Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 02:06 PM EST

PDB ID	:	2CSB
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:

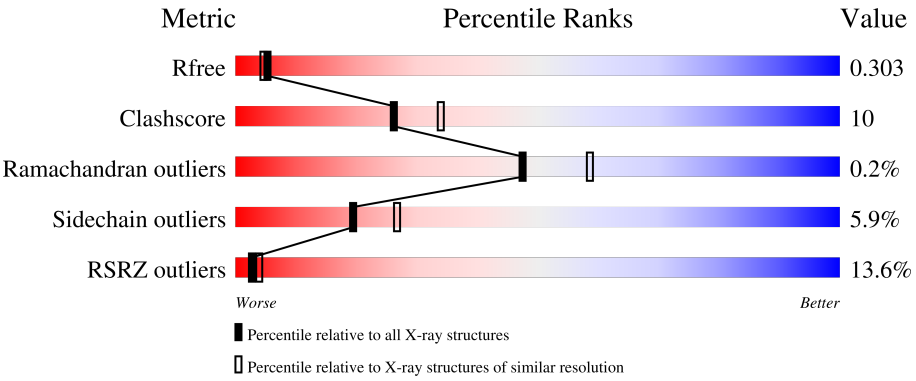
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	9% 76% 21% .
1	B	519	18% 66% 31% .

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
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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

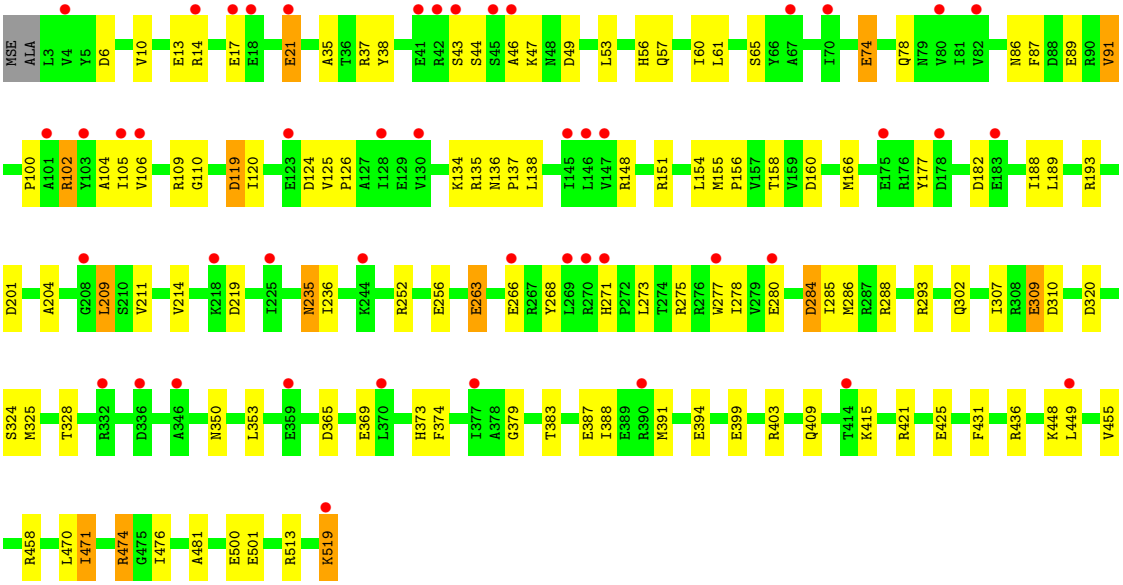
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	277	Total O 277 277	0	0
3	B	239	Total O 239 239	0	0

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.

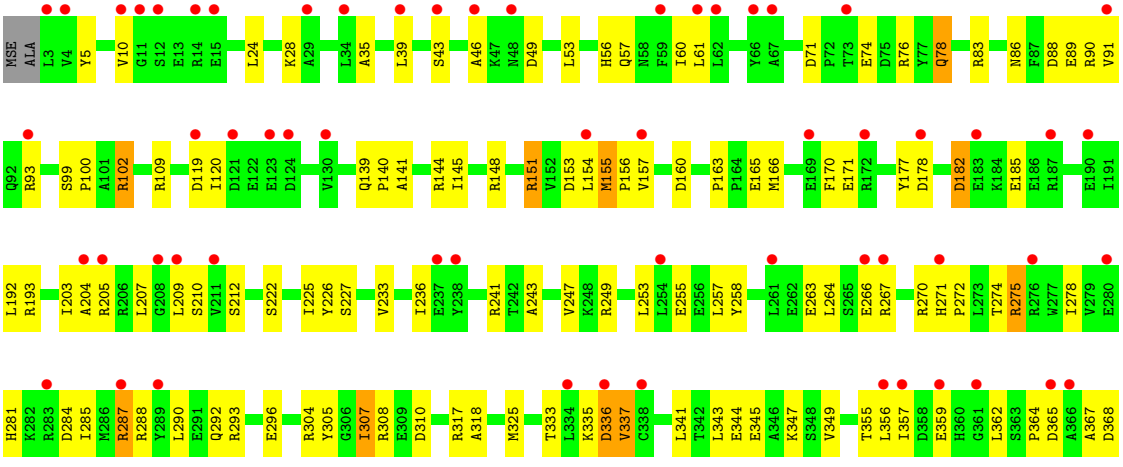
• Molecule 1: Topoisomerase V

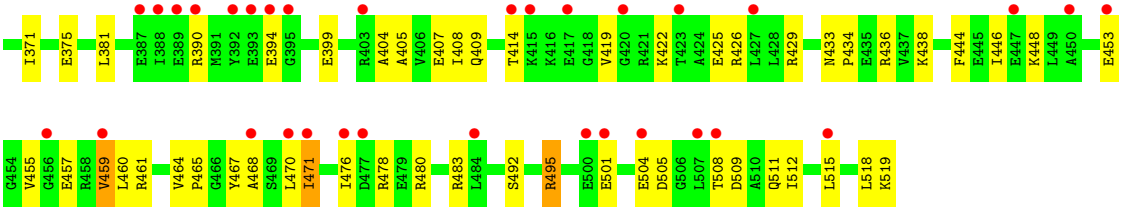
Chain A:



• Molecule 1: Topoisomerase V

Chain B:




I371
E375
L381
E387
I388
E389
R390
M391
Y392
E393
E394
G395
E399
R403
A404
A405
V406
E407
I408
Q409
T414
K415
K416
E417
G418
V419
G420
R421
K422
T423
A424
E425
R426
L427
L428
R429
N433
P434
E435
R436
V437
K438
F444
E445
I446
E447
K448
L449
A450
E453
G454
V455
G456
E457
R458
V459
L460
R461
V464
P465
G466
Y467
A468
S469
L470
I471
I476
D477
R478
E479
R480
R483
L484
S492
R495
E500
E501
E504
D505
G506
L507
T508
D509
A510
Q511
I512
L515
L518
K519

4 Data and refinement statistics (i)

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 27.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.9 (26.44-2.30) 100.0 (27.77-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1841.48 (at 2.24Å)	Xtriage
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	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9026	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage'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.*

[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: 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	0.82	0/4375	0.94	14/5884 (0.2%)
1	B	0.84	4/4338 (0.1%)	0.92	14/5835 (0.2%)
All	All	0.83	4/8713 (0.0%)	0.93	28/11719 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	453[A]	GLU	CD-OE2	14.97	1.42	1.25
1	B	453[B]	GLU	CD-OE2	14.97	1.42	1.25
1	B	453[A]	GLU	CD-OE1	6.01	1.32	1.25
1	B	453[B]	GLU	CD-OE1	6.01	1.32	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	182	ASP	CB-CG-OD2	7.64	125.17	118.30
1	B	368	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	124	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	219	ASP	CB-CG-OD2	7.24	124.82	118.30
1	A	365[A]	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	365[B]	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	310	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	284	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	151	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	505	ASP	CB-CG-OD2	6.37	124.04	118.30
1	B	119	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	284	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	160	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	49	ASP	CB-CG-OD2	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	151	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	178	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	119	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	160	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	509	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	201	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	249	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	153	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	182	ASP	CB-CA-C	-5.05	100.30	110.40
1	A	102	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	365	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	209	LEU	CA-CB-CG	5.01	126.83	115.30

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	4265	0	4271	74	0
1	B	4244	0	4258	104	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	177	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 10.

All (177) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:287:ARG:HG3	1:B:288:ARG:N	2.31	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: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:106:VAL:HG12	1:A:106:VAL:O	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:76:ARG:CD	3:B:742:HOH:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34	42
All	All	1050/1038 (101%)	1015 (97%)	33 (3%)	2 (0%)	47	58

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%)	440 (96%)	20 (4%)	29 40
1	B	456/442 (103%)	421 (92%)	35 (8%)	13 16
All	All	916/884 (104%)	861 (94%)	55 (6%)	19 26

All (55) 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	37	ARG
1	A	74	GLU
1	A	78	GLN
1	A	91	VAL
1	A	119	ASP
1	A	148	ARG
1	A	235	ASN
1	A	263	GLU
1	A	271	HIS
1	A	280	GLU
1	A	307	ILE
1	A	309	GLU
1	A	394	GLU
1	A	449	LEU
1	A	471	ILE
1	A	474	ARG
1	A	519	LYS
1	B	10	VAL
1	B	39	LEU
1	B	74	GLU
1	B	78	GLN
1	B	148	ARG
1	B	155	MSE
1	B	157	VAL
1	B	205	ARG
1	B	210	SER
1	B	212	SER
1	B	270	ARG
1	B	275	ARG
1	B	287	ARG

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Mol	Chain	Res	Type
1	B	290	LEU
1	B	307	ILE
1	B	310	ASP
1	B	317	ARG
1	B	337	VAL
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	483	ARG
1	B	492	SER
1	B	495	ARG
1	B	512	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	235	ASN
1	A	373	HIS
1	B	78	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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	511/519 (98%)	0.71	47 (9%) 9 12	22, 35, 47, 67	0
1	B	511/519 (98%)	1.14	92 (18%) 1 1	27, 42, 57, 66	0
All	All	1022/1038 (98%)	0.92	139 (13%) 3 4	22, 38, 54, 67	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	GLY	8.6
1	B	450	ALA	8.5
1	B	14	ARG	7.0
1	B	459	VAL	6.1
1	B	48	ASN	6.1
1	B	10	VAL	5.9
1	B	390	ARG	5.6
1	A	270[A]	ARG	5.4
1	B	395	GLY	5.2
1	B	468	ALA	5.1
1	B	477	ASP	4.8
1	B	12	SER	4.7
1	A	271	HIS	4.6
1	B	157	VAL	4.5
1	A	45	SER	4.4
1	A	42	ARG	4.4
1	A	175	GLU	4.3
1	B	403[A]	ARG	4.2
1	A	4	VAL	4.2
1	B	508	THR	4.1
1	A	130	VAL	4.1
1	B	414	THR	4.1
1	A	244	LYS	3.9
1	B	93[A]	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLU	3.8
1	B	476[A]	ILE	3.7
1	B	393	GLU	3.6
1	A	101	ALA	3.6
1	A	105	ILE	3.6
1	B	420	GLY	3.6
1	B	183	GLU	3.5
1	A	106	VAL	3.5
1	B	415	LYS	3.4
1	B	169	GLU	3.4
1	B	336	ASP	3.4
1	B	121	ASP	3.4
1	B	287	ARG	3.4
1	B	356	LEU	3.3
1	A	103	TYR	3.3
1	A	266[A]	GLU	3.3
1	B	338[A]	CYS	3.2
1	B	359	GLU	3.2
1	A	46	ALA	3.2
1	B	417	GLU	3.2
1	B	204	ALA	3.2
1	B	365	ASP	3.2
1	A	128	ILE	3.1
1	A	183	GLU	3.1
1	B	271	HIS	3.1
1	B	172	ARG	3.1
1	B	237	GLU	3.1
1	A	67	ALA	3.1
1	A	17	GLU	3.1
1	B	266	GLU	3.1
1	B	190	GLU	3.1
1	B	471	ILE	3.1
1	B	500	GLU	3.0
1	A	147	VAL	3.0
1	B	73	THR	3.0
1	B	11	GLY	3.0
1	B	238	TYR	2.9
1	A	43	SER	2.9
1	B	334	LEU	2.9
1	A	14	ARG	2.9
1	B	119	ASP	2.9
1	B	456	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	267	ARG	2.9
1	A	269	LEU	2.8
1	B	387	GLU	2.8
1	A	519	LYS	2.7
1	B	501	GLU	2.7
1	B	504	GLU	2.7
1	B	388	ILE	2.7
1	B	15	GLU	2.7
1	B	357	ILE	2.7
1	B	261	LEU	2.7
1	A	359	GLU	2.7
1	B	211	VAL	2.6
1	B	124	ASP	2.6
1	B	178	ASP	2.6
1	A	414	THR	2.5
1	A	208	GLY	2.5
1	B	394	GLU	2.5
1	A	218	LYS	2.5
1	B	276	ARG	2.5
1	B	205	ARG	2.5
1	B	361	GLY	2.5
1	A	336	ASP	2.5
1	B	484	LEU	2.5
1	A	18	GLU	2.4
1	A	41	GLU	2.4
1	A	277	TRP	2.4
1	B	187	ARG	2.4
1	B	470	LEU	2.4
1	B	4	VAL	2.4
1	A	390	ARG	2.4
1	A	145	ILE	2.4
1	A	146	LEU	2.4
1	B	366	ALA	2.4
1	B	392	TYR	2.3
1	A	449	LEU	2.3
1	B	61	LEU	2.3
1	A	82	VAL	2.3
1	B	423	THR	2.3
1	B	389	GLU	2.3
1	A	280	GLU	2.3
1	B	289	TYR	2.3
1	A	346	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	LEU	2.2
1	B	427	LEU	2.2
1	B	453[A]	GLU	2.2
1	B	130	VAL	2.2
1	A	178	ASP	2.2
1	B	29	ALA	2.2
1	B	67	ALA	2.2
1	B	3	LEU	2.2
1	B	283	ARG	2.2
1	A	70	ILE	2.2
1	A	370	LEU	2.2
1	B	507	LEU	2.2
1	B	91	VAL	2.1
1	B	39	LEU	2.1
1	B	66	TYR	2.1
1	A	80	VAL	2.1
1	A	332[A]	ARG	2.1
1	B	123	GLU	2.1
1	B	515	LEU	2.1
1	B	43	SER	2.1
1	B	46	ALA	2.1
1	B	59	PHE	2.1
1	B	447	GLU	2.0
1	A	377	ILE	2.0
1	B	62	LEU	2.0
1	B	254	LEU	2.0
1	A	123	GLU	2.0
1	B	280	GLU	2.0
1	A	225	ILE	2.0
1	B	34	LEU	2.0
1	B	154	LEU	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 monosaccharides in this entry.

6.4 Ligands

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, 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	B-factors(Å^2)	Q<0.9
2	MG	A	3052	1/1	0.96	0.16	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.