



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:59 pm GMT

PDB ID : 1OUM  
Title : M64V PNP +Talo  
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Deposited on : 2003-03-24  
Resolution : 2.40 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 : trunk28620  
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) : recalc28949

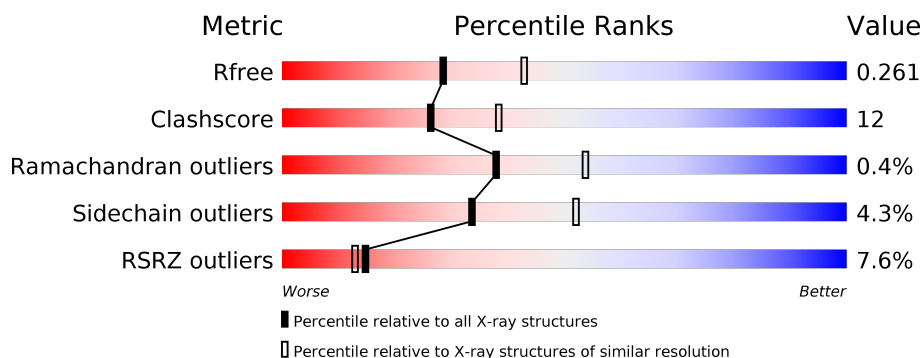
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	238	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>24%</div> </div> </div>
1	B	238	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>•</div> </div> </div>
1	C	238	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5638 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.

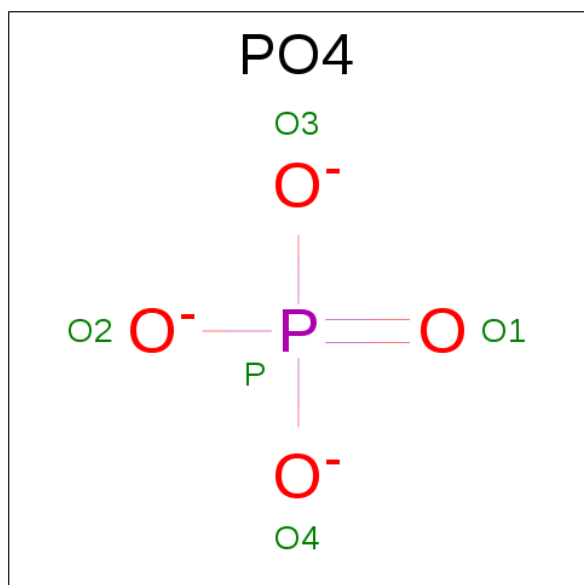
- Molecule 1 is a protein called Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1792	1132	307	339	14			
1	B	237	Total	C	N	O	S	0	0	0
			1792	1132	307	339	14			
1	C	237	Total	C	N	O	S	0	0	0
			1792	1132	307	339	14			

There are 3 discrepancies between the modelled and reference sequences:

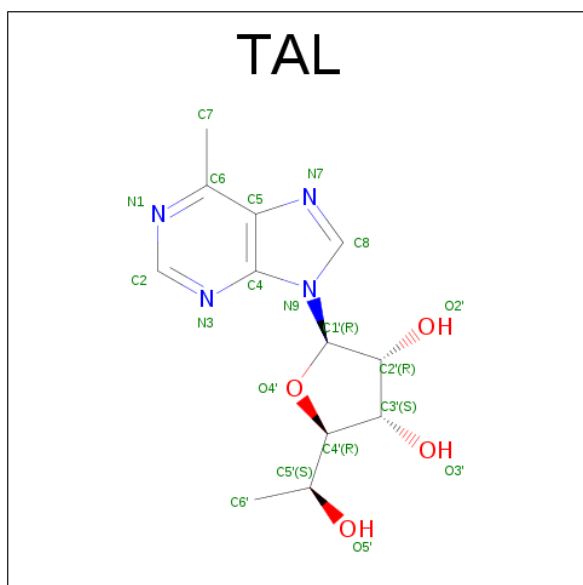
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	VAL	MET	ENGINEERED	UNP P0ABP8
B	64	VAL	MET	ENGINEERED	UNP P0ABP8
C	64	VAL	MET	ENGINEERED	UNP P0ABP8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is 9-(6-DEOXY-ALPHA-L-TALOFURANOSYL)-6-METHYLPURINE (three-letter code: TAL) (formula: C<sub>12</sub>H<sub>16</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	12	4	4		
3	B	1	Total	C	N	O	0	0
			20	12	4	4		
3	C	1	Total	C	N	O	0	0
			20	12	4	4		

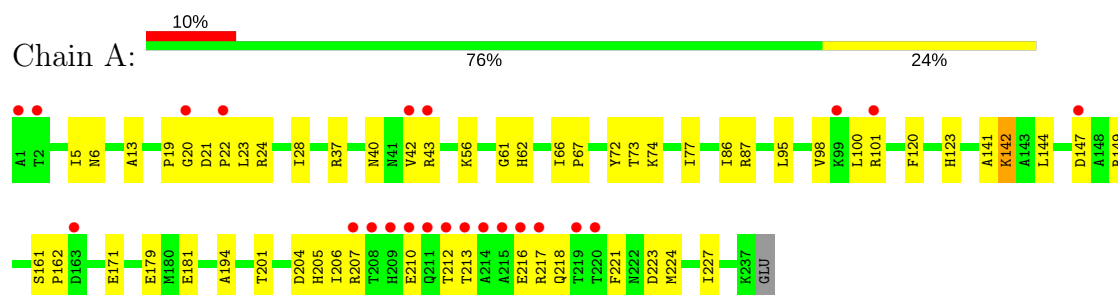
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	77	Total	O	0	0
			77	77		
4	C	60	Total	O	0	0
			60	60		

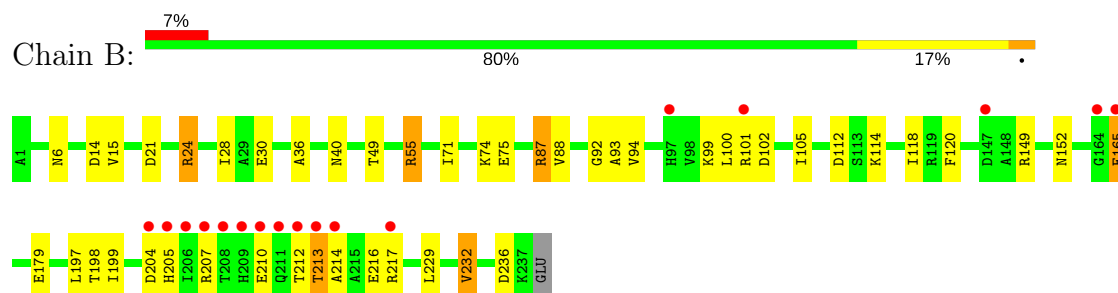
### 3 Residue-property plots [i](#)

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.

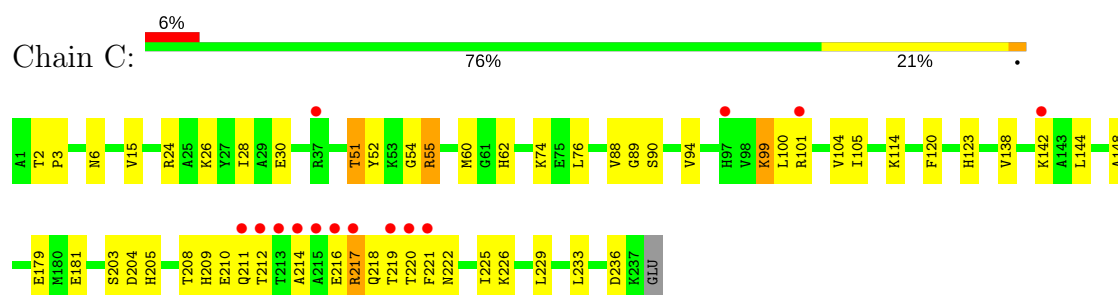
#### • Molecule 1: Purine nucleoside phosphorylase



#### • Molecule 1: Purine nucleoside phosphorylase



#### • Molecule 1: Purine nucleoside phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.94Å 120.94Å 241.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.90 – 2.40 37.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.90-2.40) 99.8 (37.77-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.21 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.228 , 0.260 0.227 , 0.261	Depositor DCC
$R_{free}$ test set	4216 reflections (10.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5638	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 5.29% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAL, PO4

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	0.38	1/1821 (0.1%)	0.95	5/2457 (0.2%)
1	B	0.36	0/1821	0.62	0/2457
1	C	0.33	0/1821	0.61	0/2457
All	All	0.36	1/5463 (0.0%)	0.74	5/7371 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ASP	N-CA	-5.50	1.35	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	C-N-CD	-32.87	48.28	120.60
1	A	21	ASP	C-N-CA	9.00	159.78	122.00
1	A	21	ASP	N-CA-C	-6.64	93.06	111.00
1	A	20	GLY	O-C-N	6.64	133.32	122.70
1	A	20	GLY	CA-C-N	-5.07	106.05	117.20

There are no chirality outliers.

There are no planarity outliers.

### 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	1792	0	1791	40	0
1	B	1792	0	1791	41	0
1	C	1792	0	1791	48	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	20	0	16	0	0
3	B	20	0	16	1	0
3	C	20	0	16	1	0
4	A	55	0	0	1	0
4	B	77	0	0	4	0
4	C	60	0	0	1	0
All	All	5638	0	5421	127	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 12.

All (127) 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:87:ARG:CD	1:B:198:THR:HG23	1.83	1.09
1:B:87:ARG:HD3	1:B:198:THR:HG23	1.33	1.07
1:B:87:ARG:CG	1:B:198:THR:HG23	1.92	0.99
1:A:42:VAL:HG12	1:A:43:ARG:HD2	1.41	0.98
1:C:101:ARG:O	1:C:220:THR:HG21	1.64	0.95
1:B:87:ARG:HD3	1:B:198:THR:CG2	1.96	0.93
1:C:90:SER:HB2	1:C:203:SER:HB2	1.53	0.90
1:A:142:LYS:HE3	1:A:142:LYS:HA	1.55	0.88
1:B:87:ARG:HG2	1:B:198:THR:HG23	1.55	0.84
1:A:144:LEU:HD12	1:A:227:ILE:HD13	1.66	0.78
1:A:100:LEU:HD22	1:A:210:GLU:HB2	1.68	0.74
1:C:219:THR:HA	1:C:222:ASN:HD22	1.57	0.70
1:C:204:ASP:HB3	1:C:211:GLN:HA	1.74	0.70
1:B:229:LEU:O	1:B:232:VAL:HG13	1.93	0.69
1:C:138:VAL:O	1:C:142:LYS:HG2	1.94	0.68
1:A:141:ALA:HA	1:A:227:ILE:HD12	1.75	0.67
1:A:23:LEU:HD21	1:A:221:PHE:CG	2.29	0.67
1:B:205:HIS:ND1	1:B:207:ARG:HB2	2.11	0.66
1:C:221:PHE:O	1:C:225:ILE:HG12	1.96	0.66
1:B:87:ARG:CD	1:B:198:THR:CG2	2.64	0.65
1:B:101:ARG:NH1	1:B:216:GLU:HB3	2.10	0.65
1:A:101:ARG:NH1	1:A:216:GLU:HB3	2.12	0.65
1:B:87:ARG:HG2	1:B:198:THR:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:O	1:B:102:ASP:HB2	1.98	0.62
1:C:100:LEU:HD11	1:C:204:ASP:HA	1.82	0.62
1:C:24:ARG:NH2	1:C:89:GLY:HA2	2.14	0.62
1:A:73:THR:O	1:A:77:ILE:HG12	2.00	0.62
1:A:201:THR:HG23	1:A:224:MET:SD	2.39	0.61
1:A:223:ASP:O	1:A:227:ILE:HG12	2.01	0.61
1:B:213:THR:HG22	4:B:273:HOH:O	2.00	0.61
1:B:214:ALA:HB1	4:B:254:HOH:O	2.02	0.60
1:A:141:ALA:HA	1:A:227:ILE:CD1	2.32	0.60
1:C:55:ARG:HD3	1:C:236:ASP:OD2	2.01	0.59
1:B:24:ARG:O	1:B:28:ILE:HG12	2.03	0.58
1:A:100:LEU:HD23	1:A:212:THR:HG23	1.86	0.58
1:A:5:ILE:HD11	1:A:72:TYR:HD1	1.68	0.57
1:C:55:ARG:HG3	1:C:233:LEU:HD23	1.84	0.57
1:C:208:THR:OG1	1:C:210:GLU:HG2	2.04	0.57
1:C:219:THR:O	1:C:222:ASN:HB2	2.04	0.57
1:A:6:ASN:H	1:A:40:ASN:ND2	2.02	0.57
1:B:105:ILE:HG12	1:B:199:ILE:HD12	1.87	0.57
1:B:87:ARG:HG2	1:B:198:THR:CG2	2.33	0.56
1:A:206:ILE:HG22	1:A:206:ILE:O	2.06	0.56
1:A:100:LEU:O	1:A:101:ARG:HB2	2.06	0.56
1:B:197:LEU:HD21	1:B:199:ILE:HD11	1.86	0.56
1:B:55:ARG:HD2	1:B:236:ASP:OD2	2.07	0.55
1:B:149:ARG:HH11	1:B:149:ARG:HG2	1.71	0.55
1:B:205:HIS:CE1	1:B:207:ARG:HB2	2.42	0.55
1:A:123:HIS:HD2	1:C:114:LYS:NZ	2.05	0.55
1:C:101:ARG:HB3	1:C:220:THR:OG1	2.07	0.54
1:B:165:GLU:OE1	1:B:165:GLU:N	2.41	0.53
1:A:100:LEU:HB2	1:A:210:GLU:OE1	2.08	0.53
1:C:90:SER:HB2	1:C:203:SER:CB	2.35	0.53
1:B:14:ASP:OD2	1:B:15:VAL:HG23	2.07	0.53
1:A:98:VAL:O	1:A:205:HIS:HE1	1.91	0.53
1:C:212:THR:HB	1:C:217:ARG:HG3	1.91	0.52
1:C:74:LYS:HD3	1:C:74:LYS:C	2.29	0.52
1:C:24:ARG:HH21	1:C:89:GLY:HA2	1.74	0.52
1:C:52:TYR:CD2	1:C:229:LEU:HD13	2.45	0.52
3:C:247:TAL:N3	3:C:247:TAL:H2'	2.24	0.52
1:C:105:ILE:HD12	1:C:105:ILE:N	2.25	0.52
1:B:213:THR:O	1:B:214:ALA:HB2	2.10	0.51
1:B:212:THR:OG1	1:B:217:ARG:HG3	2.10	0.51
1:A:141:ALA:CA	1:A:227:ILE:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:CE1	1:C:181:GLU:HG2	2.45	0.50
1:C:99:LYS:HD2	1:C:99:LYS:N	2.26	0.50
1:A:13:ALA:HB2	1:A:56:LYS:HG2	1.94	0.50
1:A:74:LYS:HD3	1:A:74:LYS:C	2.31	0.50
1:C:217:ARG:NE	4:C:255:HOH:O	2.44	0.50
1:C:219:THR:HA	1:C:222:ASN:ND2	2.26	0.49
1:B:87:ARG:HD3	1:B:198:THR:HG21	1.91	0.49
1:A:19:PRO:HD2	1:A:61:GLY:HA2	1.94	0.49
1:B:6:ASN:H	1:B:40:ASN:ND2	2.09	0.49
1:C:60:MET:CE	1:C:76:LEU:HD11	2.42	0.49
1:B:74:LYS:HD3	1:B:74:LYS:C	2.32	0.49
1:C:105:ILE:HD13	1:C:148:ALA:HB1	1.96	0.48
1:B:100:LEU:HD22	1:B:100:LEU:N	2.28	0.48
1:C:208:THR:O	1:C:209:HIS:HB2	2.12	0.48
1:C:218:GLN:HA	1:C:221:PHE:CD1	2.49	0.48
1:B:204:ASP:HA	1:B:210:GLU:O	2.13	0.48
1:C:88:VAL:O	1:C:88:VAL:HG23	2.14	0.48
1:B:88:VAL:HG23	1:B:88:VAL:O	2.14	0.47
1:A:205:HIS:C	1:A:207:ARG:H	2.15	0.47
1:C:204:ASP:CB	1:C:211:GLN:HA	2.44	0.47
1:A:213:THR:O	1:A:217:ARG:HG2	2.14	0.47
1:A:86:ILE:HD12	1:A:86:ILE:N	2.28	0.47
1:C:99:LYS:HD2	1:C:99:LYS:H	1.79	0.47
1:A:23:LEU:HD21	1:A:221:PHE:CD1	2.48	0.47
1:C:15:VAL:HG12	1:C:55:ARG:NH2	2.30	0.47
1:C:51:THR:HG23	1:C:54:GLY:H	1.80	0.47
1:C:104:VAL:C	1:C:105:ILE:HD12	2.35	0.46
1:C:214:ALA:O	1:C:217:ARG:HB2	2.15	0.46
1:C:55:ARG:HG3	1:C:233:LEU:CD2	2.45	0.46
1:A:161:SER:HA	1:A:162:PRO:HD3	1.81	0.46
1:B:36:ALA:HA	1:B:49:THR:O	2.17	0.45
1:C:2:THR:HB	1:C:3:PRO:CD	2.47	0.44
1:B:118:ILE:HD11	1:C:123:HIS:HE1	1.82	0.44
1:A:77:ILE:HD12	1:A:194:ALA:CB	2.47	0.44
1:C:100:LEU:O	1:C:101:ARG:HB2	2.18	0.44
1:A:218:GLN:OE1	1:A:218:GLN:HA	2.17	0.44
1:B:71:ILE:O	1:B:75:GLU:HG3	2.17	0.44
1:A:98:VAL:HA	1:A:149:ARG:NH2	2.33	0.43
1:B:217:ARG:HD2	4:B:287:HOH:O	2.18	0.43
1:C:205:HIS:HB3	1:C:208:THR:OG1	2.17	0.43
1:C:26:LYS:O	1:C:30:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:O	1:C:28:ILE:HG13	2.18	0.43
1:A:37:ARG:HG2	4:A:263:HOH:O	2.17	0.43
1:A:5:ILE:HD11	1:A:72:TYR:CD1	2.52	0.43
1:B:21:ASP:HB3	1:B:24:ARG:HB2	2.01	0.43
1:A:95:LEU:HD23	1:A:171:GLU:HG3	2.01	0.43
1:A:62:HIS:CE1	1:A:181:GLU:HG2	2.54	0.43
1:A:23:LEU:HD11	1:A:224:MET:CE	2.48	0.43
1:B:93:ALA:HB3	1:B:205:HIS:HA	2.02	0.42
1:C:99:LYS:HB3	1:C:99:LYS:HE3	1.83	0.42
1:B:118:ILE:CD1	1:C:123:HIS:HE1	2.33	0.42
1:C:216:GLU:O	1:C:217:ARG:O	2.38	0.42
1:A:24:ARG:O	1:A:28:ILE:HG12	2.19	0.42
1:A:23:LEU:HD21	1:A:221:PHE:HB3	2.01	0.42
1:C:214:ALA:HB1	1:C:216:GLU:OE1	2.20	0.42
1:A:66:ILE:HB	1:A:67:PRO:HD3	2.00	0.42
1:B:114:LYS:O	1:B:118:ILE:HG12	2.20	0.41
1:B:214:ALA:CB	4:B:254:HOH:O	2.66	0.41
1:C:60:MET:HE2	1:C:76:LEU:HD11	2.01	0.41
1:C:144:LEU:HD11	1:C:226:LYS:HG3	2.03	0.41
1:B:87:ARG:HG2	1:B:198:THR:CA	2.50	0.41
1:A:6:ASN:H	1:A:40:ASN:HD21	1.67	0.41
1:B:92:GLY:HA3	3:B:246:TAL:H73	2.03	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	235/238 (99%)	217 (92%)	17 (7%)	1 (0%)	38	54
1	B	235/238 (99%)	224 (95%)	10 (4%)	1 (0%)	38	54
1	C	235/238 (99%)	224 (95%)	10 (4%)	1 (0%)	38	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	705/714 (99%)	665 (94%)	37 (5%)	3 (0%)	38 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	PRO
1	C	217	ARG
1	B	213	THR

### 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	187/189 (99%)	181 (97%)	6 (3%)	44 65
1	B	187/189 (99%)	176 (94%)	11 (6%)	23 36
1	C	187/189 (99%)	180 (96%)	7 (4%)	39 59
All	All	561/567 (99%)	537 (96%)	24 (4%)	33 52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	120	PHE
1	A	142	LYS
1	A	147	ASP
1	A	179	GLU
1	A	204	ASP
1	B	24	ARG
1	B	30	GLU
1	B	55	ARG
1	B	87	ARG
1	B	94	VAL
1	B	112	ASP
1	B	120	PHE

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Mol	Chain	Res	Type
1	B	152	ASN
1	B	165	GLU
1	B	179	GLU
1	B	232	VAL
1	C	6	ASN
1	C	51	THR
1	C	55	ARG
1	C	94	VAL
1	C	99	LYS
1	C	120	PHE
1	C	179	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	116	ASN
1	A	123	HIS
1	A	205	HIS
1	B	40	ASN
1	B	152	ASN
1	B	218	GLN
1	B	222	ASN
1	C	6	ASN
1	C	116	ASN
1	C	222	ASN

### 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

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	TAL	A	245	-	19,22,22	6.83	6 (31%)	18,33,33	1.39	2 (11%)
3	TAL	B	246	-	19,22,22	6.70	4 (21%)	18,33,33	2.29	5 (27%)
2	PO4	B	248	-	4,4,4	1.48	0	6,6,6	0.38	0
3	TAL	C	247	-	19,22,22	6.62	3 (15%)	18,33,33	1.28	3 (16%)
2	PO4	C	249	-	4,4,4	1.43	0	6,6,6	0.37	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	TAL	A	245	-	-	0/4/24/24	0/3/3/3
3	TAL	B	246	-	-	0/4/24/24	0/3/3/3
2	PO4	B	248	-	-	0/0/0/0	0/0/0/0
3	TAL	C	247	-	-	0/4/24/24	0/3/3/3
2	PO4	C	249	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	245	TAL	C7-C6	-28.92	1.31	1.50
3	C	247	TAL	C7-C6	-28.35	1.32	1.50
3	B	246	TAL	C7-C6	-28.19	1.32	1.50
3	B	246	TAL	C6'-C5'	-5.05	1.35	1.51
3	A	245	TAL	C6'-C5'	-2.51	1.43	1.51
3	A	245	TAL	C8-N7	-2.06	1.30	1.34
3	A	245	TAL	C2-N3	2.07	1.35	1.32
3	B	246	TAL	C2'-C1'	2.21	1.57	1.53
3	A	245	TAL	C2'-C1'	2.49	1.57	1.53
3	C	247	TAL	C2'-C1'	2.57	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	246	TAL	C6-N1	2.72	1.35	1.32
3	C	247	TAL	C6-N1	2.74	1.35	1.32
3	A	245	TAL	C6-N1	3.24	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	246	TAL	C6'-C5'-C4'	-5.47	105.59	112.10
3	B	246	TAL	O5'-C5'-C6'	-5.46	92.64	109.70
3	C	247	TAL	C6'-C5'-C4'	2.03	114.51	112.10
3	B	246	TAL	O5'-C5'-C4'	2.16	112.75	108.91
3	C	247	TAL	O4'-C4'-C5'	2.30	113.17	109.44
3	C	247	TAL	C1'-N9-C4	2.73	131.35	126.64
3	B	246	TAL	O4'-C4'-C5'	2.89	114.14	109.44
3	A	245	TAL	O4'-C4'-C5'	3.14	114.54	109.44
3	B	246	TAL	C1'-N9-C4	3.21	132.19	126.64
3	A	245	TAL	C1'-N9-C4	3.25	132.25	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	246	TAL	1	0
3	C	247	TAL	1	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	237/238 (99%)	0.36	23 (9%) 8 8	14, 24, 62, 72	0
1	B	237/238 (99%)	0.30	17 (7%) 16 15	13, 22, 53, 76	0
1	C	237/238 (99%)	0.09	14 (5%) 23 22	13, 23, 48, 68	0
All	All	711/714 (99%)	0.25	54 (7%) 15 13	13, 23, 54, 76	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	THR	16.4
1	B	213	THR	13.6
1	A	215	ALA	13.0
1	A	209	HIS	11.3
1	B	209	HIS	11.1
1	B	211	GLN	9.9
1	C	219	THR	9.5
1	A	208	THR	9.2
1	A	212	THR	9.0
1	B	208	THR	8.9
1	C	214	ALA	8.8
1	A	214	ALA	8.5
1	A	219	THR	8.2
1	B	205	HIS	8.2
1	A	207	ARG	8.2
1	A	211	GLN	8.2
1	B	207	ARG	8.0
1	A	213	THR	7.9
1	B	210	GLU	7.8
1	C	220	THR	7.4
1	C	215	ALA	7.2
1	C	213	THR	6.8
1	A	220	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	204	ASP	6.2
1	A	216	GLU	5.9
1	C	216	GLU	5.9
1	A	210	GLU	5.7
1	A	42	VAL	5.0
1	B	206	ILE	5.0
1	B	214	ALA	4.9
1	B	97	HIS	4.8
1	A	1	ALA	4.8
1	B	165	GLU	4.5
1	C	212	THR	4.4
1	A	43	ARG	4.0
1	C	221	PHE	3.7
1	B	147	ASP	3.5
1	C	211	GLN	3.4
1	C	217	ARG	3.3
1	A	147	ASP	3.1
1	A	2	THR	2.8
1	B	101	ARG	2.7
1	C	97	HIS	2.7
1	A	217	ARG	2.6
1	A	20	GLY	2.6
1	A	163	ASP	2.6
1	A	101	ARG	2.4
1	C	142	LYS	2.4
1	B	217	ARG	2.4
1	A	99	LYS	2.4
1	C	101	ARG	2.3
1	A	22	PRO	2.2
1	B	164	GLY	2.1
1	C	37	ARG	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	TAL	C	247	20/20	0.86	0.19	1.09	32,33,36,37	0
3	TAL	B	246	20/20	0.84	0.18	0.37	42,44,45,46	0
3	TAL	A	245	20/20	0.86	0.19	0.06	30,32,35,40	0
2	PO4	C	249	5/5	0.99	0.11	-0.52	21,21,22,23	0
2	PO4	B	248	5/5	0.99	0.10	-1.12	23,23,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.