380/379 (100%)	369 (97%)	10 (3%)	1 (0%)	36	16
2	D	380/379 (100%)	369 (97%)	8 (2%)	3 (1%)	16	3
All	All	1637/1652 (99%)	1596 (98%)	36 (2%)	5 (0%)	43	16

All (5) Ramachandran outliers are listed below:

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

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%)	368 (99%)	3 (1%)	73	48
1	C	363/371 (98%)	358 (99%)	5 (1%)	59	28
2	B	328/325 (101%)	325 (99%)	3 (1%)	70	44
2	D	328/325 (101%)	327 (100%)	1 (0%)	86	72
All	All	1390/1392 (100%)	1378 (99%)	12 (1%)	78	44

All (12) 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	314	TRP
2	B	323[A]	GLN
2	B	323[B]	GLN
2	B	359	ILE
1	C	12[A]	GLN
1	C	12[B]	GLN
1	C	12[C]	GLN
1	C	228	TYR
1	C	432	VAL
2	D	376	GLU

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	390	ASN
2	B	8	GLN
2	B	98	GLN
2	B	172	ASN
2	B	324	GLN
1	C	6	ASN
1	C	435	GLN
2	D	98	GLN
2	D	150	GLN
2	D	172	ASN
2	D	324	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	BJ8	B	401	2	6,26,26	2.19	3 (50%)	-		
7	TRS	C	502[B]	-	7,7,7	0.50	0	9,9,9	0.55	0
5	SF4	A	503	1,8	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BYC	A	501	-	57,59,59	1.75	9 (15%)	81,87,87	2.53	30 (37%)
5	SF4	C	505	1,8	0,12,12	-	-	-	-	-
4	GOL	C	504[A]	-	5,5,5	1.20	0	5,5,5	0.94	0
6	BJ8	D	401	2	6,26,26	1.65	2 (33%)	-	-	-
4	GOL	A	502	-	5,5,5	1.13	0	5,5,5	0.92	0
7	TRS	B	402[A]	-	7,7,7	0.56	0	9,9,9	0.53	0
4	GOL	C	503	-	5,5,5	1.45	1 (20%)	5,5,5	0.84	0
7	TRS	C	502[A]	-	7,7,7	0.53	0	9,9,9	0.42	0
4	GOL	C	504[B]	-	5,5,5	1.20	0	5,5,5	0.95	0
3	BYC	C	501	-	57,59,59	1.79	9 (15%)	81,87,87	2.61	27 (33%)
7	TRS	B	402[B]	-	7,7,7	0.50	0	9,9,9	0.64	0

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	BJ8	B	401	2	-	-	0/12/10/10
7	TRS	C	502[B]	-	-	2/9/9/9	-
5	SF4	A	503	1,8	-	-	0/6/5/5
3	BYC	A	501	-	-	3/55/71/71	0/4/4/4
5	SF4	C	505	1,8	-	-	0/6/5/5
4	GOL	C	504[A]	-	-	4/4/4/4	-
7	TRS	C	502[A]	-	-	4/9/9/9	-
4	GOL	A	502	-	-	0/4/4/4	-
7	TRS	B	402[A]	-	-	3/9/9/9	-
4	GOL	C	503	-	-	4/4/4/4	-
6	BJ8	D	401	2	-	-	0/12/10/10
4	GOL	C	504[B]	-	-	2/4/4/4	-
3	BYC	C	501	-	-	6/55/71/71	0/4/4/4
7	TRS	B	402[B]	-	-	2/9/9/9	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	BYC	C9P-N8P	6.22	1.48	1.33
3	A	501	BYC	C9P-N8P	6.18	1.48	1.33
3	C	501	BYC	C5P-N4P	5.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	BYC	C5P-N4P	5.01	1.45	1.33
3	C	501	BYC	C6A-N6A	4.56	1.45	1.34
3	C	501	BYC	O4D-C1D	4.35	1.52	1.42
3	A	501	BYC	C6A-N6A	4.34	1.45	1.34
3	A	501	BYC	O4D-C1D	3.99	1.51	1.42
6	B	401	BJ8	S5-FE8	3.53	2.33	2.28
3	A	501	BYC	C2B-C1B	-3.34	1.43	1.49
3	C	501	BYC	C2B-C1B	-2.97	1.43	1.49
3	A	501	BYC	C2D-C3D	-2.83	1.46	1.53
3	A	501	BYC	O4D-C4D	2.82	1.51	1.45
3	C	501	BYC	C2D-C3D	-2.72	1.47	1.53
3	C	501	BYC	O4D-C4D	2.68	1.50	1.45
3	C	501	BYC	C5M-C4A	2.64	1.43	1.39
3	A	501	BYC	C5M-C4A	2.56	1.43	1.39
6	B	401	BJ8	S6-FE8	2.53	2.32	2.28
6	D	401	BJ8	S3-FE1	2.52	2.32	2.28
3	A	501	BYC	OAP-CAP	-2.52	1.37	1.42
6	B	401	BJ8	S3-FE1	2.36	2.31	2.28
6	D	401	BJ8	S5-FE8	2.27	2.31	2.28
3	C	501	BYC	OAP-CAP	-2.07	1.38	1.42
4	C	503	GOL	C1-C2	2.03	1.59	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	BYC	C4A-N9A-C8A	10.70	116.97	105.74
3	A	501	BYC	C4A-N9A-C8A	10.35	116.60	105.74
3	C	501	BYC	N9A-C8A-N7A	-7.36	103.49	113.94
3	A	501	BYC	N9A-C8A-N7A	-7.33	103.53	113.94
3	C	501	BYC	N3A-C2A-N1A	-6.95	118.06	128.58
3	C	501	BYC	N3A-C4A-N9A	6.04	137.44	127.17
3	A	501	BYC	N3A-C4A-N9A	5.82	137.07	127.17
3	A	501	BYC	N3A-C2A-N1A	-5.82	119.78	128.58
3	A	501	BYC	C5M-N7A-C8A	5.43	111.98	103.45
3	C	501	BYC	C5M-N7A-C8A	5.11	111.48	103.45
3	C	501	BYC	C2A-N1A-C6A	5.04	127.01	118.73
3	C	501	BYC	C7P-C6P-C5P	-4.34	105.16	112.39
3	A	501	BYC	C4D-O4D-C1D	-4.18	100.25	109.47
3	A	501	BYC	C5M-C4A-N3A	-4.13	121.03	126.72
3	C	501	BYC	C5M-C4A-N9A	-4.10	101.34	105.81
3	C	501	BYC	C4D-O4D-C1D	-4.01	100.61	109.47
3	C	501	BYC	C5M-C4A-N3A	-4.00	121.21	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	BYC	C2A-N1A-C6A	3.97	125.25	118.73
3	A	501	BYC	C4A-C5M-N7A	-3.97	106.04	110.58
3	A	501	BYC	C5M-C4A-N9A	-3.66	101.83	105.81
3	A	501	BYC	C7P-C6P-C5P	-3.54	106.50	112.39
3	A	501	BYC	C2P-C3P-N4P	-3.53	105.05	112.41
3	C	501	BYC	C2A-N3A-C4A	3.43	120.22	111.83
3	C	501	BYC	C4A-C5M-N7A	-3.40	106.70	110.58
3	C	501	BYC	C2P-C3P-N4P	-3.34	105.44	112.41
3	C	501	BYC	O4A-P2A-O3A	3.29	116.17	107.27
3	C	501	BYC	C2P-S1P-C1B	3.21	103.63	99.85
3	A	501	BYC	C2A-N3A-C4A	3.20	119.64	111.83
3	A	501	BYC	O2A-P1A-O3A	3.08	115.60	107.27
3	C	501	BYC	C4A-N9A-C1D	-2.90	119.85	126.63
3	A	501	BYC	C2D-C1D-N9A	2.88	120.46	113.30
3	A	501	BYC	C2P-S1P-C1B	2.79	103.13	99.85
3	A	501	BYC	C2B-C1B-S1P	2.69	119.92	114.97
3	C	501	BYC	O6A-CCP-CBP	-2.67	106.25	110.55
3	A	501	BYC	O4A-P2A-O3A	2.60	114.30	107.27
3	A	501	BYC	C6A-C5M-N7A	2.55	137.00	132.09
3	C	501	BYC	C6P-C7P-N8P	-2.51	106.66	112.00
3	A	501	BYC	C2D-C3D-C4D	2.49	107.60	103.24
3	A	501	BYC	C4A-N9A-C1D	-2.49	120.82	126.63
3	C	501	BYC	O2A-P1A-O3A	2.44	113.87	107.27
3	C	501	BYC	C2D-C3D-C4D	2.41	107.45	103.24
3	A	501	BYC	O7A-P3D-O3D	2.37	115.09	105.85
3	C	501	BYC	C2D-C1D-N9A	2.35	119.15	113.30
3	A	501	BYC	C6P-C7P-N8P	-2.34	107.03	112.00
3	C	501	BYC	C3D-C2D-C1D	2.33	105.01	99.89
3	A	501	BYC	O6A-CCP-CBP	-2.32	106.82	110.55
3	C	501	BYC	C2B-C1B-S1P	2.27	119.15	114.97
3	C	501	BYC	C6A-C5M-N7A	2.21	136.34	132.09
3	A	501	BYC	C3D-C2D-C1D	2.17	104.66	99.89
3	C	501	BYC	C3P-N4P-C5P	-2.15	118.82	122.82
3	A	501	BYC	C7P-N8P-C9P	-2.15	118.68	122.55
3	A	501	BYC	CDP-CBP-CAP	2.15	112.43	108.77
3	A	501	BYC	O3A-P2A-O5A	-2.15	104.25	110.70
3	C	501	BYC	O3D-C3D-C4D	-2.11	102.61	110.03
3	A	501	BYC	O9A-P3D-O8A	-2.06	102.81	110.83
3	A	501	BYC	C1D-N9A-C8A	-2.06	122.53	127.09
3	C	501	BYC	C7P-N8P-C9P	-2.02	118.92	122.55

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	BYC	C3P-C2P-S1P-C1B
3	C	501	BYC	C3P-C2P-S1P-C1B
4	C	503	GOL	O1-C1-C2-C3
4	C	504[A]	GOL	O1-C1-C2-C3
4	C	504[A]	GOL	C1-C2-C3-O3
7	B	402[A]	TRS	N-C-C2-O2
7	B	402[B]	TRS	N-C-C3-O3
7	C	502[A]	TRS	N-C-C3-O3
4	C	504[B]	GOL	O1-C1-C2-C3
4	C	504[A]	GOL	O1-C1-C2-O2
4	C	504[A]	GOL	O2-C2-C3-O3
7	B	402[A]	TRS	C3-C-C2-O2
4	C	503	GOL	O1-C1-C2-O2
4	C	504[B]	GOL	O1-C1-C2-O2
7	C	502[B]	TRS	N-C-C2-O2
4	C	503	GOL	C1-C2-C3-O3
3	C	501	BYC	CEP-CBP-CCP-O6A
3	C	501	BYC	CAP-CBP-CCP-O6A
3	A	501	BYC	O5P-C5P-C6P-C7P
3	A	501	BYC	N4P-C5P-C6P-C7P
7	B	402[B]	TRS	C2-C-C3-O3
7	C	502[A]	TRS	C3-C-C2-O2
7	C	502[A]	TRS	C1-C-C3-O3
4	C	503	GOL	O2-C2-C3-O3
3	C	501	BYC	N4P-C5P-C6P-C7P
3	C	501	BYC	O5P-C5P-C6P-C7P
7	B	402[A]	TRS	C1-C-C2-O2
7	C	502[B]	TRS	C1-C-C2-O2
3	C	501	BYC	CDP-CBP-CCP-O6A
7	C	502[A]	TRS	N-C-C2-O2

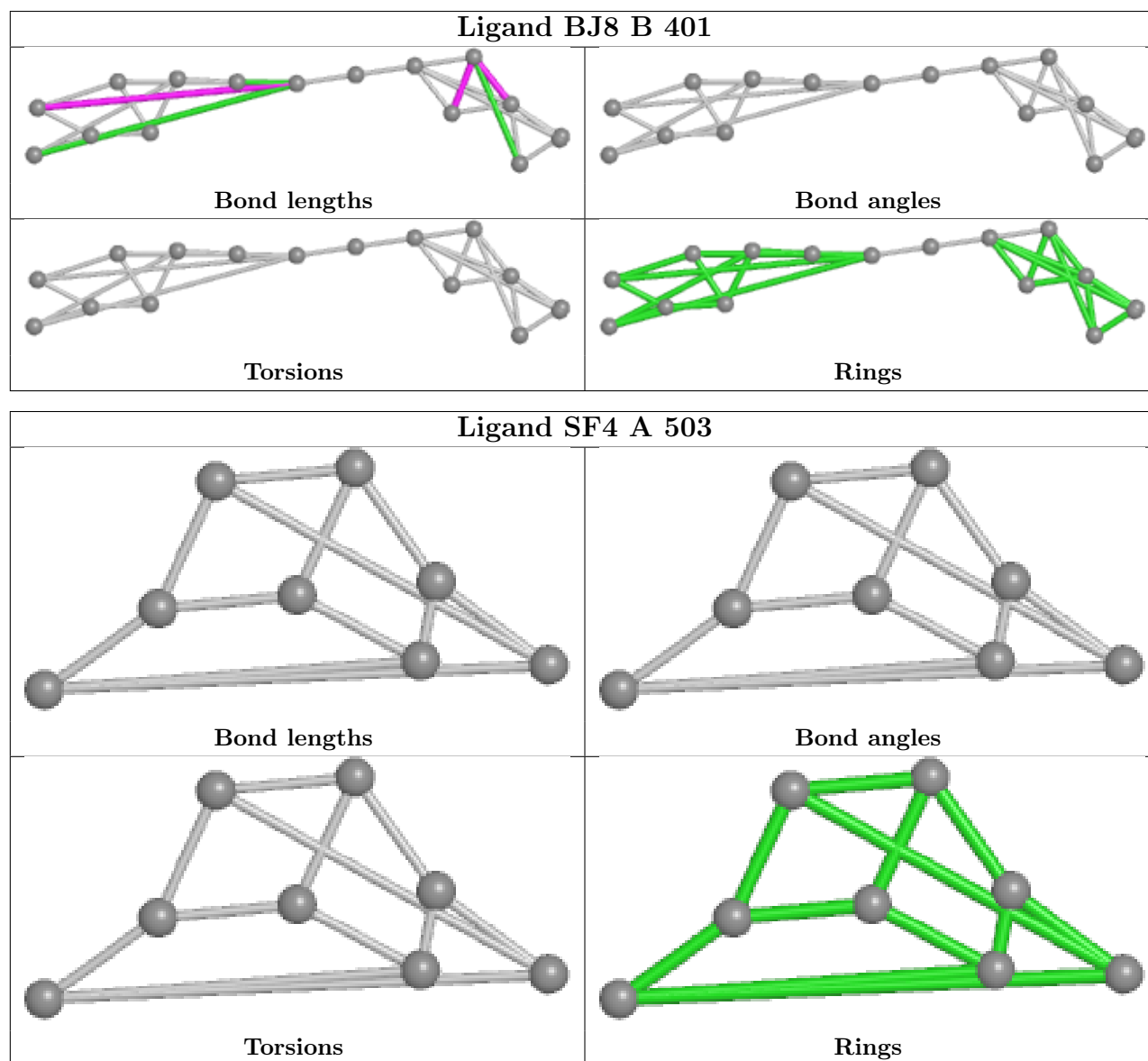
There are no ring outliers.

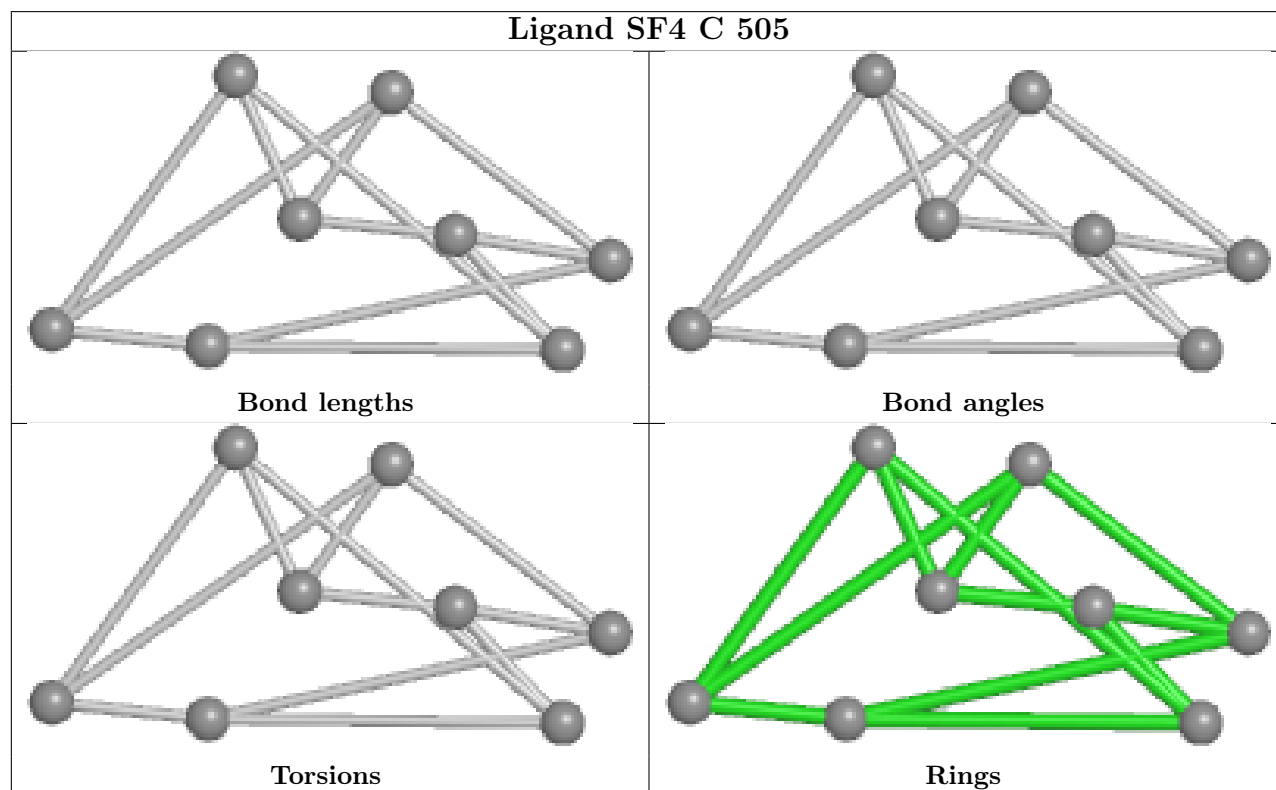
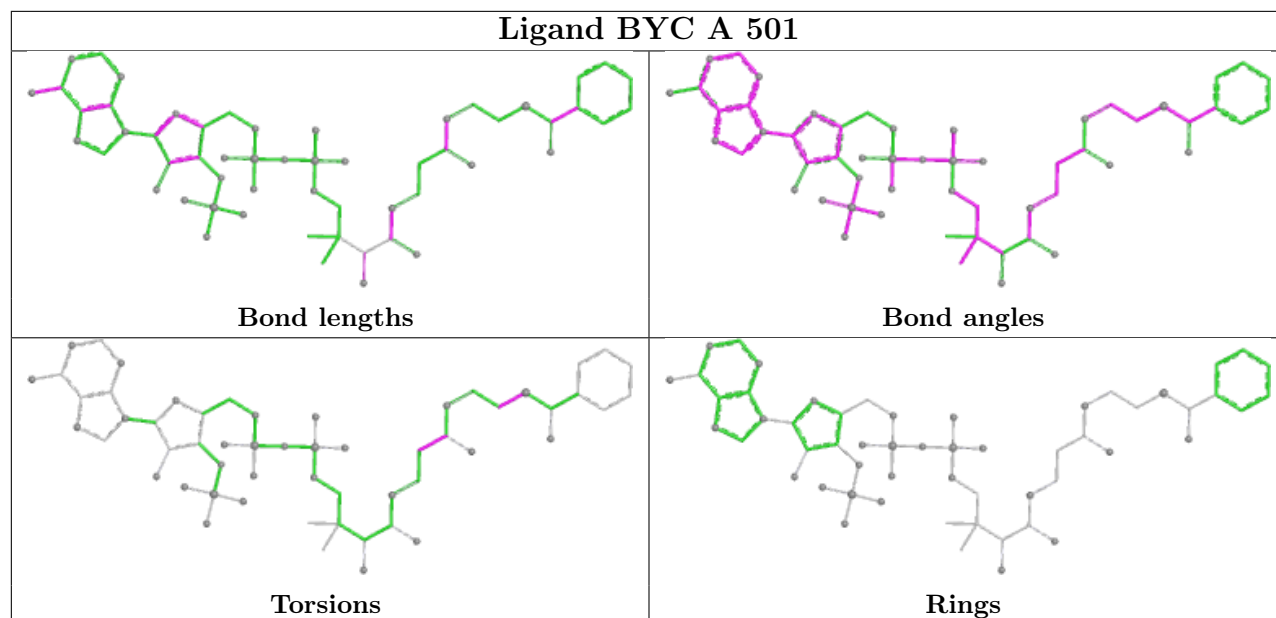
4 monomers are involved in 6 short contacts:

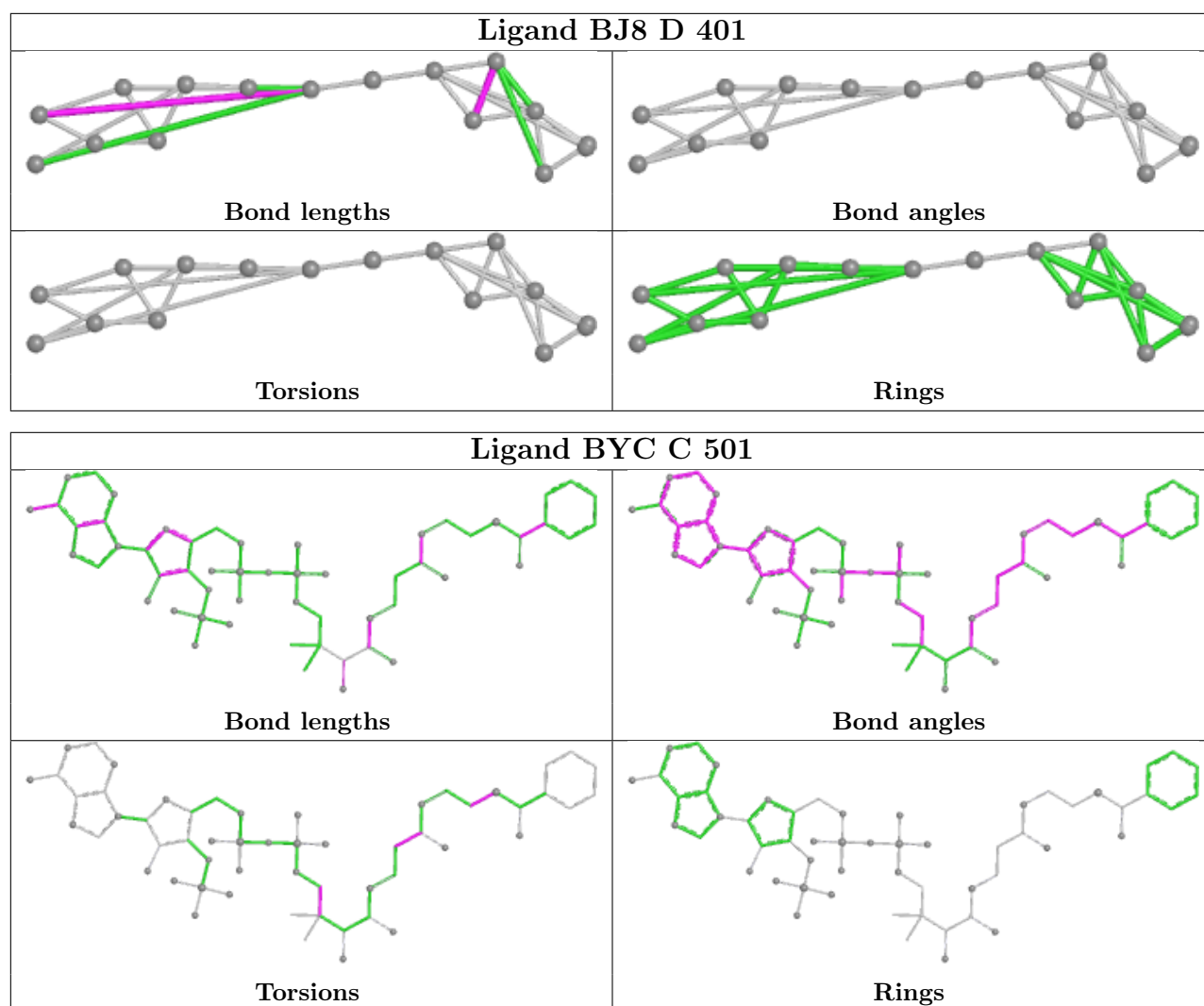
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504[A]	GOL	1	0
4	A	502	GOL	1	0
4	C	503	GOL	2	0
3	C	501	BYC	2	0

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 [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%)	0.90	50 (11%)	10 14	9, 20, 34, 65	8 (1%)
1	C	431/447 (96%)	1.03	70 (16%)	4 8	10, 22, 40, 72	3 (0%)
2	B	375/379 (98%)	1.16	68 (18%)	3 6	9, 25, 43, 64	7 (1%)
2	D	375/379 (98%)	1.33	82 (21%)	2 3	8, 25, 45, 63	7 (1%)
All	All	1619/1652 (98%)	1.09	270 (16%)	4 7	8, 22, 41, 72	25 (1%)

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279[A]	PHE	11.4
2	D	179[A]	LEU	10.1
1	A	440	TRP	10.0
1	C	436	ALA	8.2
1	A	5	ALA	7.2
2	B	244	ILE	6.5
1	C	434	ARG	5.9
1	C	277	TRP	5.9
2	D	219	ALA	5.7
1	C	8	TYR	5.7
1	A	277	TRP	5.6
2	B	2	SER	5.4
1	A	442	HIS	5.3
2	D	244	ILE	5.2
2	B	376	GLU	5.1
2	D	359	ILE	5.1
2	D	2	SER	4.8
2	B	103	TYR	4.7
1	A	282	ILE	4.7
1	A	276	PRO	4.6
2	B	218	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	372	THR	4.5
1	C	279	PHE	4.5
1	C	12[A]	GLN	4.4
1	C	16	TRP	4.4
2	D	375	GLU	4.4
2	B	179	LEU	4.4
2	D	226	VAL	4.3
1	C	432	VAL	4.3
1	C	9	PRO	4.2
1	C	433	ARG	4.2
1	A	328	ASN	4.2
1	C	417	VAL	4.1
1	C	285	TYR	4.1
2	D	218	LEU	4.1
1	A	16	TRP	4.1
2	D	5	LEU	4.0
1	A	441	SER	4.0
1	C	328	ASN	4.0
2	D	103	TYR	4.0
2	D	245	ALA	4.0
2	B	355	ILE	4.0
2	D	220	ALA	3.9
1	A	285	TYR	3.9
1	A	289	TYR	3.9
1	A	6	ASN	3.9
2	B	359	ILE	3.8
1	C	273	THR	3.8
1	C	6	ASN	3.7
1	A	288	THR	3.7
1	A	273	THR	3.7
2	D	364	ILE	3.7
1	C	431	GLY	3.6
2	D	376	GLU	3.6
2	D	246	PHE	3.6
1	C	435	GLN	3.6
2	D	3	ASP	3.6
1	A	280	LEU	3.6
1	C	267	ILE	3.6
2	D	355	ILE	3.6
1	A	327	ILE	3.5
2	D	374	SER	3.5
2	D	4	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	370	LEU	3.5
1	A	283	PHE	3.4
2	B	5	LEU	3.4
2	B	372	THR	3.4
1	C	430	LEU	3.4
1	C	289	TYR	3.4
1	C	259	ILE	3.4
2	B	358	PRO	3.4
2	B	370	LEU	3.3
1	C	288	THR	3.3
1	A	9	PRO	3.3
2	B	220	ALA	3.3
2	B	345	GLY	3.3
1	A	13	LEU	3.3
2	B	6	PHE	3.3
2	B	190	VAL	3.3
1	C	364	ILE	3.3
2	D	28	GLY	3.3
1	C	286	LEU	3.2
2	D	221	LEU	3.2
1	C	7	LYS	3.2
2	B	226	VAL	3.2
2	D	257	ILE	3.2
2	B	221	LEU	3.2
2	D	62[A]	ASN	3.1
1	C	214	VAL	3.1
2	D	253	VAL	3.1
1	C	418	ARG	3.1
2	B	208[A]	ARG	3.1
2	D	225	LYS	3.1
1	A	8	TYR	3.1
2	B	246	PHE	3.1
1	C	15	LEU	3.0
1	C	276	PRO	3.0
2	B	374	SER	3.0
2	B	234	PHE	3.0
2	D	230	THR	3.0
1	A	255	VAL	3.0
1	C	112	PHE	3.0
2	D	346	ILE	3.0
1	C	274	GLN	2.9
2	B	13	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	262	VAL	2.9
1	A	25	GLN	2.9
1	A	439	ALA	2.9
2	B	62[A]	ASN	2.9
2	D	185	ALA	2.9
2	D	25	VAL	2.9
2	D	250	VAL	2.9
2	D	6	PHE	2.8
2	B	245	ALA	2.8
2	B	253	VAL	2.8
1	C	13	LEU	2.8
1	C	280	LEU	2.8
2	B	112	LEU	2.8
2	B	353	PHE	2.8
1	A	7	LYS	2.8
1	C	10	THR	2.8
1	C	219	LEU	2.8
2	D	373	LEU	2.8
2	B	222	PRO	2.8
1	C	282	ILE	2.8
2	B	313	GLU	2.8
2	B	375	GLU	2.8
2	B	186	ALA	2.8
2	D	195	ALA	2.8
1	C	278	SER	2.7
2	B	373	LEU	2.7
2	D	55	LEU	2.7
2	D	10	LYS	2.7
2	D	259	ILE	2.7
1	A	248	TYR	2.7
2	D	182	TYR	2.7
1	C	422	ARG	2.7
1	C	17	GLY	2.7
2	D	187	ASP	2.7
2	B	217	THR	2.7
2	D	11	THR	2.7
1	A	274	GLN	2.7
1	A	286	LEU	2.7
1	C	374	LEU	2.7
1	C	421	ALA	2.6
2	D	362	PHE	2.6
2	B	223	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	17	GLY	2.6
2	D	12	TRP	2.6
2	D	227	GLU	2.6
1	C	263	PRO	2.6
2	B	225	LYS	2.6
2	D	357	ASN	2.6
2	D	356	THR	2.6
2	D	234	PHE	2.6
1	A	438	SER	2.6
2	D	222	PRO	2.6
2	D	186	ALA	2.6
1	A	275	PRO	2.6
2	D	204	PHE	2.6
2	B	154	GLY	2.5
2	B	197	TYR	2.5
2	D	231	GLY	2.5
2	D	360	GLY	2.5
2	D	168	VAL	2.5
2	B	311	ALA	2.5
1	A	434	ARG	2.5
2	D	7	ASP	2.5
1	C	414	PHE	2.5
2	D	353	PHE	2.5
2	B	21[A]	ARG	2.5
1	C	247	LEU	2.5
2	B	250	VAL	2.5
2	B	371	GLU	2.5
2	D	196	LEU	2.5
2	D	358	PRO	2.5
1	A	433	ARG	2.4
2	B	362	PHE	2.4
2	D	350	PHE	2.4
2	B	205	ILE	2.4
1	C	392	LEU	2.4
2	D	13	TYR	2.4
1	C	255	VAL	2.4
2	D	217	THR	2.4
2	B	361	PRO	2.4
1	A	217	ALA	2.4
1	A	15	LEU	2.4
2	D	112	LEU	2.4
1	C	423	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	31	VAL	2.4
2	B	168	VAL	2.4
2	D	63	VAL	2.4
2	D	111	ARG	2.4
2	B	12	TRP	2.4
2	B	3	ASP	2.4
2	D	345	GLY	2.4
2	D	269	PHE	2.4
1	A	28[A]	MET	2.3
2	B	364	ILE	2.3
2	D	27	THR	2.3
1	A	11	GLU	2.3
1	A	326	GLU	2.3
1	C	11	GLU	2.3
2	D	363	ARG	2.3
1	C	252	LYS	2.3
1	C	326	GLU	2.3
1	C	327	ILE	2.3
2	B	346	ILE	2.3
2	D	243	ASP	2.3
2	D	256	THR	2.3
1	C	319	LEU	2.3
1	C	248	TYR	2.3
2	B	360	GLY	2.3
1	C	275	PRO	2.3
1	C	57	GLU	2.3
2	B	65	GLU	2.3
2	D	36	CYS	2.3
1	A	436	ALA	2.3
2	B	23	TRP	2.3
2	D	23	TRP	2.3
1	C	25	GLN	2.3
2	B	189	LYS	2.3
1	A	192	ILE	2.3
2	B	257	ILE	2.3
1	A	324	GLY	2.3
1	A	437	ALA	2.2
2	B	323[A]	GLN	2.2
1	A	24	GLU	2.2
1	C	193	LYS	2.2
2	D	65	GLU	2.2
2	B	11	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	321	TRP	2.2
1	A	112	PHE	2.2
1	A	325	ILE	2.2
2	B	368	ALA	2.2
2	B	354	ASP	2.2
1	C	283	PHE	2.2
2	B	185	ALA	2.2
2	D	325	LYS	2.2
2	D	60	PRO	2.2
1	C	305	ILE	2.1
1	C	225	TYR	2.1
2	D	232	ALA	2.1
2	B	207	LYS	2.1
1	C	21	GLU	2.1
1	A	183	GLY	2.1
1	C	314	TRP	2.1
1	C	419	THR	2.1
2	D	223	ASN	2.1
1	C	266	ALA	2.1
2	B	283	ILE	2.1
2	D	366	ILE	2.1
2	B	193	VAL	2.1
2	D	188	PRO	2.1
2	D	229	LYS	2.1
1	C	324	GLY	2.1
2	B	175	LEU	2.1
2	D	91	ALA	2.1
1	C	387	ILE	2.1
1	C	428	GLU	2.0
1	A	33	ALA	2.0
2	B	219	ALA	2.0
2	D	255	ALA	2.0
2	B	350	PHE	2.0
1	A	12[A]	GLN	2.0
1	C	208	ILE	2.0
1	A	262	VAL	2.0
1	A	432	VAL	2.0
2	B	258	VAL	2.0
2	D	94	VAL	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](#)

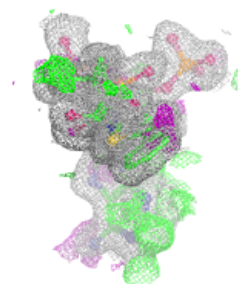
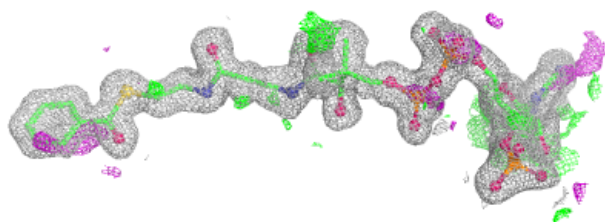
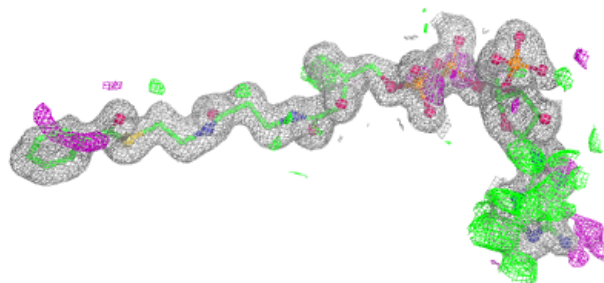
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	TRS	B	402[A]	8/8	0.70	0.16	23,27,30,31	8
7	TRS	B	402[B]	8/8	0.70	0.16	23,26,28,31	8
4	GOL	C	503	6/6	0.79	0.15	31,36,39,47	0
4	GOL	A	502	6/6	0.82	0.13	32,35,39,40	0
7	TRS	C	502[A]	8/8	0.85	0.11	22,24,26,26	8
7	TRS	C	502[B]	8/8	0.85	0.11	18,24,26,27	8
4	GOL	C	504[A]	6/6	0.87	0.13	22,25,28,32	6
4	GOL	C	504[B]	6/6	0.87	0.13	19,25,29,39	6
3	BYC	C	501	56/56	0.92	0.11	15,23,32,40	0
3	BYC	A	501	56/56	0.93	0.10	15,24,31,35	0
6	BJ8	B	401	17/17	0.99	0.03	15,16,18,19	0
6	BJ8	D	401	17/17	0.99	0.04	16,17,18,20	0
5	SF4	A	503	8/8	1.00	0.02	14,15,15,16	0
5	SF4	C	505	8/8	1.00	0.02	15,15,16,16	0

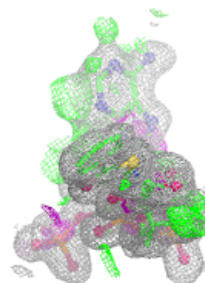
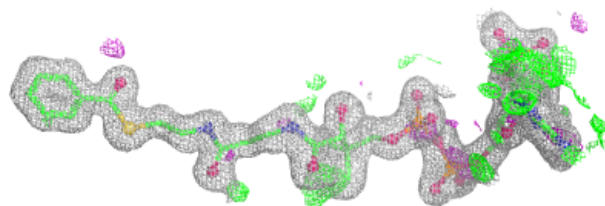
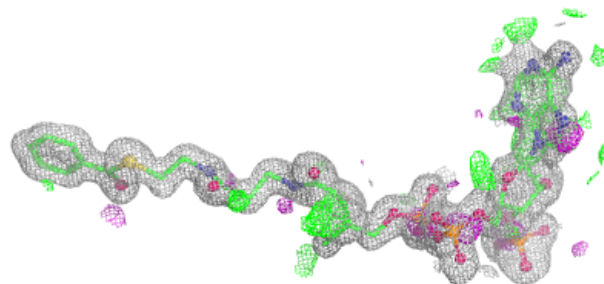
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BYC 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)

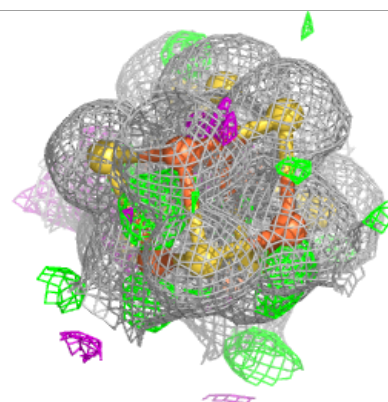
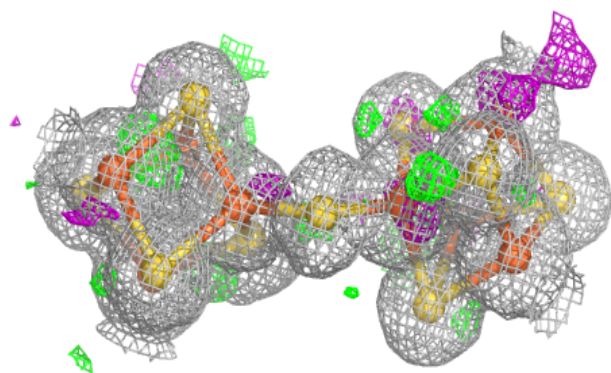
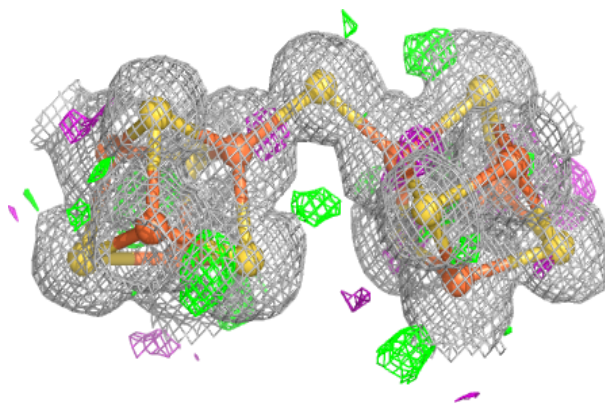
**Electron density around BYC A 501:**

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

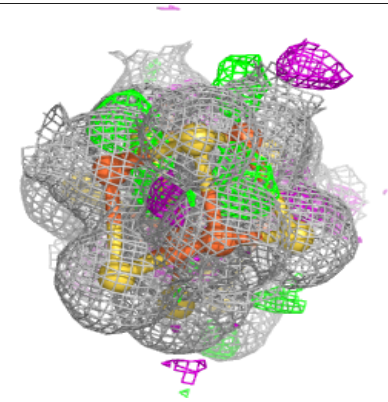
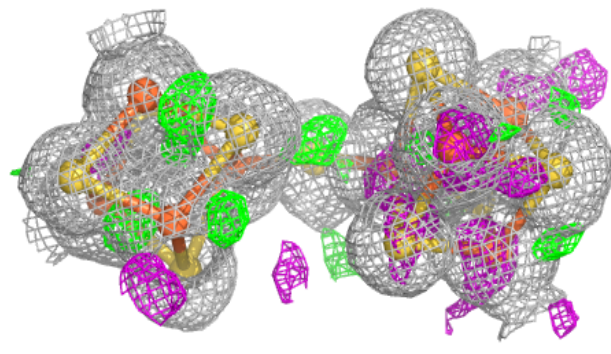
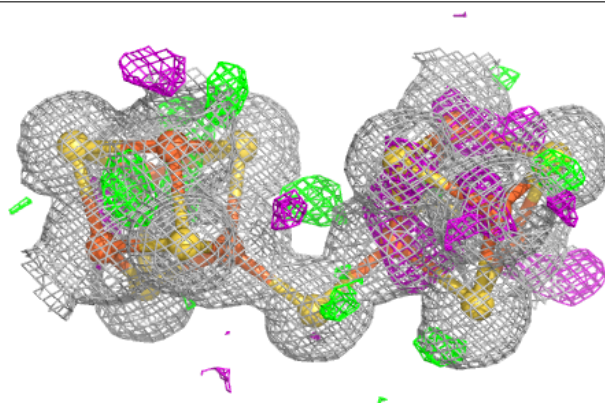


Electron density around BJ8 B 401:

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

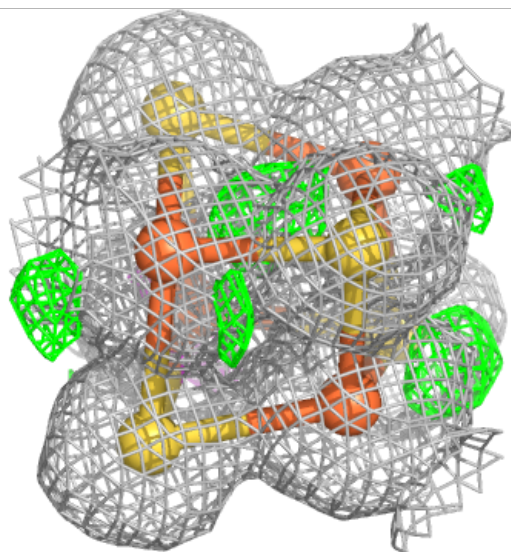
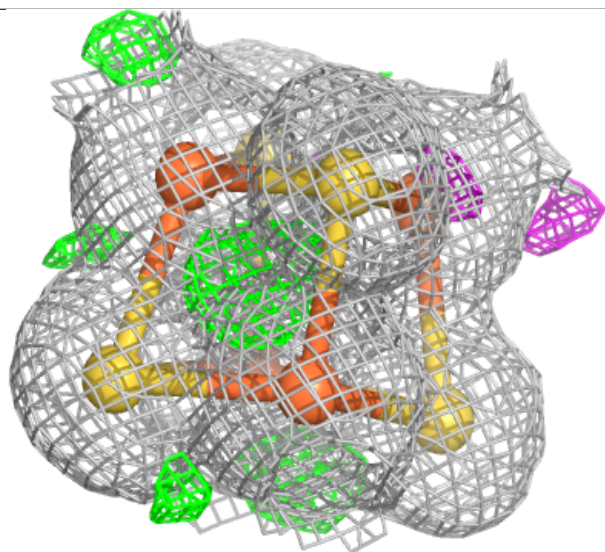
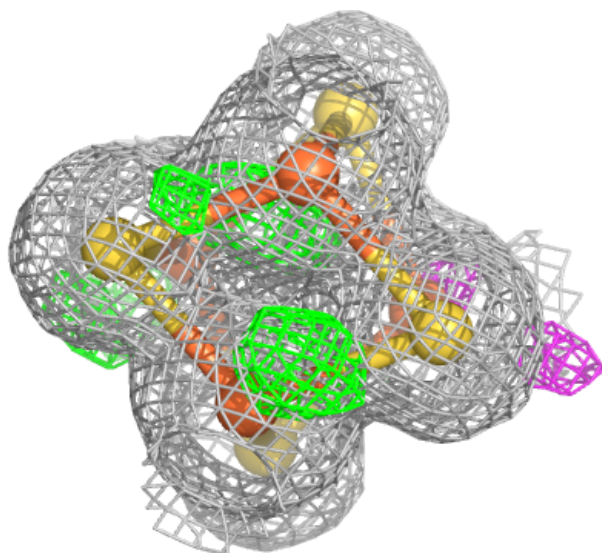
**Electron density around BJ8 D 401:**

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



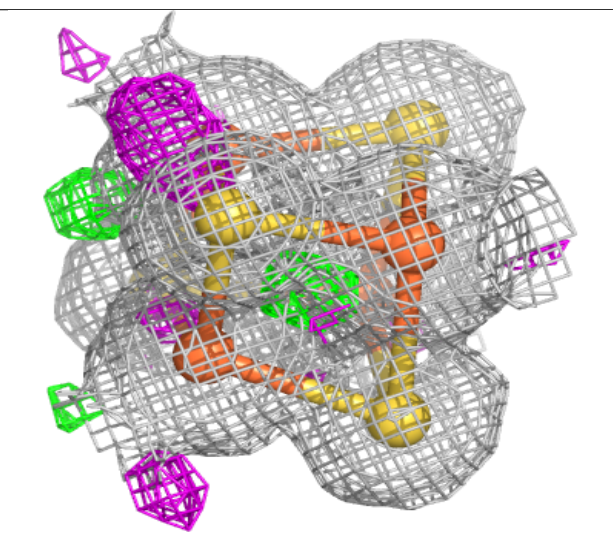
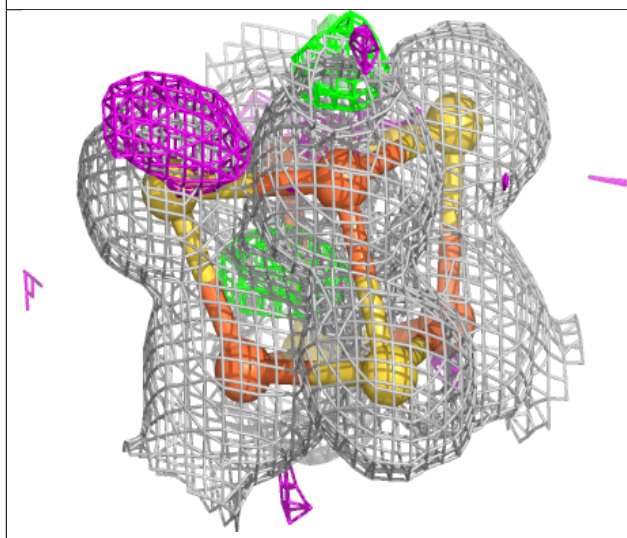
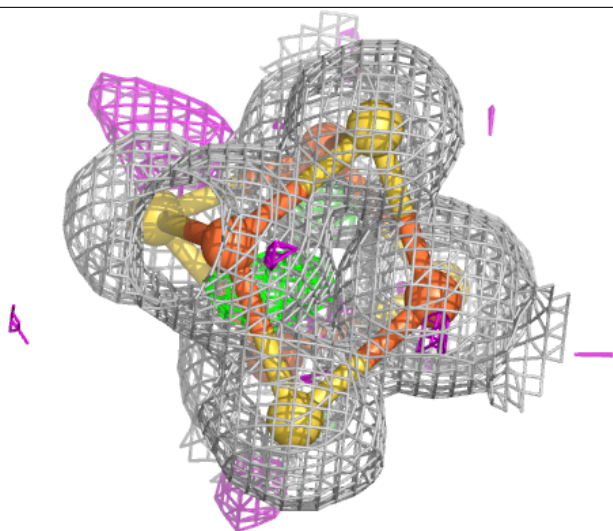
Electron density around SF4 A 503:

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



Electron density around SF4 C 505:

$2mF_o-DF_c$ (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.