



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:37 PM UTC

PDB ID : 2CSB / pdb_00002csb
Title : Crystal structure of Topoisomerase V from Methanopyrus kandleri (61 kDa fragment)
Authors : Taneja, B.; Patel, A.; Slesarev, A.; Mondragon, A.
Deposited on : 2005-05-21
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

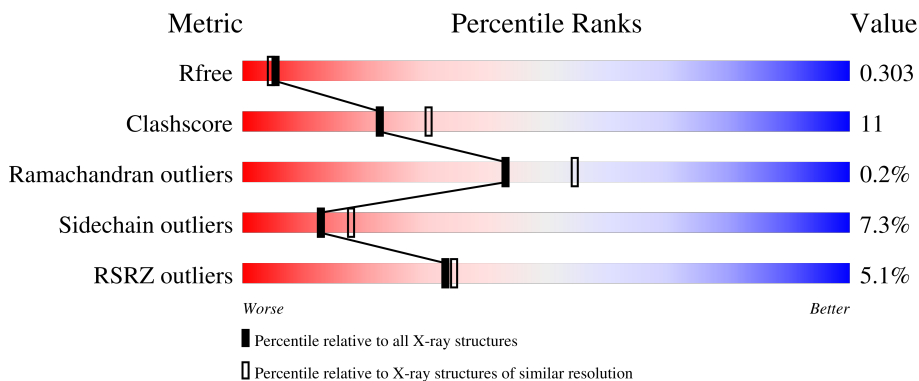
1 Overall quality at a glance

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	519	
1	B	519	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9026 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 Topoisomerase V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	517	Total	C	N	O	S	Se	0	12	0
			4265	2667	768	819	5	6			
1	B	517	Total	C	N	O	S	Se	0	8	0
			4244	2655	765	813	5	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	GB 20094872
A	40	MSE	MET	modified residue	GB 20094872
A	155	MSE	MET	modified residue	GB 20094872
A	166	MSE	MET	modified residue	GB 20094872
A	286	MSE	MET	modified residue	GB 20094872
A	325	MSE	MET	modified residue	GB 20094872
A	391	MSE	MET	modified residue	GB 20094872
B	1	MSE	MET	modified residue	GB 20094872
B	40	MSE	MET	modified residue	GB 20094872
B	155	MSE	MET	modified residue	GB 20094872
B	166	MSE	MET	modified residue	GB 20094872
B	286	MSE	MET	modified residue	GB 20094872
B	325	MSE	MET	modified residue	GB 20094872
B	391	MSE	MET	modified residue	GB 20094872

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

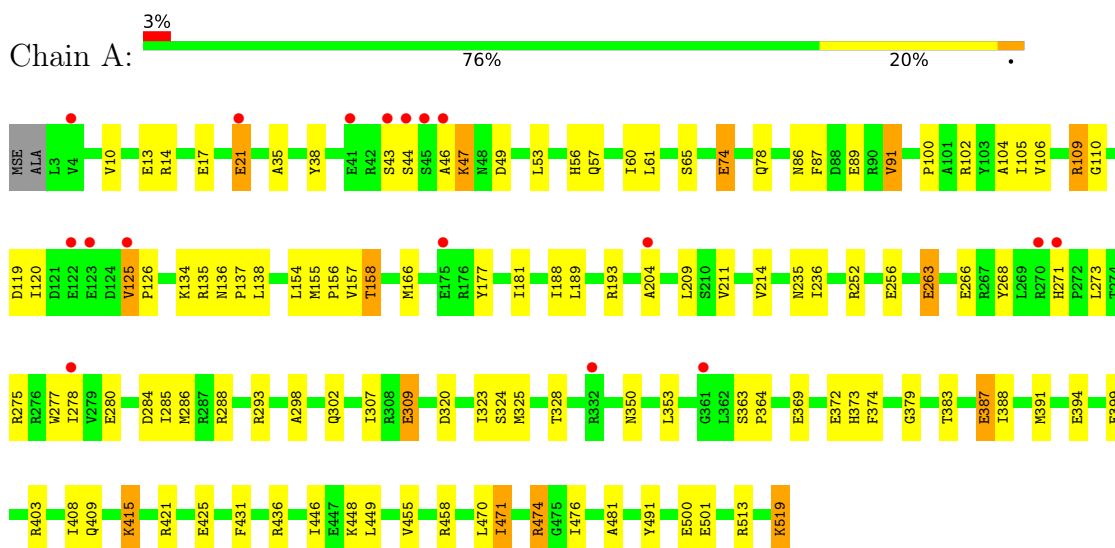
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	277	Total 277	O 277	0	0
3	B	239	Total 239	O 239	0	0

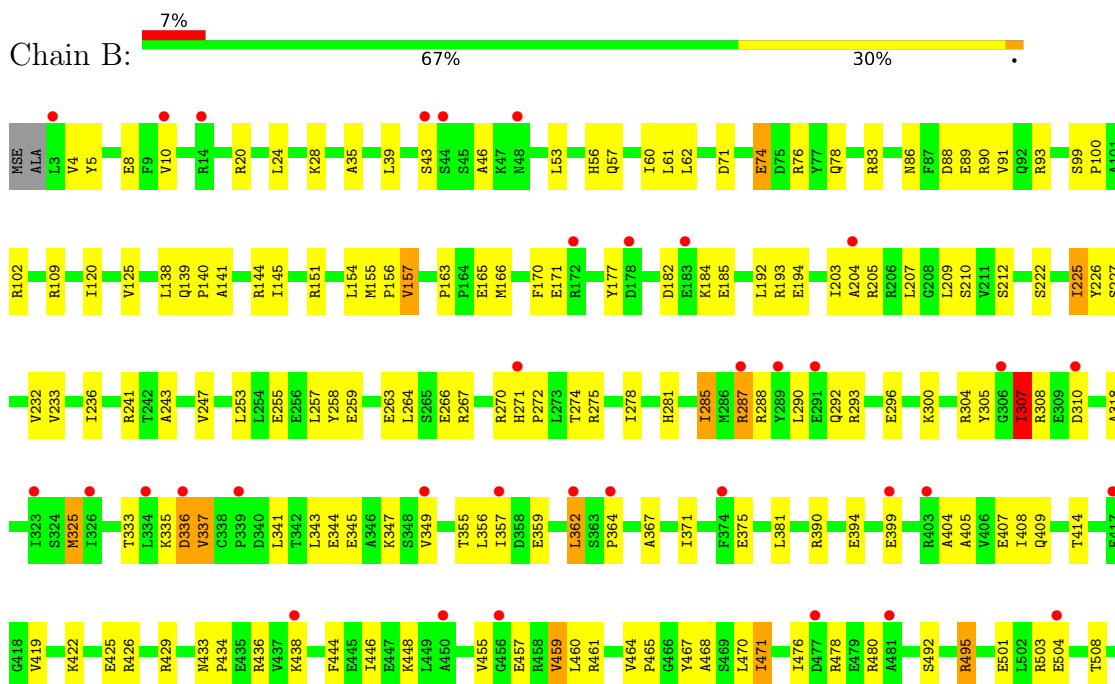
3 Residue-property plots i

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: Topoisomerase V



• Molecule 1: Topoisomerase V





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.69Å 89.77Å 189.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.44 – 2.30 26.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (26.44-2.30) 97.8 (26.44-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1841.48 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.217 , 0.292 0.231 , 0.303	Depositor DCC
R_{free} test set	2942 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9026	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: MG

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	1.00	1/4375 (0.0%)	1.14	2/5884 (0.0%)
1	B	0.93	3/4338 (0.1%)	1.13	6/5835 (0.1%)
All	All	0.96	4/8713 (0.0%)	1.14	8/11719 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ILE	CA-CB	6.07	1.61	1.54
1	B	325	MSE	SE-CE	5.82	2.12	1.95
1	B	232	VAL	CA-CB	5.71	1.61	1.54
1	A	298	ALA	CA-CB	-5.13	1.45	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	VAL	CB-CA-C	7.58	118.81	110.62
1	B	157	VAL	N-CA-C	-7.15	106.25	113.47
1	B	362	LEU	N-CA-C	6.46	118.35	110.41
1	A	157	VAL	N-CA-CB	-6.23	105.35	112.21
1	A	491	TYR	N-CA-C	5.95	117.57	111.14
1	B	62	LEU	N-CA-C	5.71	117.50	111.28
1	B	4	VAL	N-CA-C	5.12	115.72	107.98
1	B	194	GLU	N-CA-C	5.04	116.77	111.28

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	4265	0	4271	76	0
1	B	4244	0	4258	105	0
2	A	1	0	0	0	0
3	A	277	0	0	10	0
3	B	239	0	0	12	0
All	All	9026	0	8529	180	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 11.

All (180) 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:90:ARG:HG3	1:B:93[B]:ARG:NH1	1.53	1.22
1:A:388:ILE:HA	1:A:391:MSE:HE3	1.45	0.98
1:B:90:ARG:CG	1:B:93[B]:ARG:NH1	2.28	0.96
1:B:90:ARG:HG3	1:B:93[B]:ARG:HH12	1.32	0.93
1:B:61:LEU:CD2	1:B:155:MSE:HE1	1.99	0.91
1:B:61:LEU:HD23	1:B:155:MSE:HE1	1.51	0.91
1:A:293:ARG:HG3	3:A:3314:HOH:O	1.70	0.90
1:B:90:ARG:CG	1:B:93[B]:ARG:HH12	1.85	0.89
1:B:151:ARG:NH2	1:B:236:ILE:O	2.05	0.88
1:A:134:LYS:HE2	1:A:135:ARG:NH1	1.89	0.87
1:B:288:ARG:HD3	3:B:739:HOH:O	1.75	0.86
1:B:501:GLU:HG2	3:B:746:HOH:O	1.73	0.86
1:A:17:GLU:O	1:A:21:GLU:HG3	1.79	0.82
1:B:90:ARG:O	1:B:93[B]:ARG:HD3	1.80	0.82
1:B:304:ARG:HB3	3:B:755:HOH:O	1.79	0.81
1:A:519:LYS:HE2	3:A:3312:HOH:O	1.80	0.81
1:B:90:ARG:HG3	1:B:93[B]:ARG:HH11	1.47	0.79
1:B:444:PHE:O	1:B:446:ILE:HD12	1.83	0.78
1:A:263:GLU:O	1:A:266[A]:GLU:HG2	1.86	0.75
1:B:43:SER:HB3	1:B:46:ALA:HB3	1.71	0.70
1:A:87:PHE:O	1:A:91:VAL:HG23	1.92	0.70
1:A:474:ARG:HB2	3:A:3292:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:HE2	1:A:135:ARG:CZ	2.22	0.68
1:B:446:ILE:HG23	1:B:460:LEU:HD22	1.76	0.68
1:A:74:GLU:OE2	1:A:102:ARG:NH2	2.25	0.67
1:B:457:GLU:OE2	1:B:478:ARG:NH1	2.28	0.67
1:A:102:ARG:O	1:A:105:ILE:HG22	1.95	0.66
1:A:47:LYS:HG3	3:A:3261:HOH:O	1.95	0.66
1:A:399:GLU:OE2	1:A:403:ARG:HG3	1.96	0.66
1:B:171:GLU:OE1	1:B:193:ARG:NE	2.30	0.65
1:A:284:ASP:O	1:A:288:ARG:HG2	1.98	0.63
1:B:61:LEU:HD22	1:B:155:MSE:HE1	1.77	0.63
1:A:436:ARG:HG2	3:A:3302:HOH:O	1.98	0.62
1:A:273:LEU:HD21	1:A:278:ILE:HD11	1.83	0.60
1:B:53:LEU:O	1:B:57:GLN:HG3	2.02	0.60
1:B:154:LEU:O	1:B:156:PRO:HD3	2.02	0.60
1:A:109:ARG:HD2	1:A:320:ASP:OD2	2.03	0.59
1:B:467:TYR:OH	1:B:478:ARG:HD3	2.03	0.59
1:A:421:ARG:O	1:A:425:GLU:HG3	2.03	0.58
1:B:155:MSE:SE	3:B:748:HOH:O	2.71	0.57
1:B:266:GLU:HG3	1:B:272:PRO:HB3	1.86	0.57
1:B:419:VAL:HG22	1:B:459:VAL:HB	1.86	0.57
1:A:500:GLU:HG3	3:A:3247:HOH:O	2.03	0.57
1:B:336:ASP:HA	3:B:740:HOH:O	2.05	0.56
1:B:518:LEU:O	1:B:519:LYS:HB2	2.05	0.56
1:A:374:PHE:CZ	1:A:391:MSE:HE1	2.41	0.56
1:B:308:ARG:HD3	1:B:345:GLU:OE2	2.05	0.56
1:B:362:LEU:HD21	1:B:404:ALA:HB2	1.88	0.56
1:A:46:ALA:HA	1:A:268:TYR:CZ	2.42	0.55
1:B:89:GLU:O	1:B:93[A]:ARG:HD2	2.06	0.55
1:A:43:SER:OG	1:A:44:SER:N	2.39	0.55
1:B:264:LEU:CD1	1:B:267:ARG:NH1	2.70	0.54
1:B:468:ALA:HA	1:B:471:ILE:HG22	1.90	0.53
1:B:307:ILE:HD12	1:B:345:GLU:HG2	1.90	0.53
1:A:325:MSE:HE3	1:A:328:THR:OG1	2.09	0.53
1:B:109:ARG:HH22	1:B:325:MSE:HE1	1.73	0.53
1:B:222:SER:HB3	1:B:227:SER:OG	2.09	0.53
1:B:343:LEU:HG	1:B:347:LYS:HE3	1.89	0.53
1:B:24:LEU:HD21	1:B:120:ILE:HD12	1.91	0.53
1:B:405:ALA:O	1:B:409:GLN:HG3	2.09	0.53
1:A:120:ILE:HG22	1:A:126:PRO:HG3	1.91	0.53
1:A:302:GLN:NE2	1:A:309:GLU:HG2	2.24	0.52
1:A:61:LEU:O	1:A:155:MSE:HE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387[B]:GLU:HG3	1:A:391:MSE:HE2	1.92	0.52
1:A:374:PHE:O	1:A:379:GLY:HA3	2.09	0.52
1:B:204:ALA:HB1	1:B:209:LEU:O	2.10	0.51
1:A:125:VAL:HG11	1:A:286:MSE:SE	2.60	0.51
1:B:86:ASN:OD1	1:B:88:ASP:HB2	2.10	0.51
1:A:138:LEU:HD22	1:A:166:MSE:HB3	1.92	0.51
1:A:189:LEU:O	1:A:193:ARG:HG3	2.11	0.51
1:B:426:ARG:CZ	1:B:429:ARG:HG3	2.41	0.50
1:A:17:GLU:O	1:A:21:GLU:CG	2.55	0.50
1:B:281:HIS:O	1:B:285:ILE:HG12	2.11	0.50
1:B:28:LYS:NZ	1:B:255:GLU:OE2	2.45	0.50
1:B:433:ASN:OD1	1:B:436:ARG:HG3	2.12	0.50
1:B:90:ARG:HG2	1:B:93[B]:ARG:NH1	2.25	0.50
1:B:165:GLU:O	1:B:170:PHE:HA	2.11	0.50
1:B:333:THR:O	1:B:337:VAL:HG23	2.12	0.50
1:B:292:GLN:O	1:B:296:GLU:HG3	2.12	0.49
1:A:86:ASN:OD1	1:A:89:GLU:HG3	2.13	0.49
1:B:35:ALA:CB	1:B:278:ILE:HD12	2.42	0.49
1:A:211:VAL:HG11	1:A:324:SER:CB	2.42	0.49
1:B:90:ARG:HG2	1:B:93[B]:ARG:HH12	1.75	0.49
1:B:470:LEU:O	1:B:476[A]:ILE:HD11	2.13	0.49
1:A:188:ILE:HD12	1:A:214:VAL:HG13	1.94	0.48
1:B:141:ALA:O	1:B:145:ILE:HG12	2.13	0.48
1:B:192:LEU:HD11	1:B:225:ILE:HD12	1.96	0.48
1:A:399:GLU:OE2	1:A:403:ARG:NE	2.47	0.48
1:A:204:ALA:HB1	1:A:209:LEU:O	2.14	0.48
1:B:274:THR:O	1:B:278:ILE:HG12	2.14	0.48
1:B:446:ILE:HD12	1:B:446:ILE:H	1.79	0.48
1:B:367:ALA:O	1:B:371:ILE:HG12	2.14	0.48
1:A:13:GLU:HG2	1:B:436:ARG:CZ	2.44	0.47
1:A:155:MSE:HB3	1:A:155:MSE:HE3	1.47	0.47
1:A:470:LEU:O	1:A:476[B]:ILE:HG12	2.14	0.47
1:B:318:ALA:HB1	1:B:337:VAL:HG11	1.95	0.47
1:B:495:ARG:HD2	1:B:515:LEU:O	2.14	0.47
1:B:144:ARG:NH1	1:B:226:TYR:OH	2.46	0.47
1:B:28:LYS:HE3	1:B:275:ARG:HD3	1.97	0.47
1:B:344:GLU:HG2	3:B:744:HOH:O	2.15	0.46
1:B:355:THR:O	1:B:359:GLU:HB2	2.15	0.46
1:B:5:TYR:OH	1:B:83:ARG:HG3	2.15	0.46
1:A:252[B]:ARG:HD2	3:A:3142:HOH:O	2.16	0.46
1:A:374:PHE:CE2	1:A:391:MSE:HE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:O	1:A:155:MSE:CE	2.64	0.46
1:A:431:PHE:HE2	1:A:448:LYS:HZ3	1.64	0.46
1:A:211:VAL:HG11	1:A:324:SER:HB3	1.98	0.45
1:A:455:VAL:HG12	1:A:455:VAL:O	2.16	0.45
1:A:513:ARG:HH21	1:A:519:LYS:HB2	1.81	0.45
1:B:90:ARG:CG	1:B:93[B]:ARG:HH11	2.16	0.45
1:B:163:PRO:HG2	1:B:166:MSE:HG3	1.98	0.45
1:B:287:ARG:HG3	1:B:288:ARG:N	2.31	0.45
1:A:363:SER:O	1:A:364:PRO:C	2.60	0.45
1:A:53:LEU:O	1:A:57:GLN:HG3	2.16	0.44
1:A:65:SER:N	1:A:155:MSE:HE2	2.31	0.44
1:B:390:ARG:O	1:B:394:GLU:HG3	2.16	0.44
1:A:177:TYR:CE1	1:A:236:ILE:HG12	2.52	0.44
1:A:56:HIS:O	1:A:60:ILE:HG12	2.18	0.44
1:A:35:ALA:HB2	1:A:278:ILE:HD11	2.00	0.44
1:A:106:VAL:HG12	1:A:106:VAL:O	2.17	0.44
1:B:356:LEU:CD2	1:B:408:ILE:HD11	2.48	0.43
1:A:275:ARG:O	1:A:278:ILE:HB	2.19	0.43
1:B:305:TYR:CG	1:B:349:VAL:HG12	2.53	0.43
1:A:46:ALA:O	1:A:49:ASP:HB3	2.19	0.43
1:B:501:GLU:HA	1:B:504:GLU:HG2	2.00	0.43
1:A:458:ARG:HD2	3:A:3106:HOH:O	2.18	0.43
1:B:78:GLN:NE2	3:B:628:HOH:O	2.49	0.43
1:B:99:SER:HA	1:B:100:PRO:HD3	1.88	0.43
1:B:271:HIS:HA	1:B:272:PRO:HD2	1.82	0.43
1:B:381:LEU:O	1:B:434:PRO:HD2	2.18	0.43
1:A:277:TRP:HE3	1:A:278:ILE:HD13	1.83	0.43
1:B:56:HIS:NE2	1:B:60:ILE:HD11	2.34	0.43
1:B:243:ALA:O	1:B:247:VAL:HG23	2.19	0.43
1:B:471:ILE:O	1:B:471:ILE:HD13	2.19	0.43
1:B:508:THR:H	1:B:511:GLN:HE21	1.66	0.43
1:B:139:GLN:HA	1:B:140:PRO:HD3	1.91	0.42
1:B:177:TYR:CE1	1:B:236:ILE:HG12	2.54	0.42
1:B:233:VAL:HA	1:B:236:ILE:HD12	2.01	0.42
1:A:38:TYR:CD2	1:A:285:ILE:HG22	2.54	0.42
1:A:136:ASN:HA	1:A:137:PRO:HD2	1.91	0.42
1:A:104:ALA:O	1:A:110:GLY:HA3	2.20	0.42
1:A:383:THR:O	1:A:409:GLN:NE2	2.51	0.42
1:B:91:VAL:HG21	1:B:100:PRO:HA	2.01	0.42
1:B:464:VAL:HA	1:B:465:PRO:HD2	1.80	0.42
1:B:293:ARG:HD2	3:B:722:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PHE:HZ	1:A:391:MSE:HE1	1.84	0.42
1:B:455:VAL:HA	1:B:459:VAL:CG1	2.50	0.42
1:B:508:THR:H	1:B:511:GLN:NE2	2.18	0.42
1:B:241:ARG:NH1	3:B:611:HOH:O	2.53	0.42
1:B:266:GLU:CG	1:B:272:PRO:HB3	2.49	0.42
1:A:154:LEU:O	1:A:156:PRO:HD3	2.19	0.42
1:B:285:ILE:HG12	1:B:285:ILE:H	1.66	0.42
1:A:235:ASN:ND2	3:A:3295:HOH:O	2.41	0.41
1:B:61:LEU:HD22	1:B:155:MSE:CE	2.47	0.41
1:B:35:ALA:HB2	1:B:278:ILE:HD12	2.02	0.41
1:B:109:ARG:NH2	1:B:325:MSE:HE1	2.34	0.41
1:A:158:THR:HG23	3:A:3073:HOH:O	2.19	0.41
1:A:369:GLU:O	1:A:373:HIS:HD2	2.03	0.41
1:B:28:LYS:HE2	1:B:258:TYR:CE1	2.56	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.95	0.41
1:A:134:LYS:CE	1:A:135:ARG:NH1	2.73	0.41
1:B:467:TYR:OH	1:B:478:ARG:CD	2.68	0.41
1:A:91:VAL:HG21	1:A:100:PRO:HA	2.01	0.41
1:A:415[A]:LYS:HB3	1:A:415[A]:LYS:HE2	1.92	0.41
1:B:263:GLU:HG2	3:B:692:HOH:O	2.20	0.41
1:A:476[B]:ILE:HD11	1:A:481:ALA:HB2	2.02	0.41
1:B:74:GLU:CD	1:B:102:ARG:HH22	2.29	0.41
1:B:76:ARG:CD	3:B:742:HOH:O	2.69	0.41
1:B:203:ILE:O	1:B:207:LEU:HG	2.21	0.41
1:B:422:LYS:HA	1:B:425:GLU:HB2	2.04	0.41
1:A:350:ASN:O	1:A:353:LEU:HB3	2.21	0.40
1:B:71:ASP:O	1:B:102:ARG:NH2	2.50	0.40
1:B:182:ASP:HB2	1:B:185:GLU:HB2	2.03	0.40
1:B:335:LYS:HE3	1:B:341:LEU:O	2.21	0.40
1:B:337:VAL:HG12	3:B:617:HOH:O	2.21	0.40
1:B:253:LEU:O	1:B:257:LEU:HG	2.21	0.40
1:A:471:ILE:O	1:A:471:ILE:HD13	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	527/519 (102%)	514 (98%)	13 (2%)	0	100	100
1	B	523/519 (101%)	501 (96%)	20 (4%)	2 (0%)	30	38
All	All	1050/1038 (101%)	1015 (97%)	33 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	ASP
1	B	364	PRO

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	460/442 (104%)	430 (94%)	30 (6%)	15	22
1	B	456/442 (103%)	417 (91%)	39 (9%)	10	13
All	All	916/884 (104%)	847 (92%)	69 (8%)	13	17

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	14	ARG
1	A	21	GLU
1	A	47	LYS
1	A	74	GLU
1	A	78	GLN
1	A	91	VAL
1	A	109	ARG
1	A	119	ASP
1	A	125	VAL

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Mol	Chain	Res	Type
1	A	158	THR
1	A	181	ILE
1	A	263	GLU
1	A	271	HIS
1	A	280	GLU
1	A	307	ILE
1	A	309	GLU
1	A	323	ILE
1	A	372	GLU
1	A	387[A]	GLU
1	A	387[B]	GLU
1	A	394	GLU
1	A	408	ILE
1	A	415[A]	LYS
1	A	415[B]	LYS
1	A	446	ILE
1	A	449	LEU
1	A	471	ILE
1	A	474	ARG
1	A	519	LYS
1	B	8	GLU
1	B	10	VAL
1	B	20	ARG
1	B	39	LEU
1	B	74	GLU
1	B	125	VAL
1	B	138	LEU
1	B	157	VAL
1	B	184	LYS
1	B	205	ARG
1	B	210	SER
1	B	212	SER
1	B	225	ILE
1	B	259	GLU
1	B	270	ARG
1	B	285	ILE
1	B	287	ARG
1	B	290	LEU
1	B	300	LYS
1	B	307	ILE
1	B	310	ASP
1	B	337	VAL

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Mol	Chain	Res	Type
1	B	357	ILE
1	B	375	GLU
1	B	399[A]	GLU
1	B	399[B]	GLU
1	B	407	GLU
1	B	414	THR
1	B	438[A]	LYS
1	B	438[B]	LYS
1	B	448	LYS
1	B	459	VAL
1	B	461	ARG
1	B	471	ILE
1	B	480	ARG
1	B	492	SER
1	B	495	ARG
1	B	503	ARG
1	B	512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	79	ASN
1	A	235	ASN
1	A	302	GLN
1	A	373	HIS
1	B	302	GLN
1	B	511	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	511/519 (98%)	0.32	17 (3%) 49 51	18, 35, 47, 67	12 (2%)
1	B	511/519 (98%)	0.73	35 (6%) 23 25	19, 41, 57, 66	8 (1%)
All	All	1022/1038 (98%)	0.52	52 (5%) 33 35	18, 37, 54, 67	20 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	4.6
1	B	403[A]	ARG	4.3
1	A	175	GLU	4.3
1	B	477	ASP	3.3
1	A	21	GLU	3.3
1	A	45	SER	3.2
1	B	48	ASN	3.1
1	B	399[A]	GLU	3.1
1	B	456	GLY	3.0
1	A	271	HIS	2.9
1	B	306	GLY	2.9
1	B	450	ALA	2.9
1	B	10	VAL	2.9
1	A	361	GLY	2.8
1	B	3	LEU	2.8
1	B	481	ALA	2.8
1	B	44	SER	2.7
1	B	14	ARG	2.7
1	B	172	ARG	2.6
1	A	270[A]	ARG	2.6
1	A	332[A]	ARG	2.6
1	B	357	ILE	2.5
1	B	43	SER	2.5
1	B	291	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	2.5
1	B	362	LEU	2.5
1	A	41	GLU	2.4
1	B	287	ARG	2.4
1	A	43	SER	2.4
1	A	278	ILE	2.4
1	B	349	VAL	2.4
1	B	339	PRO	2.3
1	A	122	GLU	2.3
1	B	417	GLU	2.3
1	B	334	LEU	2.2
1	A	125	VAL	2.2
1	A	44	SER	2.2
1	B	310	ASP	2.1
1	B	438[A]	LYS	2.1
1	B	289	TYR	2.1
1	B	323	ILE	2.1
1	B	374	PHE	2.1
1	B	326	ILE	2.1
1	B	271	HIS	2.1
1	B	364	PRO	2.1
1	B	336	ASP	2.1
1	B	183	GLU	2.0
1	B	204	ALA	2.0
1	A	123	GLU	2.0
1	B	504	GLU	2.0
1	A	204	ALA	2.0
1	B	178	ASP	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(\AA^2)	Q<0.9
2	MG	A	3052	1/1	1.00	0.12	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.