



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 04:31 PM EST

PDB ID : 4FW6  
Title : Crystal Structure of the LpxC in complex with N-[(2S,3R)-3-HYDROXY-1-(HYDROXYAMINO)-1-OXOBUTAN-2-YL]-4-(PHENYLETHYNYL)BENZAMIDE inhibitor  
Authors : Kang, Y.N.; Stuckey, J.A.  
Deposited on : unknown  
Resolution : 1.83 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

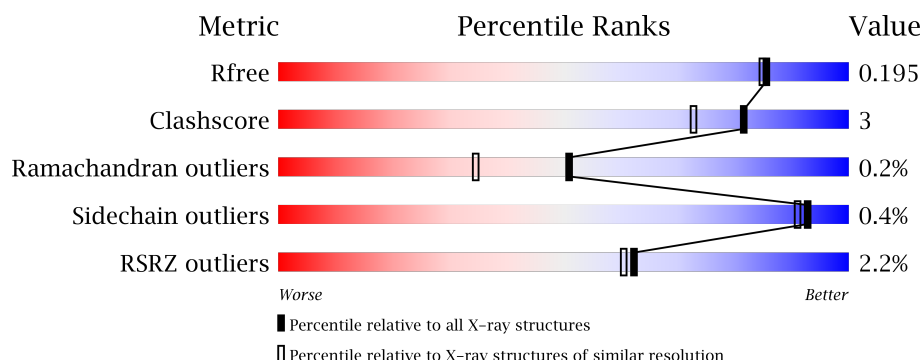
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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))
$R_{free}$	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>1%</span> <span>92%</span> <span>7%</span> </div> </div>
1	B	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 1%, green 99%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>0%</span> <span>93%</span> <span>7%</span> </div> </div>
1	C	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>4%</span> <span>92%</span> <span>7%</span> </div> </div>
1	D	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>3%</span> <span>94%</span> <span>5%</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	304	-	-	-	X
4	GOL	B	303	-	-	-	X
4	GOL	B	304	-	-	-	X
4	GOL	C	303	-	-	X	-
4	GOL	C	304	-	-	-	X
4	GOL	C	305	-	-	-	X
4	GOL	D	304	-	-	-	X
5	ACT	A	305	-	-	-	X
5	ACT	A	306	-	-	-	X
5	ACT	A	307	-	-	-	X
5	ACT	B	306	-	-	-	X
5	ACT	C	307	-	-	-	X
5	ACT	D	305	-	-	-	X
5	ACT	D	306	-	-	-	X
6	PEG	A	308	-	-	-	X
6	PEG	A	309	-	-	-	X
6	PEG	B	308	-	-	-	X
6	PEG	B	309	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10511 atoms, of which 117 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 UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	15	0
			2387	1529	400	449	9			
1	B	300	Total	C	N	O	S	0	17	0
			2404	1539	401	455	9			
1	C	302	Total	C	N	O	S	0	10	0
			2345	1497	392	450	6			
1	D	302	Total	C	N	O	S	0	8	0
			2354	1496	400	452	6			

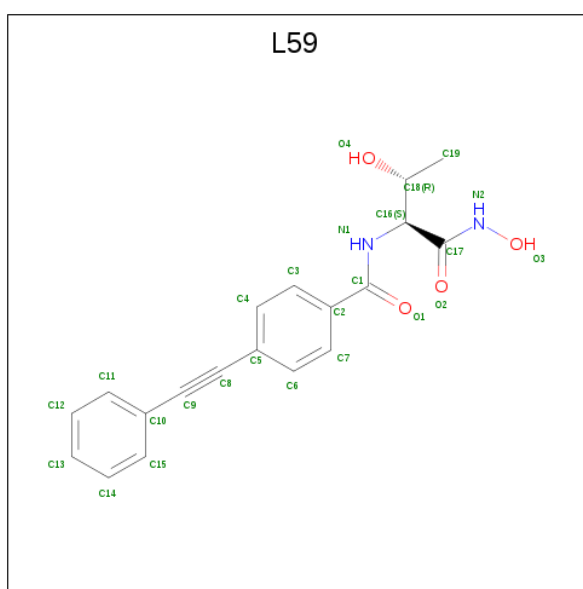
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P47205
A	-1	ASN	-	EXPRESSION TAG	UNP P47205
A	0	ALA	-	EXPRESSION TAG	UNP P47205
A	40	SER	CYS	ENGINEERED MUTATION	UNP P47205
B	-2	SER	-	EXPRESSION TAG	UNP P47205
B	-1	ASN	-	EXPRESSION TAG	UNP P47205
B	0	ALA	-	EXPRESSION TAG	UNP P47205
B	40	SER	CYS	ENGINEERED MUTATION	UNP P47205
C	-2	SER	-	EXPRESSION TAG	UNP P47205
C	-1	ASN	-	EXPRESSION TAG	UNP P47205
C	0	ALA	-	EXPRESSION TAG	UNP P47205
C	40	SER	CYS	ENGINEERED MUTATION	UNP P47205
D	-2	SER	-	EXPRESSION TAG	UNP P47205
D	-1	ASN	-	EXPRESSION TAG	UNP P47205
D	0	ALA	-	EXPRESSION TAG	UNP P47205
D	40	SER	CYS	ENGINEERED MUTATION	UNP P47205

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

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

- Molecule 3 is N-[(2S,3R)-3-hydroxy-1-(hydroxyamino)-1-oxobutan-2-yl]-4-(phenylethynyl)benzamide (three-letter code: L59) (formula: C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 43 19 18 2 4	18	0
3	B	1	Total C H N O 43 19 18 2 4	18	0
3	C	1	Total C H N O 43 19 18 2 4	18	0
3	D	1	Total C H N O 43 19 18 2 4	18	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			8	2	5	1		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	192	Total	O	0	0
			192	192		
8	B	194	Total	O	0	0
			194	194		
8	C	148	Total	O	0	0
			148	148		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	144	Total	O	0	0
			144	144		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.48 Å 89.63 Å 170.00 Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	39.64 – 1.83 38.40 – 1.83	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.64-1.83) 96.2 (38.40-1.83)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 1.83 Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.1, BUSTER 2.11.1	Depositor
R, $R_{free}$	0.163 , 0.197 0.160 , 0.195	Depositor DCC
$R_{free}$ test set	4543 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NA, L59, ACT, PEG

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	0.50	0/2472	0.63	0/3341
1	B	0.51	0/2495	0.63	0/3368
1	C	0.48	0/2413	0.62	0/3265
1	D	0.49	0/2416	0.62	0/3266
All	All	0.50	0/9796	0.63	0/13240

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	2387	0	2440	17	0
1	B	2404	0	2462	15	0
1	C	2345	0	2362	15	0
1	D	2354	0	2368	9	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
3	A	25	18	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	18	17	0	0
3	C	25	18	17	0	0
3	D	25	18	17	1	0
4	A	12	0	16	3	0
4	B	12	0	16	2	0
4	C	18	0	24	5	0
4	D	12	0	16	1	0
5	A	12	0	9	0	0
5	B	8	0	6	0	0
5	C	8	0	6	0	0
5	D	8	0	6	0	0
6	A	14	20	20	1	0
6	B	17	25	23	3	0
7	D	1	0	0	0	0
8	A	192	0	0	0	0
8	B	194	0	0	4	0
8	C	148	0	0	1	0
8	D	144	0	0	1	0
All	All	10394	117	9842	59	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 3.

All (59) 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:B:194[B]:MET:HE1	8:B:594:HOH:O	1.04	1.21
1:A:166:ARG:HG3	1:C:284[B]:VAL:HG12	1.44	0.96
1:C:253[B]:LEU:H	4:C:303:GOL:H12	1.43	0.83
1:C:253[A]:LEU:H	4:C:303:GOL:H12	1.44	0.80
6:B:308:PEG:C3	8:B:594:HOH:O	2.32	0.77
1:B:5:ARG:HD3	1:B:119[A]:LEU:HD23	1.73	0.71
1:B:111[A]:VAL:HG11	1:B:182:VAL:HG22	1.76	0.68
1:A:252:SER:HA	4:A:303:GOL:H31	1.80	0.63
1:A:253[A]:LEU:HB2	4:A:303:GOL:H32	1.82	0.62
1:C:254:ILE:HG12	1:C:294:ILE:HD12	1.82	0.62
1:C:131:ILE:HD11	1:C:253[A]:LEU:HD11	1.82	0.61
1:B:109:PRO:HA	6:B:309:PEG:H12	1.85	0.59
1:A:67[B]:VAL:HG12	1:A:72:LYS:HG2	1.85	0.58
1:C:253[B]:LEU:HD12	4:C:303:GOL:H11	1.85	0.58
1:A:145[B]:VAL:HG22	1:A:258:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG11	1:A:182:VAL:HG22	1.86	0.57
1:D:129:ILE:HD12	1:D:249[B]:LEU:HG	1.86	0.56
1:B:145[B]:VAL:HG22	1:B:258:ARG:HB2	1.87	0.56
1:A:5:ARG:NH2	1:A:297:MET:O	2.35	0.55
1:D:5:ARG:HD3	1:D:119:LEU:HD23	1.88	0.54
1:C:164:VAL:HG11	1:C:217:VAL:HG13	1.89	0.54
1:C:121:GLU:HG3	1:C:299:PRO:HG3	1.89	0.54
1:C:269:GLN:NE2	8:C:491:HOH:O	2.39	0.53
1:C:187:ARG:HG2	4:C:304:GOL:H12	1.93	0.51
1:D:242:ALA:O	1:D:246:LEU:HG	2.11	0.51
1:B:136:SER:CB	1:B:145[B]:VAL:HG12	2.42	0.50
1:A:129:ILE:HD13	1:A:249[B]:LEU:HG	1.93	0.50
1:B:136:SER:HB2	1:B:145[B]:VAL:HG12	1.92	0.50
1:A:62[B]:MET:SD	1:A:205:LEU:HD13	2.53	0.49
1:C:158:ILE:HG12	1:C:235[B]:VAL:HG22	1.94	0.49
1:A:136:SER:HB2	1:A:145[B]:VAL:HG12	1.94	0.49
1:D:5:ARG:NH2	1:D:297:MET:O	2.41	0.48
1:A:253[B]:LEU:HB2	4:A:303:GOL:H32	1.93	0.48
1:C:48:VAL:HG21	1:C:71:VAL:HG21	1.95	0.48
1:A:136:SER:CB	1:A:145[B]:VAL:HG12	2.44	0.48
1:C:5:ARG:HD3	1:C:119:LEU:HD23	1.96	0.48
1:B:243:ILE:HG23	4:B:303:GOL:H32	1.95	0.47
1:A:242:ALA:O	1:A:246:LEU:HG	2.14	0.47
1:D:48:VAL:HG21	1:D:71:VAL:HG21	1.96	0.47
1:D:133:ARG:HG3	1:D:280:ALA:HA	1.96	0.46
1:D:164:VAL:HG11	1:D:217:VAL:HG13	1.97	0.46
1:B:242:ALA:O	1:B:246:LEU:HG	2.15	0.46
1:B:111[B]:VAL:HG23	6:B:309:PEG:H41	1.99	0.45
1:B:29:LYS:HB2	1:B:92:TYR:HB2	1.97	0.45
4:D:303:GOL:H12	8:D:516:HOH:O	2.16	0.45
1:B:254:ILE:HG12	1:B:294:ILE:HD12	1.98	0.44
1:C:242:ALA:O	1:C:246:LEU:HG	2.18	0.44
1:D:27:THR:HB	1:D:94:GLU:HB2	2.00	0.44
1:A:129:ILE:CD1	1:A:249[B]:LEU:HG	2.47	0.44
1:B:294:ILE:HD13	8:B:576:HOH:O	2.17	0.43
1:A:194[B]:MET:HE1	6:A:308:PEG:C1	2.49	0.43
1:B:5:ARG:NH2	1:B:297:MET:O	2.44	0.43
1:B:64:THR:HG21	1:B:248:LEU:HD11	2.01	0.42
1:A:58:GLY:HA3	1:A:67[A]:VAL:HG23	2.01	0.42
1:A:64:THR:HG21	1:A:248:LEU:HD11	2.03	0.41
4:B:303:GOL:H12	8:B:491:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:SER:HB3	1:C:145:VAL:HG13	2.02	0.40
1:D:77:GLU:OE2	3:D:302:L59:O3	2.39	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	313/302 (104%)	304 (97%)	9 (3%)	0	100	100
1	B	315/302 (104%)	307 (98%)	8 (2%)	0	100	100
1	C	310/302 (103%)	303 (98%)	6 (2%)	1 (0%)	44	28
1	D	308/302 (102%)	302 (98%)	5 (2%)	1 (0%)	44	28
All	All	1246/1208 (103%)	1216 (98%)	28 (2%)	2 (0%)	51	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	61	THR
1	D	61	THR

### 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	263/255 (103%)	263 (100%)	0	100	100
1	B	267/255 (105%)	266 (100%)	1 (0%)	93	91
1	C	254/255 (100%)	252 (99%)	2 (1%)	85	79
1	D	255/255 (100%)	254 (100%)	1 (0%)	93	91
All	All	1039/1020 (102%)	1035 (100%)	4 (0%)	93	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	ASN
1	C	201	ARG
1	C	217	VAL
1	D	217	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 molecules 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 32 ligands modelled in this entry, 5 are monoatomic - leaving 27 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	L59	A	302	2	26,26,26	1.44	3 (11%)	33,34,34	1.13	2 (6%)
4	GOL	A	303	-	5,5,5	1.00	0	5,5,5	1.59	2 (40%)
4	GOL	A	304	-	5,5,5	0.31	0	5,5,5	0.67	0
5	ACT	A	305	-	1,3,3	1.64	0	0,3,3	0.00	-
5	ACT	A	306	-	1,3,3	1.77	0	0,3,3	0.00	-
5	ACT	A	307	-	1,3,3	1.94	0	0,3,3	0.00	-
6	PEG	A	308	-	6,6,6	0.42	0	5,5,5	0.19	0
6	PEG	A	309	-	6,6,6	0.21	0	5,5,5	0.32	0
3	L59	B	302	2	26,26,26	1.56	2 (7%)	33,34,34	1.02	2 (6%)
4	GOL	B	303	-	5,5,5	0.83	0	5,5,5	0.76	0
4	GOL	B	304	-	5,5,5	0.38	0	5,5,5	0.50	0
5	ACT	B	305	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
5	ACT	B	306	-	1,3,3	2.96	1 (100%)	0,3,3	0.00	-
6	PEG	B	307	-	6,6,6	0.13	0	5,5,5	0.18	0
6	PEG	B	308	-	2,2,6	0.12	0	1,1,5	0.26	0
6	PEG	B	309	-	6,6,6	0.35	0	5,5,5	0.42	0
3	L59	C	302	2	26,26,26	1.64	3 (11%)	33,34,34	1.22	3 (9%)
4	GOL	C	303	-	5,5,5	2.03	1 (20%)	5,5,5	2.03	2 (40%)
4	GOL	C	304	-	5,5,5	0.86	0	5,5,5	1.22	0
4	GOL	C	305	-	5,5,5	0.44	0	5,5,5	0.29	0
5	ACT	C	306	-	1,3,3	1.19	0	0,3,3	0.00	-
5	ACT	C	307	-	1,3,3	2.95	1 (100%)	0,3,3	0.00	-
3	L59	D	302	2	26,26,26	1.52	3 (11%)	33,34,34	1.31	3 (9%)
4	GOL	D	303	-	5,5,5	1.12	1 (20%)	5,5,5	0.91	0
4	GOL	D	304	-	5,5,5	0.91	0	5,5,5	1.29	0
5	ACT	D	305	-	1,3,3	2.29	1 (100%)	0,3,3	0.00	-
5	ACT	D	306	-	1,3,3	1.69	0	0,3,3	0.00	-

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	L59	A	302	2	-	0/23/23/23	0/2/2/2
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
4	GOL	A	304	-	-	0/4/4/4	0/0/0/0
5	ACT	A	305	-	-	0/0/0/0	0/0/0/0
5	ACT	A	306	-	-	0/0/0/0	0/0/0/0
5	ACT	A	307	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	308	-	-	0/4/4/4	0/0/0/0
6	PEG	A	309	-	-	0/4/4/4	0/0/0/0
3	L59	B	302	2	-	0/23/23/23	0/2/2/2
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0
4	GOL	B	304	-	-	0/4/4/4	0/0/0/0
5	ACT	B	305	-	-	0/0/0/0	0/0/0/0
5	ACT	B	306	-	-	0/0/0/0	0/0/0/0
6	PEG	B	307	-	-	0/4/4/4	0/0/0/0
6	PEG	B	308	-	-	0/0/0/4	0/0/0/0
6	PEG	B	309	-	-	0/4/4/4	0/0/0/0
3	L59	C	302	2	-	0/23/23/23	0/2/2/2
4	GOL	C	303	-	-	0/4/4/4	0/0/0/0
4	GOL	C	304	-	-	0/4/4/4	0/0/0/0
4	GOL	C	305	-	-	0/4/4/4	0/0/0/0
5	ACT	C	306	-	-	0/0/0/0	0/0/0/0
5	ACT	C	307	-	-	0/0/0/0	0/0/0/0
3	L59	D	302	2	-	0/23/23/23	0/2/2/2
4	GOL	D	303	-	-	0/4/4/4	0/0/0/0
4	GOL	D	304	-	-	0/4/4/4	0/0/0/0
5	ACT	D	305	-	-	0/0/0/0	0/0/0/0
5	ACT	D	306	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	L59	O3-N2	-3.67	1.33	1.39
3	A	302	L59	O3-N2	-3.22	1.34	1.39
3	C	302	L59	O3-N2	-3.01	1.34	1.39
3	D	302	L59	O3-N2	-2.25	1.35	1.39
5	B	305	ACT	CH3-C	2.02	1.51	1.48
4	D	303	GOL	O1-C1	2.26	1.51	1.42
5	D	305	ACT	CH3-C	2.29	1.51	1.48
3	A	302	L59	C1-N1	2.35	1.39	1.34
3	C	302	L59	C1-N1	2.47	1.39	1.34
3	D	302	L59	C1-N1	2.64	1.40	1.34
5	C	307	ACT	CH3-C	2.95	1.52	1.48
5	B	306	ACT	CH3-C	2.96	1.52	1.48
3	A	302	L59	C17-N2	3.83	1.39	1.33
4	C	303	GOL	O1-C1	4.03	1.59	1.42
3	B	302	L59	C17-N2	4.89	1.40	1.33
3	D	302	L59	C17-N2	5.18	1.41	1.33
3	C	302	L59	C17-N2	5.59	1.41	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	L59	O2-C17-N2	-5.20	116.23	123.08
3	C	302	L59	O2-C17-N2	-4.52	117.12	123.08
3	A	302	L59	O2-C17-N2	-4.11	117.66	123.08
3	B	302	L59	O2-C17-N2	-3.64	118.28	123.08
3	C	302	L59	O4-C18-C16	-2.93	102.84	109.14
3	D	302	L59	O4-C18-C16	-2.53	103.70	109.14
3	A	302	L59	O4-C18-C16	-2.28	104.25	109.14
3	B	302	L59	O4-C18-C16	-2.00	104.83	109.14
3	C	302	L59	C16-C17-N2	2.02	120.89	116.51
4	C	303	GOL	O2-C2-C1	2.06	118.55	108.84
4	A	303	GOL	O2-C2-C3	2.16	119.02	108.84
3	D	302	L59	C16-C17-N2	2.38	121.67	116.51
4	A	303	GOL	O3-C3-C2	2.59	123.12	110.07
4	C	303	GOL	O1-C1-C2	3.71	128.78	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	GOL	3	0
6	A	308	PEG	1	0
4	B	303	GOL	2	0
6	B	308	PEG	1	0
6	B	309	PEG	2	0
4	C	303	GOL	4	0
4	C	304	GOL	1	0
3	D	302	L59	1	0
4	D	303	GOL	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	300/302 (99%)	-0.31	3 (1%) 82 82	13, 23, 42, 57	0
1	B	300/302 (99%)	-0.16	1 (0%) 93 93	12, 22, 42, 58	0
1	C	302/302 (100%)	-0.08	13 (4%) 36 33	15, 28, 53, 73	0
1	D	302/302 (100%)	-0.13	9 (2%) 51 47	15, 27, 56, 73	0
All	All	1204/1208 (99%)	-0.17	26 (2%) 62 60	12, 25, 49, 73	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	PHE	4.8
1	C	165	PHE	4.5
1	D	299	PRO	3.5
1	C	219	GLU	3.4
1	D	199	TYR	3.3
1	D	297	MET	2.9
1	C	295	SER	2.8
1	C	299	PRO	2.8
1	A	299	PRO	2.7
1	C	296	TYR	2.7
1	C	297	MET	2.7
1	C	197	ILE	2.6
1	C	161	ASP	2.6
1	A	298	ARG	2.5
1	C	294	ILE	2.5
1	C	164	VAL	2.5
1	D	296	TYR	2.5
1	D	200	LEU	2.4
1	B	299	PRO	2.4
1	C	199	TYR	2.4
1	A	169	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	220	ASN	2.3
1	D	161	ASP	2.3
1	D	197	ILE	2.2
1	D	205	LEU	2.1
1	D	194	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	304	6/6	0.71	0.23	9.27	41,43,43,43	0
6	PEG	A	308	7/7	0.68	0.26	8.54	30,44,59,59	0
6	PEG	A	309	7/7	0.71	0.23	7.54	35,46,61,61	0
4	GOL	C	305	6/6	0.68	0.19	6.35	59,60,60,61	0
5	ACT	A	305	4/4	0.84	0.21	6.02	54,55,55,55	0
4	GOL	C	304	6/6	0.82	0.22	5.58	39,41,41,41	0
6	PEG	B	309	7/7	0.82	0.21	4.44	38,44,46,47	0
5	ACT	D	305	4/4	0.88	0.14	4.39	56,56,56,57	0
5	ACT	B	306	4/4	0.85	0.24	4.04	47,47,48,49	0
6	PEG	B	308	3/7	0.81	0.15	4.03	72,74,74,74	0
5	ACT	A	307	4/4	0.79	0.20	3.58	66,66,66,66	0
4	GOL	A	304	6/6	0.84	0.17	3.53	45,47,48,49	0
4	GOL	B	303	6/6	0.94	0.21	3.08	24,30,31,35	0
5	ACT	A	306	4/4	0.91	0.17	2.84	48,50,51,52	0
5	ACT	D	306	4/4	0.81	0.17	2.56	61,61,61,61	0
4	GOL	B	304	6/6	0.91	0.14	2.15	45,47,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	C	307	4/4	0.75	0.23	2.12	58,58,59,59	0
4	GOL	A	303	6/6	0.93	0.18	1.89	24,28,30,34	0
4	GOL	D	303	6/6	0.86	0.17	1.26	25,30,31,35	0
3	L59	A	302	25/25	0.95	0.11	1.06	16,20,29,36	18
5	ACT	B	305	4/4	0.84	0.13	0.99	51,52,52,53	0
5	ACT	C	306	4/4	0.92	0.15	0.71	65,66,66,66	0
4	GOL	C	303	6/6	0.95	0.12	0.67	25,28,29,34	0
6	PEG	B	307	7/7	0.83	0.13	0.62	70,72,72,72	0
3	L59	D	302	25/25	0.94	0.11	0.27	21,31,45,48	18
3	L59	C	302	25/25	0.95	0.11	0.06	21,32,47,49	18
3	L59	B	302	25/25	0.97	0.09	-0.60	13,20,30,33	18
2	ZN	D	301	1/1	0.99	0.07	-0.79	17,17,17,17	0
2	ZN	B	301	1/1	1.00	0.08	-1.14	13,13,13,13	0
2	ZN	C	301	1/1	1.00	0.06	-1.43	18,18,18,18	0
2	ZN	A	301	1/1	0.99	0.05	-1.88	14,14,14,14	0
7	NA	D	307	1/1	0.98	0.08	-	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.