



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:20 AM GMT

PDB ID : 4MDT
Title : Structure of LpxC bound to the reaction product UDP-(3-O-(R-3-hydroxymyristoyl))-glucosamine
Authors : Clayton, G.M.; Klein, D.J.; Rickert, K.W.; Patel, S.B.; Kornienko, M.; Zugay-Murphy, J.; Reid, J.C.; Tummala, S.; Sharma, S.; Singh, S.B.; Miesel, L.; Lumb, K.J.; Soisson, S.M.
Deposited on : 2013-08-23
Resolution : 2.59 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>

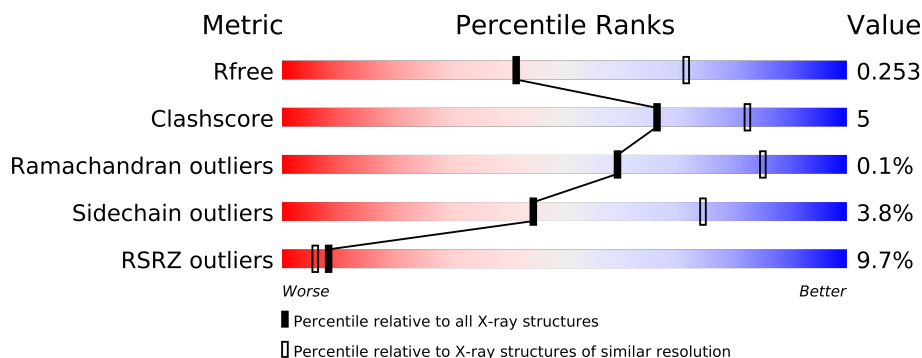
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.59 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	305	
1	B	305	
1	C	305	
1	D	305	

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	24G	A	402	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9746 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 UDP-3-O-[3-hydroxymyristoyl]N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2356	1497	408	438	13			
1	B	300	Total	C	N	O	S	0	0	0
			2356	1497	408	438	13			
1	C	299	Total	C	N	O	S	0	0	0
			2350	1494	407	436	13			
1	D	293	Total	C	N	O	S	0	0	0
			2299	1457	399	431	12			

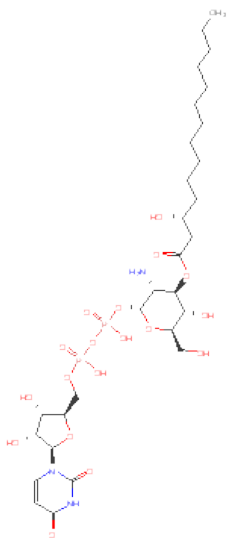
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	CYS	ENGINEERED MUTATION	UNP K0BGQ2
B	125	SER	CYS	ENGINEERED MUTATION	UNP K0BGQ2
C	125	SER	CYS	ENGINEERED MUTATION	UNP K0BGQ2
D	125	SER	CYS	ENGINEERED MUTATION	UNP K0BGQ2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

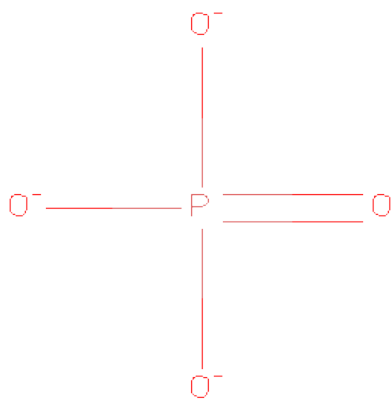
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-3-O-(R-3-HYDROXYMYRISTOYL)-GLUCOSAMINE (three-letter code: 24G) (formula: C₂₉H₅₁N₃O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			52	29	3	18	2		
3	B	1	Total	C	N	O	P	0	0
			52	29	3	18	2		
3	C	1	Total	C	N	O	P	0	0
			52	29	3	18	2		
3	D	1	Total	C	N	O	P	0	0
			52	29	3	18	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO₄) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

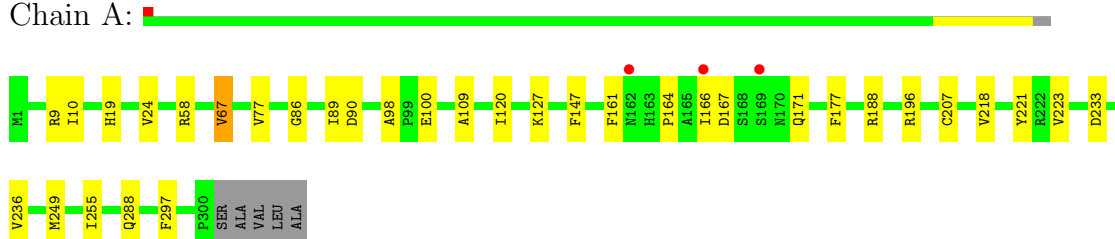
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	61	Total O 61 61	0	0
5	B	55	Total O 55 55	0	0
5	C	17	Total O 17 17	0	0
5	D	20	Total O 20 20	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

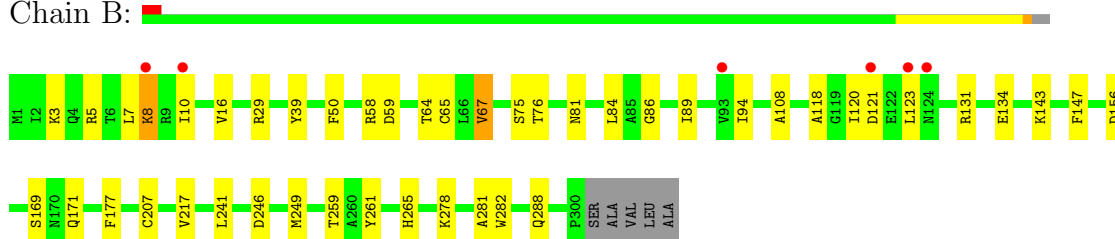
- Molecule 1: UDP-3-O-[3-hydroxymyristoyl]N-acetylglucosamine deacetylase

Chain A:



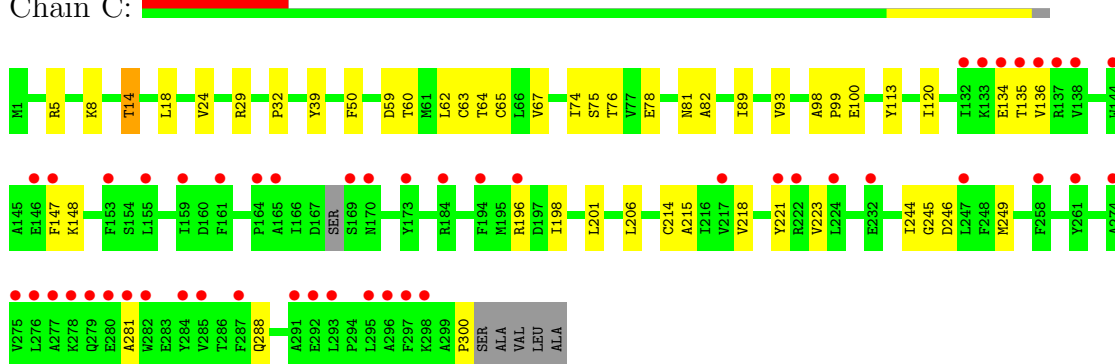
- Molecule 1: UDP-3-O-[3-hydroxymyristoyl]N-acetylglucosamine deacetylase

Chain B:



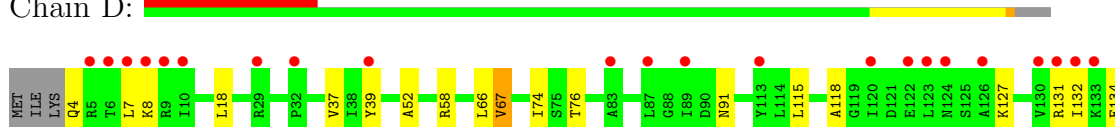
- Molecule 1: UDP-3-O-[3-hydroxymyristoyl]N-acetylglucosamine deacetylase

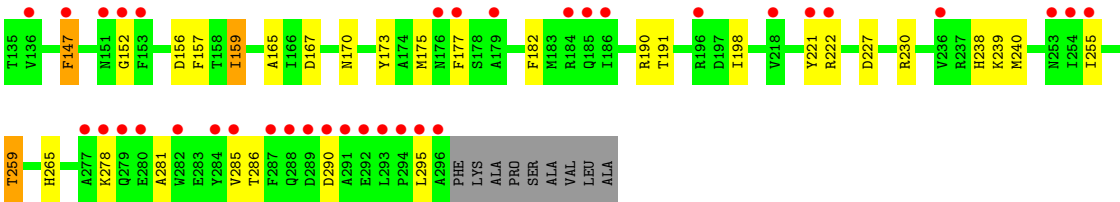
Chain C:



- Molecule 1: UDP-3-O-[3-hydroxymyristoyl]N-acetylglucosamine deacetylase

Chain D:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.97Å 103.52Å 103.97Å 90.00° 103.96° 90.00°	Depositor
Resolution (Å)	50.45 – 2.59 50.45 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.45-2.59) 95.9 (50.45-2.59)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.197 , 0.240 0.206 , 0.253	Depositor DCC
R_{free} test set	2646 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 51830 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9746	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% 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: ZN, PO4, 24G

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	0.53	0/2404	0.79	0/3255
1	B	0.52	0/2404	0.79	0/3255
1	C	0.48	0/2397	0.75	0/3244
1	D	0.48	0/2345	0.76	0/3177
All	All	0.50	0/9550	0.77	0/12931

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	2356	0	2337	20	0
1	B	2356	0	2337	23	0
1	C	2350	0	2331	28	0
1	D	2299	0	2267	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	52	0	49	0	0
3	B	52	0	49	1	0
3	C	52	0	49	3	0
3	D	52	0	49	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	2	0
5	A	61	0	0	0	0
5	B	55	0	0	0	0
5	C	17	0	0	0	0
5	D	20	0	0	0	0
All	All	9746	0	9468	97	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 5.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:39:TYR:HB2	1:B:50:PHE:HB2	1.69	0.75
1:D:134:GLU:HB2	1:D:281:ALA:HA	1.73	0.71
1:C:81:ASN:HD21	1:C:249:MET:CE	2.05	0.69
1:D:4:GLN:HB3	1:D:91:ASN:HD21	1.58	0.69
1:B:64:THR:HG21	1:B:246:ASP:OD1	1.94	0.68
1:A:89:ILE:HD11	1:A:120:ILE:HD12	1.74	0.67
1:B:8:LYS:HG2	1:B:121:ASP:HB2	1.77	0.65
1:A:77:VAL:HG21	1:A:249:MET:HE3	1.77	0.65
1:B:81:ASN:HD21	1:B:249:MET:HE2	1.66	0.61
1:B:58:ARG:HB2	1:B:67:VAL:HG13	1.82	0.61
1:A:24:VAL:HG11	1:A:100:GLU:O	2.01	0.60
1:C:134:GLU:HB2	1:C:281:ALA:HA	1.84	0.60
1:C:81:ASN:HD21	1:C:249:MET:HE3	1.66	0.59
1:A:166:ILE:HG22	1:A:171:GLN:HE21	1.68	0.58
1:B:84:LEU:HD11	1:B:94:ILE:HD11	1.85	0.58
1:C:64:THR:OG1	1:C:246:ASP:OD1	2.18	0.58
1:C:135:THR:HG23	1:C:148:LYS:HG2	1.85	0.57
1:A:58:ARG:HB2	1:A:67:VAL:HG13	1.87	0.57
1:D:191:THR:HA	1:D:238:HIS:CD2	2.39	0.57
1:B:39:TYR:OH	1:B:81:ASN:OD1	2.23	0.57
1:A:10:ILE:CD1	1:D:167:ASP:HB2	2.36	0.56
1:C:39:TYR:HB2	1:C:50:PHE:HB2	1.89	0.55
1:D:156:ASP:O	1:D:259:THR:HA	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:5:ARG:HH22	1:C:300:PRO:HD3	1.71	0.54
1:B:134:GLU:HB2	1:B:281:ALA:HA	1.89	0.54
1:C:81:ASN:HD21	1:C:249:MET:HE2	1.71	0.53
1:C:29:ARG:HB2	1:C:93:VAL:HB	1.90	0.53
1:C:59:ASP:HB3	1:C:65:CYS:HB3	1.91	0.53
1:D:265:HIS:NE2	4:D:403:PO4:O3	2.35	0.53
1:B:64:THR:HG22	1:B:265:HIS:HB3	1.91	0.53
1:A:10:ILE:HD12	1:D:167:ASP:HB2	1.91	0.53
1:A:218:VAL:HG12	1:A:223:VAL:HA	1.91	0.52
1:D:58:ARG:HB2	1:D:67:VAL:HG13	1.92	0.52
1:C:82:ALA:HA	1:C:244:ILE:HG22	1.91	0.51
1:C:24:VAL:HG11	1:C:100:GLU:O	2.10	0.51
1:B:81:ASN:HD21	1:B:249:MET:CE	2.22	0.51
1:A:164:PRO:HG2	1:A:221:TYR:HA	1.93	0.50
1:C:24:VAL:HG13	1:C:98:ALA:HB3	1.94	0.50
1:D:66:LEU:HB2	1:D:74:ILE:HG23	1.94	0.50
1:C:201:LEU:HB3	1:C:206:LEU:HB2	1.93	0.49
1:B:169:SER:O	1:B:171:GLN:NE2	2.41	0.49
3:D:402:24G:N11	4:D:403:PO4:O4	2.46	0.49
1:D:131:ARG:HD3	1:D:285:VAL:HG11	1.95	0.48
1:C:218:VAL:HG12	1:C:223:VAL:HA	1.94	0.48
1:B:86:GLY:HA2	1:B:177:PHE:HZ	1.78	0.48
1:B:108:ALA:HB2	1:B:241:LEU:HD21	1.96	0.48
1:D:7:LEU:HD21	1:D:115:LEU:HD23	1.96	0.48
1:D:157:PHE:CE2	1:D:159:ILE:HG23	2.49	0.47
1:D:165:ALA:HB2	1:D:222:ARG:HA	1.97	0.47
1:C:198:ILE:HG21	3:C:402:24G:H27	1.97	0.47
1:D:198:ILE:HG21	3:D:402:24G:H27	1.96	0.46
1:B:7:LEU:HD22	1:B:118:ALA:HB3	1.97	0.46
1:A:19:HIS:CE1	1:A:207:CYS:HG	2.33	0.46
1:A:161:PHE:H	1:A:171:GLN:HE22	1.62	0.46
1:B:3:LYS:HB3	1:B:123:LEU:O	2.16	0.46
1:B:89:ILE:HD11	1:B:120:ILE:HD12	1.98	0.46
1:A:109:ALA:HB2	1:A:188:ARG:HG2	1.97	0.46
1:C:62:LEU:HD11	1:C:206:LEU:HD13	1.98	0.45
1:A:86:GLY:HA2	1:A:177:PHE:HZ	1.81	0.45
1:B:278:LYS:HD3	1:B:281:ALA:HB2	1.98	0.45
1:D:152:GLY:H	1:D:255:ILE:HG23	1.81	0.45
1:D:4:GLN:HG3	1:D:127:LYS:HA	1.97	0.44
1:B:59:ASP:HB3	1:B:65:CYS:HB3	1.99	0.44
1:A:24:VAL:HG13	1:A:98:ALA:HB3	1.99	0.44
1:D:18:LEU:HD21	3:D:402:24G:H40	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:78:GLU:O	1:C:245:GLY:HA3	2.18	0.44
1:C:89:ILE:HD11	1:C:120:ILE:HD12	1.99	0.44
1:D:157:PHE:HE2	1:D:159:ILE:HG23	1.83	0.44
1:C:39:TYR:OH	1:C:81:ASN:OD1	2.31	0.43
1:A:24:VAL:HG22	1:A:98:ALA:HB3	1.99	0.43
1:C:18:LEU:HD11	3:C:402:24G:H36	1.99	0.43
1:D:177:PHE:CE1	1:D:182:PHE:HB2	2.53	0.43
1:C:81:ASN:ND2	1:C:249:MET:HE3	2.34	0.42
1:D:132:ILE:HG13	1:D:147:PHE:CD1	2.54	0.42
1:A:77:VAL:CG2	1:A:249:MET:HE3	2.48	0.42
1:B:10:ILE:HG12	1:B:29:ARG:HG2	2.00	0.42
1:A:233:ASP:HB2	1:A:236:VAL:HG12	2.01	0.42
1:B:156:ASP:O	1:B:259:THR:HA	2.19	0.42
1:D:278:LYS:HD3	1:D:281:ALA:HB2	2.00	0.42
1:B:131:ARG:O	1:B:282:TRP:HA	2.20	0.42
1:D:37:VAL:HB	1:D:52:ALA:HB2	2.02	0.42
1:D:39:TYR:HB3	1:D:74:ILE:HD13	2.02	0.42
1:D:173:TYR:O	1:D:240:MET:HE1	2.19	0.42
1:D:159:ILE:HG21	1:D:239:LYS:HG3	2.02	0.41
1:C:14:THR:HG23	1:D:227:ASP:OD1	2.20	0.41
1:B:217:VAL:HG21	3:B:402:24G:H30	2.01	0.41
1:C:74:ILE:HA	1:C:99:PRO:O	2.21	0.41
1:C:215:ALA:HB3	3:C:402:24G:H33	2.03	0.41
1:C:39:TYR:HB3	1:C:74:ILE:HD13	2.03	0.41
1:A:90:ASP:OD1	1:A:127:LYS:HG3	2.19	0.41
1:B:261:TYR:CG	1:C:32:PRO:HG3	2.55	0.41
1:D:190:ARG:HE	1:D:230:ARG:HG3	1.85	0.41
1:A:24:VAL:HG22	1:A:98:ALA:CB	2.50	0.41
1:A:255:ILE:HG12	1:A:297:PHE:CE2	2.56	0.41
1:C:63:CYS:SG	1:C:75:SER:HB2	2.61	0.41
1:D:173:TYR:HB3	1:D:240:MET:HE3	2.02	0.40
1:D:8:LYS:HB2	1:D:118:ALA:O	2.21	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	298/305 (98%)	286 (96%)	12 (4%)	0	100	100
1	B	298/305 (98%)	282 (95%)	16 (5%)	0	100	100
1	C	295/305 (97%)	271 (92%)	24 (8%)	0	100	100
1	D	291/305 (95%)	273 (94%)	17 (6%)	1 (0%)	50	77
All	All	1182/1220 (97%)	1112 (94%)	69 (6%)	1 (0%)	59	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	LEU

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	251/254 (99%)	245 (98%)	6 (2%)	61	87
1	B	251/254 (99%)	241 (96%)	10 (4%)	42	73
1	C	250/254 (98%)	238 (95%)	12 (5%)	35	64
1	D	245/254 (96%)	235 (96%)	10 (4%)	41	72
All	All	997/1016 (98%)	959 (96%)	38 (4%)	44	74

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	67	VAL
1	A	147	PHE
1	A	167	ASP
1	A	196	ARG
1	A	288	GLN
1	B	5	ARG
1	B	8	LYS

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Mol	Chain	Res	Type
1	B	16	VAL
1	B	67	VAL
1	B	75	SER
1	B	76	THR
1	B	143	LYS
1	B	147	PHE
1	B	207	CYS
1	B	288	GLN
1	C	8	LYS
1	C	14	THR
1	C	60	THR
1	C	67	VAL
1	C	76	THR
1	C	113	TYR
1	C	136	VAL
1	C	147	PHE
1	C	196	ARG
1	C	214	CYS
1	C	221	TYR
1	C	288	GLN
1	D	67	VAL
1	D	76	THR
1	D	147	PHE
1	D	159	ILE
1	D	170	ASN
1	D	175	MET
1	D	221	TYR
1	D	259	THR
1	D	286	THR
1	D	290	ASP

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

Mol	Chain	Res	Type
1	A	81	ASN
1	A	171	GLN
1	A	176	ASN
1	B	12	GLN
1	B	176	ASN
1	B	185	GLN
1	C	81	ASN
1	C	176	ASN

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Mol	Chain	Res	Type
1	D	91	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
3	24G	A	402	-	54,54,54	1.06	5 (9%)	72,76,76	1.41	10 (13%)
4	PO4	A	403	2	4,4,4	0.84	0	6,6,6	0.34	0
3	24G	B	402	-	54,54,54	0.93	3 (5%)	72,76,76	1.11	5 (6%)
4	PO4	B	403	2	4,4,4	1.22	0	6,6,6	0.31	0
3	24G	C	402	-	54,54,54	1.03	3 (5%)	72,76,76	1.20	6 (8%)
4	PO4	C	403	2	4,4,4	1.31	0	6,6,6	0.36	0
3	24G	D	402	-	54,54,54	1.07	3 (5%)	72,76,76	1.08	3 (4%)
4	PO4	D	403	2	4,4,4	1.80	1 (25%)	6,6,6	0.31	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
3	24G	A	402	-	-	0/40/78/78	0/3/3/3
4	PO4	A	403	2	-	0/0/0/0	0/0/0/0
3	24G	B	402	-	-	0/40/78/78	0/3/3/3
4	PO4	B	403	2	-	0/0/0/0	0/0/0/0
3	24G	C	402	-	-	0/40/78/78	0/3/3/3
4	PO4	C	403	2	-	0/0/0/0	0/0/0/0
3	24G	D	402	-	-	0/40/78/78	0/3/3/3
4	PO4	D	403	2	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	24G	P16-O17	3.39	1.64	1.51
3	D	402	24G	C36-C35	3.33	1.49	1.40
3	D	402	24G	P20-O22	3.32	1.64	1.51
3	A	402	24G	P20-O22	3.30	1.64	1.51
3	C	402	24G	P20-O22	3.28	1.63	1.51
3	C	402	24G	P16-O17	3.23	1.63	1.51
3	A	402	24G	P16-O17	3.23	1.63	1.51
3	A	402	24G	C36-C35	3.02	1.48	1.40
3	B	402	24G	P16-O17	3.01	1.62	1.51
3	B	402	24G	P20-O22	3.01	1.62	1.51
3	C	402	24G	C36-C35	2.99	1.48	1.40
3	B	402	24G	C36-C35	2.91	1.48	1.40
4	D	403	PO4	P-O1	2.86	1.67	1.52
3	A	402	24G	O29-C28	2.01	1.44	1.41
3	A	402	24G	C33-N32	2.01	1.40	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	24G	C33-N32-C28	4.08	120.77	118.21
3	A	402	24G	O5-C4-O12	3.70	116.20	111.36
3	C	402	24G	C36-C37-N32	3.66	125.35	121.21
3	A	402	24G	C36-C37-N32	3.61	125.30	121.21
3	D	402	24G	O29-C28-N32	3.07	114.55	108.06
3	C	402	24G	C33-N32-C28	3.03	120.11	118.21
3	A	402	24G	O12-C4-C3	2.95	112.61	107.91
3	C	402	24G	O5-C4-O12	2.89	115.15	111.36
3	A	402	24G	C2-O10-C13	-2.84	113.37	117.92
3	C	402	24G	C26-C27-C28	2.81	105.30	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	24G	C36-C37-N32	2.79	124.37	121.21
3	A	402	24G	C26-C27-C28	2.73	105.18	100.91
3	A	402	24G	O18-P16-O12	2.62	116.72	105.71
3	D	402	24G	O5-C4-O12	2.58	114.74	111.36
3	D	402	24G	C36-C37-N32	2.57	124.12	121.21
3	B	402	24G	N34-C33-N32	-2.49	113.90	115.97
3	A	402	24G	O10-C2-C1	2.38	113.47	107.81
3	B	402	24G	O18-P16-O19	2.35	116.27	105.14
3	B	402	24G	O21-P20-O19	2.34	116.23	105.14
3	A	402	24G	C1-C2-C3	2.27	114.87	110.97
3	B	402	24G	C2-C3-N11	-2.23	106.30	110.79
3	C	402	24G	C2-O10-C13	-2.19	114.41	117.92
3	C	402	24G	O18-P16-O12	2.14	114.71	105.71
3	A	402	24G	O21-P20-O23	2.12	119.19	108.51

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	300/305 (98%)	0.21	3 (1%) 79 81	32, 46, 69, 90	0
1	B	300/305 (98%)	0.27	6 (2%) 62 60	32, 51, 75, 95	0
1	C	299/305 (98%)	0.97	49 (16%) 2 1	42, 72, 111, 148	0
1	D	293/305 (96%)	1.20	58 (19%) 2 1	44, 74, 117, 156	0
All	All	1192/1220 (97%)	0.66	116 (9%) 8 6	32, 59, 105, 156	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	293	LEU	13.0
1	D	296	ALA	7.4
1	D	152	GLY	6.9
1	D	291	ALA	6.3
1	D	123	LEU	6.3
1	C	287	PHE	6.2
1	C	281	ALA	6.2
1	D	287	PHE	5.8
1	C	280	GLU	5.8
1	C	221	TYR	5.7
1	D	289	ASP	5.7
1	C	278	LYS	5.5
1	C	144	TRP	5.5
1	D	177	PHE	5.4
1	C	296	ALA	5.3
1	C	169	SER	5.1
1	C	222	ARG	5.1
1	D	285	VAL	5.1
1	D	288	GLN	5.0
1	D	87	LEU	4.9
1	D	196	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	134	GLU	4.8
1	D	151	ASN	4.6
1	D	278	LYS	4.6
1	C	297	PHE	4.5
1	D	10	ILE	4.4
1	D	290	ASP	4.3
1	B	124	ASN	4.3
1	C	292	GLU	4.2
1	D	294	PRO	4.2
1	D	292	GLU	4.2
1	C	276	LEU	4.1
1	D	254	ILE	4.1
1	C	170	ASN	4.0
1	C	133	LYS	4.0
1	C	285	VAL	4.0
1	D	130	VAL	4.0
1	C	298	LYS	3.9
1	C	136	VAL	3.8
1	D	295	LEU	3.7
1	D	120	ILE	3.7
1	C	135	THR	3.7
1	D	124	ASN	3.6
1	C	277	ALA	3.6
1	C	279	GLN	3.6
1	C	159	ILE	3.6
1	D	221	TYR	3.5
1	C	161	PHE	3.4
1	D	131	ARG	3.4
1	C	282	TRP	3.4
1	C	295	LEU	3.4
1	D	6	THR	3.4
1	D	132	ILE	3.4
1	D	284	TYR	3.3
1	A	169	SER	3.3
1	C	138	VAL	3.3
1	D	185	GLN	3.3
1	C	261	TYR	3.2
1	D	176	ASN	3.2
1	D	9	ARG	3.2
1	C	137	ARG	3.1
1	D	279	GLN	3.1
1	A	166	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	184	ARG	3.0
1	D	153	PHE	3.0
1	D	280	GLU	2.9
1	D	136	VAL	2.9
1	C	232	GLU	2.9
1	C	173	TYR	2.9
1	C	196	ARG	2.8
1	C	224	LEU	2.8
1	C	293	LEU	2.8
1	D	29	ARG	2.8
1	C	164	PRO	2.8
1	C	291	ALA	2.8
1	B	121	ASP	2.7
1	C	165	ALA	2.7
1	D	113	TYR	2.7
1	D	8	LYS	2.7
1	D	218	VAL	2.7
1	D	222	ARG	2.7
1	C	132	ILE	2.7
1	D	147	PHE	2.7
1	C	153	PHE	2.7
1	B	10	ILE	2.6
1	D	179	ALA	2.6
1	C	194	PHE	2.6
1	D	32	PRO	2.6
1	D	5	ARG	2.6
1	D	277	ALA	2.5
1	D	184	ARG	2.5
1	D	126	ALA	2.5
1	D	122	GLU	2.5
1	C	284	TYR	2.5
1	A	162	ASN	2.5
1	C	217	VAL	2.5
1	D	133	LYS	2.4
1	D	89	ILE	2.4
1	C	147	PHE	2.4
1	B	8	LYS	2.4
1	C	275	VAL	2.4
1	D	83	ALA	2.3
1	C	155	LEU	2.3
1	D	7	LEU	2.3
1	D	255	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	123	LEU	2.2
1	D	282	TRP	2.2
1	B	93	VAL	2.2
1	D	39	TYR	2.2
1	C	258	PHE	2.1
1	C	274	ALA	2.1
1	C	247	LEU	2.1
1	D	186	ILE	2.1
1	D	236	VAL	2.0
1	D	253	ASN	2.0
1	C	146	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
3	24G	A	402	52/52	0.26	2.45	59,70,88,89	0
3	24G	C	402	52/52	0.31	1.56	97,105,132,132	0
3	24G	D	402	52/52	0.20	0.76	55,83,90,92	0
2	ZN	A	401	1/1	0.16	0.31	39,39,39,39	0
4	PO4	D	403	5/5	0.16	0.25	42,48,52,57	0
3	24G	B	402	52/52	0.16	0.04	38,48,60,63	0
4	PO4	B	403	5/5	0.17	0.03	43,46,50,50	0
4	PO4	A	403	5/5	0.16	-0.13	43,47,50,53	0
2	ZN	C	401	1/1	0.16	-0.51	63,63,63,63	0
2	ZN	D	401	1/1	0.13	-0.58	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	401	1/1	0.15	-1.08	40,40,40,40	0
4	PO4	C	403	5/5	0.15	-1.27	62,67,68,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.