Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:27 AM GMT

PDB ID	:	2D4W
Title	:	Crystal structure of glycerol kinase from Cellulomonas sp. NT3060
Authors	:	Imada, K.; Tamura, T.; Namba, K.; Inagaki, K.
Deposited on	:	2005-10-24
Resolution	:	2.30 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 (i) symbol.

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

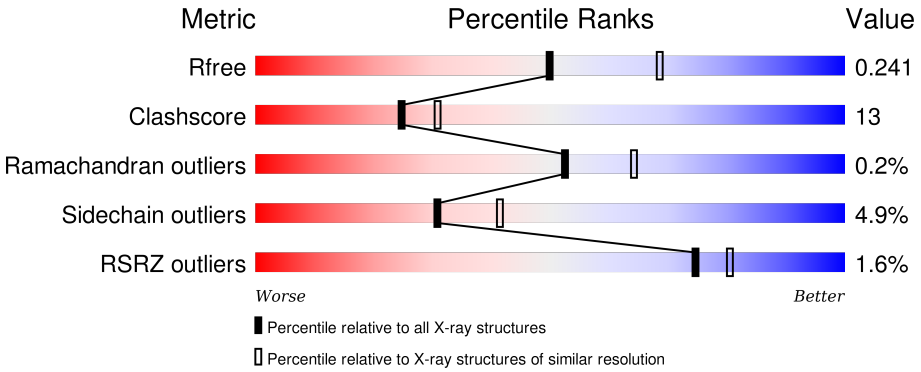
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	504	2% 76% 21%
1	B	504	% 73% 24%

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	MPD	A	1	X	-	-	X
2	MPD	A	2001	X	-	-	X
2	MPD	B	1001	X	-	X	X
2	MPD	B	3001	X	-	-	X

2 Entry composition

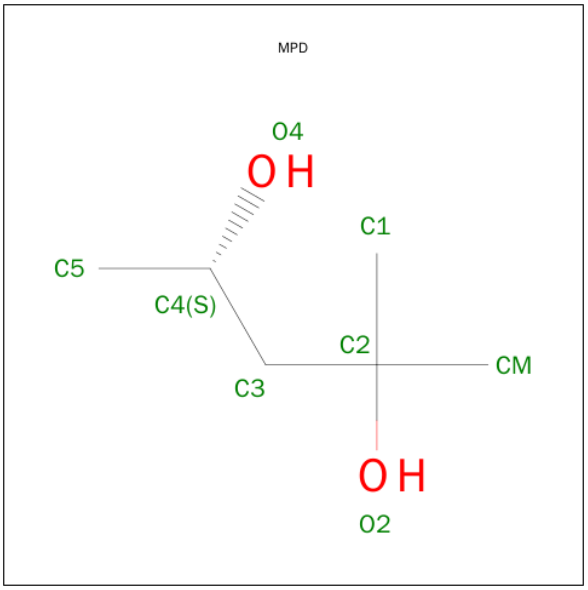
There are 3 unique types of molecules in this entry. The entry contains 8139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3877	2442	668	753	14			
1	B	503	Total	C	N	O	S	0	0	0
			3877	2442	668	753	14			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is water.

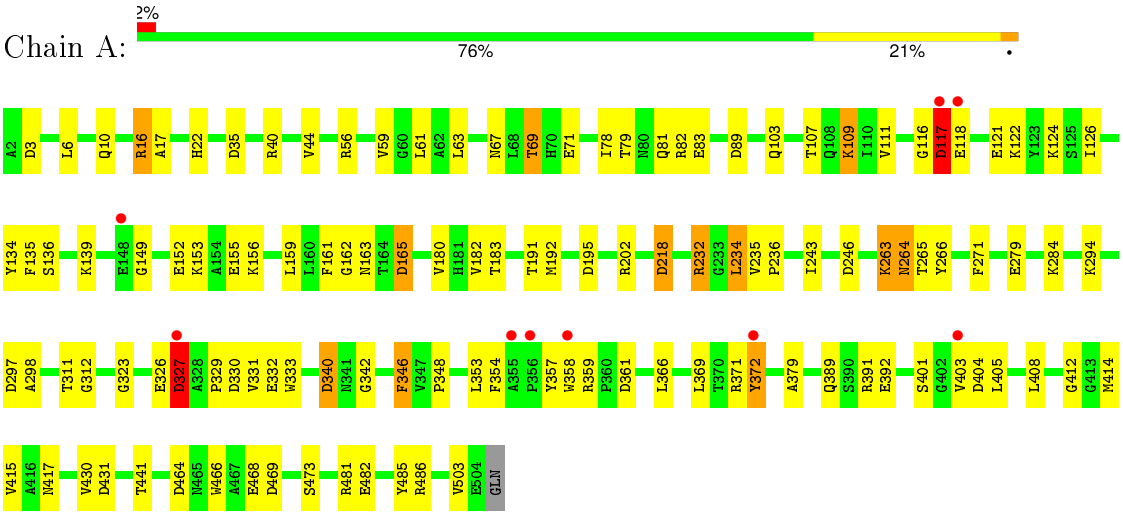
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	179	Total O 179 179	0	0
3	B	174	Total O 174 174	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

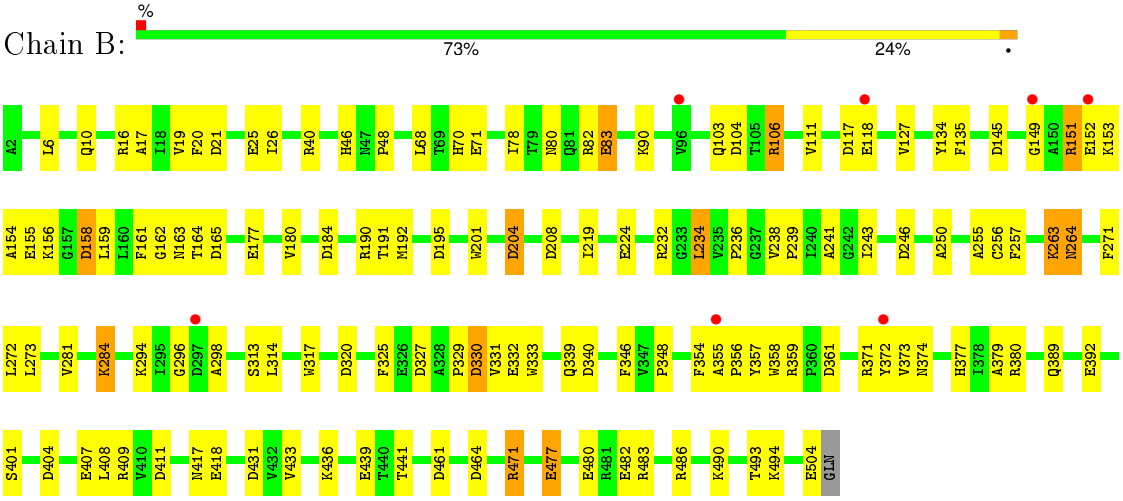
- Molecule 1: glycerol kinase

Chain A:



- Molecule 1: glycerol kinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.43Å 105.43Å 195.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 55.48 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.30) 99.2 (55.48-2.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.193 , 0.240 0.195 , 0.241	Depositor DCC
R_{free} test set	2521 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 49935 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8139	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MPD

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	0.70	1/3960 (0.0%)	0.93	15/5388 (0.3%)
1	B	0.71	0/3960	0.91	17/5388 (0.3%)
All	All	0.71	1/7920 (0.0%)	0.92	32/10776 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	ASP	CB-CG	-5.42	1.40	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	ASP	CB-CG-OD2	10.15	127.44	118.30
1	A	246	ASP	CB-CG-OD2	9.29	126.66	118.30
1	A	431	ASP	CB-CG-OD2	8.82	126.24	118.30
1	A	218	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	340	ASP	CB-CG-OD1	-7.88	111.20	118.30
1	B	208	ASP	CB-CG-OD2	7.77	125.30	118.30
1	B	195	ASP	CB-CG-OD2	7.59	125.13	118.30
1	B	145	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	330	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	361	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	340	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	464	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	297	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	461	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	195	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	404	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	204	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	464	ASP	CB-CG-OD2	5.79	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	320	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	184	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	35	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	3	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	246	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	190	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	327	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	431	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	165	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	469	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	89	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	158	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	361	ASP	CB-CG-OD2	5.19	122.97	118.30

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	3877	0	3758	94	0
1	B	3877	0	3758	98	0
2	A	16	0	26	5	0
2	B	16	0	26	17	0
3	A	179	0	0	19	0
3	B	174	0	0	23	0
All	All	8139	0	7568	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (196) 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)
2:A:1:MPD:H51	3:A:2128:HOH:O	1.14	1.25
2:B:1001:MPD:H51	3:B:3167:HOH:O	1.35	1.24
1:B:118:GLU:HB2	3:B:3050:HOH:O	1.56	1.05
1:B:486:ARG:HD2	3:B:3075:HOH:O	1.57	1.03
1:A:82:ARG:HH21	2:A:1:MPD:H13	1.25	1.01
1:A:109:LYS:HG3	3:A:2027:HOH:O	1.66	0.96
1:A:372:TYR:CD2	1:A:372:TYR:N	2.28	0.95
1:B:436:LYS:HE3	3:B:3138:HOH:O	1.68	0.94
1:A:69:THR:HG22	1:A:71:GLU:H	1.34	0.93
2:B:1001:MPD:C5	3:B:3167:HOH:O	2.01	0.92
1:A:372:TYR:HD2	1:A:372:TYR:N	1.67	0.91
1:B:271:PHE:CZ	2:B:1001:MPD:H53	2.07	0.90
1:B:271:PHE:CE1	2:B:1001:MPD:H53	2.08	0.88
1:B:317:TRP:CG	2:B:3001:MPD:H52	2.14	0.82
1:B:271:PHE:CE1	2:B:1001:MPD:C5	2.65	0.80
1:B:477:GLU:HB3	3:B:3102:HOH:O	1.81	0.80
1:B:486:ARG:HG3	3:B:3009:HOH:O	1.82	0.79
1:A:346:PHE:O	1:A:348:PRO:HD3	1.83	0.78
1:A:412:GLY:O	1:A:415:VAL:HG22	1.84	0.76
1:A:482:GLU:HG2	3:A:2114:HOH:O	1.86	0.75
1:B:374:ASN:H	1:B:377:HIS:HD2	1.35	0.74
1:B:103:GLN:NE2	3:B:3065:HOH:O	2.21	0.73
1:B:104:ASP:OD1	1:B:106:ARG:HD2	1.90	0.72
1:A:340:ASP:HB3	1:A:342:GLY:H	1.53	0.72
1:B:271:PHE:HE1	2:B:1001:MPD:C5	2.02	0.71
1:B:82:ARG:HB2	2:B:1001:MPD:O2	1.91	0.71
1:A:232:ARG:CZ	1:A:232:ARG:HB2	2.18	0.71
1:B:317:TRP:CD1	2:B:3001:MPD:H52	2.26	0.70
1:A:232:ARG:NH1	1:A:232:ARG:HB2	2.06	0.70
1:A:22:HIS:HE1	3:A:2023:HOH:O	1.73	0.70
1:A:16:ARG:HG2	1:A:16:ARG:HH11	1.56	0.69
1:B:232:ARG:HG2	3:B:3027:HOH:O	1.93	0.69
1:B:250:ALA:HB2	1:B:441:THR:HG22	1.75	0.68
1:A:149:GLY:O	1:A:152:GLU:HG2	1.95	0.67
1:A:327:ASP:N	1:A:327:ASP:OD1	2.18	0.66
1:A:126:ILE:HG21	1:A:202:ARG:HD3	1.77	0.66
1:B:371:ARG:NH1	1:B:372:TYR:OH	2.29	0.66
1:B:177:GLU:OE1	1:B:232:ARG:NH2	2.28	0.66
1:A:263:LYS:HE2	1:A:265:THR:OG1	1.97	0.65
1:A:482:GLU:HG3	3:A:2172:HOH:O	1.96	0.65
1:A:82:ARG:NH2	2:A:1:MPD:H13	2.04	0.65
1:B:371:ARG:NH1	1:B:372:TYR:CZ	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:HG3	1:B:156:LYS:NZ	2.12	0.65
1:B:271:PHE:HE1	2:B:1001:MPD:H51	1.59	0.64
1:B:356:PRO:HD3	3:B:3160:HOH:O	1.97	0.63
1:A:69:THR:CG2	1:A:71:GLU:H	2.10	0.63
1:A:354:PHE:O	1:A:358:TRP:N	2.32	0.62
1:B:355:ALA:HA	1:B:358:TRP:CZ3	2.35	0.62
1:B:356:PRO:HG3	1:B:493:THR:HG23	1.81	0.62
1:B:161:PHE:CG	1:B:162:GLY:N	2.67	0.62
1:B:127:VAL:HG11	1:B:192:MET:O	2.01	0.61
1:A:329:PRO:HD2	3:A:2169:HOH:O	2.01	0.61
1:B:482:GLU:HB3	3:B:3169:HOH:O	2.00	0.61
1:B:284:LYS:HD2	1:B:284:LYS:N	2.16	0.60
1:A:401:SER:HB2	1:A:403:VAL:HB	1.83	0.60
1:B:155:GLU:HG3	3:B:3078:HOH:O	2.01	0.60
1:A:234:LEU:C	1:A:236:PRO:HD3	2.22	0.60
1:B:329:PRO:HD2	3:B:3172:HOH:O	2.02	0.60
1:A:263:LYS:CE	1:A:265:THR:OG1	2.51	0.59
1:A:405:LEU:CD2	1:A:430:VAL:HG21	2.33	0.59
1:A:391:ARG:NH2	1:A:481:ARG:HH21	2.01	0.59
1:B:313:SER:HB3	3:B:3051:HOH:O	2.02	0.58
1:A:218:ASP:HB3	3:A:2107:HOH:O	2.02	0.58
1:B:201:TRP:CE2	1:B:219:ILE:HD11	2.39	0.58
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.20	0.57
1:B:356:PRO:CD	3:B:3160:HOH:O	2.52	0.57
1:B:331:VAL:HG13	1:B:379:ALA:HB1	1.86	0.56
1:A:271:PHE:HZ	2:A:1:MPD:H53	1.70	0.56
1:A:486:ARG:HG2	3:A:2161:HOH:O	2.05	0.56
1:B:480:GLU:OE2	1:B:483:ARG:NH1	2.36	0.56
1:A:271:PHE:CZ	2:A:1:MPD:H53	2.41	0.56
1:A:69:THR:HG22	1:A:71:GLU:N	2.12	0.56
1:A:359:ARG:HD2	3:A:2044:HOH:O	2.05	0.56
2:B:3001:MPD:C4	3:B:3051:HOH:O	2.53	0.55
1:A:235:VAL:N	1:A:236:PRO:HD3	2.21	0.55
1:B:80:ASN:HB2	1:B:164:THR:OG1	2.05	0.55
1:A:391:ARG:HG2	1:A:485:TYR:CZ	2.41	0.55
1:A:122:LYS:NZ	3:A:2071:HOH:O	2.32	0.55
1:A:372:TYR:HA	3:A:2150:HOH:O	2.06	0.55
1:A:366:LEU:HG	1:A:369:LEU:HD21	1.90	0.54
1:B:332:GLU:HB2	1:B:417:ASN:ND2	2.23	0.54
1:A:44:VAL:HG11	1:A:103:GLN:HE21	1.73	0.54
2:B:1001:MPD:C4	3:B:3167:HOH:O	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:HG13	1:A:379:ALA:HB1	1.89	0.53
1:B:355:ALA:HB2	1:B:358:TRP:CH2	2.44	0.53
1:B:317:TRP:CD1	2:B:3001:MPD:C5	2.91	0.53
1:B:152:GLU:HG3	1:B:156:LYS:HZ3	1.73	0.53
1:A:56:ARG:HG2	3:A:2065:HOH:O	2.08	0.53
1:A:333:TRP:HA	1:A:333:TRP:CE3	2.44	0.52
1:B:354:PHE:HA	1:B:358:TRP:CD1	2.46	0.51
1:A:191:THR:O	1:A:192:MET:HB2	2.10	0.51
1:B:281:VAL:HG11	1:B:401:SER:HB3	1.91	0.51
1:A:466:TRP:CZ3	1:A:468:GLU:HB3	2.46	0.51
1:B:256:CYS:SG	1:B:409:ARG:HG3	2.51	0.51
1:A:354:PHE:HA	1:A:358:TRP:CD1	2.46	0.50
1:B:6:LEU:HD11	1:B:17:ALA:HB1	1.93	0.50
1:A:83:GLU:HG2	1:A:135:PHE:HA	1.94	0.50
1:A:180:VAL:HG23	1:A:180:VAL:O	2.10	0.50
1:A:503:VAL:HG12	1:B:483:ARG:HD2	1.93	0.50
1:B:264:ASN:HB2	1:B:408:LEU:HD11	1.93	0.50
1:B:357:TYR:O	1:B:358:TRP:HB2	2.12	0.50
1:B:149:GLY:O	1:B:153:LYS:HG3	2.11	0.50
1:A:121:GLU:OE2	1:A:124:LYS:HD2	2.13	0.49
1:A:22:HIS:HD2	3:A:2037:HOH:O	1.96	0.49
1:A:152:GLU:O	1:A:156:LYS:HD3	2.13	0.49
1:B:204:ASP:N	1:B:204:ASP:OD1	2.44	0.49
1:B:224:GLU:O	1:B:241:ALA:HA	2.12	0.49
1:B:271:PHE:CZ	2:B:1001:MPD:C5	2.89	0.48
1:A:126:ILE:HD12	1:A:202:ARG:NH1	2.29	0.48
1:B:82:ARG:HH21	2:B:1001:MPD:H13	1.79	0.48
1:A:330:ASP:N	3:A:2169:HOH:O	2.42	0.48
1:B:486:ARG:NH2	3:B:3169:HOH:O	2.45	0.48
1:A:294:LYS:HE3	1:A:298:ALA:O	2.14	0.48
1:A:78:ILE:O	1:A:243:ILE:HA	2.14	0.48
1:B:46:HIS:O	1:B:48:PRO:HD3	2.13	0.48
1:B:407:GLU:OE2	1:B:471:ARG:NH2	2.47	0.48
1:B:486:ARG:O	1:B:490:LYS:HG3	2.14	0.48
1:B:78:ILE:O	1:B:243:ILE:HA	2.14	0.48
1:B:272:LEU:C	1:B:273:LEU:HD12	2.34	0.48
1:B:90:LYS:HD3	1:B:158:ASP:HA	1.97	0.47
1:A:153:LYS:HG3	1:A:159:LEU:HD11	1.97	0.47
1:A:266:TYR:HB3	1:A:414:MET:HB2	1.97	0.47
1:A:357:TYR:O	1:A:358:TRP:HB2	2.15	0.46
1:B:201:TRP:CD2	1:B:219:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:TRP:HA	1:A:333:TRP:HE3	1.79	0.46
1:B:504:GLU:C	3:B:3056:HOH:O	2.53	0.46
1:A:79:THR:HG21	1:A:441:THR:HG22	1.97	0.46
1:B:389:GLN:HA	1:B:392:GLU:HG2	1.97	0.46
1:B:155:GLU:CG	3:B:3078:HOH:O	2.63	0.46
1:B:314:LEU:HD13	2:B:3001:MPD:HM1	1.97	0.46
1:B:325:PHE:C	1:B:327:ASP:H	2.19	0.46
1:B:191:THR:O	1:B:192:MET:HB2	2.16	0.46
1:B:163:ASN:HB2	1:B:165:ASP:OD1	2.16	0.46
1:B:373:VAL:HA	1:B:377:HIS:CD2	2.51	0.46
1:A:235:VAL:N	1:A:236:PRO:CD	2.78	0.45
1:B:325:PHE:C	1:B:327:ASP:N	2.69	0.45
1:A:329:PRO:CD	3:A:2169:HOH:O	2.62	0.45
1:B:486:ARG:CZ	3:B:3169:HOH:O	2.64	0.45
1:B:152:GLU:HG3	1:B:156:LYS:HZ1	1.79	0.45
1:A:354:PHE:HE1	1:A:392:GLU:HG3	1.82	0.45
1:A:6:LEU:HD11	1:A:17:ALA:HB1	1.99	0.45
1:A:122:LYS:CE	3:A:2071:HOH:O	2.63	0.45
1:A:346:PHE:C	1:A:348:PRO:HD3	2.37	0.45
1:A:163:ASN:HB2	1:A:165:ASP:OD1	2.17	0.45
1:A:83:GLU:HB3	1:A:134:TYR:O	2.17	0.45
1:B:339:GLN:HA	1:B:339:GLN:OE1	2.15	0.44
1:B:263:LYS:HA	1:B:409:ARG:O	2.17	0.44
1:A:389:GLN:O	1:A:392:GLU:HG2	2.17	0.44
1:A:136:SER:O	1:A:139:LYS:HB2	2.17	0.44
1:B:294:LYS:HE3	1:B:298:ALA:O	2.16	0.44
1:A:405:LEU:HD23	1:A:430:VAL:HG21	2.00	0.44
1:B:161:PHE:CD2	1:B:162:GLY:N	2.86	0.44
1:A:359:ARG:CD	3:A:2044:HOH:O	2.62	0.43
1:B:154:ALA:HA	1:B:159:LEU:HB2	2.00	0.43
1:A:182:VAL:CG1	1:A:183:THR:N	2.82	0.43
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.83	0.43
1:A:69:THR:HG22	1:A:71:GLU:CB	2.49	0.43
1:A:405:LEU:HD21	1:A:430:VAL:HG21	2.01	0.43
1:B:151:ARG:HH11	1:B:151:ARG:CG	2.31	0.43
1:A:81:GLN:HG3	1:A:81:GLN:O	2.18	0.43
1:B:83:GLU:HG2	1:B:135:PHE:HA	2.00	0.42
1:A:180:VAL:CG2	1:A:180:VAL:O	2.67	0.42
1:A:116:GLY:O	1:A:117:ASP:C	2.58	0.42
1:A:69:THR:HG22	1:A:71:GLU:HB2	2.01	0.42
1:B:332:GLU:HB2	1:B:417:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ASN:H	1:B:377:HIS:CD2	2.25	0.42
1:B:20:PHE:HA	1:B:25:GLU:O	2.20	0.42
1:A:69:THR:CG2	1:A:71:GLU:HB2	2.50	0.42
1:A:264:ASN:HB2	1:A:408:LEU:HD11	2.00	0.42
1:B:294:LYS:HE2	1:B:296:GLY:O	2.19	0.42
1:B:19:VAL:HG11	1:B:68:LEU:CD1	2.50	0.42
1:A:126:ILE:HG21	1:A:202:ARG:CD	2.49	0.42
1:B:271:PHE:CE1	2:B:1001:MPD:H51	2.43	0.41
1:A:116:GLY:O	1:A:118:GLU:N	2.53	0.41
1:A:404:ASP:O	1:A:405:LEU:C	2.57	0.41
1:A:182:VAL:HG12	1:A:183:THR:N	2.36	0.41
1:A:161:PHE:CG	1:A:162:GLY:N	2.88	0.41
1:B:346:PHE:O	1:B:348:PRO:HD3	2.19	0.41
1:B:494:LYS:HD3	1:B:494:LYS:HA	1.81	0.41
1:B:83:GLU:HB3	1:B:134:TYR:O	2.21	0.41
1:B:234:LEU:C	1:B:236:PRO:HD3	2.41	0.41
1:B:238:VAL:HA	1:B:239:PRO:HD3	1.96	0.41
1:B:418:GLU:CG	3:B:3055:HOH:O	2.68	0.41
1:A:107:THR:HA	3:A:2027:HOH:O	2.21	0.41
1:B:380:ARG:HD3	3:B:3139:HOH:O	2.21	0.41
1:A:191:THR:O	1:A:192:MET:CB	2.68	0.41
1:A:323:GLY:O	1:A:326:GLU:HG3	2.20	0.41
1:B:104:ASP:CG	1:B:106:ARG:HD2	2.41	0.40
1:A:59:VAL:O	1:A:63:LEU:HG	2.21	0.40
1:A:22:HIS:CD2	3:A:2037:HOH:O	2.73	0.40
1:B:330:ASP:HB3	1:B:333:TRP:CD1	2.57	0.40
1:B:255:ALA:HA	1:B:257:PHE:CZ	2.55	0.40
1:B:70:HIS:CB	1:B:236:PRO:HD2	2.52	0.40
1:A:311:THR:HG1	1:A:312:GLY:H	1.70	0.40
1:A:332:GLU:HB2	1:A:417:ASN:ND2	2.36	0.40
1:B:26:ILE:HD11	1:B:439:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	501/504 (99%)	486 (97%)	14 (3%)	1 (0%)	52 64
1	B	501/504 (99%)	486 (97%)	14 (3%)	1 (0%)	52 64
All	All	1002/1008 (99%)	972 (97%)	28 (3%)	2 (0%)	52 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	ASP
1	B	83	GLU

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	401/402 (100%)	379 (94%)	22 (6%)	27 36
1	B	401/402 (100%)	384 (96%)	17 (4%)	36 49
All	All	802/804 (100%)	763 (95%)	39 (5%)	31 41

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	16	ARG
1	A	40	ARG
1	A	61	LEU
1	A	67	ASN
1	A	69	THR
1	A	109	LYS
1	A	111	VAL
1	A	117	ASP
1	A	155	GLU
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	234	LEU
1	A	263	LYS
1	A	264	ASN
1	A	279	GLU
1	A	284	LYS
1	A	327	ASP
1	A	346	PHE
1	A	353	LEU
1	A	371	ARG
1	A	372	TYR
1	A	473	SER
1	B	10	GLN
1	B	16	ARG
1	B	71	GLU
1	B	106	ARG
1	B	111	VAL
1	B	117	ASP
1	B	151	ARG
1	B	180	VAL
1	B	234	LEU
1	B	263	LYS
1	B	264	ASN
1	B	284	LYS
1	B	359	ARG
1	B	411	ASP
1	B	433	VAL
1	B	471	ARG
1	B	477	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	31	GLN
1	A	103	GLN
1	A	264	ASN
1	A	270	ASN
1	A	424	GLN
1	B	22	HIS
1	B	31	GLN
1	B	264	ASN
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	377	HIS
1	B	398	ASN
1	B	424	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	MPD	A	1	-	6,7,7	0.38	0	7,10,10	1.09	1 (14%)
2	MPD	A	2001	-	6,7,7	0.40	0	7,10,10	1.20	1 (14%)
2	MPD	B	1001	-	6,7,7	0.24	0	7,10,10	1.29	1 (14%)
2	MPD	B	3001	-	6,7,7	0.37	0	7,10,10	1.17	1 (14%)

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	MPD	A	1	-	1/1/2/2	0/5/5/5	0/0/0/0
2	MPD	A	2001	-	1/1/2/2	0/5/5/5	0/0/0/0
2	MPD	B	1001	-	1/1/2/2	0/5/5/5	0/0/0/0
2	MPD	B	3001	-	1/1/2/2	0/5/5/5	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3001	MPD	C2-C3-C4	2.51	128.50	116.66
2	A	1	MPD	C2-C3-C4	2.66	129.23	116.66
2	A	2001	MPD	C2-C3-C4	2.70	129.43	116.66
2	B	1001	MPD	C2-C3-C4	2.90	130.38	116.66

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3001	MPD	C4
2	A	1	MPD	C4
2	B	1001	MPD	C4
2	A	2001	MPD	C4

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MPD	5	0
2	B	1001	MPD	12	0
2	B	3001	MPD	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	503/504 (99%)	-0.26	9 (1%) 71 78	18, 28, 43, 62	0
1	B	503/504 (99%)	-0.23	7 (1%) 78 83	19, 28, 46, 62	0
All	All	1006/1008 (99%)	-0.25	16 (1%) 74 80	18, 28, 44, 62	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ASP	7.7
1	A	356	PRO	4.8
1	A	372	TYR	4.7
1	A	118	GLU	4.6
1	B	372	TYR	3.5
1	A	403	VAL	3.3
1	B	152	GLU	3.1
1	A	355	ALA	3.1
1	B	149	GLY	2.6
1	B	355	ALA	2.6
1	B	96	VAL	2.3
1	B	118	GLU	2.2
1	A	358	TRP	2.1
1	A	148	GLU	2.0
1	B	297	ASP	2.0
1	A	327	ASP	2.0

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

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^{th} 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^2)	Q<0.9
2	MPD	B	1001	8/8	0.66	0.47	23.16	67,67,71,73	0
2	MPD	A	1	8/8	0.87	0.27	10.97	64,66,68,69	0
2	MPD	B	3001	8/8	0.86	0.38	7.74	60,61,67,68	0
2	MPD	A	2001	8/8	0.93	0.27	4.47	62,64,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.