



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:39 PM EDT

PDB ID : 3PM5 / pdb_00003pm5
Title : Crystal Structure of BoxB in mixed valent state with bound benzoyl-CoA
Authors : Weinert, T.; Rather, L.; Fuchs, G.; Ermler, U.
Deposited on : 2010-11-16
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

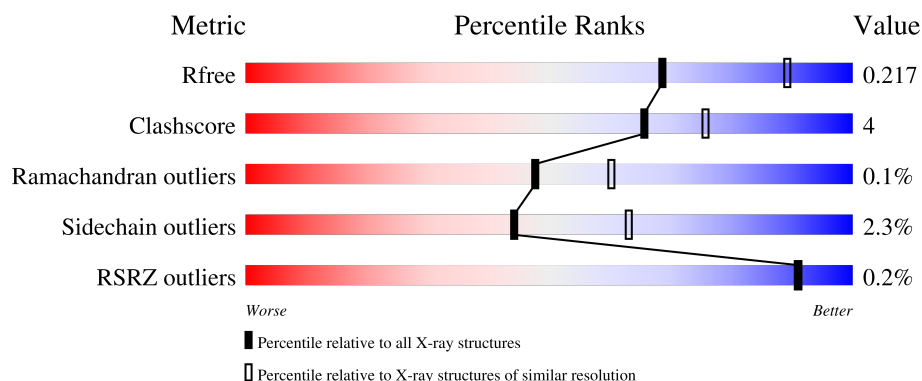
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	481	89% 9% ..
1	B	481	85% 12% ..
1	C	481	90% 8% ..
1	D	481	85% 12% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16504 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 Benzoyl-CoA oxygenase component B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	4	0
			3892	2466	690	724	12			
1	B	470	Total	C	N	O	S	0	5	0
			3887	2462	695	718	12			
1	C	475	Total	C	N	O	S	0	5	0
			3917	2484	695	725	13			
1	D	469	Total	C	N	O	S	0	5	0
			3866	2447	688	719	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	TRP	-	SEE REMARK 999	UNP Q9AIX7
A	475	SER	-	SEE REMARK 999	UNP Q9AIX7
A	476	HIS	-	SEE REMARK 999	UNP Q9AIX7
A	477	PRO	-	SEE REMARK 999	UNP Q9AIX7
A	478	GLN	-	SEE REMARK 999	UNP Q9AIX7
A	479	PHE	-	SEE REMARK 999	UNP Q9AIX7
A	480	GLU	-	SEE REMARK 999	UNP Q9AIX7
A	481	LYS	-	SEE REMARK 999	UNP Q9AIX7
B	474	TRP	-	SEE REMARK 999	UNP Q9AIX7
B	475	SER	-	SEE REMARK 999	UNP Q9AIX7
B	476	HIS	-	SEE REMARK 999	UNP Q9AIX7
B	477	PRO	-	SEE REMARK 999	UNP Q9AIX7
B	478	GLN	-	SEE REMARK 999	UNP Q9AIX7
B	479	PHE	-	SEE REMARK 999	UNP Q9AIX7
B	480	GLU	-	SEE REMARK 999	UNP Q9AIX7
B	481	LYS	-	SEE REMARK 999	UNP Q9AIX7
C	474	TRP	-	SEE REMARK 999	UNP Q9AIX7
C	475	SER	-	SEE REMARK 999	UNP Q9AIX7
C	476	HIS	-	SEE REMARK 999	UNP Q9AIX7
C	477	PRO	-	SEE REMARK 999	UNP Q9AIX7
C	478	GLN	-	SEE REMARK 999	UNP Q9AIX7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	479	PHE	-	SEE REMARK 999	UNP Q9AIX7
C	480	GLU	-	SEE REMARK 999	UNP Q9AIX7
C	481	LYS	-	SEE REMARK 999	UNP Q9AIX7
D	474	TRP	-	SEE REMARK 999	UNP Q9AIX7
D	475	SER	-	SEE REMARK 999	UNP Q9AIX7
D	476	HIS	-	SEE REMARK 999	UNP Q9AIX7
D	477	PRO	-	SEE REMARK 999	UNP Q9AIX7
D	478	GLN	-	SEE REMARK 999	UNP Q9AIX7
D	479	PHE	-	SEE REMARK 999	UNP Q9AIX7
D	480	GLU	-	SEE REMARK 999	UNP Q9AIX7
D	481	LYS	-	SEE REMARK 999	UNP Q9AIX7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

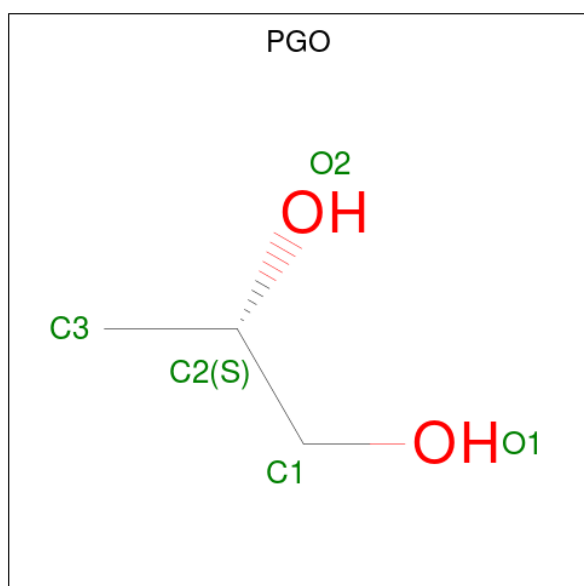
- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Fe	0	0
			2	2		
3	B	2	Total	Fe	0	0
			2	2		
3	C	2	Total	Fe	0	0
			2	2		
3	D	2	Total	Fe	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

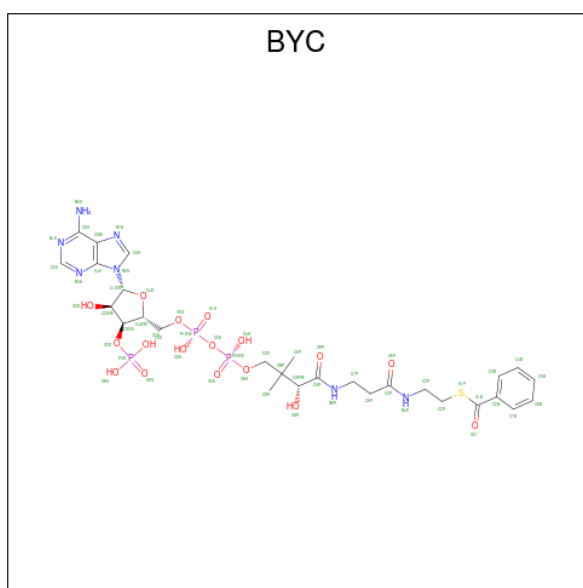
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			5	3	2		
5	B	1	Total	C	O	0	0
			5	3	2		
5	B	1	Total	C	O	0	0
			5	3	2		
5	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 6 is benzoyl coenzyme A (CCD ID: BYC) (formula: $C_{28}H_{40}N_7O_{17}P_3S$).



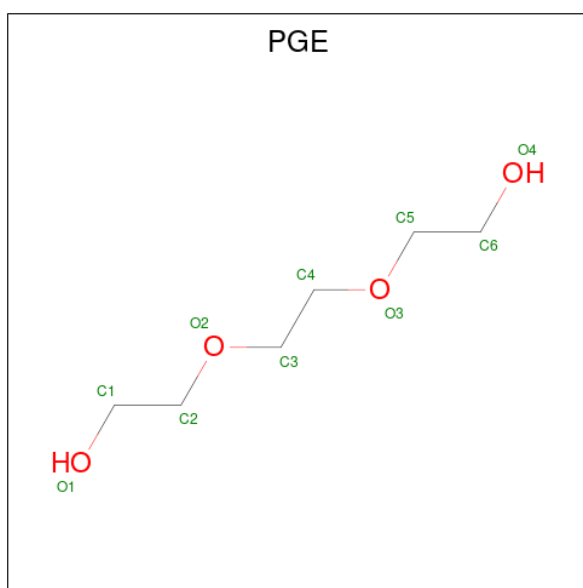
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
6	B	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
6	C	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
6	D	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			10	6	4		

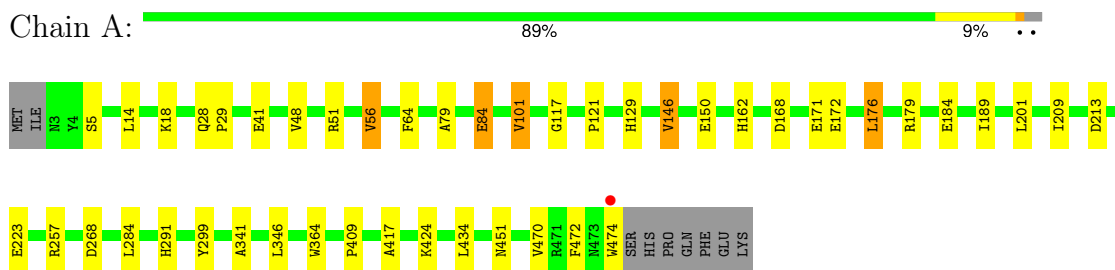
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	178	Total 178	O 178	0	0
9	B	176	Total 176	O 176	0	0
9	C	158	Total 158	O 158	0	0
9	D	117	Total 117	O 117	0	0

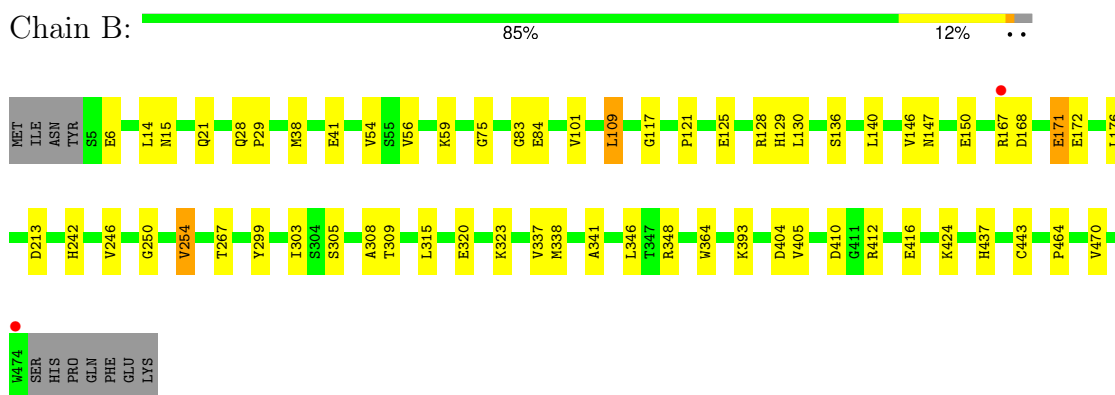
3 Residue-property plots

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

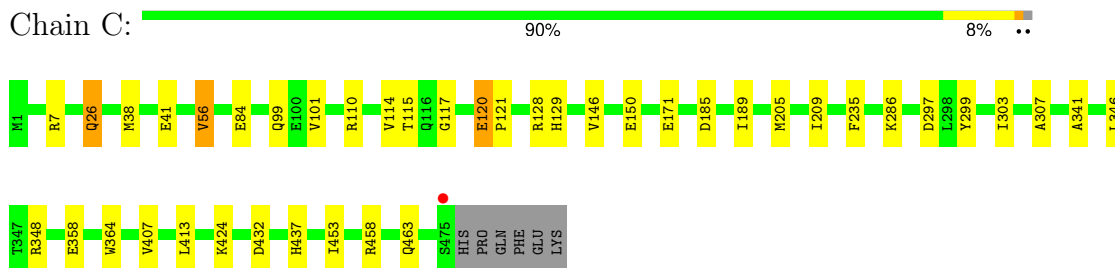
- Molecule 1: Benzoyl-CoA oxygenase component B



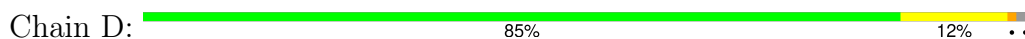
- Molecule 1: Benzoyl-CoA oxygenase component B



- Molecule 1: Benzoyl-CoA oxygenase component B



- Molecule 1: Benzoyl-CoA oxygenase component B



SER	HIS	D183	MET
PRO	ILE	L201	ILE
GLN	ASN	F208	ASN
PHE	TYR	A222	TYR
GLU	S5	A225	S5
LYS	K18	K234	K18
	R22	F235	R22
	Q26	M236	Q26
	M38	E264	M38
	S44	D268	S44
	R51	L281	R51
	V56	L284	V56
	F64	Q285	F64
	I87	K286	I87
	T88	L298	T88
	F89	Y299	F89
	H92	G314	H92
	K93	A341	K93
	V101	L346	V101
	E104	W364	E104
	Y105	A403	Y105
	R106	D404	R106
	L109	V407	L109
	T119	S408	T119
	E120	E416	E120
	P121	E430	P121
	E125	S431	E125
	L132	D432	L132
	T133	R433	T133
	A134	L434	A134
	Y138	C443	Y138
	V146	L444	V146
	E150	E445	E150
	H153	I453	H153
	E171	R458	E171
	R179	F472	R179
	R190	N473	R190
		TRP	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.18Å 76.65Å 148.20Å 90.00° 108.34° 90.00°	Depositor
Resolution (Å)	49.40 – 2.30 49.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.40-2.30) 99.2 (49.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.174 , 0.224 0.171 , 0.217	Depositor DCC
R_{free} test set	4887 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16504	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: BYC, CL, PGE, GOL, PGO, SO4, FE

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	1.16	3/3999 (0.1%)	1.04	5/5422 (0.1%)
1	B	1.17	3/3994 (0.1%)	1.06	7/5413 (0.1%)
1	C	1.18	3/4034 (0.1%)	1.04	5/5468 (0.1%)
1	D	1.15	6/3973 (0.2%)	1.05	7/5384 (0.1%)
All	All	1.16	15/16000 (0.1%)	1.05	24/21687 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	GLU	CA-C	6.80	1.61	1.52
1	C	120	GLU	N-CA	-6.50	1.42	1.46
1	D	453	ILE	CA-C	6.29	1.60	1.52
1	D	408	SER	CA-C	-6.25	1.44	1.52
1	A	189	ILE	CA-CB	6.18	1.61	1.54
1	D	134	ALA	CA-C	5.84	1.59	1.53
1	C	453	ILE	C-O	-5.55	1.18	1.23
1	D	403	ALA	CA-C	-5.47	1.45	1.52
1	B	464	PRO	CA-C	5.36	1.59	1.52
1	B	308	ALA	CA-CB	5.18	1.61	1.53
1	A	184	GLU	CA-C	5.18	1.59	1.52
1	D	281	LEU	CA-C	5.08	1.59	1.52
1	C	297	ASP	C-O	-5.07	1.17	1.24
1	D	298	LEU	C-O	-5.04	1.17	1.24
1	A	146	VAL	CA-CB	5.01	1.60	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	ILE	CB-CA-C	-7.32	104.27	111.30
1	B	267	THR	N-CA-C	6.77	119.37	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	GLU	N-CA-C	6.66	124.98	110.80
1	B	15	ASN	N-CA-C	6.40	118.79	111.11
1	A	146	VAL	N-CA-C	-6.34	104.57	110.53
1	D	445	GLU	CA-C-N	6.28	127.69	119.84
1	D	445	GLU	C-N-CA	6.28	127.69	119.84
1	D	138	TYR	N-CA-C	-6.20	104.60	111.36
1	B	254	VAL	N-CA-C	-5.96	104.70	110.72
1	B	75	GLY	N-CA-C	5.81	119.58	111.10
1	C	115	THR	N-CA-C	-5.46	105.24	111.14
1	D	208	PHE	N-CA-C	5.44	117.29	111.36
1	B	130	LEU	N-CA-C	5.34	117.98	111.78
1	C	463	GLN	CA-C-N	-5.32	114.22	119.92
1	C	463	GLN	C-N-CA	-5.32	114.22	119.92
1	D	408	SER	CA-C-N	5.21	125.52	119.47
1	D	408	SER	C-N-CA	5.21	125.52	119.47
1	A	18	LYS	N-CA-C	5.21	116.96	111.28
1	D	453	ILE	N-CA-C	5.18	115.58	108.12
1	C	205	MET	CG-SD-CE	-5.17	89.52	100.90
1	A	268	ASP	N-CA-C	-5.12	108.05	114.56
1	A	101	VAL	N-CA-C	5.11	113.03	108.63
1	B	83	GLY	N-CA-C	-5.10	105.56	112.14
1	A	209	ILE	CB-CA-C	-5.09	105.79	111.80

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	3892	0	3705	25	0
1	B	3887	0	3711	35	0
1	C	3917	0	3747	24	0
1	D	3866	0	3693	36	0
2	A	15	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	8	0	0
5	B	10	0	16	4	0
5	D	5	0	8	0	0
6	A	56	0	36	2	0
6	B	56	0	36	1	0
6	C	56	0	36	2	0
6	D	56	0	36	2	0
7	C	6	0	8	0	0
7	D	6	0	8	0	0
8	D	10	0	14	0	0
9	A	178	0	0	3	0
9	B	176	0	0	3	0
9	C	158	0	0	3	0
9	D	117	0	0	3	0
All	All	16504	0	15062	118	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 (118) 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:299:TYR:HH	1:A:364:TRP:CG	1.95	0.85
1:B:41:GLU:OE1	1:B:129[A]:HIS:ND1	2.10	0.84
1:D:444:LEU:HD13	1:D:472:PHE:CZ	2.14	0.82
1:C:299:TYR:HH	1:C:364:TRP:CG	2.00	0.78
1:D:341:ALA:CB	1:D:346:LEU:HD12	2.13	0.78
1:D:299:TYR:HH	1:D:364:TRP:CG	2.08	0.72
1:A:299:TYR:HH	1:A:364:TRP:CD1	2.07	0.70
1:A:341:ALA:CB	1:A:346:LEU:HD12	2.25	0.67
1:A:48:VAL:HG13	1:A:470:VAL:HG22	1.75	0.67
1:A:56:VAL:CG1	1:A:56:VAL:O	2.43	0.66
1:C:299:TYR:HH	1:C:364:TRP:CD1	2.14	0.65
1:D:341:ALA:HB2	1:D:346:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG13	9:D:564:HOH:O	1.99	0.63
1:D:201:LEU:HD21	1:D:284:LEU:HD23	1.81	0.63
1:A:56:VAL:O	1:A:56:VAL:HG12	2.01	0.61
1:C:101:VAL:HG12	9:C:490:HOH:O	1.99	0.61
1:B:299:TYR:HH	1:B:364:TRP:CD1	2.20	0.59
1:B:299:TYR:HH	1:B:364:TRP:CG	2.19	0.59
1:D:286:LYS:NZ	1:D:432:ASP:OD2	2.30	0.57
6:C:1003:BYC:C2A	1:D:404[B]:ASP:OD2	2.54	0.56
1:B:168:ASP:O	1:B:172:GLU:HG2	2.05	0.56
1:A:176:LEU:HD13	1:A:179:ARG:NH2	2.21	0.56
1:A:201:LEU:HD11	1:A:284:LEU:CD2	2.36	0.56
1:A:84:GLU:O	1:A:84:GLU:HG2	2.06	0.55
1:B:416:GLU:OE2	9:B:582:HOH:O	2.18	0.55
1:C:56:VAL:HG22	1:C:235:PHE:CD1	2.41	0.55
1:B:437:HIS:HE1	5:B:482:PGO:H33	1.71	0.54
1:B:437:HIS:CE1	5:B:482:PGO:H33	2.43	0.54
1:A:41:GLU:OE1	1:A:129:HIS:HD2	1.91	0.54
1:C:146:VAL:O	1:C:150[B]:GLU:HG2	2.08	0.53
1:D:119:THR:HG21	6:D:1003:BYC:H3P	1.90	0.53
1:B:140:LEU:HD23	1:B:470:VAL:HG21	1.90	0.53
1:C:41:GLU:OE1	1:C:129[A]:HIS:HD2	1.91	0.52
1:A:146:VAL:O	1:A:150[B]:GLU:HG2	2.11	0.51
1:C:120:GLU:HB2	1:C:121:PRO:CD	2.39	0.51
1:C:358:GLU:HA	1:C:358:GLU:OE1	2.10	0.51
1:B:109:LEU:CD2	1:B:315:LEU:HD22	2.40	0.51
1:A:201:LEU:HD11	1:A:284:LEU:HD21	1.92	0.51
1:C:38:MET:HE1	1:C:128[A]:ARG:CZ	2.41	0.50
1:B:117:GLY:O	1:B:121:PRO:HD2	2.11	0.50
1:D:431:SER:O	1:D:432:ASP:C	2.53	0.50
1:B:341:ALA:CB	1:B:346:LEU:HD12	2.42	0.50
5:B:483:PGO:H2	1:C:437:HIS:CE1	2.47	0.50
1:A:51:ARG:HB3	1:A:64:PHE:CE2	2.47	0.49
1:D:299:TYR:HH	1:D:364:TRP:CD1	2.29	0.49
1:B:14:LEU:HD22	1:B:21:GLN:HB2	1.94	0.49
1:D:341:ALA:CB	1:D:346:LEU:CD1	2.87	0.48
1:B:176:LEU:HD22	9:B:488:HOH:O	2.12	0.48
6:C:1003:BYC:H2A	1:D:404[B]:ASP:OD2	2.13	0.48
1:C:56:VAL:O	1:C:56:VAL:CG1	2.61	0.48
1:D:341:ALA:HB3	1:D:346:LEU:HD12	1.92	0.48
1:A:117:GLY:O	1:A:121:PRO:HD2	2.14	0.48
1:C:307:ALA:HB3	9:C:586:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PHE:CE2	1:D:314:GLY:HA2	2.49	0.47
1:D:222:ALA:O	1:D:234:LYS:NZ	2.48	0.47
1:D:132:LEU:HD23	1:D:132:LEU:N	2.29	0.47
1:B:305:SER:O	1:B:309:THR:HG23	2.14	0.46
1:D:38:MET:CE	1:D:125:GLU:HG2	2.45	0.46
1:A:213:ASP:OD2	6:A:1003:BYC:H2P	2.15	0.46
1:D:341:ALA:HB3	1:D:346:LEU:CD1	2.45	0.46
1:A:168:ASP:O	1:A:172:GLU:HG2	2.16	0.46
1:D:146:VAL:O	1:D:150[B]:GLU:HG2	2.16	0.46
6:A:1003:BYC:C2A	1:B:404:ASP:OD1	2.64	0.46
1:C:41:GLU:OE1	1:C:129[A]:HIS:CD2	2.69	0.46
1:C:99:GLN:NE2	9:C:512:HOH:O	2.45	0.45
1:D:38:MET:HE2	1:D:180[B]:ARG:HD3	1.97	0.45
1:D:458:ARG:NH1	9:D:551:HOH:O	2.47	0.45
1:A:291:HIS:HD2	9:A:545:HOH:O	1.99	0.45
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.83	0.45
1:B:320:GLU:OE1	1:B:323:LYS:HE3	2.17	0.45
1:D:180[B]:ARG:HB2	1:D:183:ASP:HB2	1.99	0.45
1:B:338:MET:HE3	1:B:393:LYS:HE3	1.98	0.45
1:C:117:GLY:O	1:C:121:PRO:HD2	2.17	0.45
6:D:1003:BYC:H4D	6:D:1003:BYC:O9A	2.17	0.45
1:B:54:VAL:HG12	9:B:634:HOH:O	2.16	0.44
1:B:136:SER:HA	1:B:443:CYS:O	2.17	0.44
9:A:608:HOH:O	1:B:171:GLU:HG2	2.16	0.44
5:B:483:PGO:H2	1:C:437:HIS:HE1	1.81	0.44
1:C:303:ILE:CD1	1:C:348[A]:ARG:NH2	2.80	0.44
1:A:472:PHE:HB3	1:A:474:TRP:CD1	2.53	0.44
1:D:268:ASP:HB2	9:D:596:HOH:O	2.17	0.44
1:B:341:ALA:HB3	1:B:346:LEU:HD12	1.99	0.44
1:B:38:MET:HE1	1:B:128[A]:ARG:CZ	2.48	0.43
1:C:110:ARG:O	1:C:114:VAL:HG23	2.18	0.43
1:D:51:ARG:HB3	1:D:64:PHE:CE2	2.53	0.43
1:D:153:HIS:CG	1:D:236:MET:HE3	2.53	0.43
1:A:257:ARG:NH2	1:A:451:ASN:OD1	2.40	0.43
1:B:242:HIS:O	1:B:246:VAL:HG23	2.18	0.43
1:A:162:HIS:HD2	9:A:610:HOH:O	2.01	0.43
1:B:28:GLN:N	1:B:29:PRO:CD	2.82	0.43
1:C:189:ILE:HD11	1:D:416:GLU:HG2	2.01	0.42
1:D:120:GLU:HB2	1:D:121:PRO:CD	2.49	0.42
1:C:407:VAL:HG22	1:C:413:LEU:HD23	2.01	0.42
1:C:286:LYS:NZ	1:C:432:ASP:OD2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:MET:HE3	1:D:125:GLU:HG2	2.01	0.42
1:D:92:HIS:O	1:D:93:LYS:C	2.63	0.42
1:D:101:VAL:HG21	1:D:106:ARG:HA	2.00	0.42
1:A:28:GLN:HB3	1:A:29:PRO:HD3	2.01	0.42
1:B:146:VAL:O	1:B:150[B]:GLU:HG2	2.19	0.42
1:B:410:ASP:OD1	1:B:412:ARG:HD3	2.19	0.42
1:B:109:LEU:HD21	1:B:315:LEU:HD22	2.02	0.41
1:C:26:GLN:HE21	1:C:26:GLN:HB2	1.58	0.41
1:B:303:ILE:CD1	1:B:348:ARG:NH2	2.83	0.41
1:D:87:ILE:HG12	1:D:225:ALA:CB	2.51	0.41
1:B:172:GLU:O	1:B:176:LEU:HD23	2.20	0.41
1:B:147:ASN:HA	1:B:150[A]:GLU:OE1	2.21	0.41
1:B:213:ASP:OD2	6:B:1003:BYC:H2P	2.21	0.41
1:B:38:MET:HE2	1:B:125:GLU:HG2	2.02	0.41
1:C:185:ASP:OD2	1:D:430:GLU:HB2	2.20	0.41
1:C:341:ALA:CB	1:C:346:LEU:HD12	2.50	0.41
1:A:417:ALA:HB2	1:B:172:GLU:HA	2.02	0.41
1:D:18:LYS:O	1:D:22:ARG:HG3	2.21	0.41
1:D:179:ARG:O	1:D:180[A]:ARG:HG3	2.21	0.41
1:A:84:GLU:O	1:A:84:GLU:CG	2.69	0.40
1:B:109:LEU:HD22	1:B:315:LEU:HD22	2.02	0.40
1:A:56:VAL:HG11	1:A:79:ALA:HA	2.03	0.40
1:B:250:GLY:O	1:B:254:VAL:HG23	2.21	0.40
1:D:407:VAL:HG12	1:D:408:SER:O	2.22	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	474/481 (98%)	459 (97%)	15 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	473/481 (98%)	461 (98%)	12 (2%)	0	100	100
1	C	478/481 (99%)	468 (98%)	10 (2%)	0	100	100
1	D	472/481 (98%)	456 (97%)	15 (3%)	1 (0%)	43	55
All	All	1897/1924 (99%)	1844 (97%)	52 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	443	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	410/415 (99%)	399 (97%)	11 (3%)	39	58
1	B	409/415 (99%)	398 (97%)	11 (3%)	39	58
1	C	414/415 (100%)	407 (98%)	7 (2%)	53	72
1	D	408/415 (98%)	397 (97%)	11 (3%)	39	58
All	All	1641/1660 (99%)	1601 (98%)	40 (2%)	44	62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	14	LEU
1	A	56	VAL
1	A	84	GLU
1	A	101	VAL
1	A	171	GLU
1	A	176	LEU
1	A	223	GLU
1	A	409	PRO
1	A	424	LYS

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Mol	Chain	Res	Type
1	A	434	LEU
1	B	6	GLU
1	B	56	VAL
1	B	59	LYS
1	B	101	VAL
1	B	109	LEU
1	B	167[A]	ARG
1	B	167[B]	ARG
1	B	171	GLU
1	B	337	VAL
1	B	405	VAL
1	B	424	LYS
1	C	7	ARG
1	C	26	GLN
1	C	56	VAL
1	C	84	GLU
1	C	171	GLU
1	C	424	LYS
1	C	458	ARG
1	D	26[A]	GLN
1	D	26[B]	GLN
1	D	44	SER
1	D	56	VAL
1	D	101	VAL
1	D	104	GLU
1	D	109	LEU
1	D	132	LEU
1	D	171	GLU
1	D	264	GLU
1	D	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	15	ASN
1	A	21	GLN
1	A	26	GLN
1	A	28	GLN
1	A	33	ASN
1	A	129	HIS
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	291	HIS
1	A	425	ASN
1	B	21	GLN
1	B	33	ASN
1	B	99	GLN
1	B	127	GLN
1	B	147	ASN
1	B	437	HIS
1	C	15	ASN
1	C	26	GLN
1	C	33	ASN
1	C	99	GLN
1	C	127	GLN
1	C	147	ASN
1	C	162	HIS
1	C	242	HIS
1	C	396	HIS
1	C	422	GLN
1	C	437	HIS
1	C	461	ASN
1	D	21	GLN
1	D	28	GLN
1	D	33	ASN
1	D	127	GLN
1	D	147	ASN
1	D	349	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SO4	A	482	-	4,4,4	0.30	0	6,6,6	0.67	0
5	PGO	B	483	-	4,4,4	0.95	0	4,4,4	1.21	0
6	BYC	C	1003	-	57,59,59	2.64	18 (31%)	81,87,87	1.90	15 (18%)
2	SO4	C	483	-	4,4,4	0.27	0	6,6,6	0.20	0
2	SO4	C	482	-	4,4,4	0.53	0	6,6,6	0.59	0
5	PGO	B	482	-	4,4,4	0.89	0	4,4,4	0.90	0
6	BYC	D	1003	-	57,59,59	2.51	20 (35%)	81,87,87	1.90	20 (24%)
2	SO4	D	482	-	4,4,4	0.24	0	6,6,6	0.25	0
7	GOL	C	486	-	5,5,5	0.51	0	5,5,5	0.92	0
5	PGO	D	484	-	4,4,4	0.66	0	4,4,4	1.29	1 (25%)
5	PGO	A	487	-	4,4,4	0.83	0	4,4,4	0.52	0
6	BYC	A	1003	-	57,59,59	2.60	19 (33%)	81,87,87	2.05	20 (24%)
6	BYC	B	1003	-	57,59,59	2.77	23 (40%)	81,87,87	2.03	22 (27%)
2	SO4	C	484	-	4,4,4	0.28	0	6,6,6	0.11	0
7	GOL	D	485	-	5,5,5	0.39	0	5,5,5	0.65	0
8	PGE	D	486	-	9,9,9	0.97	0	8,8,8	0.93	0
2	SO4	A	483	-	4,4,4	0.40	0	6,6,6	0.44	0
2	SO4	A	484	-	4,4,4	0.22	0	6,6,6	0.11	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
5	PGO	B	483	-	-	1/2/2/2	-
6	BYC	C	1003	-	-	7/55/71/71	0/4/4/4
5	PGO	B	482	-	-	2/2/2/2	-
6	BYC	D	1003	-	-	12/55/71/71	0/4/4/4
7	GOL	C	486	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGO	D	484	-	-	2/2/2/2	-
5	PGO	A	487	-	-	0/2/2/2	-
6	BYC	A	1003	-	-	7/55/71/71	0/4/4/4
7	GOL	D	485	-	-	2/4/4/4	-
8	PGE	D	486	-	-	4/7/7/7	-
6	BYC	B	1003	-	-	17/55/71/71	0/4/4/4

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1003	BYC	C2A-N3A	7.02	1.46	1.33
6	D	1003	BYC	C4A-N3A	6.70	1.46	1.34
6	C	1003	BYC	C4A-N3A	6.48	1.46	1.34
6	A	1003	BYC	C4A-N3A	6.41	1.46	1.34
6	D	1003	BYC	C2A-N3A	6.33	1.45	1.33
6	B	1003	BYC	C4A-N3A	6.33	1.46	1.34
6	A	1003	BYC	C2A-N3A	6.29	1.45	1.33
6	B	1003	BYC	C2A-N3A	6.25	1.45	1.33
6	B	1003	BYC	C4B-C3B	5.94	1.49	1.38
6	D	1003	BYC	C2A-N1A	5.88	1.44	1.33
6	B	1003	BYC	C7B-C2B	5.88	1.48	1.39
6	A	1003	BYC	C2A-N1A	5.85	1.44	1.33
6	C	1003	BYC	C4B-C3B	5.72	1.48	1.38
6	C	1003	BYC	C7B-C2B	5.72	1.48	1.39
6	B	1003	BYC	C3B-C2B	5.70	1.48	1.39
6	C	1003	BYC	C2A-N1A	5.68	1.44	1.33
6	D	1003	BYC	C3B-C2B	5.61	1.47	1.39
6	A	1003	BYC	C6B-C7B	5.61	1.48	1.38
6	B	1003	BYC	C2A-N1A	5.60	1.43	1.33
6	A	1003	BYC	C4B-C3B	5.56	1.48	1.38
6	B	1003	BYC	C9P-N8P	5.43	1.46	1.33
6	A	1003	BYC	C7B-C2B	5.35	1.47	1.39
6	C	1003	BYC	C3B-C2B	5.23	1.47	1.39
6	B	1003	BYC	C5B-C4B	5.21	1.49	1.38
6	B	1003	BYC	C6B-C7B	5.11	1.47	1.38
6	C	1003	BYC	C6B-C7B	4.96	1.47	1.38
6	A	1003	BYC	C5B-C4B	4.88	1.49	1.38
6	A	1003	BYC	C3B-C2B	4.87	1.46	1.39
6	C	1003	BYC	C9P-N8P	4.74	1.44	1.33
6	D	1003	BYC	C4B-C3B	4.68	1.46	1.38
6	C	1003	BYC	C5B-C4B	4.66	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1003	BYC	C6B-C5B	4.46	1.48	1.38
6	D	1003	BYC	C7B-C2B	4.43	1.46	1.39
6	A	1003	BYC	C9P-N8P	4.36	1.43	1.33
6	D	1003	BYC	C5B-C4B	4.28	1.47	1.38
6	D	1003	BYC	C9P-N8P	4.25	1.43	1.33
6	D	1003	BYC	C6B-C7B	4.21	1.46	1.38
6	A	1003	BYC	C6B-C5B	4.01	1.47	1.38
6	D	1003	BYC	C5M-C6A	3.95	1.52	1.41
6	C	1003	BYC	C6B-C5B	3.94	1.46	1.38
6	D	1003	BYC	C6B-C5B	3.91	1.46	1.38
6	C	1003	BYC	C5M-C6A	3.61	1.51	1.41
6	B	1003	BYC	C5P-N4P	3.41	1.41	1.33
6	A	1003	BYC	CCP-CBP	3.41	1.58	1.52
6	B	1003	BYC	C2D-C3D	-3.32	1.45	1.53
6	B	1003	BYC	C5M-C6A	3.28	1.50	1.41
6	A	1003	BYC	C5M-C6A	3.27	1.50	1.41
6	B	1003	BYC	CCP-CBP	3.21	1.57	1.52
6	C	1003	BYC	CCP-CBP	3.18	1.57	1.52
6	A	1003	BYC	C5P-N4P	3.18	1.40	1.33
6	C	1003	BYC	C2D-C3D	-3.14	1.46	1.53
6	B	1003	BYC	P1A-O3A	3.10	1.62	1.59
6	C	1003	BYC	C6A-N1A	2.91	1.43	1.35
6	C	1003	BYC	C6A-N6A	2.91	1.41	1.34
6	D	1003	BYC	C6A-N1A	2.87	1.43	1.35
6	D	1003	BYC	C5P-N4P	2.83	1.40	1.33
6	B	1003	BYC	C6A-N1A	2.82	1.43	1.35
6	B	1003	BYC	C6A-N6A	2.79	1.41	1.34
6	B	1003	BYC	C8A-N7A	2.79	1.37	1.31
6	A	1003	BYC	C6A-N1A	2.78	1.43	1.35
6	A	1003	BYC	C2D-C3D	-2.75	1.47	1.53
6	B	1003	BYC	CDP-CBP	-2.73	1.48	1.53
6	C	1003	BYC	P1A-O3A	2.71	1.62	1.59
6	D	1003	BYC	C6A-N6A	2.66	1.41	1.34
6	C	1003	BYC	C8A-N7A	2.64	1.36	1.31
6	B	1003	BYC	C1B-S1P	2.60	1.82	1.76
6	A	1003	BYC	C8A-N7A	2.58	1.36	1.31
6	D	1003	BYC	C2D-C3D	-2.57	1.47	1.53
6	B	1003	BYC	OAP-CAP	-2.56	1.37	1.42
6	D	1003	BYC	C8A-N7A	2.52	1.36	1.31
6	D	1003	BYC	C6P-C5P	2.46	1.56	1.51
6	B	1003	BYC	C5M-N7A	-2.46	1.34	1.39
6	A	1003	BYC	C6A-N6A	2.42	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1003	BYC	CCP-CBP	2.38	1.56	1.52
6	A	1003	BYC	OAP-CAP	-2.29	1.38	1.42
6	C	1003	BYC	C5M-N7A	-2.24	1.35	1.39
6	D	1003	BYC	P1A-O3A	2.20	1.61	1.59
6	A	1003	BYC	C6P-C5P	2.01	1.55	1.51
6	B	1003	BYC	C6P-C5P	2.01	1.55	1.51
6	D	1003	BYC	CDP-CBP	-2.01	1.49	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1003	BYC	C2P-S1P-C1B	7.82	109.07	99.85
6	C	1003	BYC	O4D-C1D-N9A	6.44	120.46	108.09
6	C	1003	BYC	C5M-C4A-N3A	-6.30	118.04	126.72
6	B	1003	BYC	O4D-C1D-N9A	6.03	119.66	108.09
6	D	1003	BYC	N3A-C2A-N1A	-5.85	119.73	128.58
6	B	1003	BYC	N3A-C2A-N1A	-5.80	119.80	128.58
6	B	1003	BYC	C5M-C4A-N3A	-5.59	119.01	126.72
6	A	1003	BYC	N3A-C2A-N1A	-5.33	120.51	128.58
6	D	1003	BYC	C5M-C4A-N3A	-5.27	119.47	126.72
6	A	1003	BYC	C5M-C4A-N3A	-5.21	119.54	126.72
6	A	1003	BYC	O4D-C1D-N9A	5.15	117.99	108.09
6	C	1003	BYC	N3A-C2A-N1A	-5.14	120.80	128.58
6	D	1003	BYC	O4D-C1D-N9A	4.63	116.97	108.09
6	C	1003	BYC	N3A-C4A-N9A	4.52	134.85	127.17
6	B	1003	BYC	C2P-S1P-C1B	4.39	105.02	99.85
6	D	1003	BYC	N9A-C8A-N7A	-4.08	108.15	113.94
6	A	1003	BYC	N9A-C8A-N7A	-4.00	108.26	113.94
6	D	1003	BYC	C2A-N3A-C4A	3.97	121.52	111.83
6	A	1003	BYC	N3A-C4A-N9A	3.87	133.75	127.17
6	A	1003	BYC	C7P-C6P-C5P	3.87	118.84	112.39
6	B	1003	BYC	C2A-N3A-C4A	3.86	121.25	111.83
6	C	1003	BYC	C2A-N3A-C4A	3.82	121.15	111.83
6	B	1003	BYC	N3A-C4A-N9A	3.77	133.58	127.17
6	B	1003	BYC	CDP-CBP-CAP	3.73	115.12	108.77
6	C	1003	BYC	N9A-C8A-N7A	-3.72	108.66	113.94
6	A	1003	BYC	C2P-C3P-N4P	-3.70	104.69	112.41
6	D	1003	BYC	N3A-C4A-N9A	3.65	133.38	127.17
6	A	1003	BYC	C2A-N3A-C4A	3.58	120.57	111.83
6	B	1003	BYC	C7B-C2B-C3B	3.55	123.08	118.57
6	D	1003	BYC	O6A-CCP-CBP	-3.36	105.14	110.55
6	B	1003	BYC	C4B-C3B-C2B	-3.33	117.09	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1003	BYC	N9A-C8A-N7A	-3.31	109.25	113.94
6	D	1003	BYC	C5M-N7A-C8A	3.23	108.53	103.45
6	D	1003	BYC	C2P-C3P-N4P	-3.16	105.82	112.41
6	C	1003	BYC	C5M-N7A-C8A	3.16	108.41	103.45
6	C	1003	BYC	O5P-C5P-N4P	-3.13	116.89	123.03
6	D	1003	BYC	C7B-C2B-C3B	3.12	122.54	118.57
6	C	1003	BYC	C6A-C5M-C4A	3.11	121.42	117.18
6	A	1003	BYC	C5M-N7A-C8A	2.98	108.14	103.45
6	D	1003	BYC	O5P-C5P-N4P	-2.95	117.23	123.03
6	A	1003	BYC	C5D-C4D-C3D	2.92	124.11	114.38
6	A	1003	BYC	CAP-C9P-N8P	-2.85	111.08	116.48
6	D	1003	BYC	C7P-C6P-C5P	2.82	117.10	112.39
6	D	1003	BYC	C5D-C4D-C3D	2.75	123.54	114.38
6	C	1003	BYC	C7B-C2B-C3B	2.71	122.01	118.57
6	A	1003	BYC	C7B-C2B-C3B	2.66	121.96	118.57
6	B	1003	BYC	C5M-N7A-C8A	2.60	107.54	103.45
6	B	1003	BYC	O2D-C2D-C1D	2.58	118.98	110.10
6	B	1003	BYC	C5D-C4D-C3D	2.53	122.81	114.38
6	D	1003	BYC	C4B-C3B-C2B	-2.53	117.88	120.36
6	A	1003	BYC	O2D-C2D-C1D	2.49	118.68	110.10
6	B	1003	BYC	O57-C1B-C2B	-2.49	116.13	122.24
6	B	1003	BYC	C7P-C6P-C5P	2.49	116.54	112.39
6	D	1003	BYC	C2B-C1B-S1P	2.48	119.53	114.97
6	D	1003	BYC	C4A-N9A-C8A	2.46	108.32	105.74
6	D	1003	BYC	O5P-C5P-C6P	2.42	126.41	122.02
6	D	1003	BYC	O9P-C9P-N8P	-2.40	117.90	122.98
6	D	1003	BYC	C4A-C5M-N7A	-2.39	107.84	110.58
6	B	1003	BYC	C6A-C5M-C4A	2.38	120.43	117.18
6	A	1003	BYC	C4A-N9A-C8A	2.38	108.24	105.74
6	A	1003	BYC	C4B-C3B-C2B	-2.38	118.03	120.36
6	A	1003	BYC	O4D-C1D-C2D	-2.34	101.61	106.62
6	C	1003	BYC	O2D-C2D-C1D	2.28	117.97	110.10
6	B	1003	BYC	C7P-N8P-C9P	2.28	126.64	122.55
6	B	1003	BYC	O4D-C1D-C2D	-2.22	101.86	106.62
6	A	1003	BYC	O4A-P2A-O3A	2.21	113.25	107.27
6	D	1003	BYC	O2A-P1A-O1A	2.18	122.56	112.44
6	B	1003	BYC	C6P-C7P-N8P	2.17	116.62	112.00
6	B	1003	BYC	C1D-N9A-C8A	-2.16	122.30	127.09
6	C	1003	BYC	C1D-N9A-C8A	-2.15	122.32	127.09
6	C	1003	BYC	C3P-N4P-C5P	-2.14	118.84	122.82
6	B	1003	BYC	O3D-C3D-C2D	-2.11	104.12	111.68
6	A	1003	BYC	C6A-C5M-C4A	2.08	120.02	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1003	BYC	C4A-C5M-N7A	-2.07	108.22	110.58
6	A	1003	BYC	CDP-CBP-CAP	2.04	112.24	108.77
6	B	1003	BYC	O2A-P1A-O3A	-2.04	101.77	107.27
5	D	484	PGO	O2-C2-C1	-2.03	105.01	114.99
6	C	1003	BYC	OAP-CAP-CBP	2.02	114.87	110.18

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	482	PGO	O1-C1-C2-C3
5	B	482	PGO	O1-C1-C2-O2
5	D	484	PGO	O1-C1-C2-C3
5	D	484	PGO	O1-C1-C2-O2
6	A	1003	BYC	C5D-O5D-P1A-O1A
6	A	1003	BYC	C5D-O5D-P1A-O3A
6	B	1003	BYC	C5D-O5D-P1A-O1A
6	B	1003	BYC	C5D-O5D-P1A-O3A
6	B	1003	BYC	CCP-O6A-P2A-O3A
6	B	1003	BYC	CCP-O6A-P2A-O4A
6	B	1003	BYC	CCP-O6A-P2A-O5A
6	B	1003	BYC	CAP-CBP-CCP-O6A
6	B	1003	BYC	CDP-CBP-CCP-O6A
6	B	1003	BYC	CEP-CBP-CCP-O6A
6	C	1003	BYC	C5D-O5D-P1A-O1A
6	C	1003	BYC	C5D-O5D-P1A-O3A
6	D	1003	BYC	C5D-O5D-P1A-O3A
6	D	1003	BYC	C3P-C2P-S1P-C1B
6	D	1003	BYC	CCP-O6A-P2A-O5A
7	C	486	GOL	O1-C1-C2-C3
7	C	486	GOL	C1-C2-C3-O3
6	D	1003	BYC	O4D-C4D-C5D-O5D
6	D	1003	BYC	C4D-C3D-O3D-P3D
8	D	486	PGE	O3-C5-C6-O4
7	D	485	GOL	O1-C1-C2-C3
7	C	486	GOL	O1-C1-C2-O2
6	B	1003	BYC	C2D-C3D-O3D-P3D
6	D	1003	BYC	C2D-C3D-O3D-P3D
6	B	1003	BYC	O4D-C4D-C5D-O5D
6	C	1003	BYC	O4D-C4D-C5D-O5D
7	C	486	GOL	O2-C2-C3-O3
6	A	1003	BYC	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
6	D	1003	BYC	C3D-C4D-C5D-O5D
6	A	1003	BYC	S1P-C1B-C2B-C7B
6	B	1003	BYC	P1A-O3A-P2A-O5A
7	D	485	GOL	O1-C1-C2-O2
6	A	1003	BYC	S1P-C1B-C2B-C3B
6	C	1003	BYC	C3D-C4D-C5D-O5D
8	D	486	PGE	C3-C4-O3-C5
6	D	1003	BYC	C5D-O5D-P1A-O1A
6	D	1003	BYC	CCP-O6A-P2A-O3A
6	D	1003	BYC	C2D-C1D-N9A-C8A
6	D	1003	BYC	C2D-C1D-N9A-C4A
6	B	1003	BYC	C4D-C3D-O3D-P3D
6	B	1003	BYC	O57-C1B-C2B-C3B
6	C	1003	BYC	C3D-O3D-P3D-O8A
6	D	1003	BYC	C3D-O3D-P3D-O8A
6	B	1003	BYC	O4D-C1D-N9A-C8A
6	A	1003	BYC	C2D-C3D-O3D-P3D
6	B	1003	BYC	C3D-C4D-C5D-O5D
6	A	1003	BYC	O4D-C1D-N9A-C8A
6	B	1003	BYC	O57-C1B-C2B-C7B
6	B	1003	BYC	C3D-O3D-P3D-O7A
6	C	1003	BYC	S1P-C2P-C3P-N4P
8	D	486	PGE	C6-C5-O3-C4
5	B	483	PGO	O1-C1-C2-O2
6	C	1003	BYC	O4D-C1D-N9A-C8A
8	D	486	PGE	O2-C3-C4-O3

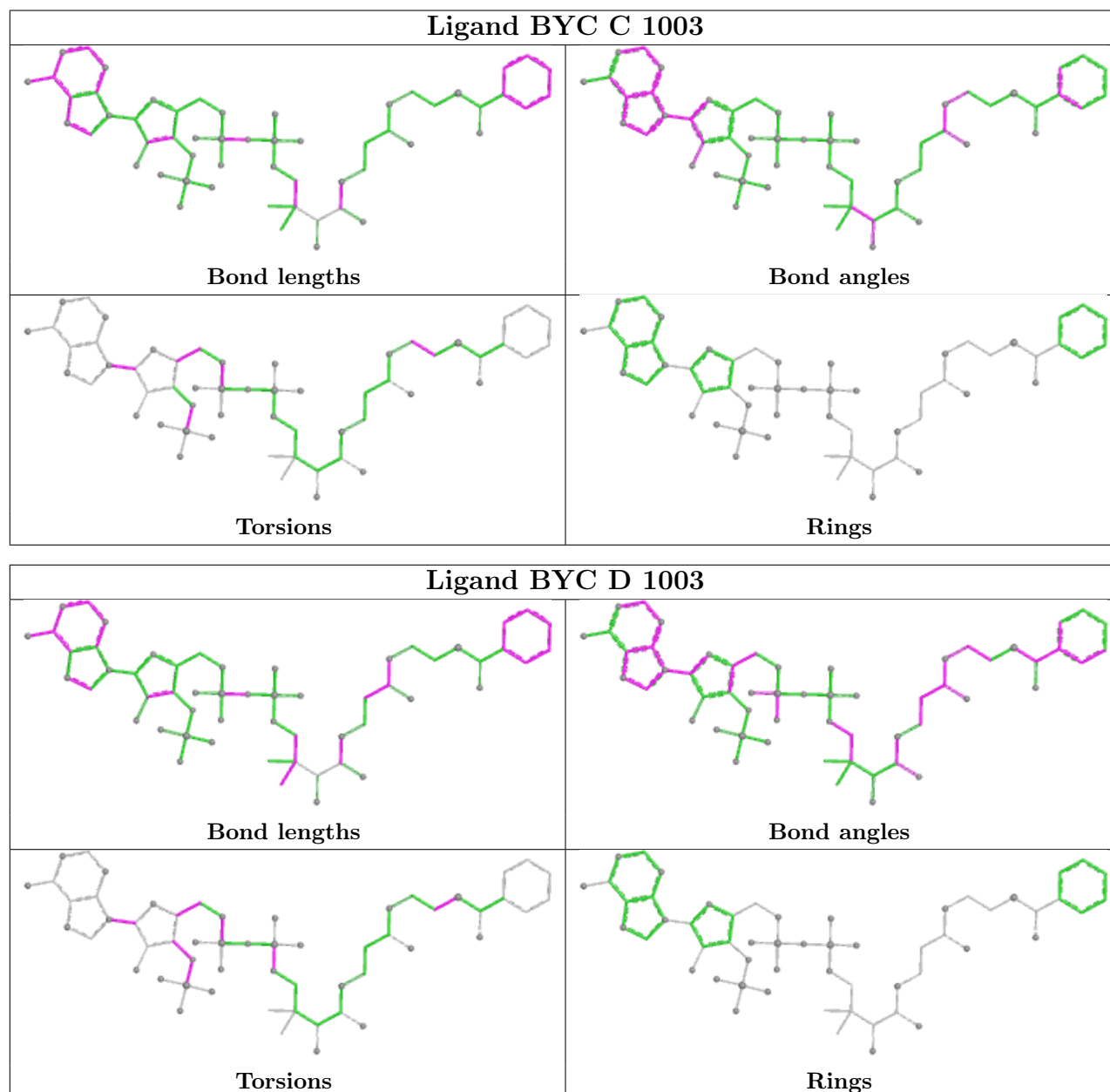
There are no ring outliers.

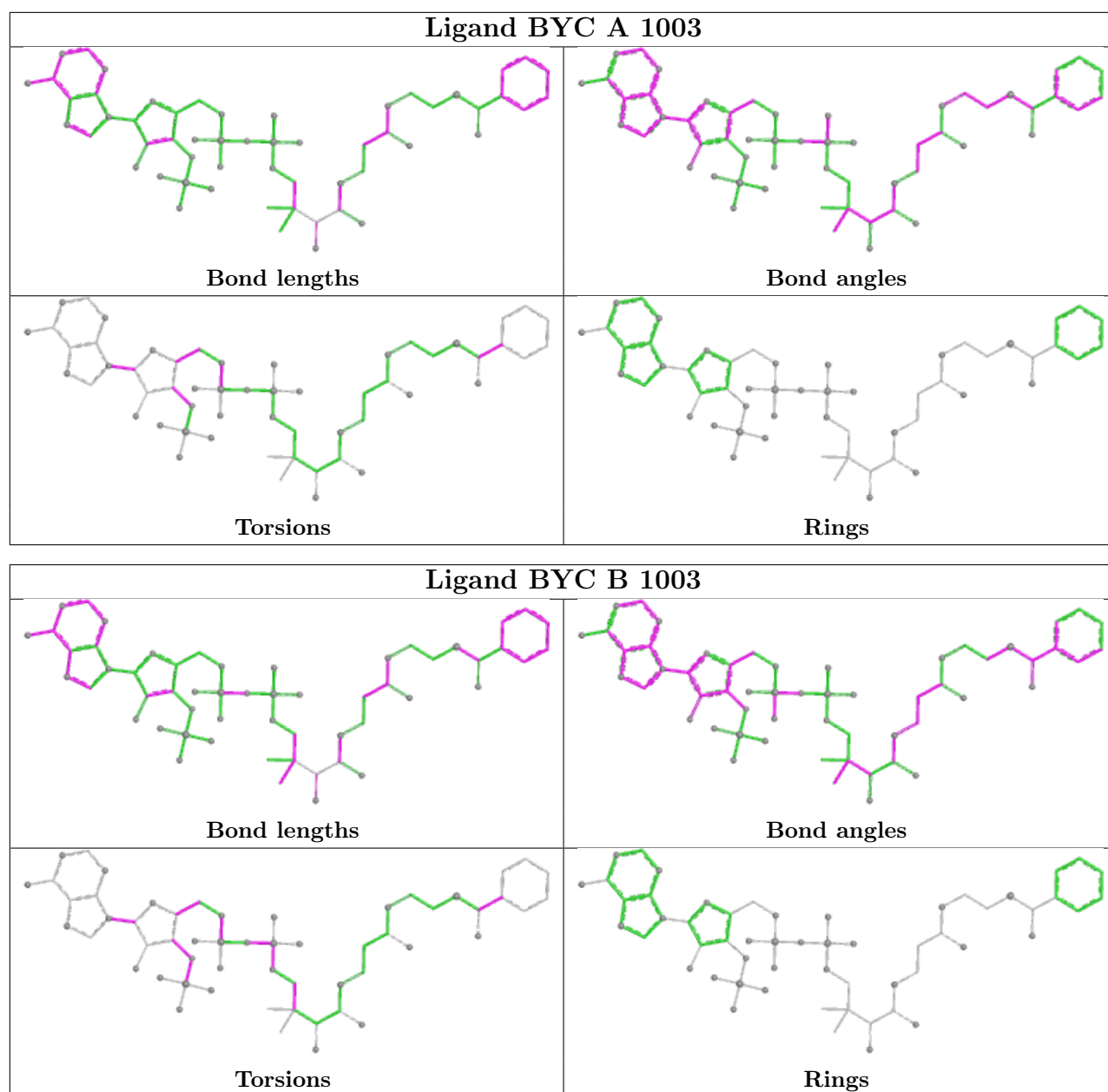
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	483	PGO	2	0
6	C	1003	BYC	2	0
5	B	482	PGO	2	0
6	D	1003	BYC	2	0
6	A	1003	BYC	2	0
6	B	1003	BYC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	472/481 (98%)	-0.43	1 (0%) 91 91	16, 42, 61, 83	4 (0%)
1	B	470/481 (97%)	-0.44	2 (0%) 88 89	17, 41, 59, 82	5 (1%)
1	C	475/481 (98%)	-0.47	1 (0%) 91 91	18, 41, 62, 79	5 (1%)
1	D	469/481 (97%)	-0.28	0 100 100	18, 47, 69, 87	5 (1%)
All	All	1886/1924 (98%)	-0.40	4 (0%) 91 91	16, 43, 63, 87	19 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	474	TRP	3.4
1	B	167[A]	ARG	2.9
1	C	475	SER	2.5
1	B	474	TRP	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](#)

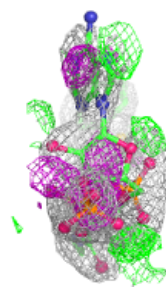
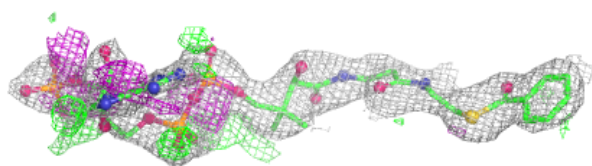
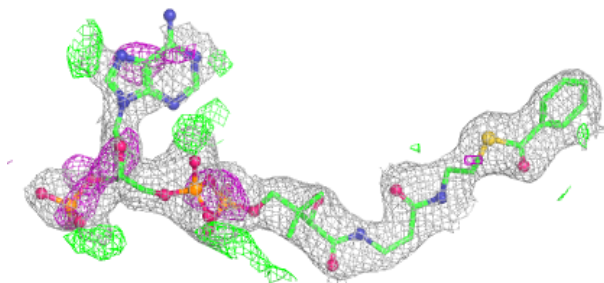
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	PGO	B	483	5/5	0.62	0.24	67,68,69,70	0
5	PGO	D	484	5/5	0.73	0.19	64,66,67,68	0
5	PGO	B	482	5/5	0.80	0.22	60,68,70,71	0
2	SO4	D	482	5/5	0.81	0.12	102,103,103,103	0
2	SO4	C	483	5/5	0.81	0.11	118,119,119,120	0
7	GOL	C	486	6/6	0.81	0.17	74,76,77,77	0
2	SO4	A	482	5/5	0.82	0.10	87,89,89,90	0
8	PGE	D	486	10/10	0.82	0.18	67,70,72,72	0
6	BYC	D	1003	56/56	0.83	0.14	49,71,103,106	0
2	SO4	A	483	5/5	0.83	0.10	96,96,96,98	0
7	GOL	D	485	6/6	0.83	0.17	86,88,89,89	0
6	BYC	A	1003	56/56	0.83	0.15	49,71,98,101	0
5	PGO	A	487	5/5	0.85	0.18	59,62,66,67	0
2	SO4	A	484	5/5	0.86	0.12	125,126,126,126	0
6	BYC	B	1003	56/56	0.87	0.14	47,69,98,99	0
6	BYC	C	1003	56/56	0.87	0.13	43,65,101,103	0
2	SO4	C	484	5/5	0.89	0.09	120,121,121,121	0
3	FE	C	1001	1/1	0.92	0.09	86,86,86,86	0
2	SO4	C	482	5/5	0.94	0.11	58,58,63,64	0
3	FE	A	1001	1/1	0.95	0.06	74,74,74,74	0
4	CL	C	485	1/1	0.97	0.06	44,44,44,44	0
3	FE	B	1001	1/1	0.97	0.05	72,72,72,72	0
3	FE	D	1001	1/1	0.97	0.04	74,74,74,74	0
4	CL	D	483	1/1	0.98	0.05	42,42,42,42	0
4	CL	A	486	1/1	0.98	0.07	39,39,39,39	0
3	FE	B	1002	1/1	0.98	0.04	63,63,63,63	0
4	CL	A	485	1/1	0.99	0.05	40,40,40,40	0
3	FE	A	1002	1/1	0.99	0.03	59,59,59,59	0
3	FE	D	1002	1/1	0.99	0.05	73,73,73,73	0
3	FE	C	1002	1/1	1.00	0.01	63,63,63,63	0

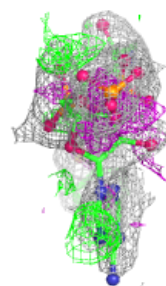
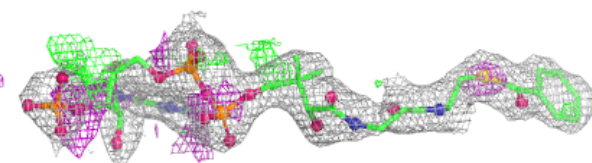
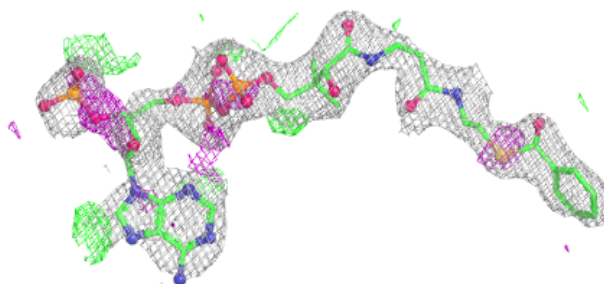
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BYC D 1003:

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

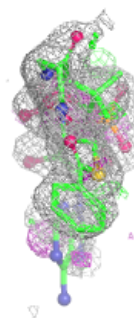
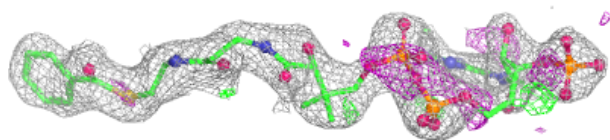
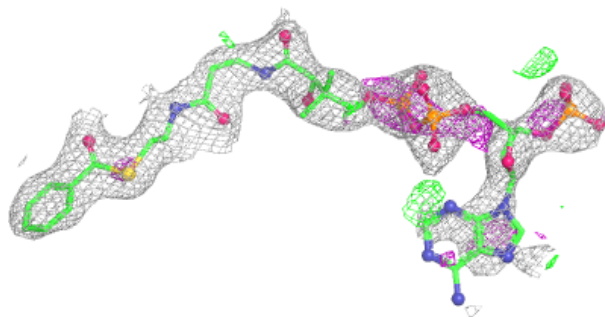
**Electron density around BYC A 1003:**

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

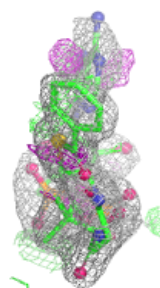
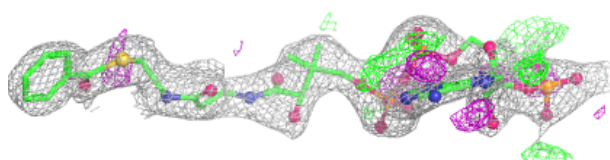
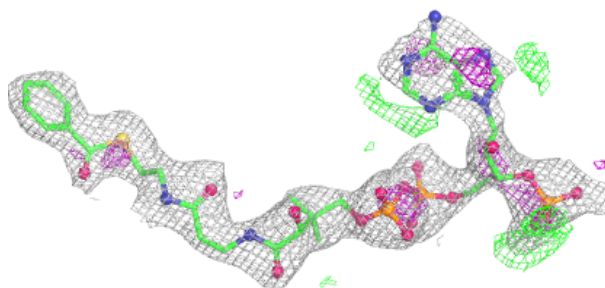


Electron density around BYC B 1003:

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

**Electron density around BYC C 1003:**

$2mF_o-DF_c$ (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.