



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:16 PM GMT

PDB ID : 4RAD  
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 : 2.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

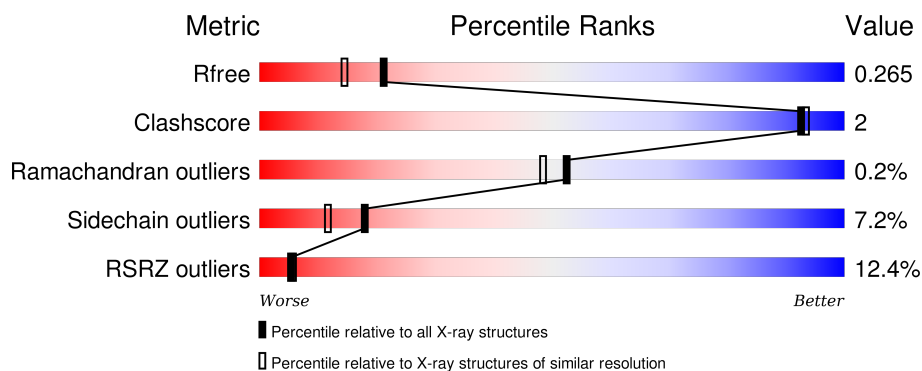
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>8%</div> <div>82%</div> <div>8%</div> <div>9%</div> </div>
1	B	217	<div> <div>8%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	C	217	<div> <div>6%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
1	D	217	<div> <div>9%</div> <div>84%</div> <div>8%</div> <div>7%</div> </div>
1	E	217	<div> <div>20%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	217	
1	G	217	
1	H	217	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3L5	C	301[A]	-	-	-	X
2	3L5	C	301[B]	-	-	-	X
3	MG	A	302	-	-	-	X
3	MG	F	302	-	-	-	X

## 2 Entry composition

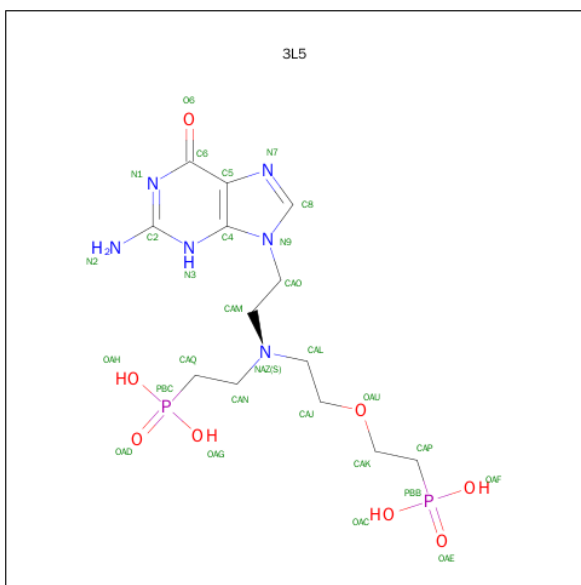
There are 4 unique types of molecules in this entry. The entry contains 26882 atoms, of which 13106 are hydrogens and 0 are deuteriums.

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	H	N	O	S	0	0	0
			3112	999	1558	259	289	7			
1	B	207	Total	C	H	N	O	S	0	0	0
			3277	1048	1644	274	304	7			
1	C	202	Total	C	H	N	O	S	0	0	0
			3210	1030	1611	268	294	7			
1	D	202	Total	C	H	N	O	S	0	0	0
			3189	1024	1597	265	296	7			
1	E	206	Total	C	H	N	O	S	0	0	0
			3238	1043	1616	269	303	7			
1	F	197	Total	C	H	N	O	S	0	0	0
			3141	1007	1581	262	284	7			
1	G	200	Total	C	H	N	O	S	0	0	0
			3171	1019	1589	264	292	7			
1	H	208	Total	C	H	N	O	S	0	0	0
			3313	1061	1663	276	306	7			

- Molecule 2 is (2-{[2-(2-AMINO-6-OXO-3,6-DIHYDRO-9H-PURIN-9-YL)ETHYL][2-(2-PHOSPHONOETHOXY)ETHYL]AMINO}ETHYL)PHOSPHONIC ACID (three-letter code: 3L5) (formula: C<sub>13</sub>H<sub>24</sub>N<sub>6</sub>O<sub>8</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 96	C 26	H 38	N 12	O 16	P 4	0	1
2	B	1	Total 48	C 13	H 19	N 6	O 8	P 2	0	0
2	C	1	Total 96	C 26	H 38	N 12	O 16	P 4	0	1
2	D	1	Total 96	C 26	H 38	N 12	O 16	P 4	0	1
2	E	1	Total 96	C 26	H 38	N 12	O 16	P 4	0	1
2	F	1	Total 48	C 13	H 19	N 6	O 8	P 2	0	0
2	G	1	Total 48	C 13	H 19	N 6	O 8	P 2	0	0
2	H	1	Total 96	C 26	H 38	N 12	O 16	P 4	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	2	Total 2	Mg 2	0	0

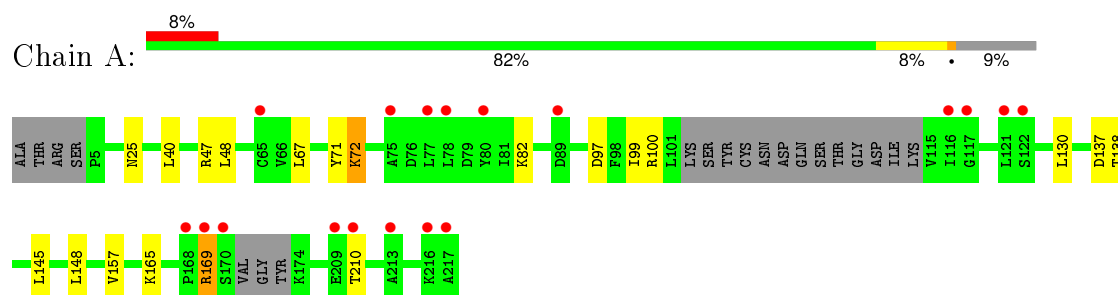
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total 78	O 78	0	0
4	B	88	Total 88	O 88	0	0
4	C	72	Total 72	O 72	0	0
4	D	94	Total 94	O 94	0	0
4	E	62	Total 62	O 62	0	0
4	F	98	Total 98	O 98	0	0
4	G	37	Total 37	O 37	0	0
4	H	69	Total 69	O 69	0	0

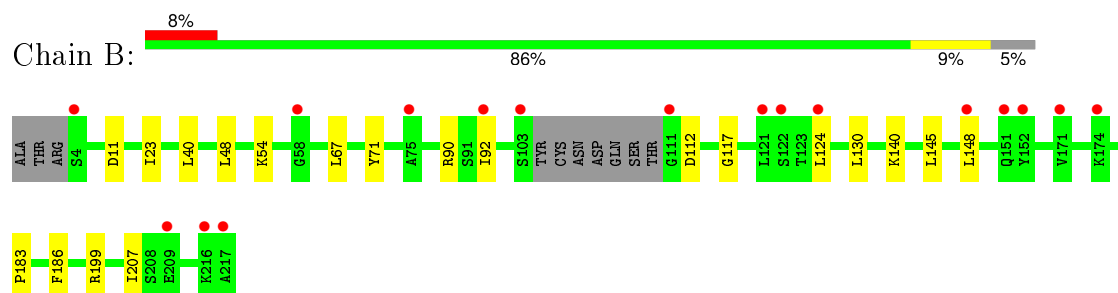
### 3 Residue-property plots [i](#)

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

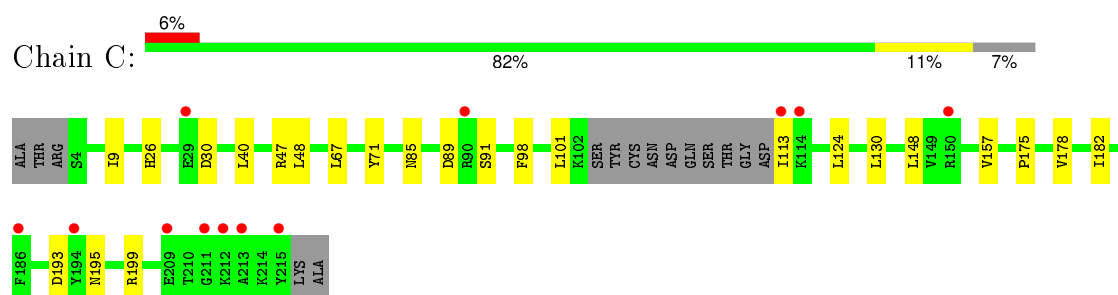
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



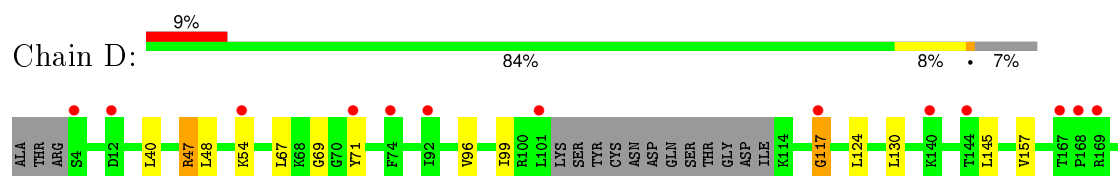
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

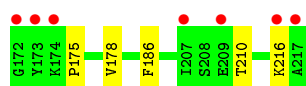


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

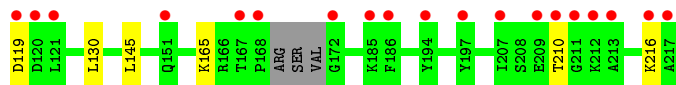
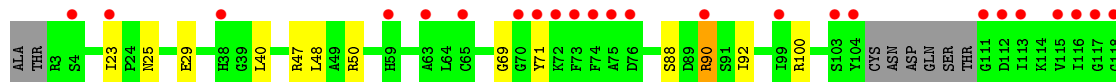
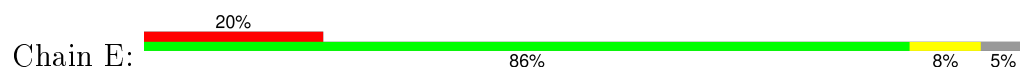


- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase

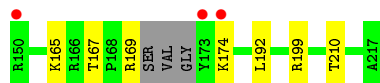
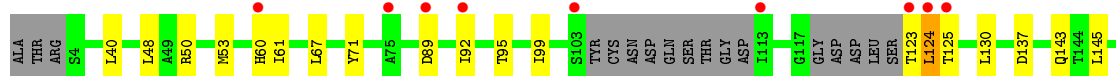
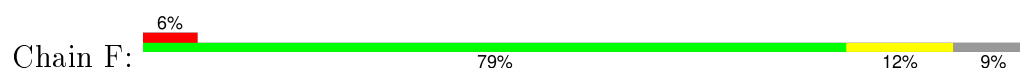




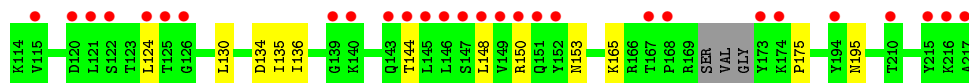
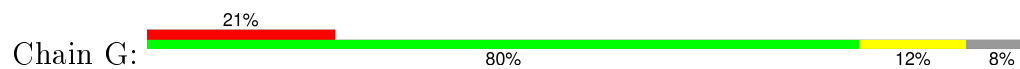
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



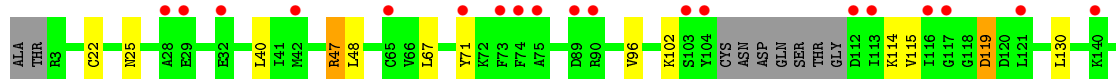
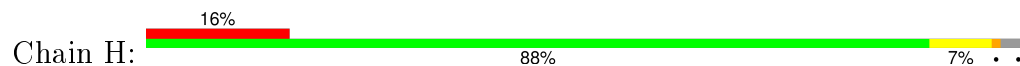
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.05Å 114.93Å 97.54Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	35.56 – 2.00 35.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.56-2.00) 98.7 (35.56-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.209 , 0.259 0.217 , 0.265	Depositor DCC
$R_{free}$ test set	2000 reflections (1.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 109336 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 3L5, MG

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	0.27	0/1583	0.52	0/2138
1	B	0.27	0/1664	0.49	0/2247
1	C	0.26	0/1630	0.50	0/2204
1	D	0.26	0/1623	0.49	0/2194
1	E	0.26	0/1653	0.47	0/2233
1	F	0.27	0/1588	0.52	0/2141
1	G	0.24	0/1612	0.46	0/2175
1	H	0.25	0/1682	0.49	0/2271
All	All	0.26	0/13035	0.49	0/17603

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	1554	1558	1558	9	0
1	B	1633	1644	1644	5	0
1	C	1599	1611	1611	9	0
1	D	1592	1597	1597	6	0
1	E	1622	1616	1616	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1560	1581	1581	8	0
1	G	1582	1589	1589	9	0
1	H	1650	1663	1663	7	0
2	A	58	38	44	0	0
2	B	29	19	22	0	0
2	C	58	38	44	2	0
2	D	58	38	44	1	0
2	E	58	38	44	1	0
2	F	29	19	22	0	0
2	G	29	19	22	0	0
2	H	58	38	44	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	78	0	0	3	0
4	B	88	0	0	1	0
4	C	72	0	0	3	0
4	D	94	0	0	3	0
4	E	62	0	0	2	0
4	F	98	0	0	0	0
4	G	37	0	0	2	0
4	H	69	0	0	1	0
All	All	13776	13106	13145	53	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 2.

All (53) 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:F:123:THR:O	1:F:125:THR:N	2.24	0.70
1:G:47:ARG:NH1	1:G:51:ASP:OD1	2.25	0.69
1:C:30:ASP:OD2	4:C:434:HOH:O	2.13	0.67
2:C:301[B]:3L5:H6	2:C:301[B]:3L5:H22	1.60	0.67
1:E:25:ASN:ND2	1:G:89:ASP:O	2.29	0.66
1:A:165:LYS:NZ	4:A:428:HOH:O	2.32	0.62
1:C:199:ARG:NH1	2:C:301[B]:3L5:OAE	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:LYS:NZ	4:G:429:HOH:O	2.34	0.60
1:B:112:ASP:N	1:B:112:ASP:OD1	2.34	0.59
1:D:117:GLY:O	4:D:444:HOH:O	2.16	0.58
1:H:47:ARG:NH2	4:H:443:HOH:O	2.37	0.58
1:C:26:HIS:O	4:C:434:HOH:O	2.17	0.57
1:A:138:THR:HA	1:A:169:ARG:CB	2.38	0.54
1:A:72:LYS:NZ	4:A:447:HOH:O	2.30	0.54
1:H:102:LYS:O	1:H:114:LYS:N	2.39	0.54
1:A:138:THR:HA	1:A:169:ARG:HB2	1.90	0.53
1:A:99:ILE:HD12	1:A:145:LEU:HD22	1.90	0.53
1:D:47:ARG:NH2	4:D:408:HOH:O	2.42	0.51
1:F:137:ASP:OD1	1:F:167:THR:HG21	2.11	0.50
1:G:134:ASP:OD1	1:G:135:ILE:N	2.45	0.50
1:F:165:LYS:O	1:F:169:ARG:NH2	2.39	0.49
1:D:175:PRO:HG2	1:D:178:VAL:HG22	1.94	0.48
1:D:186:PHE:O	4:D:461:HOH:O	2.20	0.48
1:E:69:GLY:H	2:E:301[A]:3L5:H4	1.79	0.48
1:E:50:ARG:NH2	4:E:403:HOH:O	2.43	0.47
1:B:186:PHE:HB3	1:B:207:ILE:HD11	1.96	0.47
1:F:53:MET:HA	1:F:92:ILE:HD11	1.97	0.47
1:A:82:LYS:NZ	4:A:453:HOH:O	2.48	0.46
1:A:137:ASP:OD2	1:A:169:ARG:NH2	2.49	0.46
1:F:50:ARG:NH1	1:G:86:ARG:O	2.49	0.46
1:G:165:LYS:NZ	4:G:411:HOH:O	2.49	0.46
1:F:60:HIS:NE2	1:F:95:THR:HG23	2.32	0.45
1:G:18:LEU:HB3	1:G:23:ILE:HD13	2.00	0.44
1:C:85:ASN:OD1	1:C:91:SER:OG	2.25	0.44
1:H:175:PRO:HG2	1:H:178:VAL:HG22	1.99	0.43
1:H:119:ASP:OD2	1:H:119:ASP:N	2.49	0.43
1:A:138:THR:HA	1:A:169:ARG:HG3	1.99	0.43
1:H:115:VAL:HG11	1:H:148:LEU:HD21	2.00	0.43
1:C:47:ARG:NH2	4:C:411:HOH:O	2.53	0.42
1:B:117:GLY:O	4:B:440:HOH:O	2.22	0.42
1:A:25:ASN:ND2	1:C:89:ASP:O	2.48	0.42
1:B:11:ASP:HA	1:B:183:PRO:HG3	2.01	0.42
1:C:9:ILE:HD12	1:C:182:ILE:HG22	2.02	0.42
1:F:199:ARG:HD2	1:H:96:VAL:HG22	2.01	0.41
1:F:123:THR:OG1	1:F:124:LEU:N	2.53	0.41
1:G:50:ARG:NH2	1:H:22:CYS:HA	2.35	0.41
1:E:88:SER:OG	1:E:90:ARG:NH1	2.54	0.41
1:C:175:PRO:HG2	1:C:178:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ILE:HD12	1:G:175:PRO:HG3	2.01	0.41
1:D:69:GLY:H	2:D:301[B]:3L5:H3	1.86	0.41
1:B:199:ARG:HD2	1:D:96:VAL:HG22	2.02	0.41
1:E:165:LYS:NZ	4:E:422:HOH:O	2.54	0.40
1:C:67:LEU:HD21	1:C:98:PHE:HB3	2.04	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	191/217 (88%)	185 (97%)	6 (3%)	0	100	100
1	B	203/217 (94%)	197 (97%)	6 (3%)	0	100	100
1	C	198/217 (91%)	192 (97%)	6 (3%)	0	100	100
1	D	198/217 (91%)	191 (96%)	6 (3%)	1 (0%)	34	26
1	E	200/217 (92%)	193 (96%)	7 (4%)	0	100	100
1	F	189/217 (87%)	181 (96%)	7 (4%)	1 (0%)	34	26
1	G	194/217 (89%)	186 (96%)	7 (4%)	1 (0%)	34	26
1	H	204/217 (94%)	199 (98%)	5 (2%)	0	100	100
All	All	1577/1736 (91%)	1524 (97%)	50 (3%)	3 (0%)	52	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	124	LEU
1	G	153	ASN
1	D	117	GLY

### 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	170/191 (89%)	157 (92%)	13 (8%)	16	10
1	B	179/191 (94%)	166 (93%)	13 (7%)	17	11
1	C	175/191 (92%)	164 (94%)	11 (6%)	22	16
1	D	174/191 (91%)	161 (92%)	13 (8%)	17	11
1	E	176/191 (92%)	162 (92%)	14 (8%)	15	9
1	F	170/191 (89%)	157 (92%)	13 (8%)	16	10
1	G	172/191 (90%)	159 (92%)	13 (8%)	16	10
1	H	181/191 (95%)	171 (94%)	10 (6%)	27	21
All	All	1397/1528 (91%)	1297 (93%)	100 (7%)	18	12

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	47	ARG
1	A	48	LEU
1	A	67	LEU
1	A	71	TYR
1	A	72	LYS
1	A	97	ASP
1	A	100	ARG
1	A	130	LEU
1	A	148	LEU
1	A	157	VAL
1	A	169	ARG
1	A	210	THR
1	B	23	ILE
1	B	40	LEU
1	B	48	LEU
1	B	54	LYS
1	B	67	LEU
1	B	71	TYR

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Mol	Chain	Res	Type
1	B	90	ARG
1	B	92	ILE
1	B	124	LEU
1	B	130	LEU
1	B	140	LYS
1	B	145	LEU
1	B	148	LEU
1	C	40	LEU
1	C	48	LEU
1	C	71	TYR
1	C	101	LEU
1	C	113	ILE
1	C	124	LEU
1	C	130	LEU
1	C	148	LEU
1	C	157	VAL
1	C	193	ASP
1	C	195	ASN
1	D	40	LEU
1	D	47	ARG
1	D	48	LEU
1	D	54	LYS
1	D	67	LEU
1	D	71	TYR
1	D	99	ILE
1	D	124	LEU
1	D	130	LEU
1	D	145	LEU
1	D	157	VAL
1	D	210	THR
1	D	216	LYS
1	E	23	ILE
1	E	29	GLU
1	E	40	LEU
1	E	47	ARG
1	E	48	LEU
1	E	71	TYR
1	E	90	ARG
1	E	92	ILE
1	E	100	ARG
1	E	119	ASP
1	E	130	LEU

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Mol	Chain	Res	Type
1	E	145	LEU
1	E	210	THR
1	E	216	LYS
1	F	40	LEU
1	F	48	LEU
1	F	61	ILE
1	F	67	LEU
1	F	71	TYR
1	F	89	ASP
1	F	99	ILE
1	F	130	LEU
1	F	143	GLN
1	F	145	LEU
1	F	174	LYS
1	F	192	LEU
1	F	210	THR
1	G	40	LEU
1	G	48	LEU
1	G	50	ARG
1	G	67	LEU
1	G	71	TYR
1	G	90	ARG
1	G	92	ILE
1	G	124	LEU
1	G	130	LEU
1	G	144	THR
1	G	148	LEU
1	G	150	ARG
1	G	195	ASN
1	H	25	ASN
1	H	40	LEU
1	H	47	ARG
1	H	48	LEU
1	H	67	LEU
1	H	71	TYR
1	H	119	ASP
1	H	130	LEU
1	H	145	LEU
1	H	193	ASP

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 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	3L5	A	301[A]	-	24,30,30	2.63	4 (16%)	30,43,43	1.51	4 (13%)
2	3L5	A	301[B]	-	24,30,30	2.68	4 (16%)	30,43,43	1.53	4 (13%)
2	3L5	B	301	-	24,30,30	2.46	4 (16%)	30,43,43	1.51	5 (16%)
2	3L5	C	301[A]	-	24,30,30	2.70	4 (16%)	30,43,43	1.82	6 (20%)
2	3L5	C	301[B]	-	24,30,30	2.63	4 (16%)	30,43,43	1.69	5 (16%)
2	3L5	D	301[A]	-	24,30,30	2.63	4 (16%)	30,43,43	1.58	5 (16%)
2	3L5	D	301[B]	3	24,30,30	2.58	4 (16%)	30,43,43	1.59	5 (16%)
2	3L5	E	301[A]	-	24,30,30	2.57	4 (16%)	30,43,43	1.52	4 (13%)
2	3L5	E	301[B]	-	24,30,30	2.57	4 (16%)	30,43,43	1.52	5 (16%)
2	3L5	F	301	3	24,30,30	2.53	4 (16%)	30,43,43	1.57	5 (16%)
2	3L5	G	301	-	24,30,30	2.65	4 (16%)	30,43,43	1.54	4 (13%)
2	3L5	H	301[A]	-	24,30,30	2.66	4 (16%)	30,43,43	1.69	4 (13%)
2	3L5	H	301[B]	-	24,30,30	2.62	4 (16%)	30,43,43	1.94	7 (23%)

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	3L5	A	301[A]	-	-	0/20/20/20	0/2/2/2
2	3L5	A	301[B]	-	-	0/20/20/20	0/2/2/2
2	3L5	B	301	-	-	0/20/20/20	0/2/2/2
2	3L5	C	301[A]	-	-	0/20/20/20	0/2/2/2
2	3L5	C	301[B]	-	-	0/20/20/20	0/2/2/2
2	3L5	D	301[A]	-	-	0/20/20/20	0/2/2/2
2	3L5	D	301[B]	3	-	0/20/20/20	0/2/2/2
2	3L5	E	301[A]	-	-	0/20/20/20	0/2/2/2
2	3L5	E	301[B]	-	-	0/20/20/20	0/2/2/2
2	3L5	F	301	3	-	0/20/20/20	0/2/2/2
2	3L5	G	301	-	-	0/20/20/20	0/2/2/2
2	3L5	H	301[A]	-	-	0/20/20/20	0/2/2/2
2	3L5	H	301[B]	-	-	0/20/20/20	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	3L5	PBB-CAP	4.35	1.83	1.79
2	A	301[B]	3L5	C2-N2	4.36	1.43	1.34
2	F	301	3L5	PBB-CAP	4.41	1.83	1.79
2	A	301[A]	3L5	C2-N2	4.42	1.43	1.34
2	E	301[A]	3L5	C2-N2	4.46	1.43	1.34
2	H	301[A]	3L5	C2-N2	4.50	1.43	1.34
2	D	301[B]	3L5	C2-N2	4.50	1.43	1.34
2	F	301	3L5	C2-N2	4.54	1.43	1.34
2	E	301[B]	3L5	C2-N2	4.54	1.43	1.34
2	H	301[B]	3L5	C2-N2	4.55	1.43	1.34
2	C	301[B]	3L5	C2-N2	4.55	1.43	1.34
2	G	301	3L5	C2-N2	4.55	1.43	1.34
2	C	301[A]	3L5	C2-N2	4.55	1.43	1.34
2	B	301	3L5	C2-N2	4.55	1.43	1.34
2	D	301[A]	3L5	C2-N2	4.56	1.43	1.34
2	E	301[A]	3L5	PBB-CAP	4.59	1.83	1.79
2	B	301	3L5	PBB-CAP	4.62	1.83	1.79
2	E	301[B]	3L5	PBB-CAP	4.66	1.83	1.79
2	H	301[B]	3L5	PBB-CAP	4.69	1.83	1.79
2	D	301[B]	3L5	PBB-CAP	4.70	1.83	1.79
2	H	301[A]	3L5	PBB-CAP	4.98	1.84	1.79
2	D	301[A]	3L5	PBB-CAP	5.03	1.84	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[A]	3L5	PBB-CAP	5.03	1.84	1.79
2	G	301	3L5	PBB-CAP	5.12	1.84	1.79
2	A	301[B]	3L5	PBB-CAP	5.41	1.84	1.79
2	C	301[A]	3L5	PBB-CAP	5.59	1.84	1.79
2	B	301	3L5	PBC-CAQ	5.91	1.85	1.79
2	F	301	3L5	PBC-CAQ	6.46	1.85	1.79
2	E	301[B]	3L5	PBC-CAQ	6.73	1.85	1.79
2	E	301[A]	3L5	PBC-CAQ	6.75	1.85	1.79
2	D	301[B]	3L5	PBC-CAQ	6.75	1.85	1.79
2	D	301[A]	3L5	PBC-CAQ	6.79	1.85	1.79
2	C	301[A]	3L5	PBC-CAQ	6.81	1.85	1.79
2	H	301[B]	3L5	PBC-CAQ	6.86	1.86	1.79
2	A	301[A]	3L5	PBC-CAQ	6.87	1.86	1.79
2	G	301	3L5	PBC-CAQ	7.05	1.86	1.79
2	H	301[A]	3L5	PBC-CAQ	7.05	1.86	1.79
2	C	301[B]	3L5	PBC-CAQ	7.06	1.86	1.79
2	A	301[B]	3L5	PBC-CAQ	7.15	1.86	1.79
2	B	301	3L5	O6-C6	7.48	1.42	1.24
2	F	301	3L5	O6-C6	7.56	1.42	1.24
2	G	301	3L5	O6-C6	7.60	1.42	1.24
2	E	301[B]	3L5	O6-C6	7.64	1.43	1.24
2	D	301[B]	3L5	O6-C6	7.67	1.43	1.24
2	E	301[A]	3L5	O6-C6	7.68	1.43	1.24
2	A	301[B]	3L5	O6-C6	7.69	1.43	1.24
2	A	301[A]	3L5	O6-C6	7.71	1.43	1.24
2	D	301[A]	3L5	O6-C6	7.77	1.43	1.24
2	H	301[A]	3L5	O6-C6	7.81	1.43	1.24
2	H	301[B]	3L5	O6-C6	7.81	1.43	1.24
2	C	301[B]	3L5	O6-C6	7.82	1.43	1.24
2	C	301[A]	3L5	O6-C6	7.84	1.43	1.24

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[B]	3L5	C5-C6-N1	-4.07	118.03	123.59
2	C	301[A]	3L5	C5-C6-N1	-4.05	118.06	123.59
2	H	301[A]	3L5	C5-C6-N1	-4.03	118.08	123.59
2	H	301[B]	3L5	C5-C6-N1	-4.01	118.10	123.59
2	C	301[B]	3L5	C4-C5-N7	-3.87	105.92	109.48
2	A	301[A]	3L5	C5-C6-N1	-3.79	118.41	123.59
2	D	301[B]	3L5	C5-C6-N1	-3.78	118.42	123.59
2	D	301[A]	3L5	C5-C6-N1	-3.78	118.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	3L5	C5-C6-N1	-3.72	118.50	123.59
2	A	301[B]	3L5	C5-C6-N1	-3.71	118.51	123.59
2	E	301[A]	3L5	C5-C6-N1	-3.63	118.63	123.59
2	H	301[A]	3L5	C4-C5-N7	-3.62	106.15	109.48
2	H	301[B]	3L5	C4-C5-N7	-3.62	106.15	109.48
2	C	301[A]	3L5	C4-C5-N7	-3.59	106.18	109.48
2	B	301	3L5	N3-C2-N1	-3.53	122.06	127.44
2	E	301[B]	3L5	C5-C6-N1	-3.52	118.77	123.59
2	G	301	3L5	C5-C6-N1	-3.52	118.77	123.59
2	B	301	3L5	C5-C6-N1	-3.51	118.79	123.59
2	G	301	3L5	N3-C2-N1	-3.47	122.15	127.44
2	C	301[B]	3L5	N3-C2-N1	-3.44	122.21	127.44
2	C	301[A]	3L5	N3-C2-N1	-3.43	122.22	127.44
2	A	301[A]	3L5	C4-C5-N7	-3.39	106.36	109.48
2	D	301[A]	3L5	N3-C2-N1	-3.39	122.28	127.44
2	E	301[B]	3L5	N3-C2-N1	-3.38	122.29	127.44
2	H	301[A]	3L5	N3-C2-N1	-3.36	122.32	127.44
2	D	301[B]	3L5	C4-C5-N7	-3.36	106.39	109.48
2	F	301	3L5	N3-C2-N1	-3.36	122.33	127.44
2	D	301[A]	3L5	C4-C5-N7	-3.36	106.39	109.48
2	H	301[B]	3L5	N3-C2-N1	-3.36	122.33	127.44
2	A	301[B]	3L5	C4-C5-N7	-3.34	106.40	109.48
2	D	301[B]	3L5	N3-C2-N1	-3.34	122.35	127.44
2	E	301[A]	3L5	N3-C2-N1	-3.31	122.40	127.44
2	F	301	3L5	C4-C5-N7	-3.31	106.44	109.48
2	A	301[A]	3L5	N3-C2-N1	-3.30	122.41	127.44
2	A	301[B]	3L5	N3-C2-N1	-3.25	122.50	127.44
2	E	301[A]	3L5	C4-C5-N7	-3.22	106.52	109.48
2	G	301	3L5	C4-C5-N7	-3.08	106.64	109.48
2	F	301	3L5	PBB-CAP-CAK	-3.04	110.03	114.39
2	B	301	3L5	C4-C5-N7	-3.04	106.68	109.48
2	E	301[B]	3L5	C4-C5-N7	-2.96	106.76	109.48
2	C	301[B]	3L5	PBB-CAP-CAK	-2.41	110.94	114.39
2	E	301[B]	3L5	PBB-CAP-CAK	-2.26	111.16	114.39
2	D	301[A]	3L5	PBB-CAP-CAK	-2.08	111.41	114.39
2	B	301	3L5	PBB-CAP-CAK	-2.05	111.45	114.39
2	H	301[B]	3L5	PBB-CAP-CAK	-2.02	111.50	114.39
2	D	301[B]	3L5	CAL-NAZ-CAM	2.11	116.53	111.45
2	H	301[B]	3L5	CAJ-OAU-CAK	2.42	123.72	113.31
2	C	301[A]	3L5	CAJ-OAU-CAK	3.13	126.75	113.31
2	C	301[A]	3L5	OAU-CAK-CAP	3.18	119.00	109.28
2	E	301[A]	3L5	C6-N1-C2	3.46	120.73	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301[B]	3L5	C6-N1-C2	3.46	120.74	115.94
2	G	301	3L5	C6-N1-C2	3.56	120.88	115.94
2	B	301	3L5	C6-N1-C2	3.57	120.89	115.94
2	A	301[B]	3L5	C6-N1-C2	3.57	120.90	115.94
2	D	301[A]	3L5	C6-N1-C2	3.58	120.91	115.94
2	D	301[B]	3L5	C6-N1-C2	3.60	120.93	115.94
2	A	301[A]	3L5	C6-N1-C2	3.63	120.98	115.94
2	F	301	3L5	C6-N1-C2	3.72	121.10	115.94
2	H	301[B]	3L5	CAN-NAZ-CAM	3.74	120.43	111.45
2	C	301[B]	3L5	C6-N1-C2	3.81	121.23	115.94
2	H	301[B]	3L5	C6-N1-C2	3.85	121.28	115.94
2	H	301[A]	3L5	C6-N1-C2	3.88	121.33	115.94
2	C	301[A]	3L5	C6-N1-C2	3.90	121.35	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301[B]	3L5	2	0
2	D	301[B]	3L5	1	0
2	E	301[A]	3L5	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	197/217 (90%)	0.62	18 (9%) 11 12	25, 39, 85, 107	0
1	B	207/217 (95%)	0.59	17 (8%) 14 15	26, 40, 83, 99	0
1	C	202/217 (93%)	0.36	12 (5%) 26 27	27, 43, 71, 91	0
1	D	202/217 (93%)	0.67	20 (9%) 9 10	25, 43, 67, 99	0
1	E	206/217 (94%)	1.13	43 (20%) 1 1	29, 48, 90, 134	0
1	F	197/217 (90%)	0.36	12 (6%) 25 26	24, 38, 82, 101	0
1	G	200/217 (92%)	1.27	45 (22%) 1 1	36, 66, 109, 123	0
1	H	208/217 (95%)	0.94	34 (16%) 2 3	28, 46, 86, 97	0
All	All	1619/1736 (93%)	0.74	201 (12%) 5 6	24, 44, 88, 134	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	173	TYR	11.5
1	E	121	LEU	9.0
1	C	113	ILE	7.1
1	E	117	GLY	6.9
1	G	144	THR	6.9
1	E	217	ALA	6.9
1	D	217	ALA	6.3
1	A	169	ARG	6.3
1	B	111	GLY	5.8
1	B	217	ALA	5.7
1	H	104	TYR	5.6
1	G	148	LEU	5.6
1	H	171	VAL	5.3
1	E	168	PRO	5.2
1	E	90	ARG	5.1
1	D	92	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	112	ASP	4.7
1	E	116	ILE	4.7
1	G	145	LEU	4.7
1	E	118	GLY	4.6
1	E	216	LYS	4.6
1	A	168	PRO	4.6
1	H	217	ALA	4.3
1	C	213	ALA	4.3
1	H	210	THR	4.2
1	E	210	THR	4.1
1	E	59	HIS	4.1
1	A	210	THR	4.1
1	D	4	SER	4.1
1	H	209	GLU	4.0
1	D	173	TYR	4.0
1	G	152	TYR	4.0
1	B	121	LEU	4.0
1	E	104	TYR	4.0
1	E	211	GLY	3.9
1	G	167	THR	3.9
1	E	71	TYR	3.8
1	C	211	GLY	3.8
1	B	152	TYR	3.8
1	H	169	ARG	3.8
1	G	125	THR	3.8
1	H	103	SER	3.7
1	G	143	GLN	3.7
1	G	217	ALA	3.7
1	G	58	GLY	3.6
1	E	113	ILE	3.6
1	E	209	GLU	3.5
1	E	167	THR	3.5
1	A	121	LEU	3.5
1	E	103	SER	3.5
1	G	120	ASP	3.5
1	A	209	GLU	3.4
1	G	5	PRO	3.4
1	G	89	ASP	3.4
1	G	140	LYS	3.4
1	H	211	GLY	3.4
1	F	60	HIS	3.4
1	C	90	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	117	GLY	3.4
1	C	114	LYS	3.3
1	G	121	LEU	3.3
1	E	197	TYR	3.3
1	G	113	ILE	3.2
1	D	140	LYS	3.2
1	F	92	ILE	3.2
1	A	170	SER	3.2
1	E	73	PHE	3.2
1	H	207	ILE	3.2
1	D	169	ARG	3.1
1	G	90	ARG	3.1
1	G	92	ILE	3.1
1	G	75	ALA	3.1
1	H	89	ASP	3.1
1	F	125	THR	3.1
1	F	173	TYR	3.0
1	F	124	LEU	3.0
1	H	29	GLU	3.0
1	D	172	GLY	3.0
1	E	120	ASP	3.0
1	G	150	ARG	3.0
1	B	103	SER	3.0
1	B	209	GLU	3.0
1	G	149	VAL	3.0
1	G	29	GLU	3.0
1	G	115	VAL	3.0
1	H	208	SER	3.0
1	C	150	ARG	2.9
1	G	124	LEU	2.9
1	G	98	PHE	2.9
1	D	168	PRO	2.9
1	H	173	TYR	2.9
1	E	119	ASP	2.9
1	E	207	ILE	2.9
1	E	74	PHE	2.8
1	E	72	LYS	2.8
1	C	209	GLU	2.8
1	F	89	ASP	2.8
1	B	174	LYS	2.8
1	H	216	LYS	2.8
1	G	122	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	147	SER	2.8
1	B	151	GLN	2.8
1	D	12	ASP	2.8
1	H	112	ASP	2.8
1	H	73	PHE	2.7
1	H	117	GLY	2.7
1	G	210	THR	2.7
1	G	23	ILE	2.7
1	B	148	LEU	2.7
1	C	194	TYR	2.7
1	A	89	ASP	2.7
1	G	25	ASN	2.7
1	H	168	PRO	2.7
1	E	213	ALA	2.7
1	D	216	LYS	2.6
1	D	54	LYS	2.6
1	D	74	PHE	2.6
1	H	212	LYS	2.5
1	D	71	TYR	2.5
1	D	167	THR	2.5
1	E	75	ALA	2.5
1	G	139	GLY	2.5
1	E	185	LYS	2.5
1	H	65	CYS	2.5
1	E	172	GLY	2.5
1	G	101	LEU	2.5
1	B	58	GLY	2.5
1	B	92	ILE	2.5
1	G	168	PRO	2.5
1	E	65	CYS	2.5
1	D	101	LEU	2.4
1	F	174	LYS	2.4
1	E	99	ILE	2.4
1	H	28	ALA	2.4
1	B	4	SER	2.4
1	B	216	LYS	2.4
1	H	151	GLN	2.4
1	E	186	PHE	2.4
1	D	209	GLU	2.4
1	G	215	TYR	2.4
1	E	212	LYS	2.4
1	B	171	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	215	TYR	2.4
1	A	75	ALA	2.4
1	A	213	ALA	2.4
1	G	59	HIS	2.4
1	E	63	ALA	2.3
1	F	75	ALA	2.3
1	E	111	GLY	2.3
1	A	116	ILE	2.3
1	C	212	LYS	2.3
1	G	174	LYS	2.3
1	E	4	SER	2.3
1	H	190	TYR	2.3
1	H	75	ALA	2.3
1	G	57	GLY	2.3
1	A	77	LEU	2.3
1	E	70	GLY	2.3
1	H	90	ARG	2.3
1	G	54	LYS	2.3
1	A	217	ALA	2.3
1	C	29	GLU	2.2
1	D	174	LYS	2.2
1	E	151	GLN	2.2
1	E	194	TYR	2.2
1	H	71	TYR	2.2
1	F	123	THR	2.2
1	B	75	ALA	2.2
1	H	121	LEU	2.2
1	H	140	LYS	2.2
1	H	116	ILE	2.2
1	H	213	ALA	2.2
1	A	78	LEU	2.2
1	G	146	LEU	2.2
1	G	216	LYS	2.2
1	A	122	SER	2.1
1	B	122	SER	2.1
1	G	126	GLY	2.1
1	C	186	PHE	2.1
1	D	207	ILE	2.1
1	H	113	ILE	2.1
1	F	150	ARG	2.1
1	A	65	CYS	2.1
1	F	103	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	32	GLU	2.1
1	H	42	MET	2.1
1	E	115	VAL	2.1
1	G	151	GLN	2.1
1	D	144	THR	2.1
1	E	23	ILE	2.1
1	B	124	LEU	2.1
1	G	94	MET	2.1
1	A	80	TYR	2.1
1	E	38	HIS	2.0
1	D	117	GLY	2.0
1	G	194	TYR	2.0
1	E	76	ASP	2.0
1	G	74	PHE	2.0
1	H	74	PHE	2.0
1	A	216	LYS	2.0
1	F	113	ILE	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
3	MG	A	302	1/1	0.87	0.23	3.95	69,69,69,69	0
3	MG	F	302	1/1	0.95	0.17	3.32	48,48,48,48	0
2	3L5	C	301[A]	29/29	0.85	0.24	2.58	31,45,168,170	48
2	3L5	C	301[B]	29/29	0.85	0.24	2.47	31,45,172,173	48

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3L5	E	301[B]	29/29	0.82	0.26	1.89	48,70,112,113	48
2	3L5	E	301[A]	29/29	0.82	0.26	1.76	47,68,87,112	48
2	3L5	A	301[A]	29/29	0.88	0.21	0.75	35,73,93,127	48
2	3L5	A	301[B]	29/29	0.88	0.21	0.73	34,66,90,102	48
2	3L5	D	301[A]	29/29	0.87	0.19	0.69	36,44,83,83	48
2	3L5	D	301[B]	29/29	0.87	0.19	0.65	36,44,85,86	48
2	3L5	G	301	29/29	0.85	0.22	0.36	56,83,169,169	0
2	3L5	B	301	29/29	0.93	0.14	0.06	35,48,107,107	0
2	3L5	H	301[B]	29/29	0.89	0.16	-0.07	36,44,64,64	48
2	3L5	H	301[A]	29/29	0.89	0.16	-0.12	35,42,53,54	48
3	MG	C	302	1/1	0.94	0.12	-0.17	53,53,53,53	0
2	3L5	F	301	29/29	0.97	0.12	-0.23	27,36,51,51	0
3	MG	H	302	1/1	0.88	0.14	-0.81	80,80,80,80	0
3	MG	B	302	1/1	0.92	0.10	-1.33	53,53,53,53	0
3	MG	G	302	1/1	0.97	0.10	-1.48	118,118,118,118	0
3	MG	D	302	1/1	0.82	0.10	-2.22	55,55,55,55	0
3	MG	B	303	1/1	0.71	0.15	-	78,78,78,78	0
3	MG	F	303	1/1	0.97	0.06	-	51,51,51,51	0

## 6.5 Other polymers

There are no such residues in this entry.