



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:11 am GMT

PDB ID : 2OB1  
Title : ppm1 with 1,8-ANS  
Authors : Groves, M.R.  
Deposited on : 2006-12-18  
Resolution : 1.90 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

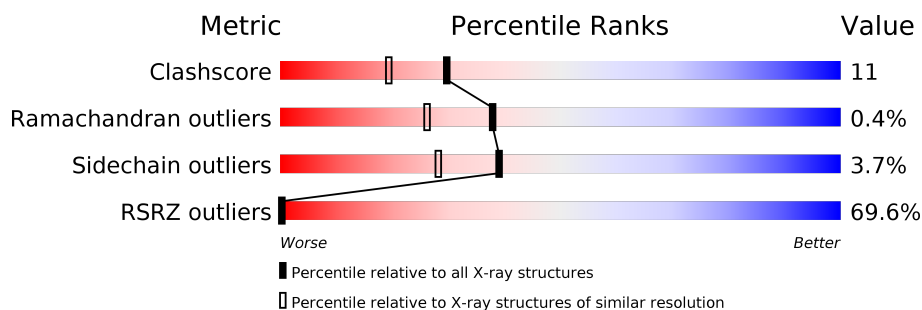
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	319	<div> <div>48%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	319	<div> <div>66%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	C	319	<div> <div>96%</div> <div> <div></div> <div>82%</div> <div>18%</div> <div>.</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	2001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	2003	-	-	-	X
2	PO4	C	2004	-	-	-	X

## 2 Entry composition [i](#)

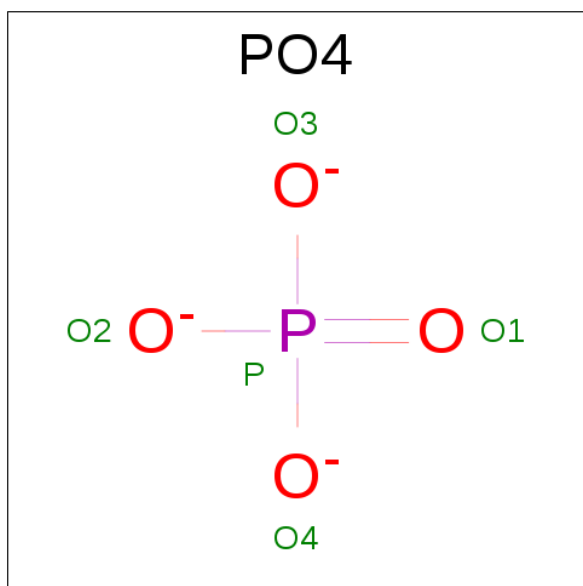
There are 3 unique types of molecules in this entry. The entry contains 8781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Leucine carboxyl methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	10	0
			2604	1663	436	485	20			
1	B	319	Total	C	N	O	S	0	12	0
			2622	1671	439	494	18			
1	C	319	Total	C	N	O	S	0	10	0
			2627	1671	443	493	20			

- 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		
2	A	1	Total	O	P	0	0
			5	4	1		

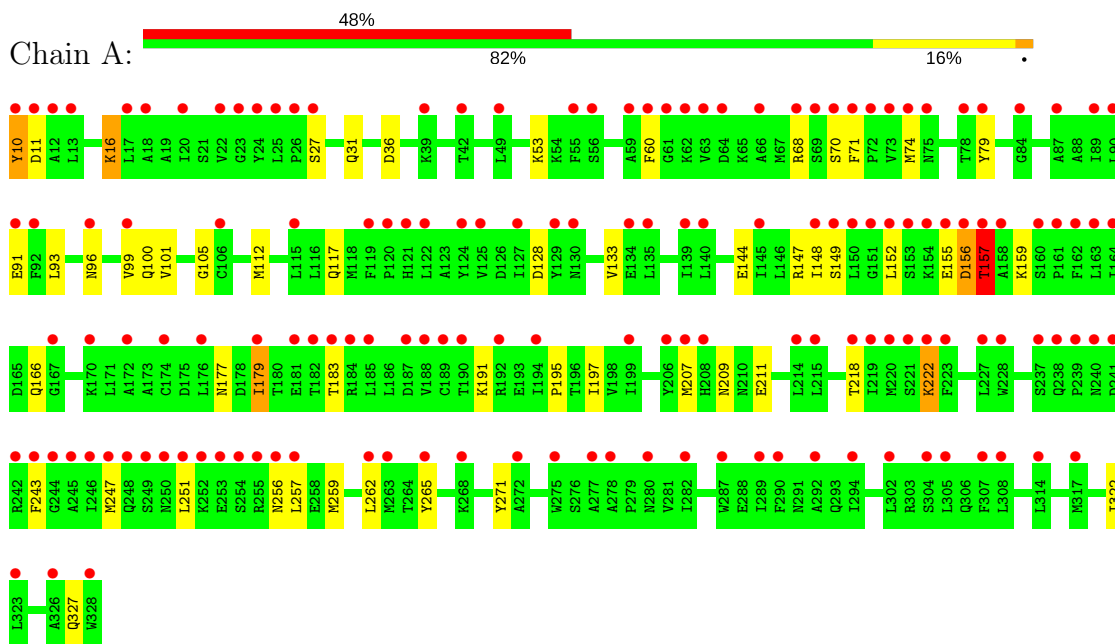
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	385	Total 385	O 385	0	0
3	B	318	Total 318	O 318	0	0
3	C	210	Total 210	O 210	0	0

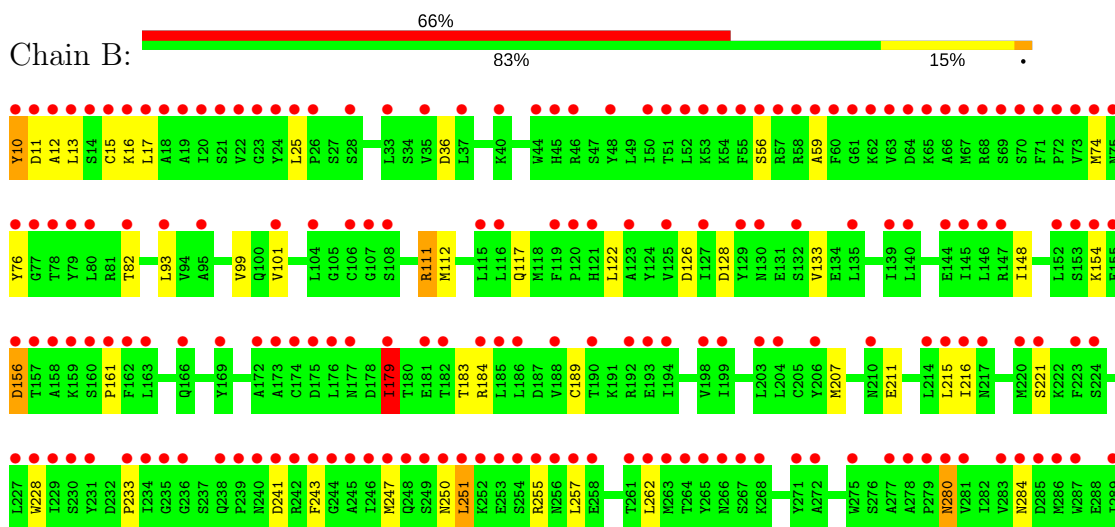
### 3 Residue-property plots

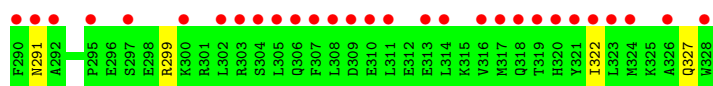
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Leucine carboxyl methyltransferase 1

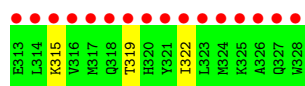
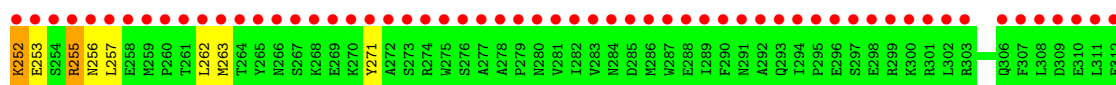
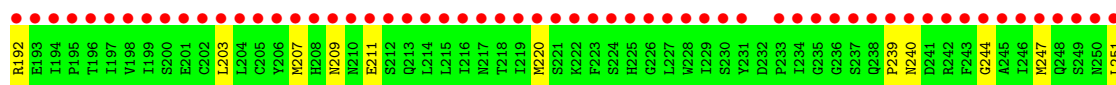
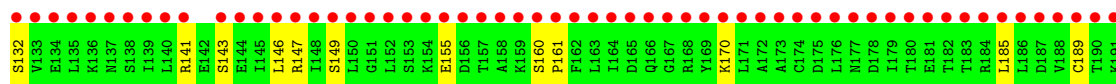
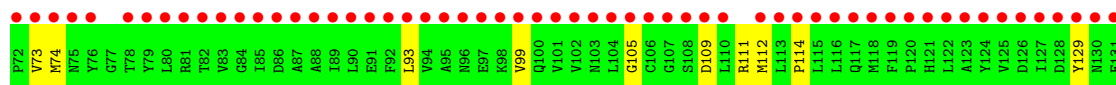
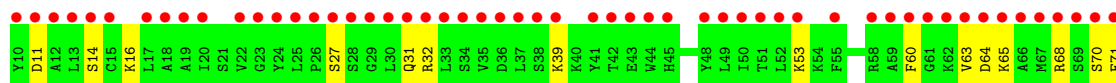
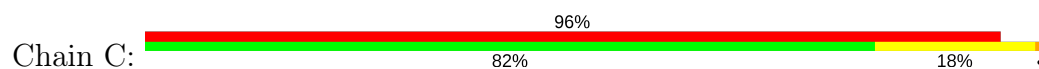


- Molecule 1: Leucine carboxyl methyltransferase 1





● Molecule 1: Leucine carboxyl methyltransferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.62Å 110.62Å 161.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.04 – 1.90 82.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (83.04-1.90) 92.6 (82.45-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.182 , 0.224 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	8781	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: 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	0.75	0/2683	0.80	0/3620
1	B	0.76	1/2695 (0.0%)	0.77	2/3640 (0.1%)
1	C	0.65	0/2682	0.70	0/3620
All	All	0.72	1/8060 (0.0%)	0.76	2/10880 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	CYS	CB-SG	-5.71	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ILE	CG1-CB-CG2	-6.13	97.92	111.40
1	B	111	ARG	CG-CD-NE	5.02	122.34	111.80

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	2604	0	2667	66	0
1	B	2622	0	2667	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2627	0	2657	55	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	385	0	0	18	1
3	B	318	0	0	14	1
3	C	210	0	0	7	0
All	All	8781	0	7991	170	1

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 11.

All (170) 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:36:ASP:HB3	3:B:2169:HOH:O	1.43	1.17
1:A:36:ASP:HB3	3:A:2324:HOH:O	1.54	1.07
1:A:179:ILE:HG22	3:A:2355:HOH:O	1.57	1.04
1:C:73:VAL:CG2	3:C:2198:HOH:O	2.05	1.03
1:A:247:MET:HE3	1:A:262:LEU:HD21	1.42	1.00
1:A:71:PHE:CE2	1:A:74[A]:MET:SD	2.58	0.97
1:C:73:VAL:HG21	3:C:2198:HOH:O	1.65	0.90
1:B:179:ILE:HD11	1:B:215:LEU:HA	1.57	0.85
1:B:93:LEU:HD22	1:B:99[A]:VAL:HG11	1.59	0.84
1:C:253:GLU:O	1:C:255:ARG:HD2	1.77	0.84
1:B:76:TYR:HE2	3:B:2299:HOH:O	1.60	0.82
1:B:243:PHE:HE2	1:B:247:MET:HE1	1.46	0.80
1:A:179:ILE:HD11	1:A:218:THR:HG21	1.62	0.80
1:A:247:MET:HE3	1:A:262:LEU:CD2	2.12	0.80
1:B:25:LEU:HD11	1:B:82[B]:THR:HG21	1.64	0.80
1:C:68:ARG:HD3	3:C:2187:HOH:O	1.82	0.80
1:A:117:GLN:HE22	1:B:36:ASP:H	1.27	0.80
1:B:179:ILE:HG12	3:B:2147:HOH:O	1.83	0.79
1:B:25:LEU:CD1	1:B:82[B]:THR:HG21	2.15	0.77
1:A:10:TYR:CD1	3:A:2094:HOH:O	2.38	0.76
1:B:161:PRO:O	3:B:2297:HOH:O	2.04	0.75
1:C:239:PRO:O	1:C:240:ASN:HB2	1.86	0.74
1:C:93:LEU:HD21	1:C:99[B]:VAL:HG21	1.68	0.72
1:B:179:ILE:O	1:B:183:THR:HG23	1.88	0.72
1:A:179:ILE:HD11	1:A:218:THR:CG2	2.19	0.72
1:A:149[A]:SER:OG	3:A:2320:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLN:NE2	1:B:36:ASP:H	1.88	0.71
1:A:36:ASP:H	1:B:117:GLN:HE22	1.38	0.71
1:C:149[B]:SER:OG	3:C:2185:HOH:O	2.08	0.71
1:A:179:ILE:HD11	1:A:218:THR:CB	2.21	0.70
1:B:101:VAL:HG23	1:B:122:LEU:HD11	1.74	0.69
1:B:243:PHE:CE2	1:B:247:MET:HE1	2.26	0.69
1:B:241:ASP:OD2	3:B:2154:HOH:O	2.10	0.69
1:B:93:LEU:CD2	1:B:99[A]:VAL:HG11	2.22	0.69
1:B:322:ILE:O	1:B:322:ILE:HD12	1.93	0.68
1:C:161:PRO:HB2	3:C:2188:HOH:O	1.92	0.67
1:C:322:ILE:O	1:C:322:ILE:HD12	1.93	0.67
1:A:27[B]:SER:H	1:A:31:GLN:HE21	1.40	0.67
1:B:221[B]:SER:OG	3:B:2087:HOH:O	2.12	0.67
1:A:11:ASP:HB3	3:A:2285:HOH:O	1.94	0.66
1:A:27[A]:SER:H	1:A:31:GLN:HE21	1.40	0.66
1:B:183:THR:HG21	3:B:2264:HOH:O	1.96	0.66
1:A:71:PHE:CZ	1:A:74[A]:MET:SD	2.91	0.64
1:B:243:PHE:CE2	1:B:247:MET:CE	2.81	0.64
1:A:247:MET:CE	1:A:262:LEU:HD21	2.26	0.63
1:A:183:THR:HG21	3:A:2173:HOH:O	1.97	0.62
1:A:10:TYR:HD1	3:A:2094:HOH:O	1.75	0.62
1:A:157:THR:HG23	3:A:2321:HOH:O	2.01	0.61
1:A:36:ASP:H	1:B:117:GLN:NE2	1.98	0.61
1:C:322:ILE:C	1:C:322:ILE:HD12	2.21	0.61
3:A:2217:HOH:O	1:C:68:ARG:CD	2.49	0.60
1:A:179:ILE:O	1:A:183:THR:HG23	2.02	0.60
1:B:243:PHE:HE2	1:B:247:MET:CE	2.13	0.60
1:A:27[B]:SER:H	1:A:31:GLN:NE2	2.00	0.59
3:A:2217:HOH:O	1:C:68:ARG:HD3	2.02	0.59
1:B:76:TYR:OH	3:B:2294:HOH:O	2.10	0.59
1:C:271:TYR:CE2	1:C:322:ILE:HD11	2.38	0.59
1:A:27[A]:SER:H	1:A:31:GLN:NE2	2.00	0.59
1:A:71:PHE:CD2	1:A:74[A]:MET:SD	2.96	0.59
1:A:144:GLU:HG2	1:A:148:ILE:HD12	1.85	0.58
1:B:76:TYR:CE2	3:B:2299:HOH:O	2.46	0.57
1:A:322:ILE:C	1:A:322:ILE:HD12	2.25	0.57
1:C:247:MET:HE2	1:C:262:LEU:CD2	2.35	0.57
1:C:32:ARG:O	1:C:32:ARG:HG2	2.05	0.57
1:B:184:ARG:HG3	3:B:2172:HOH:O	2.05	0.56
1:C:255:ARG:HD2	1:C:255:ARG:H	1.70	0.56
1:C:32:ARG:O	1:C:32:ARG:CG	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:HA	1:A:74[A]:MET:HE1	1.89	0.55
1:A:105:GLY:O	3:A:2112:HOH:O	2.18	0.55
1:B:322:ILE:C	1:B:322:ILE:HD12	2.27	0.55
1:A:179:ILE:HD11	1:A:218:THR:HB	1.87	0.54
1:C:64:ASP:O	1:C:68:ARG:HG3	2.08	0.54
1:A:93:LEU:HD22	1:A:99[B]:VAL:HG21	1.90	0.54
1:B:327:GLN:NE2	3:B:2149:HOH:O	2.36	0.53
1:C:252:LYS:HA	1:C:252:LYS:HE3	1.90	0.53
1:A:10:TYR:N	1:A:10:TYR:HD2	2.07	0.53
1:C:207:MET:HE2	1:C:211:GLU:HG3	1.90	0.53
1:C:27:SER:H	1:C:31:GLN:NE2	2.06	0.53
1:A:117:GLN:HE22	1:B:36:ASP:N	2.03	0.53
1:C:247:MET:HE2	1:C:262:LEU:HD22	1.91	0.53
1:A:27[A]:SER:HG	1:A:79:TYR:HE1	1.55	0.52
1:C:255:ARG:O	1:C:257:LEU:HB2	2.10	0.52
1:A:243:PHE:CE2	1:A:247:MET:HE2	2.45	0.52
1:B:280:ASN:ND2	3:B:2321:HOH:O	2.43	0.52
1:A:10:TYR:N	1:A:10:TYR:CD2	2.78	0.52
1:A:271:TYR:CE2	1:A:322:ILE:HD11	2.45	0.52
1:C:129:TYR:CZ	1:C:132[B]:SER:OG	2.63	0.51
1:A:27[A]:SER:OG	1:A:79:TYR:HE1	1.94	0.51
1:B:207:MET:HE2	1:B:211:GLU:HB3	1.92	0.51
1:A:36:ASP:N	1:B:117:GLN:HE22	2.08	0.51
1:A:327:GLN:NE2	3:A:2209:HOH:O	2.43	0.50
1:B:291:ASN:HA	1:B:299:ARG:NH2	2.27	0.50
1:C:149[A]:SER:HB3	3:C:2185:HOH:O	2.10	0.50
1:A:96:ASN:O	1:A:99[A]:VAL:HG23	2.12	0.50
1:C:111:ARG:O	1:C:114:PRO:HD2	2.12	0.49
1:C:247:MET:CE	1:C:262:LEU:HD21	2.43	0.49
3:A:2217:HOH:O	1:C:68:ARG:HD2	2.12	0.49
1:A:156:ASP:HB3	3:A:2028:HOH:O	2.13	0.49
1:C:93:LEU:CD2	1:C:99[B]:VAL:HG21	2.39	0.49
1:C:141:ARG:O	1:C:147:ARG:HD3	2.11	0.49
1:C:71:PHE:CE2	1:C:74[A]:MET:SD	3.06	0.48
1:B:291:ASN:HA	1:B:299:ARG:HH22	1.78	0.48
1:A:91:GLU:HG2	3:A:2329:HOH:O	2.13	0.48
1:B:15:CYS:SG	1:B:74:MET:HE3	2.54	0.48
1:B:93:LEU:CD2	1:B:99[B]:VAL:HG11	2.44	0.47
1:C:143:SER:HB3	1:C:146:LEU:HD12	1.96	0.47
1:B:280:ASN:C	1:B:280:ASN:HD22	2.19	0.46
1:C:155:GLU:CD	1:C:155:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:SER:H	1:C:31:GLN:HE21	1.63	0.46
1:A:322:ILE:O	1:A:322:ILE:HD12	2.16	0.46
1:A:209:ASN:ND2	1:A:265:TYR:OH	2.49	0.45
1:A:243:PHE:CE2	1:A:247:MET:CE	2.99	0.45
1:A:179:ILE:CG2	3:A:2355:HOH:O	2.37	0.45
1:A:99[A]:VAL:HG22	1:A:195:PRO:HB2	1.99	0.45
1:C:315:LYS:O	1:C:319:THR:HG23	2.16	0.45
1:C:239:PRO:O	1:C:240:ASN:CB	2.59	0.45
1:C:207:MET:CE	1:C:211:GLU:HG3	2.47	0.45
1:A:152:LEU:HD23	1:A:166:GLN:HG2	2.00	0.44
1:A:128:ASP:HB3	1:A:133:VAL:HG13	2.00	0.44
1:A:71:PHE:CZ	1:A:74[A]:MET:HG3	2.53	0.44
1:B:247:MET:CE	1:B:262:LEU:HD21	2.47	0.44
1:C:105:GLY:HA3	1:C:203:LEU:HD13	1.99	0.44
1:C:71:PHE:CD2	1:C:74[A]:MET:SD	3.11	0.44
1:C:251:LEU:O	1:C:255:ARG:HG2	2.18	0.44
1:B:247:MET:O	1:B:251:LEU:HB2	2.18	0.44
1:C:71:PHE:CE1	1:C:74[A]:MET:HG3	2.53	0.44
1:A:222[B]:LYS:HE2	3:A:2246:HOH:O	2.18	0.44
1:B:284:ASN:ND2	3:B:2316:HOH:O	2.46	0.44
1:A:70:SER:HA	1:A:74[A]:MET:CE	2.47	0.43
1:B:154:LYS:HE2	3:B:2306:HOH:O	2.18	0.43
1:B:25:LEU:HD11	1:B:82[B]:THR:CG2	2.42	0.43
1:C:109:ASP:OD1	1:C:111:ARG:HG2	2.18	0.43
1:C:65:LYS:HG2	1:C:68:ARG:HH21	1.83	0.43
1:A:71:PHE:CE1	1:A:74[A]:MET:HG3	2.54	0.43
1:B:10:TYR:HD2	1:B:10:TYR:C	2.22	0.43
1:B:11:ASP:HB2	1:B:255:ARG:HH21	1.83	0.43
1:C:247:MET:CE	1:C:262:LEU:CD2	2.97	0.43
1:B:13:LEU:O	1:B:17:LEU:HG	2.19	0.43
1:A:16:LYS:HB2	1:A:16:LYS:HE3	1.81	0.42
1:A:251:LEU:HD11	1:A:259:MET:SD	2.59	0.42
1:C:192:ARG:HD3	3:C:2132:HOH:O	2.17	0.42
1:A:70:SER:OG	1:A:74[B]:MET:SD	2.72	0.42
1:B:10:TYR:C	1:B:10:TYR:CD2	2.91	0.42
1:A:207:MET:HE2	1:A:211:GLU:HB3	2.00	0.42
1:B:101:VAL:CG2	1:B:122:LEU:HD11	2.46	0.42
1:A:53:LYS:HA	1:A:60:PHE:HB2	2.01	0.42
1:B:10:TYR:CE2	1:B:12:ALA:HB3	2.54	0.42
1:B:56:SER:HB3	1:B:59:ALA:HB3	2.02	0.42
1:C:143:SER:CB	1:C:146:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14[A]:SER:OG	1:C:63:VAL:HA	2.20	0.42
1:B:25:LEU:HD21	1:B:82[B]:THR:CG2	2.50	0.42
1:C:170:LYS:CD	1:C:189:CYS:HB2	2.50	0.41
1:C:247:MET:HE2	1:C:262:LEU:HD21	2.00	0.41
1:B:233:PRO:HB2	1:B:247:MET:HE1	2.01	0.41
1:C:170:LYS:HD2	1:C:189:CYS:HB2	2.01	0.41
1:A:177:ASN:HD21	1:A:207:MET:HG2	1.85	0.41
1:A:179:ILE:CD1	1:A:218:THR:HB	2.50	0.41
1:C:53:LYS:HA	1:C:60:PHE:HB2	2.02	0.41
1:B:10:TYR:HE2	1:B:13:LEU:N	2.19	0.41
1:B:128:ASP:HB3	1:B:133:VAL:HG13	2.03	0.41
1:A:68:ARG:NH1	1:C:70:SER:O	2.45	0.41
1:C:322:ILE:C	1:C:322:ILE:CD1	2.88	0.41
1:B:101:VAL:HG23	1:B:122:LEU:CD1	2.44	0.41
1:B:216:ILE:HA	1:B:228:TRP:CH2	2.56	0.41
1:C:244:GLY:HA3	1:C:263:MET:SD	2.61	0.41
1:A:101:VAL:HG22	1:A:197:ILE:HB	2.03	0.40
1:A:191:LYS:CE	3:A:2169:HOH:O	2.69	0.40
1:A:99[A]:VAL:HG12	1:A:100:GLN:N	2.36	0.40
1:B:10:TYR:HE2	1:B:13:LEU:H	1.64	0.40
1:C:16:LYS:HB2	1:C:16:LYS:HE3	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2280:HOH:O	3:B:2065:HOH:O[3_565]	2.15	0.05

## 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	327/319 (102%)	321 (98%)	4 (1%)	2 (1%)	28	16
1	B	329/319 (103%)	322 (98%)	6 (2%)	1 (0%)	44	34
1	C	327/319 (102%)	315 (96%)	11 (3%)	1 (0%)	44	34
All	All	983/957 (103%)	958 (98%)	21 (2%)	4 (0%)	38	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	256	ASN
1	A	156	ASP
1	B	156	ASP
1	A	157	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	298/288 (104%)	286 (96%)	12 (4%)	36	25
1	B	300/288 (104%)	288 (96%)	12 (4%)	36	25
1	C	298/288 (104%)	288 (97%)	10 (3%)	42	32
All	All	896/864 (104%)	862 (96%)	34 (4%)	39	27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	16	LYS
1	A	112	MET
1	A	147	ARG
1	A	155	GLU
1	A	157	THR
1	A	159	LYS
1	A	179	ILE
1	A	222[A]	LYS

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Mol	Chain	Res	Type
1	A	222[B]	LYS
1	A	256	ASN
1	A	257	LEU
1	B	10	TYR
1	B	16	LYS
1	B	111	ARG
1	B	112	MET
1	B	126	ASP
1	B	148	ILE
1	B	156	ASP
1	B	179	ILE
1	B	250	ASN
1	B	251	LEU
1	B	257	LEU
1	B	280	ASN
1	C	11	ASP
1	C	39	LYS
1	C	112	MET
1	C	160	SER
1	C	185[A]	LEU
1	C	185[B]	LEU
1	C	209	ASN
1	C	220	MET
1	C	252	LYS
1	C	255	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	117	GLN
1	A	177	ASN
1	A	209	ASN
1	A	210	ASN
1	A	256	ASN
1	A	327	GLN
1	B	117	GLN
1	B	121	HIS
1	B	177	ASN
1	B	209	ASN
1	B	210	ASN
1	B	256	ASN

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Mol	Chain	Res	Type
1	B	280	ASN
1	C	31	GLN
1	C	177	ASN
1	C	209	ASN
1	C	327	GLN

### 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](#)

3 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	$\# Z  > 2$
2	PO4	A	2001	-	4,4,4	0.97	0	6,6,6	0.47	0
2	PO4	B	2003	-	4,4,4	0.56	0	6,6,6	0.97	0
2	PO4	C	2004	-	4,4,4	1.00	0	6,6,6	1.01	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
2	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2003	-	-	0/0/0/0	0/0/0/0
2	PO4	C	2004	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	319/319 (100%)	2.34	152 (47%) <b>0</b> <b>0</b>	9, 14, 38, 61	1 (0%)
1	B	319/319 (100%)	3.04	209 (65%) <b>0</b> <b>0</b>	9, 17, 42, 62	1 (0%)
1	C	319/319 (100%)	6.78	305 (95%) <b>0</b> <b>0</b>	12, 24, 48, 68	0
All	All	957/957 (100%)	4.05	666 (69%) <b>0</b> <b>0</b>	9, 18, 43, 68	2 (0%)

All (666) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	LEU	27.5
1	A	254	SER	27.3
1	C	215	LEU	23.1
1	B	251	LEU	22.0
1	C	173	ALA	21.9
1	C	275	TRP	19.6
1	C	160	SER	19.3
1	C	247	MET	17.7
1	C	282	ILE	17.3
1	C	148	ILE	17.0
1	C	106	CYS	16.6
1	C	187	ASP	16.0
1	C	264	THR	15.8
1	C	228	TRP	15.3
1	C	229	ILE	15.2
1	C	316	VAL	14.2
1	C	281	VAL	14.2
1	C	188	VAL	14.0
1	C	129	TYR	14.0
1	C	94	VAL	13.7
1	C	89	ILE	13.6
1	C	172	ALA	13.6
1	C	245	ALA	13.5

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Mol	Chain	Res	Type	RSRZ
1	C	272	ALA	13.5
1	C	219	ILE	13.4
1	C	150	LEU	13.3
1	C	176	LEU	13.3
1	B	61	GLY	13.2
1	C	85	ILE	13.0
1	B	254	SER	12.9
1	C	286	MET	12.5
1	C	271	TYR	12.5
1	B	246	ILE	12.4
1	C	122	LEU	12.4
1	C	262	LEU	12.3
1	C	123	ALA	12.2
1	C	164	ILE	12.1
1	C	104	LEU	11.9
1	C	224	SER	11.8
1	C	174	CYS	11.8
1	C	203	LEU	11.8
1	C	121	HIS	11.7
1	C	204	LEU	11.7
1	C	138	SER	11.6
1	C	259	MET	11.6
1	B	250	ASN	11.3
1	C	127	ILE	11.2
1	A	257	LEU	11.1
1	C	225	HIS	11.1
1	C	195	PRO	11.0
1	C	198	VAL	10.9
1	C	194	ILE	10.8
1	C	120	PRO	10.8
1	C	162	PHE	10.8
1	C	237	SER	10.8
1	C	185[A]	LEU	10.7
1	C	323	LEU	10.7
1	C	251	LEU	10.7
1	C	322	ILE	10.6
1	B	238	GLN	10.6
1	C	294	ILE	10.3
1	A	156	ASP	10.2
1	C	317[A]	MET	10.1
1	C	207	MET	10.0
1	C	118	MET	9.9

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Mol	Chain	Res	Type	RSRZ
1	C	93	LEU	9.9
1	C	279	PRO	9.9
1	C	270	LYS	9.8
1	C	248	GLN	9.8
1	C	10	TYR	9.7
1	C	181	GLU	9.7
1	B	236	GLY	9.7
1	C	328	TRP	9.6
1	C	255	ARG	9.6
1	C	269	GLU	9.6
1	B	247	MET	9.6
1	C	295	PRO	9.4
1	B	71	PHE	9.4
1	C	103	ASN	9.4
1	C	199	ILE	9.3
1	C	289	ILE	9.3
1	C	280	ASN	9.2
1	B	69	SER	9.1
1	A	255	ARG	9.1
1	C	95	ALA	9.1
1	C	125	VAL	9.1
1	C	211	GLU	9.0
1	C	242	ARG	9.0
1	C	250	ASN	9.0
1	C	318	GLN	8.9
1	C	234	ILE	8.9
1	C	102	VAL	8.8
1	C	274	ARG	8.8
1	C	110	LEU	8.8
1	C	321	TYR	8.8
1	C	220	MET	8.7
1	C	66	ALA	8.6
1	C	249	SER	8.6
1	C	99[A]	VAL	8.6
1	C	268	LYS	8.6
1	C	180	THR	8.4
1	C	233	PRO	8.4
1	C	290	PHE	8.3
1	C	108[A]	SER	8.2
1	C	235	GLY	8.2
1	C	197	ILE	8.2
1	C	263	MET	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	192	ARG	8.1
1	C	206	TYR	8.0
1	A	246	ILE	8.0
1	B	308	LEU	7.9
1	C	71	PHE	7.9
1	C	170	LYS	7.9
1	C	190	THR	7.9
1	C	193	GLU	7.9
1	C	37	LEU	7.8
1	C	90	LEU	7.8
1	C	153	SER	7.8
1	B	256	ASN	7.8
1	C	308	LEU	7.7
1	B	257	LEU	7.6
1	C	201	GLU	7.6
1	C	231	TYR	7.6
1	C	217	ASN	7.6
1	C	152	LEU	7.6
1	C	261	THR	7.6
1	B	64	ASP	7.6
1	C	243	PHE	7.6
1	B	156	ASP	7.5
1	C	182	THR	7.5
1	C	221[A]	SER	7.5
1	B	304	SER	7.5
1	C	184	ARG	7.5
1	C	92	PHE	7.4
1	C	218	THR	7.4
1	C	155	GLU	7.4
1	B	129	TYR	7.4
1	C	283	VAL	7.4
1	C	260	PRO	7.4
1	C	161	PRO	7.3
1	C	119	PHE	7.3
1	C	135	LEU	7.3
1	B	307	PHE	7.2
1	C	277	ALA	7.1
1	C	324	MET	7.1
1	C	14[A]	SER	7.1
1	C	97	GLU	7.1
1	A	157	THR	7.1
1	C	265	TYR	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	242	ARG	7.1
1	C	159	LYS	7.1
1	C	158	ALA	7.0
1	C	165	ASP	7.0
1	C	223	PHE	6.9
1	B	70[A]	SER	6.9
1	C	79	TYR	6.8
1	C	320	HIS	6.8
1	C	214	LEU	6.7
1	C	273[A]	SER	6.6
1	C	189	CYS	6.6
1	C	287	TRP	6.6
1	C	166	GLN	6.6
1	B	255	ARG	6.6
1	C	12	ALA	6.6
1	C	25	LEU	6.5
1	C	139	ILE	6.4
1	C	292	ALA	6.4
1	B	153	SER	6.4
1	C	146	LEU	6.4
1	A	251	LEU	6.4
1	C	11	ASP	6.3
1	C	191	LYS	6.3
1	C	213	GLN	6.3
1	B	66	ALA	6.3
1	C	210	ASN	6.3
1	C	227	LEU	6.3
1	C	314	LEU	6.3
1	C	319	THR	6.3
1	C	278	ALA	6.3
1	C	239	PRO	6.2
1	A	245	ALA	6.2
1	C	69	SER	6.2
1	C	171	LEU	6.2
1	C	107	GLY	6.2
1	C	74[A]	MET	6.2
1	C	244	GLY	6.2
1	C	116	LEU	6.2
1	C	167	GLY	6.2
1	C	31	GLN	6.2
1	C	44	TRP	6.1
1	C	311	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	13	LEU	6.1
1	C	112	MET	6.1
1	C	178	ASP	6.1
1	C	15	CYS	6.1
1	B	309	ASP	6.1
1	C	226	GLY	6.0
1	C	291	ASN	6.0
1	C	52	LEU	6.0
1	B	290	PHE	6.0
1	C	284	ASN	5.9
1	C	35	VAL	5.9
1	C	208	HIS	5.8
1	C	124	TYR	5.8
1	C	101	VAL	5.7
1	B	57	ARG	5.7
1	B	65	LYS	5.7
1	B	67	MET	5.7
1	C	327	GLN	5.7
1	A	252	LYS	5.7
1	C	209	ASN	5.7
1	C	49	LEU	5.7
1	C	196	THR	5.7
1	B	243	PHE	5.6
1	B	239	PRO	5.6
1	B	249	SER	5.6
1	C	238	GLN	5.6
1	C	26	PRO	5.6
1	C	325	LYS	5.6
1	B	59	ALA	5.5
1	B	145[A]	ILE	5.5
1	A	256	ASN	5.4
1	C	183	THR	5.4
1	C	267	SER	5.4
1	C	128	ASP	5.4
1	C	315	LYS	5.4
1	C	133	VAL	5.4
1	B	322	ILE	5.3
1	B	14[A]	SER	5.3
1	C	45	HIS	5.3
1	A	250	ASN	5.3
1	C	252	LYS	5.3
1	B	258	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	280	ASN	5.3
1	B	60	PHE	5.3
1	C	216	ILE	5.3
1	C	117	GLN	5.3
1	C	41	TYR	5.3
1	A	68	ARG	5.3
1	B	68	ARG	5.3
1	C	82	THR	5.3
1	C	157	THR	5.3
1	C	246	ILE	5.3
1	C	30	LEU	5.2
1	B	63	VAL	5.2
1	C	175	ASP	5.2
1	C	55	PHE	5.2
1	C	88	ALA	5.2
1	B	10	TYR	5.1
1	C	20	ILE	5.1
1	C	48	TYR	5.1
1	A	66	ALA	5.1
1	B	72	PRO	5.1
1	C	163	LEU	5.0
1	B	248	GLN	5.0
1	C	140	LEU	5.0
1	A	317[A]	MET	5.0
1	A	10	TYR	4.9
1	C	326	ALA	4.9
1	C	230	SER	4.9
1	C	109	ASP	4.9
1	C	141	ARG	4.9
1	C	266	ASN	4.8
1	C	145	ILE	4.8
1	A	150	LEU	4.8
1	B	23	GLY	4.8
1	B	73	VAL	4.8
1	C	98	LYS	4.7
1	A	277	ALA	4.7
1	C	297	SER	4.7
1	C	154	LYS	4.7
1	C	256	ASN	4.7
1	C	169	TYR	4.6
1	C	84	GLY	4.5
1	C	33	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	277	ALA	4.5
1	B	55	PHE	4.5
1	A	214	LEU	4.5
1	A	249	SER	4.5
1	B	18	ALA	4.4
1	B	316	VAL	4.4
1	C	258	GLU	4.4
1	C	59	ALA	4.4
1	B	265	TYR	4.4
1	A	308	LEU	4.4
1	C	186	LEU	4.4
1	C	156	ASP	4.4
1	C	60	PHE	4.4
1	C	179	ILE	4.4
1	B	12	ALA	4.4
1	A	152	LEU	4.4
1	A	167	GLY	4.3
1	B	321	TYR	4.3
1	C	200	SER	4.3
1	B	21[A]	SER	4.3
1	A	239	PRO	4.3
1	C	212	SER	4.3
1	B	292	ALA	4.3
1	B	179	ILE	4.2
1	C	147	ARG	4.2
1	B	17	LEU	4.2
1	A	253	GLU	4.2
1	B	155	GLU	4.2
1	A	71	PHE	4.2
1	C	63	VAL	4.2
1	C	36	ASP	4.2
1	C	43	GLU	4.2
1	C	205	CYS	4.2
1	C	137	ASN	4.2
1	B	264	THR	4.2
1	A	326	ALA	4.2
1	B	245	ALA	4.2
1	A	188	VAL	4.2
1	B	76	TYR	4.1
1	A	160	SER	4.1
1	C	28	SER	4.1
1	A	129	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	306	GLN	4.1
1	B	159	LYS	4.1
1	C	254	SER	4.1
1	A	145	ILE	4.0
1	B	317	MET	4.0
1	C	236	GLY	4.0
1	B	284	ASN	4.0
1	B	311	LEU	4.0
1	B	20	ILE	4.0
1	C	76	TYR	4.0
1	C	105	GLY	4.0
1	B	300	LYS	4.0
1	B	281	VAL	4.0
1	B	235	GLY	3.9
1	C	144	GLU	3.9
1	C	149[A]	SER	3.9
1	A	74[A]	MET	3.9
1	C	62	LYS	3.9
1	A	176	LEU	3.8
1	C	222	LYS	3.8
1	B	158	ALA	3.8
1	C	18	ALA	3.8
1	B	157	THR	3.8
1	A	149[A]	SER	3.8
1	C	42	THR	3.8
1	B	233	PRO	3.7
1	B	25	LEU	3.7
1	A	282	ILE	3.7
1	C	68	ARG	3.7
1	A	238	GLN	3.7
1	B	24	TYR	3.7
1	C	96	ASN	3.7
1	B	314	LEU	3.7
1	C	113	LEU	3.7
1	C	81	ARG	3.7
1	B	44	TRP	3.6
1	C	301	ARG	3.6
1	B	50	ILE	3.6
1	B	303	ARG	3.6
1	C	253	GLU	3.6
1	C	312	GLU	3.6
1	A	243	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	194	ILE	3.6
1	B	297	SER	3.6
1	C	130	ASN	3.6
1	A	60	PHE	3.6
1	B	231	TYR	3.6
1	C	131	GLU	3.5
1	C	288	GLU	3.5
1	A	304	SER	3.5
1	C	17	LEU	3.5
1	C	293	GLN	3.5
1	C	241	ASP	3.5
1	B	252	LYS	3.5
1	A	158	ALA	3.5
1	A	240	ASN	3.5
1	A	179	ILE	3.5
1	B	217	ASN	3.5
1	A	92	PHE	3.5
1	A	162	PHE	3.5
1	A	154	LYS	3.4
1	B	22[A]	VAL	3.4
1	B	215	LEU	3.4
1	A	148	ILE	3.4
1	B	272	ALA	3.4
1	B	52	LEU	3.4
1	B	56	SER	3.4
1	B	253	GLU	3.4
1	B	206	TYR	3.4
1	B	177	ASN	3.3
1	A	174	CYS	3.3
1	B	154	LYS	3.3
1	B	135	LEU	3.3
1	C	309	ASP	3.3
1	B	13	LEU	3.3
1	C	75	ASN	3.3
1	C	132[A]	SER	3.3
1	A	263	MET	3.3
1	C	22	VAL	3.3
1	A	96	ASN	3.3
1	A	151	GLY	3.3
1	B	216	ILE	3.3
1	B	278	ALA	3.3
1	C	299	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	64	ASP	3.3
1	A	190	THR	3.2
1	B	107	GLY	3.2
1	B	328	TRP	3.2
1	B	62	LYS	3.2
1	A	289	ILE	3.2
1	B	127	ILE	3.2
1	B	139	ILE	3.2
1	B	320	HIS	3.2
1	A	272	ALA	3.2
1	B	166	GLN	3.2
1	C	83	VAL	3.2
1	B	204	LEU	3.2
1	C	80	LEU	3.2
1	B	106	CYS	3.2
1	B	283	VAL	3.2
1	B	302	LEU	3.1
1	B	203	LEU	3.1
1	A	184	ARG	3.1
1	C	87	ALA	3.1
1	C	285	ASP	3.1
1	B	19	ALA	3.1
1	B	74	MET	3.1
1	B	275	TRP	3.1
1	C	78	THR	3.1
1	B	132	SER	3.1
1	C	27	SER	3.1
1	C	24	TYR	3.1
1	A	222[A]	LYS	3.1
1	C	114	PRO	3.1
1	A	42	THR	3.1
1	C	51	THR	3.1
1	A	242	ARG	3.1
1	C	296	GLU	3.0
1	A	63	VAL	3.0
1	B	35	VAL	3.0
1	A	119	PHE	3.0
1	B	240	ASN	3.0
1	B	263	MET	3.0
1	B	182	THR	3.0
1	C	240	ASN	3.0
1	B	152	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	290	PHE	3.0
1	B	266	ASN	3.0
1	C	61	GLY	3.0
1	A	262	LEU	3.0
1	B	58	ARG	3.0
1	C	19	ALA	3.0
1	A	199	ILE	3.0
1	C	307	PHE	3.0
1	B	45	HIS	3.0
1	B	16	LYS	3.0
1	A	220	MET	3.0
1	C	100	GLN	3.0
1	B	162	PHE	3.0
1	A	328	TRP	3.0
1	B	271	TYR	3.0
1	A	87	ALA	3.0
1	B	241	ASP	3.0
1	A	122	LEU	2.9
1	C	39	LYS	2.9
1	C	70	SER	2.9
1	A	11	ASP	2.9
1	A	25	LEU	2.9
1	B	323	LEU	2.9
1	A	192	ARG	2.9
1	B	230	SER	2.9
1	A	72	PRO	2.9
1	C	29	GLY	2.9
1	C	177	ASN	2.9
1	B	125	VAL	2.9
1	B	188	VAL	2.9
1	A	135	LEU	2.9
1	C	86	ASP	2.9
1	A	91	GLU	2.9
1	A	90	LEU	2.9
1	A	115	LEU	2.9
1	A	69	SER	2.8
1	A	237	SER	2.8
1	B	28[A]	SER	2.8
1	A	153[A]	SER	2.8
1	B	108[A]	SER	2.8
1	C	126	ASP	2.8
1	C	73	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	2.8
1	B	104	LEU	2.8
1	B	227	LEU	2.8
1	B	78	THR	2.8
1	B	318	GLN	2.8
1	B	121	HIS	2.8
1	B	305	LEU	2.8
1	A	292	ALA	2.8
1	B	82[A]	THR	2.8
1	A	206	TYR	2.8
1	A	278	ALA	2.8
1	B	51	THR	2.8
1	A	170	LYS	2.8
1	C	136	LYS	2.8
1	A	121	HIS	2.8
1	A	39	LYS	2.7
1	A	241	ASP	2.7
1	B	289	ILE	2.7
1	B	15	CYS	2.7
1	C	58	ARG	2.7
1	C	38	SER	2.7
1	A	164	ILE	2.7
1	A	64	ASP	2.7
1	A	26	PRO	2.7
1	B	313	GLU	2.7
1	B	54	LYS	2.7
1	A	185	LEU	2.7
1	A	23	GLY	2.7
1	B	234	ILE	2.7
1	B	190	THR	2.7
1	A	221	SER	2.7
1	A	13	LEU	2.7
1	B	193[A]	GLU	2.7
1	A	248	GLN	2.7
1	B	214	LEU	2.7
1	B	147	ARG	2.7
1	B	295	PRO	2.7
1	B	262	LEU	2.6
1	A	73	VAL	2.6
1	B	185	LEU	2.6
1	B	220	MET	2.6
1	A	70	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	115	LEU	2.6
1	A	247	MET	2.6
1	C	310	GLU	2.6
1	B	161	PRO	2.6
1	B	261	THR	2.6
1	B	79	TYR	2.6
1	A	302	LEU	2.6
1	A	106	CYS	2.6
1	C	202	CYS	2.6
1	B	223	PHE	2.5
1	B	160	SER	2.5
1	B	291	ASN	2.5
1	C	32	ARG	2.5
1	B	163	LEU	2.5
1	C	67	MET	2.5
1	B	77	GLY	2.5
1	A	127	ILE	2.5
1	C	313	GLU	2.5
1	C	276	SER	2.5
1	B	221[A]	SER	2.5
1	B	48	TYR	2.5
1	B	176	LEU	2.5
1	B	228	TRP	2.5
1	B	53	LYS	2.5
1	C	65	LYS	2.5
1	A	17	LEU	2.5
1	A	155	GLU	2.5
1	C	303	ARG	2.5
1	C	151	GLY	2.4
1	B	324	MET	2.4
1	B	198	VAL	2.4
1	B	267	SER	2.4
1	A	79	TYR	2.4
1	B	140	LEU	2.4
1	A	20	ILE	2.4
1	C	50	ILE	2.4
1	C	34	SER	2.4
1	A	124	TYR	2.4
1	A	307	PHE	2.4
1	B	310	GLU	2.4
1	B	244	GLY	2.4
1	B	172	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	218	THR	2.4
1	A	99[A]	VAL	2.4
1	A	215	LEU	2.4
1	B	33	LEU	2.4
1	B	46	ARG	2.4
1	A	280	ASN	2.4
1	B	119	PHE	2.4
1	A	59	ALA	2.4
1	A	24	TYR	2.4
1	A	223	PHE	2.4
1	B	175	ASP	2.4
1	A	125	VAL	2.4
1	B	146	LEU	2.3
1	B	184	ARG	2.3
1	A	18	ALA	2.3
1	B	287	TRP	2.3
1	B	120	PRO	2.3
1	A	194	ILE	2.3
1	A	294	ILE	2.3
1	B	123	ALA	2.3
1	B	169	TYR	2.3
1	B	319	THR	2.3
1	A	161	PRO	2.3
1	B	285	ASP	2.3
1	C	143	SER	2.3
1	A	89	ILE	2.3
1	A	130	ASN	2.3
1	B	174	CYS	2.3
1	A	323	LEU	2.3
1	B	115	LEU	2.3
1	C	168	ARG	2.3
1	A	22	VAL	2.3
1	B	11	ASP	2.3
1	A	78	THR	2.3
1	B	116	LEU	2.3
1	B	186	LEU	2.3
1	B	95	ALA	2.3
1	B	37	LEU	2.3
1	A	207	MET	2.2
1	B	26	PRO	2.2
1	B	279	PRO	2.2
1	C	298	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	2.2
1	A	287	TRP	2.2
1	A	84	GLY	2.2
1	B	181	GLU	2.2
1	A	56	SER	2.2
1	A	139	ILE	2.2
1	A	181	GLU	2.2
1	A	228	TRP	2.2
1	B	144	GLU	2.2
1	C	302	LEU	2.2
1	B	286	MET	2.2
1	A	183	THR	2.2
1	A	208	HIS	2.2
1	A	62	LYS	2.2
1	A	314	LEU	2.2
1	C	53	LYS	2.2
1	A	305	LEU	2.2
1	C	23	GLY	2.2
1	B	210	ASN	2.2
1	B	101	VAL	2.2
1	C	306	GLN	2.2
1	A	27[A]	SER	2.1
1	B	93	LEU	2.1
1	C	134	GLU	2.1
1	A	61	GLY	2.1
1	A	172	ALA	2.1
1	B	224	SER	2.1
1	C	72	PRO	2.1
1	A	189	CYS	2.1
1	C	91	GLU	2.1
1	A	268	LYS	2.1
1	A	134	GLU	2.1
1	A	120	PRO	2.1
1	B	40	LYS	2.1
1	B	268	LYS	2.1
1	C	300	LYS	2.1
1	A	219	ILE	2.1
1	B	173	ALA	2.1
1	B	326	ALA	2.1
1	B	199	ILE	2.1
1	A	49	LEU	2.1
1	B	80	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLY	2.1
1	B	192	ARG	2.0
1	A	182	THR	2.0
1	A	187	ASP	2.0
1	A	265	TYR	2.0
1	A	275	TRP	2.0
1	A	140	LEU	2.0
1	A	227	LEU	2.0
1	B	229	ILE	2.0
1	A	55	PHE	2.0
1	A	75	ASN	2.0
1	B	75	ASN	2.0
1	B	130	ASN	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
2	PO4	A	2001	5/5	0.56	0.33	4.30	16,18,22,22	0
2	PO4	B	2003	5/5	0.81	0.36	2.48	21,26,28,29	0
2	PO4	C	2004	5/5	0.09	0.48	0.61	23,24,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.