Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 02:50 pm GMT

PDB ID	:	4ACB
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

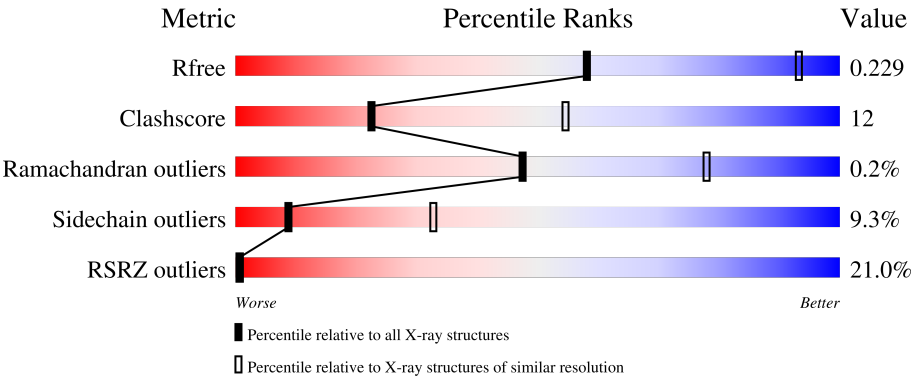
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (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 <=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	20% 67% 24% • 6%
1	B	482	15% 65% 26% • 5%
1	C	482	4% 67% 27% • •
1	D	482	41% 67% 25% 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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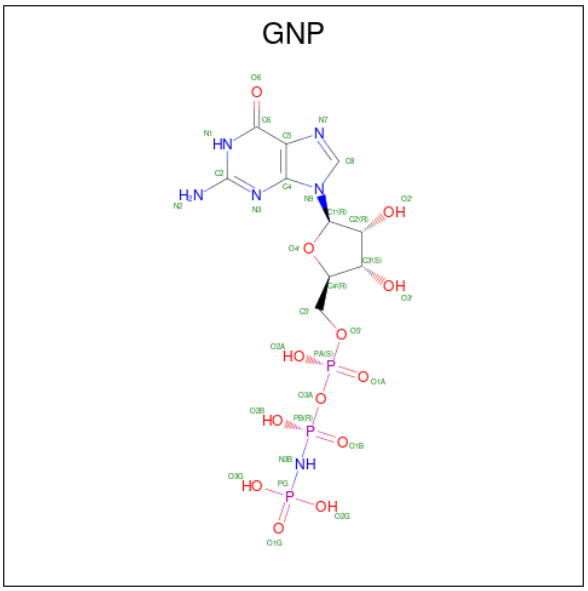
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	expression tag	UNP Q8J307
B	-5	ILE	-	expression tag	UNP Q8J307
B	-4	GLU	-	expression tag	UNP Q8J307
B	-3	GLY	-	expression tag	UNP Q8J307
B	-2	ARG	-	expression tag	UNP Q8J307
B	-1	PRO	-	expression tag	UNP Q8J307
B	0	HIS	-	expression tag	UNP Q8J307
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 (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

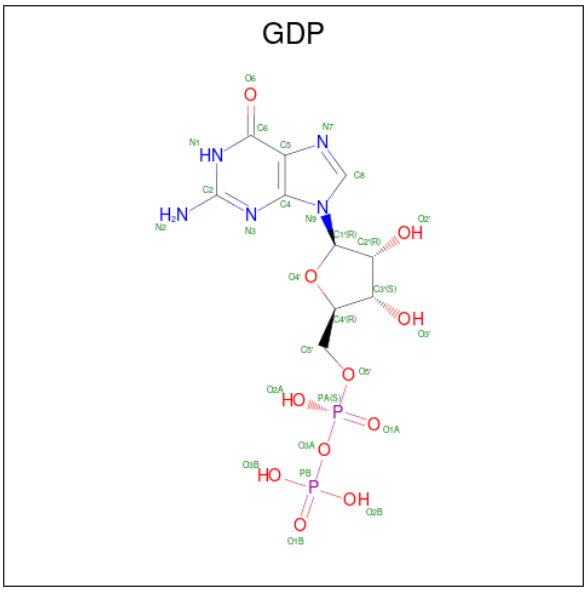


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

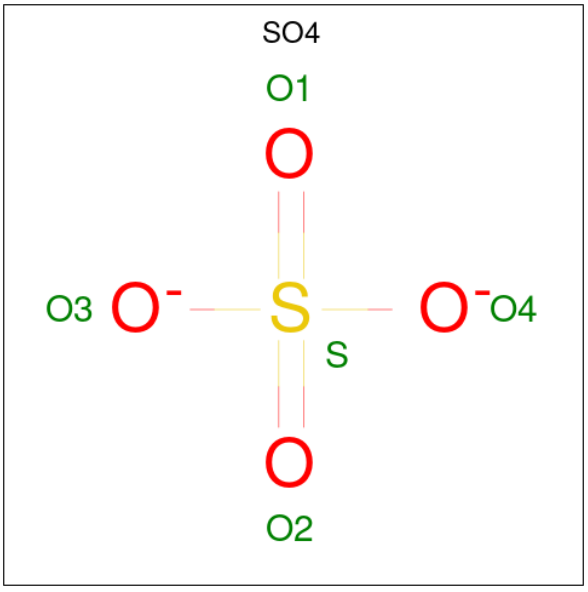
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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 (three-letter code: SO4) (formula: O_4S).



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			

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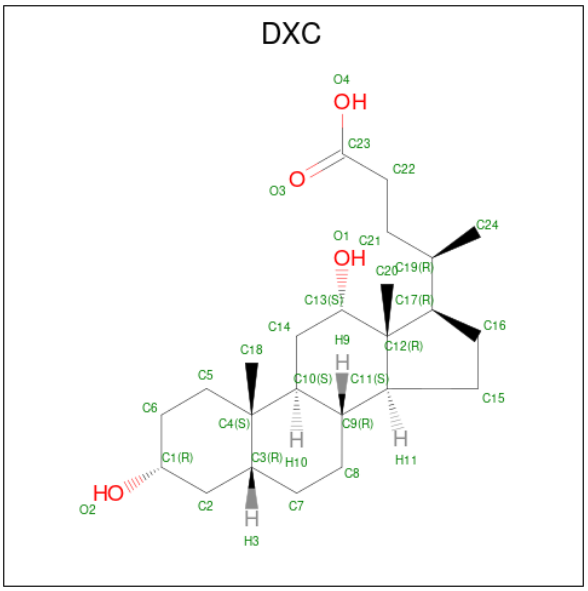
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

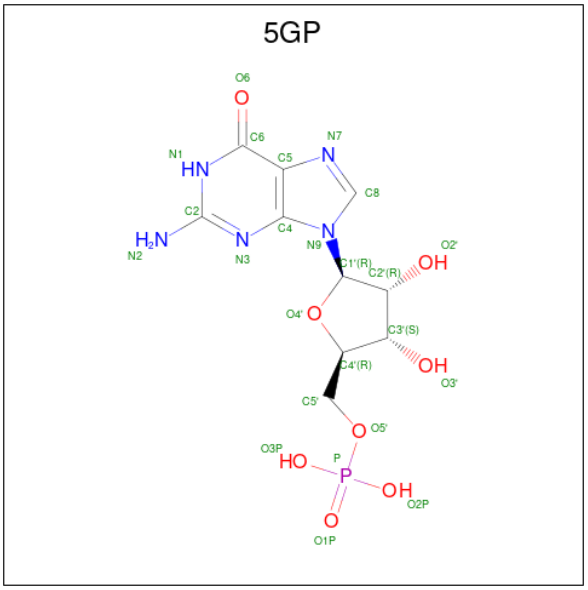
- Molecule 6 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: $C_{24}H_{40}O_4$).



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

- Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:

$C_{10}H_{14}N_5O_8P$).



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.

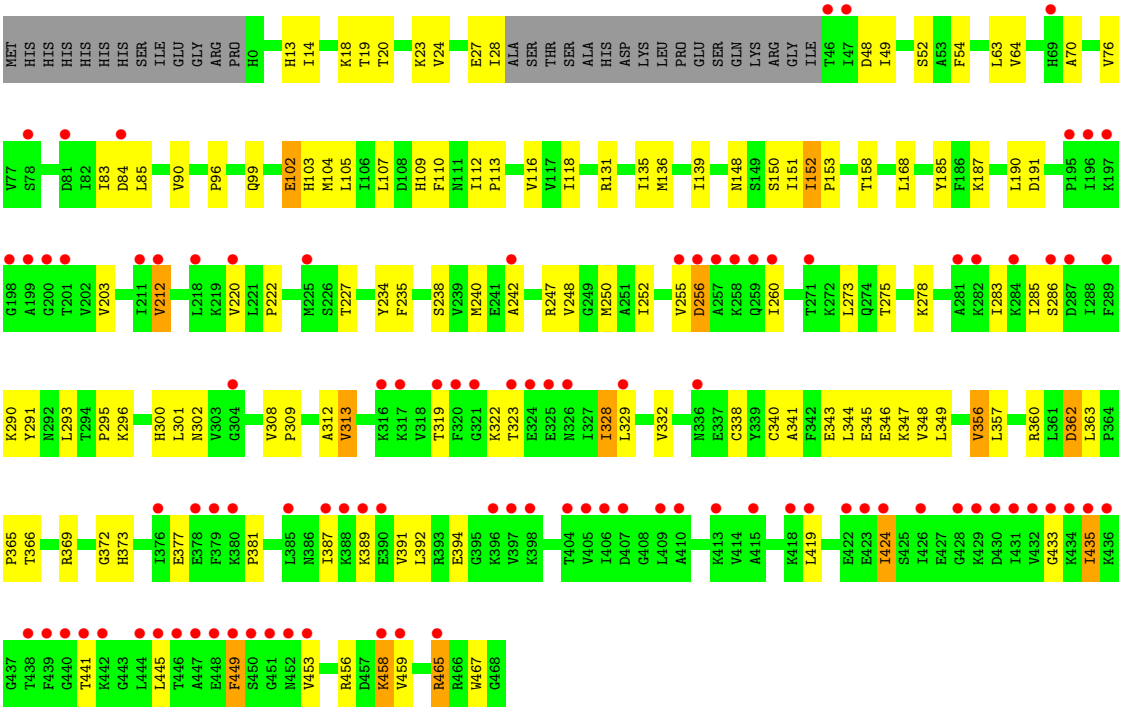
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	O	0	0
			2	2		
8	B	4	Total	O	0	0
			4	4		

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.

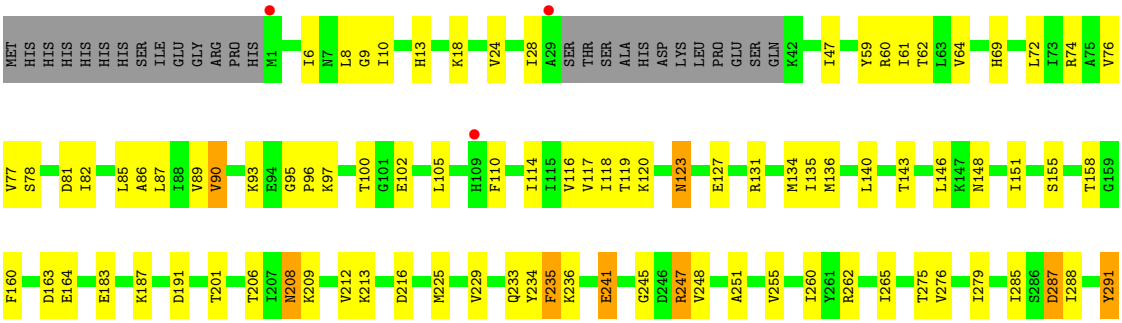
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

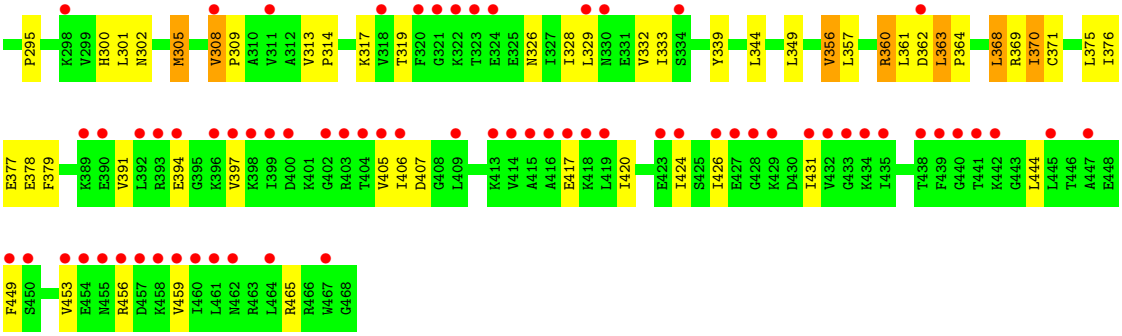
Chain A:



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

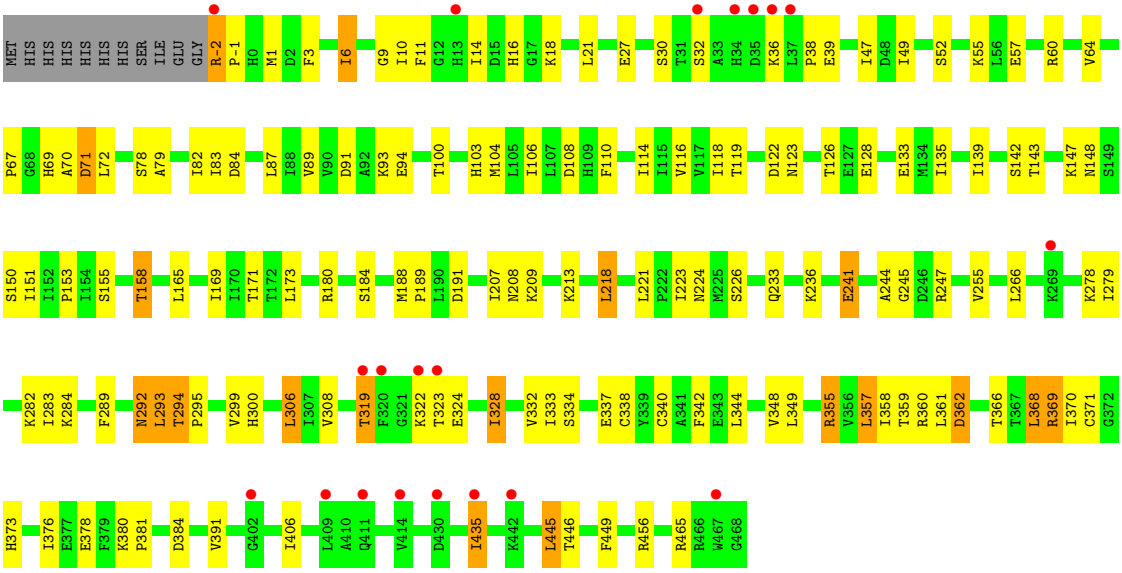
Chain B:





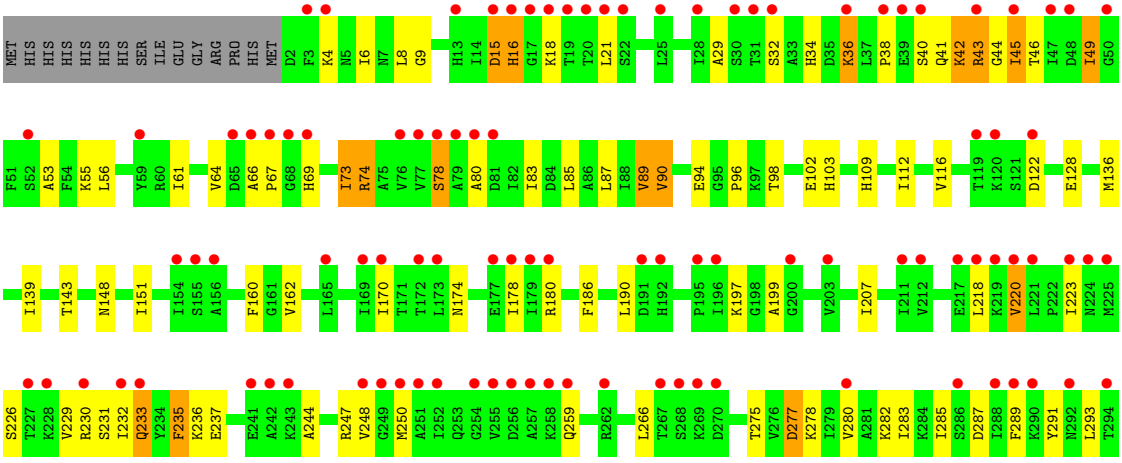
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

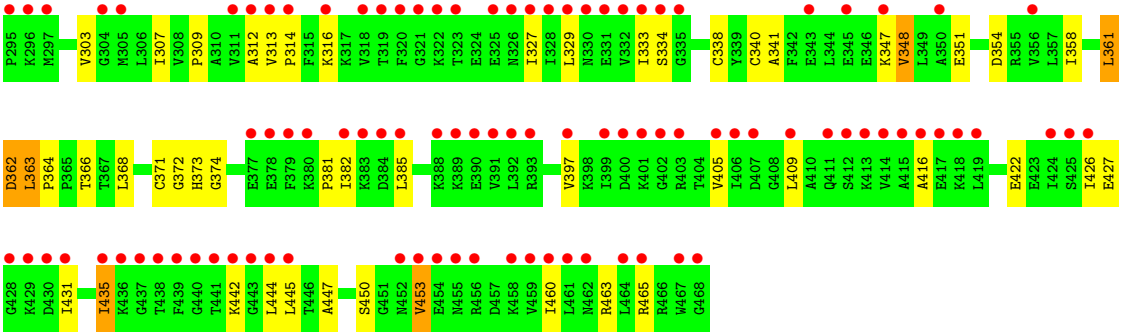
Chain C:



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

Chain D:




P295 K296 M297 V303 G304 M305 L306 I307 V308 P309 A310 V311 A312 V313 P314 F315 K316 K317 V318 T319 F320 G321 K322 T323 E324 E325 N326 I327 I328 L329 N330 E331 V332 I333 S334 G335 C338 Y339 C340 A341 F342 E343 L344 E345 E346 K347 V348 L349 A350 E351 D354 R355 V356 L357 I358 L361
D362 L363 P364 P365 T366 T367 L368 C371 G372 H373 G374 E377 E378 F379 K380 P381 I382 K383 D384 L385 K388 K389 E390 V391 L392 R393 V397 K398 I399 D400 K401 G402 R403 T404 V405 I406 D407 G408 L409 A410 Q411 S412 K413 V414 A415 A416 E417 K418 L419 E422 E423 I424 S425 I426 E427
G428 K429 D430 I431 I435 K436 G437 T438 F439 G440 T441 K442 G443 L444 L445 T446 A447 S450 G451 N452 V453 E454 N455 R456 D457 K458 V459 I460 L461 N462 R463 L464 R465 R466 W467 G468

4 Data and refinement statistics (i)

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 34.48 – 3.34	Depositor EDS
% Data completeness (in resolution range)	82.8 (19.94-3.34) 88.5 (34.48-3.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.179 , 0.223 0.188 , 0.229	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 , 153.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.31	0/3515	0.55	0/4727
1	B	0.35	0/3541	0.57	0/4760
1	C	0.40	0/3664	0.63	0/4929
1	D	0.28	0/3626	0.53	0/4878
All	All	0.34	0/14346	0.57	0/19294

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

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	73	0
1	B	3533	0	3726	84	0
1	C	3651	0	3838	82	0
1	D	3615	0	3801	107	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15362	349	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 (349) 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:B:251:ALA:HB1	1:C:1:MET:HE1	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:A:240:MET:HE1	1:B:95:GLY:HA3	1.73	0.69
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: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:D:313:VAL:HB	1:D:341:ALA:HB3	1.79	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	2.28	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:9:GLY:HA2	1:B:64:VAL:HB	1.88	0.54
5:B:1472:SO4:O2	1:C:55:LYS:NZ	2.41	0.54
1:A:96:PRO:HB3	1:A:136:MET:HE3	1.90	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: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:D:90:VAL:HG11	1:D:136:MET:HE1	1.91	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:C:1:MET:HE3	6:C:1476:DXC:H52	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:A:238:SER:H	1:B:97:LYS:HZ3	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:83:ILE:HG22	1:D:112:ILE:HD13	1.95	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:104:MET:HE2	1:C:104:MET:HB3	1.80	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: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
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: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:D:90:VAL:HG21	1:D:136:MET:HE1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:351:GLU:HG2	1:D:354:ASP:CG	2.38	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:84:ASP:CG	1:C:180:ARG:HH22	2.22	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:H221	6:C:1475:DXC:H243	1.76	0.42
6:C:1475:DXC:H71	6:C:1475:DXC:H182	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASP:CG	1:C:143:THR:HB	2.41	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
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: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: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: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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	444/482 (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%)	34 68
1	D	461/482 (96%)	435 (94%)	25 (5%)	1 (0%)	47 78
All	All	1818/1928 (94%)	1719 (95%)	96 (5%)	3 (0%)	47 78

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 (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	386/412 (94%)	352 (91%)	34 (9%)	10 36
1	B	388/412 (94%)	354 (91%)	34 (9%)	10 36
1	C	402/412 (98%)	358 (89%)	44 (11%)	6 26
1	D	398/412 (97%)	364 (92%)	34 (8%)	10 38
All	All	1574/1648 (96%)	1428 (91%)	146 (9%)	9 33

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	28	ILE
1	A	52	SER
1	A	84	ASP
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	212	VAL
1	A	235	PHE
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	348	VAL
1	A	356	VAL
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	465	ARG
1	B	47	ILE
1	B	62	THR
1	B	90	VAL
1	B	119	THR
1	B	123	ASN
1	B	136	MET
1	B	148	ASN
1	B	163	ASP
1	B	164	GLU

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Mol	Chain	Res	Type
1	B	183	GLU
1	B	208	ASN
1	B	212	VAL
1	B	225	MET
1	B	235	PHE
1	B	241	GLU
1	B	247	ARG
1	B	260	ILE
1	B	262	ARG
1	B	275	THR
1	B	287	ASP
1	B	291	TYR
1	B	300	HIS
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	394	GLU
1	B	453	VAL
1	C	-2	ARG
1	C	6	ILE
1	C	14	ILE
1	C	52	SER
1	C	71	ASP
1	C	78	SER
1	C	114	ILE
1	C	123	ASN
1	C	126	THR
1	C	142	SER
1	C	148	ASN
1	C	150	SER
1	C	158	THR
1	C	171	THR
1	C	191	ASP
1	C	218	LEU
1	C	223	ILE

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Mol	Chain	Res	Type
1	C	226	SER
1	C	241	GLU
1	C	255	VAL
1	C	278	LYS
1	C	292	ASN
1	C	293	LEU
1	C	294	THR
1	C	306	LEU
1	C	319	THR
1	C	328	ILE
1	C	332	VAL
1	C	334	SER
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
1	C	373	HIS
1	C	378	GLU
1	C	391	VAL
1	C	435	ILE
1	C	445	LEU
1	C	446	THR
1	C	456	ARG
1	D	15	ASP
1	D	16	HIS
1	D	36	LYS
1	D	41	GLN
1	D	43	ARG
1	D	45	ILE
1	D	46	THR
1	D	49	ILE
1	D	73	ILE
1	D	74	ARG
1	D	78	SER
1	D	89	VAL
1	D	90	VAL
1	D	128	GLU
1	D	139	ILE

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Mol	Chain	Res	Type
1	D	143	THR
1	D	160	PHE
1	D	162	VAL
1	D	190	LEU
1	D	220	VAL
1	D	226	SER
1	D	233	GLN
1	D	235	PHE
1	D	277	ASP
1	D	289	PHE
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	435	ILE
1	D	453	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	300	HIS
1	C	233	GLN
1	D	69	HIS
1	D	233	GLN
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	338	1	5,7,8	0.62	0	1,7,9	0.01	0
1	CMH	A	338	1	5,7,8	0.57	0	1,7,9	0.76	0
1	CMH	B	340	1	5,7,8	0.54	0	1,7,9	0.95	0
1	CMH	A	371	1	5,7,8	0.55	0	1,7,9	0.59	0
1	CMH	D	340	1	5,7,8	0.66	0	1,7,9	0.32	0
1	CMH	C	264	1	5,7,8	0.66	0	1,7,9	1.11	0
1	CMH	A	340	1	5,7,8	0.63	0	1,7,9	1.19	0
1	CMH	A	264	1	5,7,8	0.60	0	1,7,9	0.41	0
1	CMH	C	340	1	5,7,8	0.82	0	1,7,9	0.90	0
1	CMH	D	264	1	5,7,8	0.61	0	1,7,9	0.48	0
1	CMH	B	338	1	5,7,8	0.58	0	1,7,9	0.03	0
1	CMH	D	371	1	5,7,8	0.61	0	1,7,9	0.48	0
1	CMH	C	338	1	5,7,8	0.62	0	1,7,9	0.18	0
1	CMH	C	371	1	5,7,8	0.68	0	1,7,9	0.45	0
1	CMH	B	371	1	5,7,8	0.54	0	1,7,9	1.29	0
1	CMH	B	264	1	5,7,8	0.75	0	1,7,9	1.33	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	340	1	-	0/0/6/8	-
1	CMH	A	371	1	-	0/0/6/8	-
1	CMH	D	340	1	-	0/0/6/8	-
1	CMH	C	264	1	-	0/0/6/8	-
1	CMH	A	340	1	-	0/0/6/8	-
1	CMH	A	264	1	-	0/0/6/8	-
1	CMH	C	340	1	-	0/0/6/8	-
1	CMH	D	264	1	-	0/0/6/8	-
1	CMH	B	338	1	-	0/0/6/8	-
1	CMH	D	371	1	-	0/0/6/8	-
1	CMH	C	338	1	-	0/0/6/8	-
1	CMH	C	371	1	-	0/0/6/8	-
1	CMH	B	371	1	-	0/0/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CMH	B	264	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	D	340	CMH	4	0
1	A	340	CMH	2	0
1	C	340	CMH	2	0
1	D	371	CMH	2	0
1	C	338	CMH	1	0
1	C	371	CMH	3	0
1	B	371	CMH	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	B	1472	-	4,4,4	0.14	0	6,6,6	0.15	0
6	DXC	C	1478	-	31,31,31	1.34	5 (16%)	49,49,49	1.85	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	1.53	8 (25%)	49,49,49	2.15	17 (34%)
2	GNP	A	1469	3	29,34,34	1.74	6 (20%)	33,54,54	2.36	8 (24%)
5	SO4	C	1481	-	4,4,4	0.17	0	6,6,6	0.12	0
6	DXC	C	1477	-	31,31,31	1.59	6 (19%)	49,49,49	1.86	13 (26%)
6	DXC	C	1480	-	31,31,31	1.61	7 (22%)	49,49,49	2.06	16 (32%)
5	SO4	C	1471	-	4,4,4	0.27	0	6,6,6	0.72	0
6	DXC	C	1476	-	31,31,31	1.48	5 (16%)	49,49,49	1.79	13 (26%)
5	SO4	C	1472	-	4,4,4	0.25	0	6,6,6	0.20	0
5	SO4	B	1471	-	4,4,4	0.15	0	6,6,6	0.08	0
6	DXC	C	1475	-	31,31,31	1.58	5 (16%)	49,49,49	2.22	18 (36%)
7	5GP	B	1474	-	22,26,26	1.22	2 (9%)	26,40,40	1.41	5 (19%)
6	DXC	B	1473	-	31,31,31	1.33	3 (9%)	49,49,49	2.07	15 (30%)
5	SO4	C	1473	-	4,4,4	0.15	0	6,6,6	0.11	0
4	GDP	B	1469	3	24,30,30	0.93	1 (4%)	30,47,47	1.19	3 (10%)

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	1478	-	-	4/9/71/71	0/4/4/4
6	DXC	C	1479	-	-	7/9/71/71	0/4/4/4
2	GNP	A	1469	3	-	5/14/38/38	0/3/3/3
6	DXC	C	1477	-	-	6/9/71/71	0/4/4/4
6	DXC	C	1480	-	-	4/9/71/71	0/4/4/4
6	DXC	C	1476	-	-	4/9/71/71	0/4/4/4
6	DXC	C	1475	-	-	6/9/71/71	0/4/4/4
7	5GP	B	1474	-	-	2/6/26/26	0/3/3/3
6	DXC	B	1473	-	-	2/9/71/71	0/4/4/4
4	GDP	B	1469	3	-	7/12/32/32	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1469	GNP	PB-O3A	-4.75	1.53	1.59
6	C	1475	DXC	C12-C13	-4.61	1.47	1.54
7	B	1474	5GP	C5-C6	-3.93	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1469	GNP	C6-N1	3.90	1.39	1.33
6	C	1477	DXC	C18-C4	-3.87	1.47	1.54
6	C	1477	DXC	C12-C13	-3.85	1.48	1.54
6	C	1480	DXC	C18-C4	-3.80	1.47	1.54
2	A	1469	GNP	PG-O1G	3.51	1.51	1.46
6	C	1476	DXC	C12-C13	-3.40	1.49	1.54
6	C	1479	DXC	C18-C4	-3.31	1.48	1.54
6	C	1476	DXC	O1-C13	-3.13	1.38	1.43
6	C	1478	DXC	C18-C4	-3.11	1.48	1.54
6	C	1480	DXC	C12-C13	-3.06	1.49	1.54
6	B	1473	DXC	C12-C13	-3.03	1.49	1.54
6	C	1477	DXC	C4-C10	-3.02	1.50	1.56
6	C	1479	DXC	C12-C13	-2.94	1.50	1.54
6	B	1473	DXC	C18-C4	-2.93	1.49	1.54
2	A	1469	GNP	PB-O2B	-2.90	1.49	1.56
6	C	1475	DXC	O1-C13	-2.88	1.38	1.43
6	C	1476	DXC	C12-C11	-2.88	1.50	1.55
6	C	1475	DXC	C12-C11	-2.84	1.50	1.55
6	C	1480	DXC	C5-C4	-2.76	1.49	1.54
6	C	1476	DXC	C20-C12	-2.74	1.49	1.54
6	C	1475	DXC	C20-C12	-2.73	1.49	1.54
6	C	1480	DXC	C12-C11	-2.71	1.50	1.55
7	B	1474	5GP	C6-N1	-2.64	1.33	1.37
6	C	1477	DXC	C20-C12	-2.60	1.50	1.54
6	B	1473	DXC	C4-C10	-2.59	1.51	1.56
6	C	1478	DXC	C12-C11	-2.57	1.51	1.55
6	C	1479	DXC	C4-C3	-2.46	1.51	1.55
6	C	1479	DXC	O1-C13	-2.41	1.39	1.43
6	C	1476	DXC	C18-C4	-2.40	1.50	1.54
6	C	1480	DXC	C4-C10	-2.38	1.51	1.56
6	C	1478	DXC	C12-C13	-2.38	1.50	1.54
6	C	1478	DXC	O1-C13	-2.37	1.39	1.43
6	C	1480	DXC	C4-C3	-2.34	1.51	1.55
6	C	1479	DXC	C12-C11	-2.24	1.51	1.55
6	C	1477	DXC	O1-C13	-2.23	1.39	1.43
2	A	1469	GNP	C8-N7	-2.22	1.30	1.34
6	C	1479	DXC	C4-C10	-2.19	1.52	1.56
6	C	1479	DXC	C20-C12	-2.17	1.50	1.54
6	C	1480	DXC	O1-C13	-2.15	1.40	1.43
4	B	1469	GDP	C6-N1	-2.11	1.34	1.37
6	C	1475	DXC	C18-C4	-2.11	1.50	1.54
6	C	1477	DXC	C12-C11	-2.07	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1478	DXC	C20-C12	-2.06	1.50	1.54
2	A	1469	GNP	PG-O2G	-2.02	1.51	1.56
6	C	1479	DXC	C12-C17	-2.01	1.52	1.55

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1469	GNP	C5-C6-N1	-8.63	111.63	123.43
6	C	1478	DXC	C10-C14-C13	-5.61	106.89	114.30
2	A	1469	GNP	C2-N1-C6	5.61	124.85	115.93
6	C	1475	DXC	C15-C11-C12	-5.37	98.29	103.55
6	C	1479	DXC	C18-C4-C3	-5.14	101.64	110.36
6	C	1479	DXC	C6-C5-C4	-4.95	104.30	112.78
6	C	1475	DXC	C3-C2-C1	-4.91	105.55	112.76
6	C	1479	DXC	C24-C19-C17	-4.86	105.49	112.92
6	C	1480	DXC	C20-C12-C13	4.78	113.93	109.07
6	B	1473	DXC	C5-C6-C1	-4.78	104.34	110.47
6	C	1477	DXC	C10-C14-C13	-4.64	108.17	114.30
6	C	1476	DXC	C18-C4-C3	-4.64	102.49	110.36
6	C	1480	DXC	C18-C4-C5	-4.60	100.84	108.26
6	B	1473	DXC	C10-C4-C3	4.53	114.94	108.58
6	B	1473	DXC	C6-C5-C4	-4.51	105.05	112.78
6	C	1477	DXC	C14-C13-C12	-4.41	106.72	111.24
6	C	1478	DXC	C7-C8-C9	-4.36	104.96	112.14
6	C	1475	DXC	C17-C12-C13	-4.32	113.73	117.67
6	B	1473	DXC	C11-C9-C10	-4.22	103.45	109.09
6	C	1475	DXC	C5-C6-C1	-4.08	105.23	110.47
6	C	1477	DXC	C7-C8-C9	-4.04	105.49	112.14
6	C	1475	DXC	O1-C13-C12	-3.97	104.31	111.03
6	C	1475	DXC	C18-C4-C10	3.88	116.53	111.18
6	C	1477	DXC	C11-C9-C10	-3.85	103.93	109.09
6	B	1473	DXC	C14-C10-C4	-3.74	109.86	113.73
6	C	1475	DXC	C18-C4-C3	-3.63	104.20	110.36
6	C	1479	DXC	C7-C8-C9	-3.63	106.16	112.14
6	C	1476	DXC	C10-C4-C3	3.62	113.66	108.58
6	C	1476	DXC	C4-C10-C9	-3.61	108.63	112.42
2	A	1469	GNP	O3G-PG-O1G	-3.57	104.47	113.45
2	A	1469	GNP	O2B-PB-O1B	3.53	117.33	109.92
6	C	1476	DXC	C7-C8-C9	-3.42	106.51	112.14
6	C	1480	DXC	C7-C8-C9	-3.39	106.56	112.14
6	C	1480	DXC	C24-C19-C21	-3.34	105.13	110.36
6	C	1480	DXC	C17-C12-C13	-3.32	114.64	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1479	DXC	C10-C4-C3	3.31	113.24	108.58
7	B	1474	5GP	C5-C6-N1	3.31	119.79	113.95
6	C	1475	DXC	C11-C9-C10	-3.30	104.67	109.09
6	C	1480	DXC	C16-C15-C11	-3.29	98.61	105.13
6	C	1480	DXC	C11-C12-C13	-3.29	104.34	107.40
6	C	1476	DXC	C10-C14-C13	-3.27	109.98	114.30
6	B	1473	DXC	C18-C4-C3	-3.24	104.87	110.36
6	C	1477	DXC	C11-C12-C13	-3.21	104.42	107.40
6	B	1473	DXC	C5-C4-C10	-3.20	106.32	111.35
6	C	1480	DXC	C10-C14-C13	-3.18	110.10	114.30
6	C	1480	DXC	C5-C4-C10	3.17	116.34	111.35
6	C	1476	DXC	C8-C9-C10	3.17	114.42	110.49
6	C	1479	DXC	C5-C4-C3	3.15	112.43	107.77
6	C	1478	DXC	C12-C17-C19	-3.13	115.76	119.50
6	C	1479	DXC	C15-C11-C9	-3.11	113.95	119.08
6	C	1475	DXC	C6-C5-C4	-3.11	107.45	112.78
6	C	1475	DXC	C17-C12-C11	3.09	103.21	100.09
6	C	1479	DXC	C11-C9-C10	-3.06	104.99	109.09
2	A	1469	GNP	O2G-PG-O3G	3.06	115.78	107.64
6	C	1478	DXC	C3-C2-C1	-3.05	108.29	112.76
6	B	1473	DXC	C22-C21-C19	-3.04	108.97	114.52
6	C	1476	DXC	C22-C21-C19	-3.03	108.98	114.52
6	C	1477	DXC	C17-C12-C11	3.02	103.14	100.09
6	C	1479	DXC	C14-C10-C4	-3.01	110.62	113.73
2	A	1469	GNP	C2-N3-C4	-2.99	111.94	115.36
6	C	1479	DXC	C8-C9-C10	2.89	114.08	110.49
6	B	1473	DXC	C20-C12-C11	2.88	115.72	111.21
6	C	1477	DXC	C10-C4-C3	2.82	112.55	108.58
6	C	1480	DXC	C4-C10-C9	-2.81	109.47	112.42
6	C	1478	DXC	C16-C15-C11	-2.79	99.60	105.13
6	B	1473	DXC	C24-C19-C21	-2.79	105.99	110.36
6	C	1477	DXC	C2-C3-C7	-2.77	106.66	111.74
2	A	1469	GNP	PB-O3A-PA	-2.73	122.99	132.62
6	C	1476	DXC	C17-C12-C13	2.73	120.16	117.67
6	C	1476	DXC	C5-C6-C1	2.72	113.95	110.47
6	C	1477	DXC	C20-C12-C11	2.70	115.44	111.21
6	C	1479	DXC	C12-C17-C19	-2.70	116.27	119.50
6	C	1479	DXC	C4-C10-C9	-2.69	109.59	112.42
6	C	1475	DXC	C2-C1-C6	-2.65	107.39	110.55
6	C	1478	DXC	C24-C19-C21	-2.63	106.24	110.36
6	C	1479	DXC	C10-C14-C13	-2.63	110.83	114.30
6	C	1479	DXC	C14-C13-C12	-2.62	108.56	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1476	DXC	C15-C11-C12	-2.61	101.00	103.55
6	C	1480	DXC	O1-C13-C12	-2.56	106.70	111.03
6	C	1479	DXC	C18-C4-C10	2.56	114.71	111.18
6	C	1478	DXC	C10-C4-C3	2.55	112.16	108.58
6	C	1478	DXC	C6-C5-C4	-2.55	108.42	112.78
6	C	1480	DXC	C3-C2-C1	-2.54	109.03	112.76
6	C	1479	DXC	C15-C11-C12	-2.52	101.08	103.55
6	C	1478	DXC	C8-C9-C10	2.51	113.61	110.49
6	C	1475	DXC	C16-C15-C11	-2.48	100.21	105.13
6	C	1475	DXC	C18-C4-C5	-2.47	104.28	108.26
6	C	1480	DXC	C10-C4-C3	2.43	111.99	108.58
2	A	1469	GNP	N3-C2-N1	-2.40	124.02	127.22
4	B	1469	GDP	C8-N7-C5	2.37	107.50	102.99
4	B	1469	GDP	PA-O3A-PB	-2.35	124.76	132.83
7	B	1474	5GP	C8-N7-C5	2.35	107.46	102.99
6	C	1475	DXC	C2-C3-C4	-2.34	110.17	112.66
7	B	1474	5GP	C2-N1-C6	-2.33	120.81	125.10
6	C	1477	DXC	C16-C15-C11	-2.32	100.54	105.13
7	B	1474	5GP	O5'-P-O1P	-2.30	100.01	106.47
6	B	1473	DXC	C15-C11-C12	2.30	105.81	103.55
6	C	1476	DXC	C3-C2-C1	-2.27	109.43	112.76
6	C	1478	DXC	C2-C1-C6	-2.27	107.85	110.55
6	C	1480	DXC	O2-C1-C2	2.25	114.33	109.85
6	C	1479	DXC	C11-C12-C13	2.24	109.49	107.40
6	C	1478	DXC	C2-C3-C7	-2.24	107.63	111.74
4	B	1469	GDP	C5-C6-N1	2.24	117.90	113.95
6	C	1478	DXC	C21-C19-C17	2.21	114.85	110.28
6	C	1476	DXC	C15-C11-C9	-2.15	115.54	119.08
6	C	1478	DXC	C22-C21-C19	-2.14	110.60	114.52
6	C	1477	DXC	C12-C11-C9	2.14	117.08	114.71
6	C	1478	DXC	C18-C4-C3	-2.14	106.74	110.36
6	C	1475	DXC	C12-C17-C19	-2.13	116.96	119.50
6	C	1480	DXC	C8-C9-C10	2.11	113.11	110.49
6	C	1478	DXC	C8-C7-C3	-2.11	107.62	111.84
6	B	1473	DXC	C2-C3-C4	2.10	114.88	112.66
6	C	1476	DXC	C16-C17-C19	-2.09	108.91	112.15
6	C	1475	DXC	C12-C11-C9	2.07	117.00	114.71
6	C	1475	DXC	C14-C10-C4	2.07	115.86	113.73
6	B	1473	DXC	O4-C23-C22	2.07	120.68	114.03
6	C	1475	DXC	C24-C19-C21	-2.06	107.13	110.36
6	C	1477	DXC	C20-C12-C13	-2.05	106.98	109.07
7	B	1474	5GP	O2P-P-O5'	-2.05	101.27	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1478	DXC	O4-C23-C22	2.03	120.56	114.03
6	B	1473	DXC	C14-C10-C9	2.02	114.10	110.82
6	B	1473	DXC	C4-C10-C9	-2.02	110.30	112.42
6	C	1477	DXC	O4-C23-C22	2.02	120.52	114.03
6	C	1480	DXC	C2-C3-C4	-2.01	110.52	112.66

There are no chirality outliers.

All (47) 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-O1B
2	A	1469	GNP	PA-O3A-PB-O2B
4	B	1469	GDP	PA-O3A-PB-O3B
4	B	1469	GDP	C5'-O5'-PA-O1A
4	B	1469	GDP	C5'-O5'-PA-O2A
7	B	1474	5GP	C3'-C4'-C5'-O5'
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
6	C	1479	DXC	C16-C17-C19-C21
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
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
4	B	1469	GDP	PB-O3A-PA-O1A
6	C	1475	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-C24
6	C	1478	DXC	C16-C17-C19-C21
6	C	1475	DXC	C16-C17-C19-C21

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Mol	Chain	Res	Type	Atoms
6	B	1473	DXC	C21-C22-C23-O3
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	1479	DXC	C19-C21-C22-C23
4	B	1469	GDP	C5'-O5'-PA-O3A
4	B	1469	GDP	C4'-C5'-O5'-PA
6	C	1477	DXC	C21-C22-C23-O4
6	C	1477	DXC	C21-C22-C23-O3
6	C	1477	DXC	C12-C17-C19-C24

There are no ring outliers.

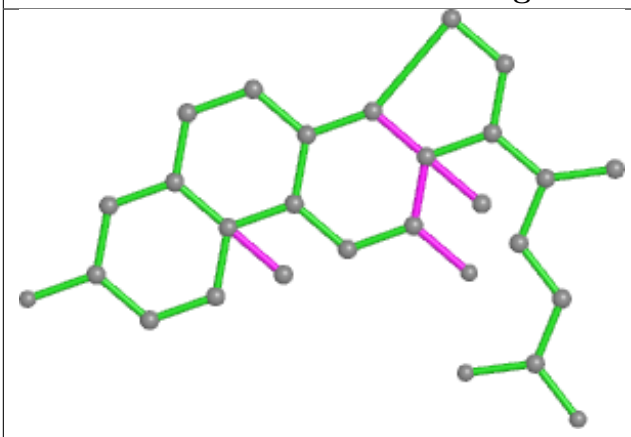
14 monomers are involved in 29 short contacts:

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

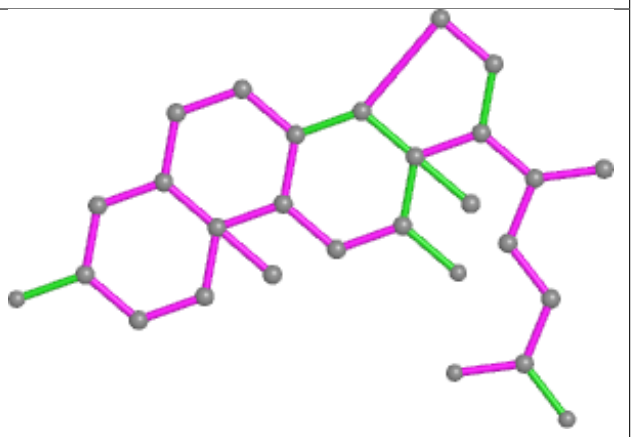
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

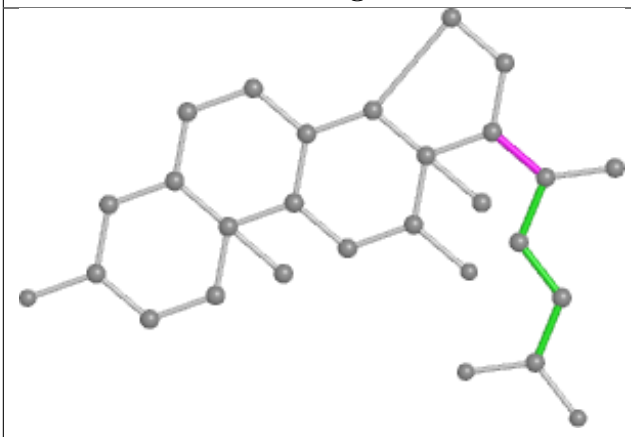
Ligand DXC C 1478



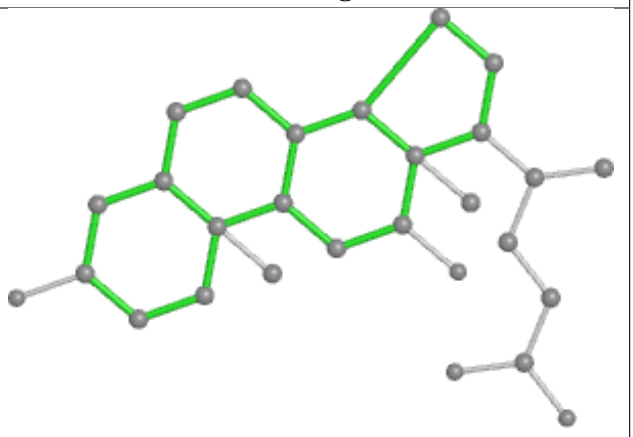
Bond lengths



Bond angles

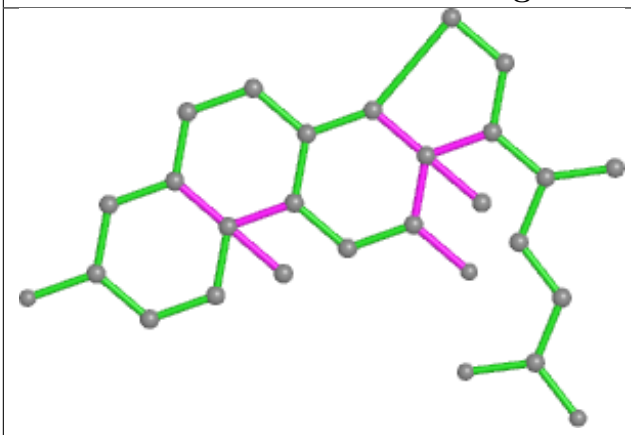


Torsions

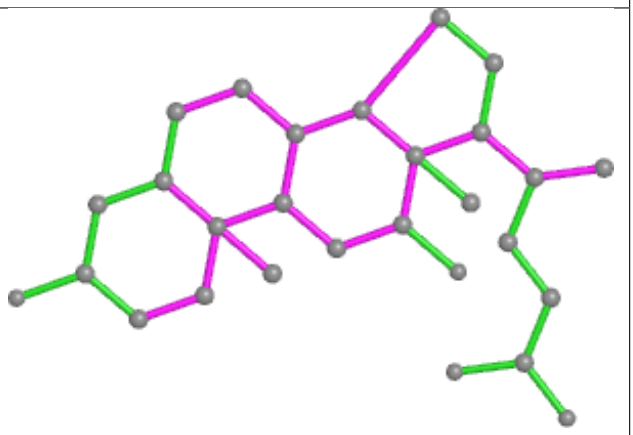


Rings

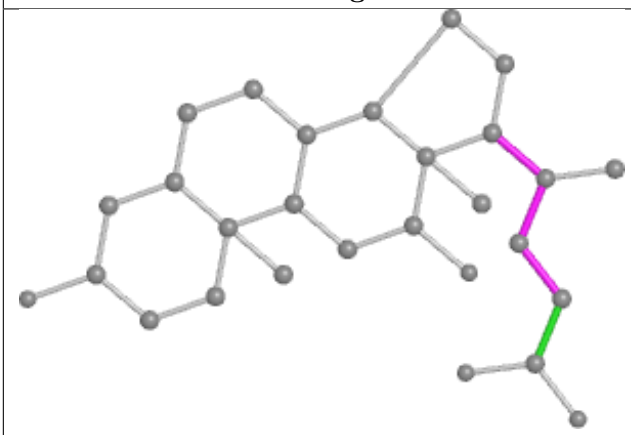
Ligand DXC C 1479



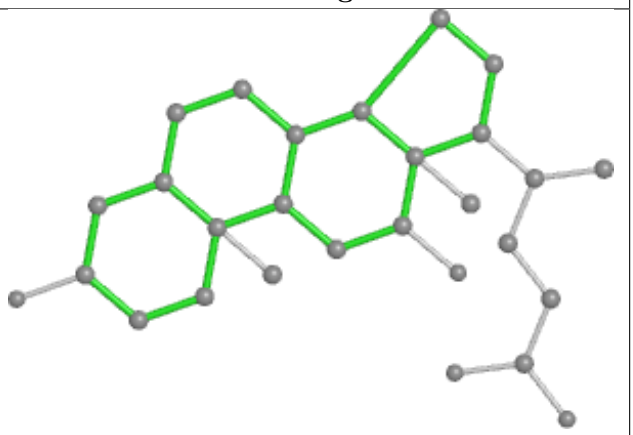
Bond lengths



Bond angles

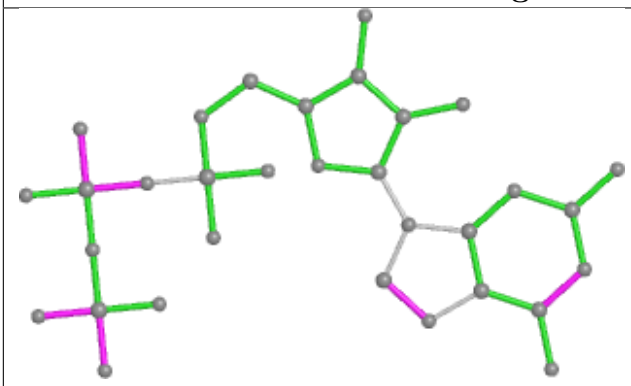


Torsions

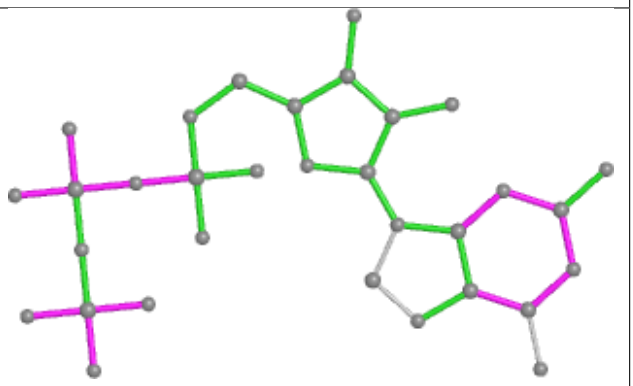


Rings

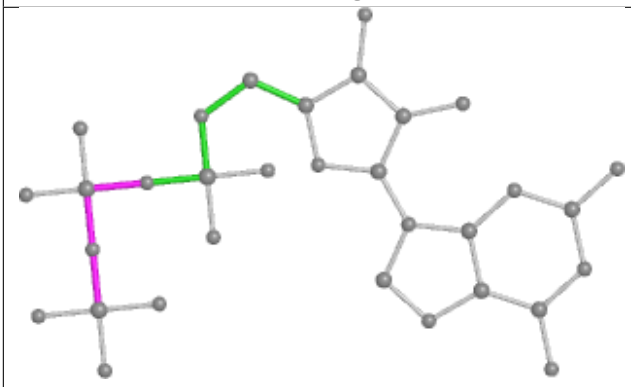
Ligand GNP A 1469



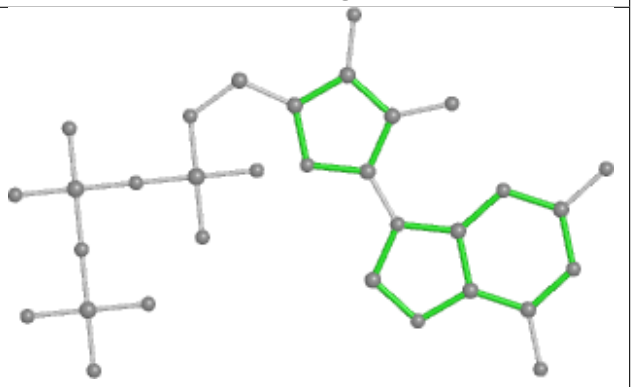
Bond lengths



Bond angles

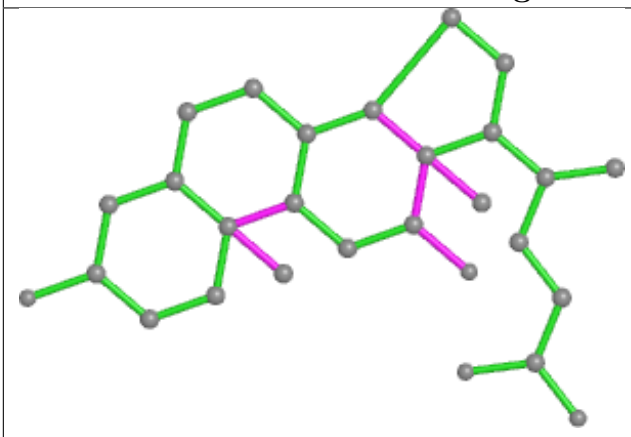


Torsions

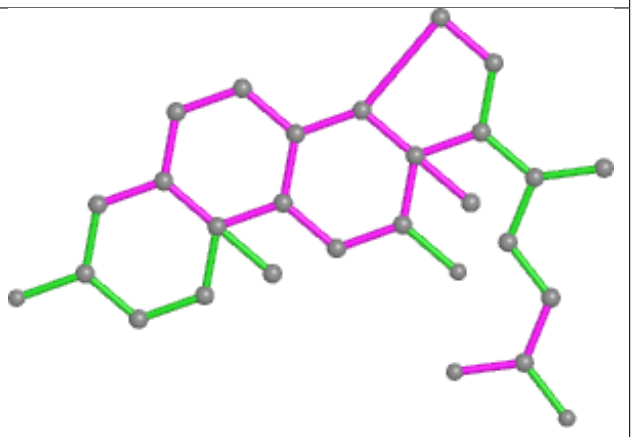


Rings

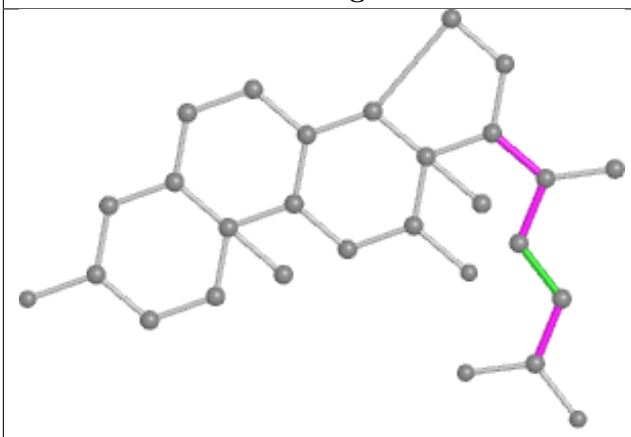
Ligand DXC C 1477



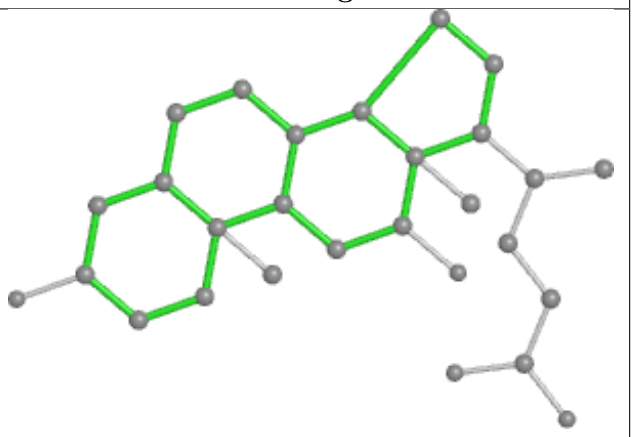
Bond lengths



Bond angles

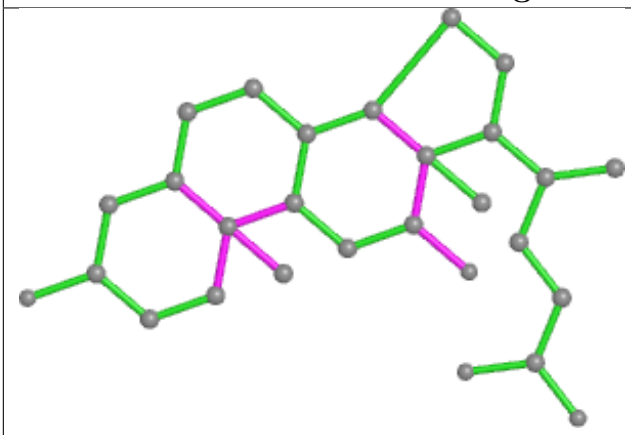


Torsions

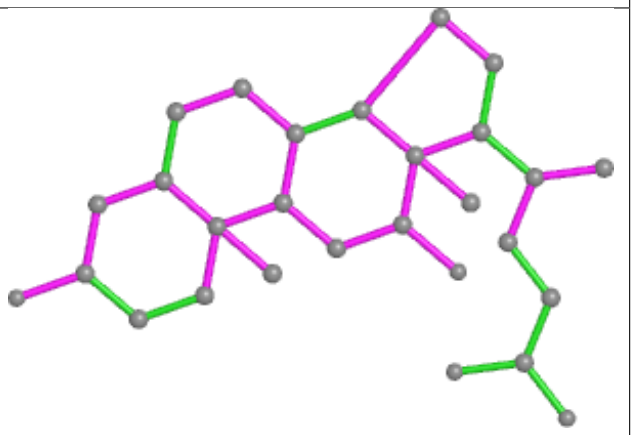


Rings

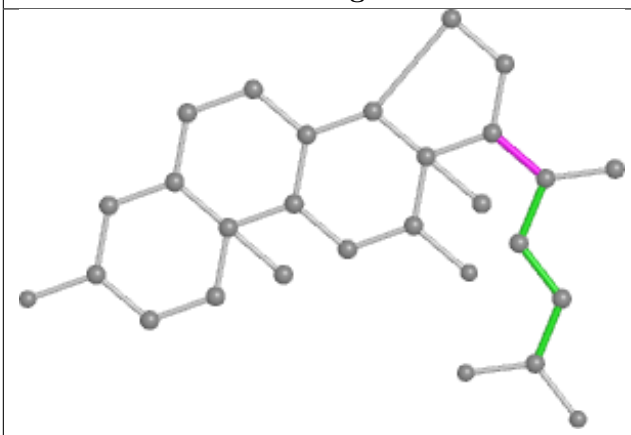
Ligand DXC C 1480



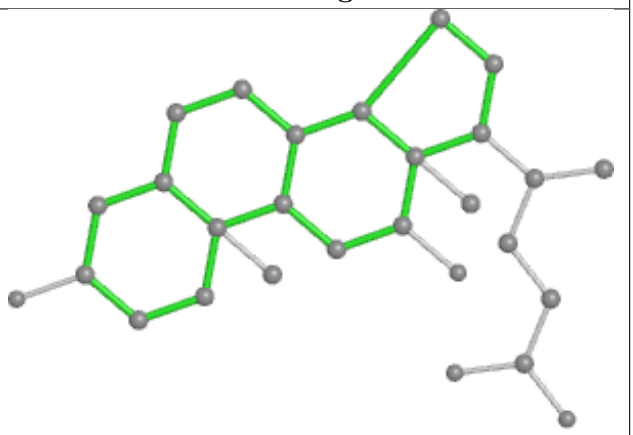
Bond lengths



Bond angles

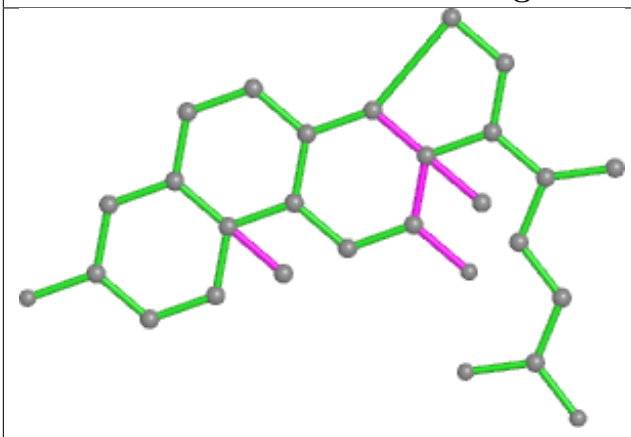


Torsions

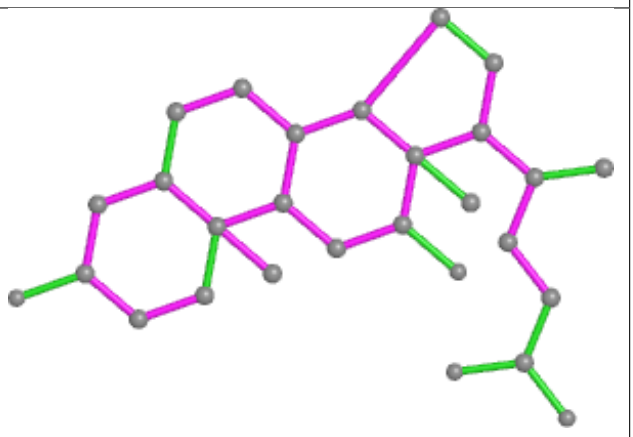


Rings

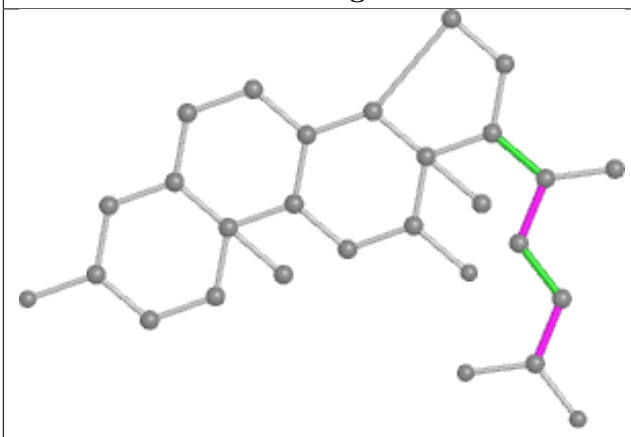
Ligand DXC C 1476



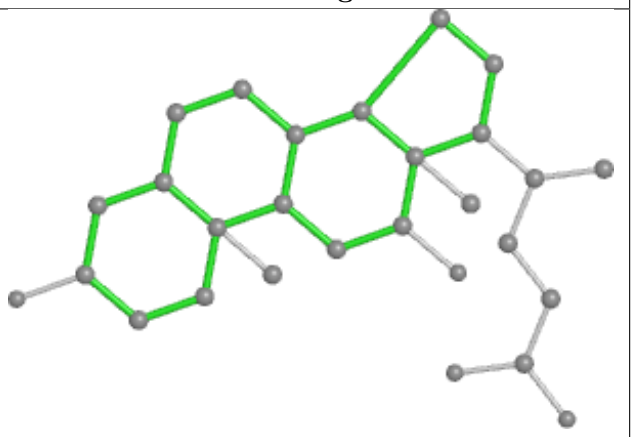
Bond lengths



Bond angles

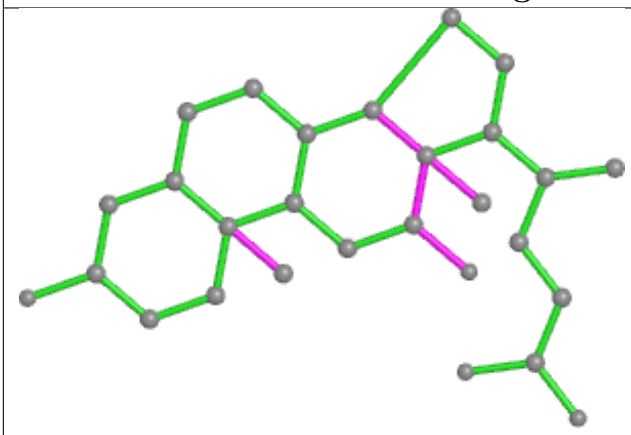


Torsions

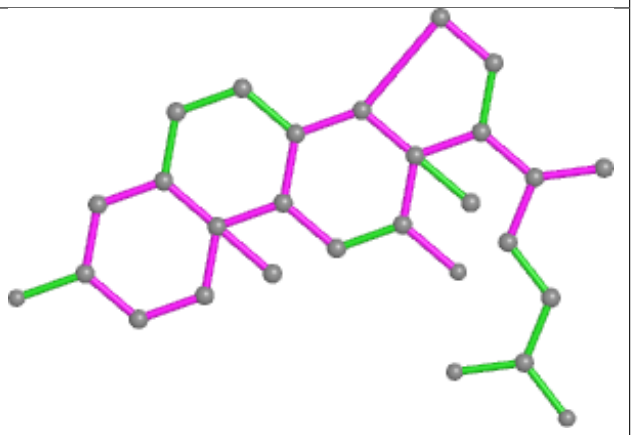


Rings

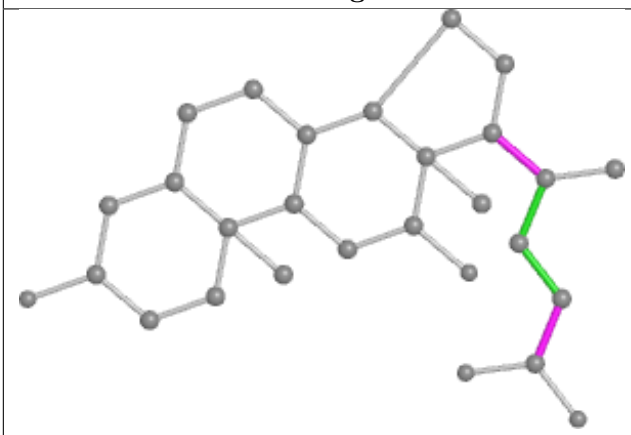
Ligand DXC C 1475



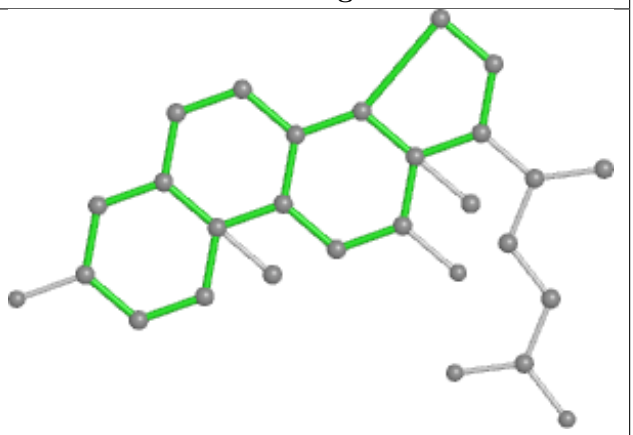
Bond lengths



Bond angles

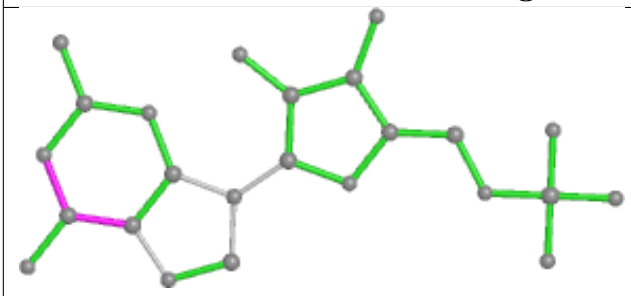


Torsions

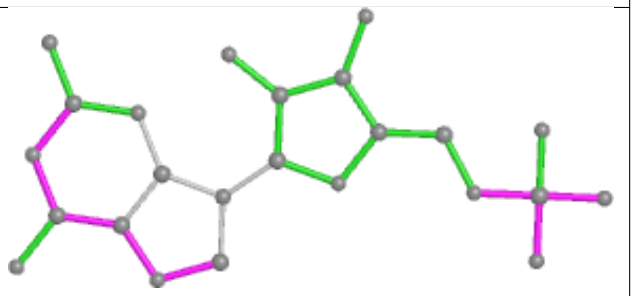


Rings

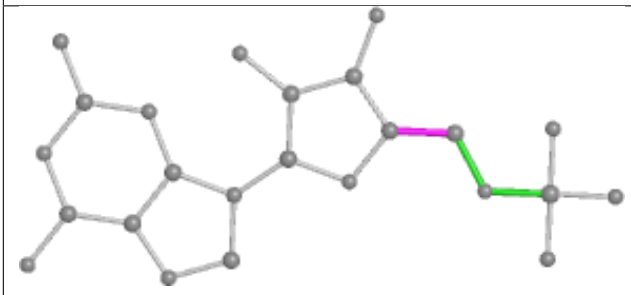
Ligand 5GP B 1474



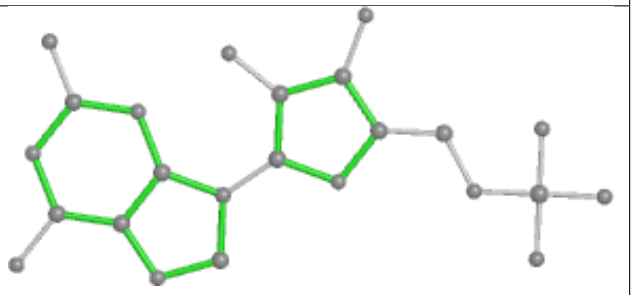
Bond lengths



Bond angles

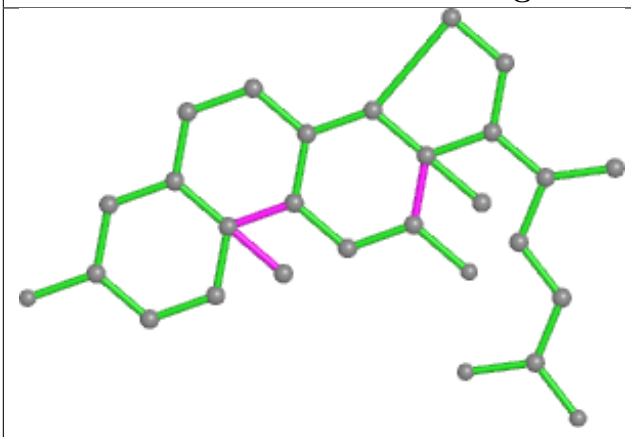


Torsions

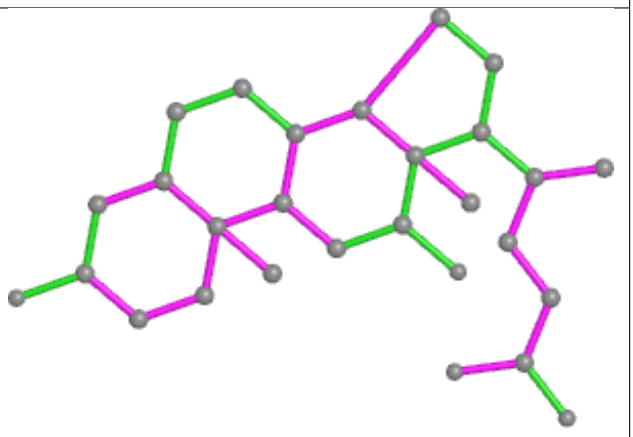


Rings

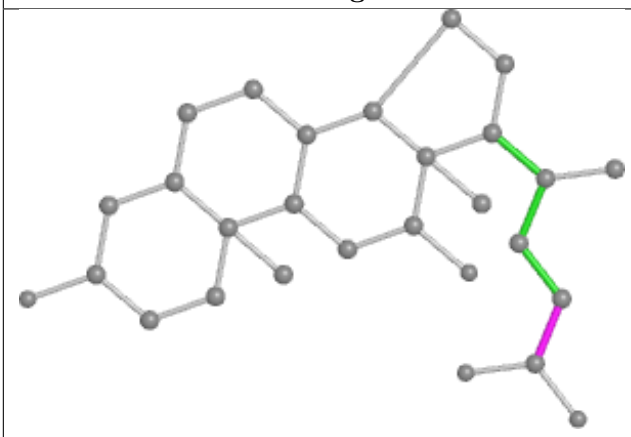
Ligand DXC B 1473



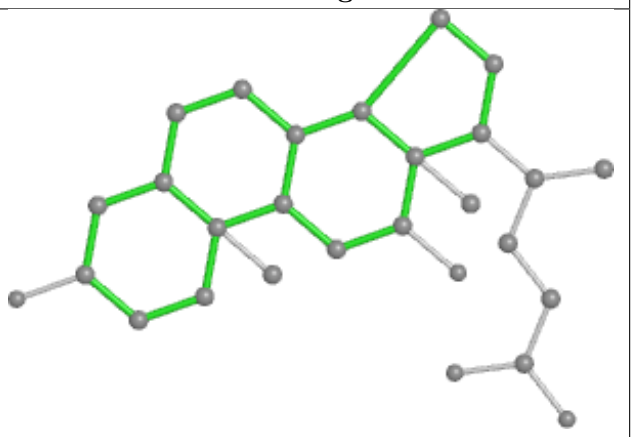
Bond lengths



Bond angles

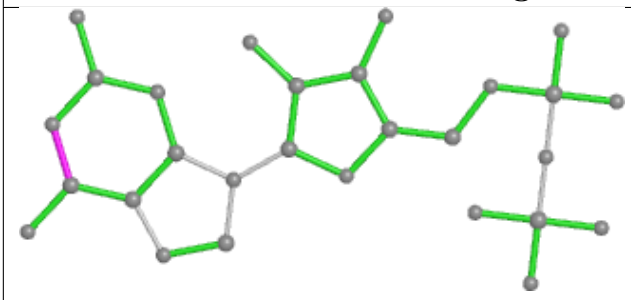


Torsions

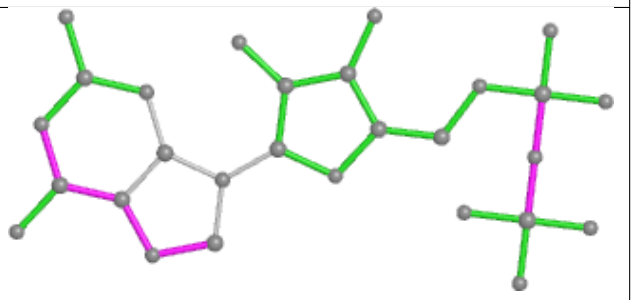


Rings

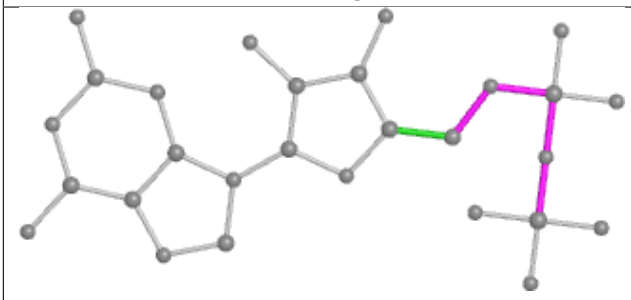
Ligand GDP B 1469



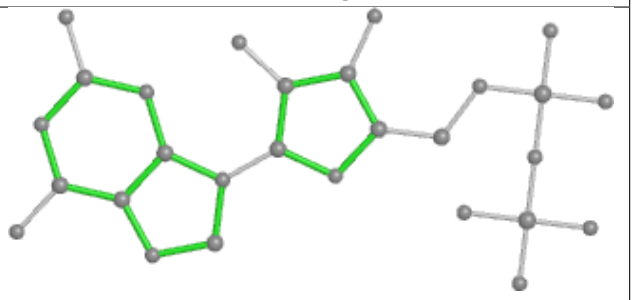
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	1.04	97 (21%) 0 0	107, 205, 299, 372	0
1	B	452/482 (93%)	0.75	71 (15%) 2 1	80, 152, 347, 414	0
1	C	467/482 (96%)	0.24	20 (4%) 35 36	74, 123, 227, 308	0
1	D	463/482 (96%)	2.14	197 (42%) 0 0	140, 274, 369, 416	0
All	All	1830/1928 (94%)	1.04	385 (21%) 1 1	74, 188, 338, 416	0

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	453	VAL	13.2
1	D	401	LYS	11.9
1	B	432	VAL	11.2
1	D	442	LYS	10.9
1	D	78	SER	10.9
1	D	438	THR	10.6
1	A	81	ASP	10.5
1	D	441	THR	10.2
1	B	404	THR	10.1
1	D	250	MET	10.1
1	D	412	SER	10.0
1	B	418	LYS	9.1
1	D	333	ILE	9.0
1	D	399	ILE	8.8
1	D	304	GLY	8.5
1	D	79	ALA	8.5
1	D	65	ASP	8.4
1	D	467	TRP	8.3
1	B	441	THR	8.1
1	D	390	GLU	8.1
1	D	406	ILE	7.9

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Mol	Chain	Res	Type	RSRZ
1	D	242	ALA	7.9
1	A	449	PHE	7.8
1	D	402	GLY	7.7
1	D	382	ILE	7.5
1	A	405	VAL	7.5
1	B	461	LEU	7.4
1	D	392	LEU	7.3
1	D	320	PHE	7.2
1	D	414	VAL	7.2
1	D	416	ALA	7.1
1	D	69	HIS	7.1
1	B	330	ASN	7.1
1	D	400	ASP	7.0
1	D	251	ALA	6.9
1	D	330	ASN	6.9
1	A	406	ILE	6.8
1	D	391	VAL	6.8
1	D	431	ILE	6.7
1	B	405	VAL	6.6
1	B	450	SER	6.6
1	A	404	THR	6.6
1	D	311	VAL	6.6
1	D	16	HIS	6.6
1	D	415	ALA	6.4
1	D	179	ILE	6.4
1	D	31	THR	6.4
1	D	256	ASP	6.4
1	D	66	ALA	6.3
1	D	38	PRO	6.3
1	D	426	ILE	6.3
1	A	257	ALA	6.3
1	B	428	GLY	6.2
1	D	405	VAL	6.2
1	A	434	LYS	6.2
1	D	425	SER	6.2
1	B	433	GLY	6.2
1	A	441	THR	6.1
1	B	396	LYS	6.0
1	B	460	ILE	6.0
1	D	322	LYS	6.0
1	D	417	GLU	5.9
1	D	173	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	332	VAL	5.8
1	D	411	GLN	5.6
1	B	449	PHE	5.6
1	D	17	GLY	5.5
1	D	429	LYS	5.5
1	D	172	THR	5.5
1	D	329	LEU	5.5
1	D	452	ASN	5.4
1	D	295	PRO	5.4
1	C	35	ASP	5.4
1	A	433	GLY	5.4
1	A	225	MET	5.4
1	D	318	VAL	5.3
1	D	413	LYS	5.2
1	A	304	GLY	5.2
1	D	428	GLY	5.2
1	B	427	GLU	5.1
1	D	40	SER	5.1
1	A	448	GLU	5.1
1	A	259	GLN	5.0
1	D	312	ALA	5.0
1	B	397	VAL	5.0
1	A	198	GLY	5.0
1	B	439	PHE	4.9
1	D	462	ASN	4.9
1	D	439	PHE	4.9
1	D	45	ILE	4.9
1	B	392	LEU	4.8
1	A	435	ILE	4.7
1	D	343	GLU	4.7
1	A	47	ILE	4.7
1	A	256	ASP	4.7
1	D	403	ARG	4.7
1	D	464	LEU	4.7
1	A	424	ILE	4.6
1	A	397	VAL	4.6
1	D	233	GLN	4.6
1	D	15	ASP	4.6
1	D	292	ASN	4.5
1	D	334	SER	4.5
1	D	316	LYS	4.5
1	A	46	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	422	GLU	4.5
1	D	48	ASP	4.5
1	A	196	ILE	4.5
1	D	331	GLU	4.5
1	D	200	GLY	4.5
1	D	430	ASP	4.4
1	B	440	GLY	4.4
1	D	440	GLY	4.4
1	A	426	ILE	4.4
1	D	444	LEU	4.4
1	D	39	GLU	4.4
1	A	439	PHE	4.4
1	A	452	ASN	4.4
1	A	389	LYS	4.4
1	A	220	VAL	4.3
1	A	429	LYS	4.3
1	B	424	ILE	4.3
1	D	47	ILE	4.3
1	C	34	HIS	4.3
1	D	455	ASN	4.3
1	B	415	ALA	4.3
1	D	178	ILE	4.2
1	A	287	ASP	4.2
1	D	212	VAL	4.2
1	D	259	GLN	4.2
1	D	195	PRO	4.2
1	D	456	ARG	4.2
1	A	69	HIS	4.2
1	D	81	ASP	4.1
1	A	465	ARG	4.1
1	D	321	GLY	4.1
1	D	241	GLU	4.1
1	B	429	LYS	4.1
1	C	32	SER	4.1
1	B	445	LEU	4.1
1	A	445	LEU	4.1
1	D	384	ASP	4.1
1	B	409	LEU	4.0
1	D	258	LYS	4.0
1	D	289	PHE	4.0
1	D	424	ILE	4.0
1	A	258	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	417	GLU	3.9
1	D	255	VAL	3.9
1	D	465	ARG	3.9
1	B	414	VAL	3.9
1	B	321	GLY	3.9
1	A	284	LYS	3.9
1	A	450	SER	3.8
1	D	169	ILE	3.8
1	D	445	LEU	3.8
1	D	328	ILE	3.8
1	D	323	THR	3.8
1	D	249	GLY	3.8
1	A	398	LYS	3.8
1	D	154	ILE	3.8
1	A	380	LYS	3.8
1	D	67	PRO	3.7
1	D	388	LYS	3.7
1	A	218	LEU	3.7
1	D	327	ILE	3.7
1	D	325	GLU	3.7
1	C	430	ASP	3.7
1	D	36	LYS	3.7
1	D	305	MET	3.7
1	D	223	ILE	3.7
1	A	432	VAL	3.6
1	D	389	LYS	3.6
1	D	436	LYS	3.6
1	B	438	THR	3.6
1	D	220	VAL	3.6
1	A	329	LEU	3.6
1	D	21	LEU	3.6
1	D	219	LYS	3.6
1	B	399	ILE	3.5
1	A	197	LYS	3.5
1	D	22	SER	3.5
1	D	68	GLY	3.5
1	C	36	LYS	3.5
1	B	413	LYS	3.5
1	B	455	ASN	3.4
1	D	225	MET	3.4
1	C	323	THR	3.4
1	B	431	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	323	THR	3.3
1	B	318	VAL	3.3
1	D	409	LEU	3.3
1	D	19	THR	3.3
1	A	428	GLY	3.3
1	D	122	ASP	3.3
1	A	413	LYS	3.3
1	D	269	LYS	3.3
1	D	221	LEU	3.3
1	D	13	HIS	3.3
1	D	461	LEU	3.3
1	B	322	LYS	3.3
1	B	323	THR	3.3
1	A	324	GLU	3.2
1	B	426	ILE	3.2
1	D	380	LYS	3.2
1	D	30	SER	3.2
1	D	4	LYS	3.2
1	D	454	GLU	3.2
1	A	407	ASP	3.2
1	D	397	VAL	3.2
1	B	447	ALA	3.2
1	D	218	LEU	3.2
1	B	362	ASP	3.1
1	A	451	GLY	3.1
1	A	396	LYS	3.1
1	A	436	LYS	3.1
1	D	155	SER	3.1
1	D	407	ASP	3.1
1	A	282	LYS	3.1
1	A	388	LYS	3.1
1	D	290	LYS	3.1
1	D	232	ILE	3.1
1	D	345	GLU	3.1
1	B	398	LYS	3.1
1	A	336	ASN	3.0
1	D	313	VAL	3.0
1	D	28	ILE	3.0
1	D	437	GLY	3.0
1	D	393	ARG	3.0
1	A	242	ALA	3.0
1	C	402	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	446	THR	3.0
1	B	1	MET	3.0
1	A	447	ALA	3.0
1	A	423	GLU	3.0
1	A	286	SER	3.0
1	A	260	ILE	3.0
1	D	170	ILE	3.0
1	D	120	LYS	3.0
1	A	326	ASN	3.0
1	B	394	GLU	3.0
1	B	403	ARG	2.9
1	A	200	GLY	2.9
1	D	314	PRO	2.9
1	A	419	LEU	2.9
1	A	78	SER	2.9
1	B	393	ARG	2.9
1	A	319	THR	2.8
1	D	119	THR	2.8
1	A	195	PRO	2.8
1	B	402	GLY	2.8
1	D	443	GLY	2.8
1	D	419	LEU	2.8
1	D	294	THR	2.8
1	D	326	ASN	2.8
1	B	434	LYS	2.8
1	A	321	GLY	2.8
1	D	191	ASP	2.8
1	D	335	GLY	2.8
1	A	255	VAL	2.8
1	D	211	ILE	2.8
1	D	59	TYR	2.8
1	A	438	THR	2.7
1	B	467	TRP	2.7
1	A	459	VAL	2.7
1	B	406	ILE	2.7
1	D	20	THR	2.7
1	D	385	LEU	2.7
1	D	377	GLU	2.7
1	C	37	LEU	2.7
1	B	308	VAL	2.7
1	C	414	VAL	2.7
1	D	459	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	416	ALA	2.7
1	D	217	GLU	2.7
1	B	453	VAL	2.7
1	B	435	ILE	2.7
1	D	468	GLY	2.7
1	D	230	ARG	2.6
1	A	458	LYS	2.6
1	B	320	PHE	2.6
1	D	254	GLY	2.6
1	A	317	LYS	2.6
1	D	243	LYS	2.6
1	A	211	ILE	2.6
1	C	322	LYS	2.6
1	B	458	LYS	2.6
1	A	281	ALA	2.6
1	B	459	VAL	2.6
1	D	3	PHE	2.5
1	D	156	ALA	2.5
1	B	324	GLU	2.5
1	D	43	ARG	2.5
1	D	180	ARG	2.5
1	A	320	PHE	2.5
1	A	431	ILE	2.5
1	D	177	GLU	2.5
1	B	457	ASP	2.5
1	A	444	LEU	2.5
1	D	350	ALA	2.5
1	A	212	VAL	2.5
1	A	289	PHE	2.5
1	B	109	HIS	2.5
1	B	389	LYS	2.5
1	D	383	LYS	2.5
1	A	199	ALA	2.5
1	B	456	ARG	2.5
1	A	440	GLY	2.4
1	A	410	ALA	2.4
1	B	334	SER	2.4
1	A	201	THR	2.4
1	A	390	GLU	2.4
1	C	435	ILE	2.4
1	D	418	LYS	2.4
1	C	409	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	356	VAL	2.4
1	A	379	PHE	2.4
1	A	442	LYS	2.4
1	B	311	VAL	2.4
1	C	442	LYS	2.4
1	D	228	LYS	2.4
1	A	271	THR	2.4
1	D	378	GLU	2.4
1	D	268	SER	2.4
1	D	50	GLY	2.4
1	B	454	GLU	2.4
1	D	80	ALA	2.4
1	D	76	VAL	2.4
1	D	267	THR	2.3
1	D	460	ILE	2.3
1	D	77	VAL	2.3
1	A	409	LEU	2.3
1	D	347	LYS	2.3
1	B	298	LYS	2.3
1	D	270	ASP	2.3
1	C	411	GLN	2.3
1	D	25	LEU	2.3
1	A	430	ASP	2.3
1	B	423	GLU	2.3
1	D	286	SER	2.3
1	C	13	HIS	2.3
1	D	196	ILE	2.3
1	D	32	SER	2.3
1	C	269	LYS	2.3
1	B	400	ASP	2.3
1	A	418	LYS	2.3
1	D	257	ALA	2.3
1	A	453	VAL	2.3
1	B	464	LEU	2.2
1	D	280	VAL	2.2
1	D	379	PHE	2.2
1	D	52	SER	2.2
1	A	387	ILE	2.2
1	C	467	TRP	2.2
1	D	288	ILE	2.2
1	D	252	ILE	2.2
1	B	462	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	-2	ARG	2.2
1	D	192	HIS	2.2
1	D	458	LYS	2.2
1	A	385	LEU	2.2
1	D	248	VAL	2.2
1	B	29	ALA	2.2
1	C	320	PHE	2.1
1	D	203	VAL	2.1
1	B	329	LEU	2.1
1	D	319	THR	2.1
1	A	84	ASP	2.1
1	D	435	ILE	2.1
1	D	165	LEU	2.1
1	B	442	LYS	2.1
1	D	297	MET	2.1
1	B	390	GLU	2.1
1	D	262	ARG	2.1
1	A	316	LYS	2.1
1	A	325	GLU	2.1
1	A	376	ILE	2.1
1	A	378	GLU	2.0
1	B	419	LEU	2.0
1	A	415	ALA	2.0
1	D	18	LYS	2.0
1	D	296	LYS	2.0
1	C	319	THR	2.0
1	D	227	THR	2.0
1	D	224	ASN	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, 95^{th} 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	0.81	0.11	180,242,266,268	2
1	CMH	A	371	8/9	0.87	0.35	168,213,225,228	2
1	CMH	D	340	8/9	0.90	0.21	207,306,312,317	2
1	CMH	B	338	8/9	0.92	0.28	151,200,232,276	2
1	CMH	D	264	8/9	0.92	0.26	241,255,280,281	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CMH	B	371	8/9	0.93	0.31	174,197,251,332	2
1	CMH	C	338	8/9	0.96	0.18	74,109,174,331	2
1	CMH	A	338	8/9	0.96	0.14	174,190,268,307	2
1	CMH	A	264	8/9	0.97	0.17	171,215,224,235	2
1	CMH	A	340	8/9	0.98	0.19	169,213,226,240	2
1	CMH	B	340	8/9	0.98	0.25	160,194,264,332	0
1	CMH	C	340	8/9	0.98	0.24	69,99,124,131	2
1	CMH	D	371	8/9	0.98	0.19	145,181,227,234	2
1	CMH	C	264	8/9	0.99	0.16	70,108,137,210	0
1	CMH	C	371	8/9	0.99	0.25	78,109,123,156	2
1	CMH	B	264	8/9	1.00	0.17	73,89,99,112	2

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	SO4	B	1471	5/5	0.79	0.17	205,213,271,283	0
5	SO4	B	1472	5/5	0.80	0.90	139,226,336,344	0
7	5GP	B	1474	24/24	0.82	0.38	242,294,308,311	0
5	SO4	C	1473	5/5	0.83	0.15	164,166,220,230	5
5	SO4	C	1481	5/5	0.90	1.65	172,210,221,235	5
6	DXC	C	1476	28/28	0.92	0.33	159,168,217,253	0
4	GDP	B	1469	28/28	0.92	0.21	126,197,212,235	0
6	DXC	C	1479	28/28	0.93	0.29	82,104,174,196	28
5	SO4	C	1472	5/5	0.93	0.19	133,154,189,210	0
6	DXC	C	1477	28/28	0.94	0.31	91,111,162,182	0
6	DXC	B	1473	28/28	0.95	0.28	68,97,134,143	0
6	DXC	C	1475	28/28	0.95	0.27	61,95,139,146	0
6	DXC	C	1478	28/28	0.96	0.24	93,118,158,196	0
2	GNP	A	1469	32/32	0.97	0.12	120,165,202,249	0
6	DXC	C	1480	28/28	0.97	0.23	63,85,106,127	0
5	SO4	C	1471	5/5	0.97	0.22	101,149,159,220	0
3	MG	B	1470	1/1	0.98	0.20	342,342,342,342	0

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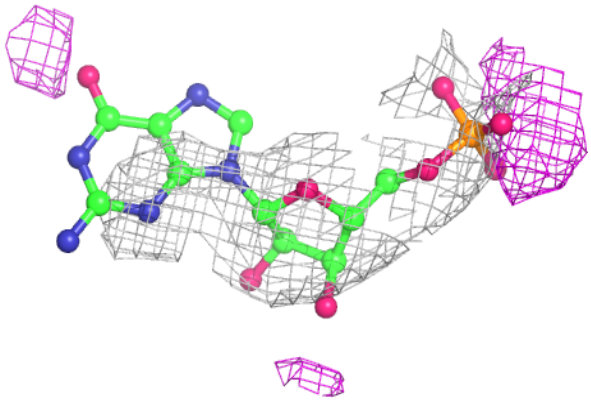
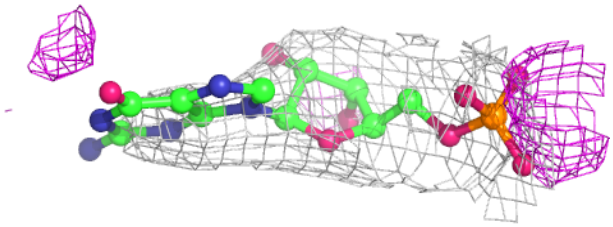
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1470	1/1	0.98	0.08	244,244,244,244	0

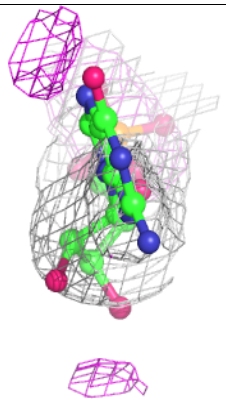
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

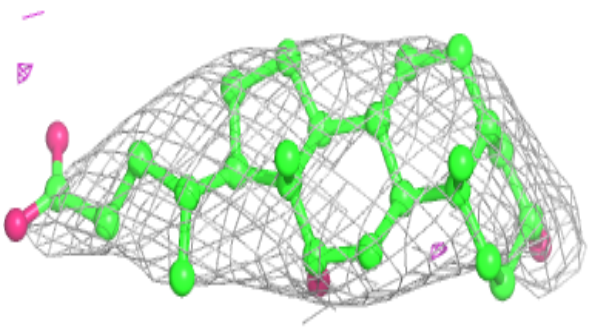


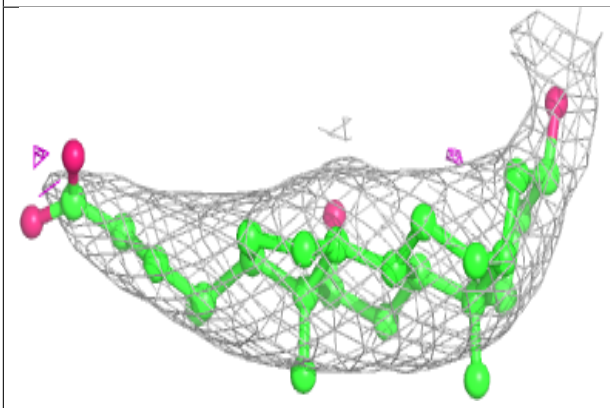


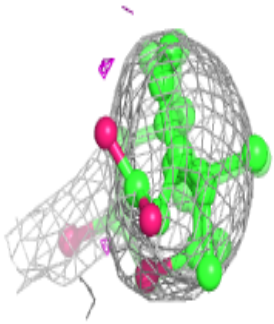


Electron density around DXC C 1476:

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

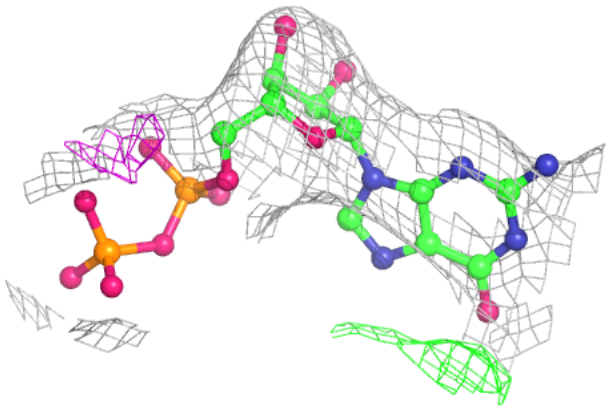


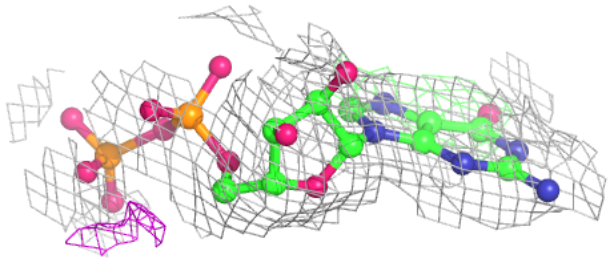


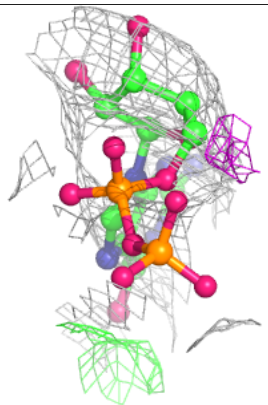


Electron density around GDP B 1469:

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

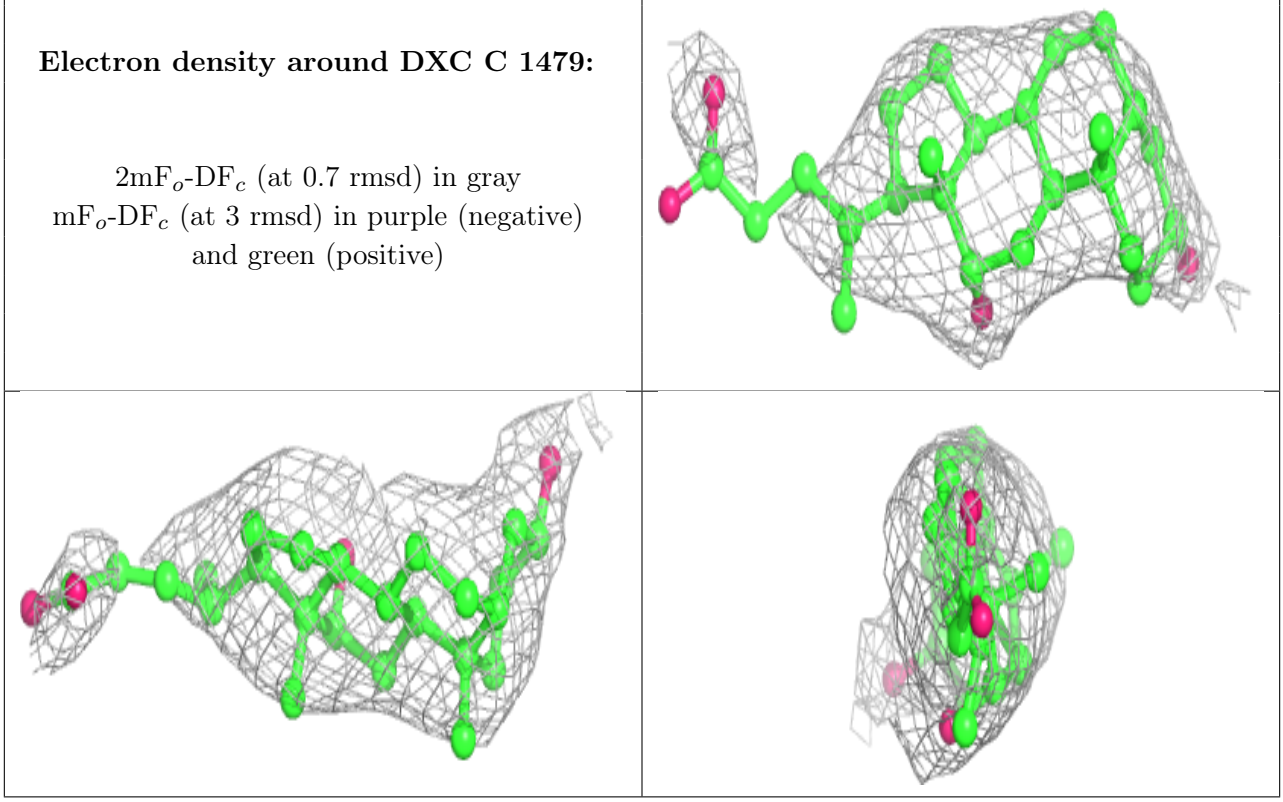






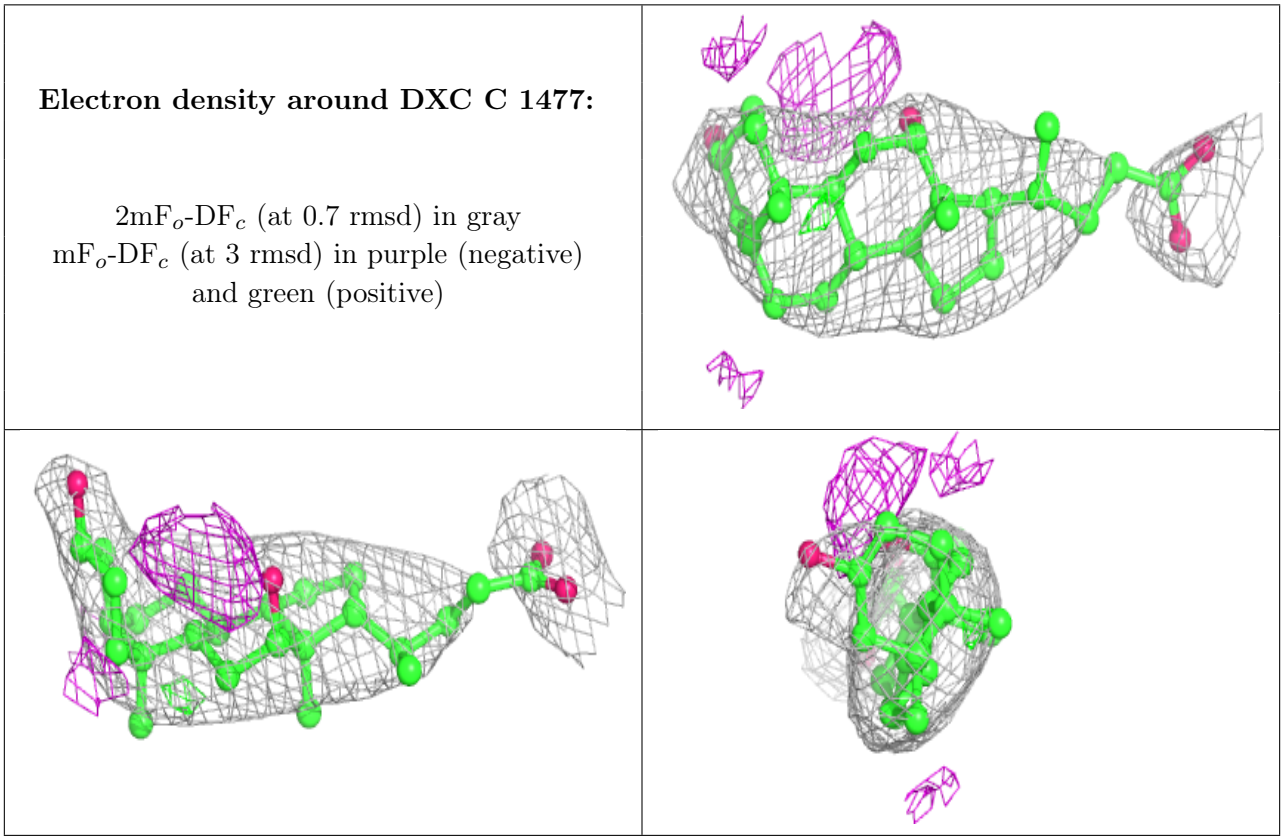
Electron density around DXC C 1479:

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



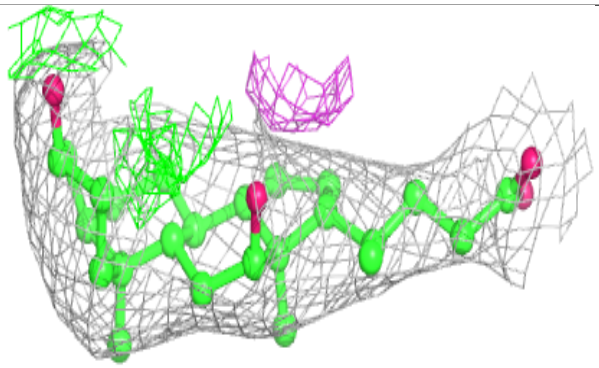
Electron density around DXC C 1477:

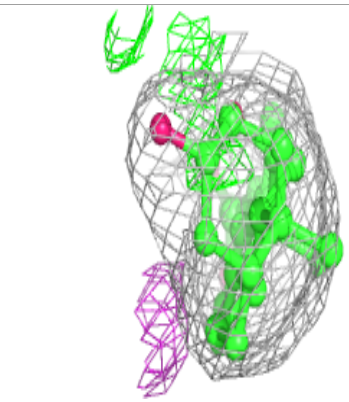
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

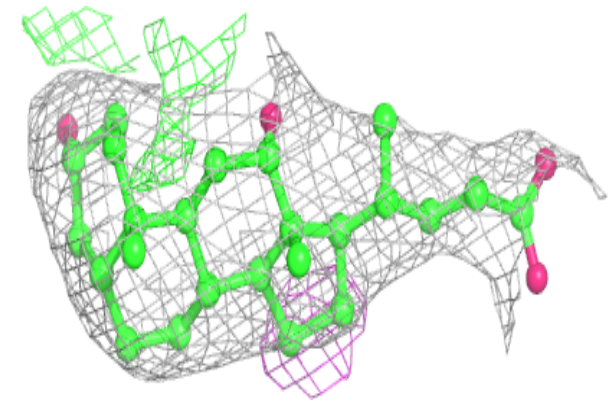


Electron density around DXC B 1473:

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

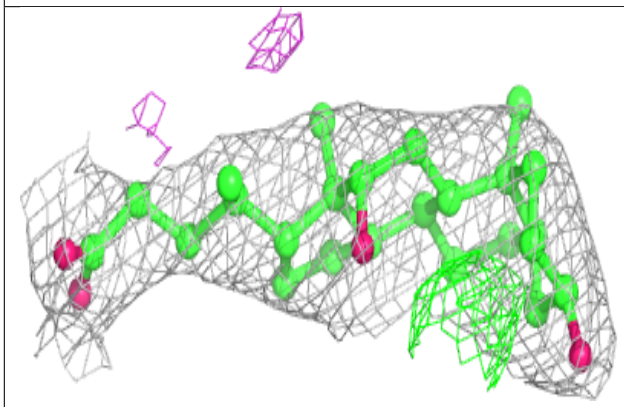


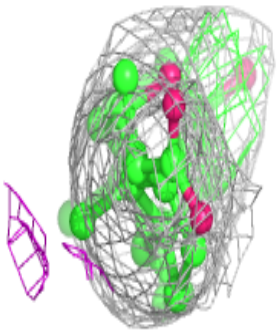


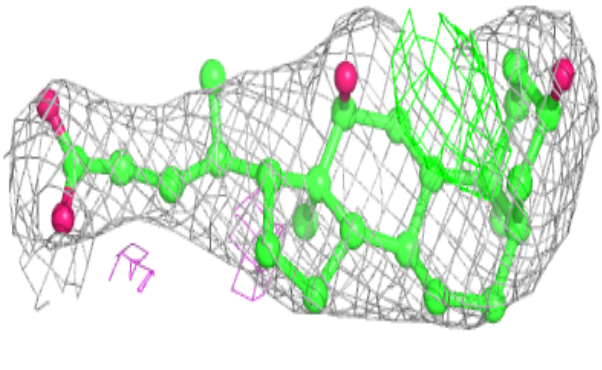


Electron density around DXC C 1475:

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

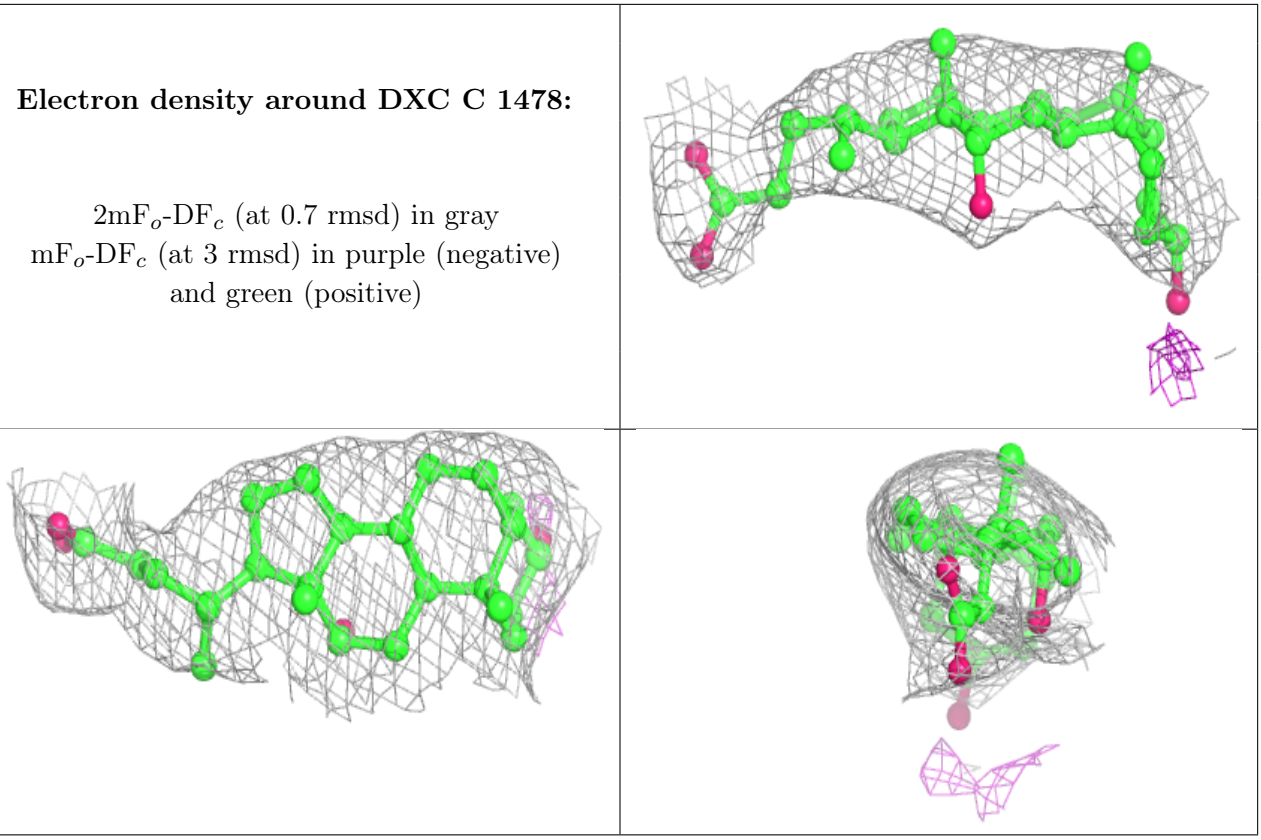






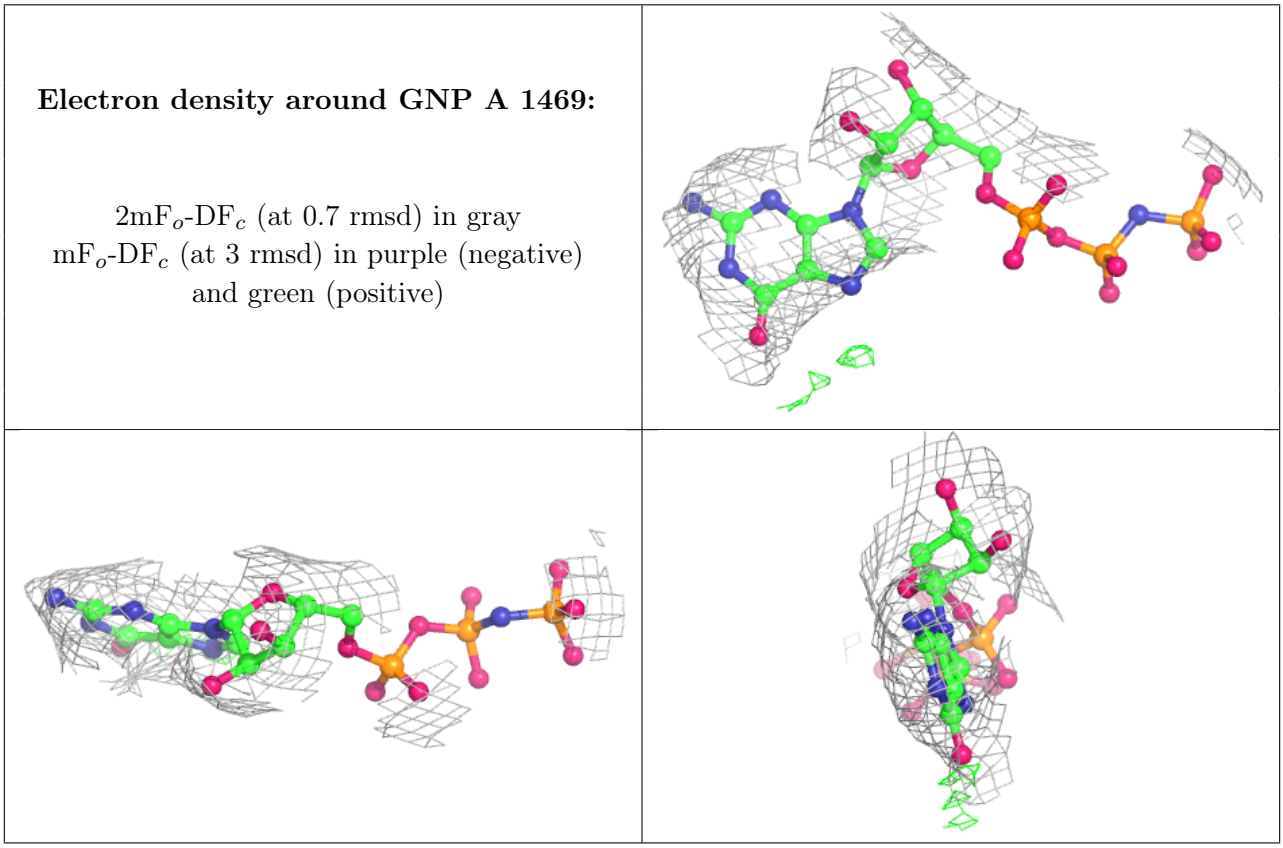
Electron density around DXC C 1478:

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



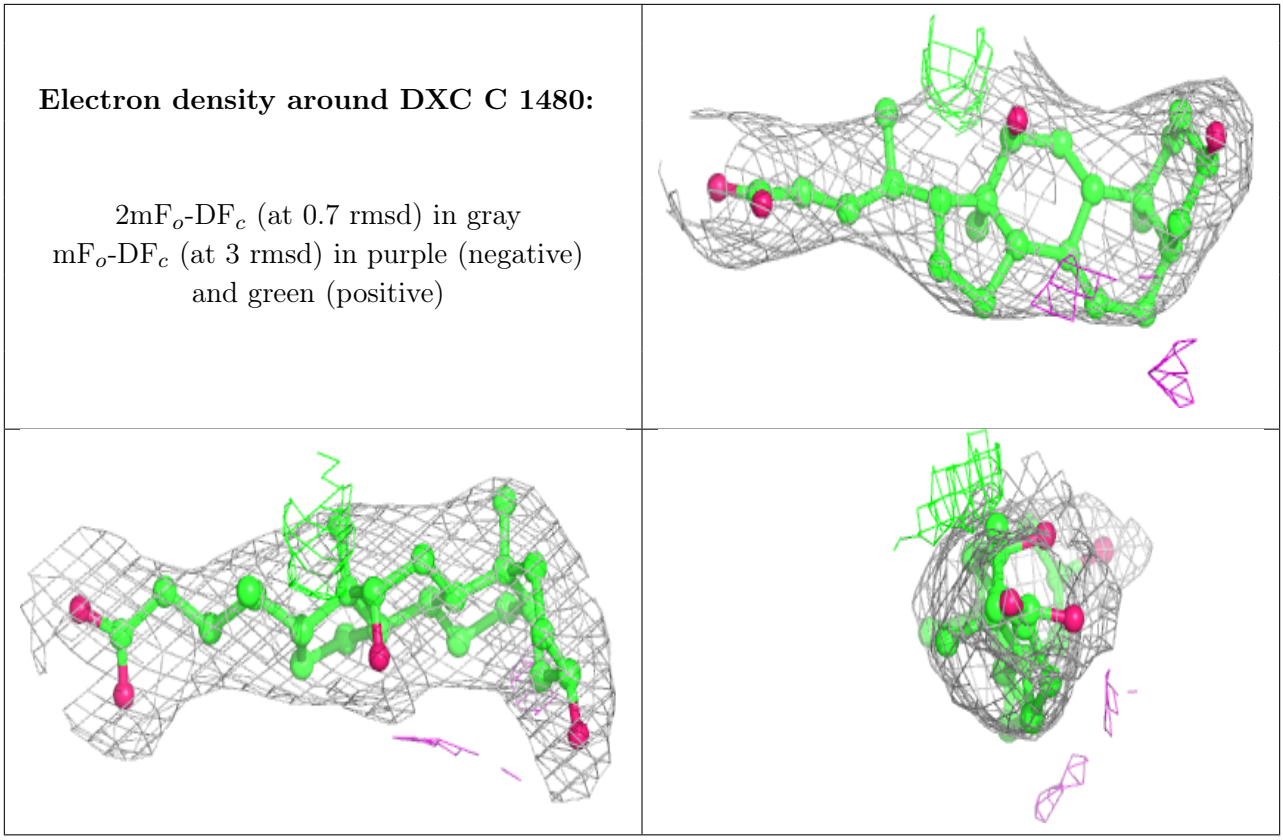
Electron density around GNP A 1469:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.