



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 AM UTC

PDB ID : 4ACB / pdb_00004acb
Title : CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR
SELB FROM METHANOCOCCUS MARIPALUDIS IN COMPLEX WITH
THE GTP ANALOGUE GPPNHP
Authors : Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on : 2011-12-14
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

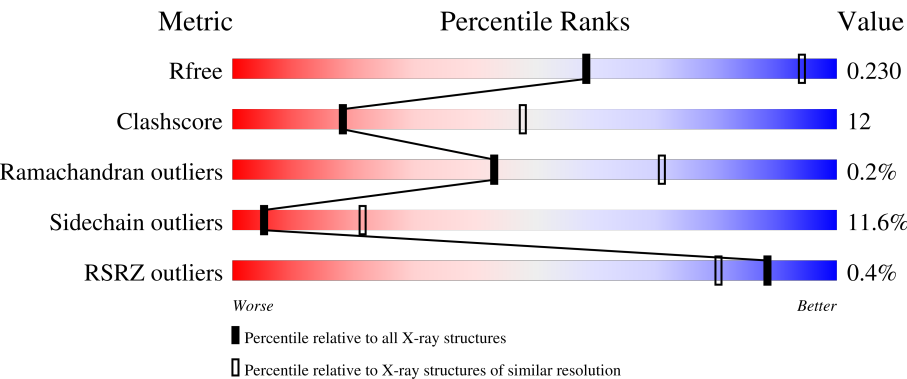
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	482	% 66% 24% • 6%
1	B	482	64% 27% • 5%
1	C	482	64% 29% 5% •
1	D	482	% 64% 27% 5% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CMH	D	340	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14623 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 TRANSLATION ELONGATION FACTOR SELB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	Hg	N	O	S	0	0	0
			3506	2240	4	597	651	14			
1	B	456	Total	C	Hg	N	O	S	0	0	0
			3533	2257	4	603	655	14			
1	C	471	Total	C	Hg	N	O	S	0	0	0
			3651	2327	4	627	679	14			
1	D	467	Total	C	Hg	N	O	S	0	0	0
			3615	2305	4	618	675	13			

There are 56 discrepancies between the modelled and reference sequences:

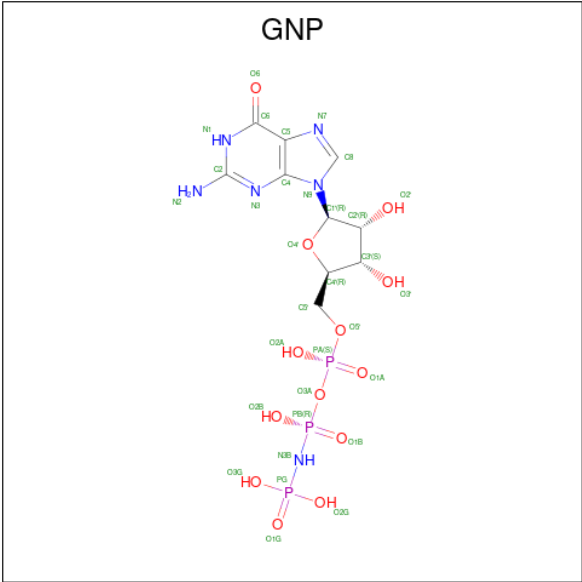
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8J307
A	-12	HIS	-	expression tag	UNP Q8J307
A	-11	HIS	-	expression tag	UNP Q8J307
A	-10	HIS	-	expression tag	UNP Q8J307
A	-9	HIS	-	expression tag	UNP Q8J307
A	-8	HIS	-	expression tag	UNP Q8J307
A	-7	HIS	-	expression tag	UNP 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 PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

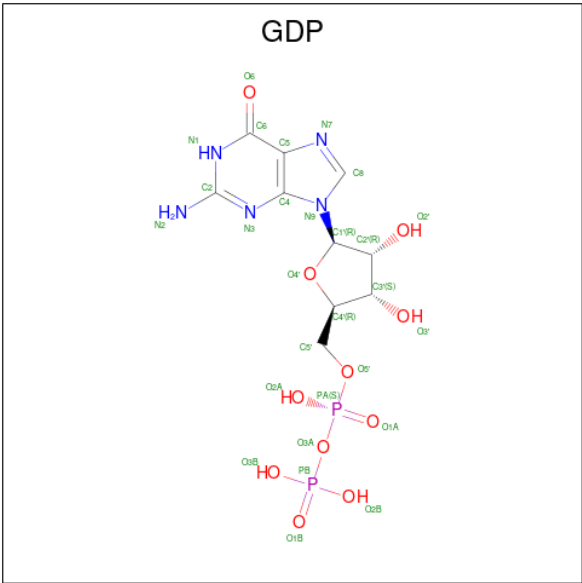


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

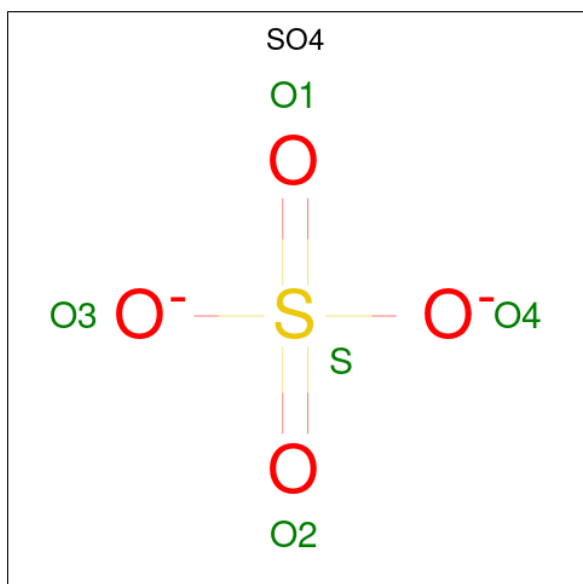
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



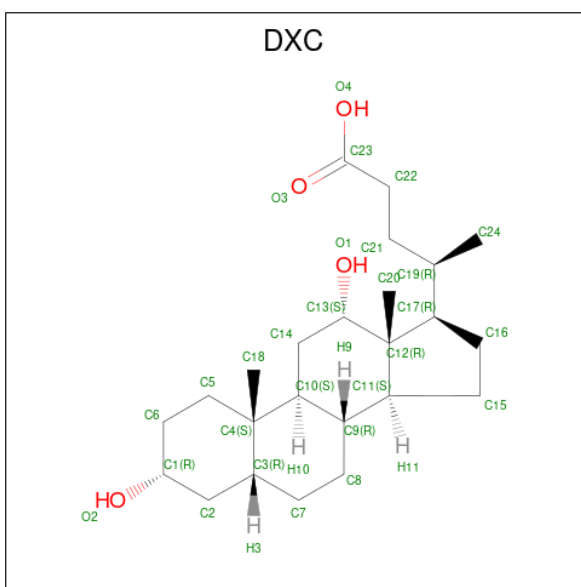
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



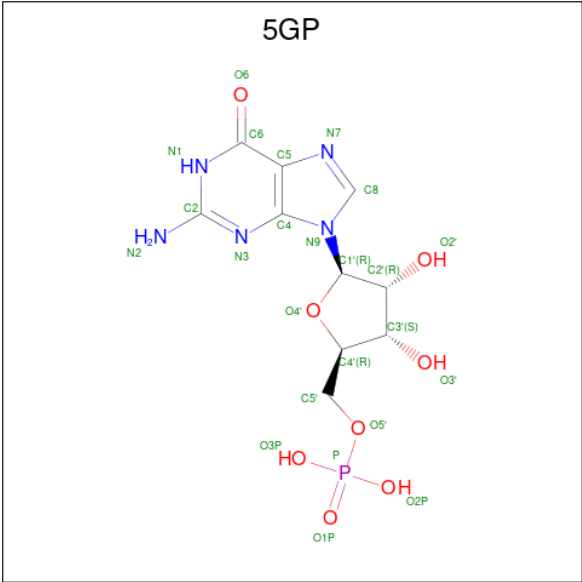
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (CCD ID: DXC) (formula: C₂₄H₄₀O₄).



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

- Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



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

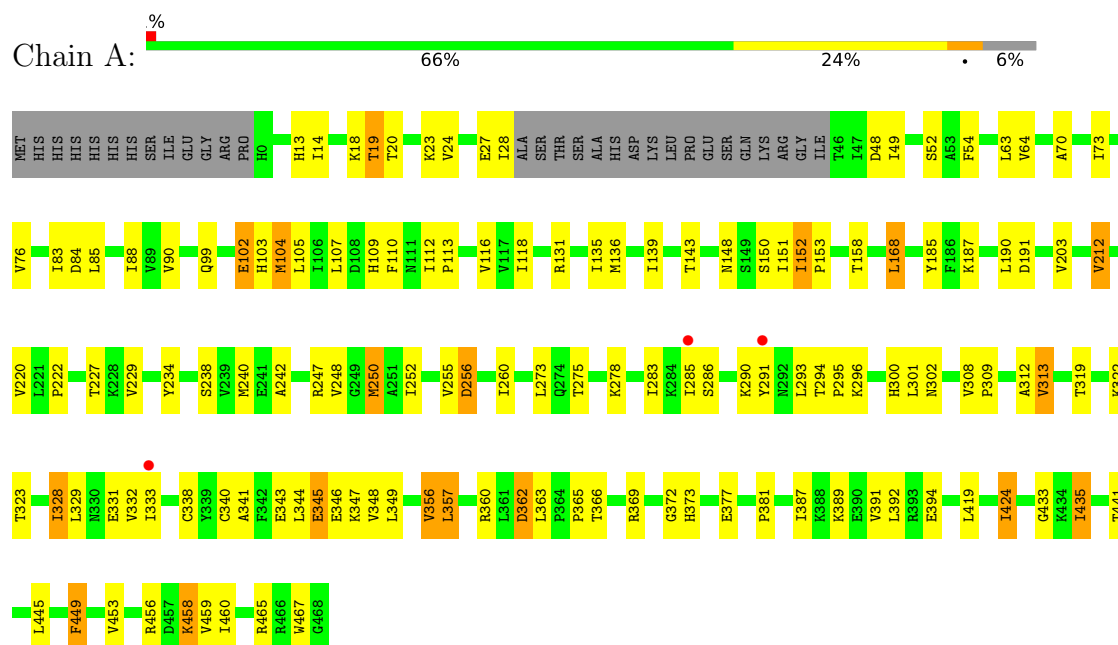
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total O	0	0
			2 2		
8	B	4	Total O	0	0
			4 4		

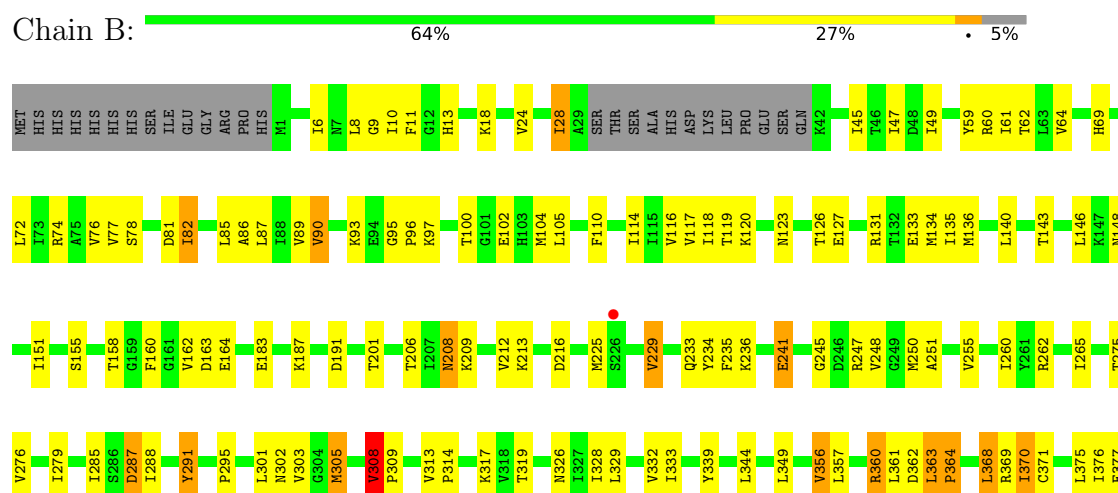
3 Residue-property plots [i](#)

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: TRANSLATION ELONGATION FACTOR SELB

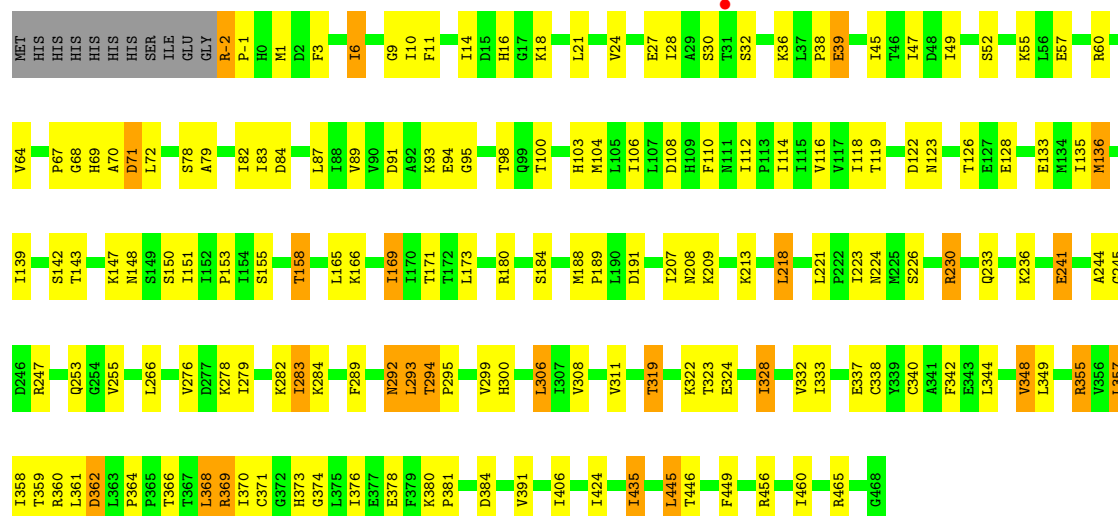


• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

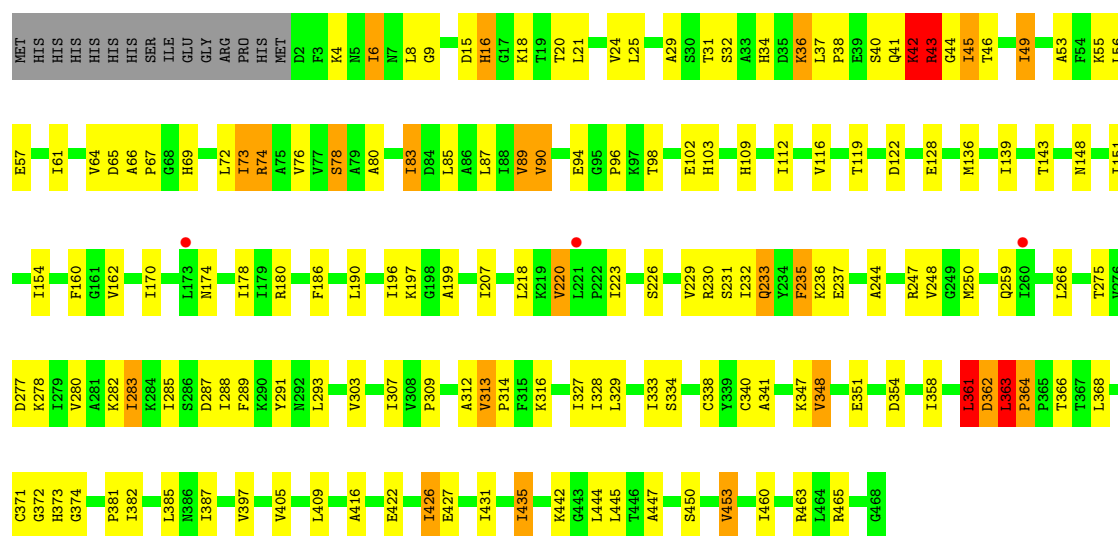




- Molecule 1: TRANSLATION ELONGATION FACTOR SELB



- Molecule 1: TRANSLATION ELONGATION FACTOR SELB



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	146.63Å 146.63Å 297.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.34 19.94 – 3.34	Depositor EDS
% Data completeness (in resolution range)	82.8 (19.94-3.34) 88.0 (19.94-3.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.179 , 0.223 0.189 , 0.230	Depositor DCC
R_{free} test set	2214 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	110.2	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 174.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14623	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DXC, 5GP, GDP, MG, CMH, SO4, GNP

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	0.41	0/3515	0.89	2/4727 (0.0%)
1	B	0.47	0/3541	0.91	5/4760 (0.1%)
1	C	0.53	0/3664	0.96	8/4929 (0.2%)
1	D	0.38	0/3626	0.90	13/4878 (0.3%)
All	All	0.45	0/14346	0.91	28/19294 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	363	LEU	CA-C-N	9.75	130.42	120.38
1	D	363	LEU	C-N-CA	9.75	130.42	120.38
1	D	364	PRO	N-CA-C	7.71	120.10	110.70
1	D	283	ILE	N-CA-C	7.26	118.35	107.75
1	B	308	VAL	N-CA-C	6.89	115.81	107.61
1	C	68	GLY	N-CA-C	6.65	121.34	110.77
1	D	364	PRO	CA-C-N	-6.40	113.10	119.56
1	D	364	PRO	C-N-CA	-6.40	113.10	119.56
1	A	294	THR	CA-C-N	6.15	126.50	119.92
1	A	294	THR	C-N-CA	6.15	126.50	119.92
1	D	43	ARG	N-CA-C	-5.96	105.31	113.30
1	C	364	PRO	CA-C-N	5.92	126.03	119.87
1	C	364	PRO	C-N-CA	5.92	126.03	119.87
1	C	95	GLY	CA-C-N	5.75	125.70	119.78
1	C	95	GLY	C-N-CA	5.75	125.70	119.78
1	D	361	LEU	N-CA-C	-5.73	105.49	112.88
1	D	37	LEU	CA-C-N	-5.60	113.45	120.51
1	D	37	LEU	C-N-CA	-5.60	113.45	120.51
1	D	313	VAL	CA-C-N	5.34	126.52	119.84
1	D	313	VAL	C-N-CA	5.34	126.52	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	PRO	CA-C-N	5.30	125.02	119.82
1	B	364	PRO	C-N-CA	5.30	125.02	119.82
1	C	112	ILE	CA-C-N	5.27	125.28	119.90
1	C	112	ILE	C-N-CA	5.27	125.28	119.90
1	B	229	VAL	CB-CA-C	-5.17	104.70	110.96
1	D	288	ILE	N-CA-C	5.16	116.62	111.00
1	B	11	PHE	N-CA-C	5.10	117.43	109.52
1	C	374	GLY	N-CA-C	5.05	117.43	110.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3506	0	3687	79	0
1	B	3533	0	3727	88	0
1	C	3651	0	3838	84	0
1	D	3615	0	3801	110	0
2	A	32	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	28	0	12	2	0
5	B	10	0	0	2	0
5	C	20	0	0	2	0
6	B	28	0	39	4	0
6	C	168	0	234	15	0
7	B	24	0	12	2	0
8	A	2	0	0	0	0
8	B	4	0	0	0	0
All	All	14623	0	15363	363	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 12.

All (363) 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:C:6:ILE:HD12	1:C:173:LEU:HD13	1.54	0.90
1:C:338:CMH:HB3	1:C:340:CMH:CM	2.05	0.86
1:D:43:ARG:HD3	1:D:45:ILE:HD11	1.57	0.85
1:D:283:ILE:HG13	1:D:340:CMH:HB3	1.61	0.82
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.61	0.80
1:C:27:GLU:HB3	1:C:32:SER:HB2	1.63	0.79
1:C:306:LEU:HD13	1:C:348:VAL:HG22	1.65	0.79
1:D:45:ILE:HB	1:D:233:GLN:HE22	1.47	0.78
1:D:416:ALA:HB1	1:D:445:LEU:HD21	1.65	0.77
1:A:234:TYR:HB2	1:A:248:VAL:HG12	1.68	0.76
1:A:116:VAL:HB	1:A:151:ILE:HG12	1.68	0.75
1:D:43:ARG:HB3	1:D:45:ILE:HG13	1.67	0.75
1:C:283:ILE:HD13	1:C:340:CMH:HB3	1.70	0.73
1:D:67:PRO:HA	1:D:78:SER:HB2	1.71	0.72
1:B:361:LEU:HD23	1:B:369:ARG:HD2	1.71	0.72
1:A:54:PHE:HE1	1:A:63:LEU:HD13	1.57	0.70
1:C:368:LEU:HD12	1:C:370:ILE:H	1.56	0.69
1:D:293:LEU:HD21	1:D:340:CMH:CM	2.23	0.68
1:B:251:ALA:HB1	1:C:1:MET:HE1	1.75	0.68
1:A:99:GLN:NE2	1:A:102:GLU:OE2	2.27	0.67
1:D:74:ARG:HH22	1:D:309:PRO:HD3	1.57	0.67
1:A:435:ILE:HD11	1:A:445:LEU:HD22	1.75	0.66
1:D:427:GLU:HG2	1:D:460:ILE:HG13	1.78	0.66
1:C:289:PHE:CE2	1:C:371:CMH:HB2	2.31	0.66
1:A:152:ILE:HD11	1:A:168:LEU:HD22	1.77	0.65
1:A:104:MET:HE1	1:A:143:THR:HG21	1.78	0.65
1:D:313:VAL:HB	1:D:341:ALA:HB3	1.79	0.65
1:A:362:ASP:N	1:A:362:ASP:OD1	2.28	0.64
1:B:158:THR:HG23	1:D:363:LEU:HB3	1.80	0.64
1:B:302:ASN:HB2	1:B:357:LEU:HB3	1.79	0.64
1:D:45:ILE:HB	1:D:233:GLN:NE2	2.12	0.63
1:C:308:VAL:HG21	1:C:344:LEU:HD13	1.80	0.63
1:A:433:GLY:HA3	1:A:449:PHE:HB3	1.80	0.63
1:D:422:GLU:H	1:D:435:ILE:HG22	1.63	0.63
1:D:338:CMH:CM	1:D:340:CMH:SG	2.87	0.63
1:B:191:ASP:OD2	1:B:247:ARG:NH1	2.25	0.62
1:A:136:MET:HE2	1:A:139:ILE:HD12	1.80	0.62
1:B:363:LEU:HD13	1:B:364:PRO:HD2	1.82	0.62
1:D:409:LEU:HD12	1:D:445:LEU:HD12	1.81	0.62
1:A:70:ALA:O	1:A:369:ARG:NH2	2.32	0.62
1:C:293:LEU:HD22	1:C:371:CMH:CM	2.30	0.62
1:D:36:LYS:HB3	1:D:236:LYS:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:THR:O	1:C:104:MET:HG3	2.01	0.61
1:A:278:LYS:HD2	1:A:343:GLU:HG2	1.82	0.60
1:D:74:ARG:HG2	1:D:361:LEU:HD13	1.82	0.60
1:C:283:ILE:HG12	1:C:358:ILE:HD11	1.82	0.60
1:A:313:VAL:HG23	1:A:341:ALA:HB3	1.82	0.60
1:D:435:ILE:HG13	1:D:447:ALA:HB2	1.83	0.60
1:C:435:ILE:HD12	1:C:445:LEU:HD13	1.83	0.59
1:B:10:ILE:HD13	1:B:87:LEU:HB2	1.84	0.59
1:B:216:ASP:O	1:B:229:VAL:HG23	2.02	0.59
1:B:287:ASP:OD1	1:B:287:ASP:N	2.28	0.59
1:B:187:LYS:HB3	1:B:209:LYS:HG3	1.84	0.59
1:B:233:GLN:HE21	1:B:236:LYS:HA	1.67	0.59
1:D:316:LYS:N	1:D:327:ILE:O	2.35	0.58
1:B:90:VAL:HG13	1:B:118:ILE:HG12	1.84	0.58
1:A:222:PRO:HB3	1:A:349:LEU:HD21	1.85	0.58
1:A:312:ALA:HB1	1:A:340:CMH:SG	2.42	0.58
1:B:288:ILE:HB	7:B:1474:5GP:HN22	1.68	0.58
1:D:43:ARG:HD3	1:D:45:ILE:CD1	2.33	0.58
1:A:18:LYS:NZ	2:A:1469:GNP:O1B	2.33	0.57
1:C:381:PRO:HD2	1:C:384:ASP:HB2	1.84	0.57
1:D:314:PRO:HB3	1:D:338:CMH:CM	2.34	0.57
1:A:295:PRO:HG3	1:A:328:ILE:HD11	1.84	0.57
1:A:391:VAL:HG21	1:A:465:ARG:HD3	1.86	0.57
1:A:240:MET:HE1	1:B:95:GLY:HA3	1.87	0.57
1:C:10:ILE:HG22	1:C:18:LYS:HG3	1.87	0.57
1:D:116:VAL:HG11	1:D:136:MET:HG2	1.86	0.57
1:B:233:GLN:OE1	6:B:1473:DXC:H10	2.05	0.56
1:A:308:VAL:HG21	1:A:344:LEU:HD13	1.88	0.56
1:A:76:VAL:HG11	1:A:103:HIS:CD2	2.41	0.56
1:A:387:ILE:HG23	1:A:467:TRP:HB3	1.87	0.56
1:C:295:PRO:HG2	1:C:328:ILE:HD11	1.88	0.56
1:D:8:LEU:HD11	1:D:87:LEU:HG	1.87	0.55
1:A:256:ASP:OD1	1:A:256:ASP:N	2.30	0.55
1:D:232:ILE:HG12	1:D:250:MET:HG2	1.87	0.55
1:C:36:LYS:HE3	1:C:38:PRO:HB3	1.87	0.55
1:C:69:HIS:CD2	1:C:70:ALA:H	2.24	0.55
1:B:301:LEU:HD11	1:B:356:VAL:HG13	1.88	0.55
1:D:397:VAL:HG11	1:D:453:VAL:HB	1.88	0.55
1:A:238:SER:H	1:B:97:LYS:NZ	2.05	0.55
1:B:74:ARG:NH2	5:B:1471:SO4:O4	2.40	0.55
1:D:15:ASP:HA	1:D:18:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLY:HA2	1:B:64:VAL:HB	1.88	0.54
1:A:300:HIS:CE1	1:A:309:PRO:HG3	2.42	0.54
1:B:116:VAL:HB	1:B:151:ILE:HG12	1.90	0.54
1:D:313:VAL:O	1:D:341:ALA:N	2.41	0.54
1:B:78:SER:HB2	1:B:305:MET:HG2	1.89	0.53
1:C:16:HIS:NE2	1:C:94:GLU:OE2	2.42	0.53
1:B:69:HIS:NE2	1:B:102:GLU:OE1	2.26	0.53
1:D:74:ARG:HH11	1:D:307:ILE:HG22	1.73	0.53
1:B:13:HIS:H	1:B:100:THR:HG22	1.74	0.53
1:B:229:VAL:HG13	1:B:250:MET:HE3	1.90	0.53
1:B:426:ILE:HB	1:B:431:ILE:HG23	1.91	0.53
1:D:285:ILE:HD11	1:D:291:TYR:HB2	1.90	0.53
1:A:285:ILE:HG12	1:A:291:TYR:CE2	2.44	0.53
1:B:82:ILE:HD13	1:B:206:THR:HG22	1.90	0.53
1:D:303:VAL:HB	1:D:348:VAL:HG11	1.91	0.53
1:D:180:ARG:HB3	1:D:244:ALA:HB3	1.91	0.52
1:B:314:PRO:HA	1:B:339:TYR:O	2.10	0.52
1:D:34:HIS:N	1:D:53:ALA:O	2.42	0.52
1:B:391:VAL:HB	1:B:465:ARG:HD3	1.92	0.52
1:C:279:ILE:HD13	1:C:376:ILE:HD11	1.89	0.52
1:D:277:ASP:HB3	1:D:347:LYS:HE2	1.91	0.52
1:A:13:HIS:ND1	1:A:99:GLN:HG2	2.24	0.52
1:D:218:LEU:HD11	1:D:229:VAL:HG22	1.90	0.52
1:D:287:ASP:HB2	1:D:291:TYR:HE1	1.75	0.52
1:B:251:ALA:HB1	1:C:1:MET:CE	2.39	0.52
1:C:10:ILE:HD12	1:C:21:LEU:HD23	1.92	0.52
1:C:322:LYS:HG3	1:C:323:THR:H	1.75	0.52
1:C:91:ASP:HB3	1:C:94:GLU:HG2	1.90	0.52
1:A:238:SER:H	1:B:97:LYS:HZ2	1.57	0.51
1:D:316:LYS:HB2	1:D:329:LEU:HD13	1.92	0.51
1:C:11:PHE:CE1	1:C:72:LEU:HD22	2.44	0.51
1:D:43:ARG:HH11	1:D:231:SER:HB3	1.74	0.51
1:D:283:ILE:HA	1:D:373:HIS:O	2.11	0.51
1:A:109:HIS:HD2	1:A:373:HIS:HB3	1.76	0.51
1:D:21:LEU:HD22	1:D:89:VAL:HG11	1.92	0.51
1:A:191:ASP:OD2	1:A:247:ARG:NH2	2.43	0.51
1:B:201:THR:OG1	1:B:255:VAL:O	2.18	0.51
1:D:382:ILE:HA	1:D:385:LEU:HD12	1.92	0.51
1:C:27:GLU:HA	1:C:30:SER:HB3	1.93	0.51
1:C:82:ILE:HG23	1:C:245:GLY:HA2	1.92	0.51
1:A:360:ARG:HG2	1:A:363:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HG22	1:B:61:ILE:HG23	1.92	0.50
1:C:49:ILE:HD11	6:C:1475:DXC:H161	1.94	0.50
1:D:4:LYS:NZ	1:D:178:ILE:O	2.44	0.50
1:B:13:HIS:CE1	1:B:97:LYS:HG3	2.47	0.50
1:C:110:PHE:CD1	1:C:355:ARG:HD2	2.47	0.50
1:D:29:ALA:HB2	1:D:56:LEU:HG	1.93	0.50
5:B:1472:SO4:O2	1:C:55:LYS:NZ	2.41	0.50
1:D:40:SER:O	1:D:44:GLY:HA2	2.12	0.50
1:D:69:HIS:CE1	1:D:103:HIS:CE1	2.99	0.50
1:A:389:LYS:HB3	1:A:465:ARG:HB3	1.94	0.50
1:B:81:ASP:OD2	1:B:208:ASN:ND2	2.45	0.50
1:D:218:LEU:HD13	1:D:266:LEU:HD11	1.94	0.50
1:D:282:LYS:O	1:D:374:GLY:HA3	2.12	0.50
1:B:72:LEU:O	1:B:76:VAL:HG23	2.12	0.50
1:B:160:PHE:CZ	1:D:98:THR:HG23	2.47	0.50
1:D:122:ASP:OD1	1:D:122:ASP:N	2.45	0.50
1:B:8:LEU:HD12	1:B:85:LEU:O	2.12	0.49
1:C:342:PHE:HZ	1:C:358:ILE:HD13	1.75	0.49
1:D:43:ARG:HH12	1:D:230:ARG:HB3	1.76	0.49
1:D:66:ALA:HB1	1:D:69:HIS:ND1	2.26	0.49
1:D:38:PRO:HB3	1:D:42:LYS:HD2	1.94	0.49
1:B:233:GLN:OE1	6:B:1473:DXC:H61	2.13	0.49
1:A:275:THR:HG22	1:A:347:LYS:HD2	1.95	0.49
1:C:11:PHE:HB3	1:C:103:HIS:ND1	2.27	0.49
1:D:42:LYS:HE2	1:D:237:GLU:HA	1.95	0.49
1:D:358:ILE:HG22	1:D:371:CMH:HB2	1.95	0.49
1:A:49:ILE:HG21	1:A:64:VAL:HG13	1.94	0.49
1:A:110:PHE:CZ	1:A:357:LEU:HD13	2.47	0.49
1:A:424:ILE:HG13	1:A:459:VAL:HG13	1.95	0.48
1:D:351:GLU:HG2	1:D:354:ASP:CG	2.38	0.48
1:D:15:ASP:OD1	1:D:16:HIS:ND1	2.46	0.48
1:A:48:ASP:OD1	1:A:49:ILE:N	2.41	0.48
1:B:317:LYS:HG2	1:B:326:ASN:OD1	2.14	0.48
1:C:122:ASP:OD2	1:C:155:SER:OG	2.29	0.48
1:B:82:ILE:HG23	1:B:245:GLY:HA2	1.96	0.48
1:B:265:ILE:HG13	1:B:349:LEU:HD12	1.95	0.48
1:B:329:LEU:HB3	1:B:332:VAL:HB	1.95	0.48
1:D:73:ILE:O	1:D:74:ARG:HG3	2.13	0.48
1:D:90:VAL:HG21	1:D:136:MET:HE1	1.95	0.48
1:D:277:ASP:HB3	1:D:347:LYS:HG2	1.95	0.48
1:B:102:GLU:HG2	1:B:368:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ILE:HG22	1:D:112:ILE:HD13	1.95	0.48
1:A:136:MET:HE2	1:A:136:MET:HA	1.96	0.47
1:D:405:VAL:CG1	1:D:444:LEU:HB3	2.44	0.47
1:D:248:VAL:HG12	1:D:250:MET:HG3	1.96	0.47
1:A:23:LYS:O	1:A:27:GLU:HG2	2.14	0.47
1:B:406:ILE:HD11	1:B:449:PHE:HZ	1.80	0.47
1:C:1:MET:HE3	6:C:1476:DXC:H52	1.96	0.47
1:C:84:ASP:CG	1:C:180:ARG:HH22	2.22	0.47
1:C:213:LYS:HE2	1:C:241:GLU:OE1	2.14	0.47
1:B:93:LYS:HE3	1:B:123:ASN:O	2.14	0.47
1:D:431:ILE:HB	1:D:450:SER:O	2.14	0.47
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.73	0.47
1:B:86:ALA:HB3	1:B:114:ILE:HG22	1.97	0.47
1:C:233:GLN:OE1	6:C:1475:DXC:H11	2.14	0.47
1:D:280:VAL:HG21	1:D:385:LEU:HD21	1.97	0.47
1:A:105:LEU:O	1:A:109:HIS:ND1	2.44	0.47
1:B:377:GLU:HG2	1:B:378:GLU:HG3	1.97	0.47
1:B:208:ASN:HB3	1:B:209:LYS:HG2	1.96	0.47
1:C:106:ILE:HG12	1:C:357:LEU:HD21	1.97	0.47
1:D:278:LYS:HD3	1:D:381:PRO:HA	1.97	0.47
1:B:120:LYS:HD3	4:B:1469:GDP:C4	2.50	0.46
1:B:291:TYR:HD1	1:B:333:ILE:HG22	1.79	0.46
1:B:362:ASP:OD1	1:B:363:LEU:N	2.48	0.46
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.81	0.46
1:D:102:GLU:HB2	1:D:366:THR:HG22	1.97	0.46
1:D:197:LYS:HB3	1:D:199:ALA:H	1.79	0.46
1:B:105:LEU:HD12	1:B:368:LEU:HD22	1.97	0.46
1:C:108:ASP:CG	1:C:143:THR:HB	2.41	0.46
1:B:133:GLU:HG2	1:B:134:MET:HE2	1.97	0.46
1:C:233:GLN:HE21	1:C:236:LYS:HA	1.81	0.46
1:A:227:THR:HG21	1:A:255:VAL:HG22	1.96	0.46
1:B:213:LYS:HG2	1:B:241:GLU:HB2	1.97	0.46
1:B:234:TYR:HB2	1:B:248:VAL:HG12	1.97	0.46
1:A:20:THR:O	1:A:24:VAL:HG23	2.15	0.46
1:A:283:ILE:HD12	1:A:340:CMH:HB3	1.98	0.46
1:C:133:GLU:HG3	1:C:151:ILE:HG21	1.98	0.46
1:D:69:HIS:CE1	1:D:103:HIS:NE2	2.84	0.46
1:A:13:HIS:HD1	1:A:99:GLN:HG2	1.81	0.46
1:D:116:VAL:HB	1:D:151:ILE:HG12	1.96	0.46
1:D:358:ILE:HB	1:D:372:GLY:N	2.31	0.46
1:A:107:LEU:HD23	1:A:112:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:PHE:CD2	1:C:371:CMH:HB2	2.51	0.46
1:D:109:HIS:HB3	1:D:373:HIS:CE1	2.51	0.46
1:C:158:THR:HG21	6:C:1478:DXC:O2	2.15	0.46
1:C:282:LYS:HE2	1:C:337:GLU:HG2	1.97	0.46
1:C:333:ILE:HD12	6:C:1480:DXC:H203	1.98	0.46
1:B:155:SER:HB3	1:B:160:PHE:HB3	1.99	0.45
6:B:1473:DXC:H10	6:B:1473:DXC:H61	1.60	0.45
1:C:10:ILE:O	1:C:18:LYS:HE3	2.16	0.45
1:C:93:LYS:HG3	1:C:128:GLU:OE1	2.16	0.45
1:A:456:ARG:O	1:A:458:LYS:NZ	2.35	0.45
1:A:283:ILE:HB	1:A:338:CMH:O	2.17	0.45
1:B:279:ILE:HG23	1:B:376:ILE:HG23	1.99	0.45
1:B:295:PRO:HB3	1:B:328:ILE:HD11	1.98	0.45
1:D:57:GLU:CD	1:D:170:ILE:HD13	2.42	0.45
1:C:116:VAL:HB	1:C:151:ILE:HG12	1.99	0.45
1:C:118:ILE:HB	1:C:153:PRO:HA	1.99	0.45
1:D:312:ALA:HB1	1:D:340:CMH:CM	2.47	0.45
1:B:288:ILE:CB	7:B:1474:5GP:HN22	2.30	0.45
1:B:407:ASP:HB2	1:B:444:LEU:HD22	1.98	0.45
1:D:69:HIS:HE1	1:D:103:HIS:CE1	2.35	0.45
1:B:285:ILE:HD13	1:B:291:TYR:HB3	1.99	0.45
1:C:10:ILE:HD13	1:C:87:LEU:HB2	1.98	0.45
1:D:80:ALA:HB1	1:D:112:ILE:HD11	1.99	0.45
1:D:275:THR:HG22	1:D:347:LYS:HD3	1.98	0.45
1:C:135:ILE:O	1:C:139:ILE:HG13	2.16	0.45
1:A:345:GLU:HG2	1:A:346:GLU:HG3	1.99	0.45
6:C:1480:DXC:H243	6:C:1480:DXC:H221	1.72	0.45
1:D:363:LEU:HA	1:D:364:PRO:HD3	1.77	0.45
1:A:419:LEU:HD12	1:A:445:LEU:HD11	1.98	0.44
1:A:136:MET:CE	1:A:139:ILE:HD12	2.47	0.44
1:A:278:LYS:HG3	1:A:381:PRO:HB3	2.00	0.44
1:A:118:ILE:HB	1:A:153:PRO:HA	1.99	0.44
1:A:190:LEU:HD22	1:A:203:VAL:HB	2.00	0.44
1:D:96:PRO:HG3	1:D:136:MET:HE1	1.99	0.44
1:A:212:VAL:HG23	1:A:242:ALA:HB3	1.99	0.44
1:B:131:ARG:O	1:B:135:ILE:HG13	2.17	0.44
1:C:319:THR:HA	1:C:324:GLU:HA	1.99	0.44
6:C:1477:DXC:H161	6:C:1477:DXC:H212	1.74	0.44
1:A:83:ILE:HG13	1:A:112:ILE:HD13	1.99	0.44
1:A:296:LYS:HE2	1:A:296:LYS:HB3	1.66	0.44
1:B:89:VAL:HA	1:B:117:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1477:DXC:H82	6:C:1477:DXC:H22	1.83	0.44
1:D:313:VAL:HA	1:D:314:PRO:HD3	1.78	0.44
1:A:131:ARG:O	1:A:135:ILE:HG13	2.18	0.44
1:A:185:TYR:CE2	1:A:187:LYS:HB2	2.52	0.44
1:B:276:VAL:HG11	1:B:379:PHE:CD1	2.53	0.44
1:B:405:VAL:HG11	1:B:444:LEU:HD13	2.00	0.44
1:C:360:ARG:O	1:C:369:ARG:HB3	2.18	0.44
1:D:109:HIS:CG	1:D:373:HIS:CE1	3.06	0.44
1:D:405:VAL:HG11	1:D:444:LEU:HB3	1.98	0.44
1:A:286:SER:OG	1:A:372:GLY:HA2	2.17	0.44
1:B:6:ILE:HD13	1:B:59:TYR:HD1	1.82	0.44
1:C:9:GLY:HA2	1:C:64:VAL:HB	2.00	0.44
1:C:136:MET:HE2	1:C:136:MET:HA	1.99	0.44
1:C:406:ILE:HD11	1:C:449:PHE:CZ	2.53	0.44
1:B:397:VAL:O	1:B:456:ARG:N	2.51	0.43
1:C:300:HIS:ND1	1:C:361:LEU:HD12	2.33	0.43
1:A:70:ALA:CB	1:A:365:PRO:HB3	2.48	0.43
1:A:329:LEU:C	1:A:331:GLU:H	2.26	0.43
1:D:186:PHE:HE1	1:D:207:ILE:HD13	1.82	0.43
1:C:292:ASN:OD1	1:C:294:THR:HG22	2.18	0.43
1:A:220:VAL:HG11	1:A:260:ILE:HD11	2.00	0.43
1:D:43:ARG:HH22	1:D:230:ARG:HD3	1.82	0.43
1:D:426:ILE:HB	1:D:431:ILE:HG12	2.00	0.43
1:A:328:ILE:HG21	1:A:467:TRP:CD1	2.53	0.43
1:C:221:LEU:HD23	1:C:224:ASN:HA	2.01	0.43
1:D:463:ARG:HE	1:D:465:ARG:CZ	2.31	0.43
1:C:36:LYS:O	1:C:38:PRO:HD3	2.19	0.43
1:C:79:ALA:O	1:C:83:ILE:HG13	2.19	0.43
1:C:380:LYS:HA	1:C:381:PRO:HD3	1.87	0.43
1:B:360:ARG:NH1	1:B:371:CMH:SG	2.92	0.43
6:C:1479:DXC:H61	6:C:1479:DXC:H10	1.78	0.43
1:D:442:LYS:HA	1:D:442:LYS:HD3	1.73	0.43
1:B:305:MET:HE3	1:B:305:MET:HB3	1.77	0.43
1:C:293:LEU:HD11	1:C:299:VAL:HG11	2.00	0.43
1:D:9:GLY:HA2	1:D:64:VAL:O	2.18	0.43
1:B:24:VAL:O	1:B:28:ILE:HG22	2.19	0.43
1:C:82:ILE:HD11	1:C:208:ASN:HA	1.99	0.43
1:C:284:LYS:HE3	5:C:1471:SO4:O1	2.19	0.43
1:D:34:HIS:NE2	1:D:235:PHE:O	2.51	0.43
1:D:220:VAL:HG13	1:D:266:LEU:HD13	1.99	0.43
1:C:39:GLU:H	1:C:39:GLU:HG2	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ARG:HG2	5:C:1473:SO4:O1	2.19	0.42
1:B:18:LYS:HB2	4:B:1469:GDP:O2B	2.19	0.42
1:C:67:PRO:HG2	1:C:71:ASP:OD2	2.19	0.42
1:B:143:THR:HG21	1:B:146:LEU:HB2	2.02	0.42
1:A:135:ILE:O	1:A:139:ILE:HG13	2.20	0.42
1:A:293:LEU:HD13	1:A:329:LEU:HD23	2.02	0.42
1:A:301:LEU:HD11	1:A:356:VAL:HG13	2.02	0.42
1:C:247:ARG:HG3	1:C:247:ARG:HH11	1.84	0.42
6:C:1475:DXC:H71	6:C:1475:DXC:H182	1.87	0.42
6:C:1475:DXC:H221	6:C:1475:DXC:H243	1.76	0.42
1:C:218:LEU:HD12	1:C:266:LEU:HD21	2.01	0.42
1:D:36:LYS:HA	1:D:236:LYS:HB3	2.02	0.42
1:B:308:VAL:HA	1:B:309:PRO:HD3	1.84	0.42
6:C:1476:DXC:H142	6:C:1476:DXC:H201	1.87	0.42
1:D:34:HIS:CD2	1:D:236:LYS:HB2	2.55	0.42
1:B:105:LEU:HB3	1:B:370:ILE:HD11	2.02	0.42
1:B:424:ILE:HD12	1:B:459:VAL:HG11	2.01	0.42
1:C:165:LEU:O	1:C:169:ILE:HG13	2.20	0.42
1:B:60:ARG:HD3	1:B:235:PHE:CE2	2.54	0.42
1:B:134:MET:SD	1:D:94:GLU:HG2	2.60	0.42
1:B:285:ILE:HG13	1:B:371:CMH:O	2.19	0.42
6:B:1473:DXC:H242	6:B:1473:DXC:H13	2.02	0.42
1:C:207:ILE:HG22	1:C:244:ALA:HA	2.01	0.42
1:C:230:ARG:HD2	1:C:253:GLN:CD	2.45	0.42
1:A:322:LYS:HG3	1:A:323:THR:H	1.84	0.42
1:C:188:MET:HA	1:C:189:PRO:HD2	1.92	0.42
1:A:285:ILE:HG23	1:A:291:TYR:CD2	2.55	0.41
1:D:6:ILE:HD11	1:D:61:ILE:HG12	2.00	0.41
1:D:74:ARG:O	1:D:307:ILE:HB	2.20	0.41
1:A:240:MET:CE	1:B:96:PRO:HD2	2.50	0.41
1:B:140:LEU:O	1:B:143:THR:HB	2.19	0.41
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.86	0.41
1:B:376:ILE:HG21	1:B:379:PHE:CE1	2.54	0.41
1:C:360:ARG:NH2	1:C:362:ASP:OD2	2.48	0.41
1:D:293:LEU:HG	1:D:314:PRO:HG3	2.02	0.41
1:A:449:PHE:CE1	1:A:453:VAL:HG21	2.55	0.41
1:D:170:ILE:HG22	1:D:174:ASN:ND2	2.35	0.41
1:D:362:ASP:O	1:D:364:PRO:HD3	2.20	0.41
1:B:77:VAL:HA	1:B:110:PHE:CE2	2.55	0.41
1:C:147:LYS:HE2	1:C:147:LYS:HB2	1.77	0.41
1:D:148:ASN:OD1	1:D:148:ASN:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:O	1:C:173:LEU:HG	2.21	0.41
6:C:1478:DXC:H61	6:C:1478:DXC:H10	1.89	0.41
1:A:85:LEU:HD12	1:A:113:PRO:O	2.21	0.41
1:D:32:SER:O	1:D:55:LYS:N	2.46	0.41
1:D:247:ARG:HA	1:D:247:ARG:HD2	1.90	0.41
1:A:360:ARG:CZ	1:A:363:LEU:HD21	2.51	0.41
1:C:-2:ARG:HA	1:C:-1:PRO:HD3	1.91	0.41
1:C:104:MET:HE2	1:C:104:MET:HB3	1.65	0.41
1:C:184:SER:OG	1:C:209:LYS:HB2	2.20	0.41
1:C:406:ILE:HD11	1:C:449:PHE:HZ	1.86	0.41
6:C:1477:DXC:H201	6:C:1477:DXC:H142	1.63	0.41
1:D:49:ILE:H	1:D:49:ILE:HG12	1.61	0.41
1:A:70:ALA:HB1	1:A:369:ARG:NH2	2.36	0.41
1:B:361:LEU:HA	1:B:369:ARG:HD2	2.02	0.41
1:B:363:LEU:HD22	1:B:363:LEU:HA	1.94	0.41
1:D:8:LEU:HD12	1:D:85:LEU:O	2.21	0.41
1:D:43:ARG:HD2	1:D:231:SER:HB2	2.03	0.41
1:D:136:MET:HB2	1:D:136:MET:HE2	1.68	0.41
1:D:358:ILE:HD13	1:D:371:CMH:CM	2.51	0.41
1:C:3:PHE:HB2	1:C:60:ARG:CZ	2.51	0.40
1:D:72:LEU:C	1:D:74:ARG:H	2.28	0.40
1:A:240:MET:CE	1:B:95:GLY:HA3	2.50	0.40
1:A:302:ASN:HB2	1:A:357:LEU:HB3	2.03	0.40
1:B:127:GLU:O	1:B:131:ARG:HG3	2.21	0.40
1:C:89:VAL:HB	1:C:119:THR:HG21	2.03	0.40
6:C:1475:DXC:H161	6:C:1475:DXC:H211	1.81	0.40
1:D:96:PRO:HG3	1:D:136:MET:SD	2.61	0.40
1:D:80:ALA:HB1	1:D:112:ILE:CD1	2.51	0.40
1:A:19:THR:HB	2:A:1469:GNP:O2B	2.20	0.40
1:A:229:VAL:HG11	1:A:250:MET:HE2	2.03	0.40
1:B:417:GLU:O	1:B:420:ILE:HG12	2.21	0.40
1:C:300:HIS:CE1	1:C:361:LEU:HD12	2.57	0.40
1:D:73:ILE:H	1:D:73:ILE:HG13	1.62	0.40
1:D:361:LEU:H	1:D:361:LEU:HG	1.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/482 (92%)	420 (95%)	24 (5%)	0	100	100
1	B	448/482 (93%)	429 (96%)	19 (4%)	0	100	100
1	C	465/482 (96%)	435 (94%)	28 (6%)	2 (0%)	30	59
1	D	461/482 (96%)	435 (94%)	25 (5%)	1 (0%)	43	71
All	All	1818/1928 (94%)	1719 (95%)	96 (5%)	3 (0%)	43	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	C	57	GLU
1	C	47	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/412 (94%)	346 (90%)	40 (10%)	7	26
1	B	388/412 (94%)	350 (90%)	38 (10%)	7	29
1	C	402/412 (98%)	344 (86%)	58 (14%)	3	14
1	D	398/412 (97%)	351 (88%)	47 (12%)	5	21
All	All	1574/1648 (96%)	1391 (88%)	183 (12%)	5	21

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	19	THR
1	A	28	ILE
1	A	52	SER
1	A	73	ILE
1	A	84	ASP
1	A	88	ILE
1	A	90	VAL
1	A	102	GLU
1	A	104	MET
1	A	148	ASN
1	A	150	SER
1	A	152	ILE
1	A	158	THR
1	A	168	LEU
1	A	212	VAL
1	A	250	MET
1	A	252	ILE
1	A	256	ASP
1	A	273	LEU
1	A	313	VAL
1	A	319	THR
1	A	328	ILE
1	A	332	VAL
1	A	333	ILE
1	A	345	GLU
1	A	348	VAL
1	A	356	VAL
1	A	357	LEU
1	A	362	ASP
1	A	366	THR
1	A	377	GLU
1	A	392	LEU
1	A	394	GLU
1	A	424	ILE
1	A	435	ILE
1	A	441	THR
1	A	449	PHE
1	A	458	LYS
1	A	460	ILE
1	B	28	ILE
1	B	45	ILE
1	B	47	ILE

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Mol	Chain	Res	Type
1	B	49	ILE
1	B	62	THR
1	B	82	ILE
1	B	90	VAL
1	B	104	MET
1	B	119	THR
1	B	126	THR
1	B	136	MET
1	B	148	ASN
1	B	162	VAL
1	B	163	ASP
1	B	164	GLU
1	B	183	GLU
1	B	208	ASN
1	B	212	VAL
1	B	225	MET
1	B	241	GLU
1	B	260	ILE
1	B	262	ARG
1	B	275	THR
1	B	287	ASP
1	B	291	TYR
1	B	303	VAL
1	B	305	MET
1	B	308	VAL
1	B	313	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	370	ILE
1	B	431	ILE
1	B	453	VAL
1	C	-2	ARG
1	C	6	ILE
1	C	14	ILE
1	C	24	VAL
1	C	28	ILE
1	C	39	GLU
1	C	45	ILE

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Mol	Chain	Res	Type
1	C	52	SER
1	C	71	ASP
1	C	78	SER
1	C	98	THR
1	C	114	ILE
1	C	123	ASN
1	C	126	THR
1	C	136	MET
1	C	142	SER
1	C	148	ASN
1	C	150	SER
1	C	158	THR
1	C	166	LYS
1	C	169	ILE
1	C	171	THR
1	C	191	ASP
1	C	218	LEU
1	C	223	ILE
1	C	226	SER
1	C	230	ARG
1	C	241	GLU
1	C	255	VAL
1	C	276	VAL
1	C	278	LYS
1	C	283	ILE
1	C	292	ASN
1	C	293	LEU
1	C	294	THR
1	C	306	LEU
1	C	311	VAL
1	C	319	THR
1	C	328	ILE
1	C	332	VAL
1	C	348	VAL
1	C	349	LEU
1	C	355	ARG
1	C	357	LEU
1	C	359	THR
1	C	362	ASP
1	C	366	THR
1	C	368	LEU
1	C	369	ARG

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Mol	Chain	Res	Type
1	C	373	HIS
1	C	378	GLU
1	C	391	VAL
1	C	424	ILE
1	C	435	ILE
1	C	445	LEU
1	C	446	THR
1	C	456	ARG
1	C	460	ILE
1	D	6	ILE
1	D	16	HIS
1	D	20	THR
1	D	24	VAL
1	D	25	LEU
1	D	31	THR
1	D	36	LYS
1	D	41	GLN
1	D	42	LYS
1	D	43	ARG
1	D	45	ILE
1	D	46	THR
1	D	49	ILE
1	D	65	ASP
1	D	73	ILE
1	D	74	ARG
1	D	76	VAL
1	D	78	SER
1	D	83	ILE
1	D	89	VAL
1	D	90	VAL
1	D	119	THR
1	D	128	GLU
1	D	139	ILE
1	D	143	THR
1	D	154	ILE
1	D	160	PHE
1	D	162	VAL
1	D	190	LEU
1	D	196	ILE
1	D	220	VAL
1	D	226	SER
1	D	233	GLN

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Mol	Chain	Res	Type
1	D	235	PHE
1	D	289	PHE
1	D	328	ILE
1	D	333	ILE
1	D	334	SER
1	D	348	VAL
1	D	361	LEU
1	D	362	ASP
1	D	363	LEU
1	D	368	LEU
1	D	387	ILE
1	D	426	ILE
1	D	435	ILE
1	D	453	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	300	HIS
1	B	462	ASN
1	C	181	ASN
1	C	233	GLN
1	D	58	ASN
1	D	69	HIS
1	D	233	GLN
1	D	373	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	338	1	5,7,8	0.64	0	1,7,9	0.39	0
1	CMH	A	338	1	5,7,8	0.58	0	1,7,9	0.21	0
1	CMH	B	338	1	5,7,8	0.59	0	1,7,9	0.72	0
1	CMH	C	340	1	5,7,8	0.84	0	1,7,9	0.47	0
1	CMH	C	371	1	5,7,8	0.69	0	1,7,9	0.43	0
1	CMH	C	264	1	5,7,8	0.68	0	1,7,9	0.21	0
1	CMH	A	264	1	5,7,8	0.61	0	1,7,9	0.54	0
1	CMH	D	340	1	5,7,8	0.67	0	1,7,9	0.78	0
1	CMH	D	371	1	5,7,8	0.63	0	1,7,9	0.23	0
1	CMH	A	340	1	5,7,8	0.65	0	1,7,9	0.44	0
1	CMH	B	264	1	5,7,8	0.77	0	1,7,9	0.46	0
1	CMH	A	371	1	5,7,8	0.56	0	1,7,9	0.68	0
1	CMH	D	264	1	5,7,8	0.62	0	1,7,9	0.14	0
1	CMH	B	371	1	5,7,8	0.55	0	1,7,9	0.30	0
1	CMH	B	340	1	5,7,8	0.55	0	1,7,9	0.51	0
1	CMH	C	338	1	5,7,8	0.64	0	1,7,9	0.22	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
1	CMH	D	338	1	-	0/0/6/8	-
1	CMH	A	338	1	-	0/0/6/8	-
1	CMH	B	338	1	-	0/0/6/8	-
1	CMH	C	340	1	-	0/0/6/8	-
1	CMH	C	371	1	-	0/0/6/8	-
1	CMH	C	264	1	-	0/0/6/8	-
1	CMH	A	264	1	-	0/0/6/8	-
1	CMH	D	340	1	-	0/0/6/8	-
1	CMH	D	371	1	-	0/0/6/8	-
1	CMH	A	340	1	-	0/0/6/8	-
1	CMH	B	264	1	-	0/0/6/8	-
1	CMH	A	371	1	-	0/0/6/8	-
1	CMH	D	264	1	-	0/0/6/8	-
1	CMH	B	371	1	-	0/0/6/8	-
1	CMH	B	340	1	-	0/0/6/8	-
1	CMH	C	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.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	338	CMH	2	0
1	A	338	CMH	1	0
1	C	340	CMH	2	0
1	C	371	CMH	3	0
1	D	340	CMH	4	0
1	D	371	CMH	2	0
1	A	340	CMH	2	0
1	B	371	CMH	2	0
1	C	338	CMH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	SO4	C	1481	-	4,4,4	0.29	0	6,6,6	0.07	0
5	SO4	C	1472	-	4,4,4	0.36	0	6,6,6	0.14	0
6	DXC	C	1475	-	31,31,31	1.62	5 (16%)	49,49,49	2.23	18 (36%)
2	GNP	A	1469	3	34,34,34	1.81	6 (17%)	47,54,54	1.07	3 (6%)
5	SO4	B	1471	-	4,4,4	0.27	0	6,6,6	0.10	0
6	DXC	C	1478	-	31,31,31	1.38	5 (16%)	49,49,49	1.87	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DXC	C	1479	-	31,31,31	1.57	8 (25%)	49,49,49	2.19	19 (38%)
6	DXC	C	1480	-	31,31,31	1.66	7 (22%)	49,49,49	2.08	16 (32%)
4	GDP	B	1469	3	29,30,30	1.23	3 (10%)	45,47,47	1.80	7 (15%)
5	SO4	C	1473	-	4,4,4	0.26	0	6,6,6	0.09	0
6	DXC	C	1477	-	31,31,31	1.64	6 (19%)	49,49,49	1.89	13 (26%)
7	5GP	B	1474	-	26,26,26	0.97	1 (3%)	39,40,40	1.76	10 (25%)
5	SO4	B	1472	-	4,4,4	0.24	0	6,6,6	0.11	0
6	DXC	B	1473	-	31,31,31	1.37	3 (9%)	49,49,49	2.08	15 (30%)
6	DXC	C	1476	-	31,31,31	1.51	5 (16%)	49,49,49	1.82	13 (26%)
5	SO4	C	1471	-	4,4,4	0.36	0	6,6,6	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DXC	C	1475	-	-	6/9/71/71	0/4/4/4
2	GNP	A	1469	3	-	5/18/38/38	0/3/3/3
6	DXC	C	1478	-	-	4/9/71/71	0/4/4/4
6	DXC	C	1479	-	-	7/9/71/71	0/4/4/4
6	DXC	C	1480	-	-	4/9/71/71	0/4/4/4
4	GDP	B	1469	3	-	8/16/32/32	0/3/3/3
6	DXC	C	1477	-	-	6/9/71/71	0/4/4/4
7	5GP	B	1474	-	-	2/10/26/26	0/3/3/3
6	DXC	B	1473	-	-	2/9/71/71	0/4/4/4
6	DXC	C	1476	-	-	4/9/71/71	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1469	GNP	PA-O3A	-6.55	1.52	1.59
2	A	1469	GNP	PB-O3A	-4.82	1.53	1.59
6	C	1475	DXC	C12-C13	-4.70	1.47	1.54
6	C	1477	DXC	C18-C4	-4.07	1.47	1.54
6	C	1480	DXC	C18-C4	-4.00	1.47	1.54
6	C	1477	DXC	C12-C13	-3.92	1.48	1.54
2	A	1469	GNP	PG-O1G	3.66	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1479	DXC	C18-C4	-3.48	1.48	1.54
6	C	1476	DXC	C12-C13	-3.46	1.49	1.54
6	C	1478	DXC	C18-C4	-3.27	1.48	1.54
6	C	1476	DXC	O1-C13	-3.16	1.38	1.43
6	C	1477	DXC	C4-C10	-3.16	1.50	1.56
4	B	1469	GDP	C5-C4	3.12	1.47	1.38
6	C	1480	DXC	C12-C13	-3.12	1.49	1.54
6	B	1473	DXC	C12-C13	-3.08	1.49	1.54
6	B	1473	DXC	C18-C4	-3.08	1.49	1.54
6	C	1479	DXC	C12-C13	-2.99	1.50	1.54
2	A	1469	GNP	PB-O2B	-2.96	1.49	1.56
4	B	1469	GDP	PA-O3A	2.93	1.62	1.59
6	C	1476	DXC	C12-C11	-2.93	1.50	1.55
6	C	1475	DXC	O1-C13	-2.91	1.38	1.43
6	C	1475	DXC	C12-C11	-2.89	1.50	1.55
6	C	1480	DXC	C5-C4	-2.84	1.49	1.54
6	C	1476	DXC	C20-C12	-2.83	1.49	1.54
6	C	1475	DXC	C20-C12	-2.82	1.49	1.54
6	C	1480	DXC	C12-C11	-2.76	1.50	1.55
6	B	1473	DXC	C4-C10	-2.71	1.51	1.56
6	C	1477	DXC	C20-C12	-2.69	1.50	1.54
7	B	1474	5GP	C6-N1	-2.63	1.33	1.38
6	C	1478	DXC	C12-C11	-2.61	1.51	1.55
6	C	1479	DXC	C4-C3	-2.56	1.51	1.55
6	C	1476	DXC	C18-C4	-2.52	1.50	1.54
6	C	1480	DXC	C4-C10	-2.49	1.51	1.56
6	C	1480	DXC	C4-C3	-2.44	1.51	1.55
6	C	1479	DXC	O1-C13	-2.43	1.39	1.43
6	C	1478	DXC	C12-C13	-2.42	1.50	1.54
6	C	1478	DXC	O1-C13	-2.39	1.39	1.43
6	C	1479	DXC	C4-C10	-2.29	1.52	1.56
6	C	1479	DXC	C12-C11	-2.28	1.51	1.55
6	C	1477	DXC	O1-C13	-2.24	1.39	1.43
6	C	1479	DXC	C20-C12	-2.24	1.50	1.54
6	C	1475	DXC	C18-C4	-2.21	1.50	1.54
4	B	1469	GDP	C6-N1	-2.20	1.34	1.38
6	C	1480	DXC	O1-C13	-2.16	1.40	1.43
6	C	1478	DXC	C20-C12	-2.13	1.50	1.54
6	C	1477	DXC	C12-C11	-2.11	1.52	1.55
2	A	1469	GNP	PG-O2G	-2.06	1.51	1.56
6	C	1479	DXC	C12-C17	-2.04	1.52	1.55
2	A	1469	GNP	PG-O3G	-2.00	1.51	1.56

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1469	GDP	C5-C4-N3	-6.11	118.67	128.39
6	C	1478	DXC	C10-C14-C13	-5.66	106.89	114.29
7	B	1474	5GP	C5-C4-N3	-5.47	119.69	128.39
6	C	1475	DXC	C15-C11-C12	-5.41	98.29	103.54
6	C	1479	DXC	C18-C4-C3	-5.26	101.64	110.44
4	B	1469	GDP	C2-N3-C4	5.22	121.29	112.30
6	C	1479	DXC	C6-C5-C4	-5.00	104.30	112.74
6	C	1479	DXC	C24-C19-C17	-4.93	105.49	112.88
6	C	1480	DXC	C20-C12-C13	4.87	113.93	109.06
6	C	1476	DXC	C18-C4-C3	-4.76	102.49	110.44
6	C	1475	DXC	C3-C2-C1	-4.75	105.55	112.71
6	C	1480	DXC	C18-C4-C5	-4.69	100.84	108.31
6	C	1477	DXC	C10-C14-C13	-4.68	108.17	114.29
6	B	1473	DXC	C5-C6-C1	-4.64	104.34	110.48
6	B	1473	DXC	C10-C4-C3	4.63	114.94	108.51
6	B	1473	DXC	C6-C5-C4	-4.55	105.05	112.74
6	C	1478	DXC	C7-C8-C9	-4.51	104.96	112.16
6	C	1477	DXC	C14-C13-C12	-4.47	106.72	111.26
4	B	1469	GDP	N9-C4-N3	4.45	134.85	125.95
6	C	1475	DXC	C17-C12-C13	-4.38	113.73	117.67
6	B	1473	DXC	C11-C9-C10	-4.32	103.45	109.09
7	B	1474	5GP	C2-N3-C4	4.23	119.59	112.30
6	C	1477	DXC	C7-C8-C9	-4.18	105.49	112.16
6	C	1475	DXC	C18-C4-C10	3.98	116.53	111.18
6	C	1475	DXC	O1-C13-C12	-3.97	104.31	111.02
6	C	1475	DXC	C5-C6-C1	-3.96	105.23	110.48
6	C	1477	DXC	C11-C9-C10	-3.95	103.93	109.09
6	B	1473	DXC	C14-C10-C4	-3.78	109.86	113.70
6	C	1479	DXC	C7-C8-C9	-3.76	106.16	112.16
6	C	1476	DXC	C4-C10-C9	-3.74	108.63	112.43
6	C	1475	DXC	C18-C4-C3	-3.73	104.20	110.44
6	C	1476	DXC	C10-C4-C3	3.71	113.66	108.51
2	A	1469	GNP	O3G-PG-O1G	-3.58	104.47	113.45
6	C	1476	DXC	C7-C8-C9	-3.54	106.51	112.16
6	C	1480	DXC	C7-C8-C9	-3.51	106.56	112.16
2	A	1469	GNP	O2B-PB-O1B	3.48	117.33	109.87
7	B	1474	5GP	N9-C4-N3	3.41	132.77	125.95
6	C	1479	DXC	C10-C4-C3	3.40	113.24	108.51
6	C	1475	DXC	C11-C9-C10	-3.38	104.67	109.09
6	C	1480	DXC	C17-C12-C13	-3.37	114.64	117.67
6	C	1480	DXC	C24-C19-C21	-3.36	105.13	110.34
6	C	1480	DXC	C11-C12-C13	-3.36	104.34	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1469	GDP	C6-C5-N7	3.35	136.38	130.29
6	C	1480	DXC	C16-C15-C11	-3.34	98.61	105.14
6	B	1473	DXC	C18-C4-C3	-3.33	104.87	110.44
6	C	1476	DXC	C10-C14-C13	-3.29	109.98	114.29
6	C	1477	DXC	C11-C12-C13	-3.28	104.42	107.42
6	C	1479	DXC	C5-C4-C3	3.26	112.43	107.75
6	C	1476	DXC	C8-C9-C10	3.25	114.42	110.52
6	B	1473	DXC	C5-C4-C10	-3.23	106.32	111.34
6	C	1479	DXC	C15-C11-C9	-3.23	113.95	119.10
6	C	1480	DXC	C5-C4-C10	3.22	116.34	111.34
6	C	1480	DXC	C10-C14-C13	-3.21	110.10	114.29
6	C	1475	DXC	C6-C5-C4	-3.14	107.45	112.74
6	C	1479	DXC	C11-C9-C10	-3.13	104.99	109.09
6	C	1475	DXC	C17-C12-C11	3.09	103.21	100.11
6	C	1478	DXC	C12-C17-C19	-3.07	115.76	119.48
2	A	1469	GNP	O2G-PG-O3G	3.05	115.78	107.59
6	C	1479	DXC	C14-C10-C4	-3.04	110.62	113.70
6	C	1477	DXC	C17-C12-C11	3.02	103.14	100.11
6	C	1479	DXC	C8-C9-C10	2.97	114.08	110.52
6	B	1473	DXC	C22-C21-C19	-2.94	108.97	114.46
6	C	1476	DXC	C22-C21-C19	-2.93	108.98	114.46
6	C	1477	DXC	C2-C3-C7	-2.93	106.66	111.73
6	C	1478	DXC	C3-C2-C1	-2.93	108.29	112.71
6	C	1480	DXC	C4-C10-C9	-2.92	109.47	112.43
6	C	1477	DXC	C10-C4-C3	2.90	112.55	108.51
6	B	1473	DXC	C20-C12-C11	2.88	115.72	111.20
6	C	1478	DXC	C16-C15-C11	-2.83	99.60	105.14
6	B	1473	DXC	C24-C19-C21	-2.81	105.99	110.34
6	C	1479	DXC	C4-C10-C9	-2.80	109.59	112.43
6	C	1476	DXC	C17-C12-C13	2.77	120.16	117.67
6	C	1477	DXC	C20-C12-C11	2.70	115.44	111.20
4	B	1469	GDP	C4-C5-N7	-2.68	106.42	110.67
6	C	1479	DXC	C14-C13-C12	-2.66	108.56	111.26
6	C	1479	DXC	C12-C17-C19	-2.65	116.27	119.48
6	C	1478	DXC	C24-C19-C21	-2.65	106.24	110.34
6	C	1479	DXC	C10-C14-C13	-2.65	110.83	114.29
6	C	1475	DXC	C2-C1-C6	-2.64	107.39	110.62
6	C	1479	DXC	C18-C4-C10	2.63	114.71	111.18
6	C	1476	DXC	C15-C11-C12	-2.62	101.00	103.54
6	C	1478	DXC	C10-C4-C3	2.62	112.16	108.51
6	C	1476	DXC	C5-C6-C1	2.62	113.95	110.48
6	C	1478	DXC	C8-C9-C10	2.58	113.61	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1474	5GP	C5-C6-N1	2.57	119.79	113.25
6	C	1478	DXC	C6-C5-C4	-2.56	108.42	112.74
6	C	1480	DXC	O1-C13-C12	-2.56	106.70	111.02
6	C	1479	DXC	C15-C11-C12	-2.54	101.08	103.54
6	C	1475	DXC	C18-C4-C5	-2.53	104.28	108.31
6	C	1475	DXC	C16-C15-C11	-2.52	100.21	105.14
6	C	1480	DXC	C10-C4-C3	2.50	111.99	108.51
6	C	1480	DXC	C3-C2-C1	-2.44	109.03	112.71
7	B	1474	5GP	O5'-P-O1P	-2.38	100.01	106.44
7	B	1474	5GP	C2-N1-C6	-2.37	120.81	125.11
6	C	1478	DXC	C2-C3-C7	-2.37	107.63	111.73
6	C	1477	DXC	C16-C15-C11	-2.35	100.54	105.14
7	B	1474	5GP	N9-C8-N7	-2.34	109.06	113.40
6	B	1473	DXC	C15-C11-C12	2.34	105.81	103.54
6	C	1475	DXC	C2-C3-C4	-2.34	110.17	112.66
4	B	1469	GDP	O2A-PA-O3A	2.29	113.46	107.27
6	C	1478	DXC	C2-C1-C6	-2.27	107.85	110.62
6	C	1479	DXC	C11-C12-C13	2.27	109.49	107.42
6	C	1480	DXC	O2-C1-C2	2.25	114.33	109.84
6	C	1476	DXC	C15-C11-C9	-2.23	115.54	119.10
6	C	1477	DXC	C12-C11-C9	2.22	117.08	114.69
6	C	1478	DXC	C18-C4-C3	-2.21	106.74	110.44
6	C	1478	DXC	C8-C7-C3	-2.18	107.62	111.84
6	C	1478	DXC	C21-C19-C17	2.18	114.85	110.33
6	C	1476	DXC	C3-C2-C1	-2.17	109.43	112.71
6	C	1480	DXC	C8-C9-C10	2.17	113.11	110.52
6	C	1476	DXC	C16-C17-C19	-2.16	108.91	112.18
7	B	1474	5GP	O6-C6-C5	-2.16	120.83	126.53
6	C	1475	DXC	C12-C11-C9	2.15	117.00	114.69
4	B	1469	GDP	O6-C6-C5	-2.13	120.91	126.53
6	C	1475	DXC	C14-C10-C4	2.13	115.86	113.70
6	C	1479	DXC	C7-C3-C4	-2.11	108.76	112.31
6	B	1473	DXC	O4-C23-C22	2.11	120.68	114.00
6	B	1473	DXC	C4-C10-C9	-2.10	110.30	112.43
6	B	1473	DXC	C2-C3-C4	2.09	114.88	112.66
6	C	1475	DXC	C12-C17-C19	-2.09	116.96	119.48
6	C	1477	DXC	C20-C12-C13	-2.08	106.98	109.06
6	C	1478	DXC	O4-C23-C22	2.08	120.56	114.00
6	C	1475	DXC	C24-C19-C21	-2.07	107.13	110.34
6	B	1473	DXC	C14-C10-C9	2.07	114.10	110.81
7	B	1474	5GP	O2P-P-O5'	-2.07	101.27	106.67
6	C	1478	DXC	C22-C21-C19	-2.07	110.60	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1477	DXC	O4-C23-C22	2.06	120.52	114.00
6	C	1479	DXC	C18-C4-C5	-2.04	105.06	108.31
7	B	1474	5GP	C4-C5-N7	-2.02	107.47	110.67
6	C	1480	DXC	C2-C3-C4	-2.01	110.52	112.66

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1469	GNP	PB-N3B-PG-O1G
2	A	1469	GNP	PG-N3B-PB-O1B
2	A	1469	GNP	PG-N3B-PB-O3A
2	A	1469	GNP	PA-O3A-PB-O2B
4	B	1469	GDP	PA-O3A-PB-O3B
4	B	1469	GDP	C5'-O5'-PA-O3A
4	B	1469	GDP	C5'-O5'-PA-O1A
4	B	1469	GDP	C5'-O5'-PA-O2A
6	C	1479	DXC	C16-C17-C19-C24
6	C	1479	DXC	C12-C17-C19-C24
6	C	1479	DXC	C12-C17-C19-C21
6	C	1476	DXC	C24-C19-C21-C22
7	B	1474	5GP	C3'-C4'-C5'-O5'
6	C	1477	DXC	C24-C19-C21-C22
6	C	1479	DXC	C24-C19-C21-C22
6	C	1477	DXC	C17-C19-C21-C22
6	C	1476	DXC	C17-C19-C21-C22
6	C	1479	DXC	C16-C17-C19-C21
7	B	1474	5GP	O4'-C4'-C5'-O5'
6	C	1480	DXC	C16-C17-C19-C24
6	C	1475	DXC	C12-C17-C19-C24
6	C	1480	DXC	C12-C17-C19-C24
6	C	1478	DXC	C12-C17-C19-C24
6	C	1475	DXC	C12-C17-C19-C21
6	C	1475	DXC	C16-C17-C19-C24
4	B	1469	GDP	PB-O3A-PA-O1A
6	C	1478	DXC	C16-C17-C19-C24
6	C	1479	DXC	C17-C19-C21-C22
6	C	1480	DXC	C16-C17-C19-C21
6	C	1478	DXC	C12-C17-C19-C21
6	C	1478	DXC	C16-C17-C19-C21
6	C	1475	DXC	C16-C17-C19-C21
6	B	1473	DXC	C21-C22-C23-O3

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Mol	Chain	Res	Type	Atoms
6	B	1473	DXC	C21-C22-C23-O4
6	C	1480	DXC	C12-C17-C19-C21
6	C	1475	DXC	C21-C22-C23-O4
6	C	1476	DXC	C21-C22-C23-O4
4	B	1469	GDP	PA-O3A-PB-O1B
6	C	1477	DXC	C16-C17-C19-C21
6	C	1475	DXC	C21-C22-C23-O3
6	C	1476	DXC	C21-C22-C23-O3
6	C	1477	DXC	C21-C22-C23-O4
4	B	1469	GDP	C4'-C5'-O5'-PA
2	A	1469	GNP	PA-O3A-PB-O1B
4	B	1469	GDP	O4'-C4'-C5'-O5'
6	C	1477	DXC	C21-C22-C23-O3
6	C	1479	DXC	C19-C21-C22-C23
6	C	1477	DXC	C12-C17-C19-C24

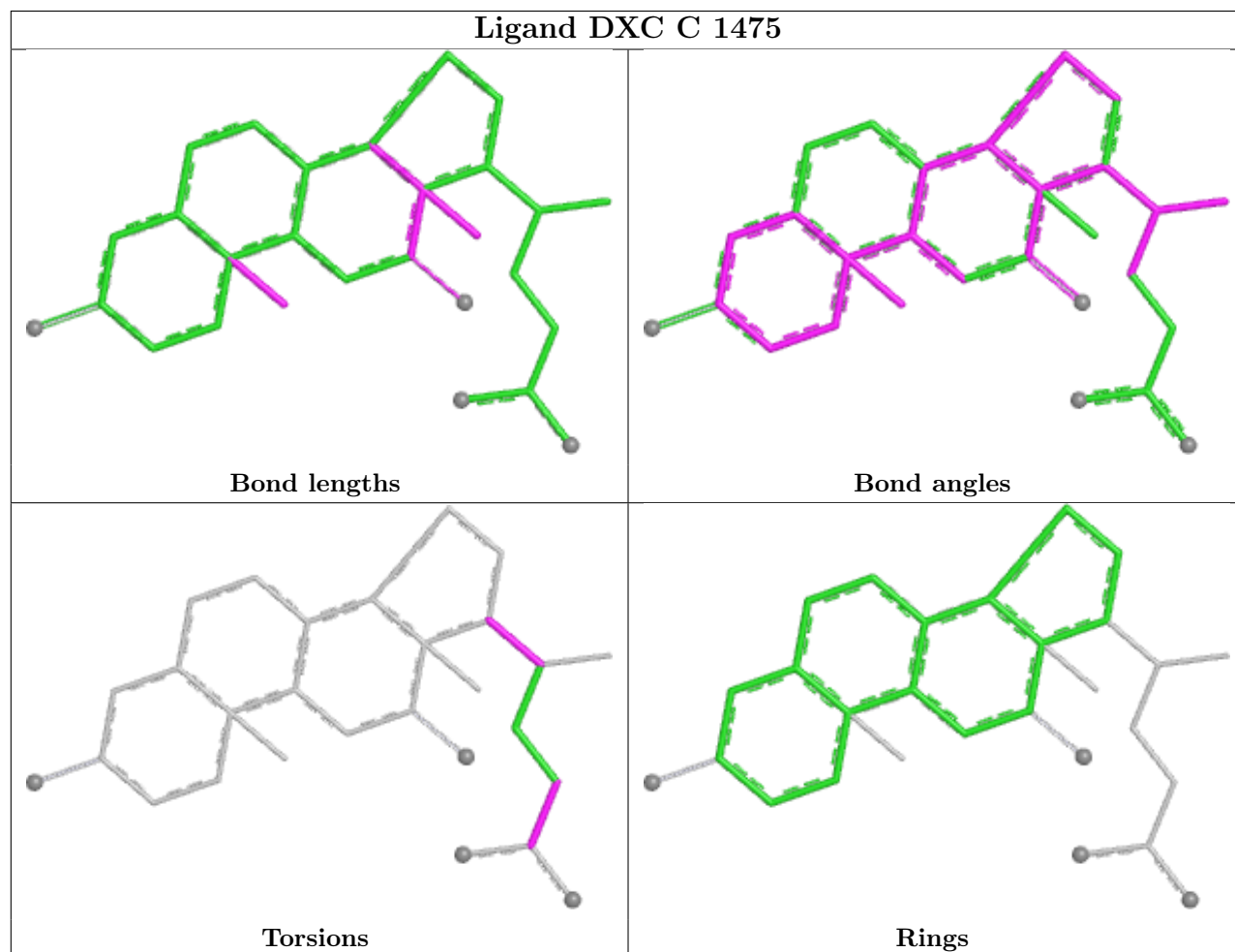
There are no ring outliers.

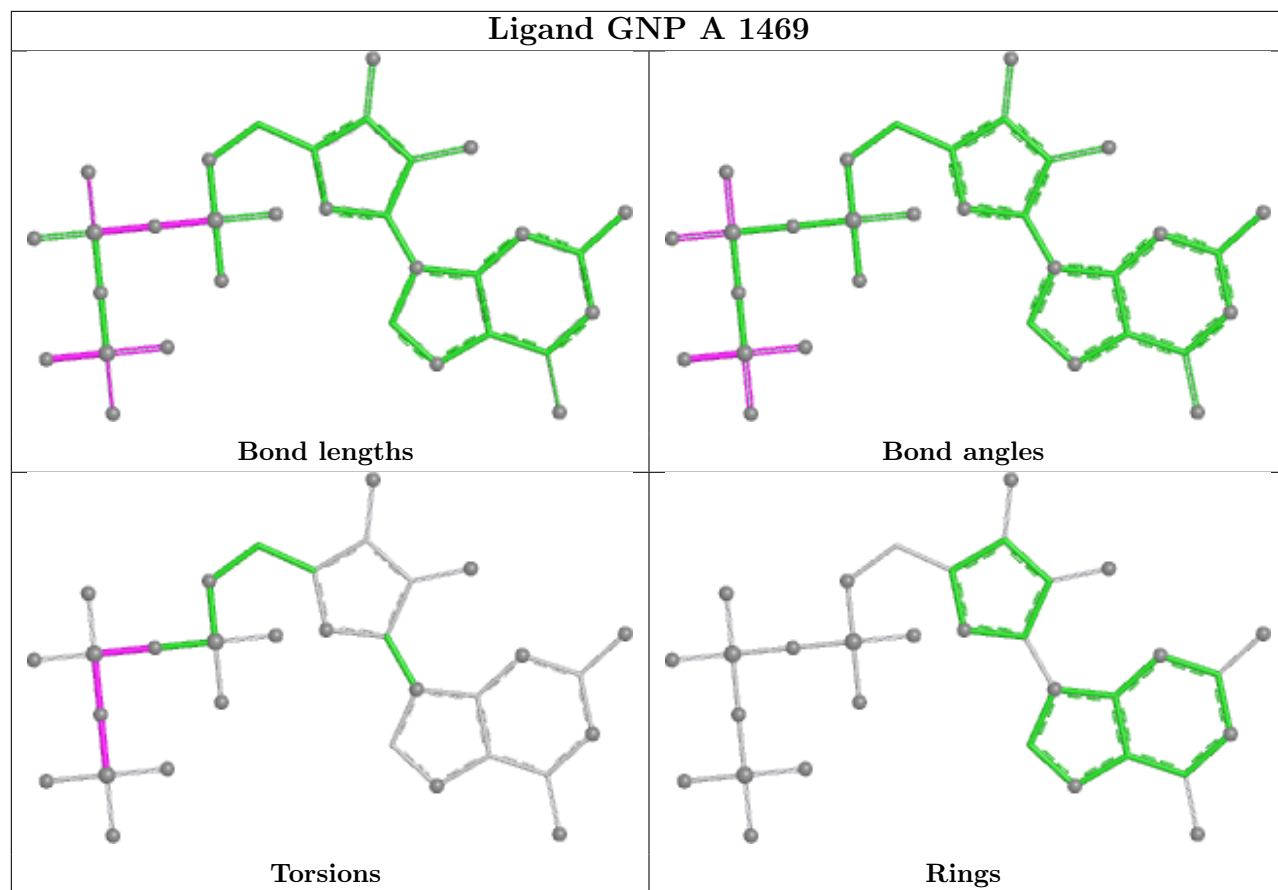
14 monomers are involved in 29 short contacts:

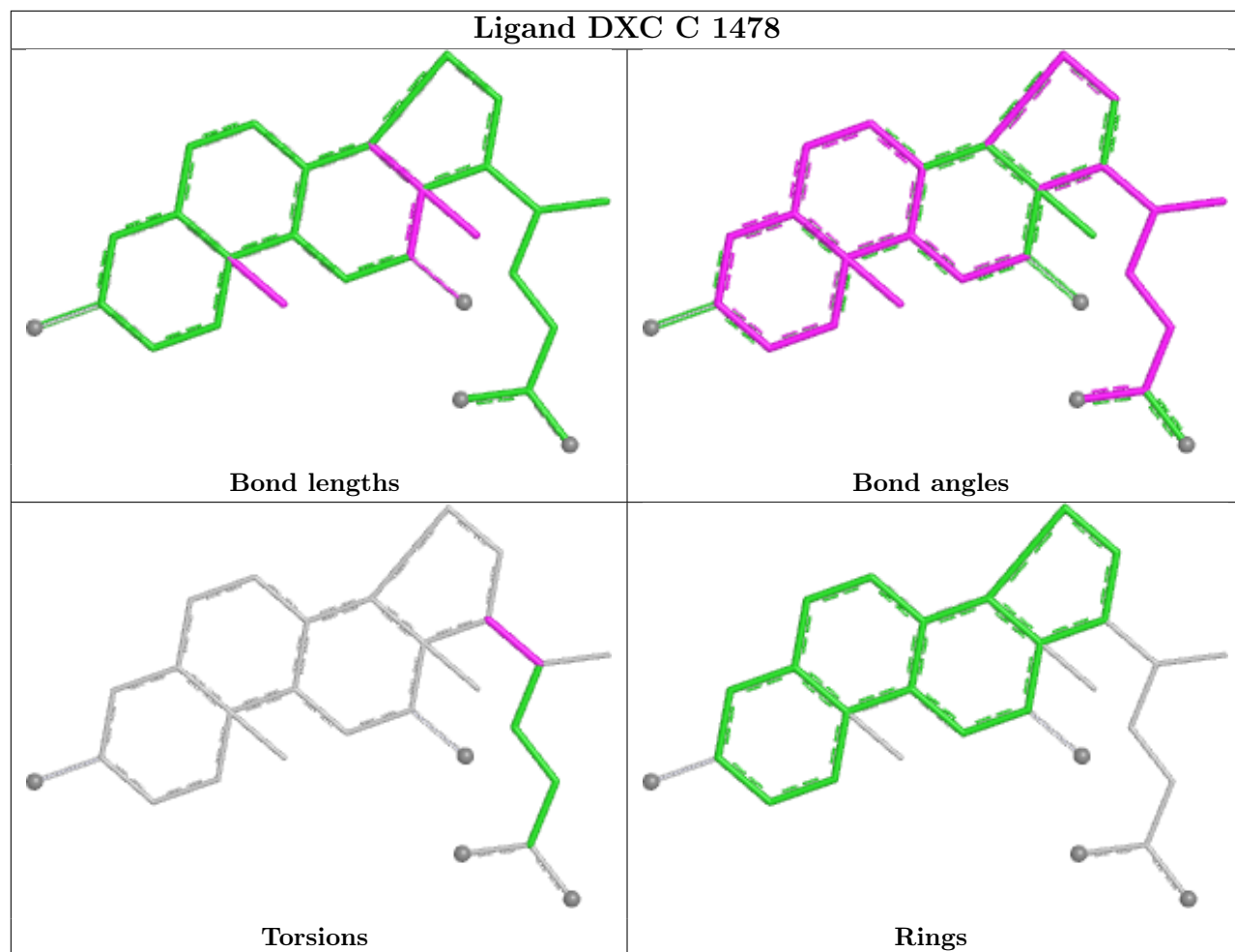
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1475	DXC	5	0
2	A	1469	GNP	2	0
5	B	1471	SO4	1	0
6	C	1478	DXC	2	0
6	C	1479	DXC	1	0
6	C	1480	DXC	2	0
4	B	1469	GDP	2	0
5	C	1473	SO4	1	0
6	C	1477	DXC	3	0
7	B	1474	5GP	2	0
5	B	1472	SO4	1	0
6	B	1473	DXC	4	0
6	C	1476	DXC	2	0
5	C	1471	SO4	1	0

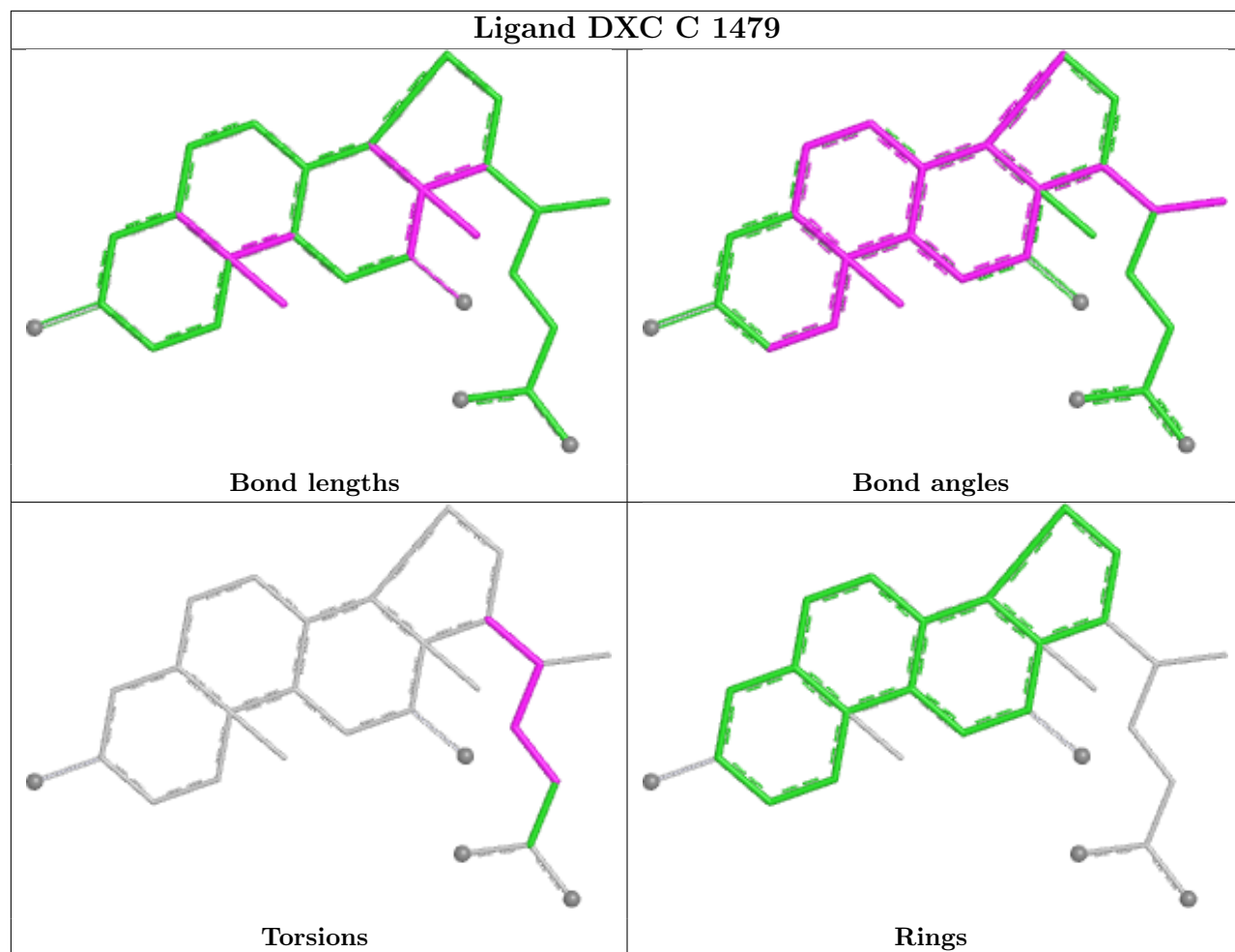
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

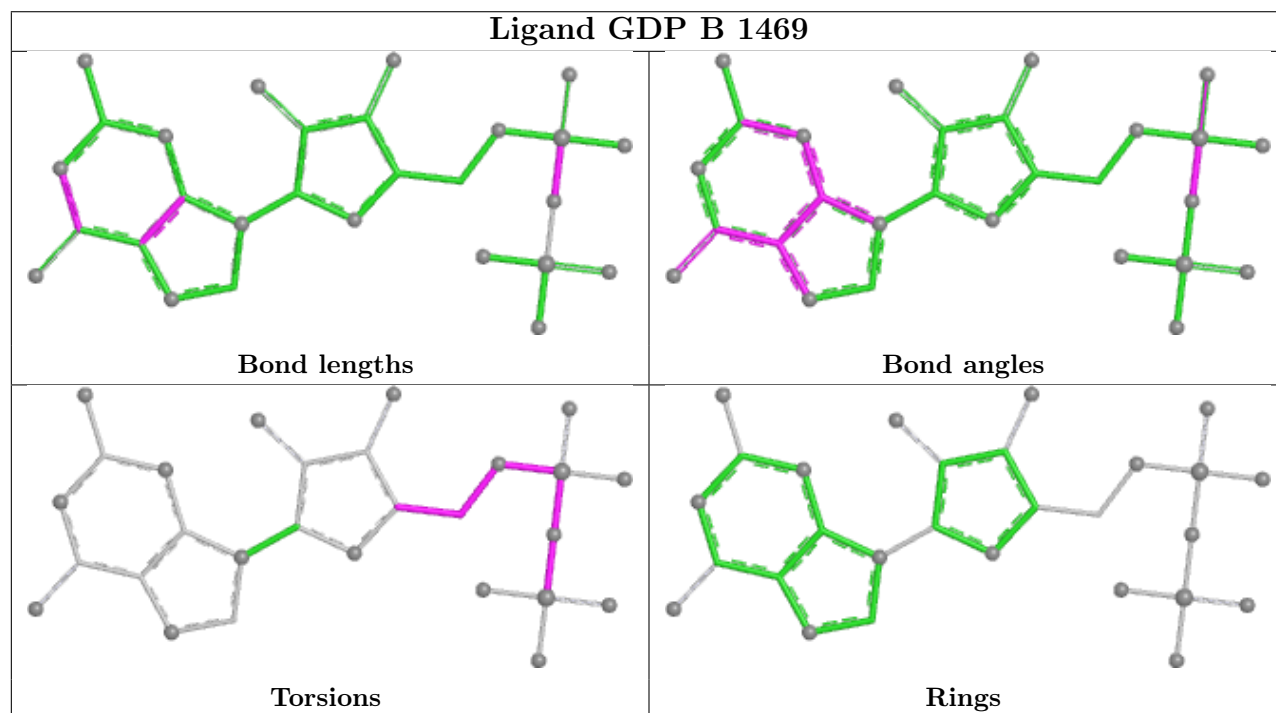
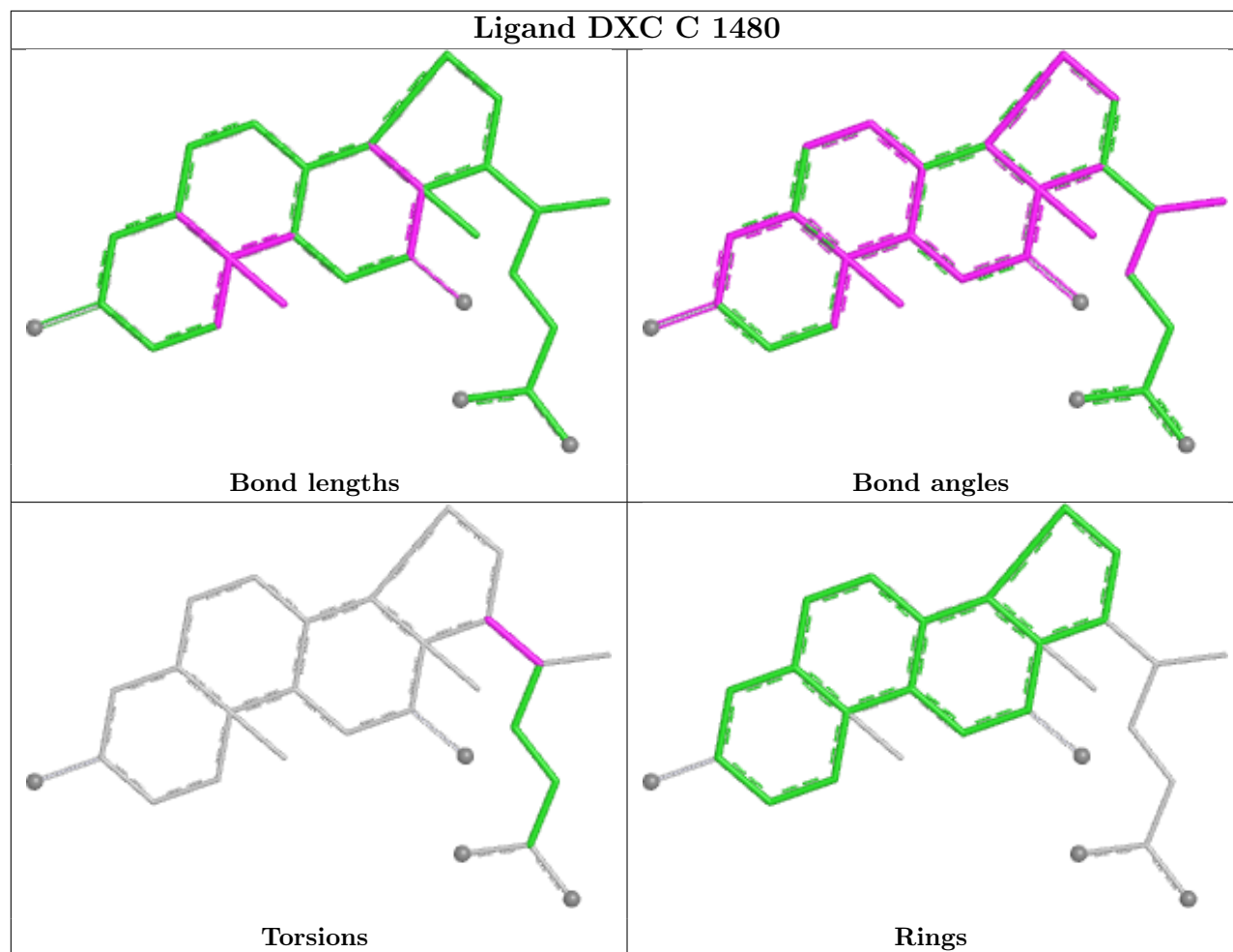
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



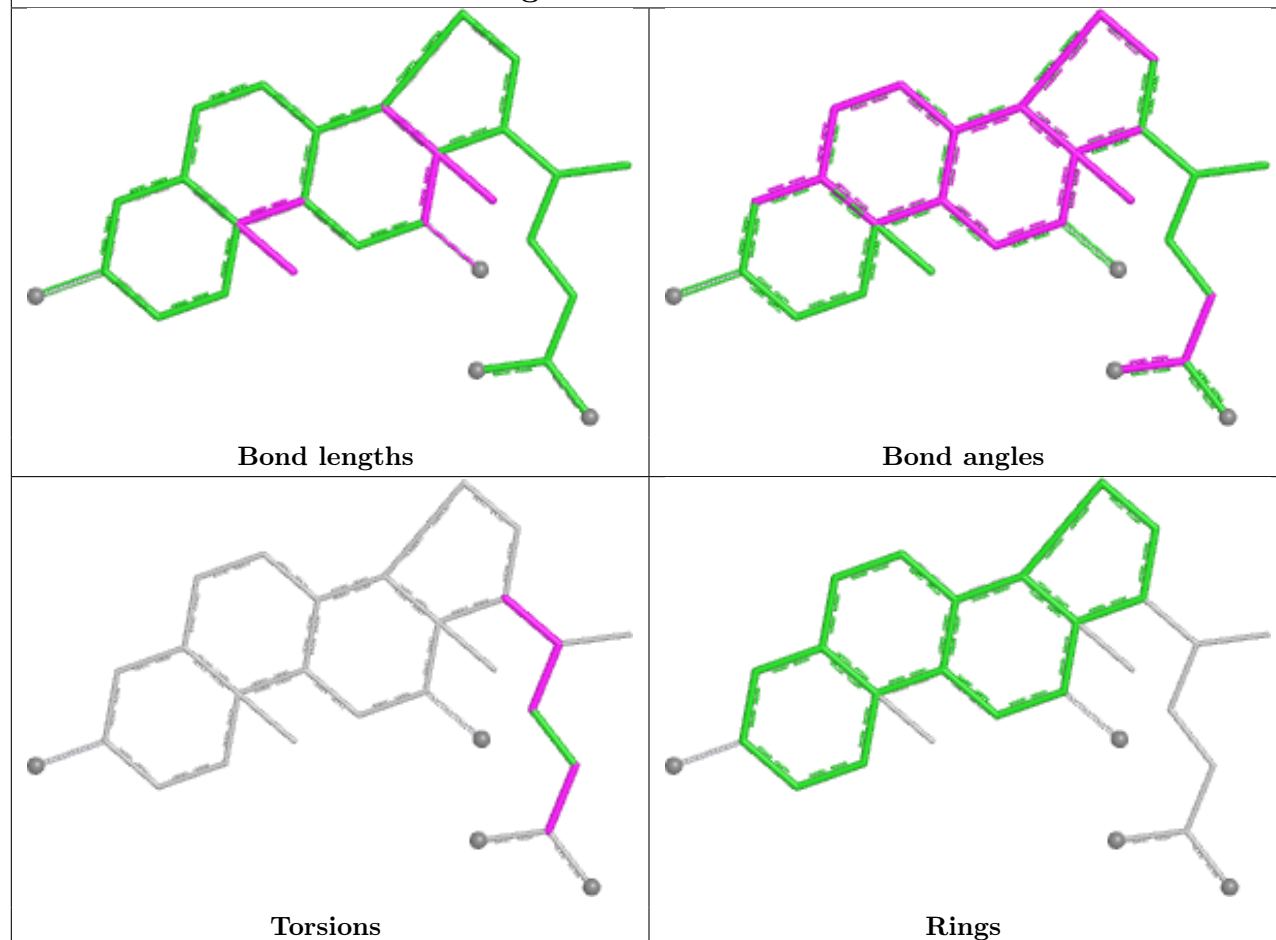




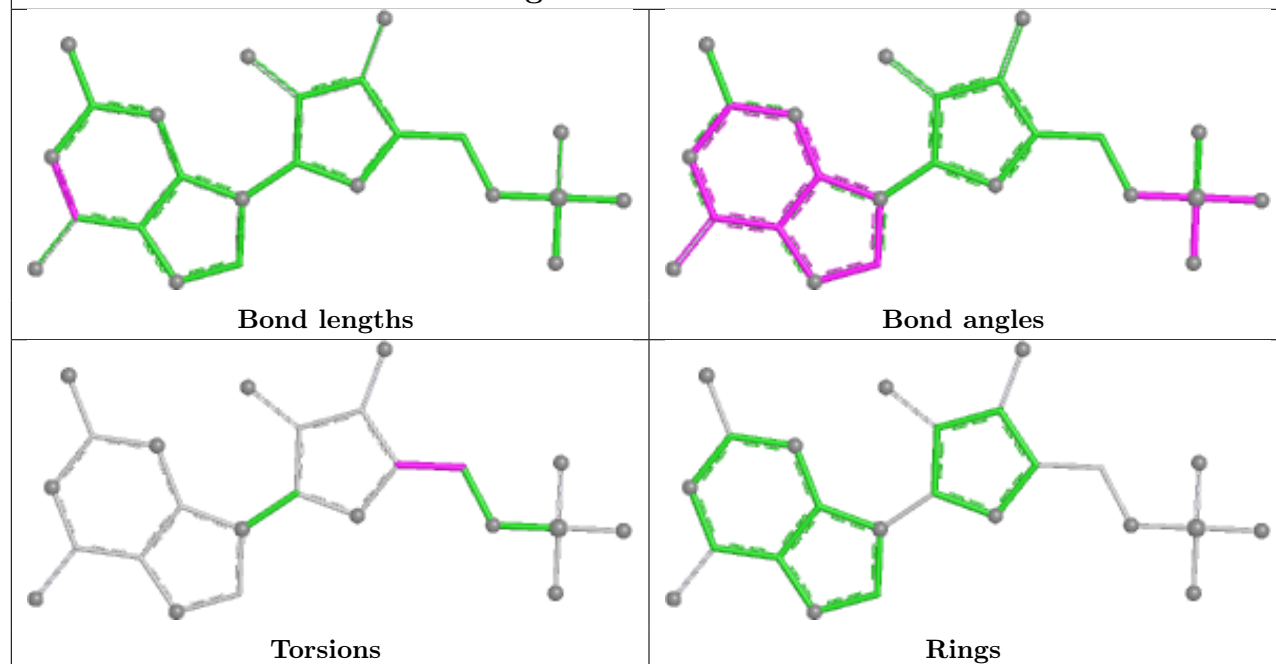


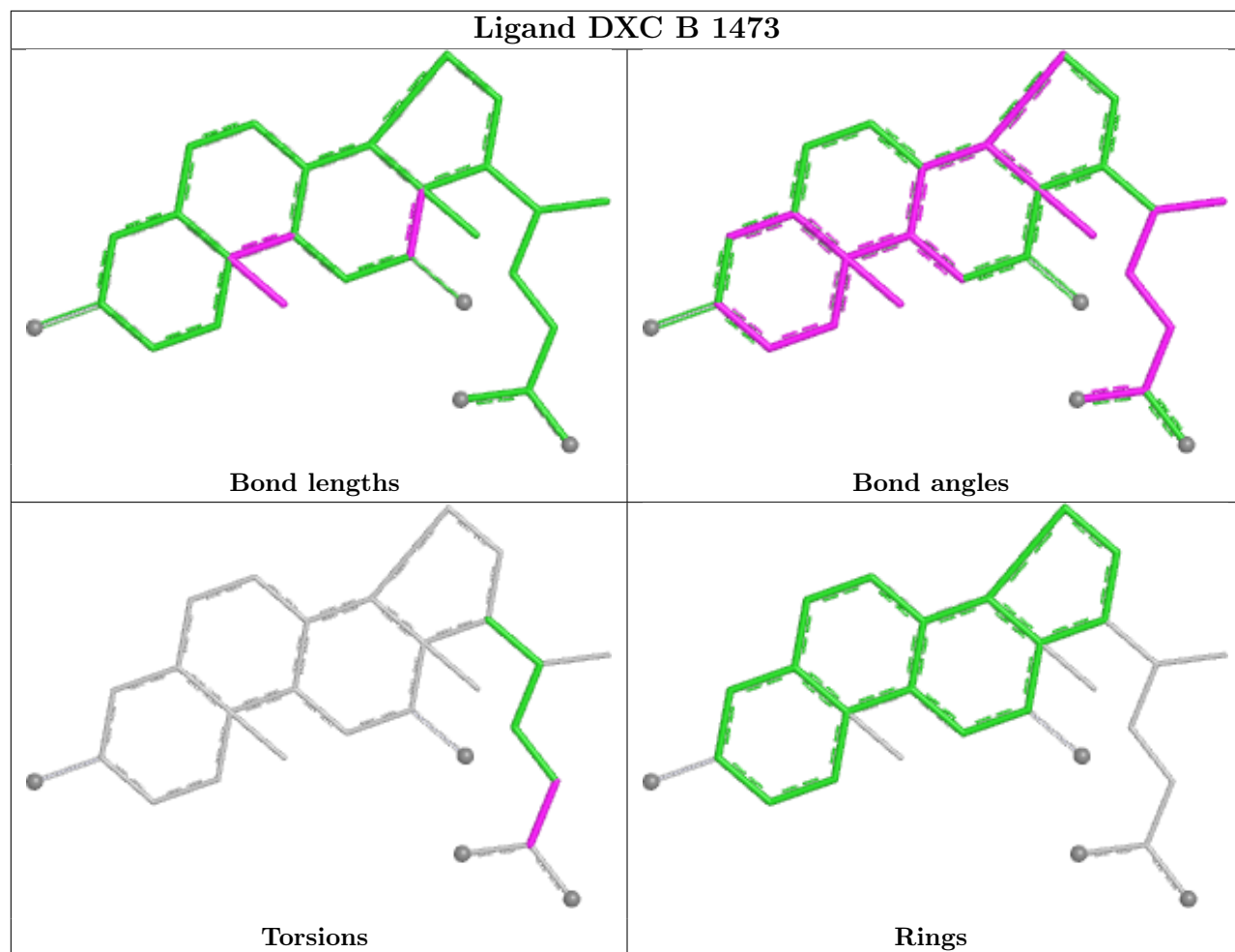


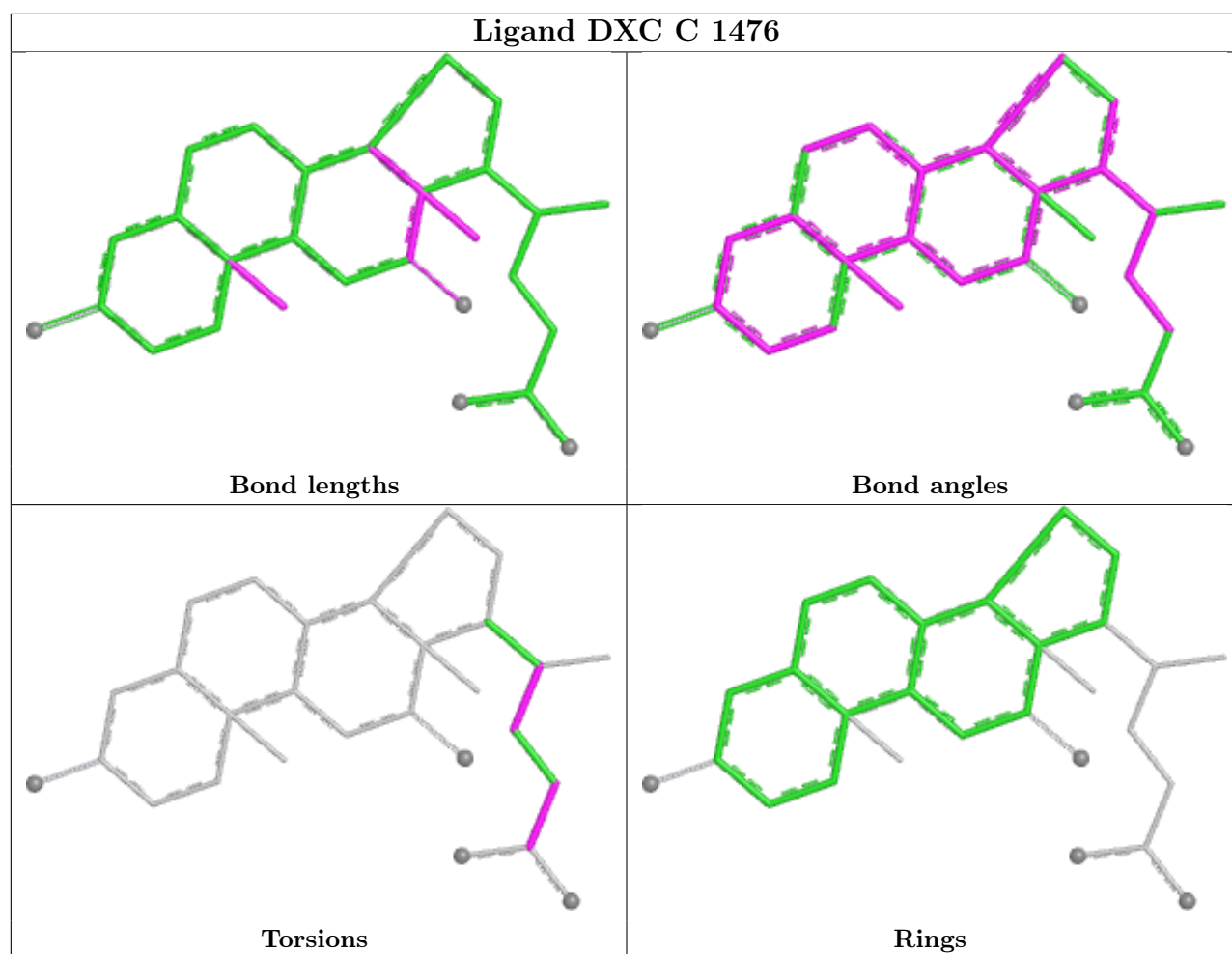
Ligand DXC C 1477



Ligand 5GP B 1474







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	448/482 (92%)	-0.47	3 (0%) 84 71	107, 205, 299, 372	0
1	B	452/482 (93%)	-0.48	1 (0%) 91 87	80, 152, 347, 414	0
1	C	467/482 (96%)	-0.53	1 (0%) 91 87	74, 123, 227, 308	0
1	D	463/482 (96%)	-0.23	3 (0%) 85 74	140, 274, 369, 416	0
All	All	1830/1928 (94%)	-0.43	8 (0%) 88 80	74, 188, 338, 416	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	ILE	2.8
1	A	291	TYR	2.7
1	A	333	ILE	2.6
1	D	260	ILE	2.3
1	B	226	SER	2.3
1	C	31	THR	2.2
1	D	173	LEU	2.2
1	D	221	LEU	2.1

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	A	338	8/9	0.81	0.15	174,190,268,307	2
1	CMH	B	338	8/9	0.82	0.17	151,200,232,276	2
1	CMH	A	371	8/9	0.83	0.13	168,213,225,228	2
1	CMH	B	371	8/9	0.86	0.11	174,197,251,332	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CMH	D	338	8/9	0.88	0.08	180,242,266,268	2
1	CMH	D	264	8/9	0.95	0.08	241,255,280,281	2
1	CMH	D	340	8/9	0.95	0.12	207,306,312,317	2
1	CMH	D	371	8/9	0.96	0.12	145,181,227,234	2
1	CMH	C	338	8/9	0.97	0.10	74,109,174,331	2
1	CMH	C	371	8/9	0.97	0.12	78,109,123,156	2
1	CMH	B	340	8/9	0.97	0.11	160,194,264,332	0
1	CMH	C	340	8/9	0.98	0.11	69,99,124,131	2
1	CMH	A	340	8/9	0.98	0.09	169,213,226,240	2
1	CMH	A	264	8/9	0.98	0.08	171,215,224,235	2
1	CMH	C	264	8/9	1.00	0.04	70,108,137,210	0
1	CMH	B	264	8/9	1.00	0.06	73,89,99,112	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

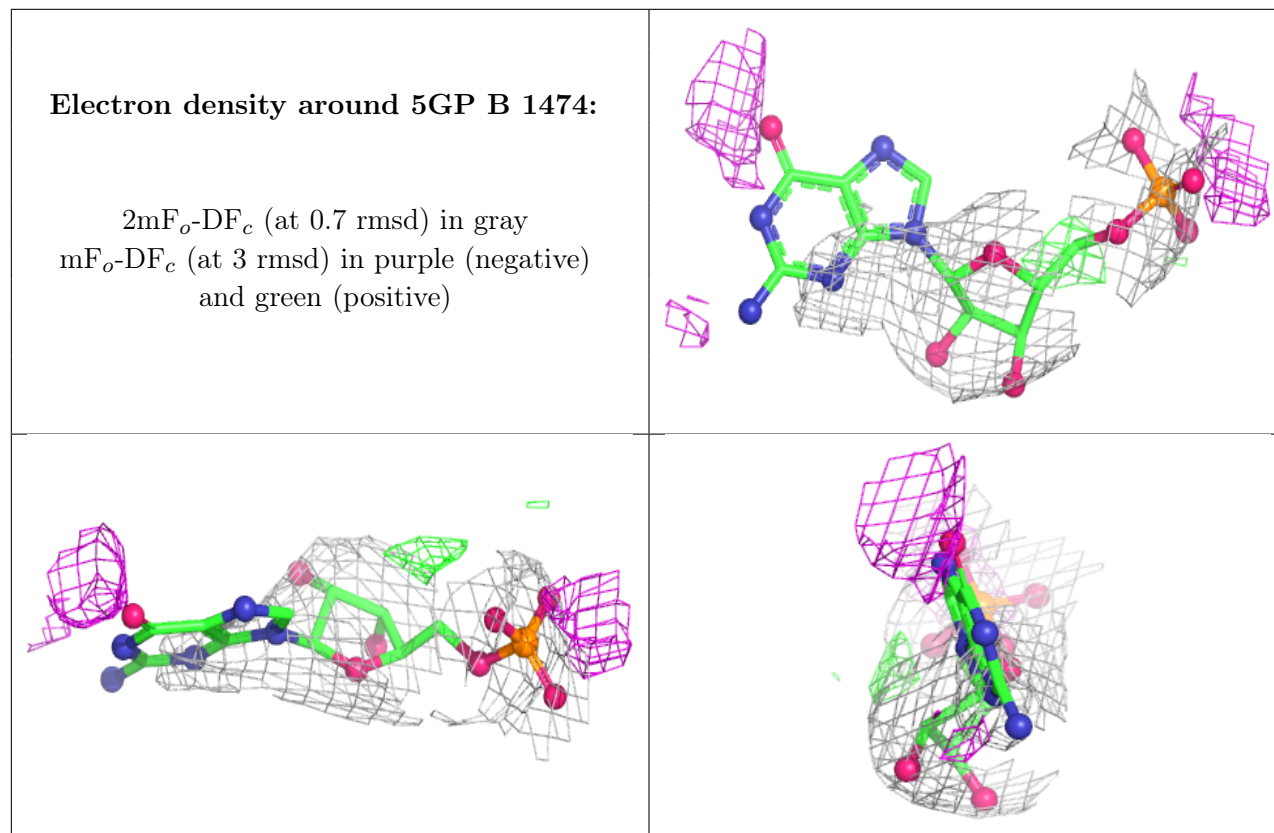
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	1481	5/5	0.77	0.08	172,210,221,235	5
3	MG	B	1470	1/1	0.81	0.14	342,342,342,342	0
5	SO4	B	1471	5/5	0.82	0.13	205,213,271,283	0
7	5GP	B	1474	24/24	0.82	0.16	242,294,308,311	0
4	GDP	B	1469	28/28	0.85	0.09	126,197,212,235	0
5	SO4	C	1473	5/5	0.88	0.04	164,166,220,230	5
5	SO4	C	1472	5/5	0.92	0.13	133,154,189,210	0
5	SO4	B	1472	5/5	0.93	0.07	139,226,336,344	0
2	GNP	A	1469	32/32	0.94	0.06	120,165,202,249	0
6	DXC	B	1473	28/28	0.94	0.10	68,97,134,143	0
5	SO4	C	1471	5/5	0.94	0.07	101,149,159,220	0
6	DXC	C	1477	28/28	0.96	0.07	91,111,162,182	0
6	DXC	C	1480	28/28	0.96	0.07	63,85,106,127	0
6	DXC	C	1476	28/28	0.96	0.10	159,168,217,253	0
6	DXC	C	1478	28/28	0.97	0.07	93,118,158,196	0
6	DXC	C	1479	28/28	0.97	0.08	82,104,174,196	28

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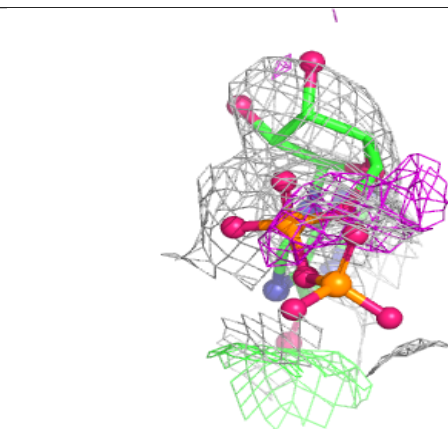
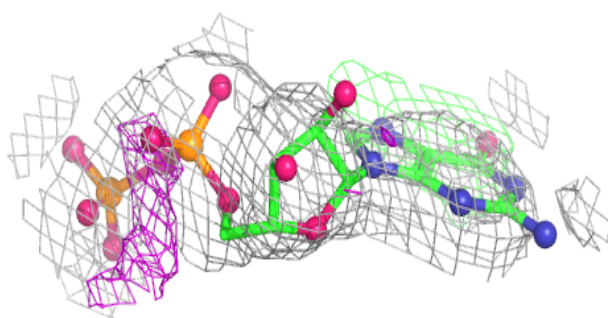
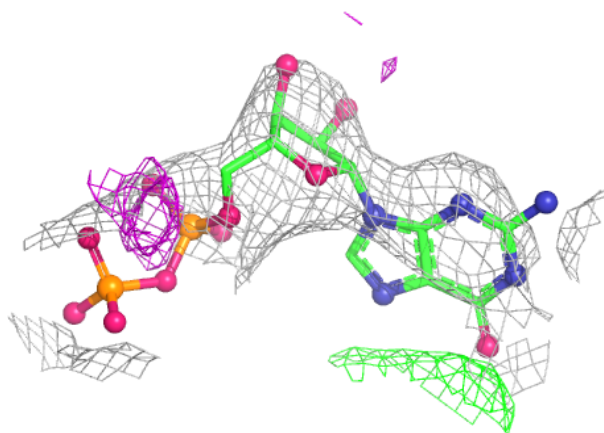
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1470	1/1	0.97	0.05	244,244,244,244	0
6	DXC	C	1475	28/28	0.97	0.07	61,95,139,146	0

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.

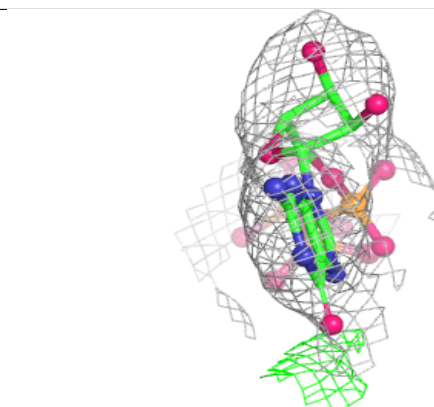
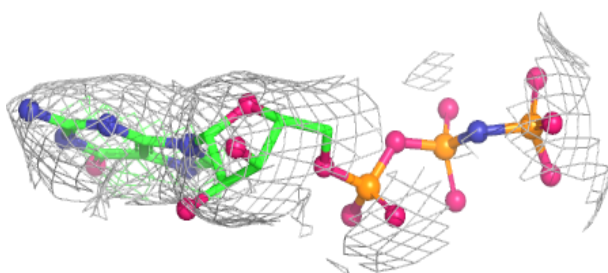
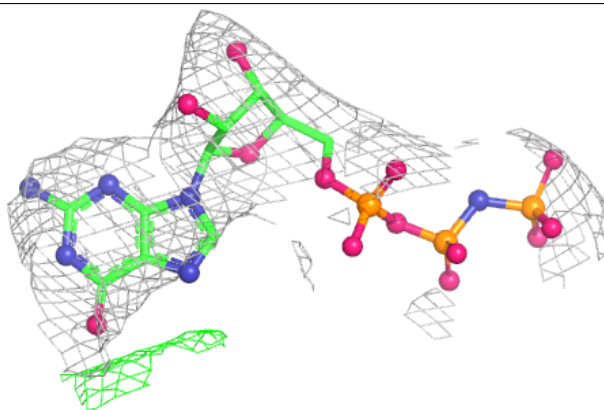


Electron density around GDP B 1469:

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

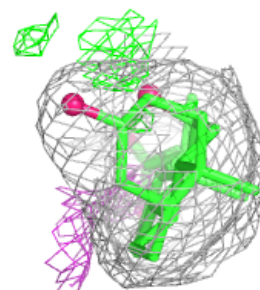
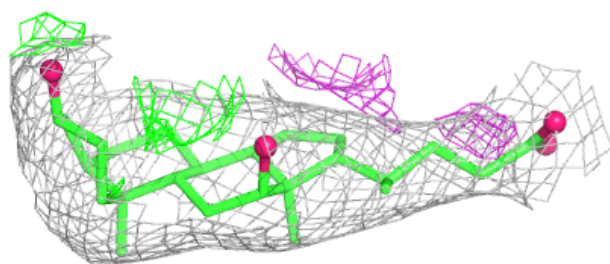
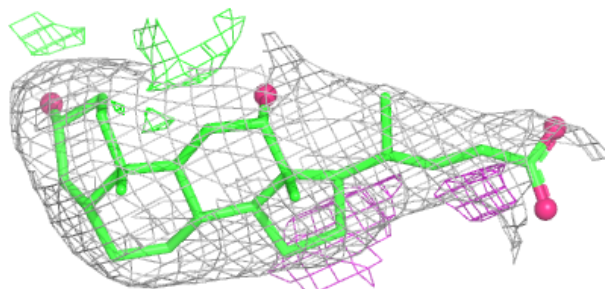
**Electron density around GNP A 1469:**

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

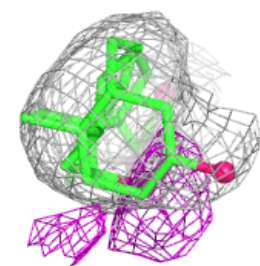
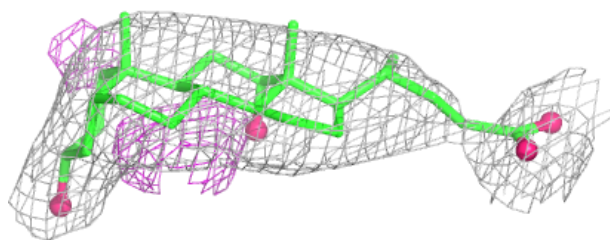
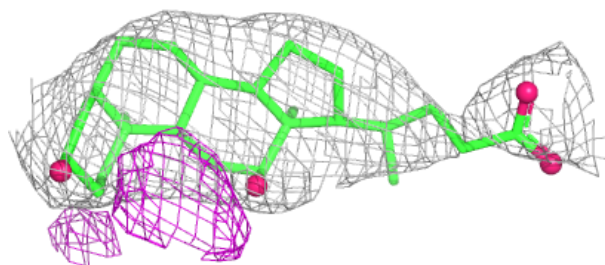


Electron density around DXC B 1473:

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

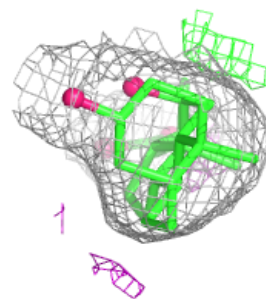
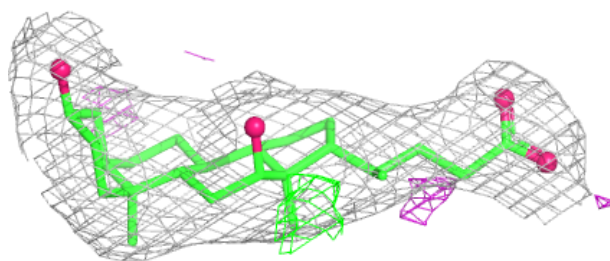
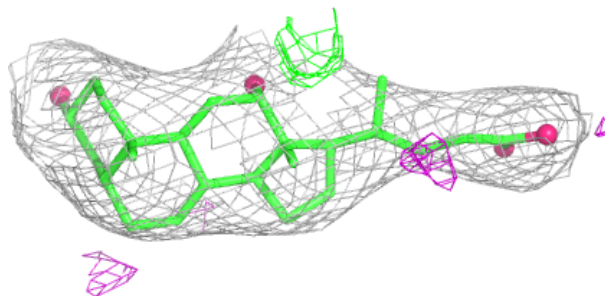
**Electron density around DXC C 1477:**

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

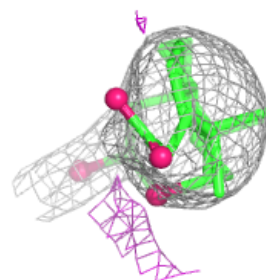
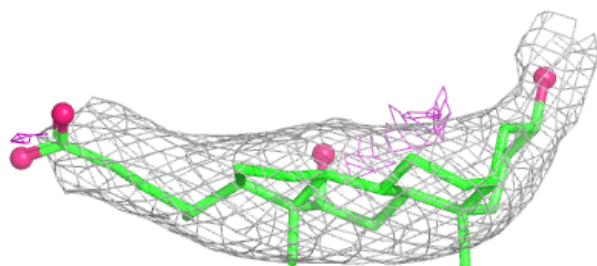
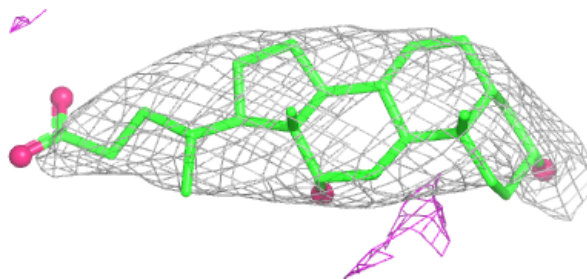


Electron density around DXC C 1480:

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and green (positive)

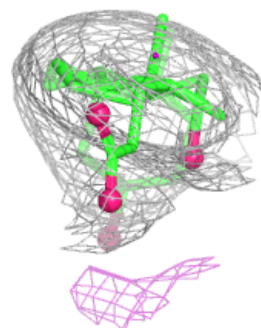
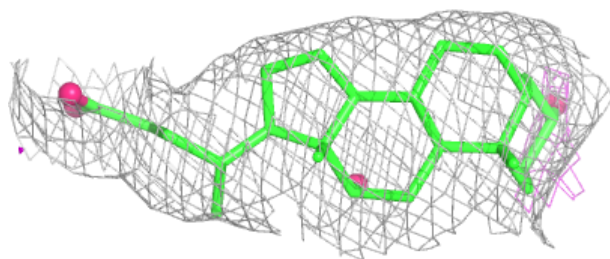
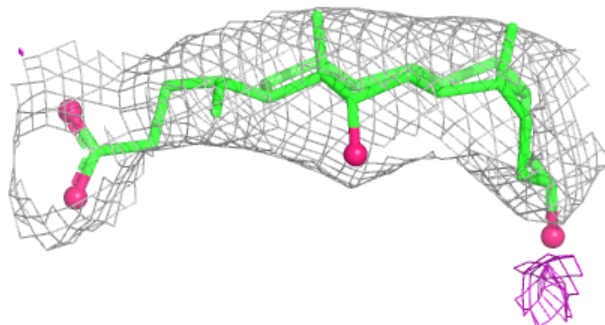
**Electron density around DXC C 1476:**

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

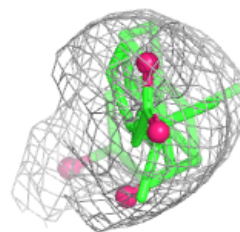
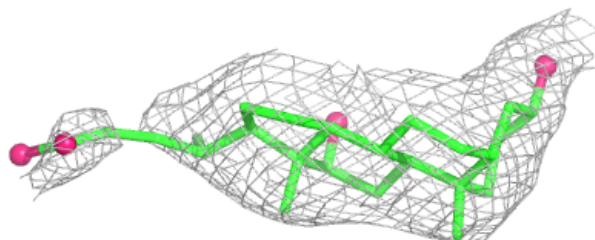
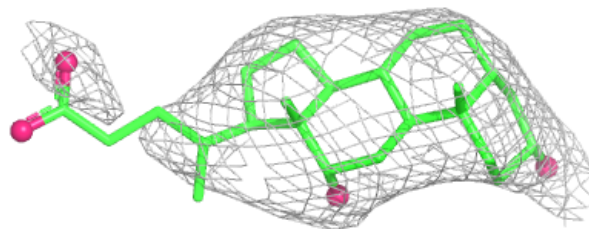


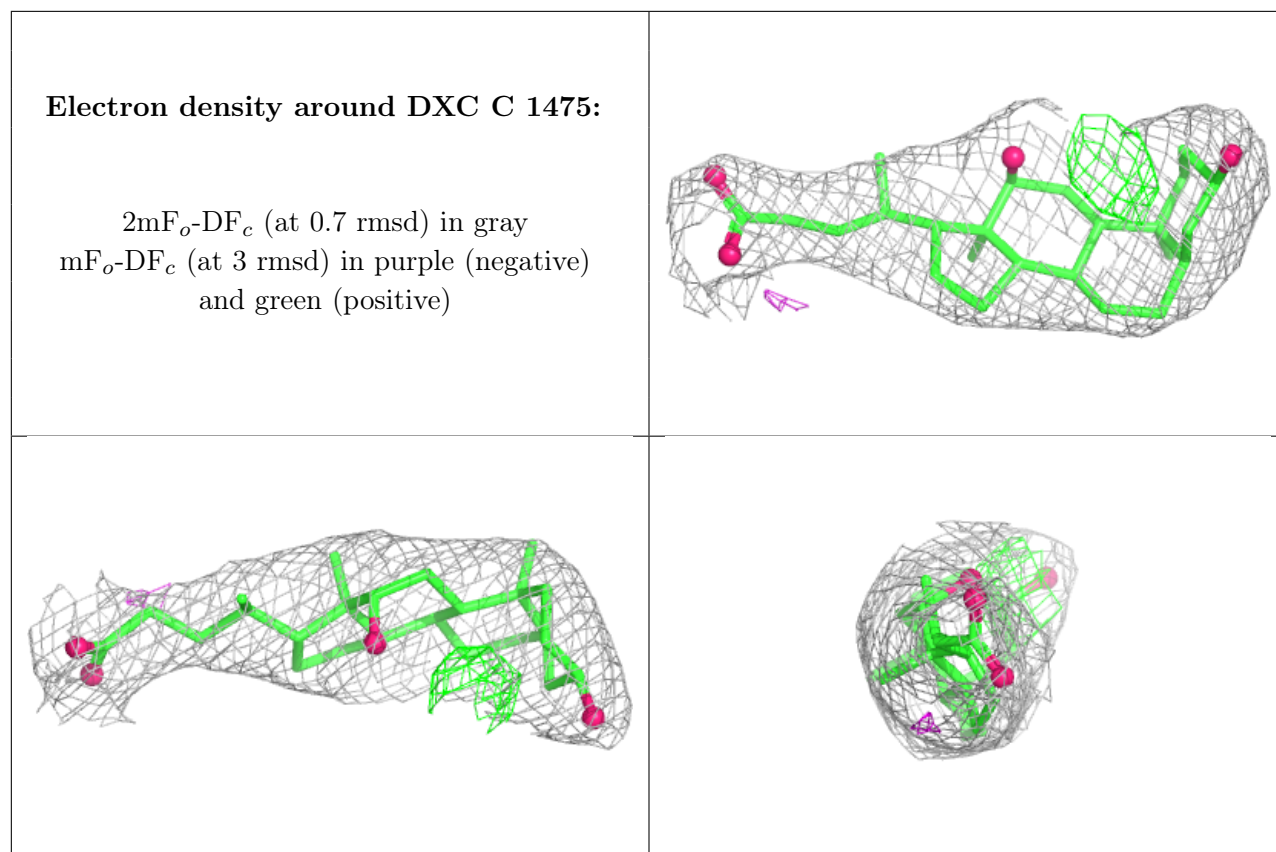
Electron density around DXC C 1478:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.