



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:05 PM UTC

PDB ID : 2D4W / pdb_00002d4w
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

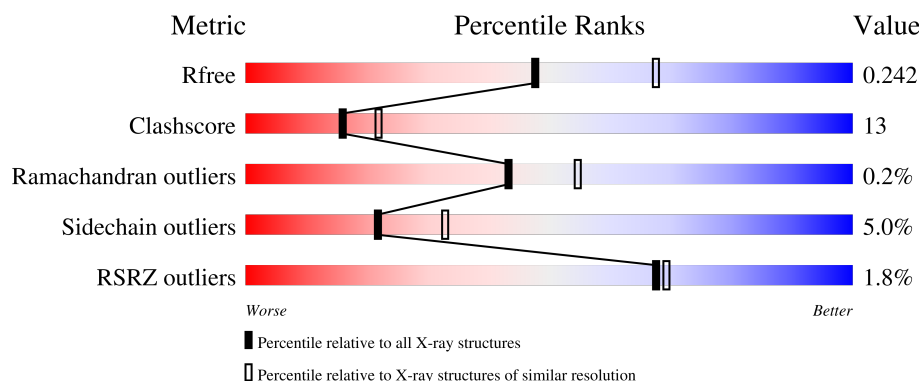
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	504	
1	B	504	

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

2 Entry composition [i](#)

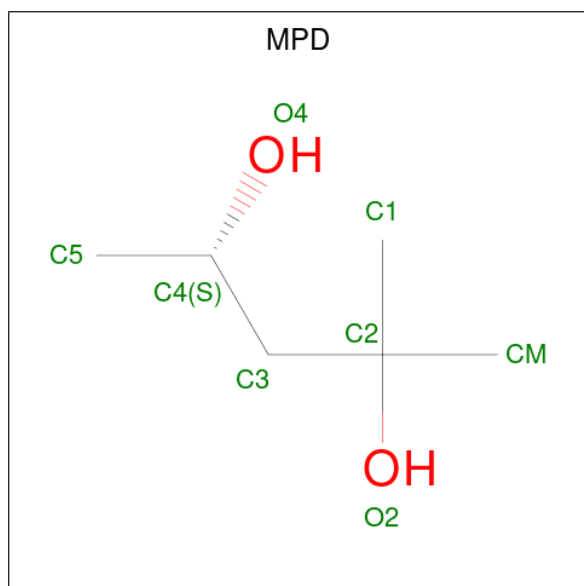
There are 3 unique types of molecules in this entry. The entry contains 8139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

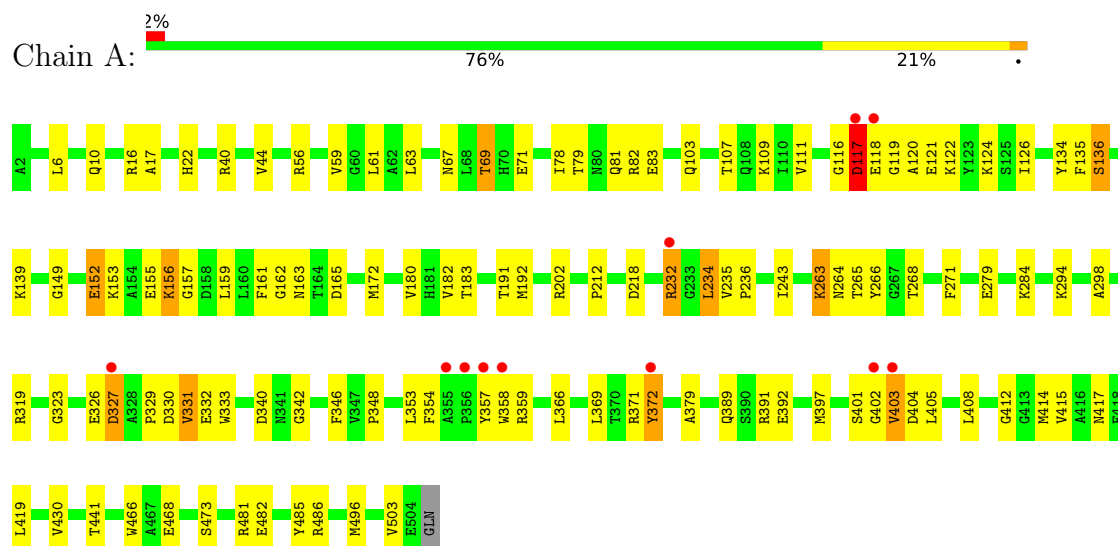
- Molecule 3 is water.

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

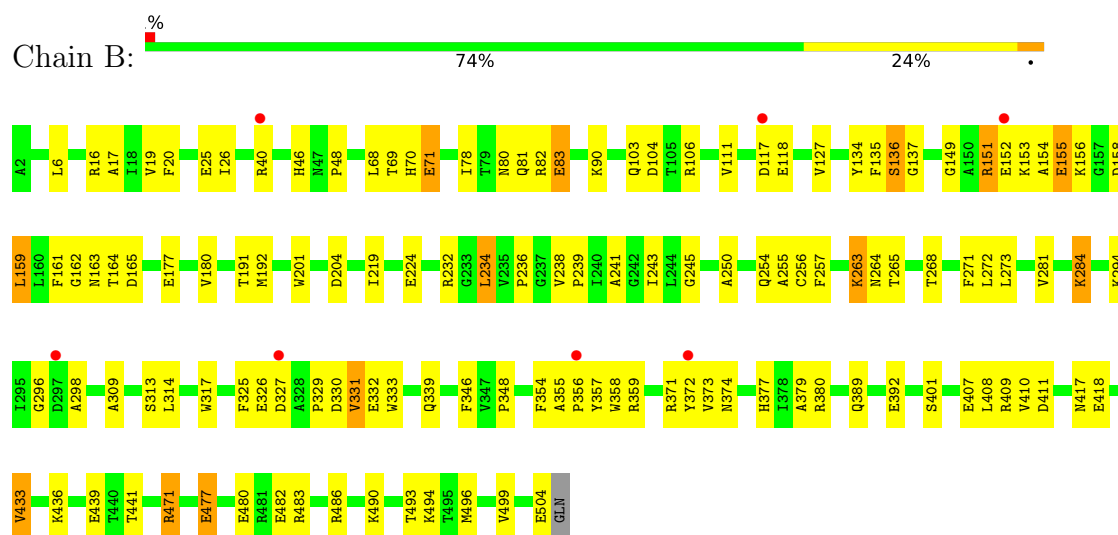
3 Residue-property plots [i](#)

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 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



• Molecule 1: glycerol kinase



4 Data and refinement statistics

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 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.30) 99.7 (20.00-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.193 , 0.240 0.196 , 0.242	Depositor DCC
R_{free} test set	2529 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.86	2/3960 (0.1%)	1.11	8/5388 (0.1%)
1	B	0.89	0/3960	1.10	9/5388 (0.2%)
All	All	0.88	2/7920 (0.0%)	1.11	17/10776 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	MET	SD-CE	6.93	1.96	1.79
1	A	397	MET	SD-CE	5.77	1.94	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	SER	N-CA-C	7.53	119.13	111.07
1	B	136	SER	N-CA-C	7.49	119.09	111.07
1	A	402	GLY	N-CA-C	-7.38	105.13	115.32
1	B	326	GLU	N-CA-C	-6.63	105.06	113.01
1	B	410	VAL	N-CA-C	6.30	117.55	108.48
1	B	245	GLY	N-CA-C	-5.94	105.10	111.93
1	B	268	THR	N-CA-C	-5.82	105.07	111.82
1	A	403	VAL	N-CA-C	-5.73	98.17	106.88
1	A	403	VAL	CA-C-N	-5.51	115.11	122.72
1	A	403	VAL	C-N-CA	-5.51	115.11	122.72
1	A	157	GLY	N-CA-C	-5.43	107.52	115.72
1	B	81	GLN	N-CA-C	-5.37	102.45	110.23
1	B	254	GLN	N-CA-C	-5.33	106.55	113.16
1	B	309	ALA	N-CA-C	5.27	116.71	111.07
1	B	433	VAL	N-CA-C	5.21	115.98	108.48
1	A	212	PRO	CA-C-O	-5.20	115.41	121.34
1	A	268	THR	N-CA-C	-5.20	105.73	111.71

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	3877	0	3758	96	0
1	B	3877	0	3758	102	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	202	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 (202) 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:N	1:A:372:TYR:HD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:232:ARG:CZ	1:A:232:ARG:HB2	2.18	0.71
1:B:82:ARG:HB2	2:B:1001:MPD:O2	1.91	0.71
1:B:271:PHE:HE1	2:B:1001:MPD:C5	2.02	0.71
1:B:317:TRP:CD1	2:B:3001:MPD:H52	2.26	0.70
1:A:232:ARG:HB2	1:A:232:ARG:NH1	2.06	0.70
1:A:22:HIS:HE1	3:A:2023:HOH:O	1.73	0.70
1:A:16:ARG:HH11	1:A:16:ARG:HG2	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:OD1	1:A:327:ASP:N	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:A:234:LEU:C	1:A:236:PRO:HD3	2.22	0.65
1:B:371:ARG:NH1	1:B:372:TYR:CZ	2.65	0.65
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:N	1:B:284:LYS:HD2	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:B:329:PRO:HD2	3:B:3172:HOH:O	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:CE	1:A:265:THR:OG1	2.51	0.59
1:A:391:ARG:NH2	1:A:481:ARG:HH21	2.01	0.59
1:A:405:LEU:CD2	1:A:430:VAL:HG21	2.33	0.59
1:B:313:SER:HB3	3:B:3051:HOH:O	2.02	0.58
1:B:496:MET:HA	1:B:496:MET:HE2	1.84	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
1:A:235:VAL:N	1:A:236:PRO:HD3	2.21	0.55
2:B:3001:MPD:C4	3:B:3051:HOH:O	2.53	0.55
1:B:80:ASN:HB2	1:B:164:THR:OG1	2.05	0.55
1:A:122:LYS:NZ	3:A:2071:HOH:O	2.32	0.55
1:A:391:ARG:HG2	1:A:485:TYR:CZ	2.41	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
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:152:GLU:HG3	1:B:156:LYS:HZ3	1.73	0.53
1:B:317:TRP:CD1	2:B:3001:MPD:C5	2.91	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:272:LEU:C	1:B:273:LEU:HD12	2.34	0.52
1:B:504:GLU:C	3:B:3056:HOH:O	2.53	0.51
1:B:354:PHE:HA	1:B:358:TRP:CD1	2.46	0.51
1:B:325:PHE:C	1:B:327:ASP:N	2.69	0.51
1:A:191:THR:O	1:A:192:MET:HB2	2.10	0.51
1:A:466:TRP:CZ3	1:A:468:GLU:HB3	2.46	0.51
1:B:281:VAL:HG11	1:B:401:SER:HB3	1.91	0.51
1:B:256:CYS:SG	1:B:409:ARG:HG3	2.51	0.51
1:B:325:PHE:C	1:B:327:ASP:H	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:149:GLY:O	1:B:153:LYS:HG3	2.11	0.50
1:B:357:TYR:O	1:B:358:TRP:HB2	2.12	0.50
1:A:346:PHE:C	1:A:348:PRO:HD3	2.37	0.49
1:A:180:VAL:O	1:A:180:VAL:HG23	2.10	0.49
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:224:GLU:O	1:B:241:ALA:HA	2.12	0.49
1:A:126:ILE:HD12	1:A:202:ARG:NH1	2.29	0.48
1:B:271:PHE:CZ	2:B:1001:MPD:C5	2.89	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:A:294:LYS:HE3	1:A:298:ALA:O	2.14	0.48
1:B:486:ARG:NH2	3:B:3169:HOH:O	2.45	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:78:ILE:O	1:B:243:ILE:HA	2.14	0.48
1:B:486:ARG:O	1:B:490:LYS:HG3	2.14	0.48
1:B:204:ASP:N	1:B:204:ASP:OD1	2.44	0.47
1:A:116:GLY:O	1:A:117:ASP:C	2.58	0.47
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:333:TRP:HA	1:A:333:TRP:HE3	1.79	0.46
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
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:A:404:ASP:O	1:A:405:LEU:C	2.57	0.46
1:B:314:LEU:HD13	2:B:3001:MPD:HM1	1.97	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:234:LEU:C	1:B:236:PRO:HD3	2.41	0.46
1:B:373:VAL:HA	1:B:377:HIS:CD2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:N	1:A:236:PRO:CD	2.78	0.45
1:B:104:ASP:CG	1:B:106:ARG:HD2	2.41	0.45
1:A:329:PRO:CD	3:A:2169:HOH:O	2.62	0.45
1:A:354:PHE:HE1	1:A:392:GLU:HG3	1.82	0.45
1:B:152:GLU:HG3	1:B:156:LYS:HZ1	1.79	0.45
1:B:486:ARG:CZ	3:B:3169:HOH:O	2.64	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: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:OE1	1:B:339:GLN:HA	2.15	0.44
1:B:263:LYS:HA	1:B:409:ARG:O	2.17	0.44
1:B:265:THR:OG1	1:B:411:ASP:OD1	2.30	0.44
1:A:136:SER:O	1:A:139:LYS:HB2	2.17	0.44
1:A:389:GLN:O	1:A:392:GLU:HG2	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:136:SER:O	1:B:137:GLY:C	2.61	0.43
1:A:182:VAL:CG1	1:A:183:THR:N	2.82	0.43
1:B:154:ALA:HA	1:B:159:LEU:HB2	2.00	0.43
1:A:496:MET:HA	1:A:496:MET:HE2	2.01	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:81:GLN:O	1:A:81:GLN:HG3	2.18	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:B:69:THR:C	1:B:71:GLU:N	2.75	0.42
1:B:83:GLU:HG2	1:B:135:PHE:HA	2.00	0.42
1:A:180:VAL:O	1:A:180:VAL:CG2	2.67	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
1:B:20:PHE:HA	1:B:25:GLU:O	2.20	0.42
1:B:374:ASN:H	1:B:377:HIS:CD2	2.25	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:A:116:GLY:O	1:A:118:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CE1	2:B:1001:MPD:H51	2.43	0.41
1:A:119:GLY:O	1:A:120:ALA:C	2.63	0.41
1:A:161:PHE:CG	1:A:162:GLY:N	2.88	0.41
1:A:182:VAL:HG12	1:A:183:THR:N	2.36	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: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: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:255:ALA:HA	1:B:257:PHE:CZ	2.55	0.40
1:B:330:ASP:HB3	1:B:333:TRP:CD1	2.57	0.40
1:A:69:THR:C	1:A:71:GLU:N	2.77	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
1:B:70:HIS:CB	1:B:236:PRO:HD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	55
1	B	501/504 (99%)	486 (97%)	14 (3%)	1 (0%)	43	55
All	All	1002/1008 (99%)	972 (97%)	28 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

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

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	401/402 (100%)	378 (94%)	23 (6%)	18	27
1	B	401/402 (100%)	384 (96%)	17 (4%)	26	40
All	All	802/804 (100%)	762 (95%)	40 (5%)	22	33

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	40	ARG
1	A	61	LEU
1	A	67	ASN
1	A	69	THR
1	A	111	VAL
1	A	117	ASP
1	A	152	GLU
1	A	155	GLU
1	A	156	LYS
1	A	232	ARG
1	A	234	LEU
1	A	263	LYS
1	A	279	GLU
1	A	284	LYS
1	A	319	ARG
1	A	327	ASP
1	A	331	VAL
1	A	353	LEU
1	A	371	ARG
1	A	372	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	419	LEU
1	A	473	SER
1	B	16	ARG
1	B	71	GLU
1	B	111	VAL
1	B	117	ASP
1	B	151	ARG
1	B	155	GLU
1	B	159	LEU
1	B	180	VAL
1	B	234	LEU
1	B	263	LYS
1	B	284	LYS
1	B	331	VAL
1	B	359	ARG
1	B	433	VAL
1	B	471	ARG
1	B	477	GLU
1	B	499	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	31	GLN
1	A	103	GLN
1	A	163	ASN
1	A	264	ASN
1	A	270	ASN
1	A	316	GLN
1	A	424	GLN
1	B	22	HIS
1	B	31	GLN
1	B	163	ASN
1	B	264	ASN
1	B	270	ASN
1	B	377	HIS
1	B	389	GLN
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 oligosaccharides 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	B	3001	-	7,7,7	0.51	0	9,10,10	1.29	1 (11%)
2	MPD	A	2001	-	7,7,7	0.55	0	9,10,10	1.27	1 (11%)
2	MPD	A	1	-	7,7,7	0.42	0	9,10,10	1.34	2 (22%)
2	MPD	B	1001	-	7,7,7	0.27	0	9,10,10	1.34	2 (22%)

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	B	3001	-	1/1/2/2	2/5/5/5	-
2	MPD	A	2001	-	1/1/2/2	4/5/5/5	-
2	MPD	A	1	-	1/1/2/2	4/5/5/5	-
2	MPD	B	1001	-	1/1/2/2	4/5/5/5	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MPD	O4-C4-C3	3.02	123.35	111.35
2	A	2001	MPD	O4-C4-C3	2.67	121.99	111.35
2	B	1001	MPD	C5-C4-C3	2.49	123.22	111.67
2	B	3001	MPD	O4-C4-C3	2.48	121.20	111.35
2	A	1	MPD	C5-C4-C3	2.27	122.23	111.67
2	B	1001	MPD	O4-C4-C3	2.23	120.23	111.35

All (4) chirality outliers are listed below:

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

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	MPD	C1-C2-C3-C4
2	A	1	MPD	O2-C2-C3-C4
2	A	2001	MPD	C1-C2-C3-C4
2	A	2001	MPD	O2-C2-C3-C4
2	B	1001	MPD	C1-C2-C3-C4
2	B	1001	MPD	O2-C2-C3-C4
2	B	1001	MPD	C2-C3-C4-C5
2	A	1	MPD	CM-C2-C3-C4
2	A	2001	MPD	CM-C2-C3-C4
2	A	1	MPD	C2-C3-C4-C5
2	A	2001	MPD	C2-C3-C4-C5
2	B	3001	MPD	C2-C3-C4-C5
2	B	1001	MPD	CM-C2-C3-C4
2	B	3001	MPD	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 22 short contacts:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	MPD	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	503/504 (99%)	-0.25	11 (2%) 62 64	18, 28, 43, 62	0
1	B	503/504 (99%)	-0.20	7 (1%) 73 75	19, 28, 46, 62	0
All	All	1006/1008 (99%)	-0.23	18 (1%) 67 69	18, 28, 44, 62	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ASP	7.8
1	A	372	TYR	5.1
1	A	118	GLU	4.1
1	A	356	PRO	4.0
1	B	327	ASP	3.7
1	A	403	VAL	3.6
1	A	355	ALA	3.4
1	A	327	ASP	3.4
1	B	372	TYR	3.3
1	A	402	GLY	2.8
1	B	152	GLU	2.8
1	B	297	ASP	2.7
1	A	232	ARG	2.7
1	A	357	TYR	2.6
1	B	117	ASP	2.4
1	B	356	PRO	2.3
1	A	358	TRP	2.1
1	B	40	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	B	1001	8/8	0.62	0.29	67,67,71,73	0
2	MPD	A	1	8/8	0.77	0.24	64,66,68,69	0
2	MPD	B	3001	8/8	0.86	0.30	60,61,67,68	0
2	MPD	A	2001	8/8	0.88	0.26	62,64,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.