



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:49 pm BST

PDB ID : 4AC9
Title : CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR
SELB FROM METHANOCOCCUS MARIPALUDIS IN COMPLEX WITH
GDP
Authors : Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on : 2011-12-14
Resolution : 3.03 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

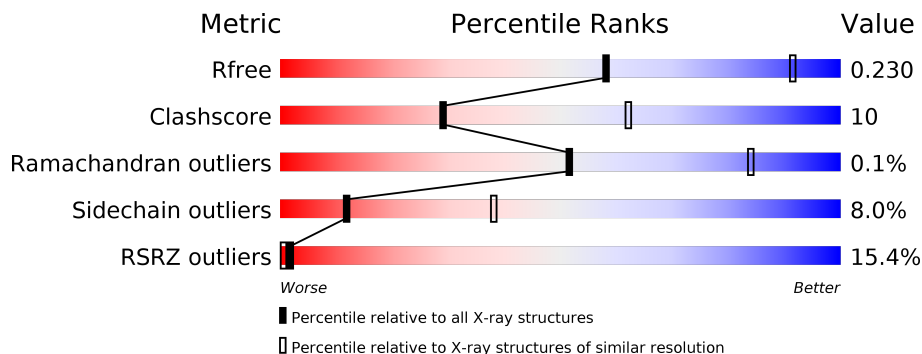
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 on 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	482	
1	B	482	
1	C	482	
1	D	482	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	1474	-	-	-	X
4	SO4	C	1481	-	-	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14628 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 MJ0495-LIKE PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	Hg	N	O	S			
1	A	448	3475	2220	4	593	644	14	0	0	0
1	B	456	3533	2257	4	603	655	14	0	0	0
1	C	471	3651	2327	4	627	679	14	0	0	0
1	D	467	3615	2305	4	618	675	13	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

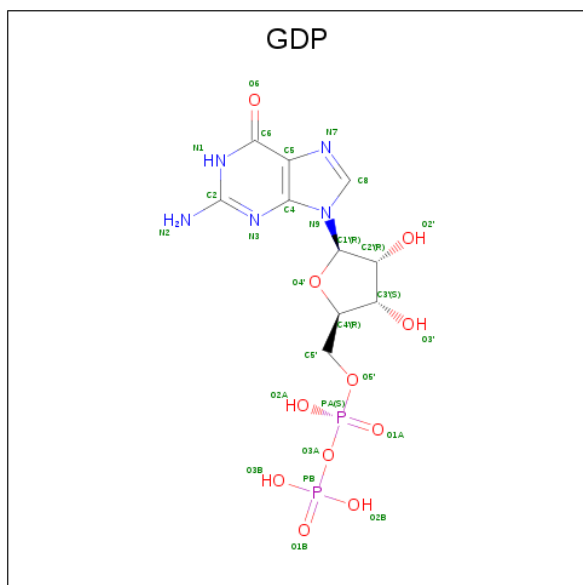
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8J307
A	-12	HIS	-	expression tag	UNP Q8J307
A	-11	HIS	-	expression tag	UNP Q8J307
A	-10	HIS	-	expression tag	UNP Q8J307
A	-9	HIS	-	expression tag	UNP Q8J307
A	-8	HIS	-	expression tag	UNP Q8J307
A	-7	HIS	-	expression tag	UNP Q8J307
A	-6	SER	-	expression tag	UNP Q8J307
A	-5	ILE	-	expression tag	UNP Q8J307
A	-4	GLU	-	expression tag	UNP Q8J307
A	-3	GLY	-	expression tag	UNP Q8J307
A	-2	ARG	-	expression tag	UNP Q8J307
A	-1	PRO	-	expression tag	UNP Q8J307
A	0	HIS	-	expression tag	UNP Q8J307
B	-13	MET	-	expression tag	UNP Q8J307
B	-12	HIS	-	expression tag	UNP Q8J307
B	-11	HIS	-	expression tag	UNP Q8J307
B	-10	HIS	-	expression tag	UNP Q8J307
B	-9	HIS	-	expression tag	UNP Q8J307
B	-8	HIS	-	expression tag	UNP Q8J307
B	-7	HIS	-	expression tag	UNP Q8J307

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	expression tag	UNP Q8J307
B	-5	ILE	-	expression tag	UNP Q8J307
B	-4	GLU	-	expression tag	UNP Q8J307
B	-3	GLY	-	expression tag	UNP Q8J307
B	-2	ARG	-	expression tag	UNP Q8J307
B	-1	PRO	-	expression tag	UNP Q8J307
B	0	HIS	-	expression tag	UNP Q8J307
C	-13	MET	-	expression tag	UNP Q8J307
C	-12	HIS	-	expression tag	UNP Q8J307
C	-11	HIS	-	expression tag	UNP Q8J307
C	-10	HIS	-	expression tag	UNP Q8J307
C	-9	HIS	-	expression tag	UNP Q8J307
C	-8	HIS	-	expression tag	UNP Q8J307
C	-7	HIS	-	expression tag	UNP Q8J307
C	-6	SER	-	expression tag	UNP Q8J307
C	-5	ILE	-	expression tag	UNP Q8J307
C	-4	GLU	-	expression tag	UNP Q8J307
C	-3	GLY	-	expression tag	UNP Q8J307
C	-2	ARG	-	expression tag	UNP Q8J307
C	-1	PRO	-	expression tag	UNP Q8J307
C	0	HIS	-	expression tag	UNP Q8J307
D	-13	MET	-	expression tag	UNP Q8J307
D	-12	HIS	-	expression tag	UNP Q8J307
D	-11	HIS	-	expression tag	UNP Q8J307
D	-10	HIS	-	expression tag	UNP Q8J307
D	-9	HIS	-	expression tag	UNP Q8J307
D	-8	HIS	-	expression tag	UNP Q8J307
D	-7	HIS	-	expression tag	UNP Q8J307
D	-6	SER	-	expression tag	UNP Q8J307
D	-5	ILE	-	expression tag	UNP Q8J307
D	-4	GLU	-	expression tag	UNP Q8J307
D	-3	GLY	-	expression tag	UNP Q8J307
D	-2	ARG	-	expression tag	UNP Q8J307
D	-1	PRO	-	expression tag	UNP Q8J307
D	0	HIS	-	expression tag	UNP Q8J307

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0
2	B	1	28	10	5	11	2	0	0
2	C	1	28	10	5	11	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

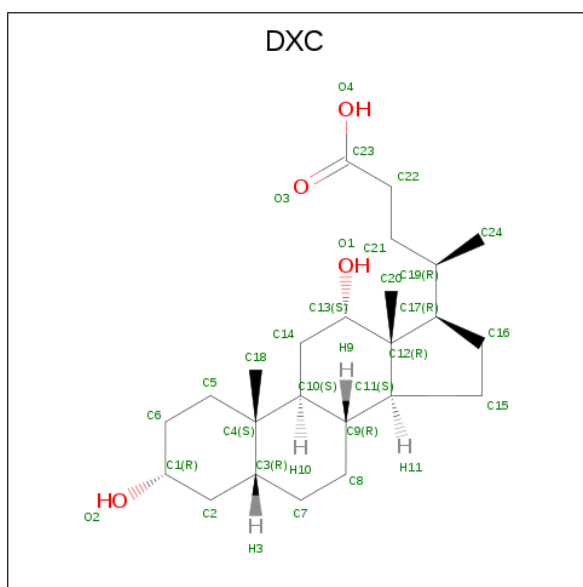
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0
3	A	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



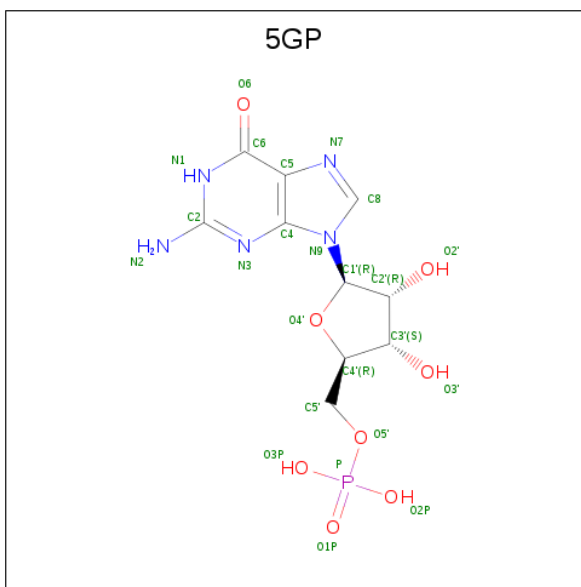
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: C₂₄H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			28	24	4		
5	C	1	Total	C	O	0	0
			28	24	4		
5	C	1	Total	C	O	0	0
			28	24	4		
5	C	1	Total	C	O	0	0
			28	24	4		
5	C	1	Total	C	O	0	0
			28	24	4		
5	C	1	Total	C	O	0	0
			28	24	4		

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	24	10	5	8	1	0	0

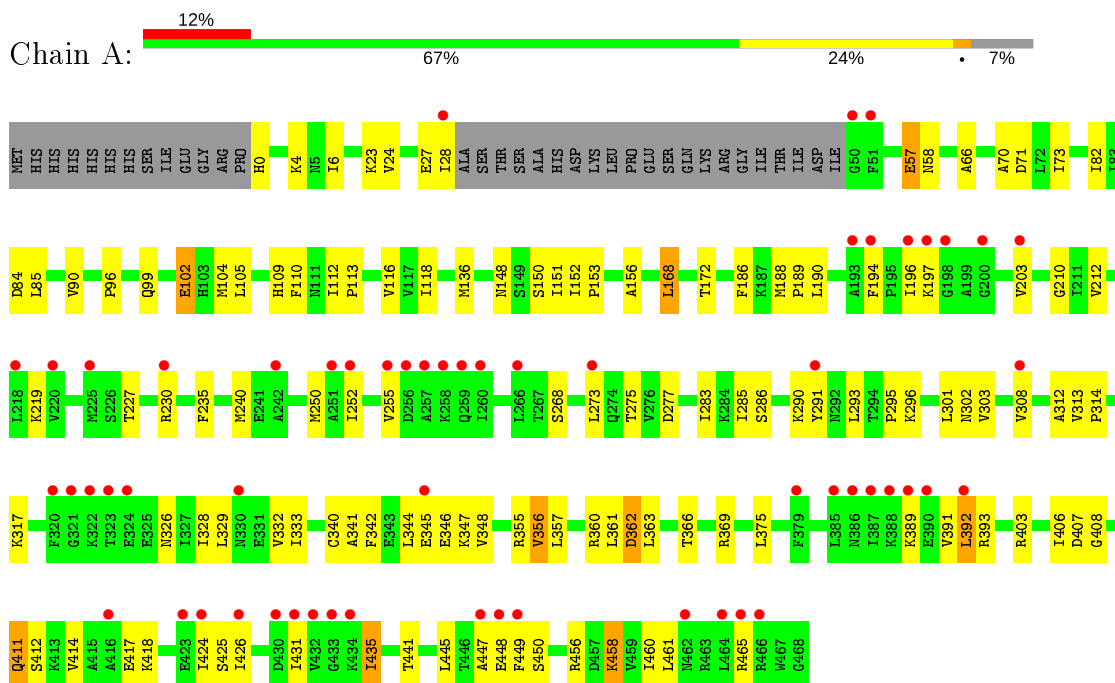
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		
7	B	4	Total	O	0	0
			4	4		
7	C	4	Total	O	0	0
			4	4		

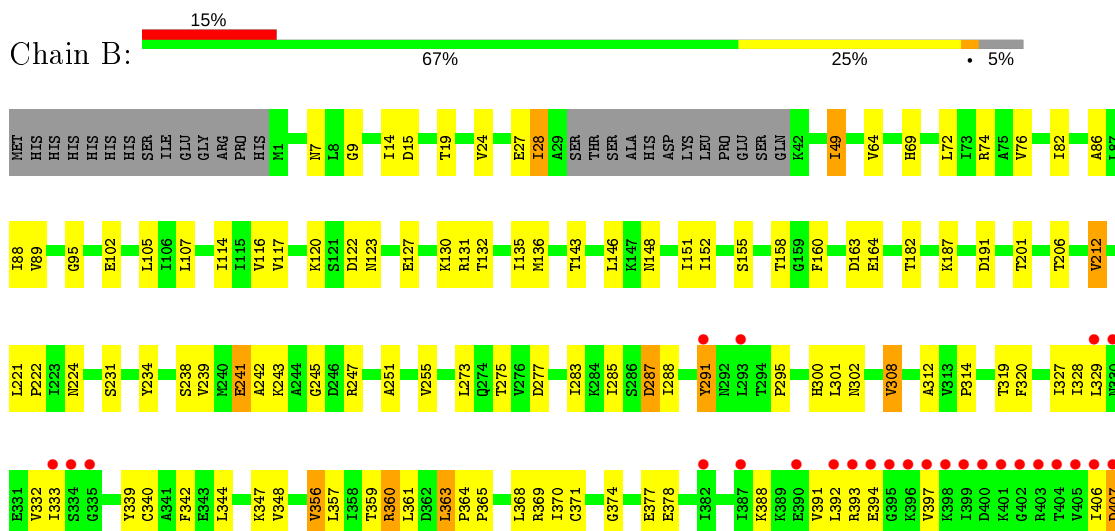
3 Residue-property plots [i](#)

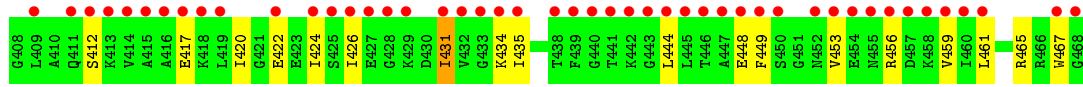
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: MJ0495-LIKE PROTEIN

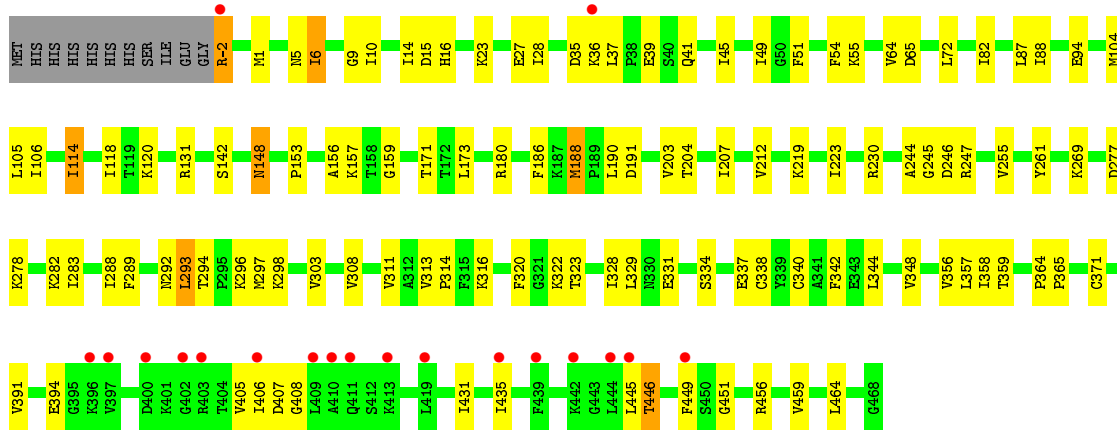


- Molecule 1: MJ0495-LIKE PROTEIN

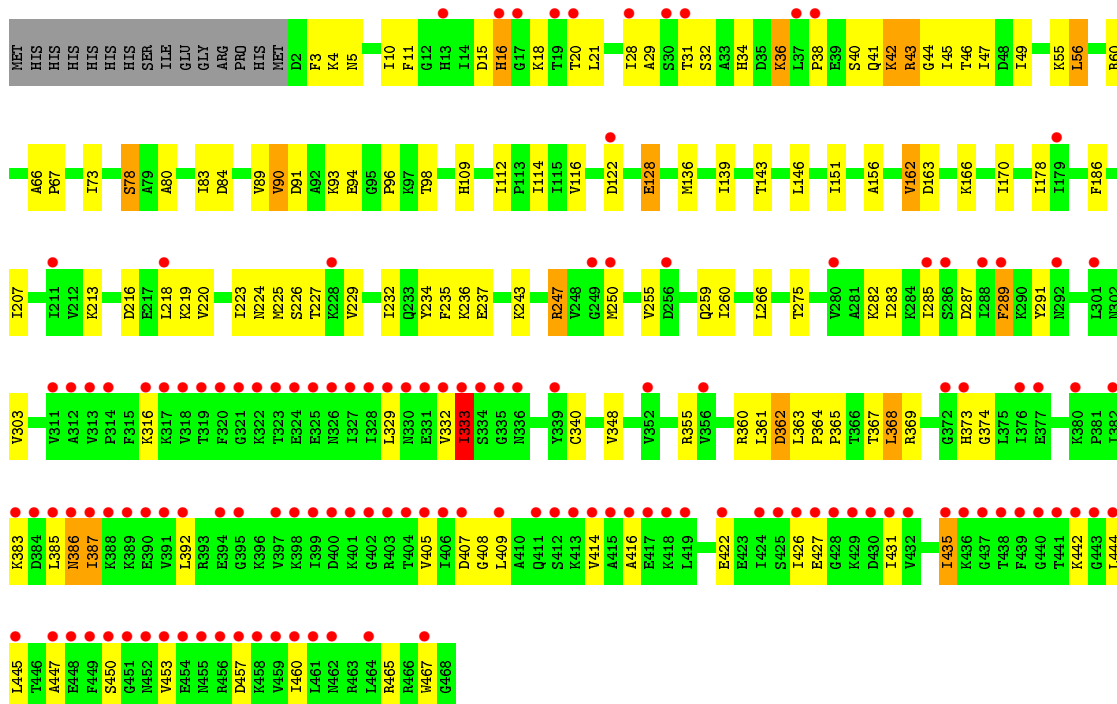




● Molecule 1: MJ0495-LIKE PROTEIN



● Molecule 1: MJ0495-LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	146.92Å 146.92Å 297.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.03 48.09 – 3.03	Depositor EDS
% Data completeness (in resolution range)	89.1 (19.98-3.03) 92.3 (48.09-3.03)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.190 , 0.222 0.198 , 0.230	Depositor DCC
R_{free} test set	2985 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtrriage
Anisotropy	0.373	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 101.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14628	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: GDP, MG, CMH, SO4, 5GP, DXC

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	0.25	0/3484	0.50	0/4684
1	B	0.25	0/3541	0.49	0/4760
1	C	0.24	0/3664	0.49	0/4929
1	D	0.26	0/3626	0.52	0/4878
All	All	0.25	0/14315	0.50	0/19251

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3475	0	3655	69	0
1	B	3533	0	3727	76	0
1	C	3651	0	3837	65	0
1	D	3615	0	3799	78	0
2	A	28	0	12	0	0
2	B	28	0	12	2	0
2	C	28	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	B	10	0	0	2	0
4	C	25	0	0	0	0
5	B	28	0	39	1	0
5	C	168	0	234	10	0
6	B	24	0	12	2	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
All	All	14628	0	15339	288	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 10.

All (288) 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:D:283:ILE:HG13	1:D:340:CMH:HB3	1.50	0.91
1:C:283:ILE:HG12	1:C:358:ILE:HD11	1.58	0.85
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.57	0.84
1:C:283:ILE:HD13	1:C:340:CMH:HB3	1.66	0.78
1:C:36:LYS:HB2	1:C:156:ALA:O	1.84	0.77
1:A:313:VAL:HG23	1:A:341:ALA:HB3	1.66	0.77
1:B:105:LEU:HB3	1:B:370:ILE:HD11	1.67	0.75
1:B:191:ASP:OD2	1:B:247:ARG:NH1	2.19	0.73
1:D:116:VAL:HG11	1:D:136:MET:HG2	1.70	0.73
1:B:82:ILE:HG23	1:B:245:GLY:HA2	1.70	0.73
1:A:152:ILE:HD11	1:A:168:LEU:HD22	1.70	0.73
1:D:416:ALA:HB1	1:D:445:LEU:HD21	1.71	0.73
1:B:422:GLU:H	1:B:435:ILE:HG22	1.54	0.72
1:A:435:ILE:HD11	1:A:445:LEU:HD22	1.73	0.71
1:A:426:ILE:HB	1:A:431:ILE:HG23	1.74	0.70
1:B:377:GLU:HG2	1:B:378:GLU:HG3	1.73	0.69
1:A:66:ALA:HB1	1:A:71:ASP:HB3	1.75	0.69
1:C:308:VAL:HG21	1:C:344:LEU:HD13	1.75	0.68
1:A:360:ARG:HG2	1:A:363:LEU:HG	1.76	0.67
1:D:29:ALA:HB2	1:D:56:LEU:HG	1.75	0.67
1:B:69:HIS:NE2	1:B:102:GLU:OE1	2.22	0.66
1:D:43:ARG:HB3	1:D:45:ILE:HG12	1.76	0.66
1:C:82:ILE:HG23	1:C:245:GLY:HA2	1.79	0.65
1:C:6:ILE:HD12	1:C:173:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:N	1:A:362:ASP:OD1	2.27	0.65
4:B:1472:SO4:O2	1:C:55:LYS:NZ	2.30	0.64
1:B:302:ASN:HB2	1:B:357:LEU:HB3	1.79	0.63
1:A:283:ILE:HD12	1:A:340:CMH:HB3	1.80	0.63
1:B:407:ASP:HB2	1:B:444:LEU:HD22	1.81	0.63
1:C:188:MET:HG3	1:C:207:ILE:HG12	1.81	0.63
1:B:361:LEU:HD23	1:B:369:ARG:HD2	1.82	0.62
1:A:393:ARG:NH2	1:A:411:GLN:OE1	2.33	0.61
1:C:191:ASP:OD2	1:C:247:ARG:NH1	2.30	0.61
1:B:158:THR:HG23	1:D:363:LEU:HB3	1.83	0.61
1:C:292:ASN:HD22	1:C:331:GLU:HG3	1.64	0.61
1:D:56:LEU:HD22	1:D:170:ILE:HD11	1.81	0.60
1:C:-2:ARG:HE	5:C:1476:DXC:H21	1.66	0.60
1:B:360:ARG:NH1	1:B:371:CMH:SG	2.75	0.60
1:B:391:VAL:HB	1:B:465:ARG:HD3	1.83	0.59
1:B:288:ILE:HB	6:B:1474:5GP:HN22	1.66	0.59
1:D:93:LYS:HA	1:D:128:GLU:HG2	1.83	0.59
1:C:36:LYS:HD2	1:C:157:LYS:HA	1.84	0.59
1:C:15:ASP:O	1:C:120:LYS:NZ	2.30	0.59
1:B:426:ILE:HB	1:B:431:ILE:HG23	1.84	0.59
1:D:387:ILE:HG13	1:D:467:TRP:HB3	1.85	0.59
1:A:240:MET:HE1	1:B:95:GLY:HA3	1.85	0.59
1:B:114:ILE:HG12	1:B:146:LEU:HD22	1.85	0.58
1:D:3:PHE:HE2	1:D:55:LYS:HE3	1.68	0.58
1:A:295:PRO:HG3	1:A:328:ILE:HD11	1.84	0.58
1:B:224:ASN:ND2	1:B:224:ASN:O	2.35	0.58
1:A:116:VAL:HB	1:A:151:ILE:HG12	1.84	0.58
1:C:118:ILE:HB	1:C:153:PRO:HA	1.86	0.57
1:C:105:LEU:HD11	1:C:288:ILE:HD11	1.86	0.57
1:D:36:LYS:HB3	1:D:236:LYS:HD2	1.87	0.57
1:D:422:GLU:H	1:D:435:ILE:HG22	1.69	0.57
1:B:86:ALA:HB3	1:B:114:ILE:HG22	1.86	0.57
1:B:287:ASP:OD1	1:B:287:ASP:N	2.31	0.57
1:C:338:CMH:HB3	1:C:340:CMH:CM	2.35	0.57
1:D:122:ASP:N	1:D:122:ASP:OD1	2.39	0.56
1:A:105:LEU:O	1:A:109:HIS:ND1	2.33	0.56
1:D:387:ILE:HD12	1:D:467:TRP:HE3	1.69	0.56
1:B:116:VAL:HB	1:B:151:ILE:HG12	1.88	0.55
1:C:49:ILE:HD11	5:C:1475:DXC:H161	1.88	0.55
1:C:88:ILE:HD13	1:C:104:MET:HG2	1.88	0.55
1:C:219:LYS:HE2	1:C:269:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:NE2	1:A:286:SER:OG	2.30	0.55
1:C:88:ILE:HD12	1:C:114:ILE:HD13	1.88	0.55
1:D:218:LEU:HD11	1:D:229:VAL:HG22	1.88	0.55
1:D:409:LEU:HD12	1:D:445:LEU:HD12	1.88	0.55
1:C:407:ASP:OD1	1:C:408:GLY:N	2.41	0.54
1:D:21:LEU:HD22	1:D:89:VAL:HG11	1.89	0.54
1:D:28:ILE:HG22	1:D:162:VAL:HG13	1.89	0.54
1:A:190:LEU:HD13	1:A:203:VAL:HG11	1.89	0.54
1:D:34:HIS:CD2	1:D:236:LYS:HB2	2.42	0.54
1:B:340:CMH:HB2	1:B:342:PHE:CE2	2.43	0.54
1:B:361:LEU:HA	1:B:369:ARG:HD2	1.89	0.53
1:A:361:LEU:HA	1:A:369:ARG:HD2	1.89	0.53
1:B:74:ARG:NH2	4:B:1471:SO4:O4	2.40	0.53
1:D:83:ILE:HG22	1:D:112:ILE:HD13	1.91	0.53
1:B:143:THR:HG21	1:B:146:LEU:HB2	1.91	0.53
1:D:218:LEU:HD13	1:D:266:LEU:HD11	1.89	0.53
1:B:329:LEU:HB3	1:B:332:VAL:HB	1.91	0.52
1:D:67:PRO:HA	1:D:78:SER:HB2	1.91	0.52
1:C:23:LYS:O	1:C:27:GLU:HB2	2.09	0.52
1:C:406:ILE:HD11	1:C:449:PHE:HZ	1.74	0.52
1:B:231:SER:HB3	1:B:251:ALA:HB3	1.91	0.52
1:B:239:VAL:HG12	1:B:241:GLU:H	1.74	0.52
1:B:388:LYS:HA	1:B:467:TRP:H	1.74	0.52
1:C:431:ILE:HG12	1:C:451:GLY:HA3	1.92	0.52
1:B:72:LEU:O	1:B:76:VAL:HG23	2.10	0.51
1:D:303:VAL:HB	1:D:348:VAL:HG11	1.93	0.51
1:B:201:THR:OG1	1:B:255:VAL:O	2.18	0.51
1:A:345:GLU:HG2	1:A:346:GLU:HG3	1.92	0.51
1:B:314:PRO:HA	1:B:339:TYR:O	2.10	0.51
1:C:282:LYS:HE2	1:C:337:GLU:HG2	1.93	0.50
1:B:285:ILE:HG13	1:B:371:CMH:O	2.11	0.50
1:C:289:PHE:CZ	1:C:371:CMH:HB2	2.46	0.50
1:D:225:MET:SD	1:D:255:VAL:HG13	2.52	0.50
1:B:9:GLY:HA2	1:B:64:VAL:HB	1.94	0.50
1:D:232:ILE:HG12	1:D:250:MET:HG2	1.93	0.50
1:D:435:ILE:HG13	1:D:447:ALA:HB2	1.93	0.50
1:C:186:PHE:CZ	1:C:188:MET:HB2	2.47	0.50
1:C:5:ASN:ND2	1:C:246:ASP:OD1	2.32	0.50
1:D:360:ARG:HD3	1:D:362:ASP:HB2	1.93	0.50
1:D:363:LEU:HD13	1:D:369:ARG:HH11	1.75	0.50
1:A:230:ARG:NH2	6:B:1474:5GP:O2'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ILE:HD12	1:B:459:VAL:HG11	1.93	0.49
1:C:16:HIS:NE2	1:C:94:GLU:OE2	2.44	0.49
1:D:3:PHE:CE2	1:D:55:LYS:HE3	2.48	0.49
1:D:40:SER:O	1:D:44:GLY:HA2	2.13	0.49
1:A:99:GLN:HA	1:A:102:GLU:HG3	1.95	0.49
1:A:308:VAL:HG21	1:A:344:LEU:HD13	1.95	0.48
1:C:303:VAL:HG22	1:C:356:VAL:HG22	1.95	0.48
1:C:28:ILE:HG22	1:C:54:PHE:HB2	1.95	0.48
1:C:320:PHE:CZ	1:C:464:LEU:HD11	2.48	0.48
1:A:219:LYS:HE2	1:A:268:SER:O	2.14	0.48
1:B:234:TYR:HB3	1:B:239:VAL:HG21	1.95	0.48
1:B:363:LEU:HD13	1:B:364:PRO:HD2	1.96	0.48
1:D:367:THR:HG22	1:D:368:LEU:HG	1.95	0.48
1:A:110:PHE:HD1	1:A:355:ARG:HD2	1.77	0.48
1:B:24:VAL:O	1:B:28:ILE:HG22	2.14	0.48
1:A:328:ILE:HG22	1:A:389:LYS:HA	1.95	0.48
1:A:70:ALA:HA	1:A:73:ILE:HD12	1.94	0.48
1:D:282:LYS:O	1:D:374:GLY:HA3	2.14	0.48
1:D:15:ASP:OD1	1:D:16:HIS:ND1	2.47	0.48
1:B:160:PHE:CZ	1:D:98:THR:HG23	2.49	0.48
1:A:24:VAL:HG21	1:A:156:ALA:HB1	1.96	0.47
1:C:106:ILE:HG12	1:C:357:LEU:HD21	1.96	0.47
1:D:4:LYS:NZ	1:D:178:ILE:O	2.47	0.47
1:D:20:THR:HG23	1:D:156:ALA:HB2	1.95	0.47
1:D:427:GLU:HG2	1:D:460:ILE:HG13	1.94	0.47
5:C:1479:DXC:H161	5:C:1479:DXC:H212	1.54	0.47
1:D:10:ILE:HD13	1:D:21:LEU:HD23	1.96	0.47
1:B:212:VAL:HG23	1:B:242:ALA:HB3	1.96	0.47
1:C:131:ARG:NH2	5:C:1477:DXC:O4	2.41	0.47
1:B:152:ILE:HD11	1:B:164:GLU:HB2	1.97	0.47
5:C:1479:DXC:H19	5:C:1479:DXC:H203	1.74	0.47
1:D:80:ALA:HB1	1:D:112:ILE:HD12	1.96	0.47
1:B:187:LYS:HD2	1:B:273:LEU:HD11	1.97	0.47
1:B:397:VAL:O	1:B:456:ARG:N	2.45	0.47
1:B:49:ILE:N	5:B:1473:DXC:O3	2.47	0.47
1:C:316:LYS:HD3	1:C:329:LEU:HD21	1.97	0.46
1:D:109:HIS:CG	1:D:373:HIS:CE1	3.03	0.46
1:A:118:ILE:HB	1:A:153:PRO:HA	1.96	0.46
1:A:328:ILE:HG21	1:A:389:LYS:HD2	1.97	0.46
1:D:15:ASP:HA	1:D:18:LYS:HE2	1.97	0.46
1:C:156:ALA:N	2:C:1469:GDP:O6	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ILE:HD11	1:C:449:PHE:CZ	2.49	0.46
1:B:283:ILE:HD13	1:B:374:GLY:HA3	1.97	0.46
1:D:114:ILE:HG12	1:D:146:LEU:HD22	1.96	0.46
1:A:285:ILE:HG23	1:A:291:TYR:CD2	2.50	0.46
1:A:4:LYS:HG2	1:A:6:ILE:HD11	1.96	0.46
1:C:322:LYS:HG3	1:C:323:THR:H	1.80	0.46
1:C:36:LYS:CD	1:C:157:LYS:HA	2.46	0.46
1:D:91:ASP:HB3	1:D:94:GLU:HB2	1.97	0.46
1:D:11:PHE:CE2	1:D:66:ALA:HB1	2.51	0.46
1:A:285:ILE:HG12	1:A:291:TYR:CE2	2.51	0.46
1:B:393:ARG:HB2	1:B:461:LEU:HD23	1.97	0.46
1:C:296:LYS:H	1:C:313:VAL:HG12	1.80	0.46
1:A:431:ILE:HD11	1:A:450:SER:O	2.15	0.46
5:C:1475:DXC:H221	5:C:1475:DXC:H243	1.69	0.46
1:C:289:PHE:CE1	1:C:371:CMH:HB2	2.51	0.46
1:D:56:LEU:HD21	1:D:166:LYS:HG3	1.97	0.46
1:A:23:LYS:O	1:A:27:GLU:HG2	2.16	0.45
1:D:90:VAL:HG21	1:D:136:MET:HE1	1.97	0.45
1:C:35:ASP:HA	1:C:159:GLY:HA3	1.99	0.45
1:C:9:GLY:HA2	1:C:64:VAL:HB	1.97	0.45
1:A:314:PRO:O	1:A:328:ILE:HD12	2.17	0.45
1:A:196:ILE:HG23	1:A:197:LYS:H	1.81	0.45
1:D:116:VAL:HB	1:D:151:ILE:HG12	1.99	0.45
1:A:227:THR:HG21	1:A:255:VAL:HG22	1.99	0.45
1:A:456:ARG:O	1:A:458:LYS:NZ	2.32	0.45
1:B:122:ASP:HA	1:D:365:PRO:HD3	1.99	0.45
1:D:84:ASP:O	1:D:112:ILE:HG23	2.17	0.45
1:B:301:LEU:HD11	1:B:356:VAL:HG13	1.98	0.45
1:A:275:THR:HG22	1:A:347:LYS:HD2	1.98	0.44
1:B:130:LYS:HA	1:B:130:LYS:HD2	1.74	0.44
1:C:49:ILE:HD12	1:C:204:THR:HG21	1.99	0.44
1:B:312:ALA:HB1	1:B:340:CMH:SG	2.57	0.44
5:C:1478:DXC:H241	5:C:1478:DXC:H222	1.55	0.44
1:D:73:ILE:H	1:D:73:ILE:HG13	1.60	0.44
1:B:114:ILE:HD13	1:B:146:LEU:HD13	2.00	0.44
1:B:406:ILE:HD11	1:B:449:PHE:HZ	1.83	0.44
1:B:295:PRO:HB3	1:B:328:ILE:HD11	2.00	0.44
1:C:49:ILE:HG13	1:C:51:PHE:CD1	2.53	0.44
1:D:287:ASP:HB2	1:D:291:TYR:HE1	1.83	0.44
1:A:312:ALA:HB1	1:A:340:CMH:SG	2.58	0.44
1:C:293:LEU:HD22	1:C:371:CMH:CM	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ASN:HD22	1:D:243:LYS:HE3	1.82	0.43
1:C:28:ILE:CG2	1:C:54:PHE:HB2	2.48	0.43
1:D:405:VAL:HG11	1:D:444:LEU:HB3	2.00	0.43
1:A:110:PHE:HE1	1:A:355:ARG:HB3	1.82	0.43
1:A:85:LEU:HD13	1:A:172:THR:HG21	2.00	0.43
1:A:392:LEU:HA	1:A:461:LEU:O	2.17	0.43
1:C:180:ARG:HB3	1:C:244:ALA:HB3	2.00	0.43
1:C:405:VAL:HG22	1:C:446:THR:HG23	1.99	0.43
1:D:223:ILE:HD13	1:D:259:GLN:O	2.18	0.43
1:D:407:ASP:OD1	1:D:408:GLY:N	2.51	0.43
1:D:442:LYS:HA	1:D:442:LYS:HD3	1.79	0.43
1:A:313:VAL:CG2	1:A:341:ALA:HB3	2.43	0.43
1:B:89:VAL:HA	1:B:117:VAL:O	2.18	0.43
1:B:120:LYS:HD3	2:B:1469:GDP:C4	2.54	0.43
1:B:221:LEU:HG	1:B:222:PRO:HA	2.01	0.43
1:C:10:ILE:HD13	1:C:87:LEU:HB2	2.01	0.43
1:D:316:LYS:HB2	1:D:329:LEU:HD13	1.99	0.43
1:D:5:ASN:OD1	1:D:234:TYR:OH	2.27	0.43
1:A:406:ILE:HD11	1:A:449:PHE:CZ	2.54	0.43
1:B:360:ARG:O	1:B:369:ARG:HB3	2.19	0.43
1:A:317:LYS:HG2	1:A:326:ASN:OD1	2.19	0.43
1:B:82:ILE:HD13	1:B:206:THR:HG22	2.01	0.43
1:A:302:ASN:HB2	1:A:357:LEU:HB3	2.00	0.43
1:A:303:VAL:HG22	1:A:356:VAL:HG22	2.00	0.43
1:C:148:ASN:OD1	1:C:148:ASN:N	2.51	0.43
1:C:39:GLU:H	1:C:39:GLU:HG2	1.66	0.43
1:D:247:ARG:HD2	1:D:247:ARG:HA	1.76	0.43
1:A:105:LEU:HD22	1:A:109:HIS:HE1	1.84	0.42
1:A:406:ILE:HD11	1:A:449:PHE:HZ	1.83	0.42
1:A:186:PHE:HA	1:A:210:GLY:HA3	2.01	0.42
1:D:213:LYS:O	1:D:216:ASP:HB2	2.19	0.42
1:B:364:PRO:HA	1:B:365:PRO:HD3	1.80	0.42
1:C:313:VAL:HA	1:C:314:PRO:HD3	1.81	0.42
1:D:223:ILE:HD11	1:D:260:ILE:HG12	2.01	0.42
1:B:417:GLU:O	1:B:420:ILE:HG12	2.19	0.42
1:B:392:LEU:HA	1:B:461:LEU:O	2.20	0.42
1:B:88:ILE:HD11	1:B:107:LEU:HD12	2.01	0.42
1:C:364:PRO:HA	1:C:365:PRO:HD3	1.77	0.42
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.82	0.42
1:A:355:ARG:HG2	1:A:375:LEU:HD23	2.02	0.42
1:A:96:PRO:HB3	1:A:136:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASN:ND2	1:B:245:GLY:O	2.50	0.42
1:B:434:LYS:O	1:B:448:GLU:HG2	2.19	0.42
1:B:130:LYS:NZ	1:D:96:PRO:O	2.34	0.42
1:A:84:ASP:O	1:A:113:PRO:HG2	2.19	0.42
1:B:127:GLU:O	1:B:131:ARG:HG3	2.19	0.42
1:A:414:VAL:HG12	1:A:418:LYS:HE3	2.01	0.42
1:B:243:LYS:HB3	1:B:243:LYS:HE2	1.72	0.42
1:C:39:GLU:OE2	1:C:41:GLN:NE2	2.53	0.42
1:D:45:ILE:HB	1:D:47:ILE:HG13	2.00	0.42
1:A:340:CMH:HB2	1:A:342:PHE:CE2	2.55	0.42
1:A:407:ASP:OD1	1:A:408:GLY:N	2.53	0.42
1:A:431:ILE:HG13	1:A:450:SER:HB2	2.02	0.42
1:D:332:VAL:HG12	1:D:333:ILE:O	2.20	0.42
1:D:363:LEU:HA	1:D:364:PRO:HD3	1.84	0.42
1:D:426:ILE:HB	1:D:431:ILE:HG12	2.01	0.42
1:B:132:THR:HA	1:B:135:ILE:HD12	2.01	0.42
5:C:1480:DXC:H243	5:C:1480:DXC:H221	1.66	0.42
1:A:188:MET:HA	1:A:189:PRO:HD3	1.87	0.41
1:B:277:ASP:HB2	1:B:347:LYS:HE3	2.02	0.41
1:B:363:LEU:HA	1:B:363:LEU:HD22	1.92	0.41
1:C:277:ASP:O	1:C:344:LEU:HG	2.20	0.41
1:A:112:ILE:HA	1:A:113:PRO:HD2	1.84	0.41
1:D:5:ASN:OD1	1:D:60:ARG:HD3	2.19	0.41
1:A:293:LEU:HD13	1:A:329:LEU:HD23	2.02	0.41
1:A:57:GLU:HB3	1:A:58:ASN:H	1.56	0.41
1:B:291:TYR:HD1	1:B:333:ILE:HG22	1.85	0.41
1:C:298:LYS:HE3	1:C:311:VAL:HG22	2.01	0.41
1:D:362:ASP:O	1:D:364:PRO:HD3	2.20	0.41
1:D:431:ILE:HB	1:D:450:SER:O	2.21	0.41
1:C:49:ILE:HG12	5:C:1475:DXC:H222	2.01	0.41
1:D:392:LEU:HD11	1:D:460:ILE:HG23	2.01	0.41
1:B:155:SER:HB3	1:B:160:PHE:HB3	2.03	0.41
1:A:150:SER:HB2	1:A:168:LEU:HD21	2.01	0.41
1:B:308:VAL:HG21	1:B:348:VAL:HG21	2.03	0.41
1:C:1:MET:HB2	5:C:1476:DXC:C6	2.50	0.41
1:C:357:LEU:HA	1:C:357:LEU:HD12	1.89	0.41
1:A:301:LEU:HD23	1:A:344:LEU:HD21	2.02	0.41
1:C:340:CMH:HB2	1:C:342:PHE:CZ	2.55	0.41
1:C:36:LYS:HG2	1:C:37:LEU:N	2.36	0.41
1:D:186:PHE:HE1	1:D:207:ILE:HD13	1.85	0.41
1:D:285:ILE:HD11	1:D:291:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:LEU:O	1:D:386:ASN:OD1	2.39	0.41
1:A:296:LYS:HB3	1:A:296:LYS:HE2	1.80	0.41
1:C:190:LEU:HD22	1:C:203:VAL:HB	2.02	0.41
1:C:36:LYS:HG2	1:C:37:LEU:H	1.85	0.41
1:B:320:PHE:CE2	1:B:327:ILE:HD11	2.56	0.41
1:A:293:LEU:HD22	1:A:329:LEU:HD23	2.02	0.40
1:A:425:SER:HB2	1:A:460:ILE:HG13	2.04	0.40
1:B:363:LEU:HD22	1:B:364:PRO:HD2	2.03	0.40
1:D:163:ASP:OD1	1:D:163:ASP:N	2.54	0.40
1:D:219:LYS:HE3	1:D:224:ASN:OD1	2.21	0.40
1:A:329:LEU:HA	1:A:329:LEU:HD12	1.85	0.40
1:A:391:VAL:HG21	1:A:465:ARG:HD3	2.03	0.40
1:A:447:ALA:HB3	1:A:449:PHE:CE2	2.57	0.40
1:B:300:HIS:HB2	1:B:359:THR:O	2.22	0.40
1:B:15:ASP:N	2:B:1469:GDP:O1B	2.55	0.40
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.97	0.40
1:D:289:PHE:HA	1:D:289:PHE:HD1	1.76	0.40
1:D:38:PRO:HB3	1:D:42:LYS:HD2	2.02	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	440/482 (91%)	428 (97%)	12 (3%)	0	100	100
1	B	448/482 (93%)	433 (97%)	15 (3%)	0	100	100
1	C	465/482 (96%)	452 (97%)	13 (3%)	0	100	100
1	D	461/482 (96%)	440 (95%)	19 (4%)	2 (0%)	34	69
All	All	1814/1928 (94%)	1753 (97%)	59 (3%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	D	333	ILE

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	382/412 (93%)	350 (92%)	32 (8%)	11	36
1	B	388/412 (94%)	360 (93%)	28 (7%)	14	43
1	C	402/412 (98%)	372 (92%)	30 (8%)	13	41
1	D	398/412 (97%)	362 (91%)	36 (9%)	9	33
All	All	1570/1648 (95%)	1444 (92%)	126 (8%)	12	38

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	28	ILE
1	A	57	GLU
1	A	82	ILE
1	A	90	VAL
1	A	102	GLU
1	A	104	MET
1	A	148	ASN
1	A	168	LEU
1	A	194	PHE
1	A	212	VAL
1	A	235	PHE
1	A	250	MET
1	A	252	ILE
1	A	273	LEU
1	A	277	ASP
1	A	332	VAL
1	A	333	ILE
1	A	348	VAL
1	A	356	VAL

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Mol	Chain	Res	Type
1	A	362	ASP
1	A	366	THR
1	A	392	LEU
1	A	403	ARG
1	A	411	GLN
1	A	412	SER
1	A	417	GLU
1	A	424	ILE
1	A	435	ILE
1	A	441	THR
1	A	448	GLU
1	A	458	LYS
1	B	14	ILE
1	B	19	THR
1	B	27	GLU
1	B	28	ILE
1	B	49	ILE
1	B	123	ASN
1	B	136	MET
1	B	148	ASN
1	B	163	ASP
1	B	182	THR
1	B	212	VAL
1	B	238	SER
1	B	241	GLU
1	B	275	THR
1	B	287	ASP
1	B	291	TYR
1	B	308	VAL
1	B	319	THR
1	B	344	LEU
1	B	356	VAL
1	B	360	ARG
1	B	363	LEU
1	B	368	LEU
1	B	394	GLU
1	B	407	ASP
1	B	412	SER
1	B	431	ILE
1	B	453	VAL
1	C	-2	ARG
1	C	6	ILE

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Mol	Chain	Res	Type
1	C	14	ILE
1	C	45	ILE
1	C	65	ASP
1	C	114	ILE
1	C	142	SER
1	C	148	ASN
1	C	171	THR
1	C	188	MET
1	C	212	VAL
1	C	223	ILE
1	C	230	ARG
1	C	255	VAL
1	C	261	TYR
1	C	278	LYS
1	C	293	LEU
1	C	294	THR
1	C	297	MET
1	C	328	ILE
1	C	334	SER
1	C	348	VAL
1	C	359	THR
1	C	391	VAL
1	C	394	GLU
1	C	435	ILE
1	C	445	LEU
1	C	446	THR
1	C	456	ARG
1	C	459	VAL
1	D	16	HIS
1	D	31	THR
1	D	32	SER
1	D	36	LYS
1	D	41	GLN
1	D	43	ARG
1	D	46	THR
1	D	49	ILE
1	D	56	LEU
1	D	78	SER
1	D	90	VAL
1	D	128	GLU
1	D	139	ILE
1	D	143	THR

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Mol	Chain	Res	Type
1	D	162	VAL
1	D	220	VAL
1	D	226	SER
1	D	227	THR
1	D	235	PHE
1	D	237	GLU
1	D	247	ARG
1	D	275	THR
1	D	289	PHE
1	D	333	ILE
1	D	355	ARG
1	D	361	LEU
1	D	362	ASP
1	D	368	LEU
1	D	383	LYS
1	D	386	ASN
1	D	387	ILE
1	D	414	VAL
1	D	435	ILE
1	D	453	VAL
1	D	457	ASP
1	D	465	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	292	ASN
1	D	373	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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
1	CMH	D	371	1	5,7,8	0.61	0	1,7,9	0.57	0
1	CMH	C	371	1	5,7,8	0.61	0	1,7,9	0.54	0
1	CMH	A	264	1	5,7,8	0.57	0	1,7,9	0.02	0
1	CMH	C	264	1	5,7,8	0.59	0	1,7,9	0.73	0
1	CMH	D	340	1	5,7,8	0.58	0	1,7,9	0.19	0
1	CMH	B	340	1	5,7,8	0.75	0	1,7,9	0.32	0
1	CMH	C	340	1	5,7,8	0.72	0	1,7,9	0.53	0
1	CMH	A	338	1	5,7,8	0.63	0	1,7,9	0.65	0
1	CMH	B	371	1	5,7,8	0.55	0	1,7,9	0.88	0
1	CMH	D	264	1	5,7,8	0.57	0	1,7,9	0.60	0
1	CMH	C	338	1	5,7,8	0.57	0	1,7,9	0.72	0
1	CMH	A	371	1	5,7,8	0.54	0	1,7,9	0.56	0
1	CMH	A	340	1	5,7,8	0.71	0	1,7,9	0.62	0
1	CMH	B	338	1	5,7,8	0.69	0	1,7,9	0.65	0
1	CMH	B	264	1	5,7,8	0.60	0	1,7,9	0.96	0
1	CMH	D	338	1	5,7,8	0.58	0	1,7,9	1.00	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CMH	D	371	1	-	0/0/6/8	-
1	CMH	C	371	1	-	0/0/6/8	-
1	CMH	A	264	1	-	0/0/6/8	-
1	CMH	C	264	1	-	0/0/6/8	-
1	CMH	D	340	1	-	0/0/6/8	-
1	CMH	B	340	1	-	0/0/6/8	-
1	CMH	C	340	1	-	0/0/6/8	-
1	CMH	A	338	1	-	0/0/6/8	-
1	CMH	B	371	1	-	0/0/6/8	-
1	CMH	D	264	1	-	0/0/6/8	-
1	CMH	C	338	1	-	0/0/6/8	-
1	CMH	A	371	1	-	0/0/6/8	-
1	CMH	A	340	1	-	0/0/6/8	-
1	CMH	B	338	1	-	0/0/6/8	-
1	CMH	B	264	1	-	0/0/6/8	-
1	CMH	D	338	1	-	0/0/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	371	CMH	3	0
1	D	340	CMH	1	0
1	B	340	CMH	2	0
1	C	340	CMH	3	0
1	B	371	CMH	2	0
1	C	338	CMH	1	0
1	A	340	CMH	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 3 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	$\# Z > 2$
5	DXC	C	1479	-	28,31,31	1.71	6 (21%)	46,49,49	1.52	8 (17%)
4	SO4	C	1474	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	1473	-	4,4,4	0.14	0	6,6,6	0.04	0
5	DXC	C	1476	-	28,31,31	1.73	6 (21%)	46,49,49	1.47	8 (17%)
2	GDP	A	1469	3	24,30,30	1.19	2 (8%)	31,47,47	1.98	8 (25%)
5	DXC	C	1480	-	28,31,31	1.75	6 (21%)	46,49,49	1.54	10 (21%)
5	DXC	B	1473	-	28,31,31	1.72	6 (21%)	46,49,49	1.43	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DXC	C	1478	-	28,31,31	1.71	6 (21%)	46,49,49	1.66	9 (19%)
5	DXC	C	1475	-	28,31,31	1.76	6 (21%)	46,49,49	1.58	10 (21%)
4	SO4	C	1472	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	1471	-	4,4,4	0.15	0	6,6,6	0.04	0
2	GDP	C	1469	3	24,30,30	1.20	2 (8%)	31,47,47	2.01	8 (25%)
5	DXC	C	1477	-	28,31,31	1.72	6 (21%)	46,49,49	1.47	8 (17%)
2	GDP	B	1469	3	24,30,30	1.19	2 (8%)	31,47,47	1.98	9 (29%)
4	SO4	B	1472	-	4,4,4	0.14	0	6,6,6	0.04	0
6	5GP	B	1474	-	22,26,26	0.58	0	27,40,40	1.75	5 (18%)
4	SO4	C	1471	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	1481	-	4,4,4	0.13	0	6,6,6	0.05	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	DXC	C	1479	-	-	6/7/71/71	0/4/4/4
5	DXC	C	1478	-	-	2/7/71/71	0/4/4/4
5	DXC	C	1476	-	-	2/7/71/71	0/4/4/4
2	GDP	A	1469	3	-	6/12/32/32	0/3/3/3
5	DXC	C	1480	-	-	4/7/71/71	0/4/4/4
5	DXC	B	1473	-	-	0/7/71/71	0/4/4/4
6	5GP	B	1474	-	-	3/6/26/26	0/3/3/3
5	DXC	C	1475	-	-	0/7/71/71	0/4/4/4
5	DXC	C	1477	-	-	2/7/71/71	0/4/4/4
2	GDP	C	1469	3	-	5/12/32/32	0/3/3/3
2	GDP	B	1469	3	-	6/12/32/32	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1469	GDP	C6-C5	4.29	1.48	1.41
2	B	1469	GDP	C6-C5	4.23	1.48	1.41
2	A	1469	GDP	C6-C5	4.21	1.48	1.41
5	C	1480	DXC	C12-C13	-4.12	1.48	1.54
5	C	1475	DXC	C12-C13	-4.02	1.48	1.54
5	C	1477	DXC	C12-C13	-3.92	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1473	DXC	C12-C13	-3.82	1.48	1.54
5	C	1478	DXC	C12-C13	-3.80	1.48	1.54
5	C	1476	DXC	C12-C13	-3.78	1.48	1.54
5	C	1479	DXC	C12-C13	-3.69	1.48	1.54
5	C	1476	DXC	C12-C11	-3.27	1.49	1.55
5	C	1476	DXC	C18-C4	-3.22	1.48	1.54
5	C	1475	DXC	C20-C12	-3.20	1.49	1.54
5	C	1477	DXC	C18-C4	-3.19	1.48	1.54
5	C	1479	DXC	C20-C12	-3.18	1.49	1.54
5	C	1478	DXC	C20-C12	-3.17	1.49	1.54
5	B	1473	DXC	C18-C4	-3.12	1.48	1.54
5	C	1479	DXC	C12-C11	-3.11	1.50	1.55
5	B	1473	DXC	C20-C12	-3.10	1.49	1.54
5	C	1475	DXC	C18-C4	-3.09	1.48	1.54
5	C	1480	DXC	C18-C4	-3.08	1.49	1.54
5	C	1479	DXC	C18-C4	-3.04	1.49	1.54
5	C	1480	DXC	C12-C11	-3.02	1.50	1.55
5	C	1475	DXC	C12-C11	-3.01	1.50	1.55
5	C	1476	DXC	C20-C12	-3.00	1.49	1.54
5	C	1480	DXC	C20-C12	-2.99	1.49	1.54
5	C	1478	DXC	C18-C4	-2.99	1.49	1.54
5	C	1477	DXC	C12-C11	-2.98	1.50	1.55
5	B	1473	DXC	O1-C13	-2.95	1.38	1.43
5	C	1480	DXC	O1-C13	-2.94	1.38	1.43
5	C	1475	DXC	O1-C13	-2.93	1.38	1.43
5	C	1478	DXC	O1-C13	-2.87	1.38	1.43
5	C	1477	DXC	C20-C12	-2.87	1.49	1.54
5	C	1479	DXC	O1-C13	-2.85	1.38	1.43
5	C	1477	DXC	O1-C13	-2.83	1.38	1.43
5	C	1476	DXC	O1-C13	-2.81	1.38	1.43
5	B	1473	DXC	C12-C11	-2.80	1.50	1.55
5	C	1478	DXC	C12-C11	-2.72	1.50	1.55
5	C	1476	DXC	C4-C10	-2.61	1.51	1.56
5	C	1477	DXC	C4-C10	-2.55	1.51	1.56
5	B	1473	DXC	C4-C10	-2.45	1.51	1.56
2	C	1469	GDP	C5-C4	2.45	1.47	1.40
2	A	1469	GDP	C5-C4	2.44	1.47	1.40
5	C	1478	DXC	C4-C10	-2.41	1.51	1.56
2	B	1469	GDP	C5-C4	2.40	1.47	1.40
5	C	1475	DXC	C4-C10	-2.37	1.51	1.56
5	C	1480	DXC	C4-C10	-2.32	1.51	1.56
5	C	1479	DXC	C4-C10	-2.25	1.52	1.56

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1478	DXC	C22-C21-C19	-5.19	107.73	114.72
2	B	1469	GDP	C2-N3-C4	4.99	121.05	115.36
2	A	1469	GDP	C2-N3-C4	4.94	120.99	115.36
2	C	1469	GDP	C2-N3-C4	4.93	120.98	115.36
6	B	1474	5GP	N3-C2-N1	-4.58	121.12	127.22
6	B	1474	5GP	C2-N3-C4	4.11	120.06	115.36
5	C	1475	DXC	C22-C21-C19	-4.11	109.18	114.72
2	A	1469	GDP	C6-N1-C2	4.06	122.39	115.93
2	C	1469	GDP	C6-N1-C2	4.02	122.32	115.93
2	B	1469	GDP	C6-N1-C2	4.02	122.32	115.93
2	C	1469	GDP	C6-C5-C4	-3.96	117.02	120.80
2	B	1469	GDP	C5-C6-N1	-3.94	118.05	123.43
2	A	1469	GDP	C5-C6-N1	-3.93	118.06	123.43
2	C	1469	GDP	C5-C6-N1	-3.91	118.08	123.43
2	A	1469	GDP	C6-C5-C4	-3.89	117.08	120.80
2	B	1469	GDP	C6-C5-C4	-3.85	117.13	120.80
2	C	1469	GDP	PA-O3A-PB	-3.75	119.95	132.83
5	C	1480	DXC	C22-C21-C19	-3.72	109.71	114.72
5	C	1479	DXC	C8-C9-C10	3.62	114.98	110.49
5	C	1478	DXC	C11-C9-C10	-3.51	104.39	109.09
5	C	1476	DXC	C18-C4-C5	-3.41	102.76	108.26
5	C	1478	DXC	C8-C9-C10	3.41	114.72	110.49
5	C	1476	DXC	C8-C9-C10	3.38	114.68	110.49
2	B	1469	GDP	N3-C2-N1	-3.37	122.73	127.22
5	C	1477	DXC	C18-C4-C5	-3.37	102.83	108.26
2	A	1469	GDP	N3-C2-N1	-3.37	122.73	127.22
5	C	1479	DXC	C18-C4-C5	-3.31	102.93	108.26
2	C	1469	GDP	N3-C2-N1	-3.31	122.81	127.22
2	A	1469	GDP	PA-O3A-PB	-3.25	121.68	132.83
5	C	1480	DXC	C18-C4-C5	-3.25	103.03	108.26
5	C	1475	DXC	C18-C4-C5	-3.23	103.06	108.26
5	C	1479	DXC	C12-C17-C19	-3.19	115.69	119.50
5	C	1475	DXC	C8-C9-C10	3.16	114.41	110.49
6	B	1474	5GP	C6-N1-C2	3.13	120.90	115.93
5	B	1473	DXC	C10-C14-C13	-3.12	110.18	114.30
5	C	1475	DXC	C11-C9-C10	-3.12	104.92	109.09
5	C	1478	DXC	C18-C4-C5	-3.09	103.28	108.26
5	C	1477	DXC	C8-C9-C10	3.06	114.28	110.49
5	B	1473	DXC	C18-C4-C5	-3.02	103.39	108.26
5	C	1477	DXC	C10-C4-C3	2.88	112.62	108.58
5	C	1476	DXC	C10-C4-C3	2.87	112.61	108.58
2	C	1469	GDP	C4-C5-N7	-2.86	106.42	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1477	DXC	C14-C10-C4	-2.86	110.78	113.73
6	B	1474	5GP	C5-C6-N1	-2.86	119.52	123.43
5	B	1473	DXC	C22-C21-C19	-2.81	110.94	114.72
2	B	1469	GDP	PA-O3A-PB	-2.81	123.19	132.83
5	C	1479	DXC	C18-C4-C3	-2.78	105.64	110.36
2	A	1469	GDP	C4-C5-N7	-2.77	106.52	109.40
5	C	1479	DXC	C11-C9-C10	-2.75	105.40	109.09
5	C	1480	DXC	C8-C9-C10	2.72	113.87	110.49
6	B	1474	5GP	O3P-P-O5'	-2.71	99.51	106.73
2	B	1469	GDP	C4-C5-N7	-2.70	106.59	109.40
5	C	1480	DXC	C10-C4-C3	2.69	112.36	108.58
2	C	1469	GDP	C3'-C2'-C1'	2.65	104.97	100.98
5	C	1480	DXC	C18-C4-C3	-2.64	105.88	110.36
5	C	1477	DXC	C11-C9-C10	-2.63	105.57	109.09
5	C	1478	DXC	C10-C4-C3	2.63	112.27	108.58
5	C	1475	DXC	C10-C14-C13	-2.61	110.85	114.30
5	C	1475	DXC	C18-C4-C3	-2.61	105.94	110.36
5	C	1476	DXC	C18-C4-C3	-2.55	106.03	110.36
5	C	1476	DXC	C11-C9-C10	-2.55	105.68	109.09
2	B	1469	GDP	C3'-C2'-C1'	2.54	104.80	100.98
5	B	1473	DXC	C8-C9-C10	2.53	113.64	110.49
5	C	1477	DXC	C17-C12-C11	2.49	102.60	100.09
5	C	1475	DXC	C10-C4-C3	2.48	112.06	108.58
5	C	1479	DXC	C21-C22-C23	-2.46	108.29	113.59
5	C	1475	DXC	C24-C19-C21	-2.45	106.52	110.36
5	C	1478	DXC	C24-C19-C21	-2.43	106.56	110.36
5	C	1479	DXC	C10-C4-C3	2.41	111.96	108.58
5	B	1473	DXC	C18-C4-C3	-2.40	106.30	110.36
5	C	1477	DXC	C18-C4-C3	-2.35	106.38	110.36
5	C	1478	DXC	C17-C12-C11	2.33	102.44	100.09
5	C	1480	DXC	C11-C9-C10	-2.32	105.98	109.09
2	A	1469	GDP	C3'-C2'-C1'	2.30	104.45	100.98
5	C	1479	DXC	C17-C12-C11	2.28	102.39	100.09
5	C	1480	DXC	C10-C14-C13	-2.21	111.38	114.30
5	B	1473	DXC	C11-C9-C10	-2.21	106.13	109.09
5	B	1473	DXC	C24-C19-C21	-2.19	106.92	110.36
5	C	1480	DXC	C17-C12-C11	2.19	102.30	100.09
5	C	1480	DXC	C11-C12-C13	-2.18	105.38	107.40
5	C	1476	DXC	C14-C10-C4	-2.17	111.48	113.73
5	C	1480	DXC	C21-C22-C23	-2.12	109.02	113.59
5	C	1478	DXC	C18-C4-C3	-2.12	106.77	110.36
5	C	1476	DXC	C7-C8-C9	-2.11	108.67	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	C	1475	DXC	C17-C12-C11	2.10	102.21	100.09
5	C	1476	DXC	C4-C10-C9	-2.09	110.23	112.42
2	B	1469	GDP	O3B-PB-O3A	2.08	111.59	104.64
5	C	1478	DXC	C20-C12-C11	2.07	114.45	111.21
5	C	1477	DXC	C10-C14-C13	-2.07	111.57	114.30
5	B	1473	DXC	C10-C4-C3	2.06	111.48	108.58
5	C	1475	DXC	O1-C13-C12	-2.02	107.62	111.03

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1469	GDP	C5'-O5'-PA-O1A
2	A	1469	GDP	C5'-O5'-PA-O2A
2	C	1469	GDP	C5'-O5'-PA-O1A
2	C	1469	GDP	C5'-O5'-PA-O2A
2	C	1469	GDP	O4'-C4'-C5'-O5'
2	B	1469	GDP	C5'-O5'-PA-O1A
2	B	1469	GDP	C5'-O5'-PA-O2A
6	B	1474	5GP	C3'-C4'-C5'-O5'
5	C	1479	DXC	C12-C17-C19-C24
5	C	1479	DXC	C24-C19-C21-C22
5	C	1479	DXC	C16-C17-C19-C24
5	C	1479	DXC	C12-C17-C19-C21
5	C	1476	DXC	C24-C19-C21-C22
5	C	1479	DXC	C16-C17-C19-C21
2	C	1469	GDP	C3'-C4'-C5'-O5'
5	C	1479	DXC	C17-C19-C21-C22
5	C	1477	DXC	C24-C19-C21-C22
5	C	1476	DXC	C17-C19-C21-C22
5	C	1477	DXC	C17-C19-C21-C22
2	A	1469	GDP	O4'-C4'-C5'-O5'
2	A	1469	GDP	C3'-C4'-C5'-O5'
6	B	1474	5GP	O4'-C4'-C5'-O5'
2	B	1469	GDP	PA-O3A-PB-O1B
5	C	1480	DXC	C12-C17-C19-C24
2	B	1469	GDP	PA-O3A-PB-O3B
2	B	1469	GDP	C5'-O5'-PA-O3A
5	C	1480	DXC	C12-C17-C19-C21
5	C	1480	DXC	C16-C17-C19-C24
5	C	1480	DXC	C16-C17-C19-C21
6	B	1474	5GP	C5'-O5'-P-O1P

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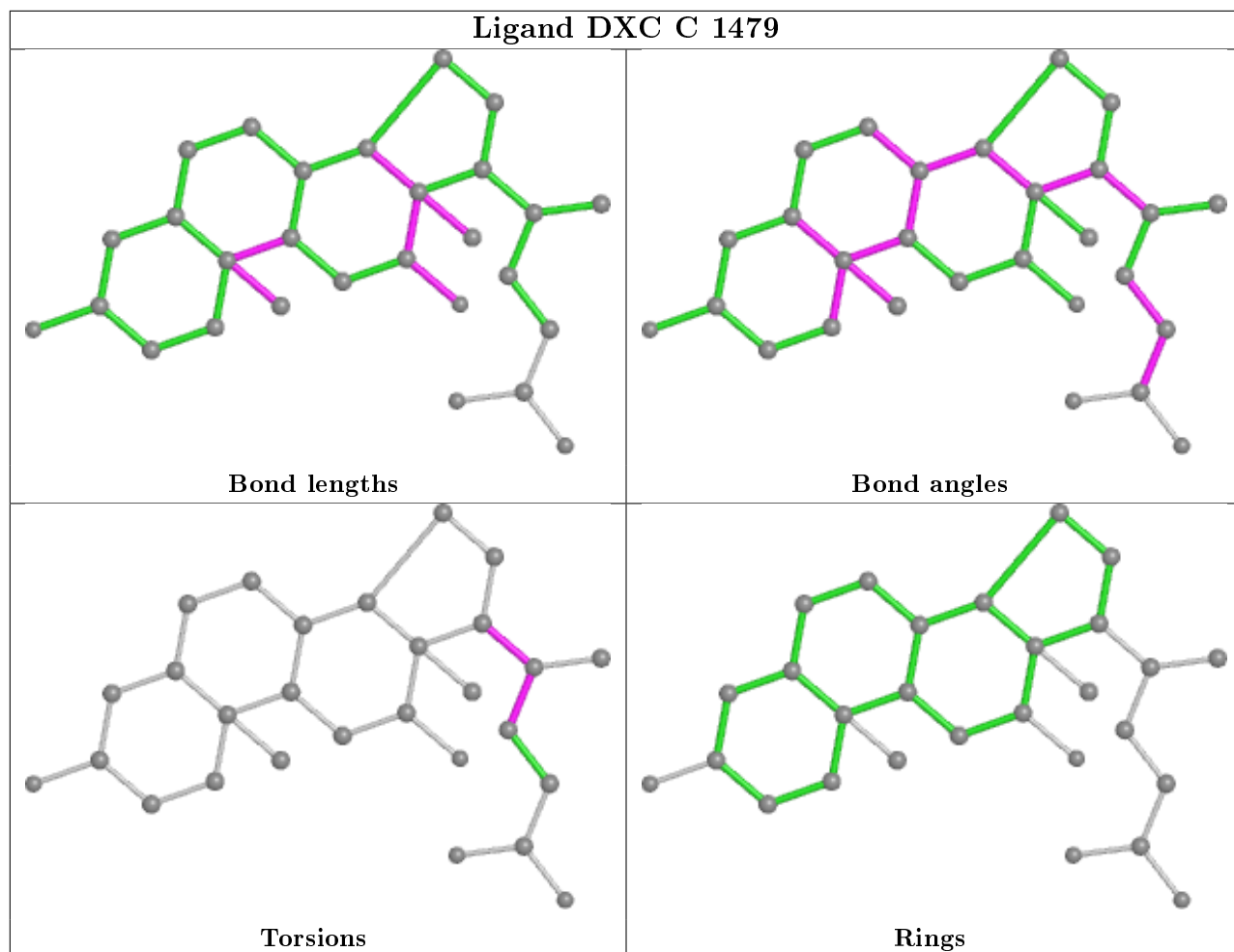
Mol	Chain	Res	Type	Atoms
2	B	1469	GDP	PB-O3A-PA-O2A
5	C	1478	DXC	C17-C19-C21-C22
5	C	1478	DXC	C12-C17-C19-C24
2	A	1469	GDP	C5'-O5'-PA-O3A
2	C	1469	GDP	C5'-O5'-PA-O3A
2	A	1469	GDP	PB-O3A-PA-O2A

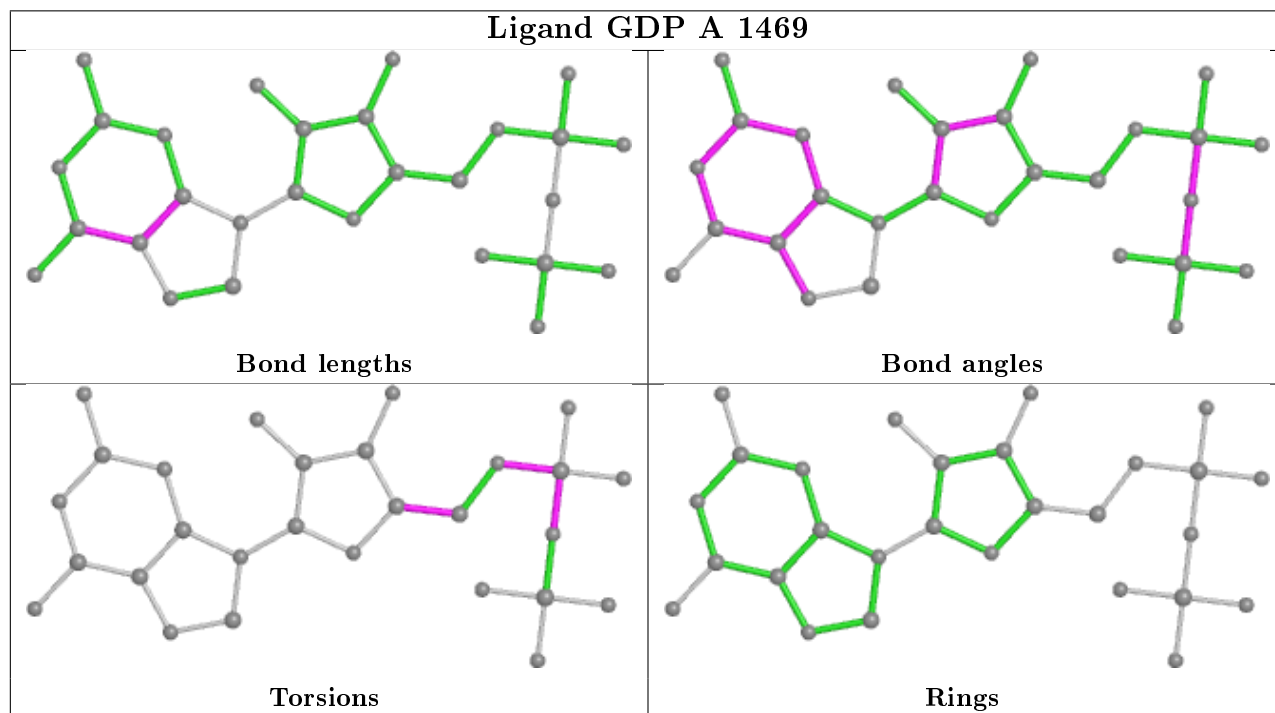
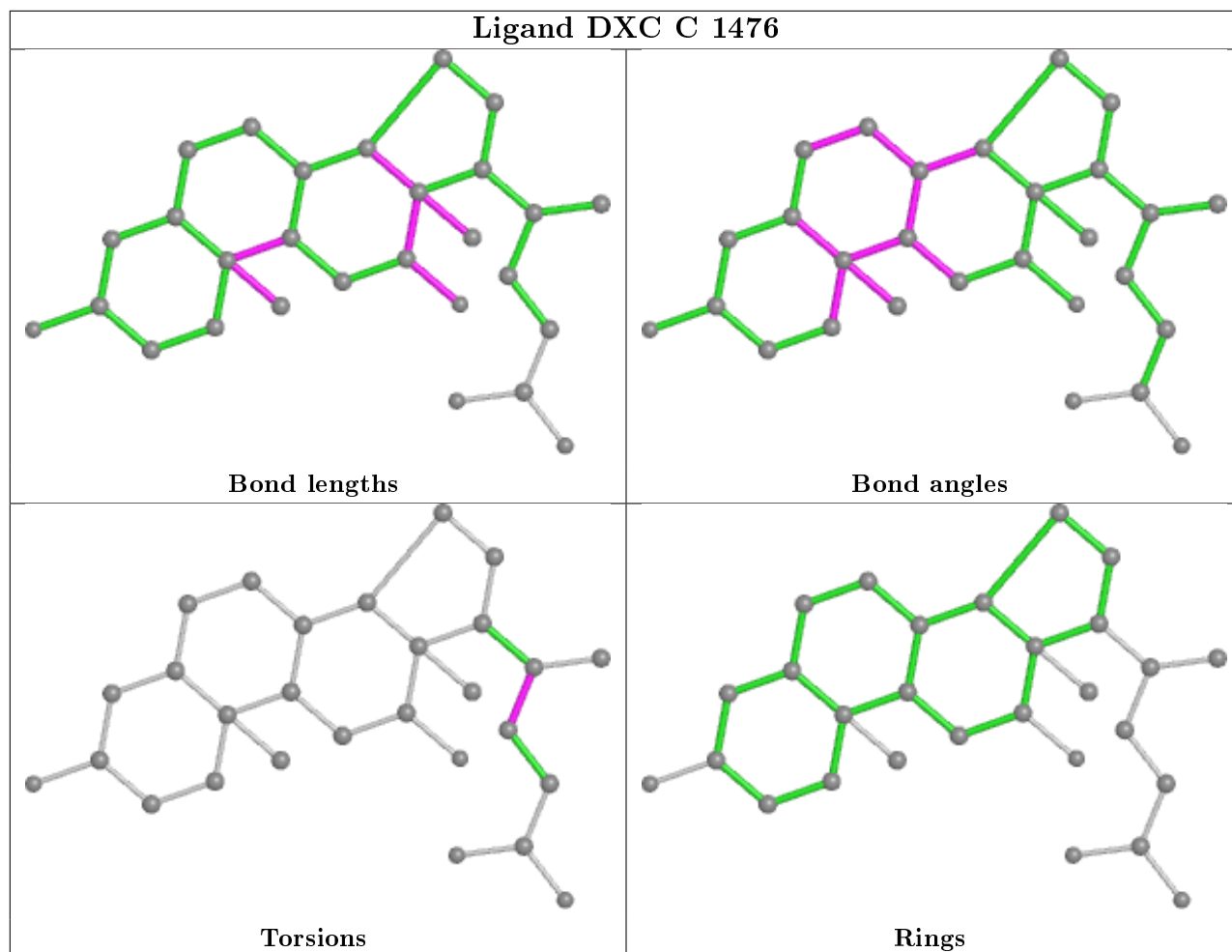
There are no ring outliers.

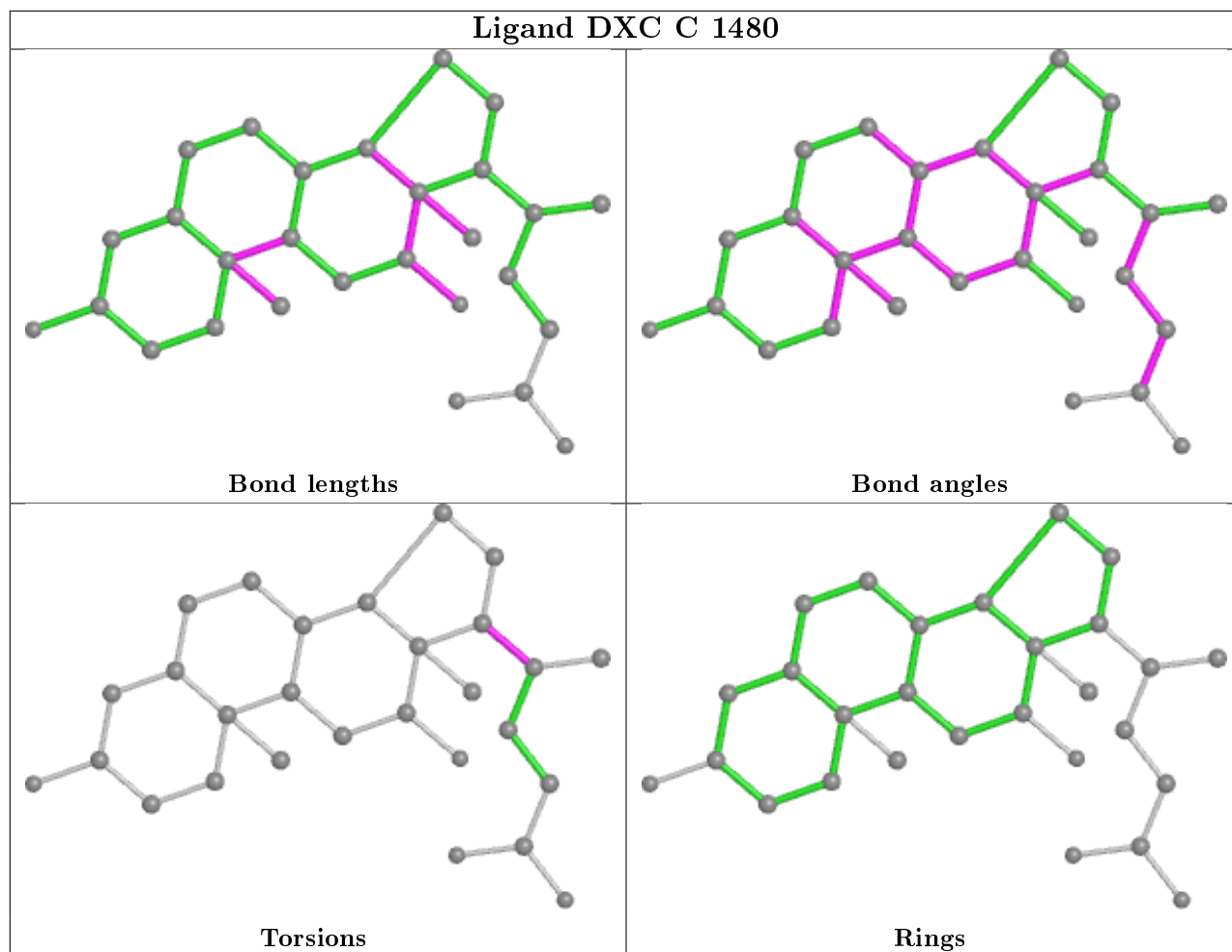
12 monomers are involved in 18 short contacts:

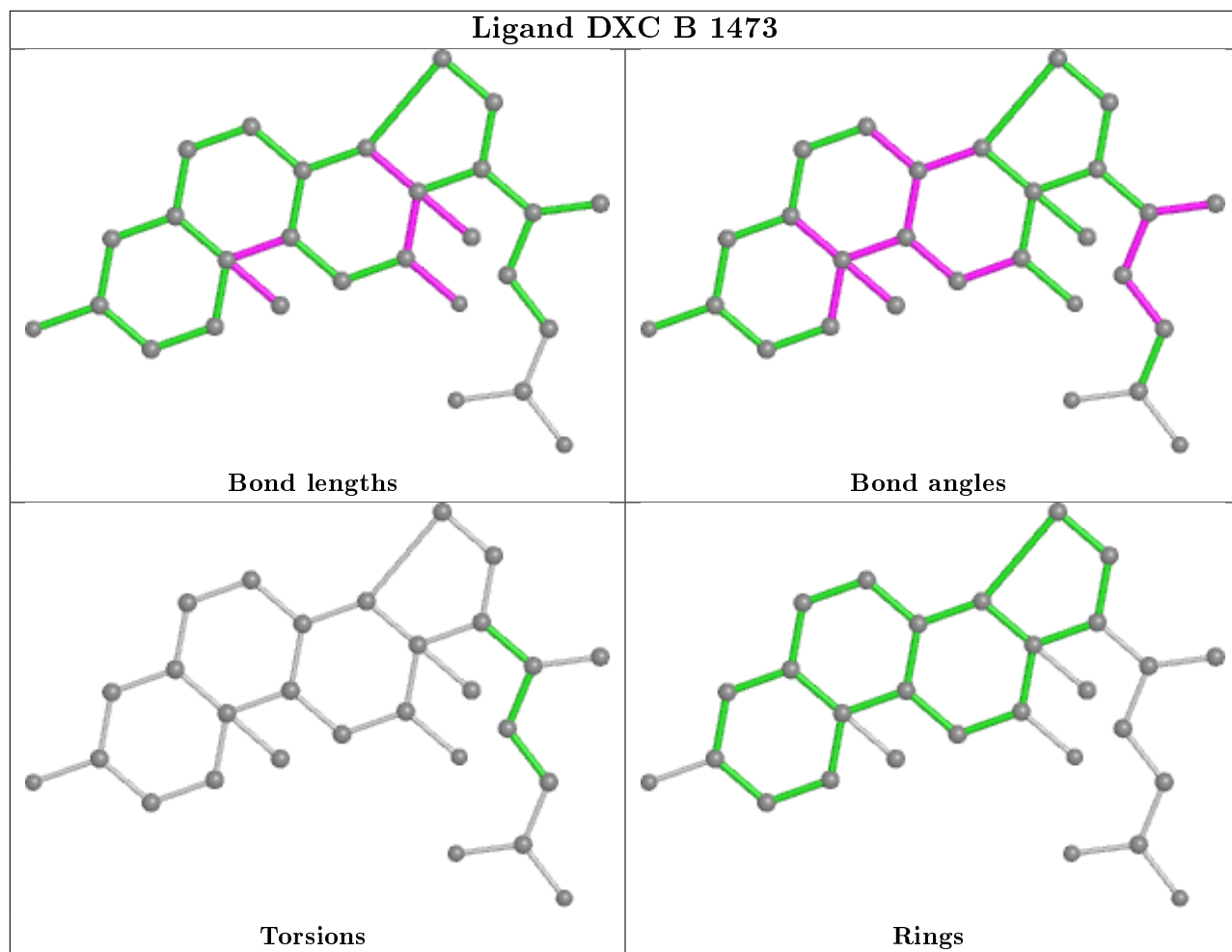
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1479	DXC	2	0
5	C	1476	DXC	2	0
5	C	1480	DXC	1	0
5	B	1473	DXC	1	0
5	C	1478	DXC	1	0
5	C	1475	DXC	3	0
4	B	1471	SO4	1	0
2	C	1469	GDP	1	0
5	C	1477	DXC	1	0
2	B	1469	GDP	2	0
4	B	1472	SO4	1	0
6	B	1474	5GP	2	0

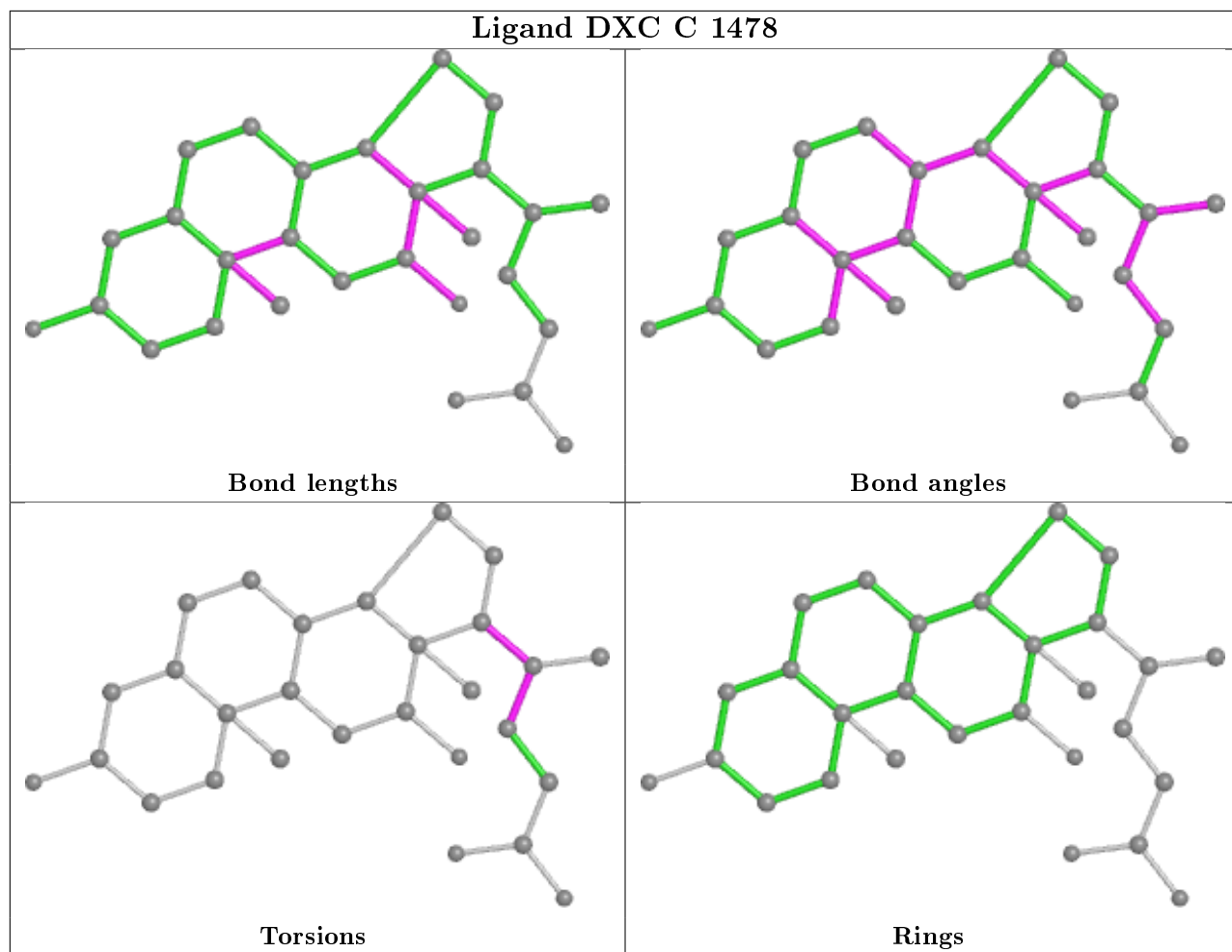
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

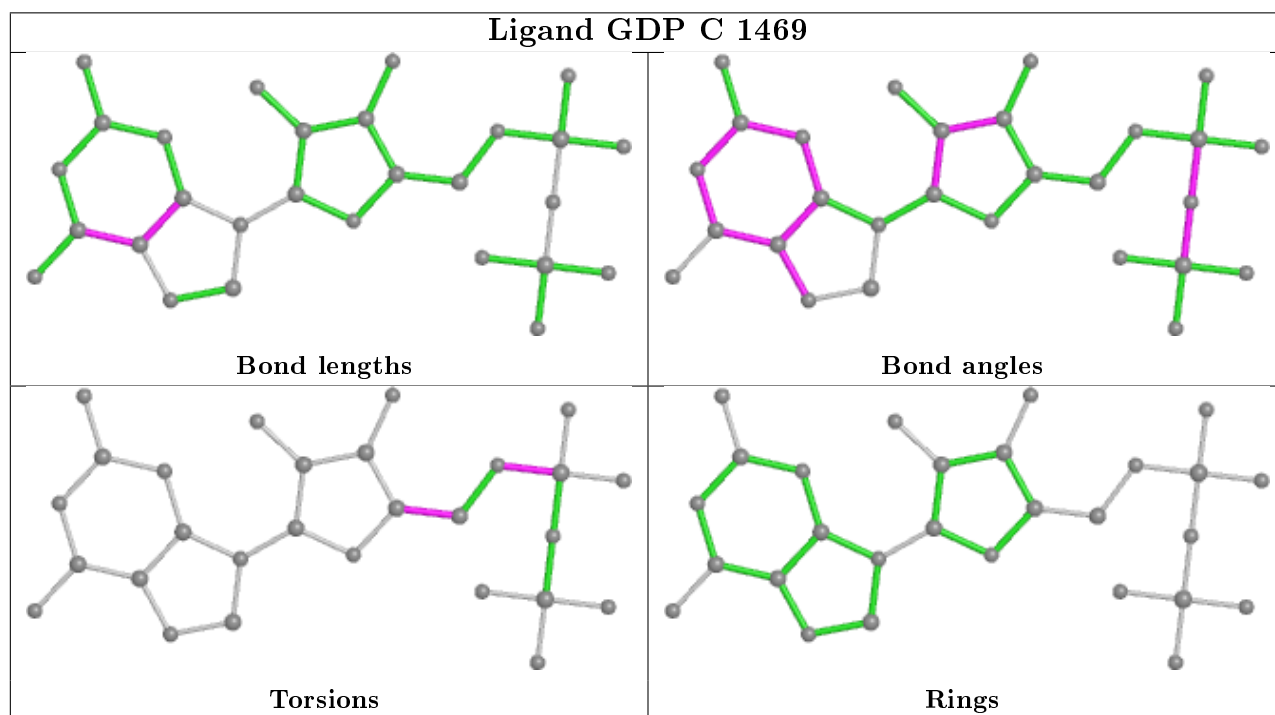
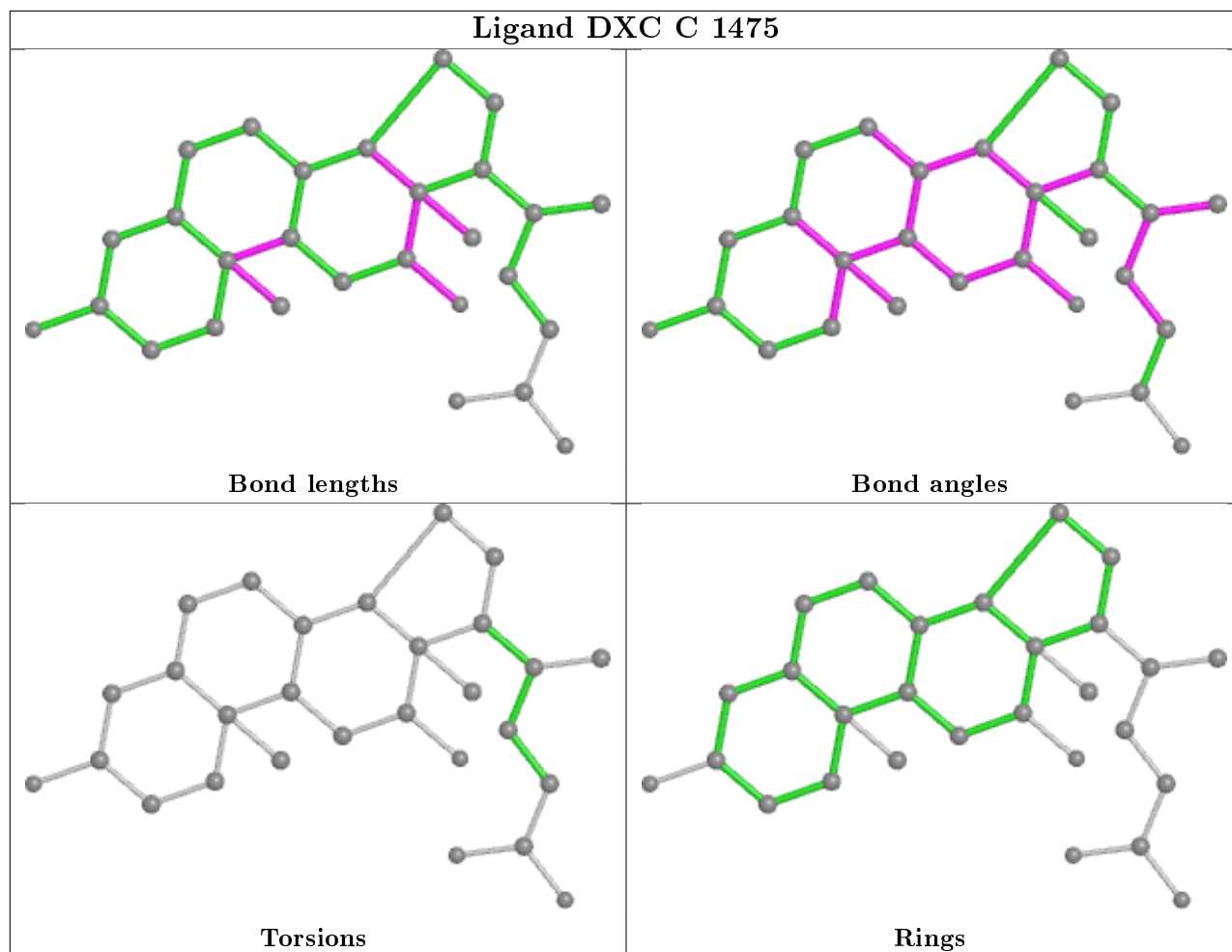


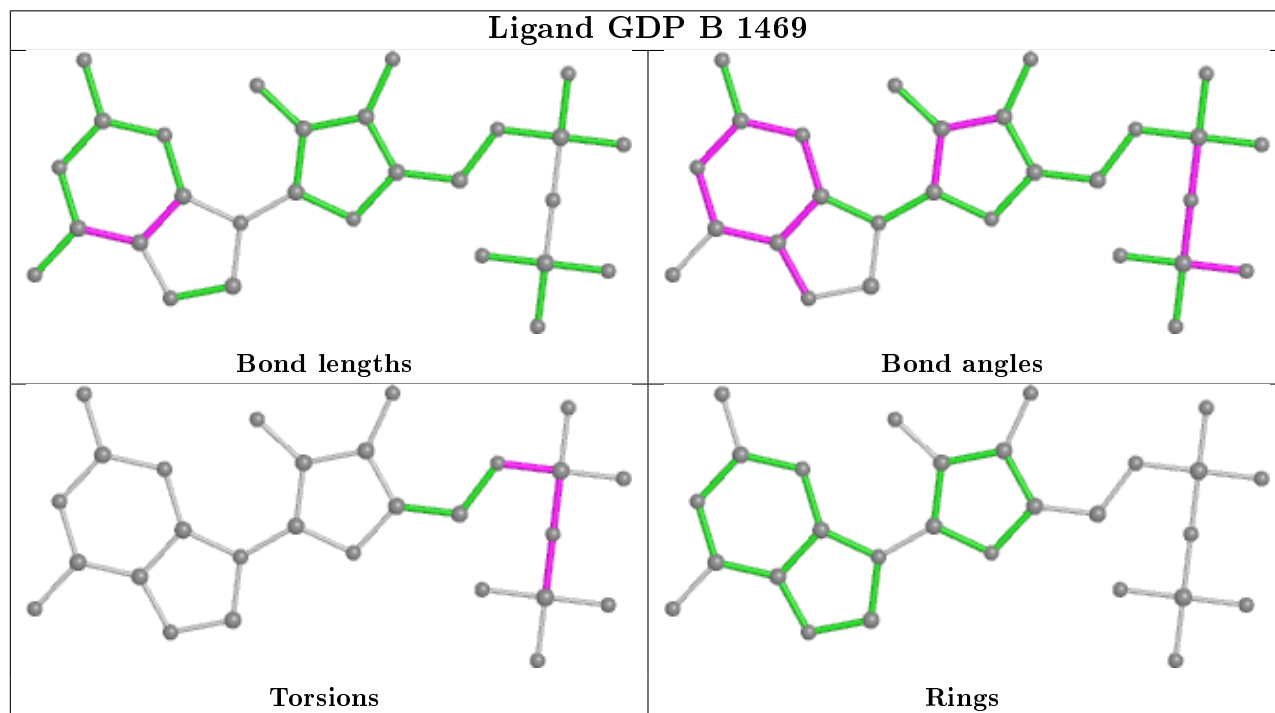
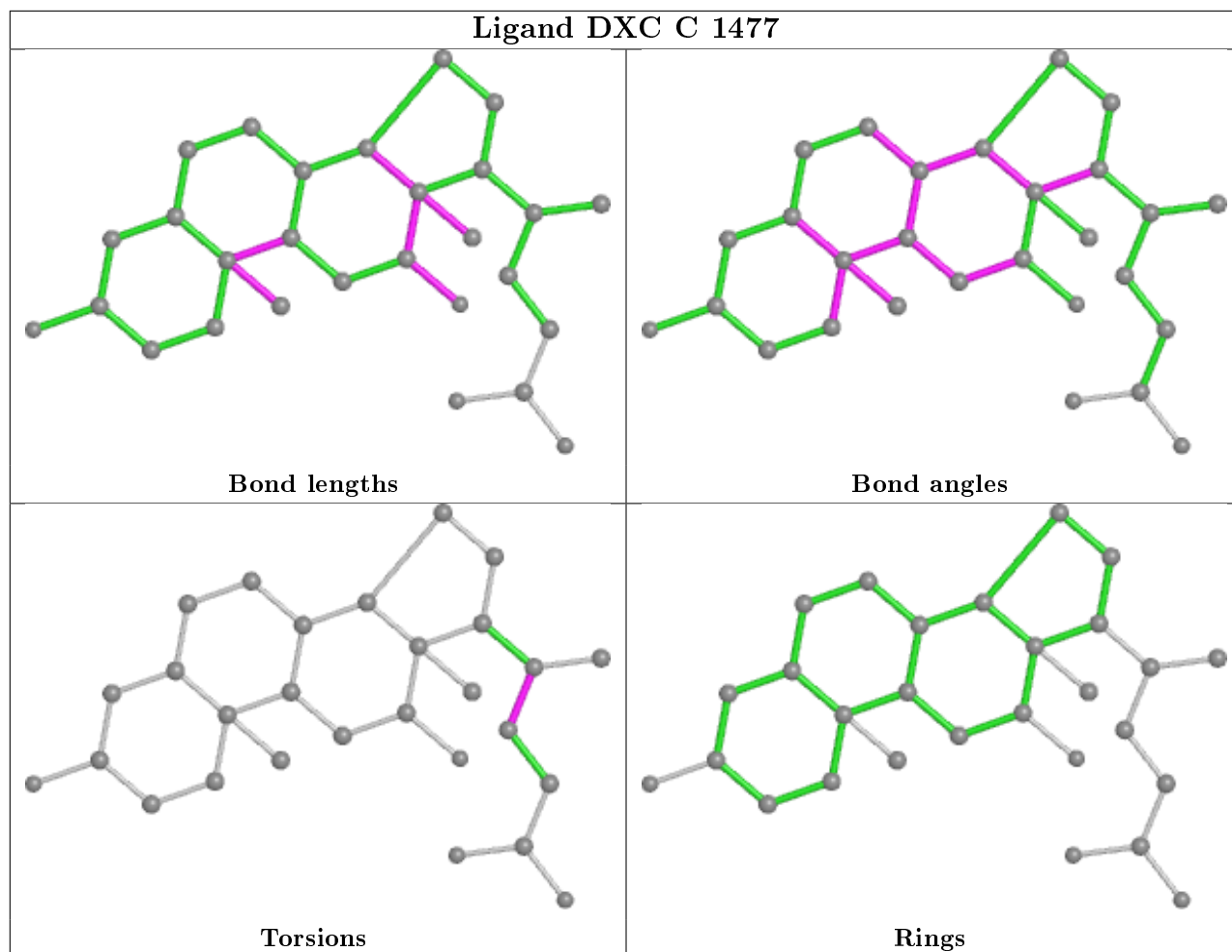


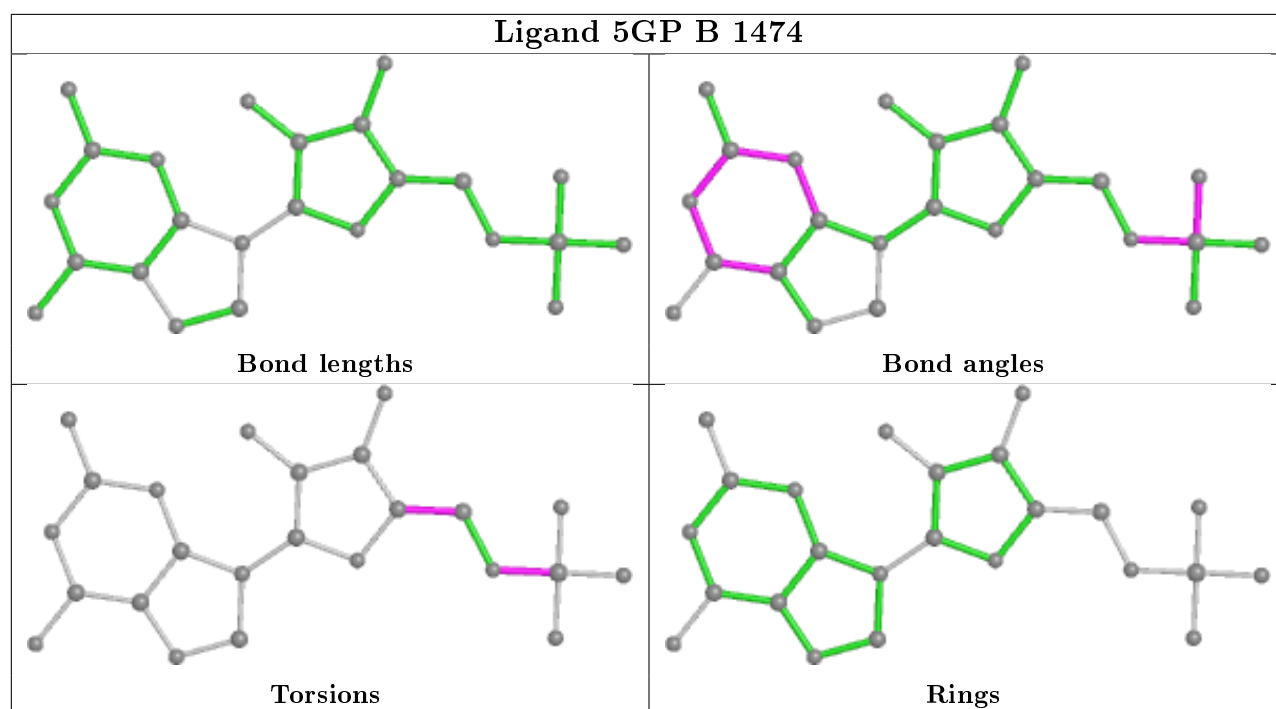












5.7 Other polymers [i](#)

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	444/482 (92%)	0.67	58 (13%) 3 1	72, 154, 219, 301	0
1	B	452/482 (93%)	0.87	73 (16%) 1 0	54, 109, 284, 316	0
1	C	467/482 (96%)	0.17	19 (4%) 37 15	53, 88, 179, 222	0
1	D	463/482 (96%)	1.44	131 (28%) 0 0	101, 187, 277, 317	0
All	All	1826/1928 (94%)	0.79	281 (15%) 2 0	53, 139, 266, 317	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	THR	16.3
1	D	453	VAL	12.2
1	B	439	PHE	10.9
1	D	441	THR	10.5
1	B	441	THR	10.5
1	B	445	LEU	9.7
1	B	460	ILE	9.6
1	D	442	LYS	9.6
1	B	450	SER	9.3
1	B	432	VAL	9.0
1	D	401	LYS	8.8
1	B	330	ASN	8.8
1	D	406	ILE	8.8
1	B	461	LEU	8.8
1	D	426	ILE	8.7
1	D	399	ILE	8.5
1	D	439	PHE	8.5
1	A	196	ILE	8.4
1	B	428	GLY	8.4
1	D	412	SER	8.2
1	D	438	THR	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	197	LYS	8.0
1	B	396	LYS	8.0
1	B	424	ILE	7.4
1	D	400	ASP	7.3
1	B	438	THR	7.2
1	B	433	GLY	7.2
1	D	415	ALA	7.1
1	D	416	ALA	7.0
1	B	440	GLY	6.9
1	B	400	ASP	6.6
1	B	397	VAL	6.5
1	D	320	PHE	6.5
1	D	462	ASN	6.4
1	A	260	ILE	6.2
1	D	402	GLY	6.2
1	B	453	VAL	6.1
1	D	414	VAL	6.1
1	D	31	THR	6.0
1	B	405	VAL	6.0
1	D	333	ILE	6.0
1	D	318	VAL	6.0
1	D	403	ARG	6.0
1	B	418	LYS	5.9
1	D	382	ILE	5.9
1	D	445	LEU	5.9
1	D	440	GLY	5.8
1	D	449	PHE	5.7
1	B	413	LYS	5.6
1	B	459	VAL	5.4
1	D	391	VAL	5.4
1	D	17	GLY	5.3
1	A	389	LYS	5.3
1	B	454	GLU	5.3
1	D	413	LYS	5.3
1	B	457	ASP	5.2
1	D	436	LYS	5.2
1	D	431	ILE	5.1
1	B	444	LEU	5.1
1	D	444	LEU	5.1
1	D	323	THR	5.0
1	D	425	SER	5.0
1	A	257	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	5.0
1	B	398	LYS	4.9
1	B	399	ILE	4.9
1	D	377	GLU	4.9
1	B	411	GLN	4.9
1	D	385	LEU	4.9
1	B	334	SER	4.9
1	D	409	LEU	4.9
1	B	446	THR	4.9
1	D	417	GLU	4.9
1	B	409	LEU	4.8
1	D	327	ILE	4.8
1	D	16	HIS	4.8
1	B	442	LYS	4.8
1	B	431	ILE	4.7
1	B	412	SER	4.6
1	B	426	ILE	4.6
1	D	397	VAL	4.6
1	B	435	ILE	4.6
1	B	407	ASP	4.6
1	D	437	GLY	4.5
1	D	322	LYS	4.5
1	D	455	ASN	4.5
1	D	314	PRO	4.5
1	B	335	GLY	4.5
1	D	467	TRP	4.5
1	B	449	PHE	4.5
1	D	389	LYS	4.4
1	A	259	GLN	4.4
1	A	449	PHE	4.4
1	D	411	GLN	4.4
1	D	452	ASN	4.4
1	D	384	ASP	4.3
1	D	218	LEU	4.3
1	D	316	LYS	4.3
1	D	428	GLY	4.3
1	A	386	ASN	4.3
1	D	330	ASN	4.2
1	D	390	GLU	4.2
1	D	19	THR	4.2
1	A	230	ARG	4.1
1	B	443	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	448	GLU	4.1
1	D	328	ILE	4.1
1	B	427	GLU	4.1
1	D	313	VAL	4.1
1	B	458	LYS	4.1
1	D	458	LYS	4.1
1	A	198	GLY	4.1
1	B	406	ILE	4.0
1	D	30	SER	4.0
1	D	459	VAL	4.0
1	B	429	LYS	4.0
1	D	392	LEU	3.9
1	B	415	ALA	3.9
1	D	372	GLY	3.9
1	D	334	SER	3.9
1	D	405	VAL	3.9
1	A	220	VAL	3.8
1	D	456	ARG	3.8
1	D	317	LYS	3.8
1	D	464	LEU	3.8
1	A	50	GLY	3.8
1	A	465	ARG	3.7
1	A	466	ARG	3.7
1	D	38	PRO	3.7
1	D	407	ASP	3.7
1	A	431	ILE	3.7
1	A	308	VAL	3.7
1	D	321	GLY	3.7
1	D	404	THR	3.6
1	D	450	SER	3.6
1	D	398	LYS	3.6
1	B	416	ALA	3.6
1	D	429	LYS	3.6
1	A	432	VAL	3.6
1	A	388	LYS	3.6
1	D	419	LEU	3.5
1	B	434	LYS	3.5
1	D	432	VAL	3.5
1	D	457	ASP	3.5
1	D	443	GLY	3.5
1	A	320	PHE	3.4
1	D	332	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	447	ALA	3.4
1	D	312	ALA	3.4
1	C	449	PHE	3.4
1	D	460	ILE	3.4
1	B	395	GLY	3.4
1	D	324	GLU	3.4
1	D	331	GLU	3.4
1	D	424	ILE	3.3
1	B	402	GLY	3.3
1	D	461	LEU	3.3
1	A	424	ILE	3.3
1	B	467	TRP	3.3
1	D	388	LYS	3.3
1	B	414	VAL	3.3
1	A	323	THR	3.2
1	A	266	LEU	3.2
1	A	433	GLY	3.2
1	A	252	ILE	3.2
1	A	225	MET	3.2
1	D	386	ASN	3.2
1	B	452	ASN	3.2
1	D	454	GLU	3.1
1	C	409	LEU	3.1
1	D	335	GLY	3.0
1	A	200	GLY	3.0
1	C	410	ALA	3.0
1	C	442	LYS	3.0
1	D	250	MET	3.0
1	D	286	SER	3.0
1	D	319	THR	3.0
1	C	402	GLY	3.0
1	C	435	ILE	2.9
1	D	435	ILE	2.9
1	A	321	GLY	2.9
1	B	394	GLU	2.9
1	A	426	ILE	2.9
1	A	218	LEU	2.9
1	D	383	LYS	2.9
1	D	448	GLU	2.9
1	D	339	TYR	2.8
1	A	255	VAL	2.8
1	B	392	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	411	GLN	2.8
1	D	326	ASN	2.8
1	D	394	GLU	2.8
1	D	228	LYS	2.8
1	C	413	LYS	2.7
1	D	288	ILE	2.7
1	D	356	VAL	2.7
1	A	392	LEU	2.7
1	D	289	PHE	2.7
1	A	322	LYS	2.7
1	A	447	ALA	2.7
1	A	28	ILE	2.7
1	B	382	ILE	2.7
1	A	464	LEU	2.7
1	B	425	SER	2.6
1	D	380	LYS	2.6
1	A	387	ILE	2.6
1	B	393	ARG	2.6
1	C	439	PHE	2.6
1	D	376	ILE	2.6
1	C	396	LYS	2.6
1	D	256	ASP	2.6
1	A	291	TYR	2.6
1	C	36	LYS	2.6
1	A	462	ASN	2.6
1	D	427	GLU	2.6
1	B	468	GLY	2.6
1	D	311	VAL	2.6
1	B	455	ASN	2.6
1	D	352	VAL	2.5
1	C	444	LEU	2.5
1	A	251	ALA	2.5
1	A	434	LYS	2.5
1	A	203	VAL	2.5
1	D	122	ASP	2.5
1	A	385	LEU	2.5
1	C	400	ASP	2.5
1	A	345	GLU	2.5
1	C	397	VAL	2.4
1	D	285	ILE	2.4
1	D	422	GLU	2.4
1	B	419	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	37	LEU	2.4
1	C	419	LEU	2.4
1	D	336	ASN	2.4
1	A	273	LEU	2.4
1	B	456	ARG	2.4
1	B	293	LEU	2.4
1	D	447	ALA	2.4
1	D	211	ILE	2.4
1	A	258	LYS	2.4
1	B	390	GLU	2.4
1	A	324	GLU	2.3
1	B	417	GLU	2.3
1	B	403	ARG	2.3
1	B	422	GLU	2.3
1	B	333	ILE	2.3
1	D	301	LEU	2.3
1	D	13	HIS	2.3
1	A	430	ASP	2.2
1	D	249	GLY	2.2
1	D	387	ILE	2.2
1	A	423	GLU	2.2
1	D	418	LYS	2.2
1	D	292	ASN	2.2
1	D	451	GLY	2.2
1	B	401	LYS	2.2
1	D	373	HIS	2.2
1	A	193	ALA	2.2
1	A	379	PHE	2.2
1	A	256	ASP	2.1
1	C	403	ARG	2.1
1	A	330	ASN	2.1
1	D	28	ILE	2.1
1	B	448	GLU	2.1
1	D	20	THR	2.1
1	B	387	ILE	2.1
1	D	179	ILE	2.1
1	B	329	LEU	2.1
1	C	445	LEU	2.1
1	A	390	GLU	2.1
1	C	406	ILE	2.1
1	A	194	PHE	2.1
1	A	51	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	280	VAL	2.1
1	D	395	GLY	2.1
1	A	416	ALA	2.0
1	D	430	ASP	2.0
1	C	-2	ARG	2.0
1	A	242	ALA	2.0
1	B	291	TYR	2.0
1	D	325	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CMH	D	338	8/9	0.75	0.18	152,222,227,253	2
1	CMH	A	371	8/9	0.82	0.33	133,164,171,190	2
1	CMH	B	338	8/9	0.88	0.14	124,171,196,199	2
1	CMH	D	340	8/9	0.90	0.34	152,216,232,249	2
1	CMH	A	338	8/9	0.93	0.24	137,150,185,236	2
1	CMH	C	338	8/9	0.94	0.15	58,83,145,240	2
1	CMH	B	371	8/9	0.94	0.17	110,130,188,228	2
1	CMH	C	340	8/9	0.96	0.19	54,75,92,110	2
1	CMH	A	340	8/9	0.97	0.23	136,173,185,199	2
1	CMH	D	371	8/9	0.97	0.17	103,144,150,163	2
1	CMH	D	264	8/9	0.97	0.17	131,162,186,191	2
1	CMH	B	340	8/9	0.98	0.15	120,138,232,238	2
1	CMH	A	264	8/9	0.98	0.13	149,163,190,206	2
1	CMH	C	264	8/9	0.99	0.17	51,90,102,105	0
1	CMH	B	264	8/9	0.99	0.21	49,64,73,84	2
1	CMH	C	371	8/9	0.99	0.20	57,94,131,132	2

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands i

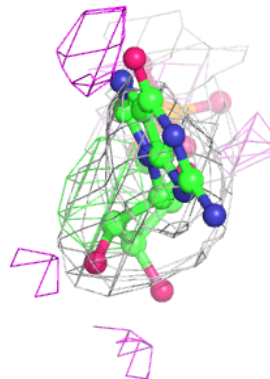
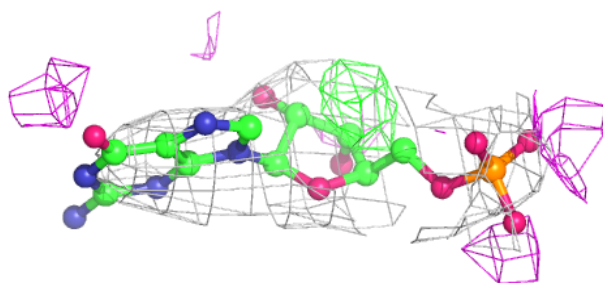
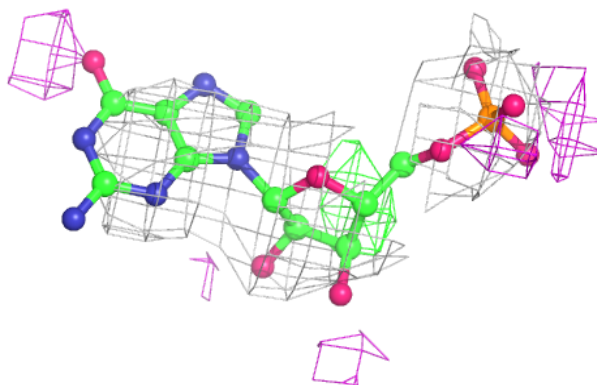
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	C	1474	5/5	0.54	0.54	125,199,203,260	5
4	SO4	C	1481	5/5	0.79	0.66	149,157,173,174	5
4	SO4	B	1472	5/5	0.84	0.41	87,206,279,300	0
6	5GP	B	1474	24/24	0.89	0.36	188,232,246,253	0
5	DXC	C	1476	28/28	0.89	0.31	101,121,161,174	0
4	SO4	B	1471	5/5	0.90	0.35	158,172,218,237	0
2	GDP	C	1469	28/28	0.90	0.27	62,99,125,141	28
4	SO4	C	1473	5/5	0.91	0.10	104,155,184,219	5
5	DXC	C	1479	28/28	0.95	0.30	48,73,147,183	28
5	DXC	C	1477	28/28	0.96	0.27	52,78,126,165	0
4	SO4	C	1472	5/5	0.96	0.16	100,129,151,170	0
4	SO4	C	1471	5/5	0.97	0.24	84,115,131,161	0
5	DXC	C	1475	28/28	0.97	0.25	51,65,105,114	0
2	GDP	B	1469	28/28	0.97	0.24	67,86,108,130	0
2	GDP	A	1469	28/28	0.97	0.18	78,92,105,106	28
5	DXC	C	1480	28/28	0.97	0.24	51,64,91,113	0
5	DXC	B	1473	28/28	0.97	0.25	51,71,101,124	0
3	MG	A	1470	1/1	0.98	0.10	147,147,147,147	1
5	DXC	C	1478	28/28	0.98	0.27	60,83,113,138	0
3	MG	B	1470	1/1	0.98	0.23	106,106,106,106	0
3	MG	C	1470	1/1	0.98	0.15	152,152,152,152	1

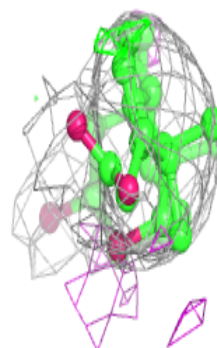
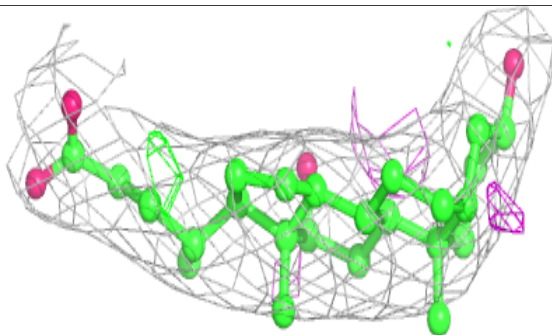
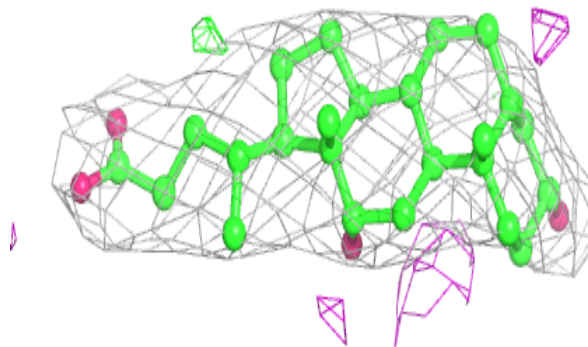
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5GP B 1474:

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

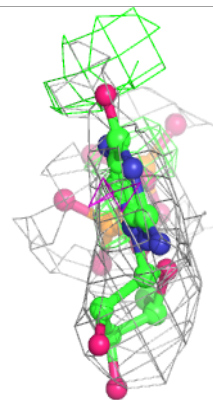
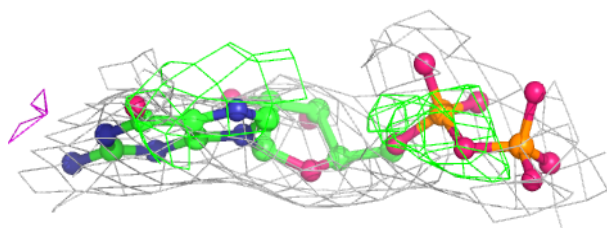
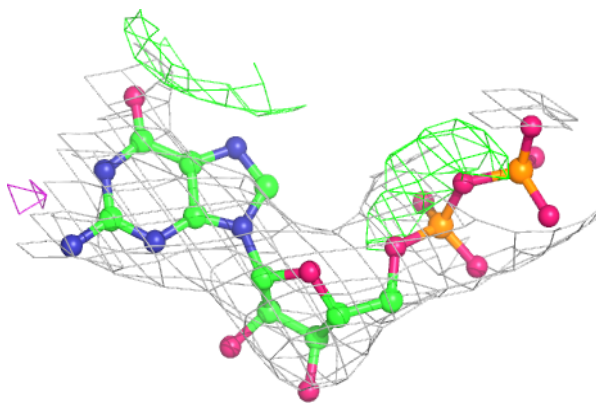
**Electron density around DXC C 1476:**

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

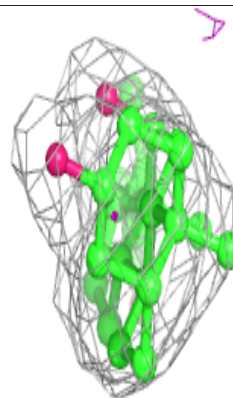
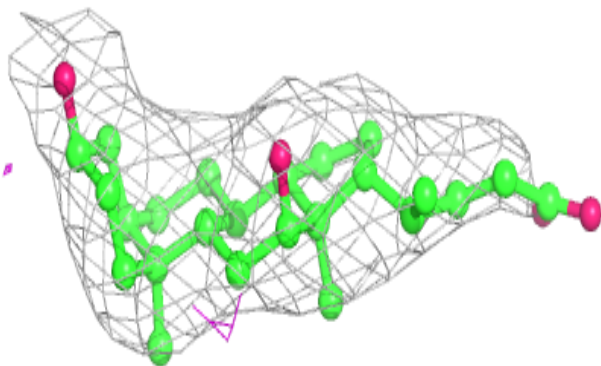
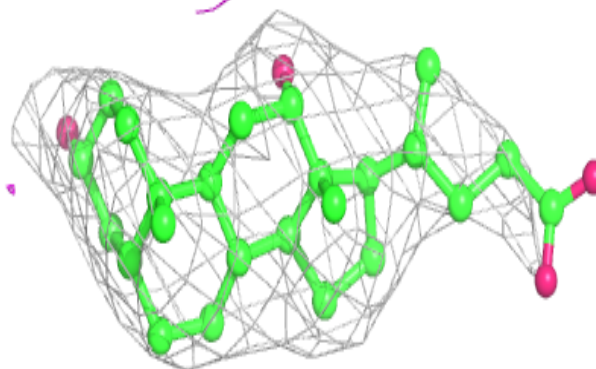


Electron density around GDP C 1469:

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

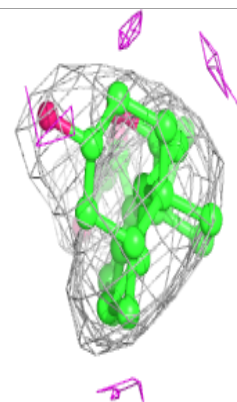
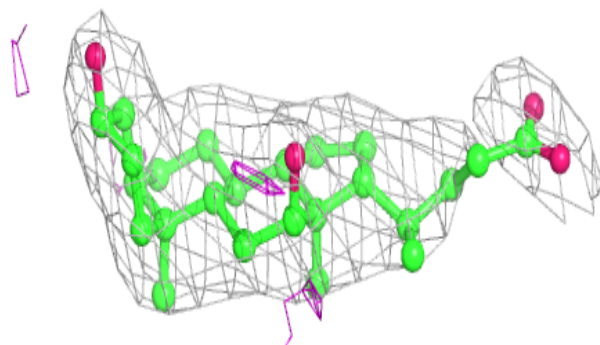
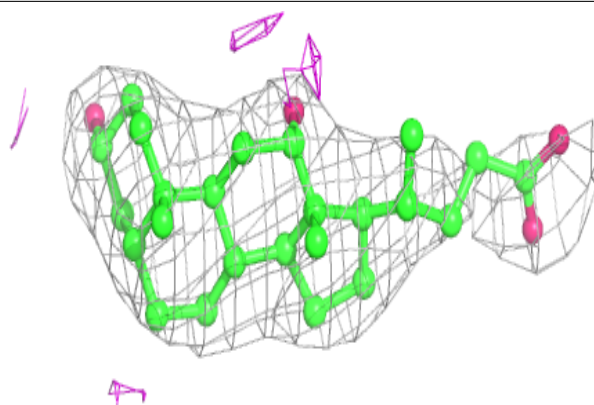
**Electron density around DXC C 1479:**

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

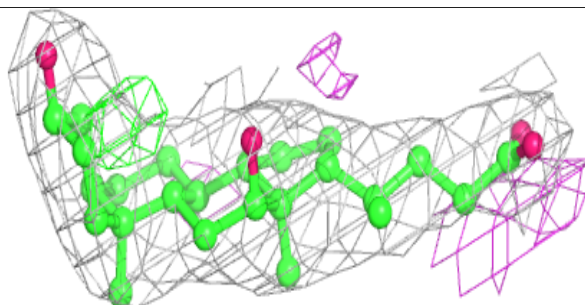
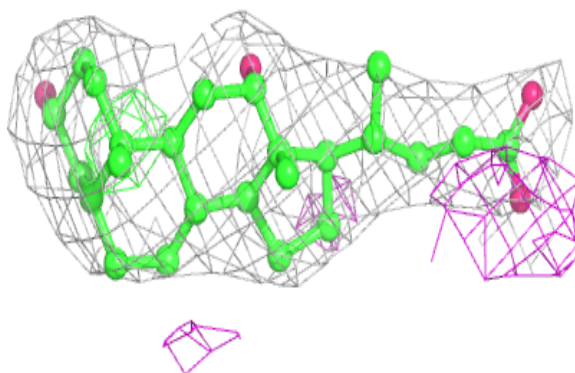


Electron density around DXC C 1477:

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

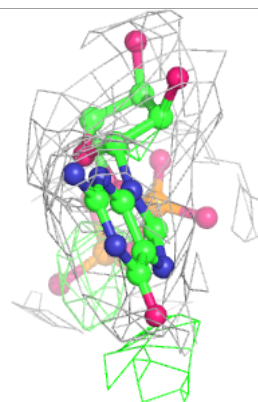
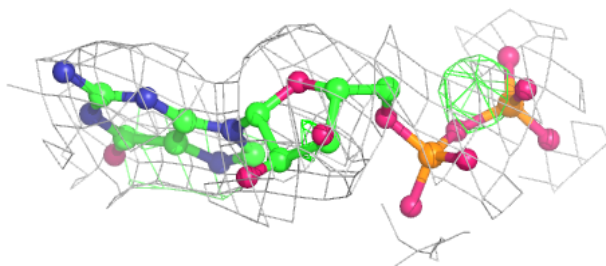
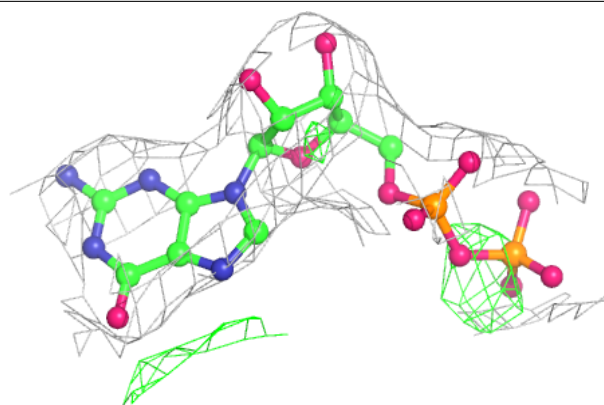
**Electron density around DXC C 1475:**

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

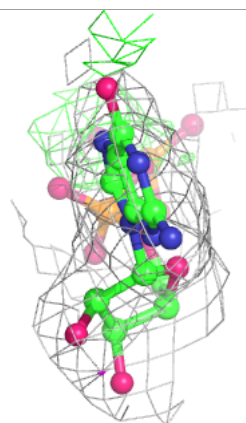
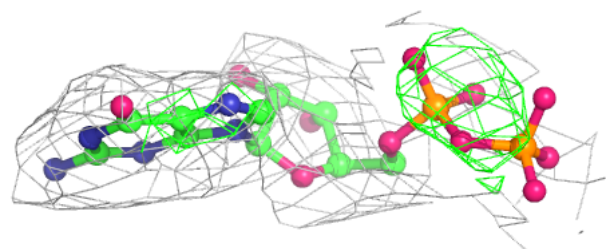
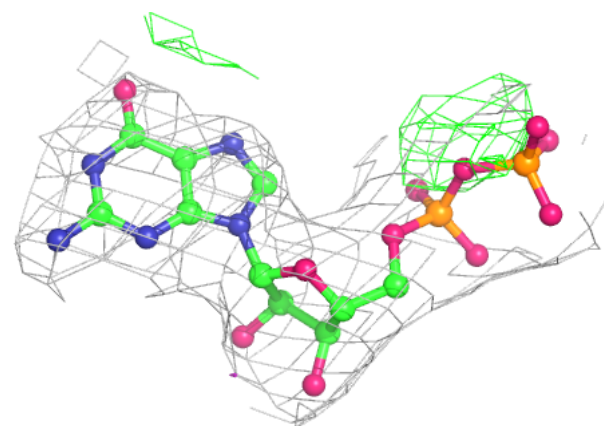


Electron density around GDP B 1469:

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

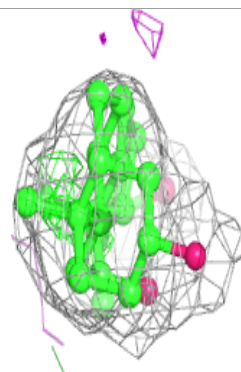
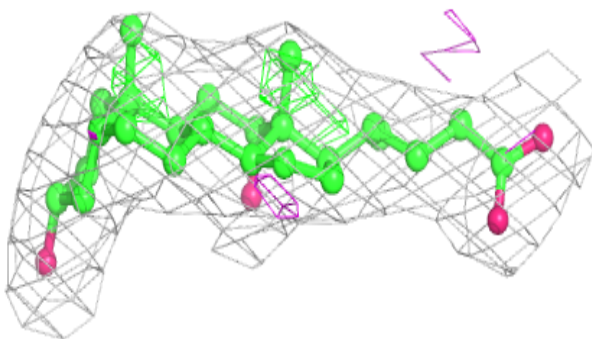
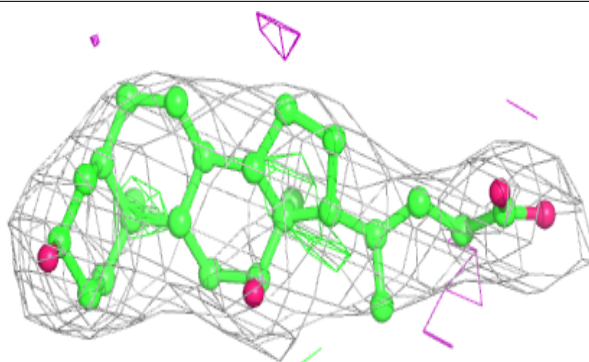
**Electron density around GDP A 1469:**

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

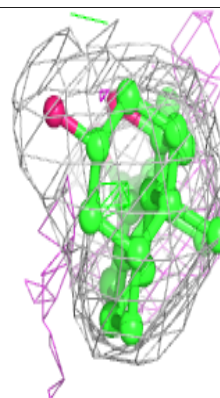
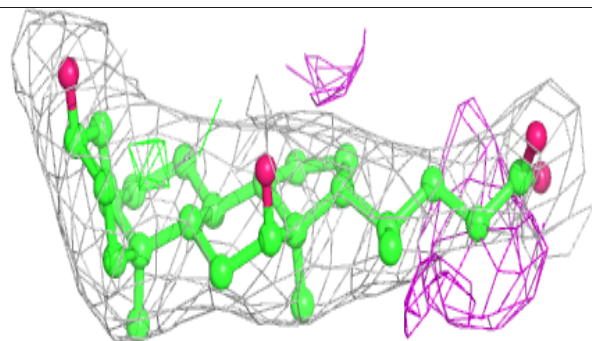
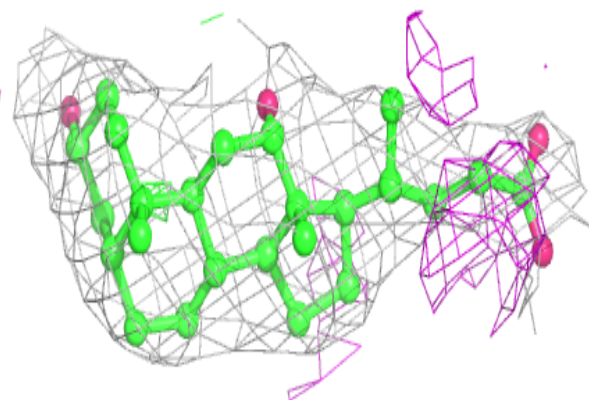


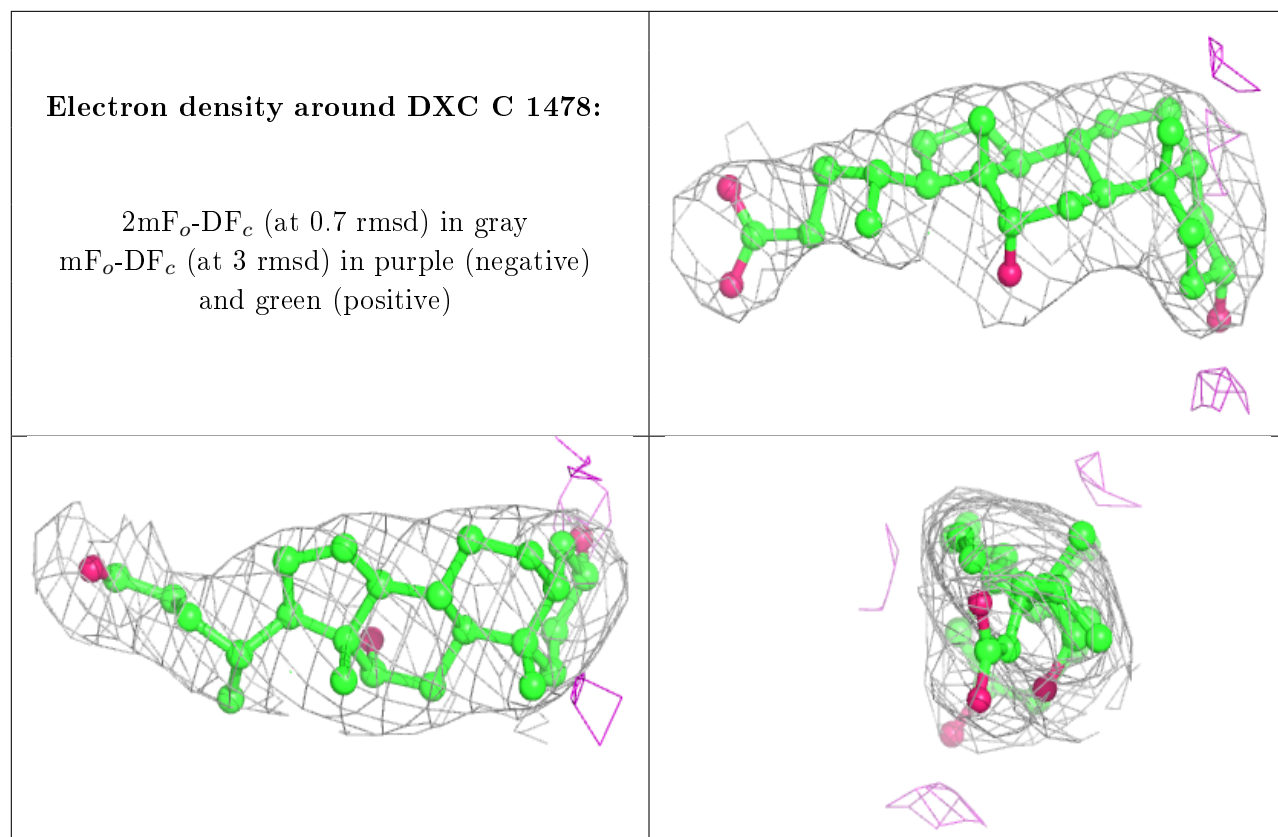
Electron density around DXC C 1480:

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

**Electron density around DXC B 1473:**

$2mF_o-DF_c$ (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.