



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

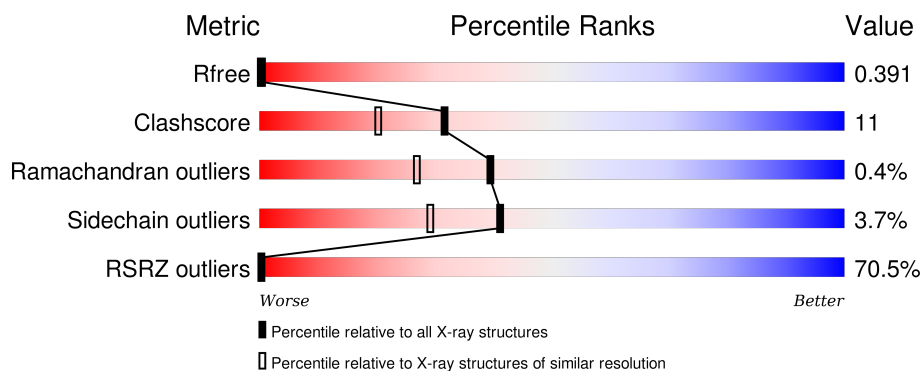
1 Overall quality at a glance

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))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 ≥ 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>49%</div> <div>82%16%•</div> </div>
1	B	319	<div> <div>66%</div> <div>83%15%•</div> </div>
1	C	319	<div> <div>96%</div> <div>82%18%•</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
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: O₄P).



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		

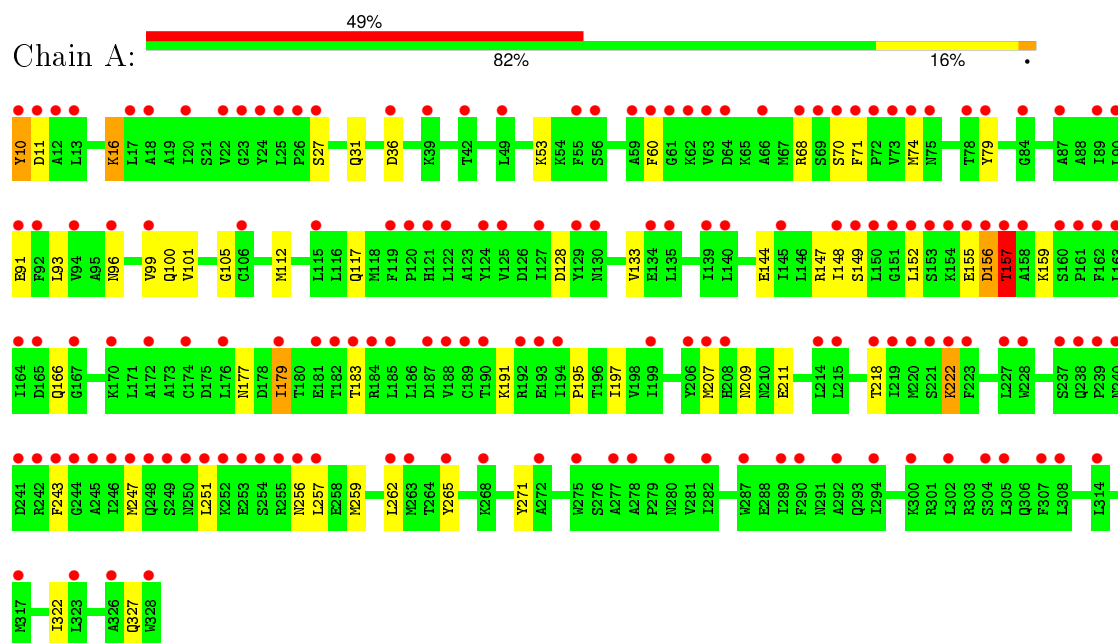
- Molecule 3 is water.

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

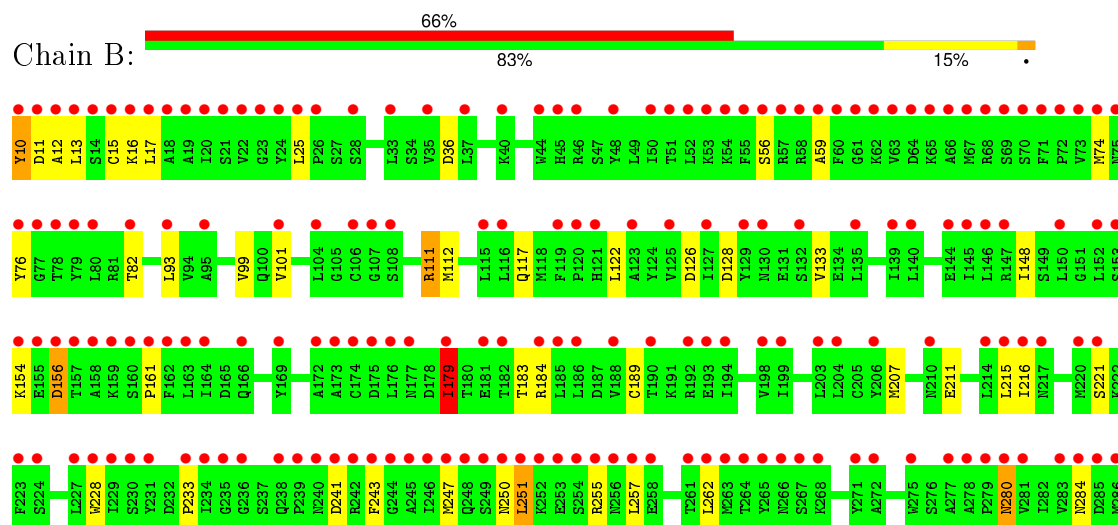
3 Residue-property plots

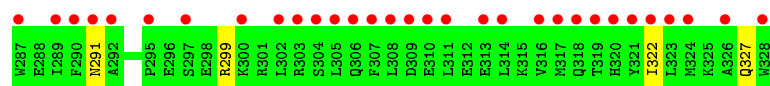
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

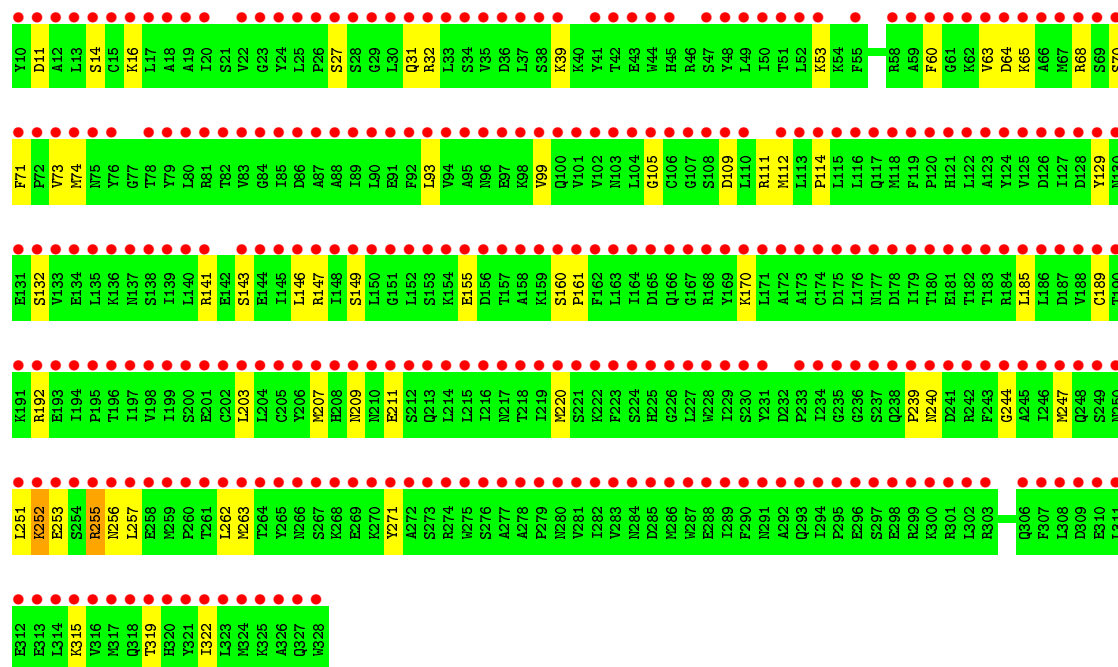
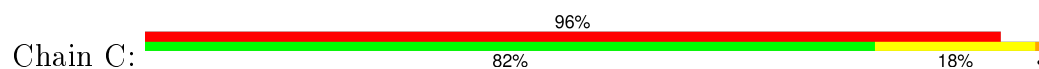


• Molecule 1: Leucine carboxyl methyltransferase 1





● Molecule 1: Leucine carboxyl methyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.182 , 0.224 0.385 , 0.391	Depositor DCC
R_{free} test set	4380 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.5	EDS
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 135135 reflections	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	8781	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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:HD12	1:C:322:ILE:O	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
3:A:2217:HOH:O	1:C:68:ARG:HD3	2.02	0.59
1:A:27[B]:SER:H	1:A:31:GLN:NE2	2.00	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:HG2	1:C:32:ARG:O	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:CG	1:C:32:ARG:O	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
3:A:2217:HOH:O	1:C:68:ARG:HD2	2.12	0.49
1:C:247:MET:CE	1:C:262:LEU:HD21	2.43	0.49
1:C:93:LEU:CD2	1:C:99[B]:VAL:HG21	2.39	0.49
1:A:156:ASP:HB3	3:A:2028:HOH:O	2.13	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:B:15:CYS:SG	1:B:74:MET:HE3	2.54	0.48
1:A:91:GLU:HG2	3:A:2329:HOH:O	2.13	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:27:SER:H	1:C:31:GLN:HE21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLU:CD	1:C:155:GLU:H	2.19	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:B:284:ASN:ND2	3:B:2316:HOH:O	2.46	0.44
1:A:222[B]:LYS:HE2	3:A:2246:HOH:O	2.18	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:65:LYS:HG2	1:C:68:ARG:HH21	1.83	0.43
1:C:109:ASP:OD1	1:C:111:ARG:HG2	2.18	0.43
1:A:71:PHE:CE1	1:A:74[A]:MET:HG3	2.54	0.43
1:C:247:MET:CE	1:C:262:LEU:CD2	2.97	0.43
1:B:11:ASP:HB2	1:B:255:ARG:HH21	1.83	0.43
1:B:10:TYR:HD2	1:B:10:TYR:C	2.22	0.43
1:B:13:LEU:O	1:B:17:LEU:HG	2.19	0.43
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:16:LYS:HB2	1:A:16:LYS:HE3	1.81	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:C:143:SER:CB	1:C:146:LEU:HD12	2.50	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:A:53:LYS:HA	1:A:60:PHE:HB2	2.01	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:247:MET:HE2	1:C:262:LEU:HD21	2.00	0.41
1:C:170:LYS:CD	1:C:189:CYS:HB2	2.50	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:179:ILE:CD1	1:A:218:THR:HB	2.50	0.41
1:A:177:ASN:HD21	1:A:207:MET:HG2	1.85	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:191:LYS:CE	3:A:2169:HOH:O	2.69	0.40
1:A:101:VAL:HG22	1:A:197:ILE:HB	2.03	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%)	30	17
1	B	329/319 (103%)	322 (98%)	6 (2%)	1 (0%)	46	35
1	C	327/319 (102%)	315 (96%)	11 (3%)	1 (0%)	46	35
All	All	983/957 (103%)	958 (98%)	21 (2%)	4 (0%)	39	27

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%)	38	26
1	B	300/288 (104%)	288 (96%)	12 (4%)	38	26
1	C	298/288 (104%)	288 (97%)	10 (3%)	44	33
All	All	896/864 (104%)	862 (96%)	34 (4%)	41	28

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	0.25	0	6,6,6	0.27	0
2	PO4	B	2003	-	4,4,4	0.41	0	6,6,6	0.31	0
2	PO4	C	2004	-	4,4,4	0.45	0	6,6,6	0.32	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, 95th 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 ²)	Q<0.9
1	A	319/319 (100%)	2.40	157 (49%) 0 0	9, 14, 38, 61	1 (0%)
1	B	319/319 (100%)	3.11	211 (66%) 0 0	9, 17, 42, 62	1 (0%)
1	C	319/319 (100%)	6.89	307 (96%) 0 0	12, 24, 48, 68	0
All	All	957/957 (100%)	4.13	675 (70%) 0 0	9, 18, 43, 68	2 (0%)

All (675) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	LEU	28.0
1	A	254	SER	27.7
1	C	215	LEU	23.6
1	B	251	LEU	22.4
1	C	173	ALA	22.3
1	C	275	TRP	19.8
1	C	160	SER	19.5
1	C	247	MET	17.7
1	C	282	ILE	17.7
1	C	148	ILE	17.3
1	C	106	CYS	16.8
1	C	187	ASP	16.3
1	C	264	THR	16.0
1	C	229	ILE	15.5
1	C	228	TRP	15.5
1	C	316	VAL	14.5
1	C	281	VAL	14.5
1	C	188	VAL	14.3
1	C	129	TYR	14.1
1	C	94	VAL	14.0
1	C	89	ILE	13.9
1	C	172	ALA	13.8
1	C	245	ALA	13.8

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Mol	Chain	Res	Type	RSRZ
1	C	272	ALA	13.7
1	C	219	ILE	13.7
1	C	176	LEU	13.5
1	C	150	LEU	13.5
1	B	61	GLY	13.4
1	C	85	ILE	13.2
1	B	254	SER	13.1
1	B	246	ILE	12.6
1	C	122	LEU	12.6
1	C	271	TYR	12.6
1	C	286	MET	12.5
1	C	262	LEU	12.5
1	C	123	ALA	12.4
1	C	164	ILE	12.3
1	C	104	LEU	12.2
1	C	203	LEU	12.0
1	C	224	SER	12.0
1	C	174	CYS	12.0
1	C	204	LEU	12.0
1	C	121	HIS	11.9
1	C	138	SER	11.8
1	C	259	MET	11.6
1	C	127	ILE	11.4
1	B	250	ASN	11.4
1	A	257	LEU	11.3
1	C	225	HIS	11.3
1	C	198	VAL	11.2
1	C	195	PRO	11.1
1	C	194	ILE	11.0
1	C	162	PHE	11.0
1	C	237	SER	10.9
1	C	120	PRO	10.9
1	C	185[A]	LEU	10.9
1	C	323	LEU	10.9
1	C	322	ILE	10.9
1	C	251	LEU	10.9
1	B	238	GLN	10.7
1	C	294	ILE	10.5
1	A	156	ASP	10.4
1	C	317[A]	MET	10.2
1	C	93	LEU	10.1
1	C	279	PRO	10.0

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Mol	Chain	Res	Type	RSRZ
1	C	207	MET	10.0
1	C	118	MET	10.0
1	C	248	GLN	9.9
1	C	270	LYS	9.9
1	B	236	GLY	9.8
1	C	10	TYR	9.8
1	C	328	TRP	9.8
1	C	181	GLU	9.7
1	C	269	GLU	9.7
1	C	255	ARG	9.7
1	B	71	PHE	9.6
1	B	247	MET	9.6
1	C	295	PRO	9.6
1	C	199	ILE	9.5
1	C	289	ILE	9.5
1	C	103	ASN	9.5
1	C	125	VAL	9.3
1	C	95	ALA	9.3
1	C	280	ASN	9.3
1	B	69	SER	9.2
1	A	255	ARG	9.1
1	C	211	GLU	9.1
1	C	234	ILE	9.1
1	C	250	ASN	9.1
1	C	242	ARG	9.0
1	C	102	VAL	9.0
1	C	318	GLN	9.0
1	C	110	LEU	9.0
1	C	321	TYR	8.8
1	C	274	ARG	8.8
1	C	66	ALA	8.8
1	C	99[A]	VAL	8.8
1	C	249	SER	8.7
1	C	220	MET	8.7
1	C	268	LYS	8.6
1	C	180	THR	8.5
1	C	290	PHE	8.5
1	C	233	PRO	8.5
1	C	108[A]	SER	8.4
1	C	197	ILE	8.4
1	C	235	GLY	8.3
1	A	246	ILE	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	263	MET	8.1
1	B	308	LEU	8.1
1	C	71	PHE	8.1
1	C	192	ARG	8.1
1	C	206	TYR	8.1
1	C	37	LEU	8.0
1	C	190	THR	8.0
1	C	90	LEU	8.0
1	C	170	LYS	8.0
1	C	193	GLU	8.0
1	C	153	SER	8.0
1	B	256	ASN	7.9
1	B	257	LEU	7.8
1	C	308	LEU	7.8
1	C	152	LEU	7.8
1	C	243	PHE	7.8
1	B	64	ASP	7.7
1	C	261	THR	7.7
1	C	217	ASN	7.7
1	C	231	TYR	7.7
1	C	201	GLU	7.7
1	B	156	ASP	7.7
1	C	221[A]	SER	7.7
1	B	304	SER	7.6
1	C	182	THR	7.6
1	C	92	PHE	7.6
1	C	283	VAL	7.6
1	C	184	ARG	7.5
1	C	218	THR	7.5
1	C	119	PHE	7.5
1	C	155	GLU	7.5
1	C	260	PRO	7.5
1	B	129	TYR	7.5
1	C	161	PRO	7.5
1	C	135	LEU	7.4
1	B	307	PHE	7.4
1	C	277	ALA	7.3
1	C	14[A]	SER	7.3
1	A	157	THR	7.2
1	C	158	ALA	7.2
1	C	97	GLU	7.2
1	C	324	MET	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	265	TYR	7.1
1	C	159	LYS	7.1
1	B	242	ARG	7.1
1	C	165	ASP	7.1
1	C	223	PHE	7.0
1	B	70[A]	SER	7.0
1	C	214	LEU	6.9
1	C	79	TYR	6.9
1	C	320	HIS	6.9
1	C	273[A]	SER	6.7
1	C	189	CYS	6.7
1	C	12	ALA	6.7
1	C	287	TRP	6.7
1	C	166	GLN	6.7
1	B	255	ARG	6.6
1	C	25	LEU	6.6
1	C	139	ILE	6.6
1	C	292	ALA	6.6
1	C	146	LEU	6.6
1	B	153	SER	6.5
1	A	251	LEU	6.5
1	C	11	ASP	6.5
1	B	66	ALA	6.5
1	C	227	LEU	6.5
1	C	314	LEU	6.5
1	C	278	ALA	6.4
1	C	213	GLN	6.4
1	A	245	ALA	6.4
1	C	210	ASN	6.4
1	C	191	LYS	6.4
1	C	171	LEU	6.4
1	C	319	THR	6.4
1	C	239	PRO	6.4
1	C	107	GLY	6.3
1	C	116	LEU	6.3
1	C	69	SER	6.3
1	C	311	LEU	6.3
1	C	13	LEU	6.3
1	C	44	TRP	6.3
1	C	167	GLY	6.3
1	C	244	GLY	6.3
1	C	74[A]	MET	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	GLN	6.2
1	C	178	ASP	6.2
1	C	15	CYS	6.2
1	B	309	ASP	6.2
1	C	226	GLY	6.1
1	C	112	MET	6.1
1	C	52	LEU	6.1
1	B	290	PHE	6.1
1	C	291	ASN	6.1
1	C	35	VAL	6.0
1	C	284	ASN	6.0
1	C	208	HIS	5.9
1	C	101	VAL	5.9
1	C	124	TYR	5.8
1	C	49	LEU	5.8
1	B	65	LYS	5.8
1	C	327	GLN	5.8
1	B	243	PHE	5.8
1	C	209	ASN	5.8
1	A	252	LYS	5.8
1	B	57	ARG	5.8
1	C	196	THR	5.7
1	B	67	MET	5.7
1	B	239	PRO	5.7
1	B	249	SER	5.7
1	C	26	PRO	5.7
1	B	59	ALA	5.7
1	C	238	GLN	5.7
1	B	145[A]	ILE	5.6
1	C	325	LYS	5.6
1	C	133	VAL	5.5
1	C	267	SER	5.5
1	C	183	THR	5.5
1	A	256	ASN	5.5
1	B	322	ILE	5.5
1	C	128	ASP	5.5
1	B	60	PHE	5.4
1	B	14[A]	SER	5.4
1	C	216	ILE	5.4
1	C	315	LYS	5.4
1	C	45	HIS	5.4
1	A	250	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	280	ASN	5.4
1	C	246	ILE	5.4
1	B	258	GLU	5.4
1	C	252	LYS	5.4
1	B	63	VAL	5.4
1	C	30	LEU	5.4
1	C	117	GLN	5.4
1	C	41	TYR	5.3
1	C	82	THR	5.3
1	C	157	THR	5.3
1	B	68	ARG	5.3
1	C	55	PHE	5.3
1	A	68	ARG	5.3
1	C	175	ASP	5.3
1	C	88	ALA	5.3
1	C	20	ILE	5.2
1	B	10	TYR	5.2
1	C	163	LEU	5.2
1	A	66	ALA	5.2
1	B	72	PRO	5.1
1	C	140	LEU	5.1
1	C	48	TYR	5.1
1	B	248	GLN	5.1
1	C	326	ALA	5.0
1	A	317[A]	MET	5.0
1	C	230	SER	5.0
1	A	10	TYR	5.0
1	C	109	ASP	5.0
1	C	145	ILE	4.9
1	C	141	ARG	4.9
1	B	73	VAL	4.9
1	A	150	LEU	4.9
1	C	266	ASN	4.9
1	B	23	GLY	4.9
1	A	277	ALA	4.8
1	C	297	SER	4.8
1	C	98	LYS	4.8
1	C	256	ASN	4.7
1	C	154	LYS	4.7
1	C	169	TYR	4.7
1	C	33	LEU	4.6
1	B	277	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	84	GLY	4.6
1	B	55	PHE	4.6
1	B	316	VAL	4.6
1	A	214	LEU	4.6
1	B	18	ALA	4.6
1	A	249	SER	4.5
1	C	59	ALA	4.5
1	A	308	LEU	4.5
1	C	186	LEU	4.5
1	C	179	ILE	4.5
1	C	60	PHE	4.5
1	B	12	ALA	4.5
1	C	258	GLU	4.5
1	A	152	LEU	4.5
1	C	156	ASP	4.5
1	B	265	TYR	4.5
1	A	167	GLY	4.4
1	C	200	SER	4.4
1	B	21[A]	SER	4.4
1	B	321	TYR	4.4
1	B	179	ILE	4.4
1	C	212	SER	4.4
1	A	239	PRO	4.4
1	B	292	ALA	4.4
1	B	17	LEU	4.4
1	C	63	VAL	4.3
1	A	71	PHE	4.3
1	A	188	VAL	4.3
1	C	147	ARG	4.3
1	A	326	ALA	4.3
1	B	245	ALA	4.3
1	C	205	CYS	4.2
1	C	36	ASP	4.2
1	B	264	THR	4.2
1	A	253	GLU	4.2
1	B	155	GLU	4.2
1	C	137	ASN	4.2
1	C	43	GLU	4.2
1	A	160	SER	4.2
1	C	28	SER	4.2
1	B	76	TYR	4.2
1	A	129	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	306	GLN	4.2
1	A	145	ILE	4.2
1	C	254	SER	4.1
1	B	159	LYS	4.1
1	B	20	ILE	4.1
1	B	311	LEU	4.1
1	C	236	GLY	4.1
1	B	281	VAL	4.1
1	C	105	GLY	4.0
1	B	284	ASN	4.0
1	B	317	MET	4.0
1	C	76	TYR	4.0
1	B	300	LYS	4.0
1	B	235	GLY	4.0
1	C	149[A]	SER	4.0
1	A	176	LEU	4.0
1	C	144	GLU	4.0
1	A	74[A]	MET	3.9
1	B	158	ALA	3.9
1	C	18	ALA	3.9
1	C	62	LYS	3.9
1	C	222	LYS	3.9
1	A	149[A]	SER	3.9
1	B	157	THR	3.9
1	B	25	LEU	3.8
1	A	282	ILE	3.8
1	C	42	THR	3.8
1	B	233	PRO	3.8
1	A	238	GLN	3.8
1	B	24	TYR	3.8
1	B	314	LEU	3.8
1	C	113	LEU	3.8
1	C	68	ARG	3.8
1	C	96	ASN	3.7
1	B	50	ILE	3.7
1	B	44	TRP	3.7
1	A	60	PHE	3.7
1	A	243	PHE	3.7
1	B	194	ILE	3.7
1	C	81	ARG	3.7
1	B	297	SER	3.7
1	C	301	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	253	GLU	3.6
1	C	17	LEU	3.6
1	C	130	ASN	3.6
1	C	312	GLU	3.6
1	B	303	ARG	3.6
1	B	231	TYR	3.6
1	A	179	ILE	3.6
1	A	158	ALA	3.6
1	A	304	SER	3.6
1	C	131	GLU	3.6
1	C	241	ASP	3.6
1	C	288	GLU	3.6
1	A	92	PHE	3.6
1	A	162	PHE	3.6
1	C	293	GLN	3.6
1	B	252	LYS	3.5
1	A	148	ILE	3.5
1	B	22[A]	VAL	3.5
1	B	215	LEU	3.5
1	A	240	ASN	3.5
1	B	217	ASN	3.5
1	B	52	LEU	3.5
1	B	272	ALA	3.5
1	A	154	LYS	3.5
1	B	56	SER	3.5
1	B	135	LEU	3.4
1	B	206	TYR	3.4
1	B	253	GLU	3.4
1	A	174	CYS	3.4
1	B	13	LEU	3.4
1	B	177	ASN	3.4
1	C	22	VAL	3.4
1	C	309	ASP	3.4
1	B	154	LYS	3.4
1	B	216	ILE	3.4
1	C	132[A]	SER	3.4
1	B	278	ALA	3.3
1	C	75	ASN	3.4
1	A	151	GLY	3.3
1	A	263	MET	3.3
1	C	64	ASP	3.3
1	A	96	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	107	GLY	3.3
1	A	190	THR	3.3
1	A	289	ILE	3.3
1	B	127	ILE	3.3
1	B	139	ILE	3.3
1	C	299	ARG	3.3
1	B	328	TRP	3.3
1	C	83	VAL	3.3
1	B	204	LEU	3.3
1	C	80	LEU	3.3
1	A	272	ALA	3.3
1	B	283	VAL	3.3
1	B	302	LEU	3.2
1	B	62	LYS	3.2
1	B	106	CYS	3.2
1	B	203	LEU	3.2
1	B	320	HIS	3.2
1	B	166	GLN	3.2
1	B	19	ALA	3.2
1	C	87	ALA	3.2
1	C	285	ASP	3.2
1	C	27	SER	3.2
1	B	275	TRP	3.2
1	B	132	SER	3.2
1	A	63	VAL	3.1
1	A	184	ARG	3.1
1	B	35	VAL	3.1
1	C	78	THR	3.1
1	A	119	PHE	3.1
1	C	114	PRO	3.1
1	C	24	TYR	3.1
1	A	42	THR	3.1
1	B	74	MET	3.1
1	C	51	THR	3.1
1	B	152	LEU	3.1
1	A	290	PHE	3.1
1	A	222[A]	LYS	3.1
1	A	199	ILE	3.1
1	A	262	LEU	3.1
1	A	242	ARG	3.1
1	C	296	GLU	3.1
1	C	307	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	THR	3.1
1	B	240	ASN	3.1
1	C	19	ALA	3.1
1	C	61	GLY	3.1
1	C	240	ASN	3.1
1	B	263	MET	3.1
1	B	162	PHE	3.1
1	B	266	ASN	3.1
1	B	45	HIS	3.0
1	A	122	LEU	3.0
1	A	87	ALA	3.0
1	A	328	TRP	3.0
1	B	58	ARG	3.0
1	B	241	ASP	3.0
1	C	100	GLN	3.0
1	B	16	LYS	3.0
1	B	271	TYR	3.0
1	C	70	SER	3.0
1	A	220	MET	3.0
1	A	25	LEU	3.0
1	B	323	LEU	3.0
1	B	125	VAL	3.0
1	B	188	VAL	3.0
1	A	11	ASP	3.0
1	A	135	LEU	3.0
1	C	39	LYS	3.0
1	B	230	SER	3.0
1	A	72	PRO	3.0
1	C	29	GLY	3.0
1	A	90	LEU	3.0
1	A	115	LEU	3.0
1	C	73	VAL	2.9
1	C	86	ASP	2.9
1	C	177	ASN	2.9
1	A	192	ARG	2.9
1	A	91	GLU	2.9
1	A	237	SER	2.9
1	B	28[A]	SER	2.9
1	A	163	LEU	2.9
1	B	104	LEU	2.9
1	B	227	LEU	2.9
1	A	69	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	153[A]	SER	2.9
1	B	108[A]	SER	2.9
1	C	126	ASP	2.9
1	B	305	LEU	2.9
1	A	292	ALA	2.9
1	B	78	THR	2.9
1	A	278	ALA	2.9
1	B	121	HIS	2.9
1	B	318	GLN	2.8
1	B	82[A]	THR	2.8
1	B	289	ILE	2.8
1	A	206	TYR	2.8
1	B	51	THR	2.8
1	A	121	HIS	2.8
1	A	164	ILE	2.8
1	A	241	ASP	2.8
1	B	15	CYS	2.8
1	A	170	LYS	2.8
1	C	136	LYS	2.8
1	A	185	LEU	2.8
1	B	234	ILE	2.8
1	C	38	SER	2.8
1	A	39	LYS	2.8
1	A	64	ASP	2.8
1	A	26	PRO	2.8
1	A	13	LEU	2.8
1	A	23	GLY	2.8
1	C	58	ARG	2.8
1	A	221	SER	2.8
1	B	190	THR	2.7
1	B	214	LEU	2.7
1	B	313	GLU	2.7
1	B	54	LYS	2.7
1	B	262	LEU	2.7
1	A	73	VAL	2.7
1	B	193[A]	GLU	2.7
1	B	295	PRO	2.7
1	A	248	GLN	2.7
1	B	185	LEU	2.7
1	B	147	ARG	2.7
1	C	115	LEU	2.7
1	A	70	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	2.7
1	B	161	PRO	2.6
1	B	223	PHE	2.6
1	B	261	THR	2.6
1	B	220	MET	2.6
1	A	106	CYS	2.6
1	C	202	CYS	2.6
1	B	79	TYR	2.6
1	C	310	GLU	2.6
1	B	163	LEU	2.6
1	A	247	MET	2.6
1	B	160	SER	2.6
1	A	127	ILE	2.6
1	B	291	ASN	2.6
1	B	77	GLY	2.6
1	C	32	ARG	2.6
1	C	276	SER	2.6
1	B	176	LEU	2.6
1	B	221[A]	SER	2.6
1	C	67	MET	2.5
1	C	313	GLU	2.5
1	A	17	LEU	2.5
1	B	198	VAL	2.5
1	B	48	TYR	2.5
1	B	228	TRP	2.5
1	B	140	LEU	2.5
1	A	307	PHE	2.5
1	A	20	ILE	2.5
1	C	50	ILE	2.5
1	C	151	GLY	2.5
1	A	155	GLU	2.5
1	B	267	SER	2.5
1	A	99[A]	VAL	2.5
1	B	53	LYS	2.5
1	C	65	LYS	2.5
1	A	79	TYR	2.5
1	B	172	ALA	2.5
1	C	303	ARG	2.5
1	C	34	SER	2.5
1	A	215	LEU	2.5
1	B	119	PHE	2.5
1	B	244	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	2.5
1	A	124	TYR	2.5
1	A	218	THR	2.5
1	B	33	LEU	2.5
1	B	324	MET	2.4
1	A	223	PHE	2.4
1	A	125	VAL	2.4
1	B	310	GLU	2.4
1	A	280	ASN	2.4
1	B	146	LEU	2.4
1	B	175	ASP	2.4
1	A	194	ILE	2.4
1	A	294	ILE	2.4
1	B	46	ARG	2.4
1	A	24	TYR	2.4
1	A	18	ALA	2.4
1	B	123	ALA	2.4
1	B	287	TRP	2.4
1	A	89	ILE	2.4
1	B	120	PRO	2.4
1	B	285	ASP	2.4
1	A	323	LEU	2.4
1	B	115	LEU	2.4
1	A	22	VAL	2.4
1	A	161	PRO	2.4
1	B	184	ARG	2.4
1	B	319	THR	2.4
1	B	174	CYS	2.4
1	C	143	SER	2.4
1	B	169	TYR	2.4
1	A	130	ASN	2.3
1	B	11	ASP	2.3
1	B	37	LEU	2.3
1	B	116	LEU	2.3
1	B	186	LEU	2.3
1	B	95	ALA	2.3
1	A	78	THR	2.3
1	C	168	ARG	2.3
1	A	12	ALA	2.3
1	A	139	ILE	2.3
1	B	26	PRO	2.3
1	B	279	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	56	SER	2.3
1	A	287	TRP	2.3
1	C	302	LEU	2.3
1	A	84	GLY	2.3
1	C	298	GLU	2.3
1	A	228	TRP	2.3
1	A	314	LEU	2.3
1	B	181	GLU	2.3
1	A	183	THR	2.3
1	A	207	MET	2.3
1	A	208	HIS	2.2
1	A	181	GLU	2.2
1	A	305	LEU	2.2
1	B	144	GLU	2.2
1	B	101	VAL	2.2
1	B	286	MET	2.2
1	A	62	LYS	2.2
1	A	61	GLY	2.2
1	C	23	GLY	2.2
1	B	210	ASN	2.2
1	A	172	ALA	2.2
1	A	27[A]	SER	2.2
1	B	93	LEU	2.2
1	C	53	LYS	2.2
1	A	189	CYS	2.2
1	C	306	GLN	2.2
1	B	224	SER	2.2
1	A	219	ILE	2.2
1	C	72	PRO	2.2
1	C	134	GLU	2.2
1	B	173	ALA	2.2
1	B	326	ALA	2.2
1	A	120	PRO	2.2
1	B	199	ILE	2.2
1	C	91	GLU	2.2
1	A	49	LEU	2.2
1	A	268	LYS	2.2
1	A	134	GLU	2.1
1	B	40	LYS	2.1
1	B	268	LYS	2.1
1	C	300	LYS	2.1
1	B	80	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	229	ILE	2.1
1	A	140	LEU	2.1
1	A	227	LEU	2.1
1	A	244	GLY	2.1
1	A	187	ASP	2.1
1	A	182	THR	2.1
1	A	55	PHE	2.1
1	A	275	TRP	2.1
1	A	265	TYR	2.1
1	B	192	ARG	2.1
1	B	130	ASN	2.1
1	B	150	LEU	2.1
1	A	94	VAL	2.1
1	A	36	ASP	2.1
1	A	165	ASP	2.1
1	A	75	ASN	2.0
1	B	75	ASN	2.0
1	B	164	ILE	2.0
1	C	47	SER	2.0
1	A	193	GLU	2.0
1	A	300	LYS	2.0
1	C	16	LYS	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, 95th 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(\AA^2)	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.