Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 06:41 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

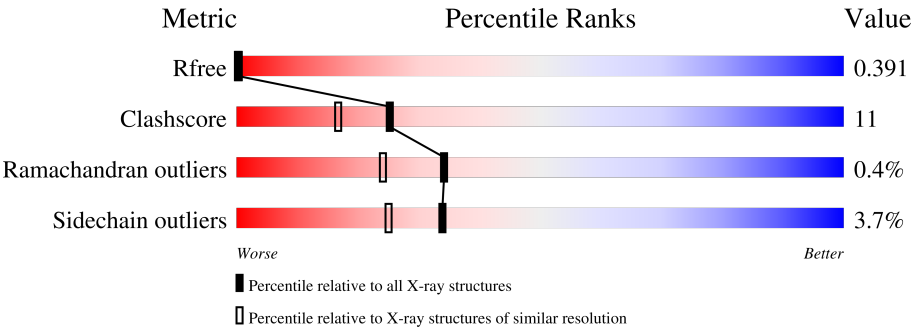
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	319	82% 16% ·
1	B	319	83% 15% ·
1	C	319	82% 18% ·

2 Entry composition (i)

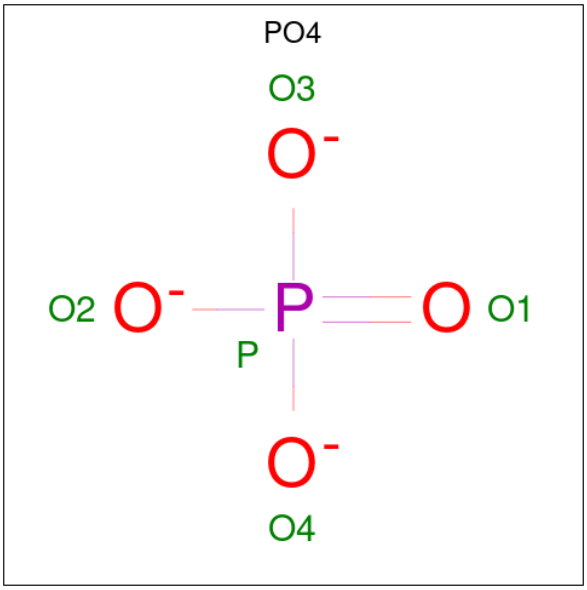
There are 3 unique types of molecules in this entry. The entry contains 8781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	P		0	0
			5	4	1			
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 water.

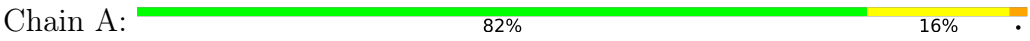
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	385	Total O 385 385	0	0
3	B	318	Total O 318 318	0	0
3	C	210	Total O 210 210	0	0

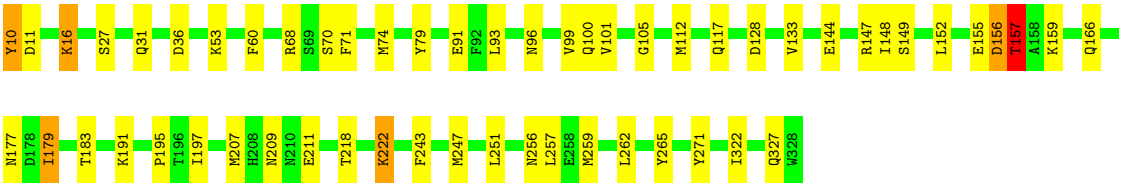
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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

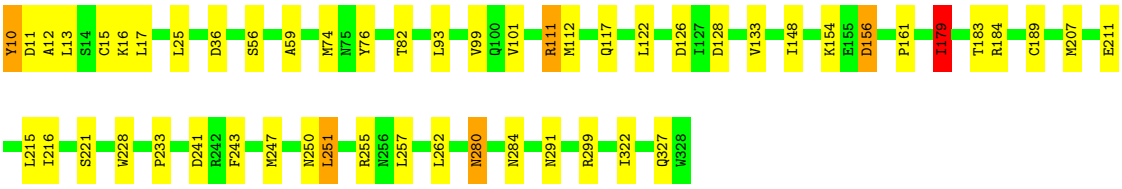
Chain A:





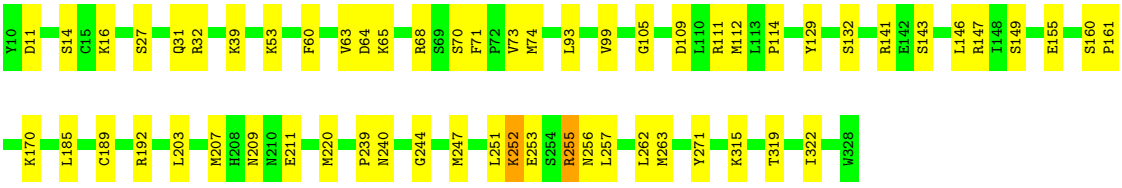
• Molecule 1: Leucine carboxyl methyltransferase 1

Chain B:



• Molecule 1: Leucine carboxyl methyltransferase 1

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	6757 reflections (5.00%)	wwPDB-VP
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 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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^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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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

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:HD12	1:B:322:ILE:O	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:HD12	1:C:322:ILE:C	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:HD12	1:A:322:ILE:C	2.25	0.57
1:C:32:ARG:HG2	1:C:32:ARG:O	2.05	0.57
1:C:247:MET:HE2	1:C:262:LEU:CD2	2.35	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:HD12	1:B:322:ILE:C	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:HE3	1:C:252:LYS:HA	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: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: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:HD12	1:A:322:ILE:O	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:99[A]:VAL:HG22	1:A:195:PRO:HB2	1.99	0.45
1:A:179:ILE:CG2	3:A:2355:HOH:O	2.37	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: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: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:A:68:ARG:NH1	1:C:70:SER:O	2.45	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: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%)	25 15
1	B	329/319 (103%)	322 (98%)	6 (2%)	1 (0%)	41 31
1	C	327/319 (102%)	315 (96%)	11 (3%)	1 (0%)	41 31
All	All	983/957 (103%)	958 (98%)	21 (2%)	4 (0%)	34 24

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	298/288 (104%)	286 (96%)	12 (4%)	31 22
1	B	300/288 (104%)	288 (96%)	12 (4%)	31 22
1	C	298/288 (104%)	288 (97%)	10 (3%)	37 28
All	All	896/864 (104%)	862 (96%)	34 (4%)	34 24

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

Sometimes 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 monosaccharides 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	B	2003	-	4,4,4	0.64	0	6,6,6	1.10	0
2	PO4	C	2004	-	4,4,4	1.02	0	6,6,6	1.15	0
2	PO4	A	2001	-	4,4,4	0.88	0	6,6,6	0.53	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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.