Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 08:09 PM JST

PDB ID	:	7YQA
Title	:	Crystal structure of D-threonine aldolase from Chlamydomonas reinhardtii
Authors	:	Hirato, Y.; Goto, M.; Mizobuchi, T.; Muramatsu, H.; Tanigawa, M.; Nishimura, K.
Deposited on	:	2022-08-05
Resolution	:	1.85 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:

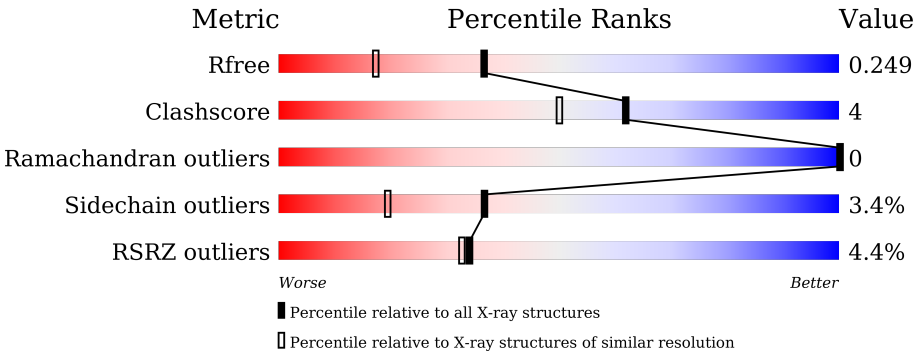
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	428	3% 82% 10% 7%
1	B	428	5% 82% 11% • 7%
1	C	428	4% 81% 11% 8%
1	D	428	4% 82% 10% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12435 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 D-threonine aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	P	S	0	6	0
			2944	1833	538	554	1	18			
1	B	398	Total	C	N	O	P	S	0	5	0
			2954	1828	549	561	1	15			
1	C	395	Total	C	N	O	P	S	0	4	0
			2934	1822	540	557	1	14			
1	D	394	Total	C	N	O	P	S	0	2	0
			2913	1803	539	555	1	15			

- 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		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

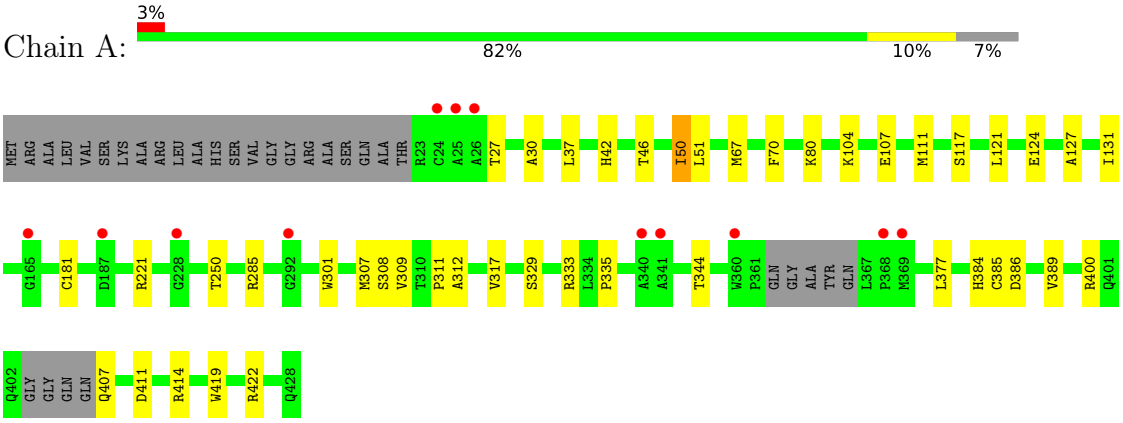
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	180	Total	O	0	0
			180	180		
3	C	171	Total	O	0	0
			171	171		
3	D	160	Total	O	0	0
			160	160		

3 Residue-property plots

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.

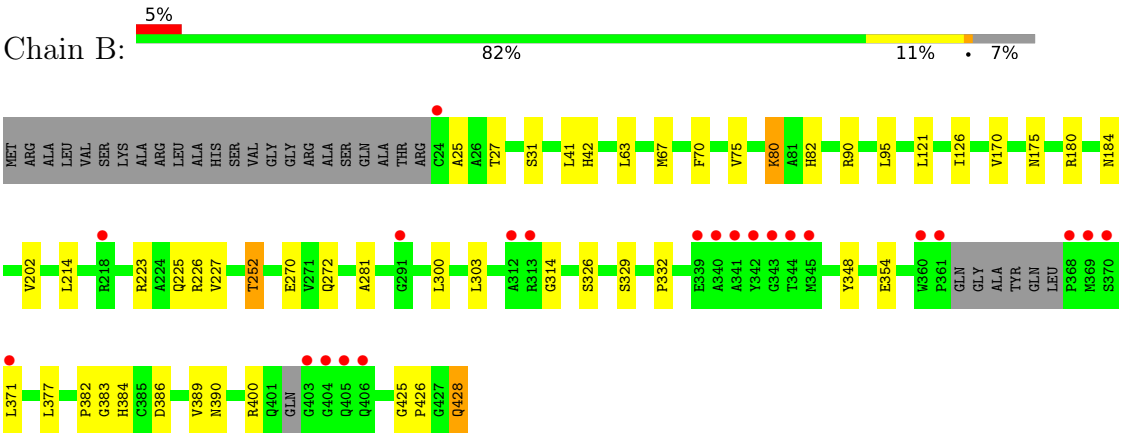
• Molecule 1: D-threonine aldolase

Chain A:



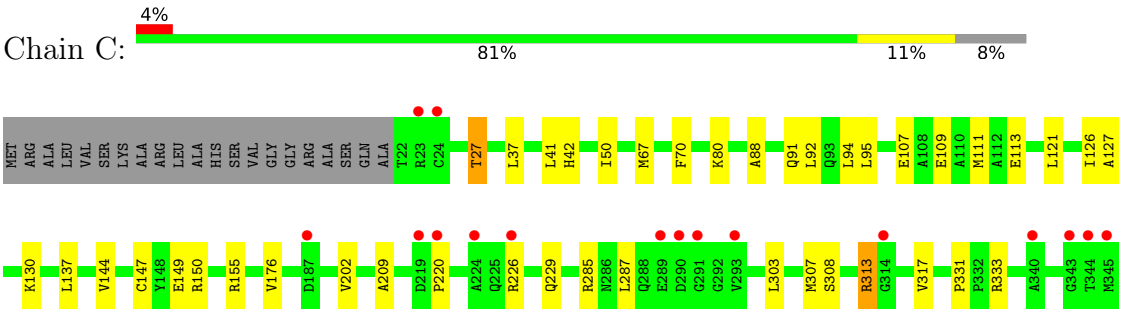
• Molecule 1: D-threonine aldolase

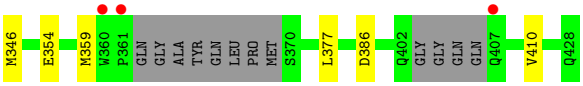
Chain B:



• Molecule 1: D-threonine aldolase

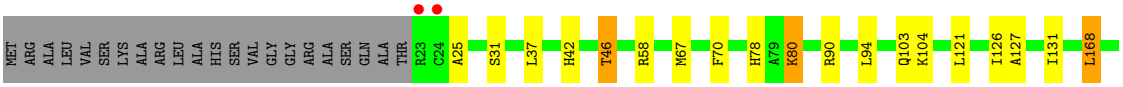
Chain C:

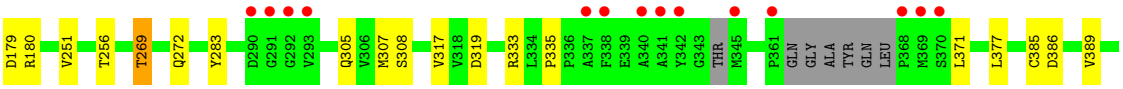




• Molecule 1: D-threonine aldolase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.79Å 74.10Å 89.94Å 77.07° 69.34° 71.93°	Depositor
Resolution (Å)	83.46 – 1.85 42.28 – 1.85	Depositor EDS
% Data completeness (in resolution range)	88.5 (83.46-1.85) 88.5 (42.28-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	5.25 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.217 , 0.249 0.217 , 0.249	Depositor DCC
R_{free} test set	5566 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12435	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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, LLP

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	0.40	0/2989	0.67	0/4060
1	B	0.41	0/2993	0.68	0/4059
1	C	0.41	0/2972	0.67	0/4036
1	D	0.41	0/2942	0.68	1/3990 (0.0%)
All	All	0.41	0/11896	0.68	1/16145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	168	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ALA	Peptide
1	B	314	GLY	Peptide

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	2944	0	2894	24	0
1	B	2954	0	2908	27	0
1	C	2934	0	2875	34	0
1	D	2913	0	2844	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	175	0	0	4	0
3	B	180	0	0	1	0
3	C	171	0	0	6	0
3	D	160	0	0	2	0
All	All	12435	0	11521	102	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 4.

All (102) 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:C:144:VAL:HG21	3:C:601:HOH:O	1.51	1.10
1:C:155[B]:ARG:HG2	1:C:155[B]:ARG:NH1	1.61	1.04
1:C:155[B]:ARG:HH11	1:C:155[B]:ARG:CG	1.72	1.02
1:C:155[B]:ARG:HG2	1:C:155[B]:ARG:HH11	0.80	0.93
1:A:51:LEU:HD23	3:A:775:HOH:O	1.77	0.84
1:C:137:LEU:HB2	3:C:601:HOH:O	1.79	0.80
1:B:390:ASN:HD21	1:B:425:GLY:H	1.30	0.80
1:B:252:THR:HG23	1:B:270:GLU:HB3	1.65	0.77
1:A:285:ARG:HG2	1:A:285:ARG:HH11	1.50	0.77
1:C:307:MET:HB2	1:D:126:ILE:HD13	1.70	0.73
1:C:130:LYS:HD2	3:C:636:HOH:O	1.88	0.70
1:D:251:VAL:H	1:D:269:THR:HB	1.58	0.68
1:A:27:THR:HG22	1:A:30:ALA:H	1.59	0.68
1:B:175:ASN:HD22	1:B:184:ASN:HD21	1.44	0.64
1:C:94:LEU:HD12	3:C:731:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:MET:HE2	1:C:70:PHE:HD2	1.62	0.63
1:B:67:MET:HE2	1:B:70:PHE:HD2	1.66	0.61
1:A:127:ALA:O	1:A:131:ILE:HG12	2.01	0.59
1:C:91:GLN:HA	3:C:731:HOH:O	2.02	0.59
1:B:426:PRO:HG2	1:B:428:GLN:HE22	1.67	0.58
1:B:63:LEU:HD21	1:B:75:VAL:HG11	1.85	0.58
1:A:67[A]:MET:HE2	1:A:70:PHE:HD2	1.70	0.57
1:D:333[A]:ARG:HH11	1:D:333[A]:ARG:HG2	1.69	0.57
1:D:46:THR:HG23	1:D:319:ASP:OD2	2.04	0.56
1:A:419:TRP:HZ3	3:A:775:HOH:O	1.88	0.56
1:A:422:ARG:HA	1:B:27[A]:THR:HA	1.88	0.55
1:B:90[B]:ARG:CZ	1:B:90[B]:ARG:CB	2.82	0.54
1:A:308:SER:HB3	1:A:317:VAL:HB	1.88	0.54
1:A:42:HIS:HA	1:A:377:LEU:HD21	1.90	0.54
1:C:308:SER:HB3	1:C:317:VAL:HB	1.90	0.54
1:C:147:CYS:HB2	3:C:604:HOH:O	2.08	0.53
1:A:67[A]:MET:HA	1:A:67[A]:MET:CE	2.39	0.53
1:B:426:PRO:HG2	1:B:428:GLN:NE2	2.23	0.52
1:A:422:ARG:HA	1:B:27[B]:THR:HA	1.90	0.51
1:A:307:MET:HA	1:B:126:ILE:HG12	1.92	0.51
1:D:25:ALA:HB3	1:D:31:SER:HB2	1.93	0.51
1:B:67:MET:HE2	1:B:70:PHE:CD2	2.45	0.51
1:D:67:MET:HE2	1:D:70:PHE:HD2	1.76	0.50
1:D:308:SER:HB3	1:D:317:VAL:HB	1.92	0.50
1:C:377:LEU:HB2	1:C:410:VAL:HG11	1.94	0.49
1:C:42:HIS:HA	1:C:377:LEU:HD21	1.95	0.49
1:D:42:HIS:HA	1:D:377:LEU:HD11	1.94	0.49
1:A:329:SER:HB2	1:A:384:HIS:HB2	1.95	0.49
1:B:41:LEU:HD13	1:B:303:LEU:HD13	1.94	0.48
1:C:155[B]:ARG:NH1	1:C:155[B]:ARG:CG	2.44	0.48
1:D:400:ARG:HH22	1:D:408:GLY:H	1.59	0.48
1:C:313:ARG:NH1	1:D:179:ASP:HB3	2.28	0.48
1:C:67:MET:HE2	1:C:70:PHE:CD2	2.46	0.47
1:C:220:PRO:HD3	1:C:287:LEU:HB2	1.96	0.47
1:C:226:ARG:HH11	1:C:229:GLN:HE22	1.61	0.47
1:A:285:ARG:HG2	1:A:285:ARG:NH1	2.25	0.47
1:C:107:GLU:O	1:C:111:MET:HG2	2.15	0.46
1:C:331:PRO:HG2	1:C:333:ARG:HH12	1.80	0.46
1:D:377:LEU:HB2	1:D:410:VAL:HG11	1.97	0.46
1:B:223:ARG:O	1:B:227:VAL:HG23	2.16	0.46
1:B:80:LLP:H6	1:B:272:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ARG:HD2	3:D:716:HOH:O	2.16	0.45
1:B:90[B]:ARG:CZ	1:B:90[B]:ARG:HB3	2.46	0.45
1:A:385:CYS:O	1:A:389:VAL:HG23	2.16	0.45
1:D:385:CYS:O	1:D:389:VAL:HG23	2.16	0.45
1:A:400:ARG:HG2	3:A:613:HOH:O	2.17	0.45
1:A:67[A]:MET:HE2	1:A:67[A]:MET:HA	2.00	0.44
1:C:27[B]:THR:HG22	3:D:646:HOH:O	2.16	0.44
1:C:126:ILE:HG12	1:D:307:MET:HA	2.00	0.44
1:D:46:THR:HG21	1:D:305:GLN:HB2	1.99	0.44
1:A:124:GLU:OE1	1:A:181[B]:CYS:SG	2.73	0.44
1:C:303:LEU:HD11	1:C:377:LEU:HD23	2.00	0.44
1:A:335:PRO:HB2	1:A:407:GLN:O	2.18	0.43
1:A:50:ILE:HG13	1:A:301:TRP:HB2	2.00	0.43
1:B:42:HIS:HA	1:B:377:LEU:HD11	2.00	0.43
1:A:309:VAL:HG12	1:A:311:PRO:HD3	2.00	0.43
1:C:27[A]:THR:HA	1:D:422:ARG:HA	2.00	0.43
1:D:90:ARG:O	1:D:94:LEU:HG	2.19	0.43
1:B:25:ALA:HB3	1:B:31[B]:SER:OG	2.17	0.43
1:D:80:LLP:H6	1:D:272:GLN:O	2.18	0.43
1:A:104[A]:LYS:NZ	1:B:354:GLU:HB3	2.33	0.43
1:C:149:GLU:HG3	1:C:150:ARG:HG3	2.00	0.43
1:D:78:HIS:CE1	1:D:80:LLP:HB2	2.54	0.42
1:D:335:PRO:HB2	1:D:407:GLN:O	2.19	0.42
1:C:285:ARG:HH12	1:C:333:ARG:HE	1.67	0.42
1:D:307:MET:HB2	1:D:307:MET:HE2	1.77	0.42
1:C:176:VAL:HG11	1:C:209:ALA:HB1	2.02	0.42
1:A:107:GLU:O	1:A:111:MET:HG2	2.20	0.42
1:C:88:ALA:O	1:C:92:LEU:HG	2.20	0.42
1:D:67:MET:HE2	1:D:70:PHE:CD2	2.53	0.42
1:D:127:ALA:O	1:D:131:ILE:HG12	2.19	0.42
1:B:329:SER:HB2	1:B:384:HIS:HB2	2.00	0.41
1:B:82:HIS:HA	1:B:389:VAL:HG11	2.01	0.41
1:B:281:ALA:HB3	1:B:383:GLY:HA2	2.03	0.41
1:B:332:PRO:HD2	1:B:348:TYR:CD1	2.56	0.41
1:B:300:LEU:HD23	1:B:382:PRO:HG2	2.03	0.41
1:D:333[A]:ARG:HG2	1:D:333[A]:ARG:NH1	2.34	0.41
1:B:170:VAL:HG21	1:B:202:VAL:HG13	2.03	0.41
1:C:109:GLU:O	1:C:113:GLU:HG2	2.21	0.41
1:C:127:ALA:HB2	1:D:305:GLN:OE1	2.21	0.41
1:D:256:THR:HB	1:D:283:TYR:CZ	2.56	0.41
1:B:180:ARG:HD2	3:B:734:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:HD22	1:B:226:ARG:HB3	2.03	0.40
1:C:346:MET:HB2	1:C:359:MET:O	2.20	0.40
1:C:354:GLU:HB3	1:D:104:LYS:HE3	2.02	0.40
1:A:46:THR:HG21	3:A:702:HOH:O	2.20	0.40
1:C:41:LEU:HD12	1:C:410:VAL:HA	2.03	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	396/428 (92%)	379 (96%)	17 (4%)	0	100	100
1	B	396/428 (92%)	380 (96%)	16 (4%)	0	100	100
1	C	392/428 (92%)	377 (96%)	15 (4%)	0	100	100
1	D	387/428 (90%)	372 (96%)	15 (4%)	0	100	100
All	All	1571/1712 (92%)	1508 (96%)	63 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	290/313 (93%)	279 (96%)	11 (4%)	33	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	291/313 (93%)	282 (97%)	9 (3%)	40	23
1	C	288/313 (92%)	278 (96%)	10 (4%)	36	18
1	D	285/313 (91%)	273 (96%)	12 (4%)	30	13
All	All	1154/1252 (92%)	1112 (96%)	42 (4%)	37	18

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	50	ILE
1	A	117	SER
1	A	121	LEU
1	A	221	ARG
1	A	250	THR
1	A	333	ARG
1	A	344	THR
1	A	386	ASP
1	A	411	ASP
1	A	414	ARG
1	B	95	LEU
1	B	121	LEU
1	B	225	GLN
1	B	252	THR
1	B	326	SER
1	B	371	LEU
1	B	386	ASP
1	B	400	ARG
1	B	428	GLN
1	C	27[A]	THR
1	C	27[B]	THR
1	C	37	LEU
1	C	50[A]	ILE
1	C	50[B]	ILE
1	C	95	LEU
1	C	121	LEU
1	C	202	VAL
1	C	313	ARG
1	C	386	ASP
1	D	37	LEU
1	D	46	THR
1	D	58	ARG

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Mol	Chain	Res	Type
1	D	103	GLN
1	D	121	LEU
1	D	168	LEU
1	D	269	THR
1	D	371	LEU
1	D	386	ASP
1	D	411	ASP
1	D	416[A]	GLU
1	D	416[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	GLN
1	B	184	ASN
1	B	225	GLN
1	B	390	ASN
1	B	428	GLN
1	C	229	GLN
1	D	103	GLN
1	D	216	HIS
1	D	288	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	LLP	C	80	1	23,24,25	2.95	5 (21%)	25,32,34	1.45	4 (16%)
1	LLP	D	80	1	23,24,25	2.96	5 (21%)	25,32,34	1.49	3 (12%)
1	LLP	A	80	1	23,24,25	2.91	5 (21%)	25,32,34	1.62	4 (16%)
1	LLP	B	80	1	23,24,25	2.83	5 (21%)	25,32,34	1.45	4 (16%)

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
1	LLP	C	80	1	-	5/16/17/19	0/1/1/1
1	LLP	D	80	1	-	5/16/17/19	0/1/1/1
1	LLP	A	80	1	-	5/16/17/19	0/1/1/1
1	LLP	B	80	1	-	5/16/17/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	LLP	C3-C2	8.89	1.49	1.40
1	D	80	LLP	C3-C2	8.85	1.49	1.40
1	A	80	LLP	C3-C2	8.80	1.49	1.40
1	B	80	LLP	C3-C2	8.28	1.49	1.40
1	C	80	LLP	C4-C5	6.63	1.50	1.42
1	A	80	LLP	C4-C5	6.56	1.50	1.42
1	D	80	LLP	C4-C5	6.43	1.50	1.42
1	B	80	LLP	C4-C5	6.18	1.49	1.42
1	D	80	LLP	C4-C3	6.06	1.49	1.40
1	B	80	LLP	C4-C3	5.60	1.49	1.40
1	A	80	LLP	C4-C3	5.57	1.49	1.40
1	C	80	LLP	C4-C3	5.56	1.49	1.40
1	B	80	LLP	C4'-NZ	5.52	1.45	1.27
1	C	80	LLP	C4'-NZ	5.40	1.45	1.27
1	D	80	LLP	C4'-NZ	5.34	1.45	1.27
1	A	80	LLP	C4'-NZ	5.29	1.45	1.27
1	D	80	LLP	C4-C4'	2.99	1.52	1.46
1	C	80	LLP	C4-C4'	2.98	1.52	1.46
1	B	80	LLP	C4-C4'	2.96	1.52	1.46
1	A	80	LLP	C4-C4'	2.95	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	LLP	C4-C3-C2	-4.65	117.31	120.19
1	C	80	LLP	C4-C3-C2	-4.47	117.42	120.19
1	D	80	LLP	C4-C3-C2	-4.29	117.53	120.19
1	A	80	LLP	C4-C4'-NZ	-3.71	107.27	124.31
1	D	80	LLP	C4-C4'-NZ	-3.54	108.04	124.31
1	B	80	LLP	C4-C3-C2	-3.46	118.05	120.19
1	B	80	LLP	C4-C4'-NZ	-3.14	109.88	124.31
1	C	80	LLP	C4-C4'-NZ	-2.77	111.57	124.31
1	A	80	LLP	C6-N1-C2	2.73	124.22	119.17
1	C	80	LLP	C6-N1-C2	2.47	123.74	119.17
1	D	80	LLP	C6-N1-C2	2.46	123.72	119.17
1	B	80	LLP	C6-N1-C2	2.38	123.58	119.17
1	A	80	LLP	O3-C3-C2	2.15	122.18	117.49
1	C	80	LLP	O3-C3-C2	2.04	121.94	117.49
1	B	80	LLP	C3-C4-C5	-2.02	116.71	118.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	80	LLP	C3-C4-C4'-NZ
1	A	80	LLP	C-CA-CB-CG
1	D	80	LLP	C-CA-CB-CG
1	A	80	LLP	C4-C4'-NZ-CE
1	D	80	LLP	C4-C4'-NZ-CE
1	B	80	LLP	C4-C4'-NZ-CE
1	C	80	LLP	C4-C4'-NZ-CE
1	D	80	LLP	CG-CD-CE-NZ
1	B	80	LLP	CG-CD-CE-NZ
1	D	80	LLP	C3-C4-C4'-NZ
1	C	80	LLP	CG-CD-CE-NZ
1	B	80	LLP	C3-C4-C4'-NZ
1	C	80	LLP	C3-C4-C4'-NZ
1	B	80	LLP	C-CA-CB-CG
1	A	80	LLP	CD-CE-NZ-C4'
1	D	80	LLP	C5-C4-C4'-NZ
1	C	80	LLP	CA-CB-CG-CD
1	B	80	LLP	C5-C4-C4'-NZ
1	C	80	LLP	C5-C4-C4'-NZ
1	A	80	LLP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	80	LLP	2	0
1	B	80	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are 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	396/428 (92%)	0.17	12 (3%)	50	48	16, 24, 39, 58	0
1	B	397/428 (92%)	0.29	22 (5%)	25	24	15, 23, 42, 62	0
1	C	394/428 (92%)	0.27	19 (4%)	30	29	15, 23, 42, 58	0
1	D	393/428 (91%)	0.12	16 (4%)	37	35	16, 24, 45, 63	0
All	All	1580/1712 (92%)	0.21	69 (4%)	34	33	15, 24, 42, 63	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	ALA	6.3
1	D	369	MET	6.2
1	C	360	TRP	6.1
1	B	341	ALA	5.9
1	B	344	THR	5.9
1	B	291	GLY	5.6
1	B	404	GLY	5.4
1	B	369	MET	5.2
1	C	361	PRO	5.1
1	D	340	ALA	5.0
1	B	345	MET	5.0
1	B	368	PRO	4.8
1	D	368	PRO	4.6
1	C	293	VAL	4.4
1	A	24	CYS	4.3
1	A	341	ALA	4.2
1	D	290	ASP	4.1
1	D	24	CYS	4.0
1	B	312	ALA	4.0
1	D	345	MET	4.0
1	D	341	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	360	TRP	3.9
1	D	23	ARG	3.8
1	B	406	GLN	3.7
1	C	289	GLU	3.4
1	D	361	PRO	3.4
1	C	344	THR	3.4
1	C	219	ASP	3.2
1	C	23	ARG	3.1
1	D	291	GLY	3.1
1	C	407	GLN	3.0
1	B	343	GLY	3.0
1	A	369	MET	2.9
1	B	342	TYR	2.9
1	C	24	CYS	2.9
1	D	337	ALA	2.9
1	B	370	SER	2.8
1	A	368	PRO	2.8
1	C	290	ASP	2.8
1	D	342	TYR	2.8
1	B	340	ALA	2.8
1	B	218	ARG	2.7
1	D	292	GLY	2.7
1	C	291	GLY	2.7
1	A	292	GLY	2.6
1	C	343	GLY	2.6
1	C	345	MET	2.6
1	A	187	ASP	2.6
1	B	361	PRO	2.6
1	A	26	ALA	2.5
1	B	403	GLY	2.5
1	A	165	GLY	2.5
1	B	371	LEU	2.3
1	B	339	GLU	2.2
1	C	340	ALA	2.2
1	B	313	ARG	2.2
1	A	228	GLY	2.2
1	A	360	TRP	2.2
1	C	314	GLY	2.2
1	D	338	PHE	2.2
1	D	370	SER	2.2
1	D	293	VAL	2.2
1	C	220	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	224	ALA	2.1
1	B	405	GLN	2.1
1	A	25	ALA	2.1
1	C	226	ARG	2.1
1	B	24	CYS	2.1
1	C	187	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	LLP	D	80	24/25	0.95	0.10	16,23,25,25	0
1	LLP	A	80	24/25	0.96	0.12	17,22,24,24	0
1	LLP	C	80	24/25	0.97	0.10	16,23,25,26	0
1	LLP	B	80	24/25	0.97	0.12	17,23,24,25	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	500	1/1	0.98	0.18	22,22,22,22	0
2	MG	D	500	1/1	0.98	0.09	22,22,22,22	0
2	MG	C	500	1/1	0.99	0.14	19,19,19,19	0
2	MG	B	500	1/1	0.99	0.14	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.