



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 09:51 AM EST

PDB ID : 4RAO  
Title : Aza-acyclic nucleoside phosphonates containing a second phosphonate group as inhibitors of the human, Plasmodium falciparum and vivax 6-oxopurine phosphoribosyltransferases and their pro-drugs as antimalarial agents  
Authors : Keough, D.T.; Hockova, D.; Janeba, Z.; Wang, T.-H.; Naesens, L.; Edstein, M.D.; Chavchich, M.; Guddat, L.W.  
Deposited on : 2014-09-10  
Resolution : 1.87 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-20030736  
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-20030736

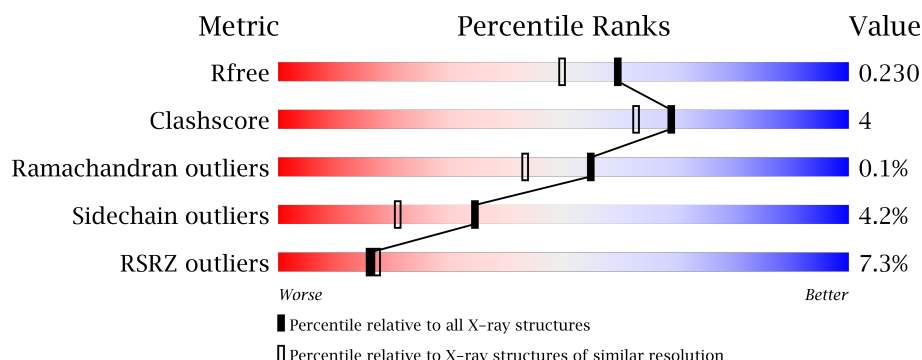
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	7505 (1.90-1.86)
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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	217	<div> <div>9%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	B	217	<div> <div>4%</div> <div>75%</div> <div>14%</div> <div>9%</div> </div>
1	C	217	<div> <div>7%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	D	217	<div> <div>7%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

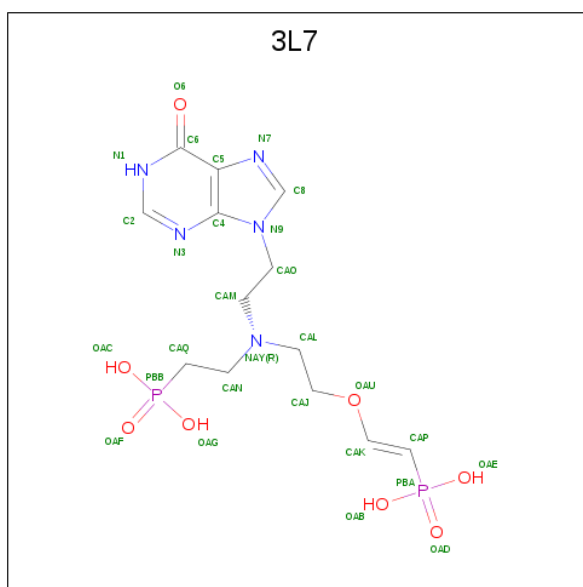
There are 4 unique types of molecules in this entry. The entry contains 6884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hypoxanthine-guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	5	0
			1585	1024	264	289	8			
1	B	198	Total	C	N	O	S	0	12	0
			1641	1060	269	302	10			
1	C	203	Total	C	N	O	S	0	6	0
			1636	1052	276	301	7			
1	D	207	Total	C	N	O	S	0	6	0
			1673	1080	277	307	9			

- Molecule 2 is (2-{[2-(6-oxo-1,6-dihydro-9H-purin-9-yl)ethyl](2-{[(E)-2-phosphonoethenyl]oxy}ethyl)amino}ethyl)phosphonic acid (three-letter code: 3L7) (formula: C<sub>13</sub>H<sub>21</sub>N<sub>5</sub>O<sub>8</sub>P<sub>2</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			28	13	5	8	2		
2	D	1	Total	C	N	O	P	0	0
			28	13	5	8	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

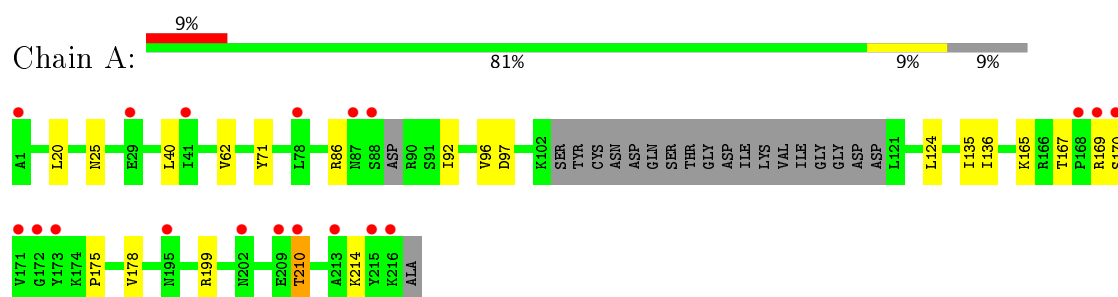
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	48	Total	O	0	0
			48	48		
4	C	53	Total	O	0	0
			53	53		
4	D	47	Total	O	0	0
			47	47		

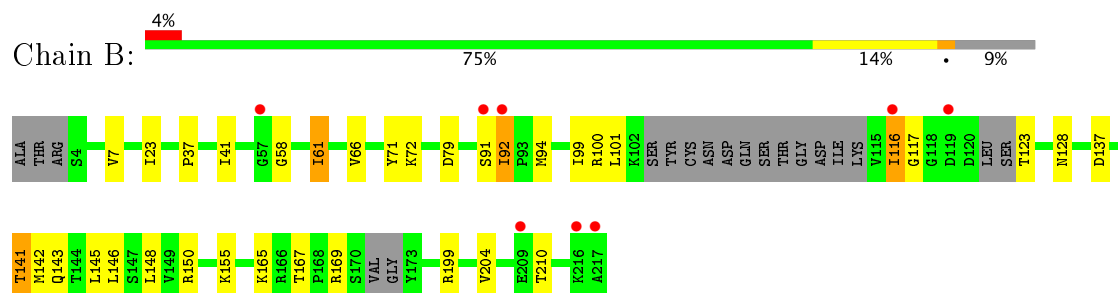
### 3 Residue-property plots [i](#)

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.

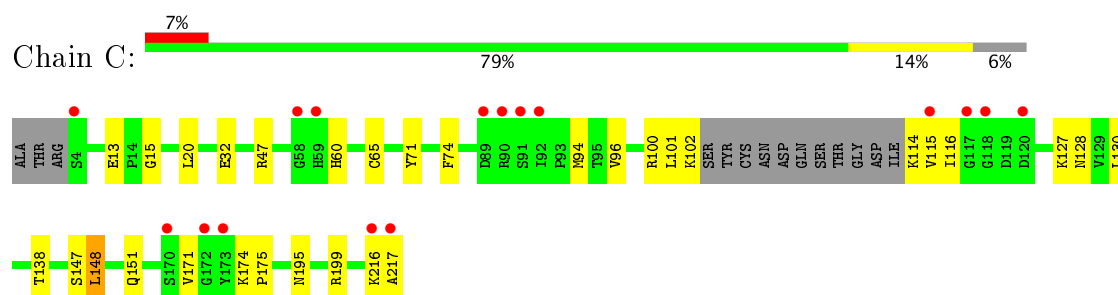
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



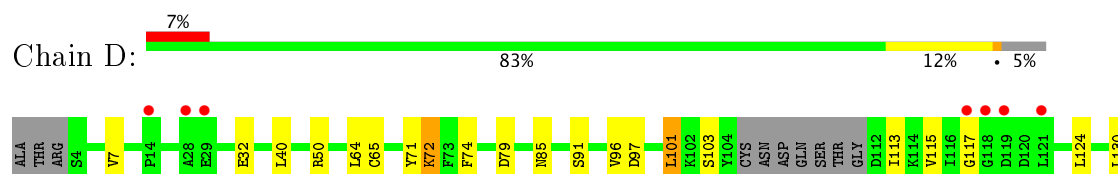
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.60Å 92.85Å 114.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.41 – 1.87 41.18 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.41-1.87) 99.8 (41.18-1.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.201 , 0.230 0.199 , 0.230	Depositor DCC
$R_{free}$ test set	2002 reflections (2.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: MG, 3L7

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	0.36	0/1629	0.55	0/2199
1	B	0.38	0/1694	0.65	2/2286 (0.1%)
1	C	0.36	0/1685	0.56	0/2274
1	D	0.35	0/1723	0.55	0/2326
All	All	0.36	0/6731	0.58	2/9085 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	92	ILE	C-N-CD	-8.02	102.95	120.60
1	B	92	ILE	C-N-CA	6.14	147.78	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	GLY	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1585	0	1616	14	0
1	B	1641	0	1654	19	0
1	C	1636	0	1658	16	0
1	D	1673	0	1706	16	0
2	A	28	0	19	0	0
2	B	56	0	36	3	0
2	C	28	0	19	2	0
2	D	28	0	19	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	53	0	0	0	0
4	B	48	0	0	1	0
4	C	53	0	0	2	0
4	D	47	0	0	0	0
All	All	6884	0	6727	57	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 4.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LEU:HB3	1:D:113:ILE:HD11	1.60	0.83
1:B:165:LYS:O	1:B:169:ARG:NH2	2.17	0.76
1:B:116:ILE:HG13	1:D:117:GLY:HA3	1.72	0.70
1:D:175:PRO:HG2	1:D:178:VAL:HG22	1.74	0.69
1:B:116:ILE:HG13	1:D:117:GLY:CA	2.31	0.60
1:B:66:VAL:HG22	1:B:99:ILE:HD11	1.85	0.58
1:C:102:LYS:O	1:C:114:LYS:N	2.40	0.55
1:B:137:ASP:OD1	1:B:167:THR:HG21	2.07	0.54
1:D:113:ILE:HG23	1:D:144:THR:HG21	1.88	0.54
1:A:97:ASP:OD1	1:C:100[A]:ARG:NH2	2.41	0.54
1:B:116:ILE:HG12	1:B:117:GLY:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:HD22	1:B:141[B]:THR:HG23	1.90	0.53
1:C:115:VAL:HG23	1:C:148:LEU:HD13	1.91	0.53
1:B:79:ASP:OD2	1:D:72:LYS:NZ	2.38	0.52
1:A:62:VAL:HG11	1:A:124:LEU:HD23	1.91	0.52
1:A:175:PRO:HG2	1:A:178:VAL:HG22	1.94	0.50
2:C:301:3L7:H4	4:C:450:HOH:O	2.11	0.50
1:D:115:VAL:HG21	1:D:148:LEU:HD23	1.94	0.49
1:A:210:THR:O	1:A:214:LYS:HB2	2.13	0.48
1:A:86:ARG:O	1:D:50:ARG:NH1	2.46	0.48
1:B:199:ARG:HD2	1:D:96:VAL:HG22	1.95	0.48
1:C:195[A]:ASN:HD21	1:C:217:ALA:HB2	1.80	0.47
1:D:64:LEU:HD12	1:D:97:ASP:HB3	1.98	0.46
1:C:216:LYS:HB2	1:C:216:LYS:HE3	1.67	0.46
1:D:85:ASN:OD1	1:D:91:SER:HB2	2.16	0.46
1:B:142[B]:MET:HE2	1:B:146:LEU:HG	1.97	0.46
1:C:94:MET:HE3	1:C:94:MET:HB3	1.69	0.45
1:C:60:HIS:HB3	1:C:127[B]:LYS:HZ3	1.81	0.45
1:A:20:LEU:HD13	1:B:7:VAL:HG22	1.99	0.45
1:D:32[B]:GLU:HB3	1:D:206:VAL:HG23	1.98	0.45
1:B:141[A]:THR:HG23	2:B:301[A]:3L7:OAG	2.17	0.45
1:C:65:CYS:HB2	1:C:74:PHE:CD1	2.52	0.44
1:A:40:LEU:HD13	1:B:37:PRO:HG2	1.98	0.44
1:B:148:LEU:O	1:B:150:ARG:N	2.46	0.44
2:B:301[B]:3L7:H6	2:B:301[B]:3L7:H10	1.84	0.44
1:A:199:ARG:HD2	1:C:96:VAL:HG22	1.99	0.44
2:B:301[A]:3L7:H18	2:B:301[A]:3L7:H11	1.40	0.43
1:A:167:THR:OG1	1:A:169:ARG:HB2	2.18	0.43
1:B:72:LYS:NZ	1:D:79:ASP:OD2	2.51	0.43
1:B:128:ASN:OD1	1:B:155:LYS:HE2	2.18	0.43
1:B:41:ILE:HD11	1:B:204:VAL:HG23	2.01	0.43
1:C:138:THR:O	1:C:171:VAL:HG22	2.18	0.43
1:A:135:ILE:HD11	1:A:165:LYS:HG3	2.01	0.42
1:C:60:HIS:O	1:C:128:ASN:HB2	2.19	0.42
1:B:61[A]:ILE:HG12	1:B:94:MET:HG2	2.02	0.41
1:C:13:GLU:HG3	1:C:15:GLY:H	1.85	0.41
1:C:174:LYS:HA	1:C:175:PRO:HD3	1.90	0.41
2:C:301:3L7:CAK	4:C:450:HOH:O	2.68	0.41
1:A:175:PRO:HG2	1:A:178:VAL:CG2	2.51	0.41
1:B:100[B]:ARG:NH2	4:B:436:HOH:O	2.24	0.41
1:D:65:CYS:HB2	1:D:74:PHE:CD1	2.55	0.41
1:A:96:VAL:HG22	1:C:199:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LEU:HD13	1:D:7:VAL:HG22	2.03	0.41
1:D:32[A]:GLU:HB3	1:D:206:VAL:HG23	2.03	0.41
1:C:147:SER:O	1:C:151:GLN:HG2	2.20	0.41
1:A:136:ILE:HD12	1:A:175:PRO:HG3	2.03	0.40
1:A:167:THR:HG23	1:A:170:SER:N	2.36	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	195/217 (90%)	190 (97%)	5 (3%)	0	100	100
1	B	203/217 (94%)	194 (96%)	8 (4%)	1 (0%)	32	19
1	C	205/217 (94%)	199 (97%)	6 (3%)	0	100	100
1	D	209/217 (96%)	206 (99%)	3 (1%)	0	100	100
All	All	812/868 (94%)	789 (97%)	22 (3%)	1 (0%)	55	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/191 (92%)	172 (98%)	4 (2%)	56	46
1	B	181/191 (95%)	169 (93%)	12 (7%)	19	8
1	C	180/191 (94%)	172 (96%)	8 (4%)	33	19
1	D	186/191 (97%)	177 (95%)	9 (5%)	30	16
All	All	723/764 (95%)	690 (95%)	33 (5%)	34	18

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	71	TYR
1	A	92	ILE
1	A	210	THR
1	B	23	ILE
1	B	61[A]	ILE
1	B	61[B]	ILE
1	B	71	TYR
1	B	91	SER
1	B	116	ILE
1	B	123	THR
1	B	141[A]	THR
1	B	141[B]	THR
1	B	143	GLN
1	B	145	LEU
1	B	210	THR
1	C	32[A]	GLU
1	C	32[B]	GLU
1	C	47	ARG
1	C	71	TYR
1	C	101	LEU
1	C	116	ILE
1	C	130	LEU
1	C	148	LEU
1	D	40[A]	LEU
1	D	40[B]	LEU
1	D	71	TYR
1	D	72	LYS
1	D	101	LEU
1	D	103	SER
1	D	124	LEU
1	D	130	LEU
1	D	207	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	3L7	A	301	3	26,29,29	3.86	10 (38%)	22,41,41	2.57	5 (22%)
2	3L7	B	301[A]	-	26,29,29	3.76	12 (46%)	22,41,41	2.60	7 (31%)
2	3L7	B	301[B]	3	26,29,29	3.74	12 (46%)	22,41,41	2.63	5 (22%)
2	3L7	C	301	3	26,29,29	3.84	10 (38%)	22,41,41	2.50	5 (22%)
2	3L7	D	301	3	26,29,29	3.75	11 (42%)	22,41,41	2.47	4 (18%)

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	3L7	A	301	3	-	0/16/20/20	0/2/2/2
2	3L7	B	301[A]	-	-	0/16/20/20	0/2/2/2
2	3L7	B	301[B]	3	-	0/16/20/20	0/2/2/2
2	3L7	C	301	3	-	0/16/20/20	0/2/2/2
2	3L7	D	301	3	-	0/16/20/20	0/2/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[A]	3L7	PBB-OAC	-3.36	1.47	1.54
2	B	301[B]	3L7	PBB-OAC	-3.33	1.47	1.54
2	A	301	3L7	PBB-OAC	-3.24	1.47	1.54
2	D	301	3L7	PBB-OAC	-2.82	1.48	1.54
2	B	301[A]	3L7	PBA-OAB	-2.72	1.50	1.54
2	B	301[A]	3L7	OAU-CAJ	-2.61	1.36	1.43
2	B	301[B]	3L7	PBA-OAB	-2.56	1.50	1.54
2	A	301	3L7	OAU-CAJ	-2.52	1.36	1.43
2	B	301[B]	3L7	OAU-CAJ	-2.49	1.36	1.43
2	C	301	3L7	OAU-CAJ	-2.44	1.36	1.43
2	C	301	3L7	PBA-OAB	-2.40	1.50	1.54
2	D	301	3L7	OAU-CAJ	-2.38	1.37	1.43
2	A	301	3L7	PBA-OAB	-2.04	1.51	1.54
2	C	301	3L7	C2-N3	2.19	1.35	1.32
2	B	301[A]	3L7	C2-N3	2.27	1.36	1.32
2	A	301	3L7	C6-N1	2.39	1.37	1.33
2	B	301[B]	3L7	C6-N1	2.39	1.37	1.33
2	B	301[B]	3L7	C2-N3	2.40	1.36	1.32
2	B	301[A]	3L7	C6-N1	2.40	1.37	1.33
2	C	301	3L7	C6-C5	2.42	1.46	1.41
2	D	301	3L7	C2-N3	2.43	1.36	1.32
2	A	301	3L7	C6-C5	2.44	1.46	1.41
2	D	301	3L7	C6-C5	2.50	1.46	1.41
2	C	301	3L7	C6-N1	2.54	1.37	1.33
2	D	301	3L7	C6-N1	2.54	1.37	1.33
2	B	301[B]	3L7	C6-C5	2.60	1.46	1.41
2	B	301[A]	3L7	C6-C5	2.62	1.46	1.41
2	B	301[B]	3L7	PBA-OAD	3.14	1.54	1.48
2	A	301	3L7	O6-C6	3.47	1.33	1.24
2	D	301	3L7	O6-C6	3.51	1.33	1.24
2	B	301[A]	3L7	PBA-OAD	3.59	1.55	1.48
2	B	301[B]	3L7	O6-C6	3.62	1.33	1.24
2	B	301[A]	3L7	O6-C6	3.63	1.33	1.24
2	B	301[B]	3L7	PBA-OAE	3.86	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	3L7	O6-C6	3.87	1.34	1.24
2	D	301	3L7	PBB-OAF	4.09	1.59	1.50
2	B	301[A]	3L7	PBA-OAE	4.28	1.60	1.54
2	D	301	3L7	PBA-OAE	4.29	1.60	1.54
2	C	301	3L7	C4-N3	4.38	1.42	1.35
2	D	301	3L7	C4-N3	4.44	1.42	1.35
2	B	301[B]	3L7	C4-N3	4.83	1.42	1.35
2	B	301[A]	3L7	C4-N3	4.87	1.42	1.35
2	A	301	3L7	C4-N3	5.05	1.43	1.35
2	C	301	3L7	PBA-OAD	6.17	1.59	1.48
2	A	301	3L7	PBA-OAD	6.70	1.60	1.48
2	B	301[A]	3L7	PBA-CAP	8.13	1.88	1.76
2	B	301[B]	3L7	PBA-CAP	8.34	1.88	1.76
2	A	301	3L7	PBA-CAP	8.41	1.88	1.76
2	D	301	3L7	PBA-CAP	8.58	1.88	1.76
2	C	301	3L7	PBA-CAP	8.99	1.89	1.76
2	B	301[A]	3L7	CAP-CAK	13.28	1.52	1.32
2	B	301[B]	3L7	CAP-CAK	13.38	1.53	1.32
2	D	301	3L7	CAP-CAK	13.49	1.53	1.32
2	A	301	3L7	CAP-CAK	13.55	1.53	1.32
2	C	301	3L7	CAP-CAK	13.78	1.53	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	3L7	N3-C2-N1	-9.66	120.45	128.86
2	B	301[B]	3L7	N3-C2-N1	-9.14	120.90	128.86
2	B	301[A]	3L7	N3-C2-N1	-9.12	120.92	128.86
2	D	301	3L7	N3-C2-N1	-8.49	121.47	128.86
2	C	301	3L7	N3-C2-N1	-8.49	121.47	128.86
2	A	301	3L7	C6-C5-C4	-2.62	118.23	120.84
2	B	301[A]	3L7	C6-C5-C4	-2.17	118.68	120.84
2	B	301[B]	3L7	C6-C5-C4	-2.10	118.76	120.84
2	C	301	3L7	C4-C5-N7	-2.07	107.41	109.41
2	B	301[A]	3L7	C4-C5-N7	-2.02	107.46	109.41
2	A	301	3L7	CAO-CAM-NAY	2.07	117.42	112.28
2	B	301[A]	3L7	OAG-PBB-CAQ	2.33	112.41	106.96
2	B	301[A]	3L7	CAO-CAM-NAY	2.48	118.45	112.28
2	D	301	3L7	CAO-CAM-NAY	2.77	119.18	112.28
2	B	301[B]	3L7	OAU-CAJ-CAL	2.81	115.85	108.56
2	C	301	3L7	CAO-CAM-NAY	2.96	119.64	112.28
2	B	301[A]	3L7	OAU-CAJ-CAL	3.14	116.72	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	3L7	OAU-CAJ-CAL	3.27	117.05	108.56
2	B	301[B]	3L7	CAO-CAM-NAY	3.51	121.00	112.28
2	D	301	3L7	OAU-CAJ-CAL	3.85	118.55	108.56
2	C	301	3L7	OAU-CAJ-CAL	3.87	118.59	108.56
2	D	301	3L7	C2-N1-C6	4.27	123.05	115.91
2	B	301[A]	3L7	C2-N1-C6	4.41	123.28	115.91
2	B	301[B]	3L7	C2-N1-C6	4.44	123.33	115.91
2	C	301	3L7	C2-N1-C6	4.51	123.44	115.91
2	A	301	3L7	C2-N1-C6	4.63	123.65	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301[A]	3L7	2	0
2	B	301[B]	3L7	1	0
2	C	301	3L7	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	197/217 (90%)	0.52	19 (9%) 9 9	22, 37, 73, 96	0
1	B	198/217 (91%)	0.36	8 (4%) 39 41	20, 34, 74, 101	0
1	C	203/217 (93%)	0.44	16 (7%) 13 15	22, 39, 70, 107	0
1	D	207/217 (95%)	0.32	16 (7%) 14 15	22, 36, 68, 88	0
All	All	805/868 (92%)	0.41	59 (7%) 16 17	20, 37, 71, 107	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ALA	7.3
1	A	171	VAL	6.9
1	A	170	SER	5.8
1	A	168	PRO	5.6
1	A	210	THR	5.2
1	D	168	PRO	4.5
1	D	171	VAL	4.5
1	C	173	TYR	4.4
1	C	217	ALA	4.3
1	A	172	GLY	4.2
1	D	213	ALA	3.9
1	C	117	GLY	3.9
1	A	215	TYR	3.9
1	A	1	ALA	3.4
1	C	91	SER	3.4
1	C	90	ARG	3.3
1	D	29	GLU	3.3
1	B	91	SER	3.1
1	D	210	THR	3.1
1	A	173	TYR	3.1
1	A	213	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	89	ASP	3.0
1	D	121	LEU	3.0
1	C	58	GLY	3.0
1	A	216	LYS	3.0
1	B	92	ILE	2.9
1	A	169	ARG	2.9
1	C	172	GLY	2.9
1	B	116	ILE	2.9
1	B	119	ASP	2.9
1	C	92	ILE	2.8
1	B	209	GLU	2.8
1	D	209	GLU	2.8
1	B	57	GLY	2.7
1	C	115	VAL	2.7
1	C	118	GLY	2.6
1	C	120	ASP	2.6
1	B	216	LYS	2.6
1	D	208	SER	2.5
1	D	169	ARG	2.5
1	C	4	SER	2.4
1	A	209	GLU	2.3
1	D	211	GLY	2.3
1	D	28	ALA	2.3
1	C	216	LYS	2.3
1	A	87	ASN	2.2
1	D	119	ASP	2.2
1	D	14	PRO	2.2
1	A	195	ASN	2.2
1	A	202[A]	ASN	2.2
1	A	88[A]	SER	2.1
1	A	29	GLU	2.1
1	D	117	GLY	2.1
1	A	78[A]	LEU	2.1
1	D	216	LYS	2.1
1	D	118	GLY	2.1
1	A	41	ILE	2.0
1	C	59	HIS	2.0
1	C	170	SER	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 [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
2	3L7	B	301[B]	28/28	0.95	0.16	1.11	26,35,41,42	28
2	3L7	B	301[A]	28/28	0.95	0.16	0.98	31,37,60,62	28
2	3L7	C	301	28/28	0.95	0.15	0.98	23,32,51,53	28
2	3L7	D	301	28/28	0.94	0.13	0.87	37,45,80,115	0
2	3L7	A	301	28/28	0.95	0.12	0.30	36,42,69,73	0
3	MG	B	302	1/1	0.86	0.13	0.00	75,75,75,75	0
3	MG	B	303	1/1	0.99	0.08	-	36,36,36,36	0
3	MG	A	302	1/1	0.97	0.12	-	28,28,28,28	0
3	MG	C	302	1/1	0.98	0.08	-	27,27,27,27	0
3	MG	D	302	1/1	0.98	0.15	-	26,26,26,26	0
3	MG	C	303	1/1	0.95	0.06	-	41,41,41,41	0
3	MG	A	303	1/1	0.95	0.14	-	45,45,45,45	0
3	MG	D	303	1/1	0.95	0.06	-	45,45,45,45	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.