Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 10:31 AM EST

PDB ID	:	3PM5
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 (i) 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 (i)) were used in the production of this report:

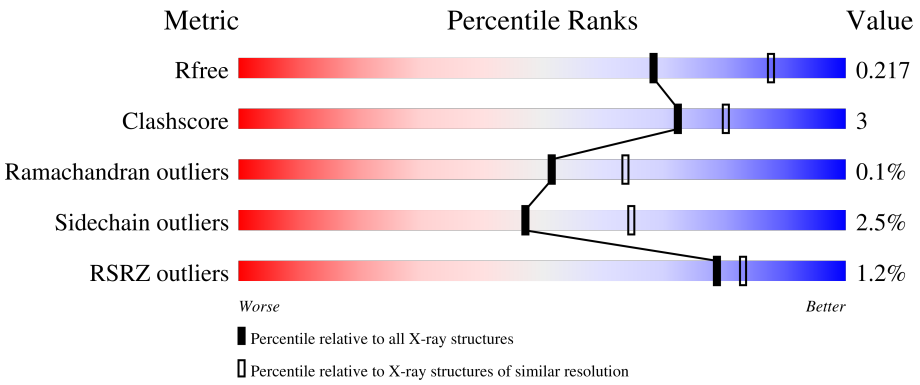
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	2% 89% 9% • •
1	B	481	% 86% 10% • •
1	C	481	91% 7% • •
1	D	481	% 87% 10% •

2 Entry composition (i)

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

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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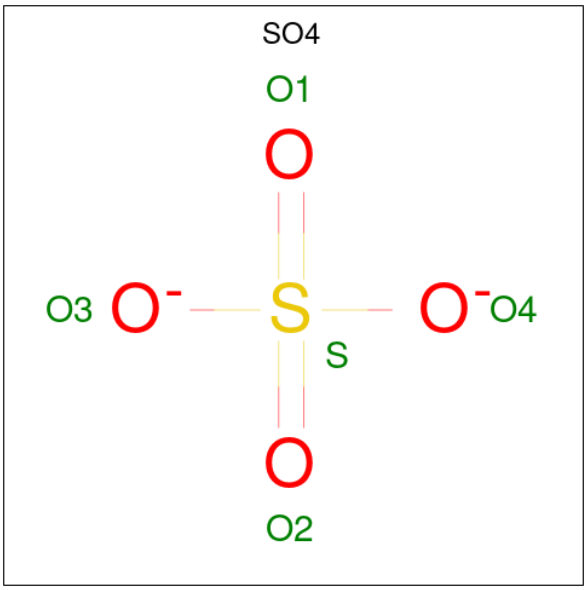
Chain	Residue	Modelled	Actual	Comment	Reference
C	479	PHE	-	SEE REMARK 999	UNP Q9AIX7
C	480	GLU	-	SEE REMARK 999	UNP Q9AIX7
C	481	LYS	-	SEE REMARK 999	UNP Q9AIX7
D	474	TRP	-	SEE REMARK 999	UNP Q9AIX7
D	475	SER	-	SEE REMARK 999	UNP Q9AIX7
D	476	HIS	-	SEE REMARK 999	UNP Q9AIX7
D	477	PRO	-	SEE REMARK 999	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 (three-letter code: SO4) (formula: O_4S).



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

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

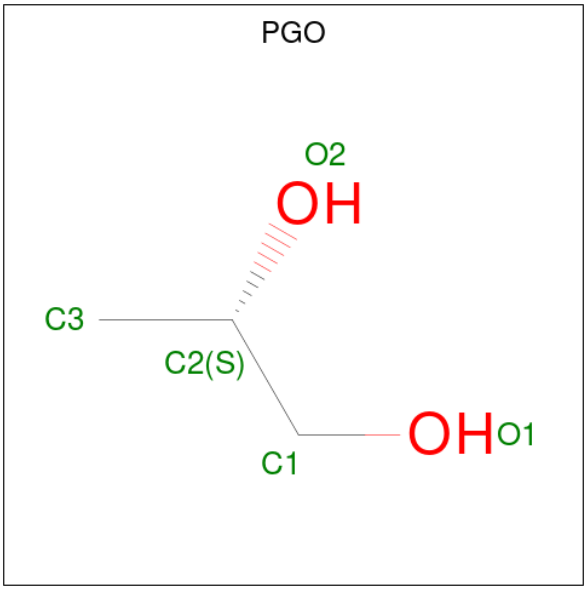
- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

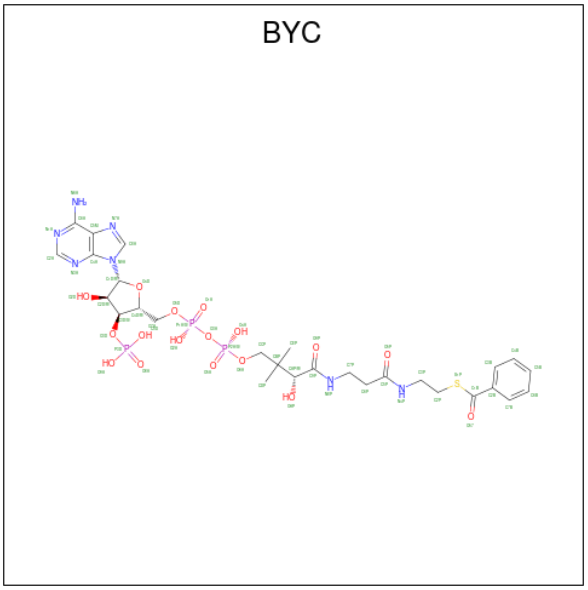
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	2	2	2	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



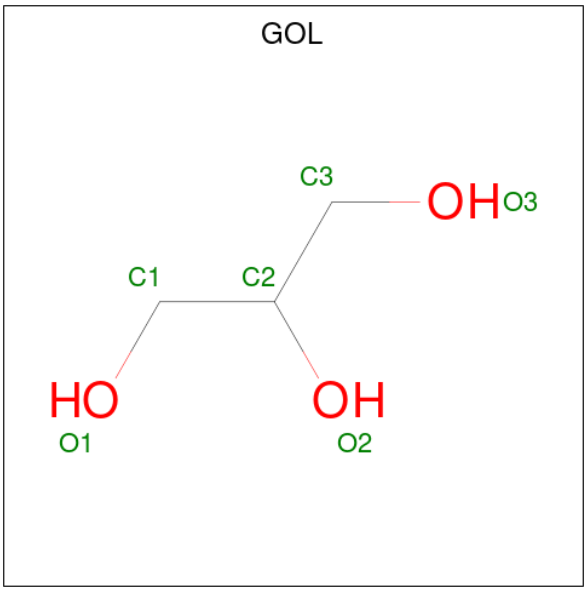
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	5	3	2		0	0
5	B	1	5	3	2		0	0
5	B	1	5	3	2		0	0
5	D	1	5	3	2		0	0

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



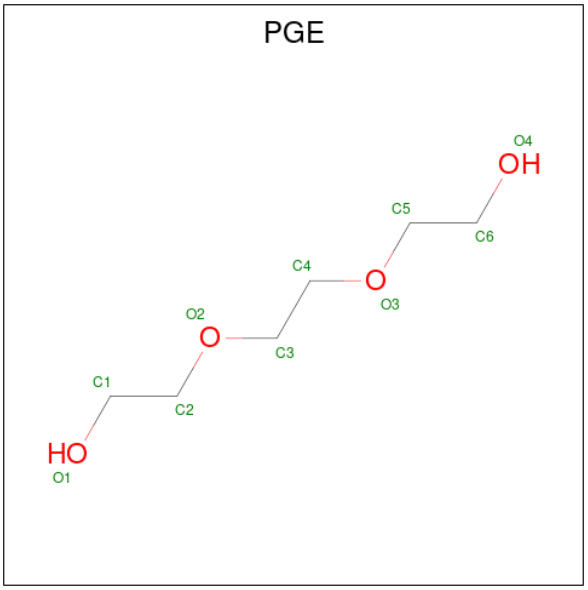
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	A	1	56	28	7	17	3	1	0	0
6	B	1	56	28	7	17	3	1	0	0
6	C	1	56	28	7	17	3	1	0	0
6	D	1	56	28	7	17	3	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 9 is water.

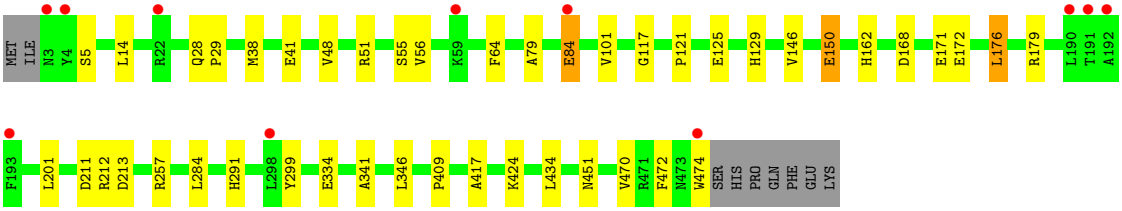
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	178	178	178	0	0
			Total	O		
9	B	176	176	176	0	0
			Total	O		
9	C	158	158	158	0	0
			Total	O		
9	D	117	117	117	0	0

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.

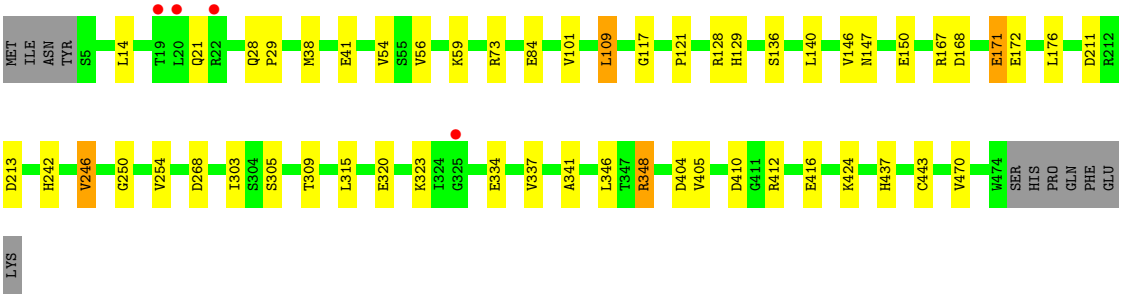
• Molecule 1: Benzoyl-CoA oxygenase component B

Chain A:



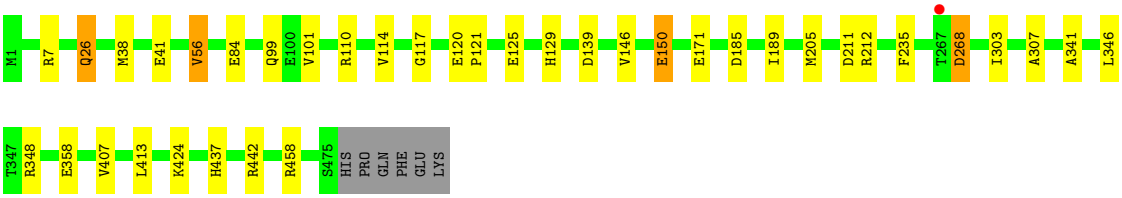
• Molecule 1: Benzoyl-CoA oxygenase component B

Chain B:



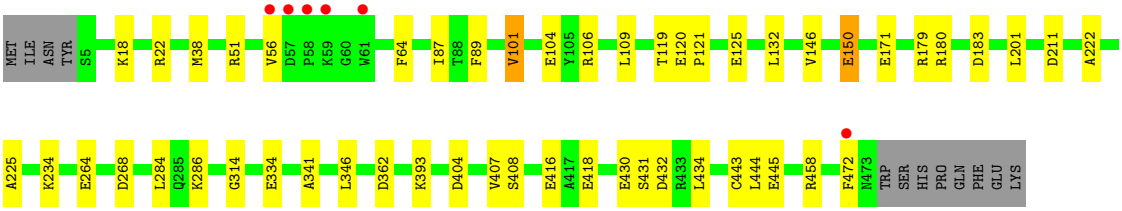
• Molecule 1: Benzoyl-CoA oxygenase component B

Chain C:



• Molecule 1: Benzoyl-CoA oxygenase component B

Chain D:


MET
ILE
ASN
TYR
S5
K18
R22
M38
R51
V56
D57
P58
K59
G60
W61
F64
I87
T88
F89
V101
E104
Y105
R106
L109
T119
E120
P121
E125
L132
V146
E150
E171
R179
R180
D183
L201
D211
A222
A225
K234
E264
D268
L284
Q285
K286
G314
E334
A341
L346
D362
K393
D404
V407
S408
E416
A417
E418
E430
S431
D432
R433
L434
C443
L444
E445
R458
F472
M473
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FE, CL, PGO, GOL, SO4, PGE, BYC

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	0.97	4/3999 (0.1%)	0.85	1/5422 (0.0%)
1	B	0.98	2/3994 (0.1%)	0.86	3/5413 (0.1%)
1	C	1.00	2/4034 (0.0%)	0.88	6/5468 (0.1%)
1	D	0.96	6/3973 (0.2%)	0.83	0/5384
All	All	0.98	14/16000 (0.1%)	0.86	10/21687 (0.0%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150[A]	GLU	CG-CD	7.02	1.62	1.51
1	C	150[B]	GLU	CG-CD	7.02	1.62	1.51
1	A	334	GLU	CB-CG	-6.45	1.39	1.52
1	D	445	GLU	CG-CD	6.26	1.61	1.51
1	A	150[A]	GLU	CG-CD	6.06	1.61	1.51
1	A	150[B]	GLU	CG-CD	6.06	1.61	1.51
1	D	445	GLU	CB-CG	5.87	1.63	1.52
1	A	299	TYR	CD1-CE1	-5.40	1.31	1.39
1	D	334	GLU	CB-CG	-5.22	1.42	1.52
1	D	150[A]	GLU	CG-CD	5.21	1.59	1.51
1	D	150[B]	GLU	CG-CD	5.21	1.59	1.51
1	B	246	VAL	CB-CG2	5.17	1.63	1.52
1	D	418	GLU	CG-CD	5.16	1.59	1.51
1	B	334	GLU	CB-CG	-5.08	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	212	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	C	205	MET	CG-SD-CE	-6.67	89.52	100.20
1	B	348	ARG	NE-CZ-NH1	6.41	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	268	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	C	139	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	B	84	GLU	N-CA-C	5.18	124.98	111.00
1	A	212	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	150[A]	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	C	150[B]	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	B	73	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3892	0	3705	24	0
1	B	3887	0	3711	31	0
1	C	3917	0	3747	21	0
1	D	3866	0	3693	32	0
2	A	15	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	106	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 3.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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:D:341:ALA:CB	1:D:346:LEU:HD12	2.13	0.78
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:D:341:ALA:HB2	1:D:346:LEU:HD12	1.78	0.65
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:C:38:MET:HE2	1:C:125:GLU:HG2	1.86	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:D:38:MET:HE2	1:D:125:GLU:HG2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:38:MET:HE2	1:A:125:GLU:HG2	1.94	0.50
1:B:117:GLY:O	1:B:121:PRO:HD2	2.11	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:B:14:LEU:HD22	1:B:21:GLN:HB2	1.94	0.49
1:D:286:LYS:NZ	1:D:432:ASP:OD2	2.30	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:CG1	1:C:56:VAL:O	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
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:A:213:ASP:OD2	6:A:1003:BYC:H2P	2.15	0.46
1:D:38:MET:CE	1:D:125:GLU:HG2	2.45	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:D:431:SER:O	1:D:432:ASP:C	2.53	0.45
1:C:99:GLN:NE2	9:C:512:HOH:O	2.45	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:362:ASP:OD1	1:D:393:LYS:NZ	2.41	0.45
1:D:180[B]:ARG:HB2	1:D:183:ASP:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:38:MET:HE1	1:B:128[A]:ARG:CZ	2.48	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: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: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: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: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
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%)	47	58
All	All	1897/1924 (99%)	1844 (97%)	52 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	443	CYS

5.3.2 Protein sidechains (i)

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%)	44	61
1	B	409/415 (99%)	397 (97%)	12 (3%)	42	58
1	C	414/415 (100%)	404 (98%)	10 (2%)	49	66
1	D	408/415 (98%)	400 (98%)	8 (2%)	55	72
All	All	1641/1660 (99%)	1600 (98%)	41 (2%)	47	65

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	14	LEU
1	A	55	SER
1	A	84	GLU
1	A	101	VAL
1	A	171	GLU
1	A	176	LEU
1	A	211	ASP
1	A	409	PRO
1	A	424	LYS
1	A	434	LEU
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	211	ASP
1	B	268	ASP
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	211	ASP
1	C	268	ASP
1	C	424	LYS
1	C	442	ARG
1	C	458	ARG
1	D	56	VAL
1	D	101	VAL
1	D	104	GLU
1	D	109	LEU
1	D	171	GLU
1	D	211	ASP
1	D	264	GLU
1	D	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	15	ASN
1	A	21	GLN
1	A	28	GLN
1	A	33	ASN
1	A	127	GLN
1	A	129	HIS
1	A	147	ASN
1	A	291	HIS
1	A	425	ASN
1	B	21	GLN
1	B	33	ASN
1	B	99	GLN
1	B	437	HIS
1	C	21	GLN
1	C	26	GLN
1	C	33	ASN
1	C	162	HIS
1	C	396	HIS
1	C	437	HIS
1	D	21	GLN
1	D	33	ASN
1	D	95	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	482	-	4,4,4	0.44	0	6,6,6	0.60	0
5	PGO	D	484	-	3,4,4	0.37	0	1,4,4	0.06	0
2	SO4	C	484	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	D	482	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	C	483	-	4,4,4	0.16	0	6,6,6	0.19	0
5	PGO	A	487	-	3,4,4	0.48	0	1,4,4	0.38	0
6	BYC	D	1003	-	51,59,59	2.58	15 (29%)	64,87,87	1.60	14 (21%)
5	PGO	B	483	-	3,4,4	0.65	0	1,4,4	0.98	0
6	BYC	A	1003	-	51,59,59	2.64	16 (31%)	64,87,87	1.79	10 (15%)
6	BYC	B	1003	-	51,59,59	2.76	17 (33%)	64,87,87	1.71	15 (23%)
7	GOL	D	485	-	5,5,5	0.38	0	5,5,5	0.60	0
2	SO4	A	483	-	4,4,4	0.30	0	6,6,6	0.40	0
8	PGE	D	486	-	9,9,9	0.96	0	8,8,8	0.94	0
7	GOL	C	486	-	5,5,5	0.49	0	5,5,5	0.86	0
5	PGO	B	482	-	3,4,4	0.36	0	1,4,4	0.32	0
2	SO4	A	482	-	4,4,4	0.19	0	6,6,6	0.68	0
2	SO4	A	484	-	4,4,4	0.11	0	6,6,6	0.15	0
6	BYC	C	1003	-	51,59,59	2.66	13 (25%)	64,87,87	1.35	6 (9%)

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	D	484	-	-	2/2/2/2	-
5	PGO	A	487	-	-	0/2/2/2	-
6	BYC	D	1003	-	-	10/51/71/71	0/4/4/4
5	PGO	B	483	-	-	1/2/2/2	-
6	BYC	B	1003	-	-	16/51/71/71	0/4/4/4
8	PGE	D	486	-	-	4/7/7/7	-
7	GOL	D	485	-	-	2/4/4/4	-
7	GOL	C	486	-	-	4/4/4/4	-
5	PGO	B	482	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BYC	A	1003	-	-	7/51/71/71	0/4/4/4
6	BYC	C	1003	-	-	6/51/71/71	0/4/4/4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1003	BYC	C2A-N3A	8.86	1.46	1.32
6	D	1003	BYC	C4A-N3A	8.18	1.46	1.35
6	D	1003	BYC	C2A-N3A	8.11	1.45	1.32
6	A	1003	BYC	C2A-N3A	8.06	1.45	1.32
6	B	1003	BYC	C2A-N3A	8.02	1.45	1.32
6	C	1003	BYC	C4A-N3A	7.89	1.46	1.35
6	A	1003	BYC	C4A-N3A	7.79	1.46	1.35
6	B	1003	BYC	C4A-N3A	7.69	1.46	1.35
6	B	1003	BYC	C9P-N8P	5.84	1.46	1.33
6	D	1003	BYC	C2A-N1A	5.63	1.44	1.33
6	A	1003	BYC	C2A-N1A	5.60	1.44	1.33
6	C	1003	BYC	C2A-N1A	5.43	1.44	1.33
6	B	1003	BYC	C2A-N1A	5.36	1.43	1.33
6	B	1003	BYC	C7B-C2B	5.27	1.48	1.39
6	C	1003	BYC	C7B-C2B	5.13	1.48	1.39
6	B	1003	BYC	C3B-C2B	5.11	1.48	1.39
6	C	1003	BYC	C9P-N8P	5.09	1.44	1.33
6	D	1003	BYC	C3B-C2B	5.03	1.47	1.39
6	B	1003	BYC	C4B-C3B	4.81	1.49	1.38
6	A	1003	BYC	C7B-C2B	4.80	1.47	1.39
6	C	1003	BYC	C3B-C2B	4.70	1.47	1.39
6	A	1003	BYC	C9P-N8P	4.69	1.43	1.33
6	C	1003	BYC	C4B-C3B	4.64	1.48	1.38
6	D	1003	BYC	C9P-N8P	4.56	1.43	1.33
6	A	1003	BYC	C6B-C7B	4.55	1.48	1.38
6	A	1003	BYC	C4B-C3B	4.51	1.48	1.38
6	B	1003	BYC	C5B-C4B	4.41	1.49	1.38
6	A	1003	BYC	C3B-C2B	4.37	1.46	1.39
6	B	1003	BYC	C6B-C7B	4.15	1.47	1.38
6	A	1003	BYC	C5B-C4B	4.13	1.49	1.38
6	C	1003	BYC	C6B-C7B	4.02	1.47	1.38
6	D	1003	BYC	C7B-C2B	3.99	1.46	1.39
6	C	1003	BYC	C5B-C4B	3.95	1.48	1.38
6	D	1003	BYC	C4B-C3B	3.79	1.46	1.38
6	B	1003	BYC	C6B-C5B	3.78	1.48	1.38
6	D	1003	BYC	C5B-C4B	3.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1003	BYC	C5P-N4P	3.56	1.41	1.33
6	D	1003	BYC	C6B-C7B	3.41	1.46	1.38
6	A	1003	BYC	C6B-C5B	3.41	1.47	1.38
6	C	1003	BYC	C6B-C5B	3.35	1.46	1.38
6	D	1003	BYC	C6B-C5B	3.33	1.46	1.38
6	A	1003	BYC	C5P-N4P	3.31	1.40	1.33
6	B	1003	BYC	C2D-C3D	-3.24	1.45	1.52
6	C	1003	BYC	C2D-C3D	-3.06	1.46	1.52
6	D	1003	BYC	C5P-N4P	2.95	1.40	1.33
6	B	1003	BYC	C1B-S1P	2.78	1.82	1.76
6	A	1003	BYC	C2D-C3D	-2.67	1.47	1.52
6	D	1003	BYC	C6P-C5P	2.59	1.56	1.51
6	B	1003	BYC	CDP-CBP	-2.58	1.48	1.53
6	D	1003	BYC	C2D-C3D	-2.50	1.47	1.52
6	B	1003	BYC	OAP-CAP	-2.45	1.37	1.42
6	D	1003	BYC	O4D-C1D	2.40	1.44	1.41
6	D	1003	BYC	C6A-C5M	2.34	1.52	1.43
6	A	1003	BYC	OAP-CAP	-2.19	1.38	1.42
6	A	1003	BYC	O4D-C1D	2.17	1.44	1.41
6	A	1003	BYC	C6P-C5P	2.11	1.55	1.51
6	B	1003	BYC	C6P-C5P	2.11	1.55	1.51
6	A	1003	BYC	C1B-S1P	2.10	1.81	1.76
6	C	1003	BYC	C6A-N6A	2.09	1.41	1.34
6	C	1003	BYC	C6A-C5M	2.08	1.51	1.43
6	B	1003	BYC	C6A-N6A	2.01	1.41	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1003	BYC	C2P-S1P-C1B	7.38	109.07	99.80
6	D	1003	BYC	N3A-C2A-N1A	-5.72	119.73	128.68
6	B	1003	BYC	N3A-C2A-N1A	-5.68	119.80	128.68
6	A	1003	BYC	N3A-C2A-N1A	-5.22	120.51	128.68
6	C	1003	BYC	N3A-C2A-N1A	-5.04	120.80	128.68
6	B	1003	BYC	C2P-S1P-C1B	4.16	105.02	99.80
6	A	1003	BYC	C7P-C6P-C5P	3.90	118.84	112.36
6	A	1003	BYC	P2A-O3A-P1A	-3.81	119.76	132.83
6	A	1003	BYC	C2P-C3P-N4P	-3.67	104.69	112.42
6	A	1003	BYC	O4D-C1D-C2D	-3.64	101.61	106.93
6	B	1003	BYC	CDP-CBP-CAP	3.63	115.12	108.82
6	B	1003	BYC	O4D-C1D-C2D	-3.47	101.86	106.93
6	D	1003	BYC	O6A-CCP-CBP	-3.36	105.14	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1003	BYC	O5P-C5P-N4P	-3.25	116.89	123.01
6	B	1003	BYC	C7B-C2B-C3B	3.15	123.08	118.59
6	D	1003	BYC	C2P-C3P-N4P	-3.14	105.82	112.42
6	D	1003	BYC	O5P-C5P-N4P	-3.06	117.23	123.01
6	D	1003	BYC	P2A-O3A-P1A	-3.05	122.38	132.83
6	A	1003	BYC	C5D-C4D-C3D	2.93	124.11	114.40
6	D	1003	BYC	C7P-C6P-C5P	2.85	117.10	112.36
6	C	1003	BYC	O4D-C1D-C2D	-2.83	102.78	106.93
6	D	1003	BYC	O4D-C1D-C2D	-2.78	102.86	106.93
6	D	1003	BYC	C7B-C2B-C3B	2.77	122.54	118.59
6	A	1003	BYC	CAP-C9P-N8P	-2.76	111.08	116.58
6	D	1003	BYC	C5D-C4D-C3D	2.76	123.54	114.40
6	B	1003	BYC	C4B-C3B-C2B	-2.75	117.09	120.34
6	B	1003	BYC	P2A-O3A-P1A	-2.61	123.88	132.83
6	B	1003	BYC	C5D-C4D-C3D	2.54	122.81	114.40
6	B	1003	BYC	C7P-C6P-C5P	2.51	116.54	112.36
6	B	1003	BYC	O57-C1B-C2B	-2.42	116.13	122.13
6	C	1003	BYC	C7B-C2B-C3B	2.41	122.01	118.59
6	D	1003	BYC	O5P-C5P-C6P	2.40	126.41	122.02
6	D	1003	BYC	O9P-C9P-N8P	-2.37	117.90	122.99
6	A	1003	BYC	C7B-C2B-C3B	2.37	121.96	118.59
6	B	1003	BYC	C6P-C7P-N8P	2.34	116.62	111.90
6	B	1003	BYC	C7P-N8P-C9P	2.27	126.64	122.59
6	D	1003	BYC	C2B-C1B-S1P	2.21	119.53	114.99
6	B	1003	BYC	O2D-C2D-C1D	2.20	118.98	110.85
6	B	1003	BYC	C1D-N9A-C4A	2.19	130.49	126.64
6	C	1003	BYC	P2A-O3A-P1A	-2.17	125.37	132.83
6	C	1003	BYC	C3P-N4P-C5P	-2.15	118.84	122.84
6	A	1003	BYC	O2D-C2D-C1D	2.12	118.68	110.85
6	D	1003	BYC	O2A-P1A-O1A	2.09	122.56	112.24
6	B	1003	BYC	O3D-C3D-C2D	-2.09	104.12	111.68
6	D	1003	BYC	C4B-C3B-C2B	-2.08	117.88	120.34

There are no chirality outliers.

All (54) 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

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Mol	Chain	Res	Type	Atoms
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	C	1003	BYC	C5D-O5D-P1A-O1A
6	C	1003	BYC	C5D-O5D-P1A-O3A
6	C	1003	BYC	C3D-O3D-P3D-O8A
6	D	1003	BYC	C5D-O5D-P1A-O3A
6	D	1003	BYC	CCP-O6A-P2A-O5A
6	D	1003	BYC	C3D-O3D-P3D-O8A
7	C	486	GOL	O1-C1-C2-C3
7	C	486	GOL	C1-C2-C3-O3
6	D	1003	BYC	O4D-C4D-C5D-O5D
8	D	486	PGE	O3-C5-C6-O4
6	D	1003	BYC	C4D-C3D-O3D-P3D
6	B	1003	BYC	CDP-CBP-CCP-O6A
6	B	1003	BYC	CEP-CBP-CCP-O6A
7	D	485	GOL	O1-C1-C2-C3
6	B	1003	BYC	C2D-C3D-O3D-P3D
6	D	1003	BYC	C2D-C3D-O3D-P3D
7	C	486	GOL	O1-C1-C2-O2
6	A	1003	BYC	S1P-C1B-C2B-C7B
6	A	1003	BYC	O4D-C4D-C5D-O5D
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	D	1003	BYC	C3D-C4D-C5D-O5D
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	A	1003	BYC	C5D-O5D-P1A-O3A
6	B	1003	BYC	C3D-O3D-P3D-O7A
6	D	1003	BYC	CCP-O6A-P2A-O3A
6	C	1003	BYC	C3D-C4D-C5D-O5D
6	D	1003	BYC	C5D-O5D-P1A-O1A
8	D	486	PGE	C3-C4-O3-C5
6	B	1003	BYC	O57-C1B-C2B-C3B
6	B	1003	BYC	C4D-C3D-O3D-P3D
6	D	1003	BYC	C3P-C2P-S1P-C1B
6	A	1003	BYC	C2D-C3D-O3D-P3D

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Mol	Chain	Res	Type	Atoms
6	B	1003	BYC	O57-C1B-C2B-C7B
6	B	1003	BYC	C3D-C4D-C5D-O5D
6	A	1003	BYC	C3D-O3D-P3D-O7A
8	D	486	PGE	C6-C5-O3-C4
8	D	486	PGE	O2-C3-C4-O3
5	B	483	PGO	O1-C1-C2-O2
6	C	1003	BYC	S1P-C2P-C3P-N4P

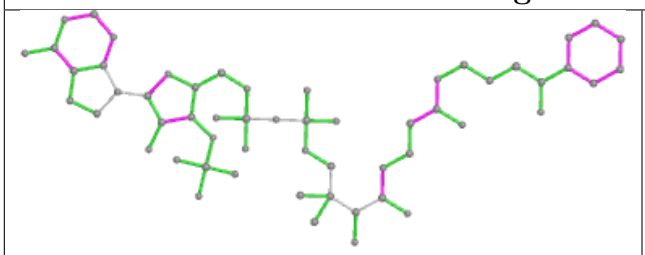
There are no ring outliers.

6 monomers are involved in 11 short contacts:

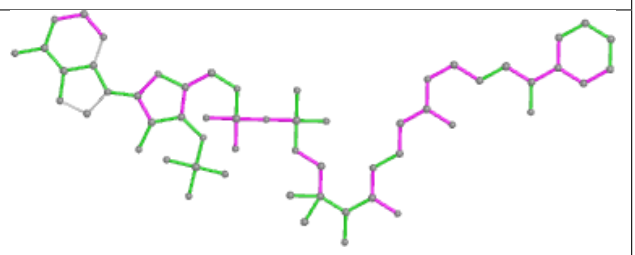
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1003	BYC	2	0
5	B	483	PGO	2	0
6	A	1003	BYC	2	0
6	B	1003	BYC	1	0
5	B	482	PGO	2	0
6	C	1003	BYC	2	0

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 then 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.

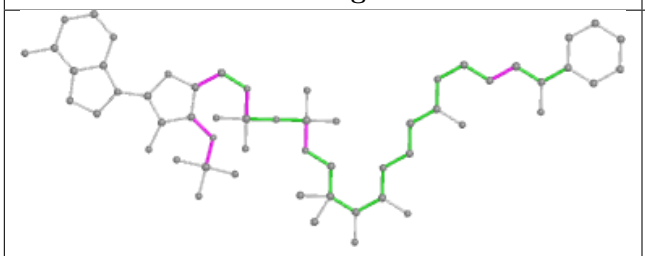
Ligand BYC D 1003



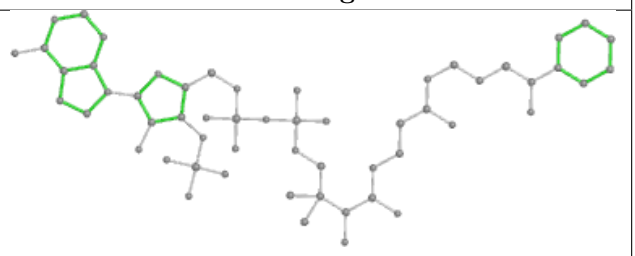
Bond lengths



Bond angles

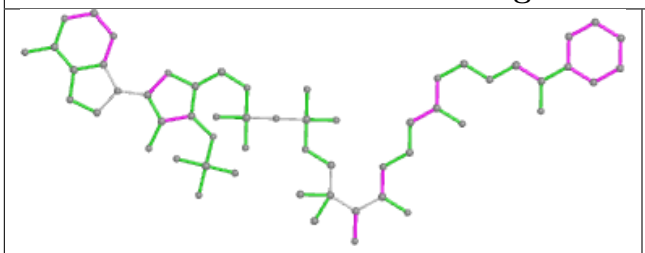


Torsions

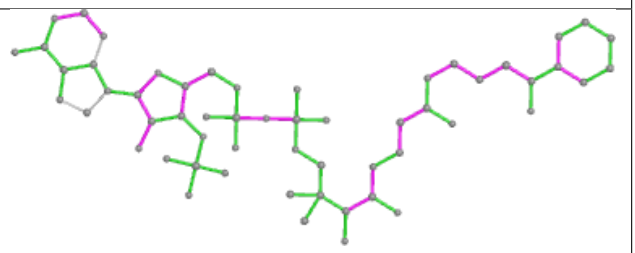


Rings

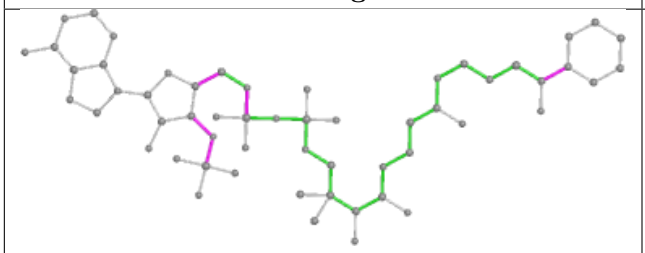
Ligand BYC A 1003



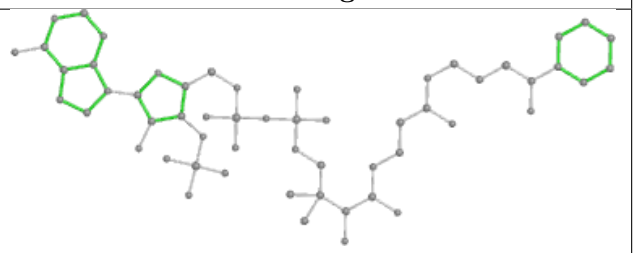
Bond lengths



Bond angles

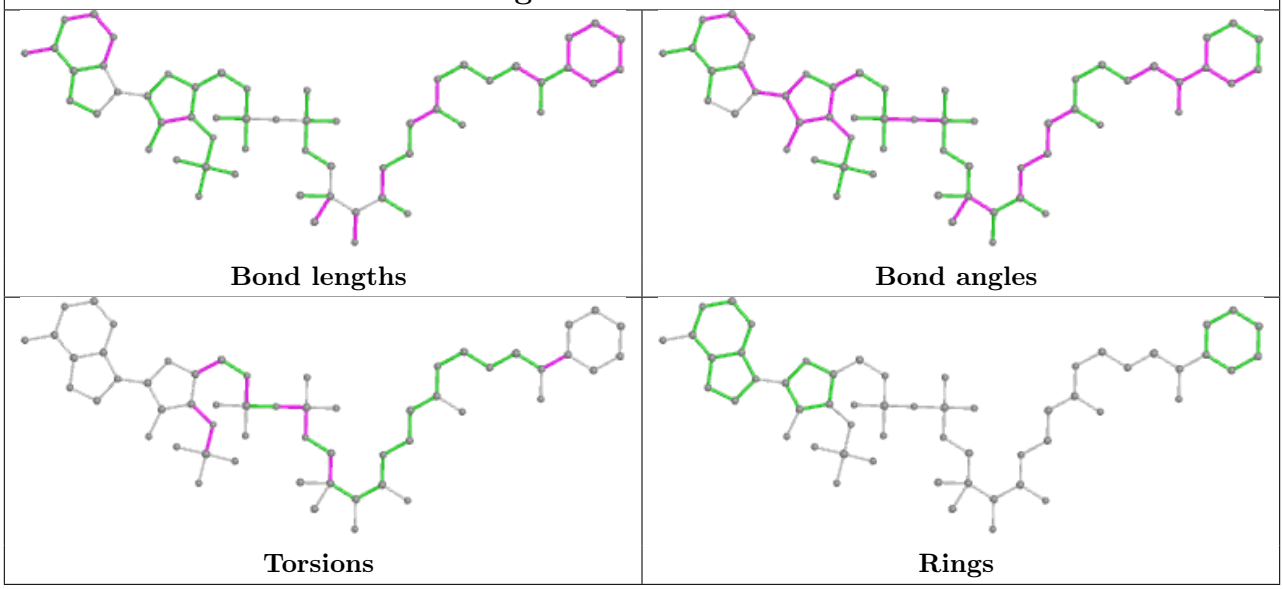


Torsions

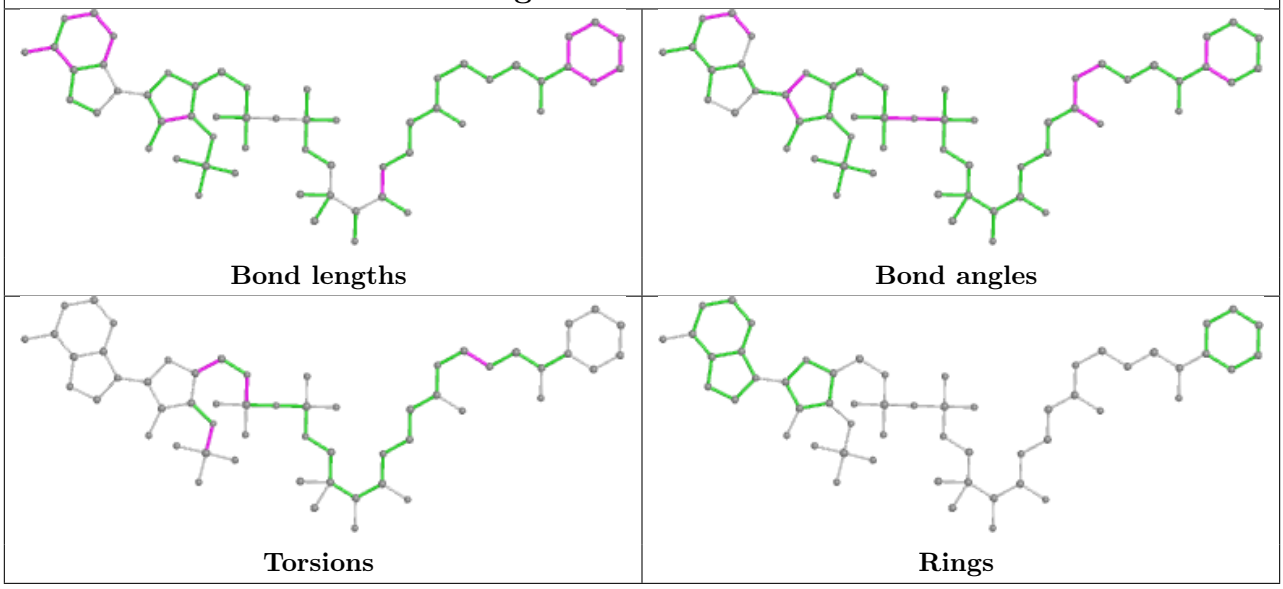


Rings

Ligand BYC B 1003



Ligand BYC C 1003



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%)	-0.02	11 (2%)	60	67	28, 42, 61, 83	0
1	B	470/481 (97%)	-0.25	4 (0%)	84	88	28, 41, 59, 82	0
1	C	475/481 (98%)	-0.22	1 (0%)	95	96	29, 42, 62, 79	0
1	D	469/481 (97%)	-0.22	6 (1%)	77	81	27, 47, 69, 87	0
All	All	1886/1924 (98%)	-0.18	22 (1%)	79	83	27, 43, 63, 87	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	LYS	4.3
1	A	474	TRP	4.3
1	A	3	ASN	3.7
1	D	58	PRO	3.6
1	A	190	LEU	3.1
1	A	84	GLU	2.7
1	D	61	TRP	2.6
1	B	325	GLY	2.6
1	A	191	THR	2.4
1	A	298	LEU	2.4
1	A	22	ARG	2.3
1	D	57	ASP	2.2
1	B	20	LEU	2.2
1	D	472	PHE	2.2
1	B	22	ARG	2.1
1	A	193	PHE	2.1
1	B	19	THR	2.1
1	A	59	LYS	2.1
1	A	4	TYR	2.1
1	C	267	THR	2.1
1	D	56	VAL	2.0
1	A	192	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PGE	D	486	10/10	0.74	0.23	67,70,72,72	0
5	PGO	B	483	5/5	0.75	0.17	67,68,69,70	0
7	GOL	C	486	6/6	0.78	0.15	74,76,77,77	0
5	PGO	D	484	5/5	0.83	0.22	64,66,67,68	0
2	SO4	C	483	5/5	0.84	0.42	118,119,119,120	0
6	BYC	D	1003	56/56	0.85	0.20	49,71,103,106	0
2	SO4	A	484	5/5	0.86	0.44	125,126,126,126	0
6	BYC	A	1003	56/56	0.87	0.23	49,71,98,101	0
2	SO4	D	482	5/5	0.87	0.38	102,103,103,103	0
2	SO4	A	482	5/5	0.89	0.15	87,89,89,90	0
5	PGO	A	487	5/5	0.90	0.16	59,62,66,67	0
2	SO4	A	483	5/5	0.90	0.32	96,96,96,98	0
7	GOL	D	485	6/6	0.90	0.14	86,88,89,89	0
6	BYC	B	1003	56/56	0.90	0.17	47,69,98,99	0
2	SO4	C	484	5/5	0.91	0.36	120,121,121,121	0
6	BYC	C	1003	56/56	0.91	0.18	43,65,101,103	0
5	PGO	B	482	5/5	0.92	0.17	60,68,70,71	0
3	FE	C	1001	1/1	0.95	0.16	86,86,86,86	0
3	FE	A	1001	1/1	0.95	0.17	74,74,74,74	0
4	CL	C	485	1/1	0.96	0.12	44,44,44,44	0
3	FE	B	1002	1/1	0.96	0.08	63,63,63,63	0
4	CL	D	483	1/1	0.97	0.16	42,42,42,42	0
3	FE	D	1002	1/1	0.97	0.05	73,73,73,73	0
3	FE	D	1001	1/1	0.98	0.06	74,74,74,74	0
2	SO4	C	482	5/5	0.98	0.10	58,58,63,64	0
4	CL	A	485	1/1	0.98	0.09	40,40,40,40	0
3	FE	B	1001	1/1	0.98	0.09	72,72,72,72	0

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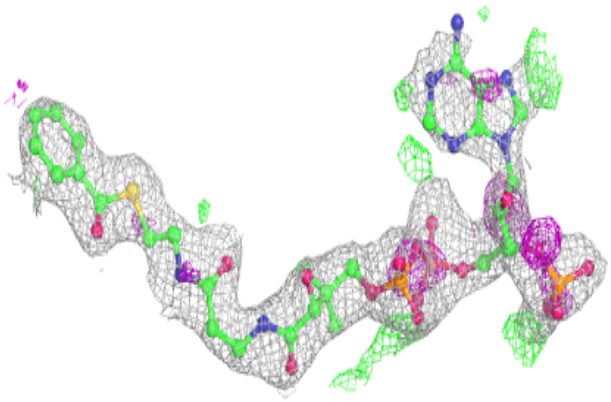
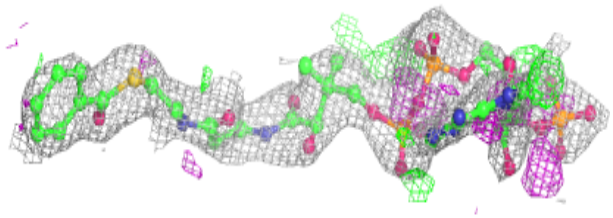
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE	A	1002	1/1	0.99	0.14	59,59,59,59	0
4	CL	A	486	1/1	0.99	0.06	39,39,39,39	0
3	FE	C	1002	1/1	0.99	0.12	63,63,63,63	0

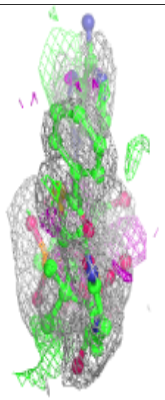
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

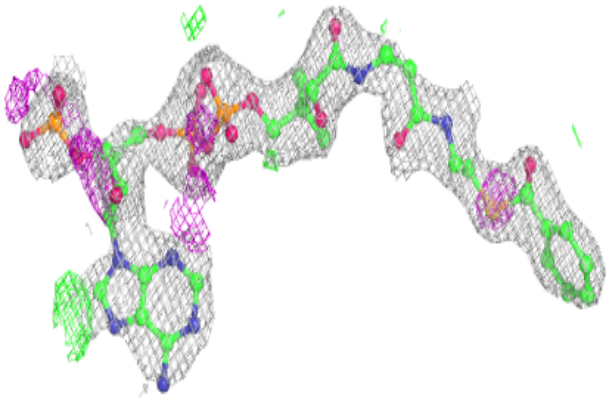


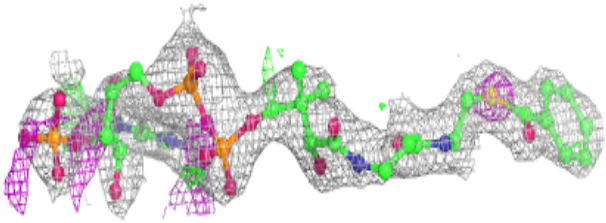


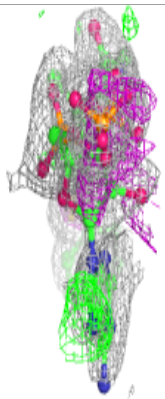


Electron density around BYC A 1003:

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

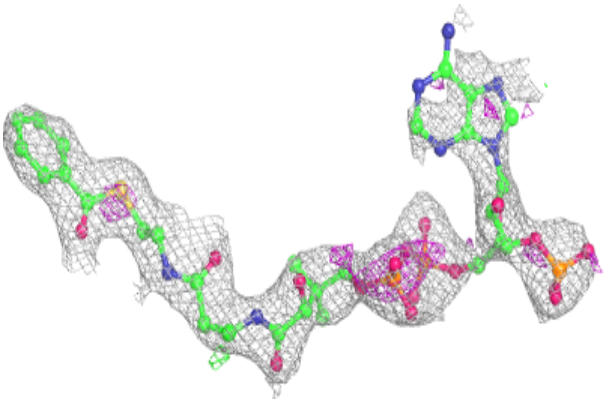


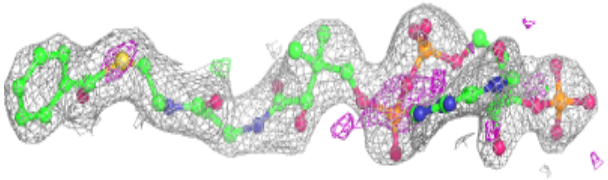


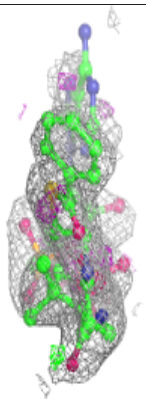


Electron density around BYC B 1003:

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

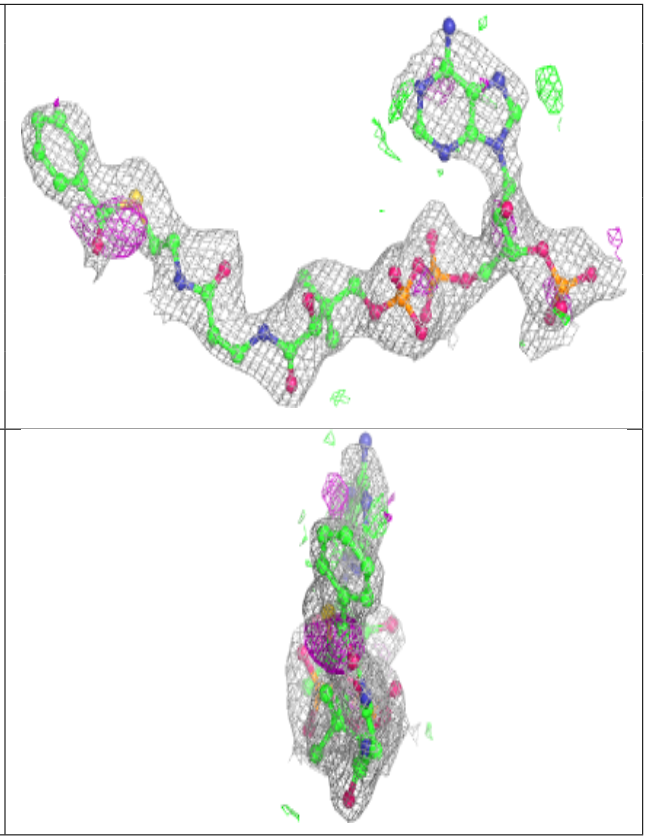






Electron density around BYC C 1003:

$2mF_o$-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.