Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:37 pm GMT

PDB ID	:	4ACA
Title	:	CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR SELB FROM METHANOCOCCUS MARIPALUDIS, APO FORM
Authors	:	Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on	:	2011-12-14
Resolution	:	3.15 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:

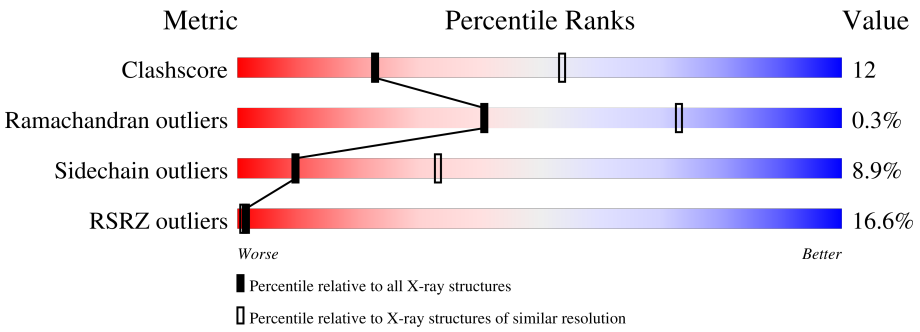
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.15 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))
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	16% 63% 27% • 7%
1	B	482	15% 65% 27% • 5%
1	C	482	4% 73% 22% • •
1	D	482	29% 65% 28% • •

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	A	340	-	-	X	-
1	CMH	B	371	-	-	X	-
2	SO4	B	1471	-	-	-	X
2	SO4	C	1474	-	-	-	X
2	SO4	C	1481	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14529 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
			Total	C	Hg	N	O	S			
1	A	448	3475	2220	4	593	644	14	0	0	0
1	B	456	3533	2257	4	603	655	14	0	0	0
1	C	471	3651	2327	4	627	679	14	0	0	0
1	D	467	3615	2305	4	618	675	13	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

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

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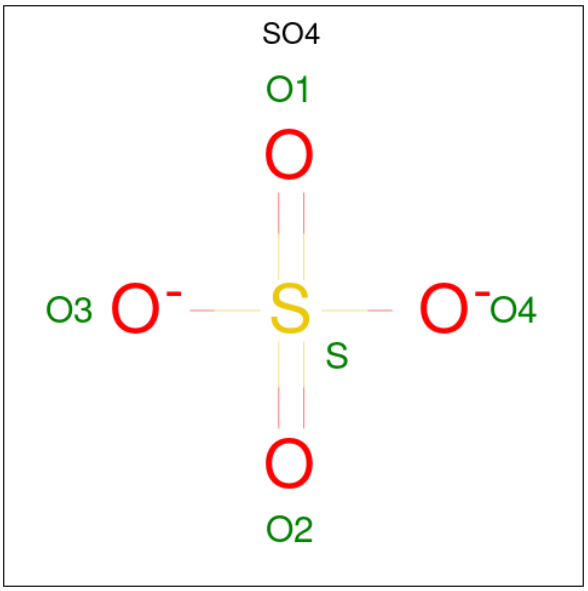
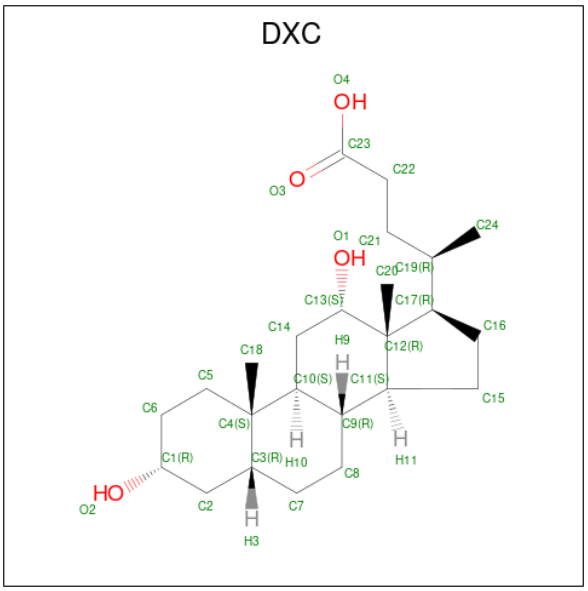
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	expression tag	UNP Q8J307
B	-5	ILE	-	expression tag	UNP Q8J307
B	-4	GLU	-	expression tag	UNP Q8J307
B	-3	GLY	-	expression tag	UNP Q8J307
B	-2	ARG	-	expression tag	UNP Q8J307
B	-1	PRO	-	expression tag	UNP Q8J307
B	0	HIS	-	expression tag	UNP Q8J307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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



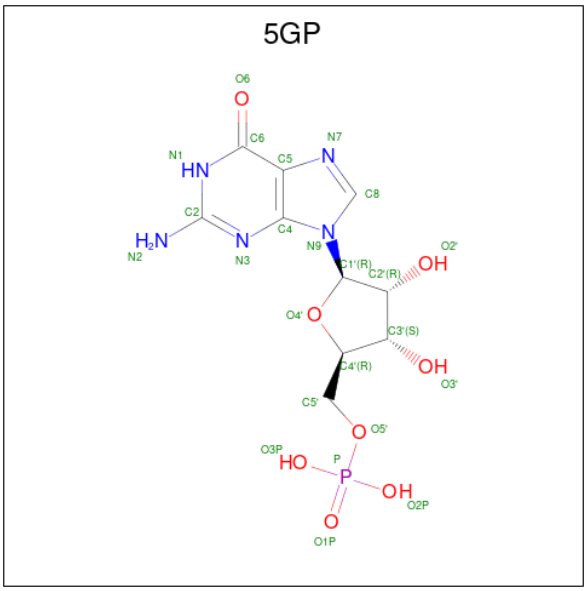
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 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
			Total	C	O			
3	B	1	28	24	4		0	0
			Total	C	O			
3	C	1	28	24	4		0	0
			Total	C	O			
3	C	1	28	24	4		0	0
			Total	C	O			
3	C	1	28	24	4		0	0
			Total	C	O			
3	C	1	28	24	4		0	0
			Total	C	O			
3	C	1	28	24	4		0	0
			Total	C	O			
3	C	1	28	24	4		0	0

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



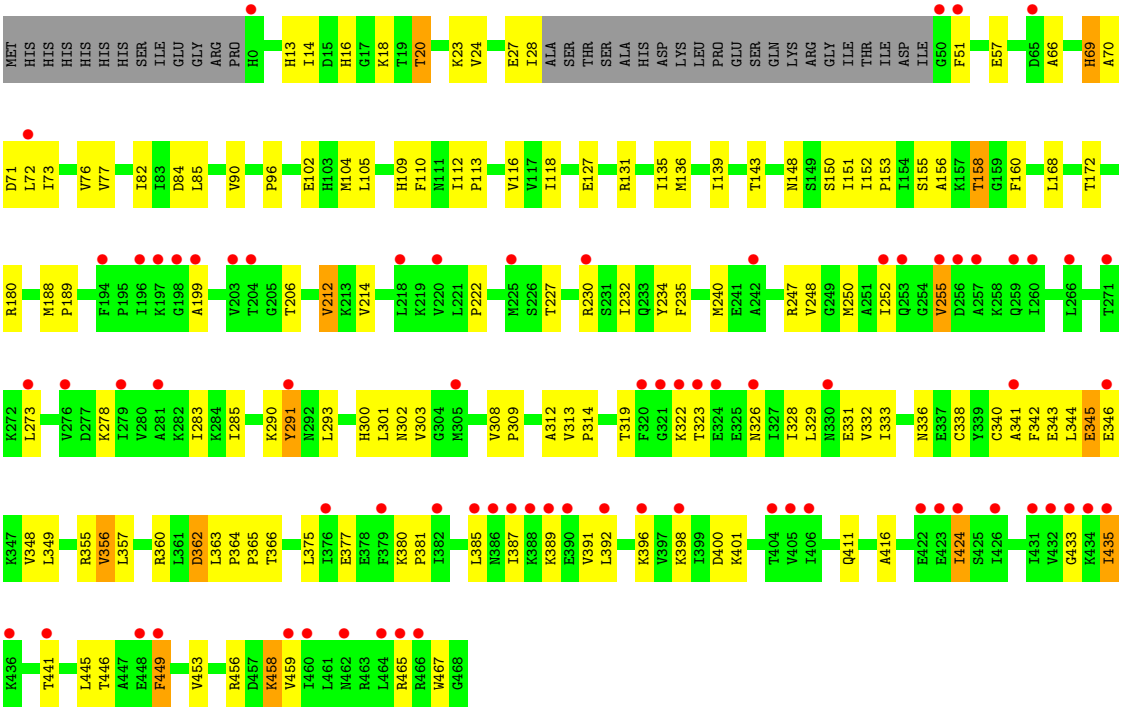
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	24	10	5	8	1	0	0

3 Residue-property plots (i)

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

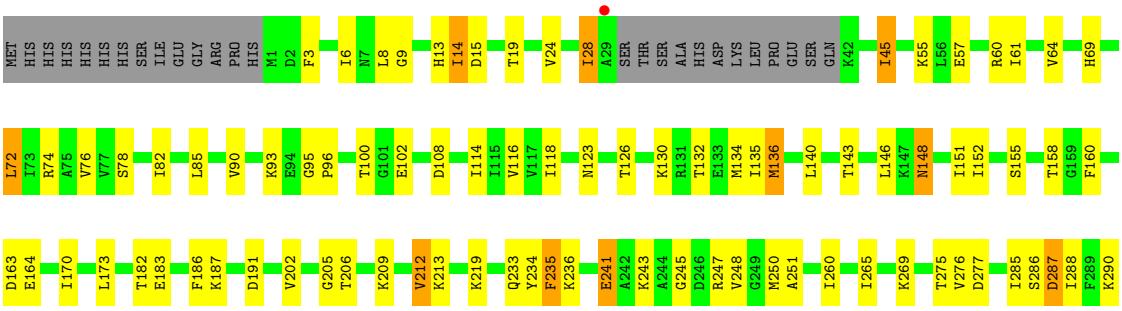
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

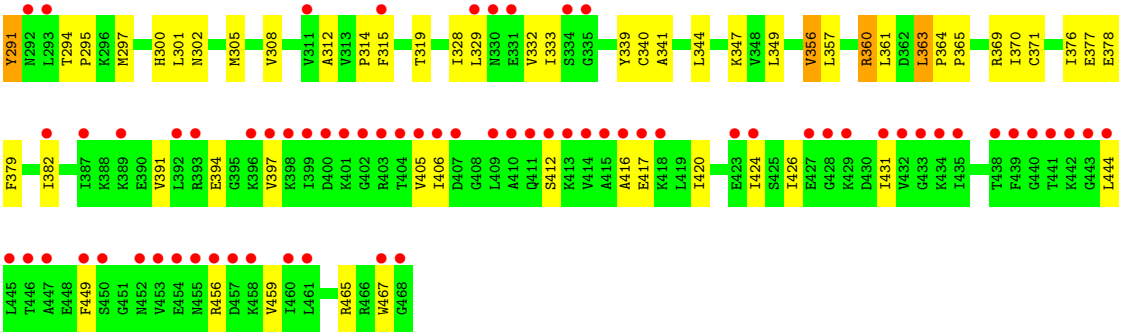
Chain A:



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

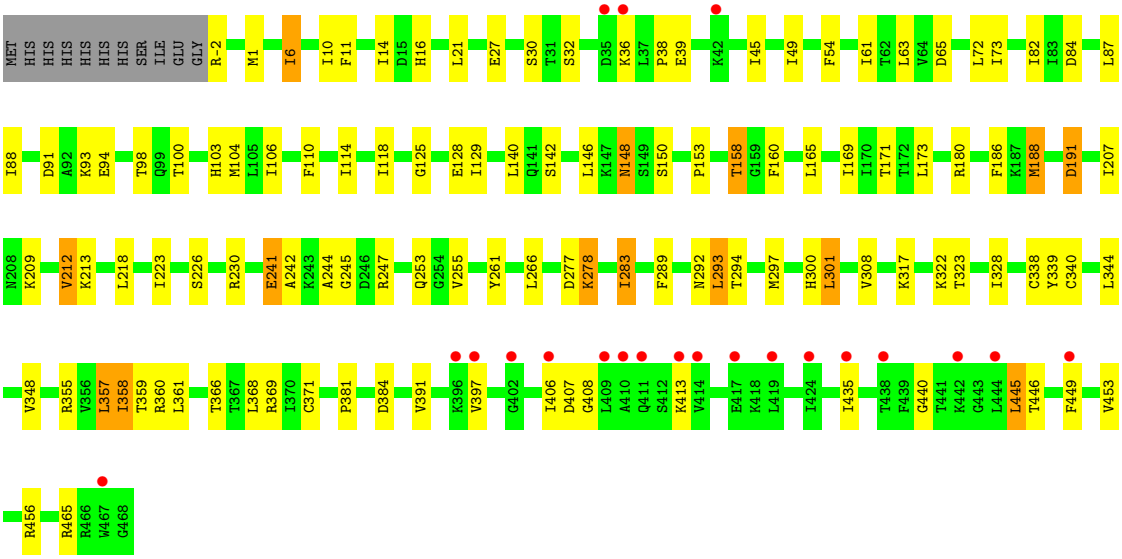
Chain B:





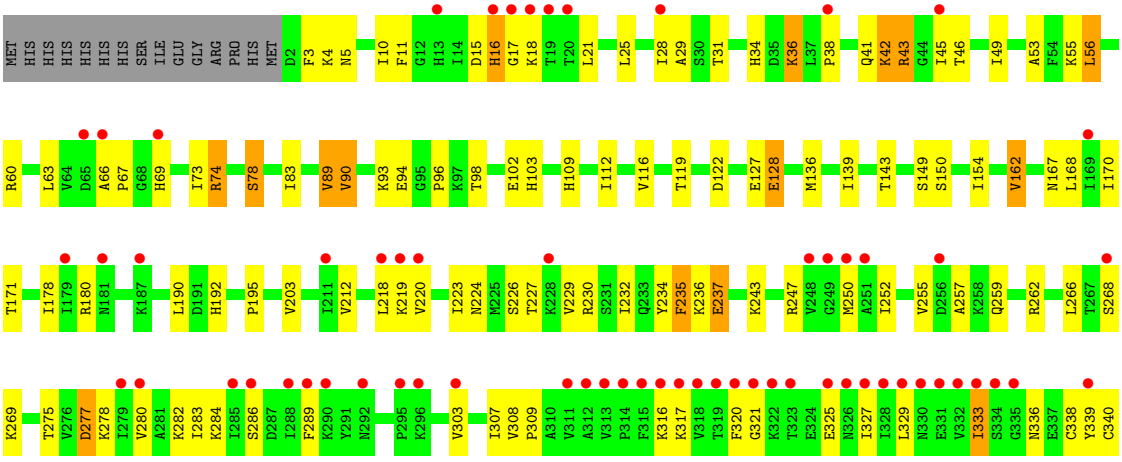
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

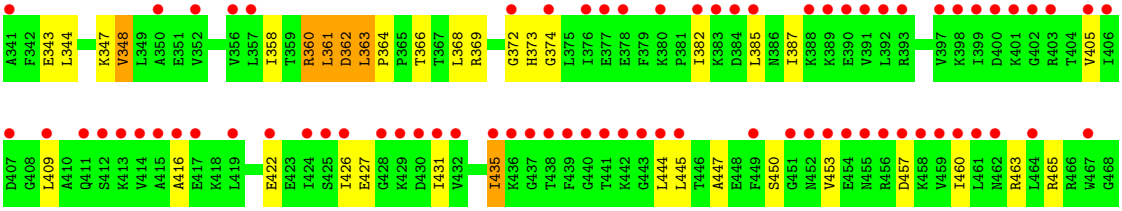
Chain C:



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

Chain D:




A341 F342 E343 L344 K347 V348 L349 A350 E351 V352 V356 L357 I358 T359 R360 L361 D362 L363 P364 P365 T366 T367 L368 R369 G372 H373 G374 L375 I376 E377 E378 F379 K380 P381 I382 K383 D384 L385 N386 I387 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 V432 I435 K436 G437 T438 F439 G440 T441 K442 G443 L444 L445 T446 A447 E448 F449 S450 G451 N452 V453 E454 N455 R456 D457 K458 V459 I460 L461 M462 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	146.86Å 146.86Å 297.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.15 48.07 – 3.15	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.97-3.15) 90.3 (48.07-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.172 , 0.215 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	100.6	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 126.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.31	0/3484	0.54	0/4684
1	B	0.34	0/3541	0.57	0/4760
1	C	0.39	0/3664	0.62	0/4929
1	D	0.29	0/3626	0.52	0/4878
All	All	0.33	0/14315	0.56	0/19251

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3475	0	3656	83	0
1	B	3533	0	3728	91	0
1	C	3651	0	3838	70	0
1	D	3615	0	3799	101	0
2	B	10	0	0	1	0
2	C	25	0	0	1	0
3	B	28	0	39	2	0
3	C	168	0	234	11	0
4	B	24	0	12	2	0
All	All	14529	0	15306	343	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 (343) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ILE:HG13	1:D:340:CMH:HB3	1.21	1.15
1:C:338:CMH:HB3	1:C:340:CMH:CM	2.03	0.86
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.58	0.85
1:D:284:LYS:HG3	1:D:336:ASN:HB2	1.63	0.81
1:D:416:ALA:HB1	1:D:445:LEU:HD21	1.61	0.79
1:C:283:ILE:HG12	1:C:358:ILE:HD11	1.70	0.74
1:C:6:ILE:HD12	1:C:173:LEU:HD13	1.71	0.73
1:B:360:ARG:NH1	1:B:371:CMH:SG	2.61	0.73
1:D:116:VAL:HG11	1:D:136:MET:HG2	1.69	0.72
1:B:158:THR:HG23	1:D:363:LEU:HB3	1.75	0.69
1:D:422:GLU:H	1:D:435:ILE:HG22	1.57	0.69
1:B:302:ASN:HB2	1:B:357:LEU:HB3	1.76	0.68
1:C:158:THR:HG22	1:C:160:PHE:H	1.58	0.68
1:D:21:LEU:HD22	1:D:89:VAL:HG11	1.76	0.67
1:D:427:GLU:HG2	1:D:460:ILE:HG13	1.76	0.67
1:B:82:ILE:HG23	1:B:245:GLY:HA2	1.76	0.67
1:B:233:GLN:HE21	1:B:236:LYS:HA	1.59	0.67
1:C:283:ILE:HD13	1:C:340:CMH:HB3	1.74	0.67
1:C:308:VAL:HG21	1:C:344:LEU:HD13	1.77	0.66
1:D:277:ASP:HB3	1:D:347:LYS:HE2	1.77	0.66
1:A:234:TYR:HB2	1:A:248:VAL:HG12	1.77	0.66
1:A:152:ILE:HD11	1:A:168:LEU:HD22	1.80	0.64
1:D:316:LYS:N	1:D:327:ILE:O	2.29	0.64
1:D:360:ARG:HD2	1:D:363:LEU:HD11	1.78	0.64
1:D:67:PRO:HA	1:D:78:SER:HB2	1.78	0.64
1:B:143:THR:HG21	1:B:146:LEU:HB2	1.80	0.63
1:A:118:ILE:HB	1:A:153:PRO:HA	1.81	0.63
1:B:361:LEU:HA	1:B:369:ARG:HD2	1.81	0.63
1:B:288:ILE:HB	4:B:1474:5GP:HN22	1.64	0.62
1:D:4:LYS:NZ	1:D:178:ILE:O	2.31	0.62
1:C:82:ILE:HG23	1:C:245:GLY:HA2	1.80	0.62
1:B:132:THR:HA	1:B:135:ILE:HD12	1.81	0.62
1:B:69:HIS:NE2	1:B:102:GLU:OE1	2.25	0.62
1:D:218:LEU:HD11	1:D:229:VAL:HG22	1.81	0.61
1:D:73:ILE:O	1:D:74:ARG:HG3	2.00	0.61
1:A:435:ILE:HD11	1:A:445:LEU:HD22	1.83	0.60
1:D:43:ARG:HB3	1:D:45:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:HA3	1:A:449:PHE:HB3	1.82	0.60
1:C:88:ILE:HD12	1:C:114:ILE:HD13	1.83	0.59
1:B:116:VAL:HB	1:B:151:ILE:HG12	1.85	0.59
1:C:88:ILE:HD13	1:C:104:MET:HG2	1.83	0.59
1:B:74:ARG:NH2	2:B:1471:SO4:O4	2.35	0.59
1:D:93:LYS:HA	1:D:128:GLU:HG2	1.84	0.58
1:D:109:HIS:CG	1:D:373:HIS:HE1	2.21	0.58
1:D:338:CMH:SG	1:D:339:TYR:N	2.75	0.58
1:B:114:ILE:HG12	1:B:146:LEU:HD22	1.86	0.58
1:C:110:PHE:CD2	1:C:355:ARG:HD2	2.37	0.58
1:D:409:LEU:HD12	1:D:445:LEU:HD12	1.85	0.58
1:C:27:GLU:HB3	1:C:32:SER:HB2	1.84	0.58
1:B:426:ILE:HB	1:B:431:ILE:HG23	1.85	0.58
1:A:362:ASP:N	1:A:362:ASP:OD1	2.32	0.57
1:B:213:LYS:HG2	1:B:241:GLU:HB2	1.86	0.57
1:D:360:ARG:HH11	1:D:363:LEU:HD21	1.67	0.57
1:C:191:ASP:OD2	1:C:247:ARG:NH1	2.31	0.57
1:B:90:VAL:HG13	1:B:118:ILE:HG12	1.87	0.57
1:C:11:PHE:HB3	1:C:103:HIS:ND1	2.20	0.57
1:C:188:MET:HG3	1:C:207:ILE:HG12	1.86	0.57
1:D:109:HIS:HB3	1:D:373:HIS:HE1	1.70	0.57
1:D:29:ALA:HB2	1:D:56:LEU:HG	1.86	0.57
1:D:83:ILE:HG22	1:D:112:ILE:HD13	1.86	0.57
1:A:96:PRO:HB3	1:A:136:MET:HE1	1.86	0.57
1:C:125:GLY:O	1:C:129:ILE:HG13	2.05	0.57
1:C:106:ILE:HG12	1:C:357:LEU:HD21	1.87	0.56
1:D:232:ILE:HG12	1:D:250:MET:HG2	1.87	0.56
1:A:158:THR:HG22	1:A:160:PHE:H	1.69	0.56
1:D:38:PRO:HB3	1:D:42:LYS:HD2	1.88	0.56
1:A:66:ALA:HB1	1:A:71:ASP:HB3	1.88	0.56
1:C:36:LYS:HE3	1:C:38:PRO:HB3	1.87	0.56
1:C:100:THR:O	1:C:104:MET:HG3	2.06	0.56
1:A:278:LYS:HD2	1:A:343:GLU:HG2	1.88	0.56
1:D:96:PRO:HG3	1:D:136:MET:SD	2.46	0.56
1:D:109:HIS:CG	1:D:373:HIS:CE1	2.94	0.56
1:D:36:LYS:HB3	1:D:236:LYS:HD2	1.88	0.55
1:B:187:LYS:HB3	1:B:209:LYS:HG3	1.89	0.55
1:B:72:LEU:O	1:B:76:VAL:HG23	2.06	0.55
1:A:313:VAL:HG23	1:A:341:ALA:HB3	1.88	0.55
1:A:345:GLU:HG2	1:A:346:GLU:HG3	1.89	0.55
1:C:283:ILE:HG21	1:C:371:CMH:CM	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PHE:CE2	1:C:72:LEU:HD22	2.42	0.55
1:A:24:VAL:HG21	1:A:156:ALA:HB1	1.89	0.54
1:C:165:LEU:O	1:C:169:ILE:HG13	2.08	0.54
1:B:8:LEU:HD12	1:B:85:LEU:O	2.08	0.54
1:D:74:ARG:HG2	1:D:361:LEU:HD13	1.88	0.54
1:D:102:GLU:HB2	1:D:366:THR:HG22	1.89	0.54
1:C:148:ASN:OD1	1:C:148:ASN:N	2.41	0.54
1:B:287:ASP:OD1	1:B:287:ASP:N	2.36	0.53
1:A:77:VAL:HG11	1:A:302:ASN:HB3	1.90	0.53
1:B:6:ILE:HG22	1:B:61:ILE:HG23	1.89	0.53
1:D:358:ILE:HD12	1:D:372:GLY:HA3	1.90	0.53
1:A:240:MET:HE1	1:B:95:GLY:HA3	1.91	0.53
1:A:14:ILE:HA	1:A:18:LYS:NZ	2.23	0.53
1:A:283:ILE:HD12	1:A:340:CMH:HB3	1.91	0.53
1:C:397:VAL:HG11	1:C:453:VAL:HG23	1.90	0.53
1:A:293:LEU:HD13	1:A:329:LEU:HD23	1.91	0.53
1:C:118:ILE:HB	1:C:153:PRO:HA	1.90	0.53
1:B:82:ILE:HD13	1:B:206:THR:HG22	1.91	0.52
1:B:363:LEU:HD13	1:B:364:PRO:HD2	1.91	0.52
1:A:110:PHE:HD1	1:A:355:ARG:HD2	1.73	0.52
1:B:155:SER:HB3	1:B:160:PHE:HB3	1.91	0.52
1:C:110:PHE:CE2	1:C:355:ARG:HD2	2.44	0.52
1:D:3:PHE:HE2	1:D:55:LYS:HE3	1.74	0.52
1:B:406:ILE:HD11	1:B:449:PHE:HZ	1.75	0.52
1:B:93:LYS:HE3	1:B:123:ASN:O	2.09	0.51
1:C:27:GLU:HA	1:C:30:SER:HB3	1.92	0.51
1:A:389:LYS:HB3	1:A:465:ARG:HB3	1.92	0.51
1:C:293:LEU:HD22	1:C:371:CMH:CM	2.40	0.51
1:D:34:HIS:CD2	1:D:236:LYS:HB2	2.45	0.51
1:D:69:HIS:CE1	1:D:103:HIS:CE1	2.98	0.51
1:A:136:MET:HE2	1:A:139:ILE:HD12	1.93	0.51
1:D:90:VAL:HG21	1:D:136:MET:HE1	1.93	0.51
1:A:300:HIS:CE1	1:A:309:PRO:HG3	2.46	0.51
1:D:282:LYS:O	1:D:374:GLY:HA2	2.11	0.51
1:C:317:LYS:HD2	1:C:339:TYR:CE2	2.46	0.50
1:D:435:ILE:HG13	1:D:447:ALA:HB2	1.93	0.50
1:B:143:THR:HG22	1:B:146:LEU:H	1.75	0.50
1:B:329:LEU:HB3	1:B:332:VAL:HB	1.93	0.50
1:D:463:ARG:HE	1:D:465:ARG:CZ	2.25	0.50
1:B:60:ARG:HD3	1:B:235:PHE:CD2	2.47	0.50
1:B:265:ILE:HG13	1:B:349:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ASP:HA	1:D:18:LYS:HE2	1.92	0.50
1:A:285:ILE:HG12	1:A:291:TYR:CE2	2.47	0.49
1:A:336:ASN:HA	1:A:338:CMH:CM	2.42	0.49
1:B:152:ILE:HD11	1:B:164:GLU:HB2	1.94	0.49
1:B:251:ALA:HB1	1:C:1:MET:HE1	1.94	0.49
1:C:213:LYS:HG2	1:C:241:GLU:HB2	1.94	0.49
1:B:140:LEU:O	1:B:143:THR:HB	2.11	0.49
1:A:70:ALA:HA	1:A:73:ILE:HD12	1.92	0.49
1:A:387:ILE:HG23	1:A:467:TRP:HB3	1.95	0.49
1:A:398:LYS:HE2	1:A:456:ARG:NH1	2.28	0.49
1:D:109:HIS:CB	1:D:373:HIS:HE1	2.26	0.49
1:A:110:PHE:HE1	1:A:355:ARG:HB3	1.77	0.49
1:A:131:ARG:O	1:A:135:ILE:HG13	2.11	0.49
1:A:285:ILE:HG23	1:A:291:TYR:CD2	2.48	0.49
1:B:148:ASN:ND2	1:D:127:GLU:HB3	2.27	0.49
1:B:294:THR:HB	1:B:297:MET:HB3	1.94	0.49
1:B:377:GLU:HG2	1:B:378:GLU:HG3	1.95	0.49
1:D:56:LEU:HD22	1:D:170:ILE:HD11	1.94	0.49
1:A:338:CMH:HB2	1:A:340:CMH:CM	2.43	0.49
1:D:34:HIS:N	1:D:53:ALA:O	2.46	0.48
1:D:303:VAL:HB	1:D:348:VAL:HG11	1.94	0.48
1:B:243:LYS:HB3	1:B:243:LYS:HE2	1.62	0.48
1:C:322:LYS:HG3	1:C:323:THR:H	1.78	0.48
1:D:360:ARG:HD3	1:D:362:ASP:HB2	1.94	0.48
1:B:301:LEU:HD11	1:B:356:VAL:HG13	1.96	0.48
1:C:10:ILE:HD13	1:C:87:LEU:HB2	1.95	0.48
1:B:160:PHE:CZ	1:D:98:THR:HG23	2.48	0.48
1:D:405:VAL:CG1	1:D:444:LEU:HB3	2.44	0.48
1:B:134:MET:SD	1:D:94:GLU:HG2	2.53	0.48
1:D:405:VAL:HG11	1:D:444:LEU:HB3	1.95	0.48
1:A:360:ARG:HG2	1:A:363:LEU:HG	1.96	0.48
1:B:285:ILE:HD12	1:B:371:CMH:CM	2.44	0.48
1:A:308:VAL:HG21	1:A:344:LEU:HD13	1.95	0.48
1:B:82:ILE:HG21	1:B:206:THR:HG21	1.96	0.48
1:B:186:PHE:CE1	1:B:212:VAL:HG22	2.49	0.48
1:A:355:ARG:HG2	1:A:375:LEU:HD23	1.96	0.47
1:B:405:VAL:HG11	1:B:444:LEU:HD13	1.96	0.47
1:D:167:ASN:O	1:D:171:THR:OG1	2.22	0.47
1:A:155:SER:OG	1:A:158:THR:HB	2.14	0.47
1:C:-2:ARG:HE	3:C:1476:DXC:H21	1.79	0.47
1:C:16:HIS:NE2	1:C:94:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LYS:HG2	1:D:343:GLU:HG2	1.96	0.47
1:A:110:PHE:CD1	1:A:355:ARG:HD2	2.50	0.47
1:A:301:LEU:HD11	1:A:356:VAL:HG13	1.95	0.47
1:D:43:ARG:HH12	1:D:230:ARG:HB3	1.78	0.47
1:A:424:ILE:HG13	1:A:459:VAL:HG13	1.97	0.47
1:B:78:SER:HB2	1:B:305:MET:HG2	1.96	0.47
1:D:5:ASN:OD1	1:D:234:TYR:OH	2.24	0.47
1:B:276:VAL:HG11	1:B:379:PHE:CD1	2.49	0.47
1:D:5:ASN:HD22	1:D:243:LYS:HE3	1.80	0.47
1:D:34:HIS:NE2	1:D:235:PHE:O	2.47	0.47
1:A:105:LEU:O	1:A:109:HIS:ND1	2.42	0.47
1:B:277:ASP:HB2	1:B:347:LYS:HE3	1.96	0.47
1:A:212:VAL:HG11	1:A:250:MET:HE1	1.96	0.46
1:D:28:ILE:HG22	1:D:162:VAL:HG13	1.98	0.46
1:D:42:LYS:HE2	1:D:237:GLU:HA	1.97	0.46
1:A:312:ALA:HB1	1:A:340:CMH:SG	2.55	0.46
1:B:3:PHE:CE1	1:B:55:LYS:HE3	2.51	0.46
1:D:17:GLY:HA2	1:D:119:THR:HG21	1.97	0.46
1:A:456:ARG:O	1:A:458:LYS:NZ	2.30	0.46
1:D:190:LEU:HG	1:D:203:VAL:HB	1.97	0.46
1:A:449:PHE:CD1	1:A:453:VAL:HG21	2.50	0.46
1:B:9:GLY:HA2	1:B:64:VAL:HB	1.98	0.46
1:D:218:LEU:HD13	1:D:266:LEU:HD11	1.97	0.46
1:C:54:PHE:HE1	1:C:63:LEU:HD21	1.80	0.46
1:D:122:ASP:OD1	1:D:122:ASP:N	2.48	0.46
1:A:230:ARG:NH2	4:B:1474:5GP:O2'	2.49	0.46
1:A:326:ASN:HD22	1:A:385:LEU:HB3	1.80	0.46
1:B:285:ILE:HD13	1:B:291:TYR:HB3	1.96	0.46
1:C:27:GLU:O	1:C:32:SER:N	2.48	0.46
1:A:240:MET:CE	1:B:96:PRO:HD2	2.46	0.45
1:B:424:ILE:HD12	1:B:459:VAL:HG11	1.99	0.45
1:D:268:SER:OG	1:D:269:LYS:N	2.49	0.45
1:A:20:THR:O	1:A:24:VAL:HG23	2.16	0.45
1:B:285:ILE:HG13	1:B:371:CMH:O	2.15	0.45
1:C:300:HIS:ND1	1:C:361:LEU:HD12	2.32	0.45
1:A:340:CMH:HB2	1:A:342:PHE:CE2	2.51	0.45
1:C:435:ILE:HD12	1:C:445:LEU:HD13	1.98	0.45
1:A:85:LEU:HD13	1:A:172:THR:HG21	1.98	0.45
1:C:186:PHE:CE1	1:C:212:VAL:HG22	2.52	0.45
1:D:219:LYS:HE3	1:D:224:ASN:OD1	2.16	0.45
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG21	1:A:255:VAL:HG22	1.99	0.45
1:D:74:ARG:O	1:D:307:ILE:HB	2.17	0.45
1:D:96:PRO:HG3	1:D:136:MET:CE	2.47	0.45
1:B:202:VAL:HA	1:B:250:MET:O	2.16	0.45
1:B:341:ALA:HB1	1:B:382:ILE:HG12	1.99	0.45
1:A:222:PRO:HB3	1:A:349:LEU:HD21	2.00	0.44
1:D:212:VAL:HG22	1:D:232:ILE:HD11	1.99	0.44
1:B:191:ASP:OD2	1:B:247:ARG:NH1	2.47	0.44
1:B:251:ALA:HB1	1:C:1:MET:CE	2.47	0.44
1:C:93:LYS:HG3	1:C:128:GLU:OE1	2.17	0.44
1:C:140:LEU:HD22	1:C:146:LEU:O	2.17	0.44
1:C:407:ASP:OD1	1:C:408:GLY:N	2.50	0.44
1:D:227:THR:HG21	1:D:252:ILE:HD12	1.99	0.44
1:B:397:VAL:O	1:B:456:ARG:N	2.47	0.44
1:D:10:ILE:HD11	1:D:63:LEU:HD11	2.00	0.44
1:D:363:LEU:HA	1:D:364:PRO:HD3	1.66	0.44
1:A:199:ALA:HB3	1:B:290:LYS:HD2	1.99	0.44
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.75	0.44
1:B:234:TYR:HB2	1:B:248:VAL:HG12	2.00	0.44
1:B:315:PHE:O	1:B:339:TYR:N	2.50	0.44
1:A:72:LEU:O	1:A:76:VAL:HG23	2.16	0.44
1:B:130:LYS:HD2	1:B:130:LYS:HA	1.77	0.44
1:A:84:ASP:OD2	1:A:180:ARG:NH2	2.51	0.44
1:A:136:MET:CE	1:A:139:ILE:HD12	2.48	0.44
1:C:158:THR:HG21	3:C:1478:DXC:O2	2.17	0.44
3:C:1479:DXC:H243	3:C:1479:DXC:H222	1.77	0.44
1:B:314:PRO:HA	1:B:339:TYR:O	2.18	0.44
1:D:283:ILE:HA	1:D:373:HIS:O	2.18	0.44
1:D:426:ILE:HB	1:D:431:ILE:HG12	1.98	0.44
1:B:364:PRO:HA	1:B:365:PRO:HD3	1.79	0.44
1:C:10:ILE:HD11	1:C:87:LEU:HD12	2.00	0.44
1:C:10:ILE:HD12	1:C:21:LEU:HD23	1.99	0.44
1:B:82:ILE:HG21	1:B:206:THR:CG2	2.48	0.43
1:C:39:GLU:H	1:C:39:GLU:HG2	1.63	0.43
1:C:406:ILE:HD11	1:C:449:PHE:CZ	2.52	0.43
1:D:329:LEU:HD22	1:D:338:CMH:CB	2.48	0.43
1:A:23:LYS:O	1:A:27:GLU:HG2	2.19	0.43
1:A:400:ASP:OD1	1:A:401:LYS:HE3	2.18	0.43
1:B:391:VAL:HB	1:B:465:ARG:HD3	2.00	0.43
1:C:1:MET:HB2	3:C:1476:DXC:H62	1.99	0.43
1:D:74:ARG:HH22	1:D:309:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLU:O	1:B:420:ILE:HG12	2.18	0.43
1:D:15:ASP:OD1	1:D:16:HIS:ND1	2.51	0.43
1:D:317:LYS:HE2	1:D:339:TYR:OH	2.18	0.43
1:C:301:LEU:CD1	1:C:358:ILE:HG23	2.48	0.43
1:D:5:ASN:OD1	1:D:60:ARG:HD3	2.18	0.43
1:A:116:VAL:HB	1:A:151:ILE:HG12	2.00	0.43
1:B:24:VAL:O	1:B:28:ILE:HG22	2.18	0.43
1:B:96:PRO:HG3	1:B:136:MET:SD	2.58	0.43
1:B:360:ARG:HH12	1:B:371:CMH:CB	2.31	0.43
1:B:416:ALA:O	1:B:420:ILE:HG23	2.19	0.43
1:A:51:PHE:CE2	1:A:247:ARG:HG2	2.53	0.43
1:A:391:VAL:HG21	1:A:465:ARG:HD3	2.01	0.43
1:B:6:ILE:HG12	1:B:173:LEU:HD13	2.00	0.43
1:B:130:LYS:HE3	1:B:134:MET:HE3	2.01	0.43
1:D:308:VAL:HG21	1:D:344:LEU:HB3	2.00	0.43
1:A:240:MET:CE	1:B:95:GLY:HA3	2.49	0.43
1:A:314:PRO:O	1:A:328:ILE:HD12	2.19	0.43
1:B:57:GLU:HG3	1:B:170:ILE:HD13	2.00	0.43
1:C:188:MET:HE3	1:C:188:MET:HB3	1.93	0.43
1:C:406:ILE:HD11	1:C:449:PHE:HZ	1.83	0.43
1:C:465:ARG:HG2	2:C:1473:SO4:O1	2.19	0.43
1:A:13:HIS:O	1:A:16:HIS:HB2	2.19	0.42
1:A:84:ASP:O	1:A:113:PRO:HG2	2.19	0.42
1:B:13:HIS:H	1:B:100:THR:HG22	1.84	0.42
1:D:431:ILE:HB	1:D:450:SER:O	2.19	0.42
1:B:219:LYS:HE2	1:B:269:LYS:HA	2.01	0.42
1:C:230:ARG:HD2	1:C:253:GLN:CD	2.40	0.42
1:B:191:ASP:OD2	1:B:205:GLY:HA2	2.20	0.42
1:D:21:LEU:O	1:D:25:LEU:HB2	2.19	0.42
1:D:192:HIS:HA	1:D:262:ARG:HD2	2.02	0.42
1:C:91:ASP:HB3	1:C:94:GLU:HG2	2.02	0.42
1:D:247:ARG:HD2	1:D:247:ARG:HA	1.77	0.42
1:A:329:LEU:C	1:A:331:GLU:H	2.22	0.42
1:C:357:LEU:HA	1:C:357:LEU:HD12	1.82	0.42
1:D:66:ALA:HB1	1:D:69:HIS:ND1	2.35	0.42
1:D:363:LEU:HD13	1:D:369:ARG:HH11	1.84	0.42
1:C:277:ASP:HB3	1:C:278:LYS:HG2	2.01	0.42
1:D:280:VAL:HG21	1:D:385:LEU:HD21	2.01	0.42
1:A:158:THR:HG22	1:A:160:PHE:N	2.35	0.42
1:A:214:VAL:HG22	1:A:232:ILE:HG13	2.01	0.42
1:A:109:HIS:HD1	1:A:109:HIS:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1478:DXC:H22	3:C:1478:DXC:H82	1.79	0.42
1:D:73:ILE:H	1:D:73:ILE:HG13	1.58	0.42
1:A:69:HIS:CD2	1:A:70:ALA:H	2.38	0.42
1:A:112:ILE:HA	1:A:113:PRO:HD2	1.90	0.41
1:A:302:ASN:HB2	1:A:357:LEU:HB3	2.02	0.41
1:A:322:LYS:HG3	1:A:323:THR:H	1.85	0.41
1:A:380:LYS:HA	1:A:381:PRO:HD3	1.90	0.41
3:C:1479:DXC:H71	3:C:1479:DXC:H182	1.86	0.41
1:D:218:LEU:CD1	1:D:229:VAL:HG22	2.50	0.41
1:D:320:PHE:HE1	1:D:325:GLU:HG3	1.85	0.41
1:B:291:TYR:HD1	1:B:333:ILE:HG22	1.85	0.41
3:B:1473:DXC:H242	3:B:1473:DXC:H13	2.02	0.41
1:C:360:ARG:O	1:C:369:ARG:HB3	2.19	0.41
1:D:150:SER:OG	1:D:168:LEU:HD21	2.20	0.41
1:B:108:ASP:CG	1:B:143:THR:HG23	2.41	0.41
1:C:218:LEU:HD12	1:C:266:LEU:HD21	2.02	0.41
1:B:14:ILE:O	1:B:15:ASP:HB2	2.20	0.41
1:B:234:TYR:CD2	1:B:235:PHE:HB2	2.55	0.41
1:C:49:ILE:HD11	3:C:1475:DXC:H161	2.03	0.41
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.86	0.41
1:C:381:PRO:HD2	1:C:384:ASP:HB2	2.03	0.41
1:D:11:PHE:CZ	1:D:67:PRO:HD2	2.55	0.41
1:D:43:ARG:HH22	1:D:230:ARG:HD3	1.85	0.41
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.76	0.41
1:A:188:MET:HA	1:A:189:PRO:HD3	1.92	0.41
1:A:206:THR:HA	1:A:247:ARG:HA	2.03	0.41
1:B:312:ALA:HB1	1:B:340:CMH:SG	2.61	0.41
1:B:328:ILE:HG21	1:B:467:TRP:CD1	2.56	0.41
1:C:84:ASP:CG	1:C:180:ARG:HH22	2.23	0.41
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.92	0.41
1:C:1:MET:HB2	3:C:1476:DXC:C6	2.51	0.41
1:D:10:ILE:HD13	1:D:21:LEU:HD23	2.02	0.41
3:C:1480:DXC:H221	3:C:1480:DXC:H243	1.70	0.41
1:D:3:PHE:CE2	1:D:55:LYS:HE3	2.54	0.41
1:A:158:THR:CG2	1:A:160:PHE:HB2	2.51	0.41
1:A:303:VAL:HG22	1:A:356:VAL:HG22	2.03	0.41
3:B:1473:DXC:H10	3:B:1473:DXC:H61	1.83	0.41
1:C:27:GLU:C	1:C:32:SER:HB2	2.41	0.41
1:C:289:PHE:CZ	1:C:371:CMH:HB2	2.56	0.41
3:C:1479:DXC:H203	3:C:1479:DXC:H19	1.81	0.41
1:D:34:HIS:HB3	1:D:53:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:LEU:HD13	1:D:266:LEU:HD21	2.03	0.41
1:B:305:MET:HE3	1:B:305:MET:HB3	1.93	0.40
1:D:227:THR:HB	1:D:255:VAL:HG23	2.03	0.40
1:B:295:PRO:HB3	1:B:328:ILE:HD11	2.01	0.40
1:C:413:LYS:HB2	1:C:440:GLY:O	2.22	0.40
1:D:5:ASN:O	1:D:180:ARG:NH2	2.49	0.40
1:B:45:ILE:HG12	1:B:45:ILE:O	2.21	0.40
1:B:376:ILE:HG21	1:B:379:PHE:CE1	2.56	0.40
1:D:74:ARG:HH11	1:D:307:ILE:HG22	1.86	0.40
1:D:195:PRO:HD3	1:D:257:ALA:HB1	2.03	0.40
1:B:78:SER:CB	1:B:305:MET:HG2	2.52	0.40
1:B:114:ILE:HD13	1:B:146:LEU:HD13	2.03	0.40
1:A:158:THR:HG22	1:A:160:PHE:HB2	2.02	0.40
1:A:416:ALA:HB1	1:A:445:LEU:HD21	2.04	0.40
1:C:158:THR:HG22	1:C:160:PHE:N	2.33	0.40
1:C:209:LYS:HA	1:C:244:ALA:HB2	2.02	0.40
1:C:212:VAL:HG23	1:C:242:ALA:HB3	2.04	0.40
3:C:1475:DXC:H221	3:C:1475:DXC:H243	1.73	0.40
1:D:223:ILE:HD13	1:D:259:GLN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/482 (91%)	420 (96%)	19 (4%)	1 (0%)	47 78
1	B	448/482 (93%)	430 (96%)	18 (4%)	0	100 100
1	C	465/482 (96%)	439 (94%)	26 (6%)	0	100 100
1	D	461/482 (96%)	433 (94%)	24 (5%)	4 (1%)	17 53
All	All	1814/1928 (94%)	1722 (95%)	87 (5%)	5 (0%)	41 73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	A	69	HIS
1	D	333	ILE
1	D	321	GLY
1	D	382	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/412 (93%)	346 (91%)	36 (9%)	8	30
1	B	388/412 (94%)	359 (92%)	29 (8%)	13	42
1	C	402/412 (98%)	364 (90%)	38 (10%)	8	30
1	D	398/412 (97%)	361 (91%)	37 (9%)	9	31
All	All	1570/1648 (95%)	1430 (91%)	140 (9%)	9	33

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	28	ILE
1	A	57	GLU
1	A	82	ILE
1	A	90	VAL
1	A	102	GLU
1	A	104	MET
1	A	127	GLU
1	A	143	THR
1	A	148	ASN
1	A	150	SER
1	A	158	THR
1	A	212	VAL
1	A	235	PHE
1	A	252	ILE

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Mol	Chain	Res	Type
1	A	255	VAL
1	A	273	LEU
1	A	291	TYR
1	A	319	THR
1	A	332	VAL
1	A	333	ILE
1	A	345	GLU
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	396	LYS
1	A	411	GLN
1	A	424	ILE
1	A	435	ILE
1	A	441	THR
1	A	446	THR
1	A	449	PHE
1	A	458	LYS
1	B	14	ILE
1	B	19	THR
1	B	28	ILE
1	B	45	ILE
1	B	72	LEU
1	B	126	THR
1	B	136	MET
1	B	148	ASN
1	B	163	ASP
1	B	182	THR
1	B	183	GLU
1	B	212	VAL
1	B	235	PHE
1	B	241	GLU
1	B	260	ILE
1	B	275	THR
1	B	286	SER
1	B	287	ASP
1	B	291	TYR
1	B	300	HIS
1	B	308	VAL

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Mol	Chain	Res	Type
1	B	319	THR
1	B	344	LEU
1	B	356	VAL
1	B	360	ARG
1	B	363	LEU
1	B	370	ILE
1	B	394	GLU
1	B	412	SER
1	C	6	ILE
1	C	14	ILE
1	C	45	ILE
1	C	61	ILE
1	C	65	ASP
1	C	73	ILE
1	C	98	THR
1	C	142	SER
1	C	148	ASN
1	C	150	SER
1	C	158	THR
1	C	171	THR
1	C	188	MET
1	C	191	ASP
1	C	212	VAL
1	C	223	ILE
1	C	226	SER
1	C	241	GLU
1	C	255	VAL
1	C	261	TYR
1	C	278	LYS
1	C	283	ILE
1	C	292	ASN
1	C	293	LEU
1	C	294	THR
1	C	297	MET
1	C	301	LEU
1	C	328	ILE
1	C	348	VAL
1	C	357	LEU
1	C	358	ILE
1	C	359	THR
1	C	366	THR
1	C	368	LEU

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Mol	Chain	Res	Type
1	C	391	VAL
1	C	445	LEU
1	C	446	THR
1	C	456	ARG
1	D	16	HIS
1	D	31	THR
1	D	36	LYS
1	D	41	GLN
1	D	43	ARG
1	D	46	THR
1	D	49	ILE
1	D	56	LEU
1	D	74	ARG
1	D	78	SER
1	D	89	VAL
1	D	90	VAL
1	D	128	GLU
1	D	139	ILE
1	D	143	THR
1	D	149	SER
1	D	154	ILE
1	D	162	VAL
1	D	220	VAL
1	D	226	SER
1	D	235	PHE
1	D	237	GLU
1	D	275	THR
1	D	277	ASP
1	D	286	SER
1	D	289	PHE
1	D	333	ILE
1	D	348	VAL
1	D	360	ARG
1	D	361	LEU
1	D	362	ASP
1	D	363	LEU
1	D	368	LEU
1	D	387	ILE
1	D	435	ILE
1	D	453	VAL
1	D	457	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	B	148	ASN
1	D	69	HIS
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	C	371	1	5,7,8	0.69	0	1,7,9	1.01	0
1	CMH	D	340	1	5,7,8	0.71	0	1,7,9	0.56	0
1	CMH	A	264	1	5,7,8	0.58	0	1,7,9	0.47	0
1	CMH	A	338	1	5,7,8	0.65	0	1,7,9	0.18	0
1	CMH	C	338	1	5,7,8	0.73	0	1,7,9	0.35	0
1	CMH	D	264	1	5,7,8	0.62	0	1,7,9	0.58	0
1	CMH	C	264	1	5,7,8	0.73	0	1,7,9	1.91	0
1	CMH	B	340	1	5,7,8	0.57	0	1,7,9	0.35	0
1	CMH	C	340	1	5,7,8	0.88	0	1,7,9	1.05	0
1	CMH	D	338	1	5,7,8	0.70	0	1,7,9	0.53	0
1	CMH	D	371	1	5,7,8	0.58	0	1,7,9	0.36	0
1	CMH	A	371	1	5,7,8	0.63	0	1,7,9	1.54	0
1	CMH	A	340	1	5,7,8	0.72	0	1,7,9	0.80	0
1	CMH	B	338	1	5,7,8	0.65	0	1,7,9	0.47	0
1	CMH	B	371	1	5,7,8	0.54	0	1,7,9	1.76	0
1	CMH	B	264	1	5,7,8	0.88	0	1,7,9	1.55	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	C	371	1	-	0/0/6/8	-
1	CMH	D	340	1	-	0/0/6/8	-
1	CMH	A	264	1	-	0/0/6/8	-
1	CMH	A	338	1	-	0/0/6/8	-
1	CMH	C	338	1	-	0/0/6/8	-
1	CMH	D	264	1	-	0/0/6/8	-
1	CMH	C	264	1	-	0/0/6/8	-
1	CMH	B	340	1	-	0/0/6/8	-
1	CMH	C	340	1	-	0/0/6/8	-
1	CMH	D	338	1	-	0/0/6/8	-
1	CMH	D	371	1	-	0/0/6/8	-
1	CMH	A	371	1	-	0/0/6/8	-
1	CMH	A	340	1	-	0/0/6/8	-
1	CMH	B	338	1	-	0/0/6/8	-
1	CMH	B	371	1	-	0/0/6/8	-
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 18 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands 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	$\#\|Z\| > 2$
4	5GP	B	1474	-	22,26,26	1.24	2 (9%)	26,40,40	1.32	5 (19%)
3	DXC	C	1479	-	31,31,31	1.52	7 (22%)	49,49,49	1.92	14 (28%)
2	SO4	C	1474	-	4,4,4	0.18	0	6,6,6	0.19	0
3	DXC	C	1480	-	31,31,31	1.84	8 (25%)	49,49,49	1.73	10 (20%)
2	SO4	C	1471	-	4,4,4	0.12	0	6,6,6	0.34	0
2	SO4	C	1473	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1471	-	4,4,4	0.14	0	6,6,6	0.07	0
3	DXC	C	1476	-	31,31,31	1.65	5 (16%)	49,49,49	1.61	9 (18%)
3	DXC	C	1477	-	31,31,31	1.61	6 (19%)	49,49,49	1.57	12 (24%)
3	DXC	C	1475	-	31,31,31	1.76	6 (19%)	49,49,49	1.80	16 (32%)
2	SO4	B	1472	-	4,4,4	0.14	0	6,6,6	0.20	0
3	DXC	B	1473	-	31,31,31	1.45	5 (16%)	49,49,49	1.66	13 (26%)
3	DXC	C	1478	-	31,31,31	1.51	7 (22%)	49,49,49	1.89	16 (32%)
2	SO4	C	1472	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	C	1481	-	4,4,4	0.15	0	6,6,6	0.06	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
4	5GP	B	1474	-	-	2/6/26/26	0/3/3/3
3	DXC	C	1479	-	-	7/9/71/71	0/4/4/4
3	DXC	C	1480	-	-	0/9/71/71	0/4/4/4
3	DXC	C	1477	-	-	4/9/71/71	0/4/4/4
3	DXC	C	1476	-	-	4/9/71/71	0/4/4/4
3	DXC	C	1475	-	-	2/9/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DXC	C	1478	-	-	1/9/71/71	0/4/4/4
3	DXC	B	1473	-	-	2/9/71/71	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1475	DXC	C12-C13	-4.68	1.47	1.54
3	C	1480	DXC	C12-C13	-4.28	1.47	1.54
3	C	1477	DXC	C12-C13	-4.01	1.48	1.54
4	B	1474	5GP	C5-C6	-4.00	1.39	1.47
3	C	1480	DXC	C18-C4	-3.94	1.47	1.54
3	C	1476	DXC	C12-C13	-3.58	1.49	1.54
3	C	1476	DXC	C12-C11	-3.38	1.49	1.55
3	C	1477	DXC	C18-C4	-3.37	1.48	1.54
3	C	1475	DXC	C20-C12	-3.34	1.48	1.54
3	C	1476	DXC	O1-C13	-3.32	1.38	1.43
3	B	1473	DXC	C12-C13	-3.15	1.49	1.54
3	C	1478	DXC	C20-C12	-3.09	1.49	1.54
3	C	1480	DXC	C5-C4	-3.08	1.48	1.54
3	C	1478	DXC	C18-C4	-3.07	1.49	1.54
3	C	1475	DXC	C12-C11	-3.05	1.50	1.55
3	B	1473	DXC	C20-C12	-2.95	1.49	1.54
3	C	1480	DXC	C12-C11	-2.94	1.50	1.55
3	C	1476	DXC	C20-C12	-2.92	1.49	1.54
3	C	1478	DXC	C12-C13	-2.90	1.50	1.54
3	C	1479	DXC	C12-C11	-2.89	1.50	1.55
3	C	1480	DXC	O1-C13	-2.87	1.38	1.43
3	C	1479	DXC	C18-C4	-2.85	1.49	1.54
3	C	1475	DXC	C18-C4	-2.83	1.49	1.54
3	C	1477	DXC	C4-C10	-2.80	1.51	1.56
3	C	1480	DXC	C4-C3	-2.80	1.50	1.55
3	C	1476	DXC	C18-C4	-2.75	1.49	1.54
3	C	1475	DXC	O1-C13	-2.71	1.39	1.43
3	B	1473	DXC	O1-C13	-2.68	1.39	1.43
4	B	1474	5GP	C6-N1	-2.64	1.33	1.37
3	C	1477	DXC	C12-C11	-2.62	1.51	1.55
3	C	1480	DXC	C4-C10	-2.56	1.51	1.56
3	C	1479	DXC	C20-C12	-2.54	1.50	1.54
3	C	1479	DXC	C12-C13	-2.53	1.50	1.54
3	B	1473	DXC	C18-C4	-2.51	1.50	1.54
3	C	1477	DXC	C20-C12	-2.47	1.50	1.54
3	C	1475	DXC	C12-C17	-2.38	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1478	DXC	C2-C1	-2.37	1.47	1.51
3	C	1480	DXC	C20-C12	-2.35	1.50	1.54
3	C	1479	DXC	O1-C13	-2.32	1.39	1.43
3	C	1477	DXC	O1-C13	-2.31	1.39	1.43
3	B	1473	DXC	C12-C11	-2.27	1.51	1.55
3	C	1478	DXC	C12-C11	-2.27	1.51	1.55
3	C	1479	DXC	C4-C3	-2.12	1.52	1.55
3	C	1478	DXC	O1-C13	-2.07	1.40	1.43
3	C	1478	DXC	C5-C4	-2.01	1.50	1.54
3	C	1479	DXC	C4-C10	-2.00	1.52	1.56

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1478	DXC	C7-C8-C9	-4.79	104.25	112.14
3	C	1480	DXC	C18-C4-C5	-4.75	100.60	108.26
3	C	1478	DXC	C10-C14-C13	-4.60	108.23	114.30
3	C	1476	DXC	C18-C4-C3	-4.55	102.64	110.36
3	C	1479	DXC	C8-C9-C10	4.41	115.97	110.49
3	C	1479	DXC	C18-C4-C3	-4.36	102.97	110.36
3	B	1473	DXC	C18-C4-C3	-4.11	103.39	110.36
3	C	1475	DXC	C18-C4-C3	-3.70	104.09	110.36
3	C	1480	DXC	C4-C10-C9	-3.69	108.54	112.42
3	C	1480	DXC	C5-C4-C10	3.65	117.09	111.35
3	C	1479	DXC	C10-C14-C13	-3.64	109.49	114.30
3	C	1476	DXC	C10-C4-C3	3.58	113.60	108.58
3	C	1475	DXC	O1-C13-C12	-3.55	105.03	111.03
3	C	1475	DXC	C11-C12-C13	-3.50	104.14	107.40
3	B	1473	DXC	C10-C14-C13	-3.47	109.72	114.30
3	C	1479	DXC	C11-C9-C10	-3.45	104.47	109.09
3	C	1475	DXC	C10-C14-C13	-3.39	109.83	114.30
3	C	1478	DXC	C15-C11-C12	-3.27	100.35	103.55
3	C	1475	DXC	C3-C2-C1	-3.21	108.05	112.76
3	C	1480	DXC	C22-C21-C19	-3.20	108.68	114.52
3	C	1479	DXC	C6-C5-C4	-3.19	107.31	112.78
4	B	1474	5GP	C5-C6-N1	3.17	119.54	113.95
3	C	1476	DXC	C10-C14-C13	-3.17	110.12	114.30
3	C	1477	DXC	C7-C8-C9	-3.16	106.93	112.14
3	C	1477	DXC	C10-C14-C13	-3.15	110.14	114.30
3	C	1476	DXC	C15-C11-C12	-3.14	100.48	103.55
3	C	1479	DXC	C15-C11-C9	-3.13	113.93	119.08
3	C	1477	DXC	C10-C4-C3	3.06	112.88	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1476	DXC	C8-C9-C10	3.05	114.28	110.49
3	C	1476	DXC	C4-C10-C9	-3.01	109.25	112.42
3	C	1477	DXC	C11-C9-C10	-3.01	105.06	109.09
3	C	1478	DXC	C6-C5-C4	-3.00	107.63	112.78
3	B	1473	DXC	C6-C5-C4	-2.98	107.66	112.78
3	B	1473	DXC	C17-C12-C13	2.97	120.38	117.67
3	C	1476	DXC	C7-C8-C9	-2.96	107.26	112.14
3	C	1480	DXC	C7-C8-C9	-2.96	107.27	112.14
3	C	1479	DXC	C12-C17-C19	-2.95	115.97	119.50
3	C	1479	DXC	C18-C4-C10	2.94	115.23	111.18
3	B	1473	DXC	C20-C12-C17	-2.88	106.71	111.21
3	C	1475	DXC	C18-C4-C5	-2.88	103.63	108.26
3	B	1473	DXC	C10-C4-C3	2.84	112.58	108.58
3	B	1473	DXC	C18-C4-C10	2.82	115.08	111.18
3	C	1478	DXC	C16-C15-C11	-2.80	99.58	105.13
3	C	1478	DXC	C2-C1-C6	-2.75	107.26	110.55
3	C	1479	DXC	C15-C11-C12	-2.72	100.88	103.55
3	C	1480	DXC	C10-C4-C3	2.69	112.36	108.58
3	C	1475	DXC	C24-C19-C21	-2.69	106.15	110.36
3	C	1477	DXC	C15-C11-C12	-2.68	100.92	103.55
3	C	1478	DXC	C3-C2-C1	-2.68	108.83	112.76
3	C	1480	DXC	C14-C13-C12	-2.67	108.50	111.24
3	C	1475	DXC	C7-C8-C9	-2.67	107.74	112.14
3	C	1475	DXC	C20-C12-C11	2.63	115.33	111.21
3	C	1478	DXC	C14-C13-C12	-2.63	108.55	111.24
3	C	1477	DXC	C14-C13-C12	-2.61	108.56	111.24
3	C	1480	DXC	C15-C11-C12	-2.56	101.04	103.55
3	C	1479	DXC	C5-C4-C3	2.55	111.55	107.77
3	C	1478	DXC	C10-C4-C3	2.55	112.16	108.58
3	C	1477	DXC	C8-C9-C10	2.47	113.56	110.49
3	C	1478	DXC	C18-C4-C3	-2.46	106.19	110.36
3	C	1476	DXC	C15-C11-C9	-2.46	115.03	119.08
3	C	1478	DXC	C24-C19-C21	-2.45	106.52	110.36
3	C	1479	DXC	C2-C3-C4	-2.45	110.06	112.66
3	B	1473	DXC	C7-C8-C9	-2.44	108.12	112.14
3	C	1480	DXC	C8-C9-C10	2.43	113.51	110.49
3	C	1477	DXC	C16-C15-C11	-2.38	100.41	105.13
3	C	1475	DXC	C17-C12-C13	-2.37	115.50	117.67
3	C	1478	DXC	O4-C23-C22	2.35	121.57	114.03
4	B	1474	5GP	C8-N7-C5	2.33	107.43	102.99
4	B	1474	5GP	C2-N1-C6	-2.31	120.85	125.10
3	C	1478	DXC	C8-C9-C10	2.30	113.35	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1479	DXC	C20-C12-C17	-2.30	107.61	111.21
4	B	1474	5GP	O2P-P-O5'	-2.26	100.73	106.73
3	C	1479	DXC	C24-C19-C17	-2.25	109.48	112.92
3	C	1477	DXC	C17-C12-C13	-2.24	115.62	117.67
3	C	1475	DXC	C18-C4-C10	2.20	114.22	111.18
3	B	1473	DXC	C20-C12-C11	2.18	114.62	111.21
3	C	1475	DXC	C2-C3-C4	-2.18	110.35	112.66
3	B	1473	DXC	O4-C23-C22	2.17	121.00	114.03
3	C	1475	DXC	C11-C9-C10	-2.14	106.23	109.09
3	C	1477	DXC	C6-C5-C4	-2.12	109.14	112.78
3	C	1478	DXC	C18-C4-C5	-2.11	104.87	108.26
3	C	1477	DXC	O1-C13-C14	2.09	113.39	109.12
3	C	1477	DXC	C2-C3-C7	-2.09	107.91	111.74
3	C	1480	DXC	C5-C4-C3	-2.06	104.72	107.77
3	B	1473	DXC	C15-C11-C9	-2.06	115.69	119.08
3	C	1479	DXC	C10-C4-C3	2.05	111.46	108.58
3	C	1476	DXC	C18-C4-C5	-2.04	104.97	108.26
3	C	1478	DXC	C2-C3-C7	-2.04	108.01	111.74
3	C	1478	DXC	C22-C21-C19	-2.02	110.83	114.52
3	C	1475	DXC	C17-C12-C11	2.02	102.13	100.09
3	B	1473	DXC	C12-C11-C9	2.02	116.94	114.71
3	C	1475	DXC	C5-C4-C10	2.01	114.51	111.35
3	C	1475	DXC	C2-C1-C6	-2.01	108.15	110.55
4	B	1474	5GP	O6-C6-C5	-2.01	120.45	124.37
3	B	1473	DXC	O4-C23-O3	-2.01	118.30	123.30

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1474	5GP	C3'-C4'-C5'-O5'
3	C	1479	DXC	C16-C17-C19-C24
3	C	1479	DXC	C12-C17-C19-C24
3	C	1476	DXC	C24-C19-C21-C22
3	C	1479	DXC	C24-C19-C21-C22
3	C	1479	DXC	C12-C17-C19-C21
3	C	1477	DXC	C24-C19-C21-C22
3	C	1479	DXC	C16-C17-C19-C21
3	C	1476	DXC	C17-C19-C21-C22
3	C	1477	DXC	C17-C19-C21-C22
4	B	1474	5GP	O4'-C4'-C5'-O5'
3	C	1478	DXC	C17-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
3	C	1479	DXC	C17-C19-C21-C22
3	C	1479	DXC	C19-C21-C22-C23
3	B	1473	DXC	C21-C22-C23-O3
3	B	1473	DXC	C21-C22-C23-O4
3	C	1476	DXC	C21-C22-C23-O4
3	C	1475	DXC	C21-C22-C23-O4
3	C	1476	DXC	C21-C22-C23-O3
3	C	1475	DXC	C21-C22-C23-O3
3	C	1477	DXC	C21-C22-C23-O4
3	C	1477	DXC	C21-C22-C23-O3

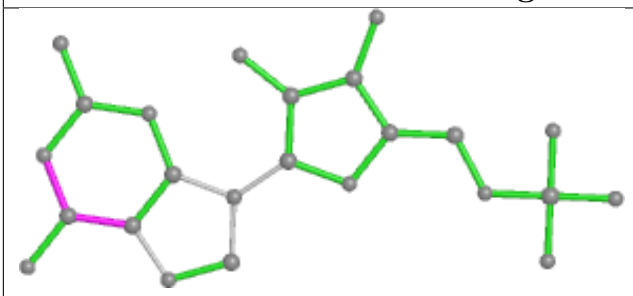
There are no ring outliers.

9 monomers are involved in 17 short contacts:

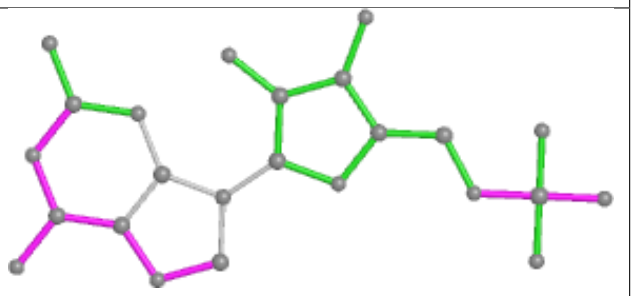
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1474	5GP	2	0
3	C	1479	DXC	3	0
3	C	1480	DXC	1	0
2	C	1473	SO4	1	0
2	B	1471	SO4	1	0
3	C	1476	DXC	3	0
3	C	1475	DXC	2	0
3	B	1473	DXC	2	0
3	C	1478	DXC	2	0

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.

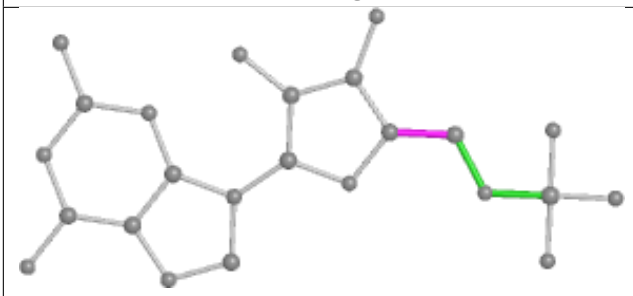
Ligand 5GP B 1474



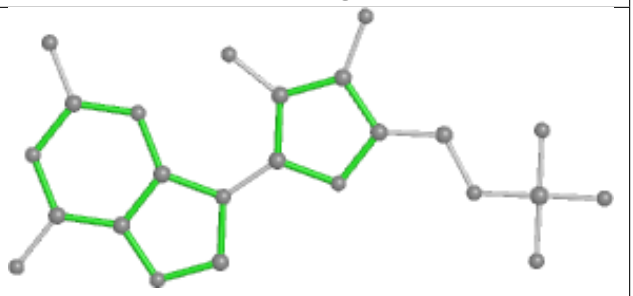
Bond lengths



Bond angles

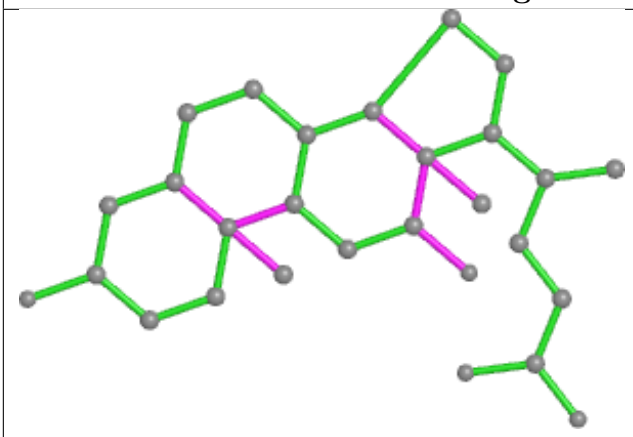


Torsions

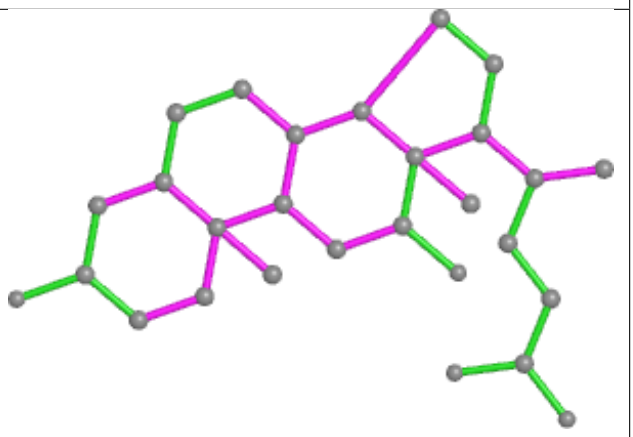


Rings

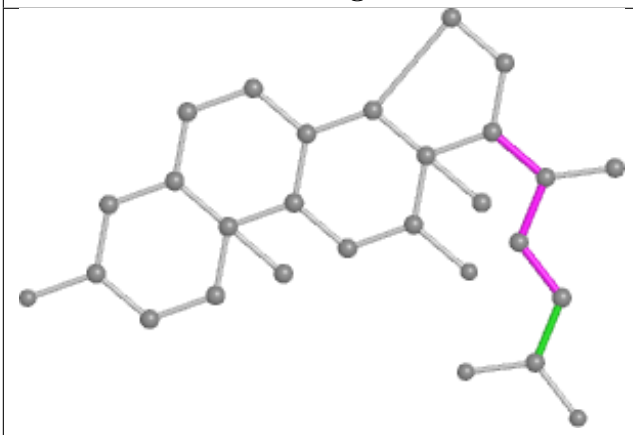
Ligand DXC C 1479



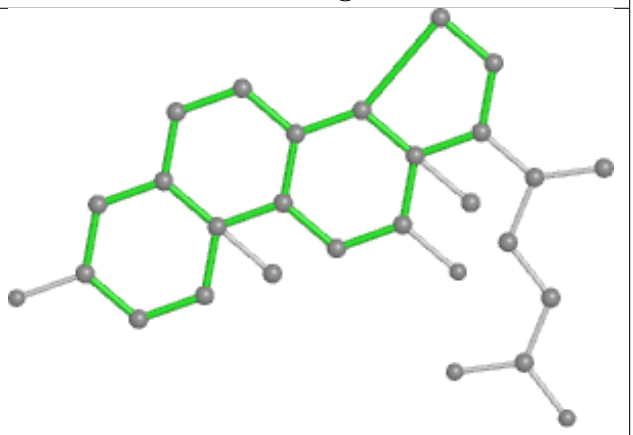
Bond lengths



Bond angles

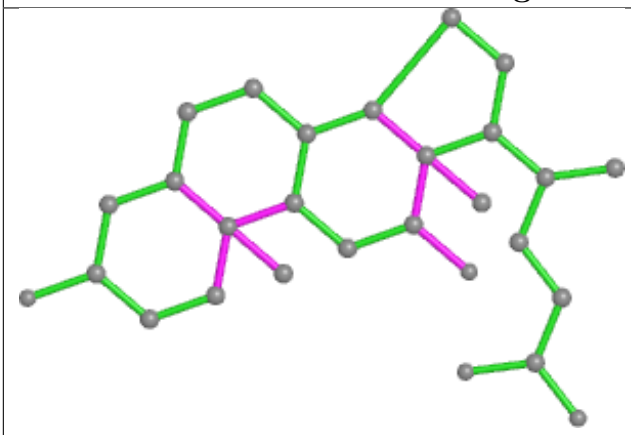


Torsions

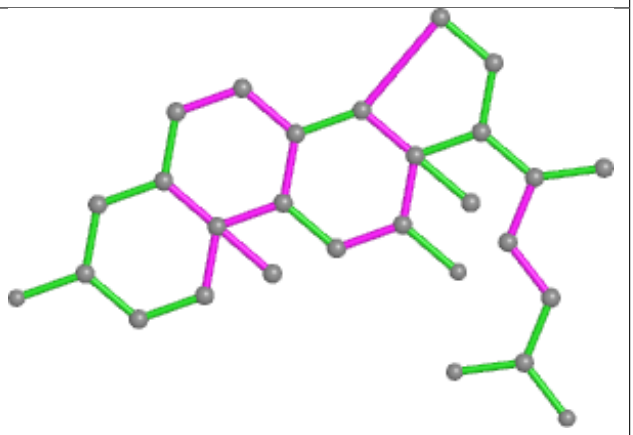


Rings

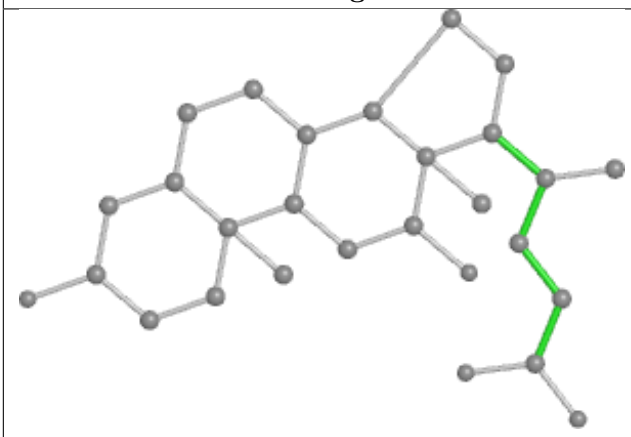
Ligand DXC C 1480



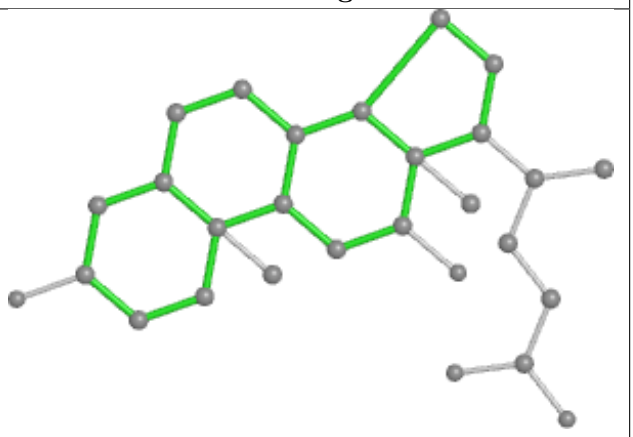
Bond lengths



Bond angles

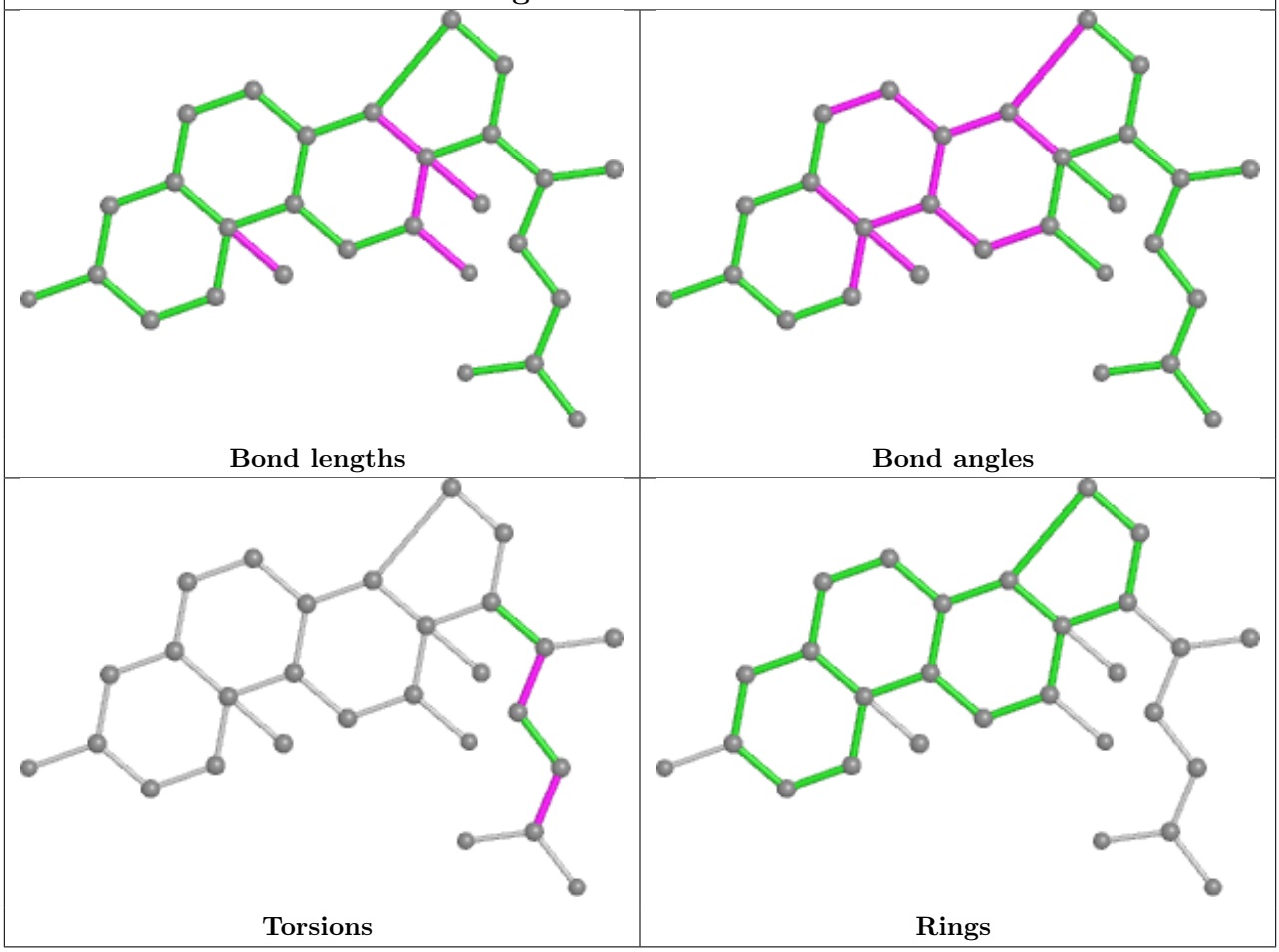


Torsions

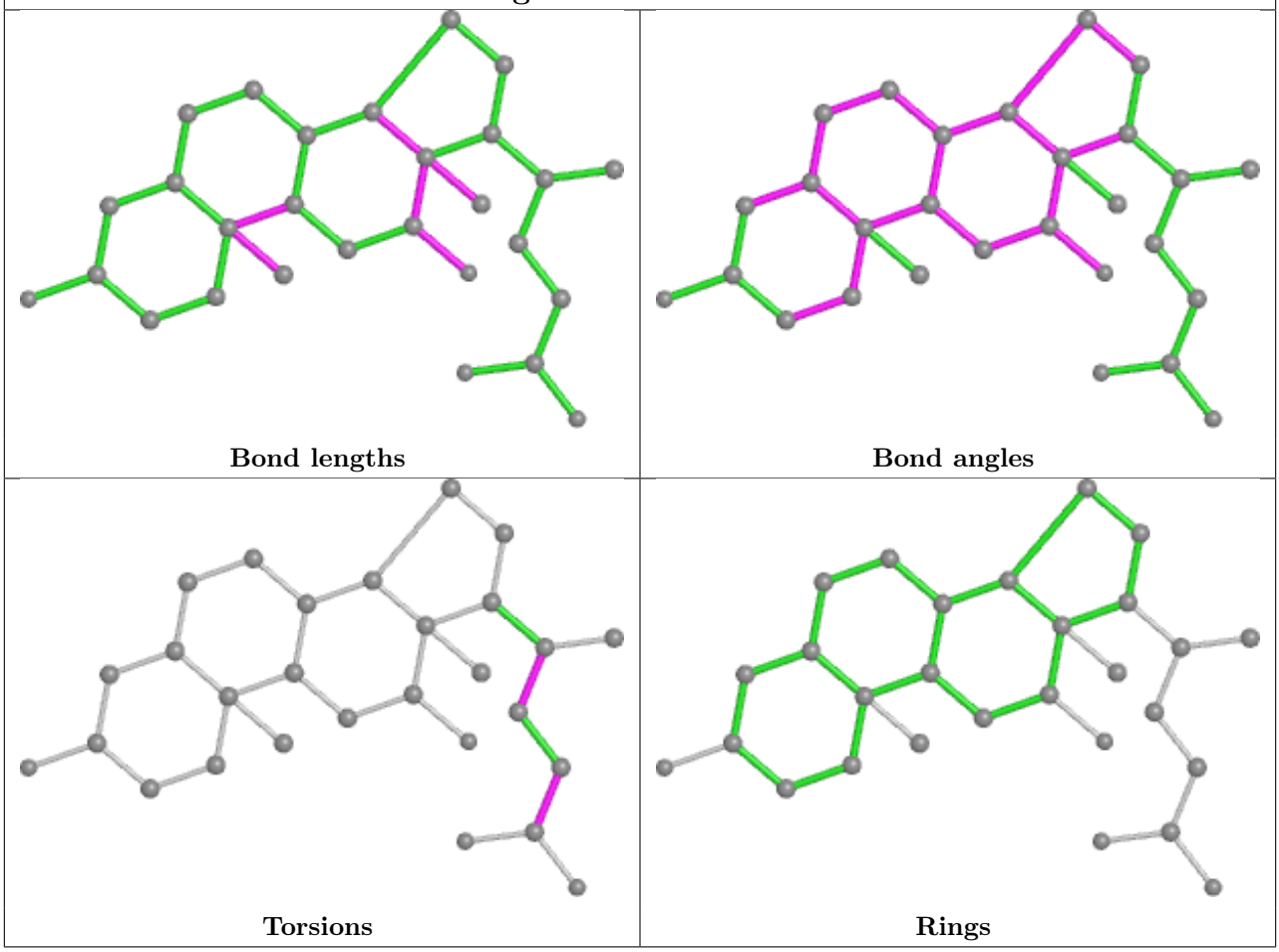


Rings

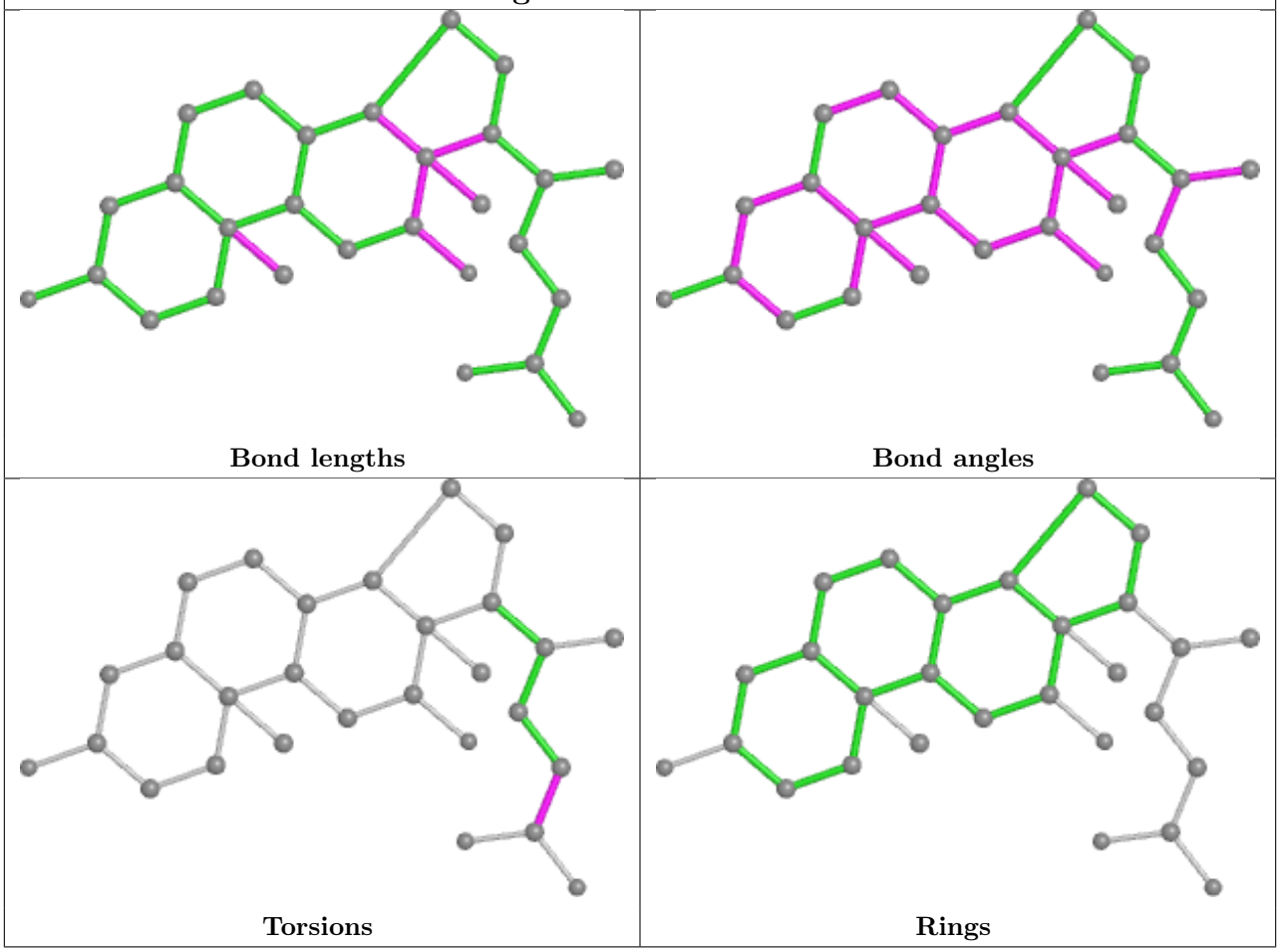
Ligand DXC C 1476



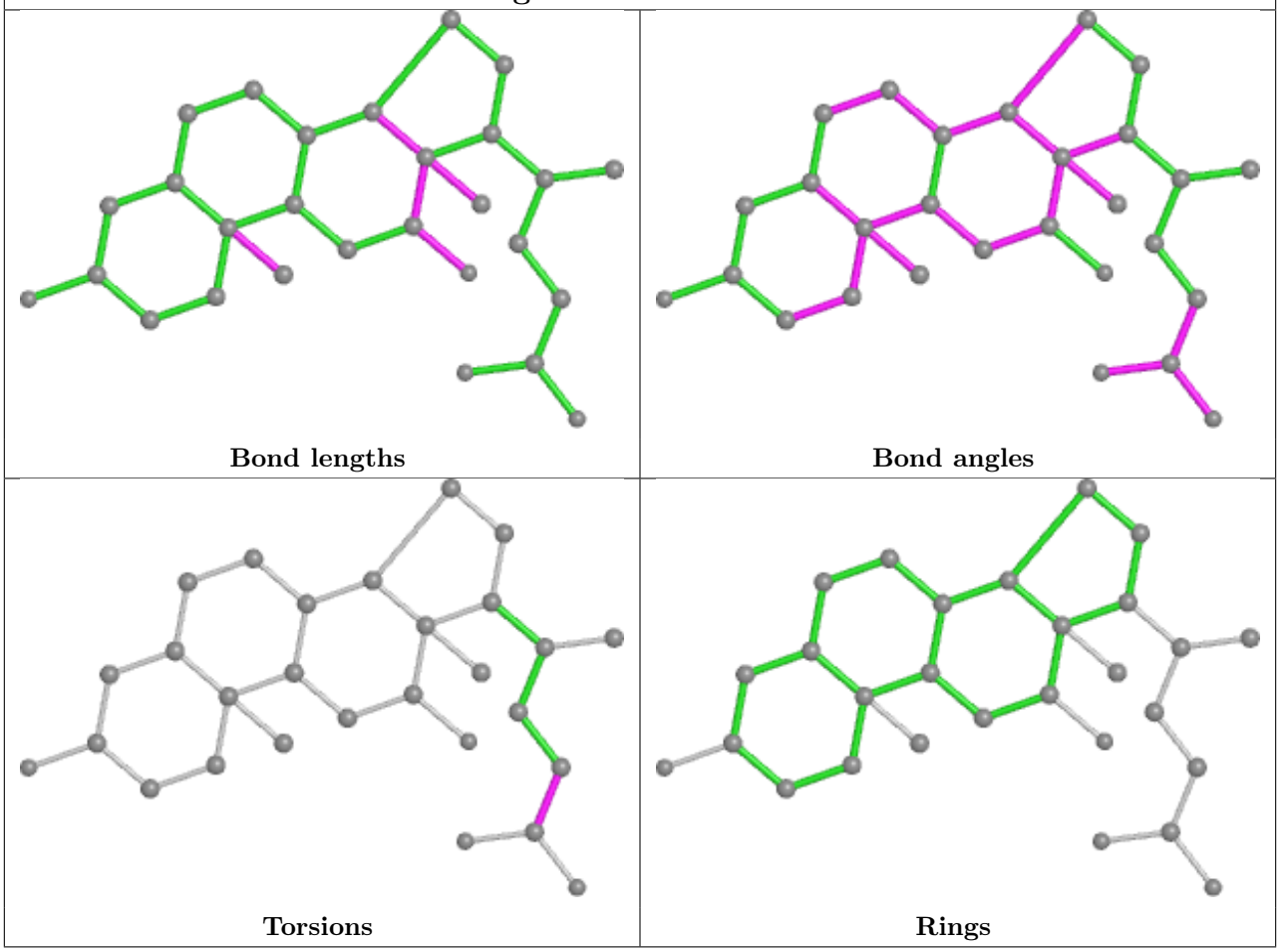
Ligand DXC C 1477



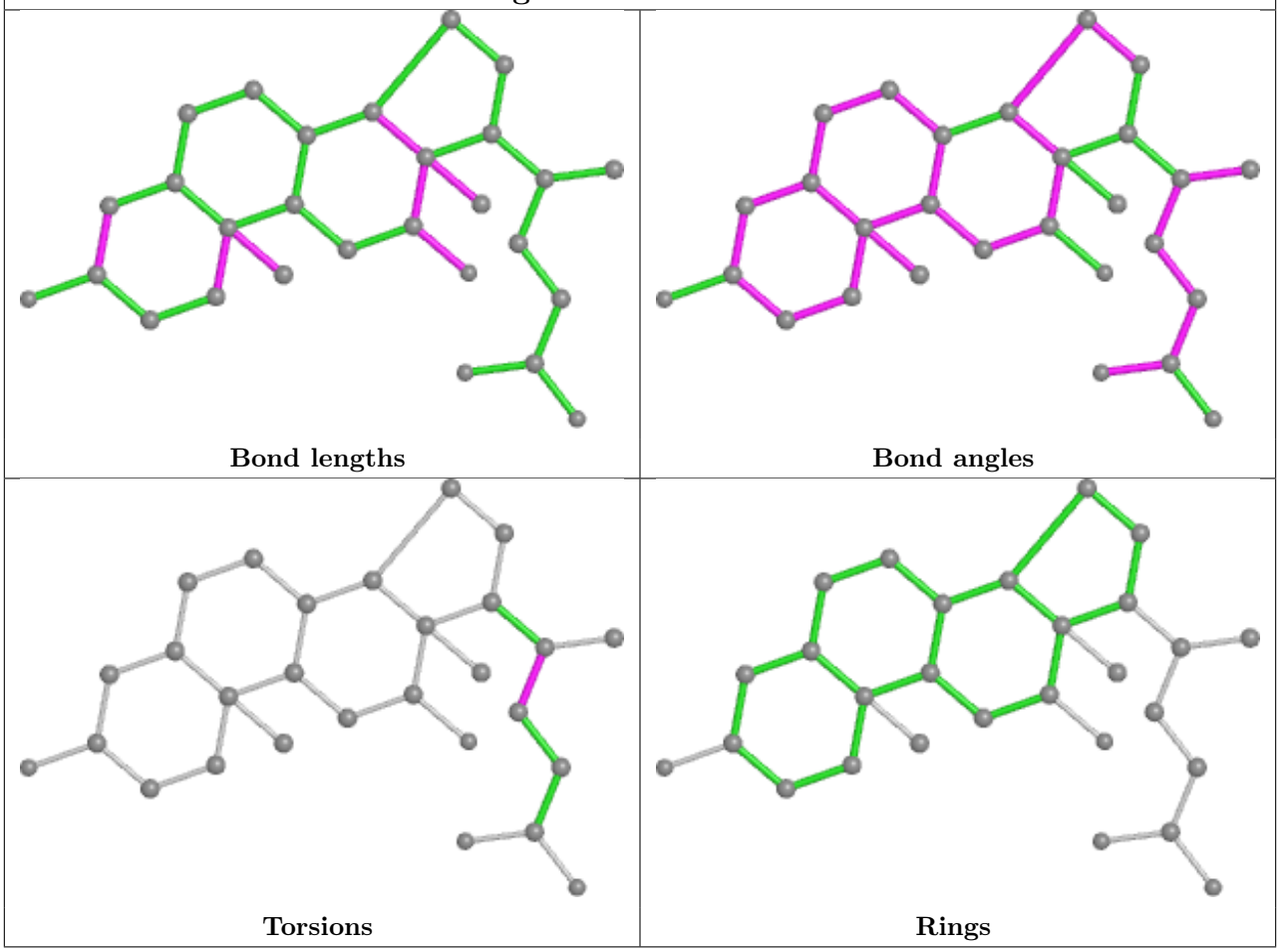
Ligand DXC C 1475



Ligand DXC B 1473



Ligand DXC C 1478



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	444/482 (92%)	0.76	75 (16%)	1	1	89, 172, 246, 330	0
1	B	452/482 (93%)	0.81	70 (15%)	2	1	67, 130, 321, 373	0
1	C	467/482 (96%)	0.24	21 (4%)	33	19	65, 105, 204, 279	0
1	D	463/482 (96%)	1.62	138 (29%)	0	0	117, 220, 320, 374	0
All	All	1826/1928 (94%)	0.86	304 (16%)	1	1	65, 163, 299, 374	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	THR	16.5
1	D	442	LYS	12.3
1	D	441	THR	12.2
1	D	453	VAL	11.4
1	B	441	THR	10.9
1	D	333	ILE	10.4
1	D	406	ILE	10.3
1	D	438	THR	10.2
1	D	412	SER	10.0
1	D	415	ALA	9.7
1	D	399	ILE	9.2
1	B	461	LEU	9.0
1	D	401	LYS	8.8
1	B	445	LEU	8.7
1	D	334	SER	8.7
1	D	428	GLY	8.6
1	D	402	GLY	8.6
1	B	330	ASN	8.5
1	D	416	ALA	8.4
1	B	450	SER	8.4
1	A	197	LYS	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	396	LYS	8.0
1	D	314	PRO	7.8
1	B	432	VAL	7.7
1	B	460	ILE	7.6
1	B	439	PHE	7.6
1	D	413	LYS	7.4
1	B	449	PHE	7.4
1	D	426	ILE	7.3
1	D	320	PHE	7.2
1	D	329	LEU	7.0
1	D	439	PHE	6.9
1	B	433	GLY	6.8
1	D	400	ASP	6.7
1	D	462	ASN	6.7
1	D	411	GLN	6.7
1	D	414	VAL	6.7
1	A	196	ILE	6.7
1	B	405	VAL	6.6
1	D	403	ARG	6.5
1	D	17	GLY	6.3
1	B	397	VAL	6.3
1	D	13	HIS	6.3
1	B	424	ILE	6.2
1	D	440	GLY	6.2
1	D	405	VAL	6.2
1	D	444	LEU	6.0
1	B	334	SER	6.0
1	D	431	ILE	5.9
1	B	400	ASP	5.9
1	D	445	LEU	5.9
1	D	467	TRP	5.9
1	D	316	LYS	5.9
1	A	230	ARG	5.8
1	D	452	ASN	5.7
1	D	330	ASN	5.7
1	D	409	LEU	5.6
1	D	318	VAL	5.6
1	B	447	ALA	5.6
1	B	418	LYS	5.5
1	B	411	GLN	5.4
1	D	437	GLY	5.3
1	A	449	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	391	VAL	5.2
1	D	454	GLU	5.2
1	B	454	GLU	5.2
1	D	449	PHE	5.2
1	D	390	GLU	5.1
1	D	397	VAL	5.1
1	D	356	VAL	5.1
1	D	425	SER	5.0
1	D	429	LYS	5.0
1	D	250	MET	5.0
1	D	377	GLU	5.0
1	D	382	ILE	4.9
1	D	417	GLU	4.9
1	B	440	GLY	4.9
1	B	402	GLY	4.9
1	D	392	LEU	4.9
1	D	419	LEU	4.8
1	A	198	GLY	4.8
1	B	403	ARG	4.8
1	B	409	LEU	4.8
1	D	311	VAL	4.7
1	D	407	ASP	4.7
1	A	218	LEU	4.7
1	A	465	ARG	4.7
1	D	376	ILE	4.6
1	B	457	ASP	4.6
1	D	327	ILE	4.6
1	D	380	LYS	4.6
1	D	432	VAL	4.6
1	D	455	ASN	4.5
1	B	446	THR	4.5
1	A	424	ILE	4.5
1	D	424	ILE	4.5
1	A	389	LYS	4.5
1	D	19	THR	4.4
1	B	453	VAL	4.4
1	D	436	LYS	4.4
1	A	260	ILE	4.2
1	B	412	SER	4.2
1	B	428	GLY	4.2
1	B	431	ILE	4.2
1	D	280	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	4.2
1	D	16	HIS	4.2
1	D	461	LEU	4.2
1	B	392	LEU	4.1
1	A	433	GLY	4.1
1	D	331	GLU	4.1
1	B	399	ILE	4.1
1	B	438	THR	4.1
1	A	422	GLU	4.0
1	D	218	LEU	4.0
1	A	259	GLN	3.9
1	A	273	LEU	3.9
1	C	36	LYS	3.9
1	D	38	PRO	3.9
1	A	225	MET	3.9
1	B	429	LYS	3.9
1	B	329	LEU	3.8
1	A	323	THR	3.8
1	C	435	ILE	3.8
1	D	312	ALA	3.8
1	D	332	VAL	3.8
1	A	423	GLU	3.7
1	D	350	ALA	3.7
1	A	220	VAL	3.7
1	B	442	LYS	3.7
1	D	248	VAL	3.7
1	D	459	VAL	3.7
1	A	434	LYS	3.7
1	D	443	GLY	3.6
1	A	388	LYS	3.6
1	C	410	ALA	3.6
1	D	249	GLY	3.6
1	A	0	HIS	3.5
1	A	322	LYS	3.5
1	D	456	ARG	3.5
1	D	398	LYS	3.5
1	A	405	VAL	3.5
1	B	414	VAL	3.5
1	D	464	LEU	3.5
1	D	323	THR	3.4
1	A	50	GLY	3.4
1	B	398	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	416	ALA	3.4
1	B	335	GLY	3.4
1	B	467	TRP	3.4
1	D	256	ASP	3.4
1	D	385	LEU	3.4
1	A	326	ASN	3.4
1	D	352	VAL	3.4
1	D	328	ILE	3.3
1	B	427	GLU	3.3
1	B	293	LEU	3.3
1	D	45	ILE	3.3
1	B	410	ALA	3.2
1	B	444	LEU	3.2
1	A	448	GLU	3.2
1	D	317	LYS	3.2
1	B	417	GLU	3.2
1	C	449	PHE	3.1
1	B	455	ASN	3.1
1	D	321	GLY	3.1
1	A	257	ALA	3.1
1	C	35	ASP	3.1
1	C	438	THR	3.1
1	D	384	ASP	3.1
1	B	401	LYS	3.0
1	D	322	LYS	3.0
1	D	378	GLU	3.0
1	D	288	ILE	3.0
1	D	451	GLY	3.0
1	A	266	LEU	3.0
1	C	409	LEU	3.0
1	D	315	PHE	3.0
1	D	372	GLY	3.0
1	A	320	PHE	3.0
1	B	382	ILE	3.0
1	D	388	LYS	3.0
1	A	460	ILE	3.0
1	A	426	ILE	3.0
1	A	255	VAL	3.0
1	B	452	ASN	3.0
1	D	339	TYR	3.0
1	D	435	ILE	3.0
1	C	402	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	18	LYS	2.9
1	B	407	ASP	2.9
1	B	413	LYS	2.9
1	A	271	THR	2.9
1	D	65	ASP	2.9
1	D	313	VAL	2.9
1	C	442	LYS	2.9
1	D	179	ILE	2.8
1	D	28	ILE	2.8
1	D	289	PHE	2.8
1	B	415	ALA	2.8
1	A	432	VAL	2.8
1	D	187	LYS	2.8
1	D	20	THR	2.8
1	D	335	GLY	2.8
1	A	385	LEU	2.8
1	A	256	ASP	2.8
1	B	443	GLY	2.8
1	D	357	LEU	2.8
1	A	252	ILE	2.7
1	D	422	GLU	2.7
1	D	211	ILE	2.7
1	C	413	LYS	2.7
1	D	383	LYS	2.7
1	A	324	GLU	2.7
1	C	396	LYS	2.7
1	B	435	ILE	2.7
1	A	281	ALA	2.7
1	D	430	ASP	2.7
1	D	220	VAL	2.7
1	A	387	ILE	2.7
1	D	389	LYS	2.6
1	A	464	LEU	2.6
1	A	321	GLY	2.6
1	C	406	ILE	2.6
1	A	203	VAL	2.6
1	C	397	VAL	2.6
1	A	435	ILE	2.6
1	C	419	LEU	2.6
1	A	441	THR	2.6
1	B	456	ARG	2.6
1	A	379	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	292	ASN	2.6
1	B	434	LYS	2.5
1	A	330	ASN	2.5
1	D	326	ASN	2.5
1	B	331	GLU	2.5
1	A	276	VAL	2.5
1	A	376	ILE	2.5
1	B	468	GLY	2.5
1	A	392	LEU	2.5
1	B	406	ILE	2.5
1	A	72	LEU	2.4
1	D	458	LYS	2.4
1	D	295	PRO	2.4
1	A	390	GLU	2.4
1	D	374	GLY	2.4
1	A	65	ASP	2.4
1	D	268	SER	2.4
1	B	387	ILE	2.4
1	D	285	ILE	2.4
1	B	311	VAL	2.4
1	B	393	ARG	2.4
1	A	341	ALA	2.4
1	A	305	MET	2.4
1	B	389	LYS	2.4
1	A	386	ASN	2.4
1	A	436	LYS	2.3
1	D	286	SER	2.3
1	A	406	ILE	2.3
1	C	424	ILE	2.3
1	A	396	LYS	2.3
1	A	279	ILE	2.3
1	D	219	LYS	2.3
1	B	292	ASN	2.3
1	A	194	PHE	2.3
1	A	466	ARG	2.3
1	D	325	GLU	2.3
1	A	346	GLU	2.3
1	C	411	GLN	2.3
1	D	66	ALA	2.3
1	A	242	ALA	2.2
1	A	204	THR	2.2
1	B	423	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	393	ARG	2.2
1	C	414	VAL	2.2
1	D	457	ASP	2.2
1	D	319	THR	2.2
1	A	431	ILE	2.2
1	D	341	ALA	2.2
1	D	181	ASN	2.2
1	D	303	VAL	2.2
1	C	417	GLU	2.2
1	A	291	TYR	2.1
1	D	228	LYS	2.1
1	D	279	ILE	2.1
1	C	467	TRP	2.1
1	A	253	GLN	2.1
1	A	462	ASN	2.1
1	B	458	LYS	2.1
1	D	169	ILE	2.1
1	D	290	LYS	2.1
1	D	296	LYS	2.1
1	A	398	LYS	2.1
1	D	251	ALA	2.1
1	D	69	HIS	2.1
1	C	444	LEU	2.1
1	B	315	PHE	2.0
1	A	404	THR	2.0
1	C	42	LYS	2.0
1	A	51	PHE	2.0
1	A	199	ALA	2.0
1	A	382	ILE	2.0
1	D	460	ILE	2.0
1	A	459	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CMH	D	338	8/9	0.75	0.17	187,264,268,302	2
1	CMH	A	371	8/9	0.91	0.34	154,165,195,202	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	0.94	0.13	141,161,218,263	2
1	CMH	A	338	8/9	0.94	0.21	149,179,204,211	2
1	CMH	B	338	8/9	0.95	0.15	157,190,227,235	2
1	CMH	D	340	8/9	0.96	0.24	155,269,276,276	2
1	CMH	D	371	8/9	0.96	0.21	129,151,184,191	2
1	CMH	C	338	8/9	0.97	0.19	72,94,152,200	2
1	CMH	C	340	8/9	0.98	0.16	58,87,108,131	2
1	CMH	D	264	8/9	0.98	0.24	164,180,206,220	2
1	CMH	B	340	8/9	0.98	0.17	141,161,259,276	2
1	CMH	A	264	8/9	0.98	0.17	166,181,195,201	2
1	CMH	A	340	8/9	0.98	0.22	150,189,198,212	2
1	CMH	C	264	8/9	1.00	0.17	61,95,114,120	0
1	CMH	C	371	8/9	1.00	0.19	55,102,148,154	2
1	CMH	B	264	8/9	1.00	0.23	57,72,95,100	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, 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
2	SO4	C	1474	5/5	0.57	0.62	156,216,245,297	5
2	SO4	C	1481	5/5	0.67	0.85	157,190,196,199	5
2	SO4	B	1471	5/5	0.73	0.41	172,203,237,246	0
4	5GP	B	1474	24/24	0.87	0.41	204,243,284,292	0
2	SO4	C	1473	5/5	0.88	0.11	138,173,210,226	5
3	DXC	C	1476	28/28	0.89	0.34	139,146,204,235	0
2	SO4	B	1472	5/5	0.91	0.42	94,222,224,320	0
3	DXC	C	1479	28/28	0.93	0.34	72,89,173,216	28
3	DXC	C	1477	28/28	0.95	0.30	67,90,157,199	0
3	DXC	C	1478	28/28	0.96	0.31	73,105,138,168	0
2	SO4	C	1472	5/5	0.96	0.17	112,131,153,180	0
2	SO4	C	1471	5/5	0.96	0.24	93,127,147,181	0
3	DXC	C	1475	28/28	0.97	0.26	64,79,119,144	0
3	DXC	C	1480	28/28	0.98	0.23	64,76,98,107	0

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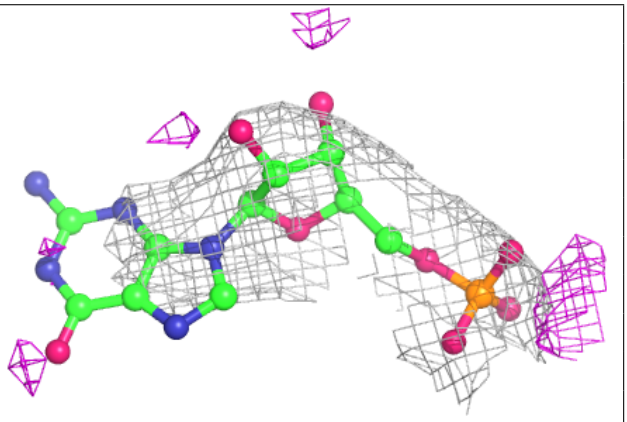
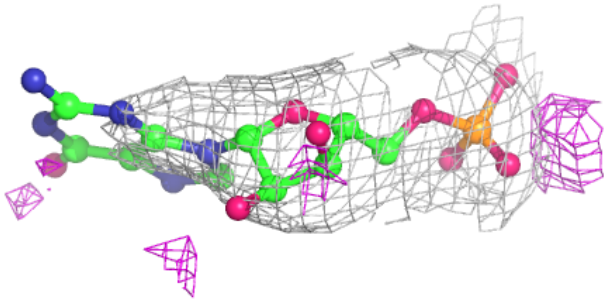
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DXC	B	1473	28/28	0.98	0.26	62,82,119,128	0

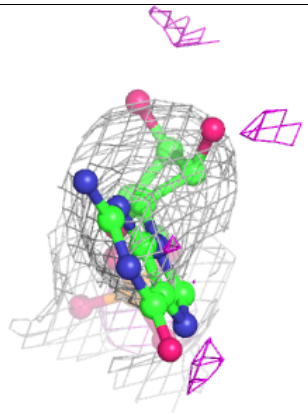
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

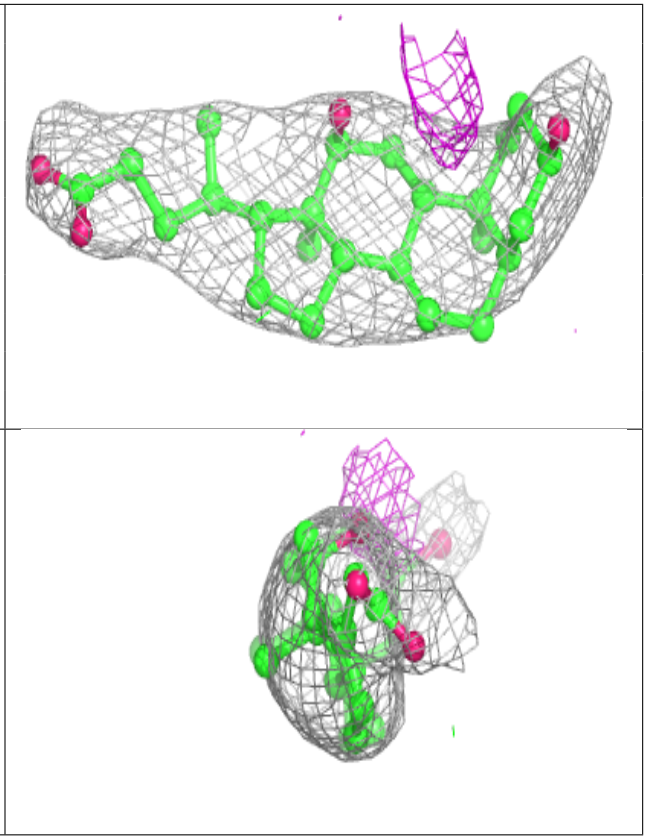






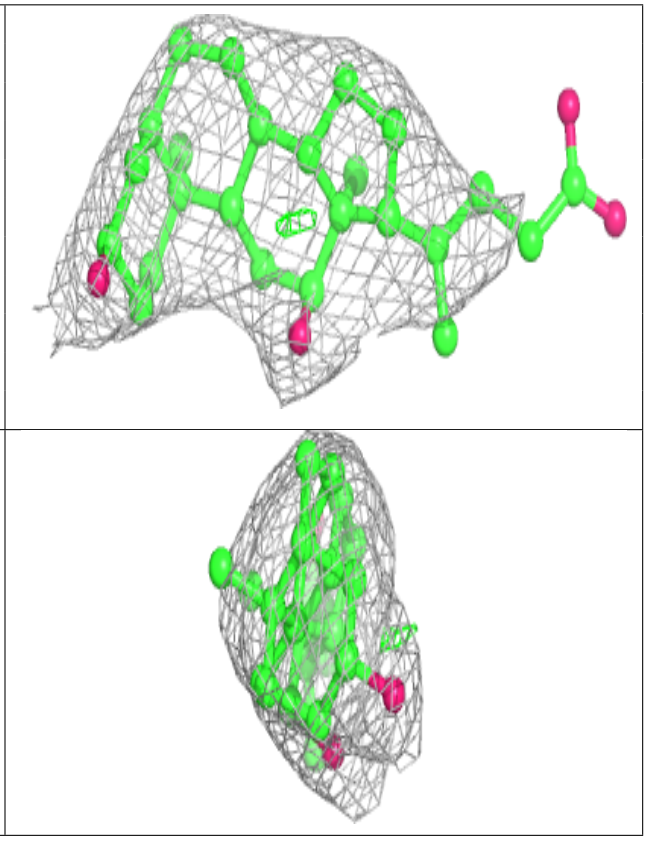
Electron density around DXC C 1476:

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



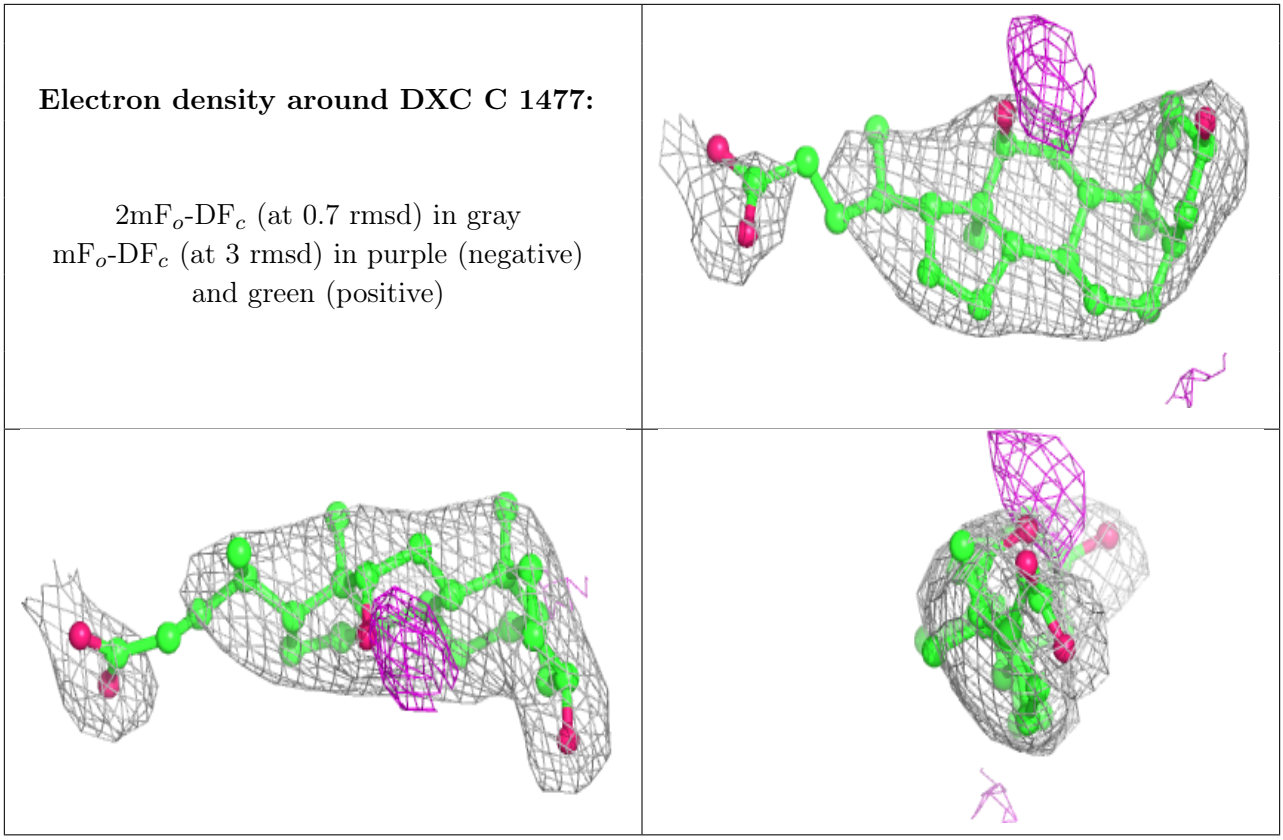
Electron density around DXC C 1479:

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



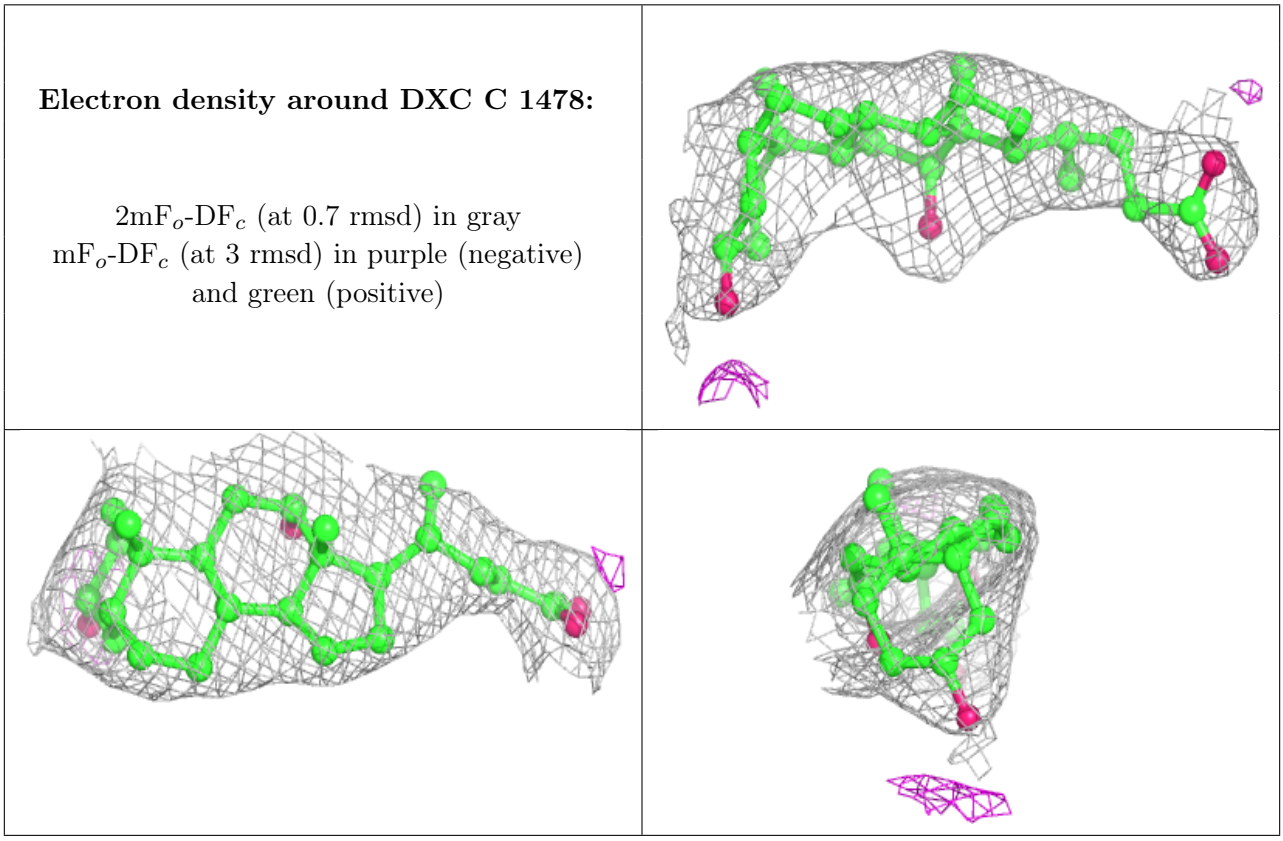
Electron density around DXC C 1477:

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



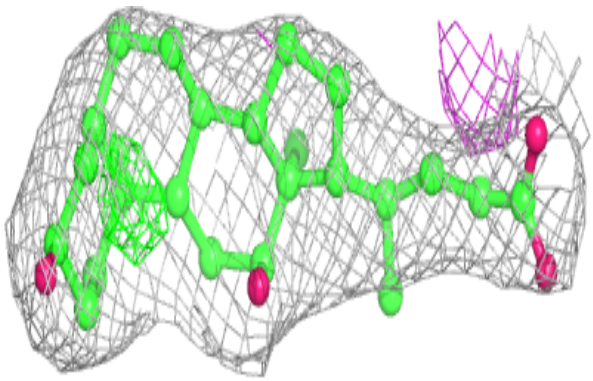
Electron density around DXC C 1478:

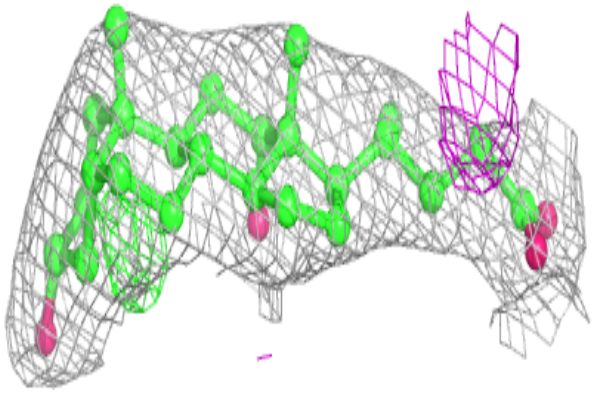
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

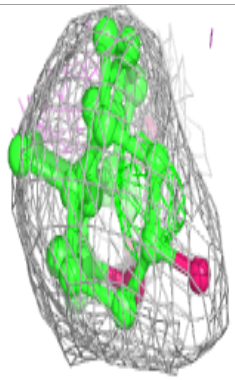


Electron density around DXC C 1475:

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

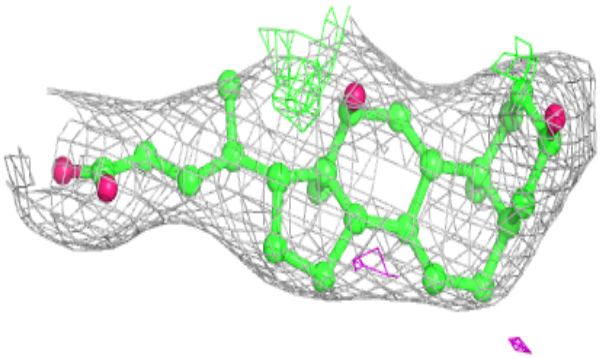


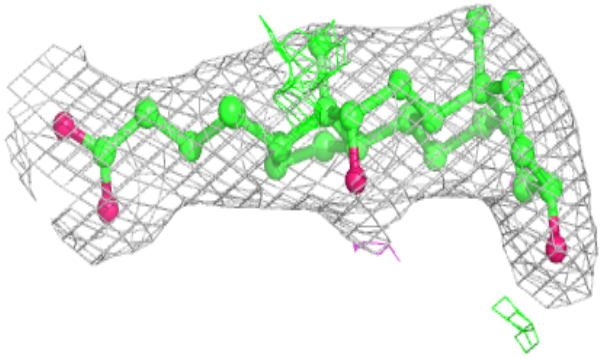


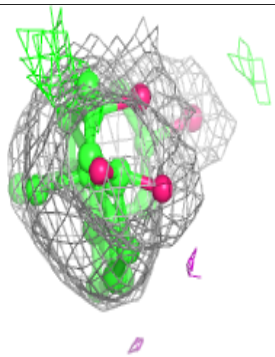


Electron density around DXC C 1480:

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

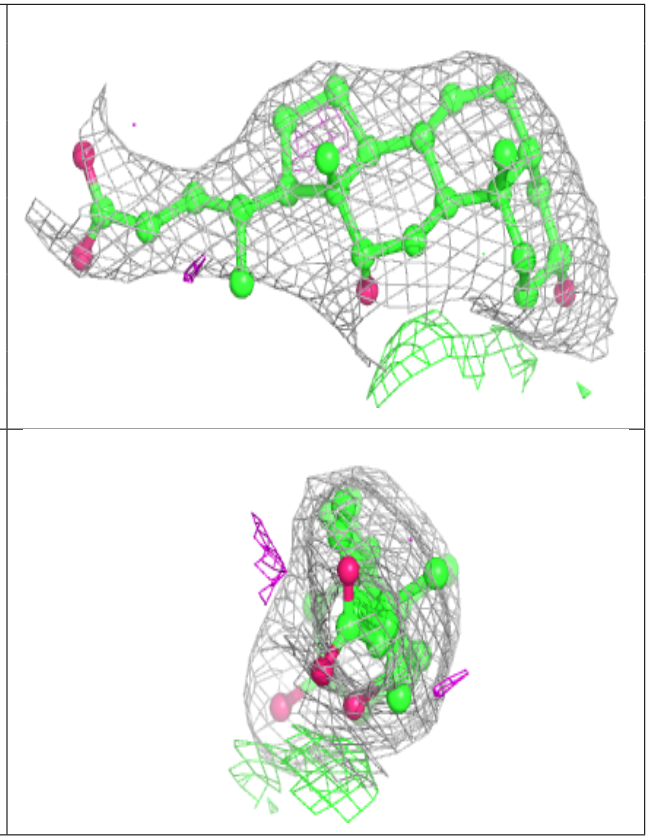






Electron density around DXC B 1473:

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



6.5 Other polymers (i)

There are no such residues in this entry.