



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:11 PM UTC

PDB ID : 3RLA / pdb_00003rla
Title : ALTERING THE BINUCLEAR MANGANESE CLUSTER OF ARGINASE
DIMINISHES THERMOSTABILITY AND CATALYTIC FUNCTION
Authors : Scolnick, L.R.; Kanyo, Z.F.; Christianson, D.W.
Deposited on : 1997-05-07
Resolution : 2.54 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

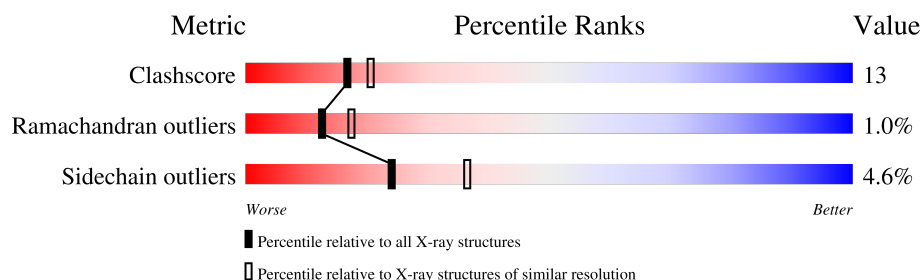
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	 69% 24% . .
1	B	323	 67% 26% . .
1	C	323	 64% 28% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7209 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 ARGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2388	1524	403	454	7			
1	B	314	Total	C	N	O	S	0	0	0
			2388	1524	403	454	7			
1	C	314	Total	C	N	O	S	0	0	0
			2388	1524	403	454	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ASN	HIS	engineered mutation	UNP P07824
B	101	ASN	HIS	engineered mutation	UNP P07824
C	101	ASN	HIS	engineered mutation	UNP P07824

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	8	Total	O	0	0
			8	8		

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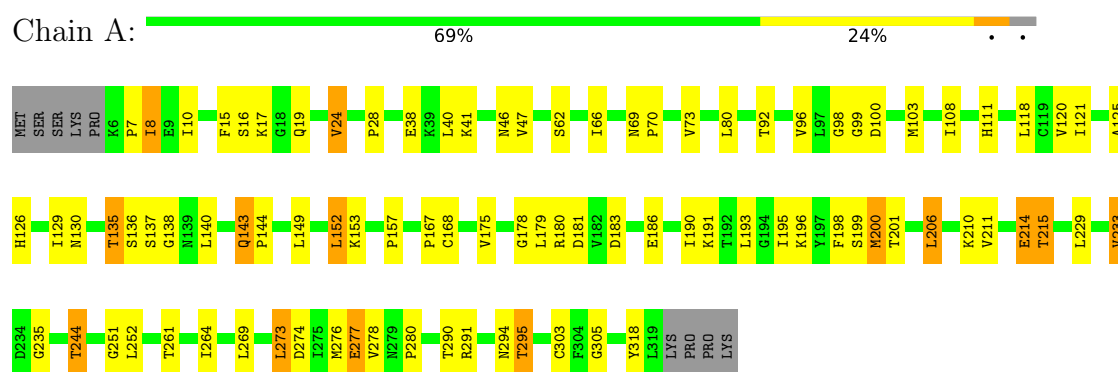
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	10	Total	O	0	0
			10	10		

3 Residue-property plots

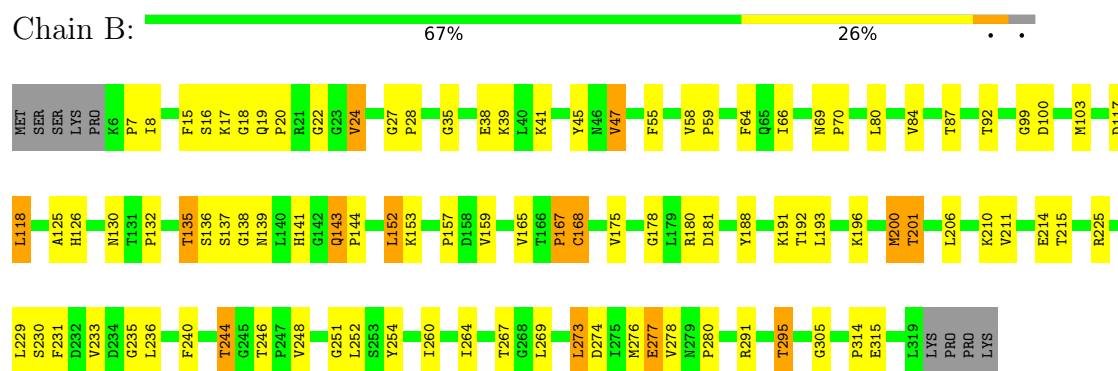
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

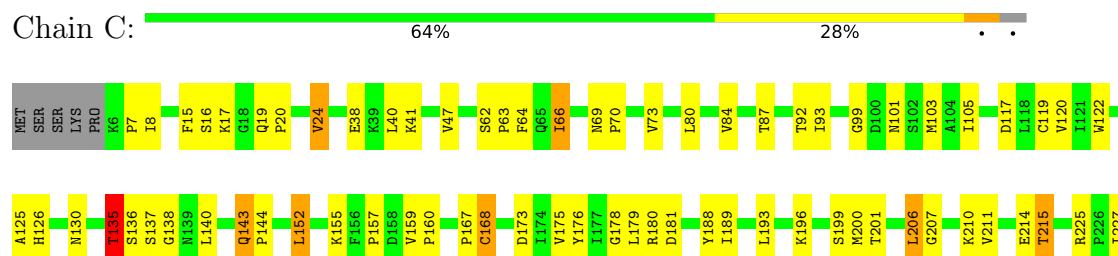
• Molecule 1: ARGINASE

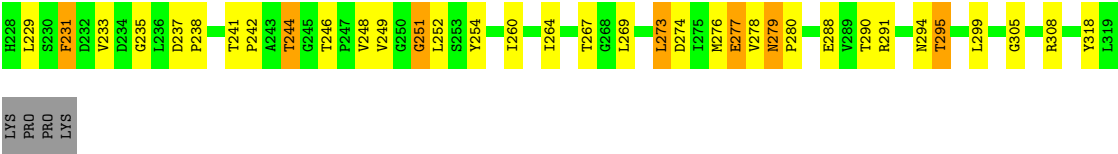


• Molecule 1: ARGINASE



• Molecule 1: ARGINASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	89.00Å 89.00Å 115.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.54	Depositor
% Data completeness (in resolution range)	74.0 (15.00-2.54)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7209	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.81	1/2440 (0.0%)	1.15	13/3314 (0.4%)
1	B	0.78	1/2440 (0.0%)	1.15	8/3314 (0.2%)
1	C	0.80	3/2440 (0.1%)	1.12	14/3314 (0.4%)
All	All	0.79	5/7320 (0.1%)	1.14	35/9942 (0.4%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	MET	SD-CE	-5.97	1.64	1.79
1	C	120	VAL	CA-CB	5.73	1.61	1.54
1	C	241	THR	CA-CB	5.61	1.59	1.53
1	C	93	ILE	CA-CB	5.47	1.59	1.53
1	B	200	MET	SD-CE	-5.10	1.66	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLU	N-CA-C	8.37	123.44	113.23
1	B	277	GLU	N-CA-C	8.26	123.31	113.23
1	C	277	GLU	N-CA-C	7.26	122.09	113.23
1	A	305	GLY	N-CA-C	6.75	121.69	113.79
1	C	305	GLY	N-CA-C	6.62	122.70	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	SER	N-CA-C	-6.56	105.32	113.38
1	A	136	SER	N-CA-C	-6.54	105.12	113.23
1	C	168	CYS	N-CA-C	6.34	121.02	113.28
1	B	305	GLY	N-CA-C	6.20	121.86	114.48
1	B	168	CYS	N-CA-C	5.83	120.39	113.28
1	A	149	LEU	N-CA-C	5.73	118.55	109.96
1	A	62	SER	CA-C-N	5.71	126.00	119.83
1	A	62	SER	C-N-CA	5.71	126.00	119.83
1	C	135	THR	N-CA-C	5.62	118.48	110.10
1	A	121	ILE	N-CA-C	-5.60	99.68	107.80
1	B	47	VAL	N-CA-C	5.54	115.86	108.11
1	B	22	GLY	N-CA-C	-5.47	104.14	112.51
1	A	8	ILE	CB-CA-C	-5.42	102.16	110.50
1	C	249	VAL	N-CA-C	5.41	117.43	109.63
1	C	279	ASN	CA-C-N	5.38	125.05	119.56
1	C	279	ASN	C-N-CA	5.38	125.05	119.56
1	C	122	TRP	N-CA-C	5.38	118.22	107.62
1	C	66	ILE	N-CA-C	-5.36	108.62	113.71
1	A	183	ASP	CA-C-N	5.25	124.88	119.05
1	A	183	ASP	C-N-CA	5.25	124.88	119.05
1	B	231	PHE	N-CA-C	5.23	117.25	107.99
1	C	251	GLY	N-CA-C	5.23	119.73	112.57
1	C	206	LEU	N-CA-C	5.19	120.61	113.97
1	A	206	LEU	N-CA-C	5.17	119.72	113.41
1	B	165	VAL	N-CA-C	5.16	115.75	109.30
1	A	168	CYS	N-CA-C	5.15	119.56	113.28
1	C	231	PHE	N-CA-C	5.10	117.02	107.99
1	A	46	ASN	N-CA-C	-5.07	101.04	109.46
1	C	136	SER	N-CA-C	-5.04	106.98	113.23
1	C	101	ASN	N-CA-C	5.01	118.89	112.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	176	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2414	55	0
1	B	2388	0	2414	66	0
1	C	2388	0	2414	69	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	21	0	0	0	0
3	B	8	0	0	1	0
3	C	10	0	0	0	0
All	All	7209	0	7242	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (185) 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:274:ASP:HB3	1:A:276:MET:HE3	1.39	1.00
1:B:38:GLU:HA	1:B:41:LYS:HE2	1.54	0.89
1:B:274:ASP:HB3	1:B:276:MET:HE3	1.59	0.85
1:A:130:ASN:HB3	1:A:135:THR:HG23	1.59	0.84
1:C:38:GLU:HA	1:C:41:LYS:HE2	1.58	0.84
1:C:7:PRO:HG2	1:C:92:THR:HG22	1.62	0.81
1:C:274:ASP:HB3	1:C:276:MET:HE3	1.62	0.80
1:A:135:THR:HG21	1:A:143:GLN:HE21	1.44	0.80
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.62	0.79
1:C:135:THR:HG21	1:C:143:GLN:HE21	1.48	0.79
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.19	0.78
1:B:7:PRO:HG2	1:B:92:THR:HG22	1.65	0.77
1:A:200:MET:HE1	1:A:252:LEU:HG	1.68	0.75
1:C:211:VAL:O	1:C:215:THR:HG23	1.87	0.73
1:A:135:THR:HB	1:A:137:SER:O	1.91	0.69
1:A:211:VAL:O	1:A:215:THR:HG23	1.92	0.68
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.74	0.68
1:A:66:ILE:O	1:A:138:GLY:HA3	1.93	0.68
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.75	0.68
1:A:16:SER:HB3	1:A:24:VAL:HG23	1.74	0.67
1:A:38:GLU:HA	1:A:41:LYS:HE2	1.76	0.67
1:B:66:ILE:O	1:B:138:GLY:HA3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:HB	1:B:137:SER:O	1.93	0.67
1:B:135:THR:HG21	1:B:143:GLN:HE21	1.61	0.66
1:C:244:THR:HG23	1:C:277:GLU:O	1.95	0.66
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.77	0.66
1:A:200:MET:HE3	1:A:251:GLY:HA2	1.77	0.66
1:C:143:GLN:N	1:C:144:PRO:HD2	2.12	0.65
1:B:200:MET:HE1	1:B:252:LEU:HG	1.77	0.65
1:A:244:THR:HG23	1:A:277:GLU:O	1.97	0.64
1:A:291:ARG:O	1:A:295:THR:HG23	1.97	0.64
1:B:291:ARG:O	1:B:295:THR:HG23	1.97	0.64
1:C:135:THR:HB	1:C:137:SER:O	1.98	0.64
1:B:211:VAL:O	1:B:215:THR:HG23	1.97	0.63
1:B:274:ASP:CB	1:B:276:MET:HE3	2.28	0.63
1:C:66:ILE:O	1:C:138:GLY:HA3	1.99	0.62
1:B:278:VAL:O	1:B:280:PRO:HD3	2.00	0.62
1:C:69:ASN:N	1:C:70:PRO:HD3	2.15	0.61
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.36	0.61
1:C:180:ARG:NH2	1:C:235:GLY:O	2.35	0.60
1:C:200:MET:HE3	1:C:251:GLY:HA2	1.83	0.60
1:A:143:GLN:N	1:A:144:PRO:HD2	2.17	0.60
1:C:80:LEU:HD22	1:C:103:MET:HE3	1.83	0.60
1:A:69:ASN:N	1:A:70:PRO:HD3	2.16	0.60
1:C:40:LEU:HB3	1:C:47:VAL:HG21	1.83	0.60
1:B:16:SER:HB3	1:B:24:VAL:HG23	1.84	0.60
1:C:278:VAL:O	1:C:280:PRO:HD3	2.02	0.59
1:B:143:GLN:N	1:B:144:PRO:HD2	2.18	0.59
1:B:8:ILE:HD12	1:B:47:VAL:HG22	1.85	0.58
1:C:260:ILE:O	1:C:264:ILE:HG12	2.04	0.58
1:C:69:ASN:O	1:C:73:VAL:HG23	2.04	0.58
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.85	0.57
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.86	0.57
1:B:16:SER:CB	1:B:24:VAL:HG23	2.36	0.56
1:B:69:ASN:N	1:B:70:PRO:HD3	2.20	0.56
1:A:278:VAL:O	1:A:280:PRO:HD3	2.05	0.56
1:B:206:LEU:HB3	1:B:210:LYS:HB3	1.88	0.55
1:B:178:GLY:O	1:B:200:MET:HE2	2.07	0.55
1:B:254:TYR:CE1	1:B:295:THR:HB	2.41	0.55
1:C:175:VAL:HA	1:C:196:LYS:O	2.07	0.55
1:B:254:TYR:HE1	1:B:295:THR:HB	1.72	0.54
1:C:229:LEU:HB3	1:C:273:LEU:HD23	1.89	0.54
1:B:15:PHE:O	1:B:99:GLY:HA2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HB3	1:A:210:LYS:HB3	1.89	0.54
1:A:274:ASP:CB	1:A:276:MET:HE3	2.28	0.54
1:A:143:GLN:N	1:A:144:PRO:CD	2.70	0.54
1:A:180:ARG:NH2	1:A:235:GLY:O	2.41	0.54
1:A:7:PRO:HG2	1:A:92:THR:HG22	1.89	0.53
1:A:80:LEU:HD22	1:A:103:MET:HE3	1.91	0.53
1:A:16:SER:CB	1:A:24:VAL:HG23	2.38	0.53
1:C:16:SER:HB3	1:C:24:VAL:HG23	1.89	0.53
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.43	0.53
1:B:200:MET:HE3	1:B:251:GLY:HA2	1.91	0.53
1:C:143:GLN:N	1:C:144:PRO:CD	2.71	0.53
1:B:153:LYS:HD3	1:B:167:PRO:HG2	1.90	0.53
1:B:15:PHE:CD2	1:B:103:MET:SD	3.02	0.52
1:B:260:ILE:O	1:B:264:ILE:HG12	2.09	0.52
1:C:16:SER:CB	1:C:24:VAL:HG23	2.39	0.52
1:A:19:GLN:OE1	1:A:100:ASP:HB2	2.10	0.52
1:C:207:GLY:O	1:C:211:VAL:HG23	2.10	0.52
1:A:130:ASN:O	1:A:143:GLN:HG2	2.09	0.52
1:C:291:ARG:O	1:C:295:THR:HG23	2.10	0.51
1:B:192:THR:HG22	1:B:193:LEU:HD12	1.91	0.51
1:B:230:SER:HA	1:B:274:ASP:HB2	1.92	0.51
1:B:18:GLY:HA3	1:B:100:ASP:OD2	2.11	0.51
1:C:200:MET:HE1	1:C:252:LEU:HG	1.94	0.50
1:B:125:ALA:HA	1:B:178:GLY:O	2.12	0.50
1:A:28:PRO:HD3	1:A:98:GLY:O	2.11	0.50
1:C:64:PHE:CD2	1:C:159:VAL:HG22	2.46	0.50
1:A:10:ILE:HD12	1:A:10:ILE:N	2.25	0.50
1:B:87:THR:HG22	1:B:92:THR:OG1	2.12	0.49
1:C:254:TYR:CE1	1:C:295:THR:HB	2.47	0.49
1:B:143:GLN:N	1:B:144:PRO:CD	2.75	0.49
1:C:173:ASP:OD1	1:C:225:ARG:NH2	2.44	0.49
1:B:201:THR:HG22	1:C:308:ARG:HB2	1.93	0.49
1:C:254:TYR:HE1	1:C:295:THR:HB	1.77	0.49
1:A:179:LEU:O	1:A:199:SER:HB2	2.13	0.49
1:A:111:HIS:ND1	1:A:118:LEU:HD22	2.28	0.49
1:A:8:ILE:HD12	1:A:47:VAL:HG22	1.95	0.49
1:B:244:THR:HG23	1:B:277:GLU:O	2.12	0.49
1:B:188:TYR:CD2	1:C:318:TYR:HB2	2.48	0.48
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.94	0.48
1:A:40:LEU:HB3	1:A:47:VAL:HG21	1.94	0.48
1:B:80:LEU:O	1:B:84:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:O	1:A:99:GLY:HA2	2.14	0.48
1:C:8:ILE:HD12	1:C:47:VAL:HG22	1.95	0.47
1:C:274:ASP:CB	1:C:276:MET:HE3	2.39	0.47
1:A:229:LEU:HD12	1:A:264:ILE:HG13	1.98	0.46
1:A:318:TYR:HB2	1:C:188:TYR:CD2	2.50	0.46
1:C:125:ALA:HA	1:C:178:GLY:O	2.15	0.46
1:B:55:PHE:HA	3:B:508:HOH:O	2.15	0.46
1:C:179:LEU:O	1:C:199:SER:HB2	2.16	0.46
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.97	0.46
1:C:80:LEU:O	1:C:84:VAL:HG23	2.15	0.46
1:A:96:VAL:HB	1:A:274:ASP:OD1	2.16	0.46
1:C:87:THR:HG22	1:C:92:THR:OG1	2.16	0.46
1:C:126:HIS:CD2	1:C:181:ASP:HB3	2.51	0.46
1:C:180:ARG:NH1	1:C:248:VAL:O	2.48	0.45
1:A:73:VAL:HG11	1:A:140:LEU:HD13	1.98	0.45
1:B:35:GLY:O	1:B:39:LYS:HG3	2.16	0.45
1:B:240:PHE:CD1	1:B:254:TYR:HB2	2.51	0.45
1:C:119:CYS:SG	1:C:227:ILE:HG12	2.57	0.45
1:C:140:LEU:HD23	1:C:143:GLN:OE1	2.17	0.45
1:C:206:LEU:HB3	1:C:210:LYS:HB3	1.98	0.45
1:A:153:LYS:HD3	1:A:167:PRO:HG2	1.98	0.45
1:C:62:SER:HA	1:C:63:PRO:HD3	1.84	0.45
1:C:80:LEU:CD2	1:C:103:MET:HE3	2.45	0.45
1:C:73:VAL:HG21	1:C:140:LEU:HD12	1.99	0.45
1:A:73:VAL:HG21	1:A:140:LEU:HD12	1.99	0.44
1:A:198:PHE:CE2	1:A:215:THR:HG22	2.52	0.44
1:B:125:ALA:HB2	1:B:180:ARG:NH2	2.32	0.44
1:A:140:LEU:HD23	1:A:143:GLN:OE1	2.17	0.44
1:C:242:PRO:HG2	1:C:288:GLU:HB3	2.00	0.44
1:B:64:PHE:CD2	1:B:159:VAL:HG22	2.53	0.44
1:B:139:ASN:HB3	1:B:141:HIS:HD2	1.82	0.44
1:A:126:HIS:CD2	1:A:181:ASP:HB3	2.53	0.44
1:B:175:VAL:HA	1:B:196:LYS:O	2.18	0.44
1:A:233:VAL:HG21	1:A:278:VAL:CG2	2.48	0.44
1:C:189:ILE:O	1:C:193:LEU:HB2	2.18	0.44
1:B:244:THR:CG2	1:B:277:GLU:O	2.66	0.43
1:B:314:PRO:O	1:B:315:GLU:HB2	2.18	0.43
1:C:180:ARG:HH22	1:C:235:GLY:C	2.26	0.43
1:A:190:ILE:HG22	1:A:195:ILE:HD12	1.99	0.43
1:C:152:LEU:O	1:C:155:LYS:HB2	2.18	0.43
1:B:236:LEU:HD23	1:B:252:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:HG3	1:C:248:VAL:HG11	2.00	0.43
1:B:117:ASP:O	1:B:225:ARG:HB2	2.19	0.43
1:C:130:ASN:O	1:C:143:GLN:HG2	2.19	0.43
1:A:180:ARG:HH22	1:A:235:GLY:C	2.26	0.42
1:B:8:ILE:HD11	1:B:45:TYR:CB	2.48	0.42
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.90	0.42
1:B:80:LEU:HD22	1:B:103:MET:HE3	2.00	0.42
1:A:210:LYS:O	1:A:214:GLU:HB2	2.19	0.42
1:B:200:MET:HB2	1:C:308:ARG:HD2	2.01	0.42
1:A:261:THR:HG22	1:A:303:CYS:SG	2.60	0.42
1:A:125:ALA:HA	1:A:178:GLY:O	2.20	0.42
1:A:191:LYS:HA	1:A:191:LYS:HD3	1.81	0.42
1:C:24:VAL:HG13	1:C:279:ASN:HB2	2.02	0.42
1:C:69:ASN:N	1:C:70:PRO:CD	2.83	0.42
1:C:237:ASP:HA	1:C:238:PRO:HD3	1.95	0.42
1:C:267:THR:O	1:C:269:LEU:HD13	2.19	0.42
1:B:126:HIS:CD2	1:B:181:ASP:HB3	2.54	0.41
1:A:290:THR:HG22	1:A:294:ASN:ND2	2.36	0.41
1:B:180:ARG:NH2	1:B:235:GLY:O	2.52	0.41
1:B:27:GLY:N	1:B:28:PRO:HD2	2.35	0.41
1:B:191:LYS:HA	1:B:191:LYS:HD3	1.78	0.41
1:A:175:VAL:HA	1:A:196:LYS:O	2.20	0.41
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.82	0.41
1:C:290:THR:HG22	1:C:294:ASN:ND2	2.36	0.41
1:A:129:ILE:HG22	1:A:186:GLU:HB3	2.02	0.41
1:B:58:VAL:HA	1:B:59:PRO:HD2	1.83	0.41
1:A:15:PHE:CD2	1:A:103:MET:SD	3.14	0.41
1:C:15:PHE:O	1:C:99:GLY:HA2	2.20	0.41
1:A:108:ILE:HD13	1:A:120:VAL:HG21	2.02	0.41
1:B:64:PHE:HD2	1:B:159:VAL:HG22	1.86	0.41
1:B:229:LEU:O	1:B:273:LEU:HA	2.21	0.41
1:C:178:GLY:O	1:C:200:MET:HE2	2.21	0.41
1:C:231:PHE:CE2	1:C:299:LEU:HD22	2.57	0.40
1:B:201:THR:CG2	1:C:308:ARG:HB2	2.51	0.40
1:C:117:ASP:O	1:C:225:ARG:HB2	2.22	0.40
1:A:229:LEU:O	1:A:273:LEU:HA	2.21	0.40
1:B:118:LEU:C	1:B:118:LEU:HD12	2.46	0.40
1:B:139:ASN:HB3	1:B:141:HIS:CD2	2.56	0.40
1:B:180:ARG:HH22	1:B:235:GLY:C	2.29	0.40
1:B:267:THR:O	1:B:269:LEU:HD13	2.21	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	312/323 (97%)	294 (94%)	16 (5%)	2 (1%)	21	29
1	B	312/323 (97%)	293 (94%)	16 (5%)	3 (1%)	12	17
1	C	312/323 (97%)	292 (94%)	16 (5%)	4 (1%)	9	12
All	All	936/969 (97%)	879 (94%)	48 (5%)	9 (1%)	12	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	PRO
1	C	157	PRO
1	A	157	PRO
1	B	143	GLN
1	C	143	GLN
1	A	143	GLN
1	B	167	PRO
1	C	167	PRO
1	C	105	ILE

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	263/273 (96%)	252 (96%)	11 (4%)	26	40
1	B	263/273 (96%)	250 (95%)	13 (5%)	22	34
1	C	263/273 (96%)	251 (95%)	12 (5%)	24	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	789/819 (96%)	753 (95%)	36 (5%)	24	36

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	135	THR
1	A	152	LEU
1	A	201	THR
1	A	214	GLU
1	A	215	THR
1	A	233	VAL
1	A	244	THR
1	A	269	LEU
1	A	273	LEU
1	A	295	THR
1	B	24	VAL
1	B	118	LEU
1	B	132	PRO
1	B	135	THR
1	B	152	LEU
1	B	168	CYS
1	B	201	THR
1	B	214	GLU
1	B	233	VAL
1	B	244	THR
1	B	246	THR
1	B	273	LEU
1	B	295	THR
1	C	24	VAL
1	C	135	THR
1	C	152	LEU
1	C	168	CYS
1	C	201	THR
1	C	214	GLU
1	C	215	THR
1	C	233	VAL
1	C	244	THR
1	C	246	THR
1	C	273	LEU
1	C	295	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	79	GLN
1	A	141	HIS
1	A	143	GLN
1	B	65	GLN
1	B	79	GLN
1	B	141	HIS
1	B	143	GLN
1	B	187	HIS
1	C	65	GLN
1	C	79	GLN
1	C	143	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 [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.