Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:14 PM GMT

PDB ID	:	1SR9
Title	:	Crystal Structure of LeuA from Mycobacterium tuberculosis
Authors	:	Koon, N.; Squire, C.J.; Baker, E.N.
Deposited on	:	2004-03-22
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

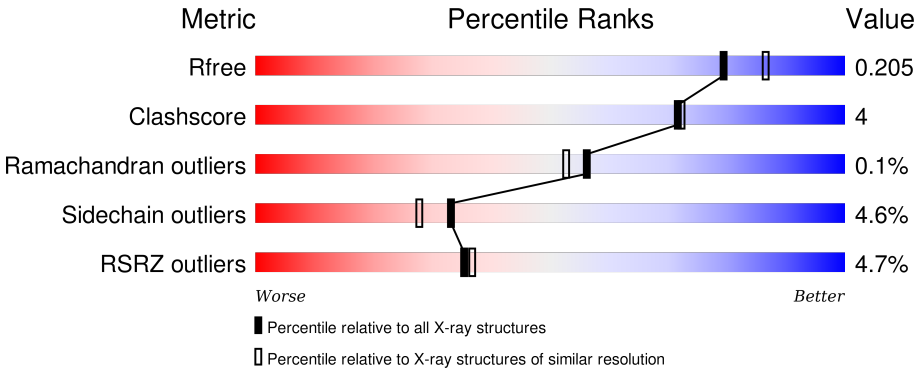
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	5% 79% 9% • 11%
1	B	644	4% 77% 10% • 10%

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
3	CL	A	705	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9153 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 2-isopropylmalate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	Se	0	0	0
			4319	2717	752	830	9	11			
1	B	577	Total	C	N	O	S	Se	0	0	0
			4349	2733	761	835	9	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	41	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	90	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	98	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	105	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	257	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	270	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	390	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	404	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	441	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	480	MSE	MET	MODIFIED RESIDUE	UNP P96420
A	559	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	1	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	41	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	90	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	98	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	105	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	257	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	270	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	390	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	404	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	441	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	480	MSE	MET	MODIFIED RESIDUE	UNP P96420
B	559	MSE	MET	MODIFIED RESIDUE	UNP P96420

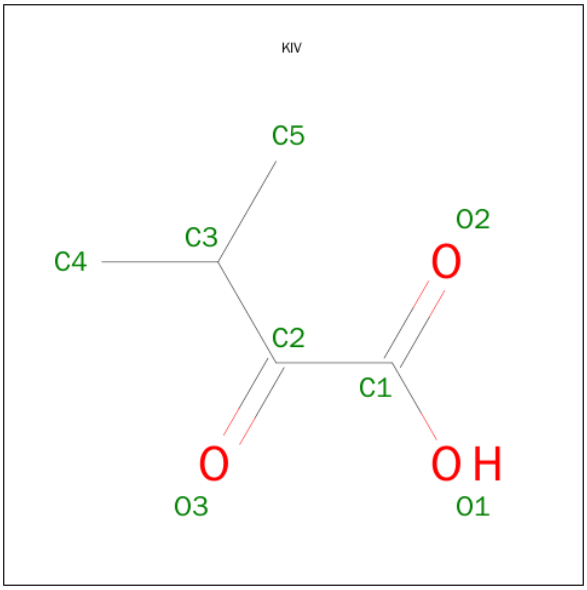
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is 3-METHYL-2-OXOBUTANOIC ACID (three-letter code: KIV) (formula: $C_5H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 5 3	0	0
4	B	1	Total C O 8 5 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	236	Total O 236 236	0	0

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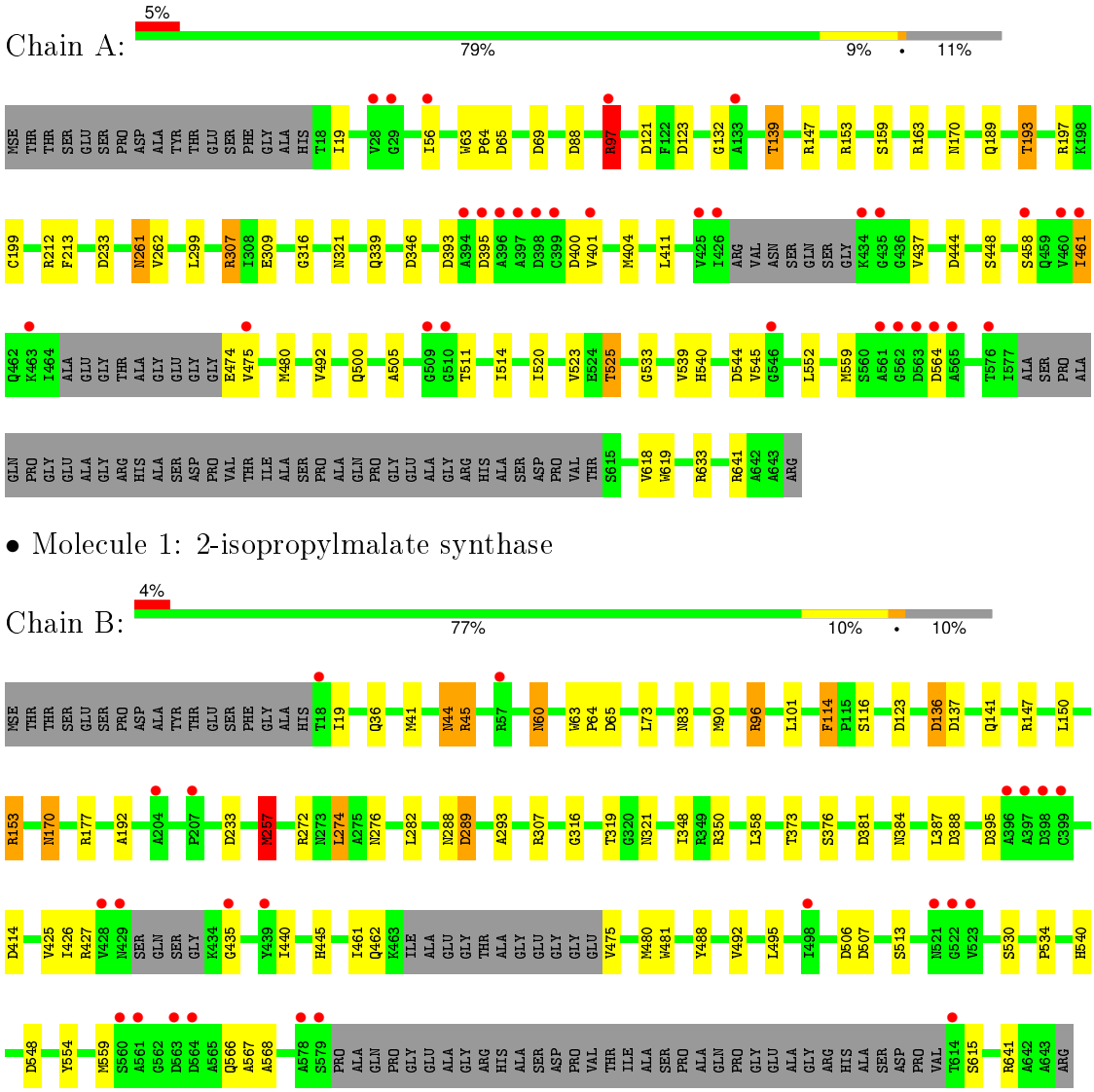
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	230	Total	O	0	0
			230	230		

3 Residue-property plots (i)

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

- Molecule 1: 2-isopropylmalate synthase

Chain A:



- Molecule 1: 2-isopropylmalate synthase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.25Å 154.73Å 68.82Å 90.00° 98.05° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 26.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 97.9 (26.44-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.197 0.181 , 0.205	Depositor DCC
R_{free} test set	3742 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 86156 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9153	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, KIV, CL

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	0.72	1/4403 (0.0%)	0.90	17/5999 (0.3%)
1	B	0.70	0/4433	0.89	19/6036 (0.3%)
All	All	0.71	1/8836 (0.0%)	0.89	36/12035 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	559	MSE	CG-SE	-5.37	1.77	1.95

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	A	307	ARG	NE-CZ-NH2	11.85	126.22	120.30
1	B	45	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	B	45	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	B	233	ASP	CB-CG-OD2	7.56	125.11	118.30
1	A	544	ASP	CB-CG-OD2	7.37	124.94	118.30
1	B	388	ASP	CB-CG-OD2	7.27	124.84	118.30
1	B	507	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	69	ASP	CB-CG-OD2	6.78	124.41	118.30
1	B	257	MSE	CG-SE-CE	-6.69	84.18	98.90
1	B	137	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	233	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	395	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	395	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	88	ASP	CB-CG-OD2	6.35	124.01	118.30
1	B	41	MSE	CG-SE-CE	-6.14	85.38	98.90
1	A	212	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	123	ASP	CB-CG-OD2	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	414	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	400	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	121	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	381	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	274	LEU	CA-CB-CG	5.89	128.85	115.30
1	B	65	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	307	ARG	CD-NE-CZ	5.73	131.62	123.60
1	A	444	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	65	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	548	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	177	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	350	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	136	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	97	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	633	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	289	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	393	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	96	ARG	NE-CZ-NH2	5.02	122.81	120.30

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	4319	0	4106	39	0
1	B	4349	0	4134	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	1	0
4	A	8	0	7	0	0
4	B	8	0	7	0	0
5	A	236	0	0	12	0
5	B	230	0	0	4	0
All	All	9153	0	8254	73	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 (73) 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:A:56:ILE:HG13	5:A:1180:HOH:O	1.71	0.88
1:A:56:ILE:HD11	1:A:262:VAL:HG13	1.58	0.85
1:A:404:MSE:O	1:B:45:ARG:HD2	1.78	0.83
1:B:141:GLN:HE22	1:B:307:ARG:HH22	1.21	0.83
1:B:83:ASN:HD21	1:B:90:MSE:H	1.27	0.82
1:A:474:GLU:OE1	5:A:1081:HOH:O	2.00	0.79
1:A:641:ARG:NH1	5:A:924:HOH:O	2.16	0.77
1:A:139:THR:HG21	5:A:1265:HOH:O	1.85	0.76
1:A:139:THR:HB	1:A:163:ARG:HG3	1.72	0.71
1:A:523:VAL:O	1:A:525:THR:HG22	1.90	0.70
5:A:1115:HOH:O	1:B:257:MSE:HE1	1.92	0.69
1:B:123:ASP:OD2	5:B:1261:HOH:O	2.11	0.67
1:B:141:GLN:HE22	1:B:307:ARG:NH2	1.93	0.67
1:A:193:THR:HG21	5:A:1121:HOH:O	1.95	0.66
1:B:440:ILE:HG22	1:B:480:MSE:HE1	1.77	0.66
1:A:505:ALA:HB2	1:A:511:THR:O	1.97	0.63
1:A:56:ILE:CD1	1:A:262:VAL:HG13	2.29	0.63
1:A:193:THR:HG23	1:A:197:ARG:HH12	1.64	0.62
1:A:193:THR:HG23	1:A:197:ARG:NH1	2.15	0.62
1:A:339:GLN:NE2	1:B:36:GLN:HE21	1.99	0.60
1:A:316:GLY:HA3	1:A:321:ASN:HD22	1.68	0.58
1:A:19:ILE:HD11	1:B:348:ILE:HG13	1.84	0.58
1:B:559:MSE:HE2	1:B:567:ALA:C	2.24	0.58
1:B:530:SER:O	1:B:540:HIS:HD2	1.86	0.58
1:A:261:ASN:HD22	1:A:261:ASN:H	1.50	0.57
1:B:44:ASN:ND2	5:B:1133:HOH:O	2.31	0.56
1:B:83:ASN:ND2	1:B:90:MSE:H	2.00	0.56
1:A:437:VAL:HG21	1:A:458:SER:HB3	1.89	0.55
1:A:520:ILE:HD11	1:A:545:VAL:CG2	2.36	0.55
1:A:307:ARG:NH1	1:A:309:GLU:OE1	2.40	0.55
1:A:500:GLN:HG3	1:A:514:ILE:HD11	1.90	0.54
1:A:339:GLN:HE21	1:B:36:GLN:HE21	1.54	0.54
1:B:150:LEU:HD13	5:B:1273:HOH:O	2.08	0.54
1:A:404:MSE:O	1:B:45:ARG:CD	2.55	0.53
1:B:559:MSE:HE3	1:B:566:GLN:CB	2.39	0.53
5:A:1195:HOH:O	1:B:19:ILE:HG12	2.09	0.53
1:B:60:ASN:ND2	1:B:272:ARG:HH22	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HD3	5:A:1251:HOH:O	2.10	0.52
1:A:193:THR:CG2	1:A:197:ARG:HH12	2.22	0.52
1:B:488:TYR:CE2	1:B:641:ARG:HD3	2.45	0.52
1:A:56:ILE:CD1	5:A:1180:HOH:O	2.57	0.51
1:B:288:ASN:HD22	1:B:293:ALA:H	1.59	0.51
1:B:384:ASN:HD21	1:B:462:GLN:NE2	2.08	0.50
1:A:619:TRP:N	5:A:924:HOH:O	2.44	0.50
1:B:114:PHE:HE2	5:B:1273:HOH:O	1.93	0.49
1:A:533:GLY:HA3	3:A:705:CL:CL	2.49	0.49
1:B:63:TRP:N	1:B:64:PRO:CD	2.77	0.48
1:B:316:GLY:HA3	1:B:321:ASN:HD22	1.79	0.47
1:A:461:ILE:CD1	1:A:480:MSE:HG3	2.44	0.47
1:B:373:THR:HG23	1:B:425:VAL:HG23	1.95	0.47
1:A:520:ILE:HD11	1:A:545:VAL:HG22	1.98	0.46
1:B:288:ASN:ND2	1:B:293:ALA:H	2.14	0.46
1:B:513:SER:OG	1:B:530:SER:OG	2.25	0.46
1:B:435:GLY:HA2	1:B:440:ILE:HD11	1.99	0.45
1:A:461:ILE:HD11	1:A:480:MSE:HG3	1.98	0.45
1:B:116:SER:HA	1:B:153:ARG:HG2	1.99	0.43
1:B:289:ASP:HA	1:B:319:THR:HG21	2.00	0.43
1:A:316:GLY:HA3	1:A:321:ASN:ND2	2.32	0.43
1:B:559:MSE:HE3	1:B:566:GLN:HB3	2.01	0.43
1:B:445:HIS:CE1	1:B:481:TRP:CD2	3.07	0.43
1:B:426:ILE:HG21	1:B:461:ILE:HG21	2.00	0.43
1:B:73:LEU:O	1:B:307:ARG:HA	2.19	0.43
1:A:139:THR:HG22	1:A:163:ARG:HD2	2.01	0.42
1:B:170:ASN:HD21	1:B:192:ALA:HB2	1.85	0.42
1:A:63:TRP:CG	1:A:64:PRO:HD3	2.56	0.41
1:B:60:ASN:HD21	1:B:272:ARG:HH22	1.66	0.41
1:A:500:GLN:O	1:B:506:ASP:HA	2.20	0.41
1:A:132:GLY:HA2	5:A:1165:HOH:O	2.21	0.41
1:A:539:VAL:HG23	1:A:540:HIS:CD2	2.56	0.41
5:A:1258:HOH:O	1:B:534:PRO:HG3	2.21	0.40
1:A:199:CYS:HB3	1:A:213:PHE:CE2	2.56	0.40
1:B:559:MSE:HE2	1:B:568:ALA:N	2.37	0.40
1:A:189:GLN:O	1:A:193:THR:HB	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	565/644 (88%)	553 (98%)	11 (2%)	1 (0%)	52 48
1	B	569/644 (88%)	553 (97%)	16 (3%)	0	100 100
All	All	1134/1288 (88%)	1106 (98%)	27 (2%)	1 (0%)	56 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	564	ASP

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	441/508 (87%)	422 (96%)	19 (4%)	35 30
1	B	443/508 (87%)	421 (95%)	22 (5%)	30 24
All	All	884/1016 (87%)	843 (95%)	41 (5%)	33 28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	139	THR
1	A	147	ARG
1	A	153	ARG
1	A	159	SER

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	193	THR
1	A	261	ASN
1	A	299	LEU
1	A	346	ASP
1	A	401	VAL
1	A	411	LEU
1	A	448	SER
1	A	461	ILE
1	A	475	VAL
1	A	492	VAL
1	A	525	THR
1	A	552	LEU
1	A	618	VAL
1	B	44	ASN
1	B	60	ASN
1	B	96	ARG
1	B	101	LEU
1	B	114	PHE
1	B	136	ASP
1	B	147	ARG
1	B	153	ARG
1	B	170	ASN
1	B	257	MSE
1	B	274	LEU
1	B	276	ASN
1	B	282	LEU
1	B	358	LEU
1	B	376	SER
1	B	387	LEU
1	B	427	ARG
1	B	475	VAL
1	B	492	VAL
1	B	495	LEU
1	B	554	TYR
1	B	615	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	230	GLN

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	261	ASN
1	A	273	ASN
1	A	321	ASN
1	A	339	GLN
1	A	357	GLN
1	B	44	ASN
1	B	60	ASN
1	B	83	ASN
1	B	119	GLN
1	B	131	GLN
1	B	141	GLN
1	B	170	ASN
1	B	276	ASN
1	B	288	ASN
1	B	321	ASN
1	B	380	GLN
1	B	445	HIS
1	B	459	GLN
1	B	462	GLN
1	B	540	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	KIV	A	701	2	4,7,7	0.43	0	4,9,9	1.26	1 (25%)
4	KIV	B	702	2	4,7,7	0.64	0	4,9,9	1.10	0

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
4	KIV	A	701	2	-	0/4/8/8	0/0/0/0
4	KIV	B	702	2	-	0/4/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	KIV	O3-C2-C3	2.05	122.32	117.64

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	562/644 (87%)	0.06	30 (5%)	30	32	25, 38, 55, 72	0
1	B	566/644 (87%)	0.06	23 (4%)	41	42	25, 37, 55, 64	0
All	All	1128/1288 (87%)	0.06	53 (4%)	35	37	25, 37, 55, 72	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	ALA	7.1
1	B	579	SER	6.9
1	A	563	ASP	6.3
1	A	562	GLY	6.2
1	A	509	GLY	5.6
1	A	28	VAL	5.5
1	A	561	ALA	5.2
1	A	564	ASP	4.8
1	A	434	LYS	4.6
1	A	461	ILE	4.6
1	B	563	ASP	4.6
1	A	395	ASP	4.2
1	B	561	ALA	4.2
1	B	435	GLY	4.0
1	A	396	ALA	4.0
1	A	458	SER	4.0
1	B	578	ALA	3.8
1	A	426	ILE	3.7
1	A	546	GLY	3.4
1	B	439	TYR	3.3
1	B	396	ALA	3.3
1	A	29	GLY	3.2
1	A	463	LYS	3.1
1	A	398	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	398	ASP	3.1
1	B	57	ARG	3.0
1	A	399	CYS	2.8
1	B	564	ASP	2.8
1	B	18	THR	2.7
1	B	522	GLY	2.7
1	A	394	ALA	2.6
1	B	614	THR	2.5
1	B	397	ALA	2.5
1	A	425	VAL	2.4
1	A	401	VAL	2.4
1	B	523	VAL	2.4
1	B	521	ASN	2.4
1	B	399	CYS	2.3
1	B	207	PRO	2.3
1	A	475	VAL	2.2
1	B	429	ASN	2.2
1	A	397	ALA	2.2
1	B	204	ALA	2.2
1	A	435	GLY	2.1
1	A	97	ARG	2.1
1	A	56	ILE	2.1
1	A	510	GLY	2.1
1	A	460	VAL	2.1
1	B	498	ILE	2.1
1	B	560	SER	2.0
1	A	133	ALA	2.0
1	A	576	THR	2.0
1	B	428	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	A	705	1/1	0.89	0.52	8.64	39,39,39,39	1
4	KIV	A	701	8/8	0.93	0.15	0.75	33,37,38,38	0
4	KIV	B	702	8/8	0.92	0.13	0.05	29,35,39,40	0
2	ZN	A	704	1/1	0.99	0.04	-	39,39,39,39	0
2	ZN	B	703	1/1	0.99	0.03	-	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.