



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:59 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

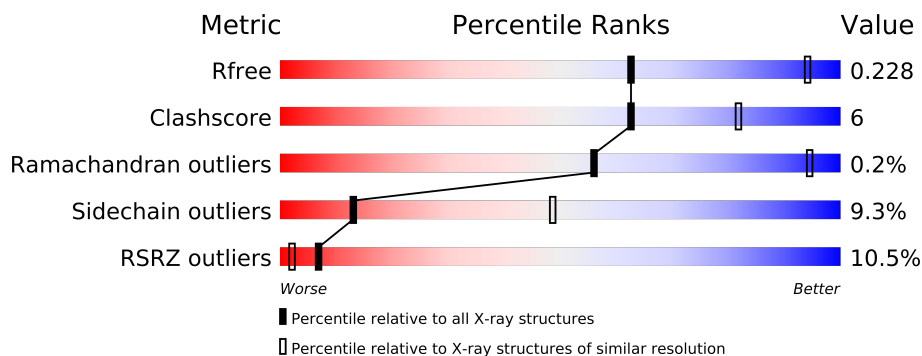
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1421 (3.48-3.20)
Clashscore	79885	1077 (3.46-3.22)
Ramachandran outliers	78287	1053 (3.46-3.22)
Sidechain outliers	78261	1052 (3.46-3.22)
RSRZ outliers	66119	1422 (3.48-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	482	
1	B	482	
1	C	482	
1	D	482	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	B	1470	-	X
5	SO4	B	1472	-	X
5	SO4	C	1481	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14623 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

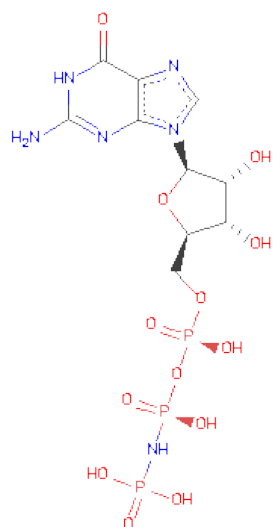
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8J307
A	-12	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-11	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-10	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-9	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-8	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-7	HIS	-	EXPRESSION TAG	UNP 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 PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

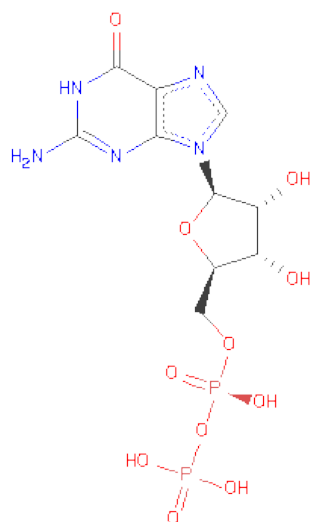


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

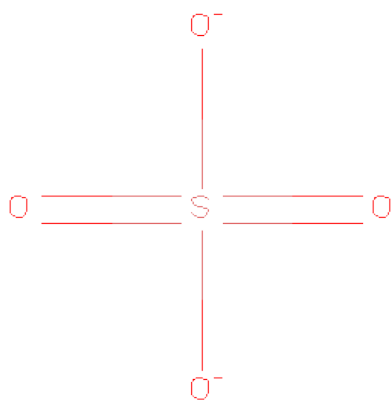
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



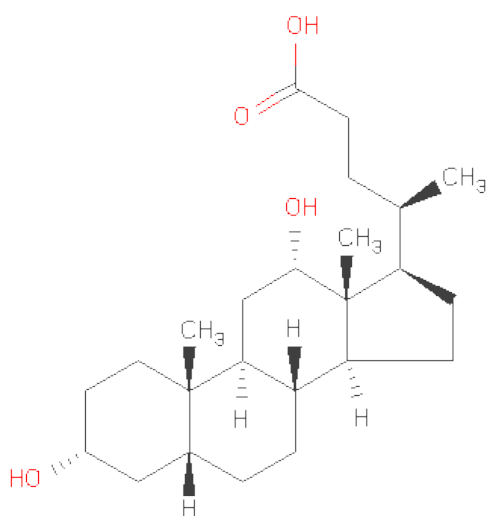
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

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

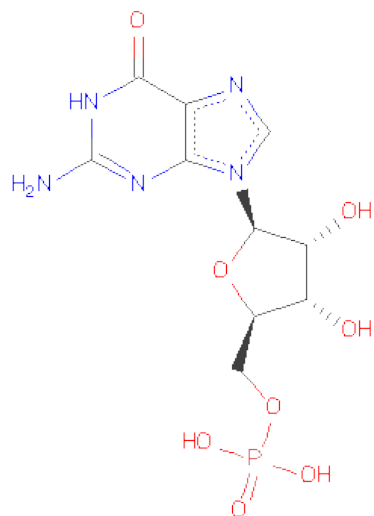
- Molecule 6 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OICACID (three-letter code: DXC) (formula: C₂₄H₄₀O₄).



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

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

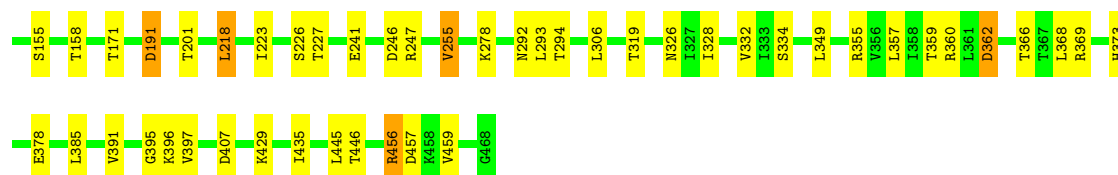
C₁₀H₁₄N₅O₈P).



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

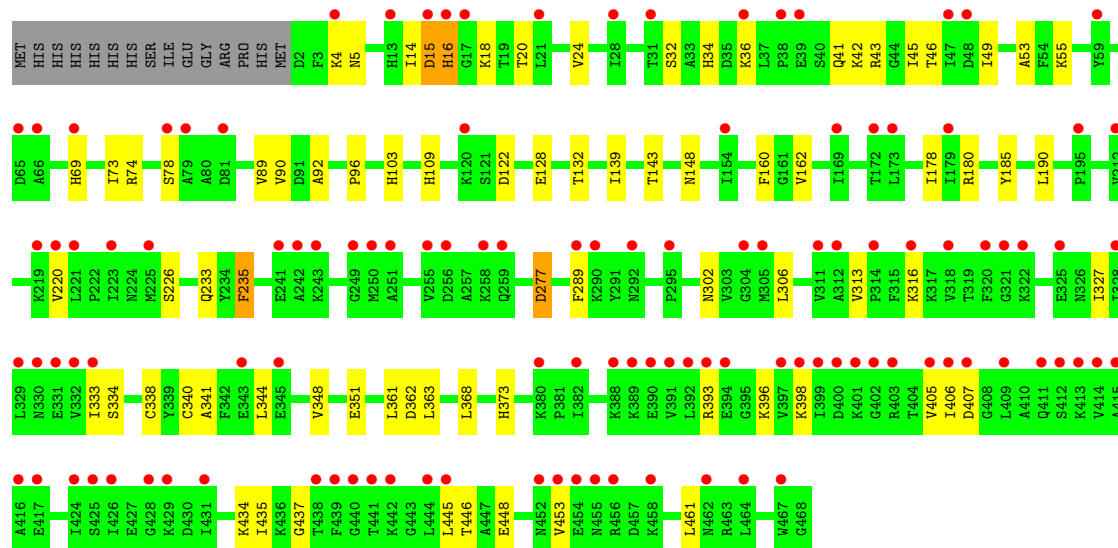
- Molecule 8 is water.

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



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	146.63Å 146.63Å 297.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.34 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
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.179 , 0.223 0.186 , 0.228	Depositor DCC
R_{free} test set	1975 reflections (4.19%)	DCC
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 , 151.7	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 53119 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.31	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3506	0	0	18	0
1	B	3533	0	0	18	0
1	C	3651	0	0	18	0
1	D	3615	0	0	29	0
2	A	32	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	10	0	0	2	0
5	C	20	0	0	0	0
6	B	28	0	0	0	0
6	C	168	0	0	0	0
7	B	24	0	0	0	0
8	A	2	0	0	0	0
8	B	4	0	0	0	0
All	All	14623	0	0	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:191:ASP:OD2	1:B:247:ARG:NH1	2.25	0.69
1:B:69:HIS:NE2	1:B:102:GLU:OE1	2.26	0.68
1:A:99:GLN:NE2	1:A:102:GLU:OE2	2.27	0.67
1:B:287:ASP:N	1:B:287:ASP:OD1	2.28	0.67
1:A:256:ASP:N	1:A:256:ASP:OD1	2.30	0.65
1:A:362:ASP:OD1	1:A:362:ASP:N	2.28	0.64
1:D:338:CMH:CM	1:D:340:CMH:SG	2.87	0.63
1:A:70:ALA:O	1:A:369:ARG:NH2	2.32	0.62
1:A:18:LYS:NZ	2:A:1469:GNP:O1B	2.33	0.61
1:B:201:THR:OG1	1:B:255:VAL:O	2.18	0.60
1:A:456:ARG:O	1:A:458:LYS:NZ	2.35	0.60
1:C:191:ASP:OD2	1:C:247:ARG:NH1	2.35	0.60
1:D:316:LYS:N	1:D:327:ILE:O	2.35	0.59
1:C:395:GLY:O	1:C:459:VAL:N	2.36	0.59
1:A:109:HIS:NE2	1:A:286:SER:OG	2.36	0.58
1:B:59:TYR:OH	1:B:174:ASN:OD1	2.22	0.58
1:B:130:LYS:NZ	1:D:96:PRO:O	2.38	0.56
1:D:20:THR:O	1:D:24:VAL:N	2.39	0.55
1:B:74:ARG:NH2	5:B:1471:SO4:O4	2.40	0.55
1:B:213:LYS:N	1:B:216:ASP:OD2	2.40	0.55
1:C:218:LEU:O	1:C:227:THR:N	2.40	0.54
1:B:186:PHE:O	1:B:267:THR:OG1	2.25	0.54
5:B:1472:SO4:O2	1:C:55:LYS:NZ	2.41	0.54
1:D:313:VAL:O	1:D:341:ALA:N	2.41	0.54
1:C:16:HIS:NE2	1:C:94:GLU:OE2	2.42	0.53
1:A:48:ASP:OD1	1:A:49:ILE:N	2.41	0.53
1:C:395:GLY:N	1:C:459:VAL:O	2.42	0.53
1:D:34:HIS:N	1:D:53:ALA:O	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:191:ASP:OD2	1:A:247:ARG:NH2	2.43	0.52
1:D:148:ASN:OD1	1:D:148:ASN:N	2.43	0.52
1:D:398:LYS:N	1:D:405:VAL:O	2.43	0.51
1:A:105:LEU:O	1:A:109:HIS:ND1	2.44	0.51
1:D:4:LYS:NZ	1:D:178:ILE:O	2.44	0.50
1:D:69:HIS:CE1	1:D:103:HIS:CE1	2.99	0.50
1:B:81:ASP:OD2	1:B:208:ASN:ND2	2.45	0.50
1:D:122:ASP:N	1:D:122:ASP:OD1	2.45	0.50
1:C:122:ASP:OD2	1:C:155:SER:OG	2.29	0.49
1:C:148:ASN:OD1	1:C:148:ASN:N	2.43	0.49
1:D:302:ASN:ND2	1:D:306:LEU:O	2.46	0.48
1:D:15:ASP:OD1	1:D:16:HIS:ND1	2.46	0.48
1:D:32:SER:O	1:D:55:LYS:N	2.46	0.48
1:D:393:ARG:N	1:D:461:LEU:O	2.48	0.47
1:D:277:ASP:O	1:D:344:LEU:N	2.47	0.47
1:B:11:PHE:N	1:B:87:LEU:O	2.48	0.47
1:C:360:ARG:NH2	1:C:362:ASP:OD2	2.48	0.47
1:B:185:TYR:OH	1:B:351:GLU:OE1	2.32	0.46
1:B:362:ASP:OD1	1:B:363:LEU:N	2.48	0.46
1:A:18:LYS:NZ	2:A:1469:GNP:O2G	2.49	0.46
1:D:69:HIS:CE1	1:D:103:HIS:NE2	2.84	0.46
1:C:396:LYS:N	1:C:407:ASP:O	2.50	0.44
1:B:7:ASN:N	1:B:84:ASP:OD2	2.50	0.44
1:A:356:VAL:N	1:A:374:GLY:O	2.51	0.44
1:C:429:LYS:NZ	1:C:457:ASP:OD2	2.51	0.44
1:D:109:HIS:CG	1:D:373:HIS:CE1	3.06	0.44
1:B:397:VAL:O	1:B:456:ARG:N	2.51	0.44
1:B:360:ARG:NH1	1:B:371:CMH:SG	2.92	0.43
1:D:185:TYR:OH	1:D:351:GLU:OE1	2.36	0.43
1:D:316:LYS:O	1:D:327:ILE:N	2.52	0.43
1:C:201:THR:OG1	1:C:255:VAL:O	2.37	0.43
1:B:11:PHE:O	1:B:89:VAL:N	2.51	0.43
1:A:155:SER:O	1:A:159:GLY:N	2.52	0.43
1:A:52:SER:O	1:A:63:LEU:N	2.52	0.43
1:D:34:HIS:NE2	1:D:235:PHE:O	2.51	0.43
1:D:437:GLY:O	1:D:446:THR:N	2.52	0.42
1:A:188:MET:O	1:A:266:LEU:N	2.52	0.42
1:D:92:ALA:O	1:D:132:THR:OG1	2.37	0.42
1:D:406:ILE:N	1:D:445:LEU:O	2.52	0.42
1:B:16:HIS:O	1:B:119:THR:OG1	2.37	0.42
1:C:397:VAL:O	1:C:456:ARG:N	2.52	0.41
1:A:121:SER:OG	1:A:154:ILE:O	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:396:LYS:N	1:D:407:ASP:O	2.53	0.41
1:C:5:ASN:ND2	1:C:246:ASP:OD1	2.54	0.41
1:D:14:ILE:O	1:D:18:LYS:N	2.54	0.41
1:C:49:ILE:O	1:C:247:ARG:NH2	2.54	0.41
1:C:56:LEU:O	1:C:59:TYR:N	2.54	0.41
1:D:434:LYS:O	1:D:448:GLU:N	2.53	0.41
1:D:5:ASN:O	1:D:180:ARG:NH2	2.54	0.41
1:A:279:ILE:O	1:A:342:PHE:N	2.54	0.40
1:C:11:PHE:N	1:C:87:LEU:O	2.53	0.40
1:C:326:ASN:ND2	1:C:385:LEU:O	2.53	0.40
1:D:434:LYS:N	1:D:448:GLU:O	2.54	0.40
1:A:101:GLY:O	1:A:105:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/482 (92%)	420 (95%)	24 (5%)	0	100	100
1	B	448/482 (93%)	429 (96%)	19 (4%)	0	100	100
1	C	465/482 (96%)	435 (94%)	28 (6%)	2 (0%)	43	89
1	D	461/482 (96%)	435 (94%)	25 (5%)	1 (0%)	56	94
All	All	1818/1928 (94%)	1719 (95%)	96 (5%)	3 (0%)	56	94

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/412 (94%)	352 (91%)	34 (9%)	14	52
1	B	388/412 (94%)	354 (91%)	34 (9%)	14	52
1	C	402/412 (98%)	358 (89%)	44 (11%)	9	38
1	D	398/412 (97%)	364 (92%)	34 (8%)	15	55
All	All	1574/1648 (96%)	1428 (91%)	146 (9%)	13	48

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CMH	A	264	1	7,7,8	6.71	2 (28%)	3,7,9	0.69	0
1	CMH	A	338	1	7,7,8	6.57	2 (28%)	3,7,9	2.95	1 (33%)
1	CMH	A	340	1	7,7,8	6.97	3 (42%)	3,7,9	1.88	2 (66%)
1	CMH	A	371	1	7,7,8	6.92	2 (28%)	3,7,9	1.04	0
1	CMH	B	264	1	7,7,8	6.82	3 (42%)	3,7,9	1.27	1 (33%)
1	CMH	B	338	1	7,7,8	6.57	1 (14%)	3,7,9	2.65	1 (33%)
1	CMH	B	340	1	7,7,8	6.76	2 (28%)	3,7,9	1.24	0
1	CMH	B	371	1	7,7,8	6.46	2 (28%)	3,7,9	1.63	1 (33%)
1	CMH	C	264	1	7,7,8	6.98	3 (42%)	3,7,9	1.37	0
1	CMH	C	338	1	7,7,8	6.48	1 (14%)	3,7,9	0.42	0
1	CMH	C	340	1	7,7,8	6.93	2 (28%)	3,7,9	4.51	1 (33%)
1	CMH	C	371	1	7,7,8	6.66	2 (28%)	3,7,9	1.67	1 (33%)
1	CMH	D	264	1	7,7,8	6.55	2 (28%)	3,7,9	0.91	0
1	CMH	D	338	1	7,7,8	6.70	3 (42%)	3,7,9	3.67	1 (33%)
1	CMH	D	340	1	7,7,8	6.93	2 (28%)	3,7,9	0.28	0
1	CMH	D	371	1	7,7,8	6.56	2 (28%)	3,7,9	0.87	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	A	264	1	-	0/2/6/8	0/0/0/0
1	CMH	A	338	1	-	0/2/6/8	0/0/0/0
1	CMH	A	340	1	-	0/2/6/8	0/0/0/0
1	CMH	A	371	1	-	0/2/6/8	0/0/0/0
1	CMH	B	264	1	-	0/2/6/8	0/0/0/0
1	CMH	B	338	1	-	0/2/6/8	0/0/0/0
1	CMH	B	340	1	-	0/2/6/8	0/0/0/0
1	CMH	B	371	1	-	0/2/6/8	0/0/0/0
1	CMH	C	264	1	-	0/2/6/8	0/0/0/0
1	CMH	C	338	1	-	0/2/6/8	0/0/0/0
1	CMH	C	340	1	-	0/2/6/8	0/0/0/0
1	CMH	C	371	1	-	0/2/6/8	0/0/0/0
1	CMH	D	264	1	-	0/2/6/8	0/0/0/0
1	CMH	D	338	1	-	0/2/6/8	0/0/0/0
1	CMH	D	340	1	-	0/2/6/8	0/0/0/0
1	CMH	D	371	1	-	0/2/6/8	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	264	CMH	O-C	18.08	1.23	1.11
1	C	340	CMH	O-C	18.08	1.23	1.11
1	A	371	CMH	O-C	18.05	1.23	1.11
1	D	340	CMH	O-C	17.86	1.23	1.11
1	A	340	CMH	O-C	17.85	1.23	1.11
1	B	340	CMH	O-C	17.68	1.23	1.11
1	A	264	CMH	O-C	17.45	1.23	1.11
1	B	264	CMH	O-C	17.36	1.23	1.11
1	D	338	CMH	O-C	17.29	1.23	1.11
1	C	371	CMH	O-C	17.25	1.23	1.11
1	B	338	CMH	O-C	17.25	1.23	1.11
1	A	338	CMH	O-C	17.18	1.23	1.11
1	D	264	CMH	O-C	17.16	1.23	1.11
1	D	371	CMH	O-C	17.08	1.23	1.11
1	C	338	CMH	O-C	16.98	1.23	1.11
1	B	371	CMH	O-C	16.94	1.23	1.11
1	A	340	CMH	SG-HG	-3.78	2.32	2.36
1	B	264	CMH	SG-HG	-3.65	2.32	2.36
1	D	340	CMH	CA-C	3.47	1.54	1.48
1	C	371	CMH	SG-HG	-3.06	2.33	2.36
1	B	264	CMH	CA-C	3.05	1.54	1.48
1	C	264	CMH	CA-C	2.88	1.53	1.48
1	A	371	CMH	CA-C	2.86	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	CMH	CA-C	2.81	1.53	1.48
1	D	338	CMH	CA-C	2.79	1.53	1.48
1	D	338	CMH	SG-HG	-2.63	2.33	2.36
1	A	340	CMH	CA-C	2.49	1.52	1.48
1	D	371	CMH	CA-C	2.44	1.52	1.48
1	C	340	CMH	CA-C	2.33	1.52	1.48
1	C	264	CMH	SG-HG	-2.33	2.33	2.36
1	B	340	CMH	CA-C	2.31	1.52	1.48
1	D	264	CMH	CA-C	2.28	1.52	1.48
1	A	338	CMH	CA-C	2.24	1.52	1.48
1	B	371	CMH	CA-C	2.16	1.52	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	CMH	C-CA-N	-7.61	106.23	113.83
1	D	338	CMH	C-CA-N	-6.27	107.57	113.83
1	A	338	CMH	C-CA-N	-4.75	109.09	113.83
1	B	338	CMH	C-CA-N	-4.38	109.46	113.83
1	C	371	CMH	C-CA-N	-2.59	111.24	113.83
1	A	340	CMH	C-CA-N	-2.55	111.29	113.83
1	B	264	CMH	CA-CB-SG	2.18	120.00	111.64
1	B	371	CMH	CA-CB-SG	2.14	119.85	111.64
1	A	340	CMH	CA-CB-SG	2.03	119.44	111.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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
2	GNP	A	1469	3	34,34,34	2.25	6 (17%)	50,54,54	5.03	8 (16%)
4	GDP	B	1469	3	30,30,30	1.50	5 (16%)	44,47,47	3.03	7 (15%)
5	SO4	B	1471	-	4,4,4	0.09	0	6,6,6	0.09	0
5	SO4	B	1472	-	4,4,4	0.17	0	6,6,6	0.16	0
6	DXC	B	1473	-	31,31,31	1.30	3 (9%)	49,49,49	2.00	14 (28%)
7	5GP	B	1474	-	26,26,26	1.02	2 (7%)	37,40,40	1.63	7 (18%)
5	SO4	C	1471	-	4,4,4	0.50	0	6,6,6	0.44	0
5	SO4	C	1472	-	4,4,4	0.19	0	6,6,6	0.16	0
5	SO4	C	1473	-	4,4,4	0.12	0	6,6,6	0.15	0
6	DXC	C	1475	-	31,31,31	1.52	4 (12%)	49,49,49	2.17	16 (32%)
6	DXC	C	1476	-	31,31,31	1.43	5 (16%)	49,49,49	1.75	12 (24%)
6	DXC	C	1477	-	31,31,31	1.55	6 (19%)	49,49,49	1.83	12 (24%)
6	DXC	C	1478	-	31,31,31	1.28	5 (16%)	49,49,49	1.81	15 (30%)
6	DXC	C	1479	-	31,31,31	1.48	8 (25%)	49,49,49	2.12	17 (34%)
6	DXC	C	1480	-	31,31,31	1.55	7 (22%)	49,49,49	2.02	15 (30%)
5	SO4	C	1481	-	4,4,4	0.07	0	6,6,6	0.10	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
2	GNP	A	1469	3	-	0/18/38/38	0/1/3/3
4	GDP	B	1469	3	-	0/16/32/32	0/1/3/3
5	SO4	B	1471	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1472	-	-	0/0/0/0	0/0/0/0
6	DXC	B	1473	-	-	0/9/71/71	0/0/4/4
7	5GP	B	1474	-	-	0/10/26/26	0/1/3/3
5	SO4	C	1471	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1472	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1473	-	-	0/0/0/0	0/0/0/0
6	DXC	C	1475	-	-	0/9/71/71	0/0/4/4
6	DXC	C	1476	-	-	0/9/71/71	0/0/4/4
6	DXC	C	1477	-	-	0/9/71/71	0/0/4/4
6	DXC	C	1478	-	-	0/9/71/71	0/0/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DXC	C	1479	-	-	0/9/71/71	0/0/4/4
6	DXC	C	1480	-	-	0/9/71/71	0/0/4/4
5	SO4	C	1481	-	-	0/0/0/0	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1469	GNP	PG-N3B	-6.84	1.58	1.64
2	A	1469	GNP	PB-N3B	-6.54	1.58	1.64
4	B	1469	GDP	C6-C5	4.68	1.48	1.41
2	A	1469	GNP	PG-O1G	4.50	1.51	1.46
6	C	1475	DXC	C12-C13	-4.49	1.47	1.54
2	A	1469	GNP	PB-O3A	-4.28	1.53	1.59
2	A	1469	GNP	PA-O3A	-4.11	1.52	1.59
6	C	1477	DXC	C12-C13	-3.75	1.48	1.54
6	C	1477	DXC	C4-C10	-3.55	1.50	1.56
6	C	1477	DXC	C18-C4	-3.53	1.47	1.54
6	C	1480	DXC	C18-C4	-3.46	1.47	1.54
6	C	1476	DXC	C12-C13	-3.30	1.49	1.54
6	B	1473	DXC	C4-C10	-3.05	1.51	1.56
4	B	1469	GDP	C5-C4	3.02	1.47	1.40
6	C	1479	DXC	C18-C4	-3.02	1.48	1.54
6	C	1476	DXC	O1-C13	-3.01	1.38	1.43
6	C	1480	DXC	C12-C13	-2.97	1.49	1.54
6	B	1473	DXC	C12-C13	-2.94	1.49	1.54
6	C	1476	DXC	C12-C11	-2.87	1.50	1.55
6	C	1479	DXC	C12-C13	-2.85	1.50	1.54
6	C	1478	DXC	C18-C4	-2.84	1.48	1.54
6	C	1475	DXC	C12-C11	-2.83	1.50	1.55
6	C	1480	DXC	C4-C10	-2.81	1.51	1.56
6	C	1475	DXC	O1-C13	-2.77	1.38	1.43
6	C	1476	DXC	C20-C12	-2.77	1.49	1.54
6	C	1475	DXC	C20-C12	-2.76	1.49	1.54
4	B	1469	GDP	C4-N9	-2.74	1.33	1.37
6	C	1480	DXC	C12-C11	-2.71	1.50	1.55
6	B	1473	DXC	C18-C4	-2.68	1.49	1.54
6	C	1477	DXC	C20-C12	-2.64	1.50	1.54
6	C	1480	DXC	C5-C4	-2.59	1.49	1.54
6	C	1479	DXC	C4-C10	-2.58	1.52	1.56
6	C	1478	DXC	C12-C11	-2.57	1.51	1.55
4	B	1469	GDP	C2-N2	2.52	1.36	1.32
7	B	1474	5GP	C4-N9	-2.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1479	DXC	O1-C13	-2.33	1.39	1.43
6	C	1479	DXC	C4-C3	-2.32	1.51	1.55
6	C	1478	DXC	C12-C13	-2.31	1.50	1.54
6	C	1478	DXC	O1-C13	-2.29	1.39	1.43
4	B	1469	GDP	C2-N3	2.28	1.36	1.33
6	C	1479	DXC	C12-C11	-2.24	1.51	1.55
6	C	1480	DXC	C4-C3	-2.21	1.51	1.55
6	C	1479	DXC	C20-C12	-2.20	1.50	1.54
6	C	1476	DXC	C18-C4	-2.20	1.50	1.54
6	C	1477	DXC	O1-C13	-2.15	1.39	1.43
2	A	1469	GNP	PB-O2B	-2.14	1.49	1.55
6	C	1478	DXC	C20-C12	-2.10	1.50	1.54
6	C	1480	DXC	O1-C13	-2.08	1.40	1.43
6	C	1477	DXC	C12-C11	-2.07	1.52	1.55
7	B	1474	5GP	C2-N2	2.02	1.35	1.32
6	C	1479	DXC	C12-C17	-2.01	1.52	1.55

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1469	GNP	C6-C5-N7	-33.92	129.57	134.14
4	B	1469	GDP	C6-C5-N7	16.66	136.38	134.14
6	C	1478	DXC	C10-C14-C13	-5.72	106.89	114.35
4	B	1469	GDP	N3-C4-N9	5.42	134.85	126.91
6	C	1475	DXC	C15-C11-C12	-5.28	98.29	103.58
2	A	1469	GNP	PB-N3B-PG	-5.12	121.46	130.07
6	C	1475	DXC	C3-C2-C1	-5.04	105.55	112.95
4	B	1469	GDP	C5-C4-N3	-5.02	118.67	125.94
6	C	1479	DXC	C18-C4-C3	-4.98	101.64	110.26
6	C	1480	DXC	C20-C12-C13	4.86	113.93	109.08
6	C	1477	DXC	C10-C14-C13	-4.74	108.17	114.35
6	C	1479	DXC	C6-C5-C4	-4.70	104.30	112.83
6	B	1473	DXC	C10-C4-C3	4.51	114.94	108.67
6	C	1476	DXC	C18-C4-C3	-4.49	102.49	110.26
4	B	1469	GDP	C2-N3-C4	4.41	121.29	115.09
6	C	1477	DXC	C14-C13-C12	-4.37	106.72	111.21
7	B	1474	5GP	C5-C4-N3	-4.32	119.69	125.94
6	C	1480	DXC	C18-C4-C5	-4.31	100.84	108.17
6	B	1473	DXC	C6-C5-C4	-4.29	105.05	112.83
6	C	1479	DXC	C24-C19-C17	-4.27	105.49	112.96
6	C	1475	DXC	C17-C12-C13	-4.27	113.73	117.67
6	C	1479	DXC	C5-C4-C3	4.21	112.43	107.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1473	DXC	C11-C9-C10	-4.21	103.45	109.04
6	C	1475	DXC	C18-C4-C10	4.15	116.53	111.17
6	C	1475	DXC	O1-C13-C12	-4.15	104.31	111.13
6	C	1478	DXC	C7-C8-C9	-4.05	104.96	112.12
7	B	1474	5GP	N3-C4-N9	4.00	132.77	126.91
6	C	1477	DXC	C11-C9-C10	-3.84	103.93	109.04
6	C	1477	DXC	C7-C8-C9	-3.75	105.49	112.12
6	B	1473	DXC	C5-C6-C1	-3.64	104.34	110.37
4	B	1469	GDP	C4-C5-N7	-3.63	106.42	109.52
6	B	1473	DXC	C14-C10-C4	-3.61	109.86	113.73
6	C	1476	DXC	C10-C4-C3	3.59	113.66	108.67
2	A	1469	GNP	O3G-PG-O1G	-3.55	104.47	113.60
6	C	1475	DXC	C18-C4-C3	-3.50	104.20	110.26
6	B	1473	DXC	C22-C21-C19	-3.46	108.97	114.46
6	C	1476	DXC	C22-C21-C19	-3.46	108.98	114.46
6	C	1479	DXC	C7-C8-C9	-3.37	106.16	112.12
6	C	1476	DXC	C4-C10-C9	-3.35	108.63	112.41
6	C	1476	DXC	C10-C14-C13	-3.35	109.98	114.35
6	C	1480	DXC	C11-C12-C13	-3.30	104.34	107.40
6	C	1475	DXC	C11-C9-C10	-3.28	104.67	109.04
6	C	1480	DXC	C17-C12-C13	-3.28	114.64	117.67
6	C	1479	DXC	C10-C4-C3	3.28	113.24	108.67
6	C	1480	DXC	C10-C14-C13	-3.26	110.10	114.35
6	C	1476	DXC	C8-C9-C10	3.23	114.42	110.47
2	A	1469	GNP	O2B-PB-O1B	3.22	117.33	109.89
6	C	1477	DXC	C11-C12-C13	-3.22	104.42	107.40
6	C	1480	DXC	C16-C15-C11	-3.22	98.61	105.14
6	B	1473	DXC	C5-C4-C10	-3.20	106.32	111.45
7	B	1474	5GP	C2-N3-C4	3.20	119.59	115.09
6	C	1479	DXC	C15-C11-C9	-3.19	113.95	119.03
6	C	1478	DXC	C3-C2-C1	-3.18	108.29	112.95
6	C	1476	DXC	C7-C8-C9	-3.17	106.51	112.12
6	C	1480	DXC	C7-C8-C9	-3.15	106.56	112.12
6	C	1478	DXC	C12-C17-C19	-3.11	115.76	119.51
6	B	1473	DXC	C18-C4-C3	-3.11	104.87	110.26
6	C	1475	DXC	C5-C6-C1	-3.10	105.23	110.37
6	C	1475	DXC	C17-C12-C11	3.07	103.21	100.07
6	C	1480	DXC	C24-C19-C21	-3.07	105.13	110.37
2	A	1469	GNP	C6-N1-C2	3.05	124.85	119.51
6	C	1480	DXC	C5-C4-C10	3.04	116.34	111.45
6	C	1479	DXC	C11-C9-C10	-3.04	104.99	109.04
6	C	1477	DXC	C17-C12-C11	3.01	103.14	100.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1475	DXC	C6-C5-C4	-2.97	107.45	112.83
6	C	1479	DXC	C8-C9-C10	2.95	114.08	110.47
6	C	1479	DXC	C14-C10-C4	-2.90	110.62	113.73
7	B	1474	5GP	C6-C5-N7	-2.89	133.75	134.14
6	B	1473	DXC	C20-C12-C11	2.83	115.72	111.22
2	A	1469	GNP	O3G-PG-O2G	2.83	115.78	107.66
6	C	1477	DXC	C10-C4-C3	2.79	112.55	108.67
6	C	1479	DXC	C18-C4-C10	2.74	114.71	111.17
6	C	1478	DXC	C16-C15-C11	-2.73	99.60	105.14
6	C	1476	DXC	C17-C12-C13	2.70	120.16	117.67
6	C	1480	DXC	O1-C13-C12	-2.70	106.70	111.13
6	C	1479	DXC	C10-C14-C13	-2.70	110.83	114.35
6	C	1479	DXC	C12-C17-C19	-2.69	116.27	119.51
6	C	1480	DXC	C3-C2-C1	-2.67	109.03	112.95
6	C	1477	DXC	C20-C12-C11	2.66	115.44	111.22
6	C	1480	DXC	C4-C10-C9	-2.60	109.47	112.41
6	C	1479	DXC	C14-C13-C12	-2.58	108.56	111.21
6	C	1476	DXC	C15-C11-C12	-2.58	101.00	103.58
2	A	1469	GNP	PA-O3A-PB	-2.58	122.99	131.81
6	C	1478	DXC	C8-C9-C10	2.57	113.61	110.47
6	B	1473	DXC	C24-C19-C21	-2.57	105.99	110.37
6	C	1477	DXC	C2-C3-C7	-2.56	106.66	111.70
6	B	1473	DXC	C5-C4-C3	2.53	110.58	107.79
6	C	1478	DXC	C10-C4-C3	2.50	112.16	108.67
6	C	1479	DXC	C15-C11-C12	-2.50	101.08	103.58
6	C	1479	DXC	C4-C10-C9	-2.50	109.59	112.41
6	C	1475	DXC	C2-C1-C6	-2.46	107.39	110.54
6	C	1478	DXC	C22-C21-C19	-2.43	110.60	114.46
6	C	1478	DXC	C6-C5-C4	-2.43	108.42	112.83
6	C	1475	DXC	C16-C15-C11	-2.43	100.21	105.14
6	C	1478	DXC	C24-C19-C21	-2.43	106.24	110.37
6	C	1476	DXC	C3-C2-C1	-2.40	109.43	112.95
7	B	1474	5GP	C4-C5-N7	-2.39	107.47	109.52
6	C	1480	DXC	C10-C4-C3	2.39	111.99	108.67
4	B	1469	GDP	PA-O3A-PB	-2.36	124.76	131.68
6	C	1475	DXC	C2-C3-C4	-2.31	110.17	112.67
6	C	1475	DXC	C18-C4-C5	-2.29	104.28	108.17
7	B	1474	5GP	O5'-P-O1P	-2.28	100.01	106.71
6	C	1477	DXC	C16-C15-C11	-2.27	100.54	105.14
6	C	1479	DXC	C11-C12-C13	2.26	109.49	107.40
4	B	1469	GDP	C8-N9-C4	2.24	108.61	106.90
2	A	1469	GNP	C2-N3-C4	-2.24	111.94	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1480	DXC	O2-C1-C2	2.23	114.33	109.87
6	B	1473	DXC	C15-C11-C12	2.22	105.81	103.58
6	C	1476	DXC	C15-C11-C9	-2.19	115.54	119.03
6	C	1480	DXC	C8-C9-C10	2.17	113.11	110.47
6	C	1476	DXC	C5-C6-C1	2.16	113.95	110.37
6	C	1477	DXC	C12-C11-C9	2.14	117.08	114.68
6	C	1475	DXC	C12-C17-C19	-2.12	116.96	119.51
6	C	1477	DXC	C20-C12-C13	-2.11	106.98	109.08
6	C	1478	DXC	C2-C1-C6	-2.10	107.85	110.54
6	C	1475	DXC	C12-C11-C9	2.07	117.00	114.68
6	C	1478	DXC	C2-C3-C7	-2.07	107.63	111.70
6	B	1473	DXC	C14-C10-C9	2.05	114.10	110.84
6	C	1478	DXC	C21-C19-C17	2.05	114.85	110.25
6	B	1473	DXC	C2-C3-C4	2.04	114.88	112.67
7	B	1474	5GP	C8-N9-C4	2.04	108.46	106.90
6	C	1478	DXC	C18-C4-C3	-2.03	106.74	110.26
6	C	1478	DXC	C8-C7-C3	-2.02	107.62	111.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	452/482 (93%)	0.49	37 (8%)	12 3	107, 205, 299, 372	3 (0%)
1	B	456/482 (94%)	0.40	36 (7%)	13 4	80, 153, 347, 414	2 (0%)
1	C	471/482 (97%)	0.06	5 (1%)	77 32	74, 123, 227, 308	0
1	D	467/482 (96%)	1.20	115 (24%)	1 1	140, 274, 369, 416	3 (0%)
All	All	1846/1928 (95%)	0.54	193 (10%)	7 2	74, 188, 338, 416	8 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	442	LYS	9.1
1	D	401	LYS	7.5
1	D	250	MET	7.4
1	D	441	THR	7.4
1	B	418	LYS	7.0
1	D	390	GLU	6.8
1	B	404	THR	6.6
1	D	453	VAL	6.4
1	D	333	ILE	5.6
1	B	461	LEU	5.4
1	D	406	ILE	5.2
1	D	392	LEU	5.0
1	D	242	ALA	5.0
1	B	460	ILE	4.7
1	B	432	VAL	4.7
1	D	438	THR	4.7
1	D	413	LYS	4.6
1	D	467	TRP	4.5
1	A	81	ASP	4.5
1	D	79	ALA	4.4
1	D	304	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	405	VAL	4.3
1	A	434	LYS	4.2
1	D	16	HIS	4.2
1	D	251	ALA	4.2
1	D	382	ILE	4.2
1	D	78	SER	4.1
1	D	69	HIS	4.1
1	D	399	ILE	4.0
1	D	322	LYS	4.0
1	D	426	ILE	4.0
1	D	429	LYS	4.0
1	D	311	VAL	4.0
1	A	404	THR	3.9
1	D	320	PHE	3.9
1	D	412	SER	3.9
1	D	414	VAL	3.9
1	A	405	VAL	3.8
1	A	449	PHE	3.8
1	B	441	THR	3.8
1	A	406	ILE	3.8
1	B	396	LYS	3.8
1	D	402	GLY	3.7
1	D	256	ASP	3.7
1	D	416	ALA	3.7
1	D	417	GLU	3.7
1	D	66	ALA	3.7
1	D	405	VAL	3.6
1	D	65	ASP	3.6
1	D	329	LEU	3.6
1	B	424	ILE	3.6
1	D	415	ALA	3.5
1	D	456	ARG	3.5
1	D	259	GLN	3.5
1	B	429	LYS	3.5
1	B	445	LEU	3.4
1	D	312	ALA	3.4
1	A	448	GLU	3.4
1	B	433	GLY	3.4
1	B	439	PHE	3.4
1	B	417	GLU	3.4
1	D	391	VAL	3.3
1	A	257	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	411	GLN	3.3
1	B	392	LEU	3.3
1	D	330	ASN	3.3
1	D	431	ILE	3.2
1	D	445	LEU	3.2
1	D	31	THR	3.2
1	D	428	GLY	3.2
1	D	316	LYS	3.1
1	D	17	GLY	3.1
1	D	258	LYS	3.1
1	D	345	GLU	3.1
1	B	438	THR	3.1
1	D	343	GLU	3.0
1	D	173	LEU	3.0
1	A	441	THR	3.0
1	A	47	ILE	3.0
1	B	330	ASN	3.0
1	D	295	PRO	3.0
1	D	403	ARG	2.9
1	D	332	VAL	2.9
1	A	398	LYS	2.9
1	B	449	PHE	2.8
1	D	444	LEU	2.8
1	D	318	VAL	2.8
1	C	34	HIS	2.8
1	B	440	GLY	2.8
1	B	398	LYS	2.8
1	D	179	ILE	2.8
1	D	38	PRO	2.8
1	C	35	ASP	2.8
1	D	400	ASP	2.8
1	B	428	GLY	2.8
1	A	429	LYS	2.8
1	D	440	GLY	2.8
1	A	225	MET	2.8
1	B	413	LYS	2.7
1	D	331	GLU	2.7
1	D	454	GLU	2.7
1	A	426	ILE	2.7
1	D	407	ASP	2.7
1	D	241	GLU	2.7
1	D	328	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	439	PHE	2.7
1	A	197	LYS	2.7
1	D	36	LYS	2.7
1	D	455	ASN	2.6
1	A	465	ARG	2.6
1	B	450	SER	2.6
1	D	425	SER	2.6
1	D	458	LYS	2.6
1	A	196	ILE	2.6
1	B	447	ALA	2.6
1	C	32	SER	2.6
1	A	433	GLY	2.6
1	A	435	ILE	2.6
1	B	415	ALA	2.6
1	D	255	VAL	2.6
1	D	48	ASP	2.6
1	D	15	ASP	2.6
1	D	321	GLY	2.6
1	A	389	LYS	2.6
1	B	409	LEU	2.5
1	A	218	LEU	2.5
1	A	304	GLY	2.5
1	D	389	LYS	2.5
1	D	225	MET	2.5
1	D	397	VAL	2.5
1	D	221	LEU	2.5
1	A	422	GLU	2.5
1	A	397	VAL	2.5
1	B	403	ARG	2.5
1	B	427	GLU	2.5
1	D	464	LEU	2.5
1	D	452	ASN	2.5
1	D	388	LYS	2.5
1	B	371	CMH	2.5
1	D	289	PHE	2.4
1	A	424	ILE	2.4
1	D	120	LYS	2.4
1	D	195	PRO	2.4
1	A	371	CMH	2.4
1	B	454	GLU	2.4
1	A	396	LYS	2.4
1	A	256	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLN	2.4
1	D	223	ILE	2.4
1	D	21	LEU	2.4
1	A	284	LYS	2.4
1	A	445	LEU	2.3
1	D	219	LYS	2.3
1	D	39	GLU	2.3
1	A	380	LYS	2.3
1	B	416	ALA	2.3
1	B	397	VAL	2.3
1	D	47	ILE	2.3
1	A	282	LYS	2.3
1	D	172	THR	2.3
1	D	249	GLY	2.3
1	D	81	ASP	2.3
1	D	393	ARG	2.3
1	B	322	LYS	2.3
1	D	154	ILE	2.3
1	B	394	GLU	2.3
1	D	305	MET	2.3
1	D	409	LEU	2.2
1	D	220	VAL	2.2
1	D	169	ILE	2.2
1	D	398	LYS	2.2
1	D	462	ASN	2.2
1	A	258	LYS	2.2
1	D	290	LYS	2.2
1	D	4	LYS	2.2
1	C	36	LYS	2.2
1	B	414	VAL	2.2
1	D	325	GLU	2.1
1	D	380	LYS	2.1
1	C	-2	ARG	2.1
1	D	212	VAL	2.1
1	D	394	GLU	2.1
1	D	28	ILE	2.1
1	D	314	PRO	2.1
1	D	424	ILE	2.1
1	D	13	HIS	2.1
1	D	243	LYS	2.1
1	A	413	LYS	2.1
1	D	59	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	220	VAL	2.1
1	D	292	ASN	2.0
1	A	439	PHE	2.0
1	B	393	ARG	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CMH	B	371	8/9	0.34	0.73	174,197,251,332	2
1	CMH	A	371	8/9	0.34	0.56	168,213,225,228	2
1	CMH	C	371	8/9	0.23	0.48	78,109,123,156	2
1	CMH	B	340	8/9	0.28	0.30	160,194,264,332	0
1	CMH	B	338	8/9	0.31	-0.11	151,200,232,276	2
1	CMH	C	340	8/9	0.23	-0.62	69,99,124,131	2
1	CMH	B	264	8/9	0.16	-0.77	73,89,99,112	2
1	CMH	A	264	8/9	0.16	-0.93	171,215,224,235	2
1	CMH	D	340	8/9	0.20	-1.06	207,306,312,317	2
1	CMH	D	371	8/9	0.19	-1.07	145,181,227,234	2
1	CMH	D	264	8/9	0.21	-1.08	241,255,280,281	2
1	CMH	C	338	8/9	0.18	-1.11	74,109,174,331	2
1	CMH	D	338	8/9	0.10	-1.21	180,242,266,268	2
1	CMH	A	340	8/9	0.18	-1.43	169,213,226,240	2
1	CMH	C	264	8/9	0.16	-1.48	70,108,137,210	0
1	CMH	A	338	8/9	0.14	-1.94	174,190,268,307	2

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	C	1481	5/5	1.73	228.23	172,210,221,235	5
3	MG	B	1470	1/1	0.24	15.20	342,342,342,342	0
5	SO4	B	1472	5/5	0.99	9.04	139,226,336,344	0
7	5GP	B	1474	24/24	0.39	1.57	242,294,308,311	0
6	DXC	C	1477	28/28	0.31	1.33	91,111,162,182	0
6	DXC	C	1479	28/28	0.28	1.07	82,104,174,196	28
6	DXC	C	1478	28/28	0.22	0.48	93,118,158,196	0
6	DXC	C	1476	28/28	0.33	0.34	159,168,217,253	0
6	DXC	B	1473	28/28	0.27	0.24	68,97,134,143	0
4	GDP	B	1469	28/28	0.21	0.14	126,197,212,235	0
6	DXC	C	1475	28/28	0.27	0.14	61,95,139,146	0
5	SO4	C	1471	5/5	0.18	-0.16	101,149,159,220	0
5	SO4	C	1472	5/5	0.16	-0.19	133,154,189,210	0
5	SO4	B	1471	5/5	0.20	-0.60	205,213,271,283	0
6	DXC	C	1480	28/28	0.22	-0.78	63,85,106,127	0
2	GNP	A	1469	32/32	0.10	-1.11	120,165,202,249	0
3	MG	A	1470	1/1	0.08	-1.23	244,244,244,244	0
5	SO4	C	1473	5/5	0.14	-5.42	164,166,220,230	5

6.5 Other polymers ⓘ

There are no such residues in this entry.