



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:40 PM UTC

PDB ID : 3MJL / pdb_00003mjl
Title : Crystal structure of human arginase I in complex with 2-aminoimidazole. Resolution 1.90 Å.
Authors : Di Costanzo, L.; Christianson, D.W.
Deposited on : 2010-04-13
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

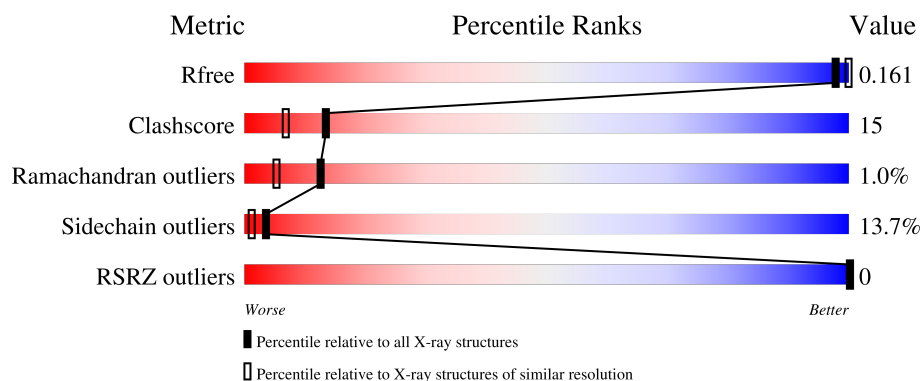
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	322	
1	B	322	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5032 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.

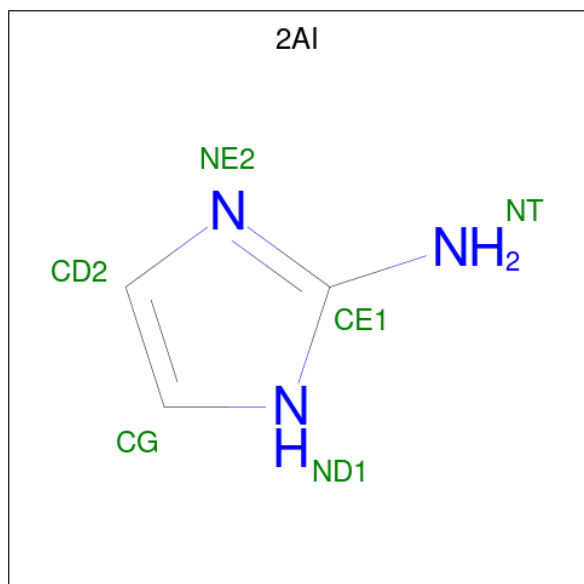
- Molecule 1 is a protein called Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2389	1523	407	453	6			
1	B	313	Total	C	N	O	S	0	0	0
			2381	1519	405	451	6			

- 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		

- Molecule 3 is 1H-imidazol-2-amine (CCD ID: 2AI) (formula: C₃H₅N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	N 3	0	0
3	B	1	Total 6	C 3	N 3	0	0

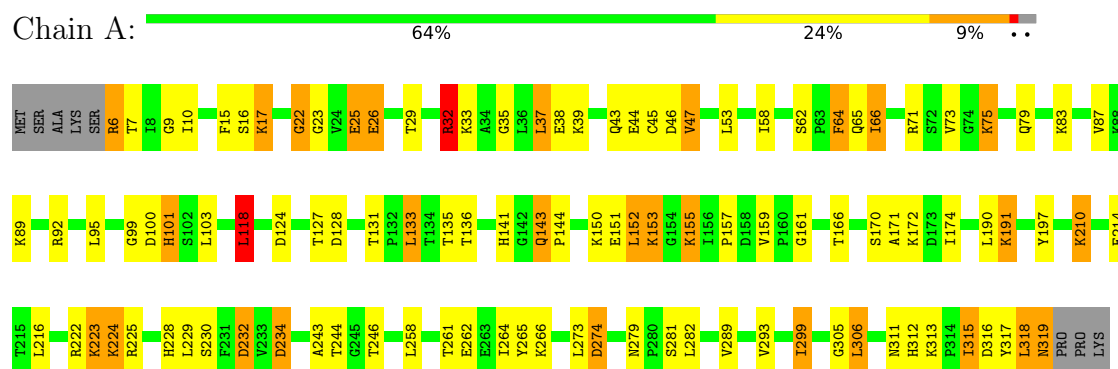
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total 143	O 143	0	0
4	B	103	Total 103	O 103	0	0

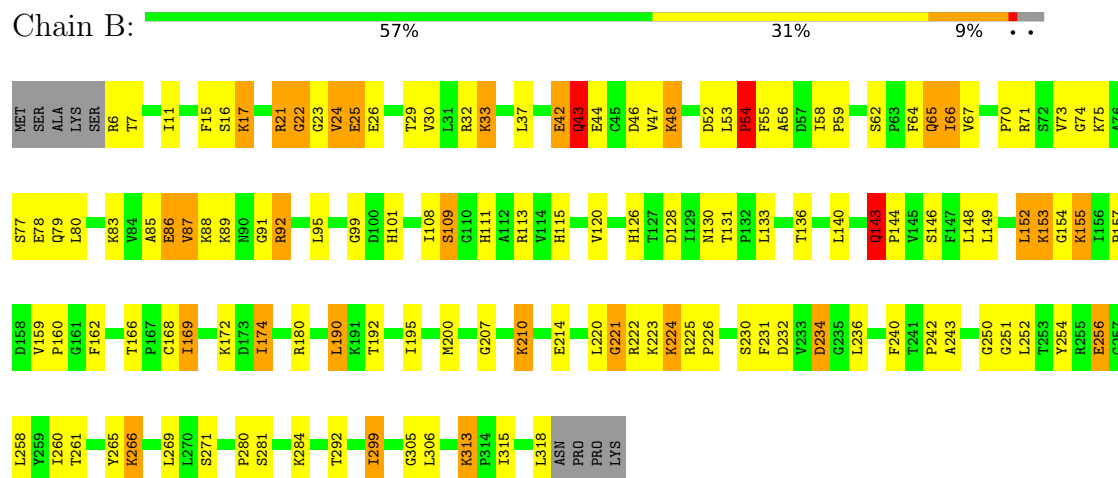
3 Residue-property plots

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: Arginase-1



• Molecule 1: Arginase-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	90.68Å 90.68Å 69.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 97.7 (50.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.90Å)	Xtriage
Refinement program	SHELXL, CNS	Depositor
R, R_{free}	0.168 , 0.176 0.132 , 0.161	Depositor DCC
R_{free} test set	2500 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.426 for -h,-k,l 0.119 for h,-h-k,-l 0.118 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5032	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 2AI

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	0.51	0/2439	1.67	36/3310 (1.1%)
1	B	0.47	0/2431	1.56	25/3299 (0.8%)
All	All	0.49	0/4870	1.62	61/6609 (0.9%)

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	CD-NE-CZ	16.40	147.36	124.40
1	A	318	LEU	CA-C-N	10.05	139.79	121.70
1	A	318	LEU	C-N-CA	10.05	139.79	121.70
1	A	311	ASN	CA-CB-CG	9.54	122.14	112.60
1	A	22	GLY	N-CA-C	9.28	124.65	112.77
1	A	234	ASP	CA-CB-CG	7.89	120.49	112.60
1	A	318	LEU	O-C-N	-7.85	110.61	122.08
1	A	274	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	232	ASP	CA-CB-CG	7.14	119.74	112.60
1	B	250	GLY	CA-C-N	6.97	131.63	121.67
1	B	250	GLY	C-N-CA	6.97	131.63	121.67
1	A	244	THR	CA-C-N	6.90	127.59	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	THR	C-N-CA	6.90	127.59	120.00
1	A	29	THR	CA-C-N	-6.67	109.70	120.64
1	A	29	THR	C-N-CA	-6.67	109.70	120.64
1	B	231	PHE	CA-CB-CG	6.54	120.34	113.80
1	B	207	GLY	CA-C-O	-6.31	116.75	122.24
1	A	161	GLY	CA-C-N	-6.29	112.68	122.37
1	A	161	GLY	C-N-CA	-6.29	112.68	122.37
1	A	159	VAL	N-CA-C	6.13	113.90	108.63
1	B	234	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	166	THR	O-C-N	6.06	128.07	121.23
1	B	126	HIS	CA-CB-CG	-6.00	107.80	113.80
1	A	282	LEU	CA-C-N	-6.00	114.64	120.34
1	A	282	LEU	C-N-CA	-6.00	114.64	120.34
1	A	141	HIS	CA-C-N	5.98	133.13	121.41
1	A	141	HIS	C-N-CA	5.98	133.13	121.41
1	B	23	GLY	N-CA-C	5.93	120.99	114.40
1	A	133	LEU	CA-C-N	-5.90	112.87	122.26
1	A	133	LEU	C-N-CA	-5.90	112.87	122.26
1	B	54	PRO	CA-C-N	5.90	130.26	122.30
1	B	54	PRO	C-N-CA	5.90	130.26	122.30
1	A	73	VAL	CA-C-N	5.85	126.60	119.99
1	A	73	VAL	C-N-CA	5.85	126.60	119.99
1	B	56	ALA	CA-C-N	-5.81	112.62	120.87
1	B	56	ALA	C-N-CA	-5.81	112.62	120.87
1	B	190	LEU	CA-C-N	5.81	128.07	120.28
1	B	190	LEU	C-N-CA	5.81	128.07	120.28
1	B	21	ARG	CA-C-O	5.78	127.07	120.54
1	A	45	CYS	N-CA-C	5.78	119.14	109.95
1	B	143	GLN	CA-C-O	-5.64	112.43	120.16
1	A	47	VAL	N-CA-C	5.56	115.86	107.75
1	B	22	GLY	O-C-N	-5.53	116.25	122.28
1	A	64	PHE	CA-C-N	-5.47	115.05	123.04
1	A	64	PHE	C-N-CA	-5.47	115.05	123.04
1	B	92	ARG	CD-NE-CZ	5.44	132.02	124.40
1	B	232	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	319	ASN	CA-CB-CG	-5.40	107.20	112.60
1	B	24	VAL	O-C-N	-5.39	116.46	121.90
1	B	78	GLU	O-C-N	5.39	127.83	122.12
1	A	143	GLN	CA-C-O	-5.38	112.79	120.16
1	A	32	ARG	CA-C-N	5.37	127.48	120.28
1	A	32	ARG	C-N-CA	5.37	127.48	120.28
1	A	6	ARG	CG-CD-NE	5.36	123.80	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	CA-C-O	5.35	126.12	119.97
1	B	256	GLU	CA-C-N	5.32	125.85	120.00
1	B	256	GLU	C-N-CA	5.32	125.85	120.00
1	A	118	LEU	CA-C-O	5.22	127.09	121.55
1	B	65	GLN	CB-CA-C	-5.13	110.26	117.23
1	A	124	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	154	GLY	N-CA-C	-5.02	108.40	114.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ASP	Sidechain
1	A	318	LEU	Mainchain
1	B	234	ASP	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	2389	0	2433	64	0
1	B	2381	0	2427	78	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	3	1	0
3	B	6	0	3	0	0
4	A	143	0	0	5	0
4	B	103	0	0	3	0
All	All	5032	0	4866	142	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 15.

All (142) 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:30:VAL:HA	1:B:33:LYS:HD3	1.47	0.97
1:B:16:SER:HB3	1:B:25:GLU:HG2	1.50	0.92
1:A:16:SER:HB3	1:A:25:GLU:HG2	1.55	0.88
1:B:29:THR:HG22	1:B:33:LYS:HD2	1.57	0.84
1:B:148:LEU:HB3	1:B:169:ILE:HD11	1.63	0.80
1:B:26:GLU:O	1:B:30:VAL:HG23	1.85	0.77
1:B:224:LYS:HG3	1:B:269:LEU:HD11	1.66	0.76
1:B:47:VAL:O	1:B:48:LYS:HD3	1.87	0.74
1:A:53:LEU:HD21	1:A:83:LYS:HG3	1.71	0.73
1:B:22:GLY:O	1:B:25:GLU:HG3	1.89	0.72
1:A:262:GLU:O	1:A:266:LYS:HD3	1.89	0.71
1:A:22:GLY:O	1:A:25:GLU:HG3	1.91	0.71
1:B:85:ALA:O	1:B:89:LYS:HG3	1.91	0.71
1:A:75:LYS:O	1:A:79:GLN:HG3	1.91	0.70
1:B:157:PRO:O	1:B:159:VAL:HG23	1.91	0.70
1:B:109:SER:O	1:B:113:ARG:HG3	1.92	0.68
1:A:136:THR:HG23	4:A:9235:HOH:O	1.94	0.67
1:A:9:GLY:HA3	1:A:87:VAL:HG11	1.76	0.67
1:B:190:LEU:HA	1:B:195:ILE:HD12	1.78	0.66
3:A:5001:2AI:HD2	4:A:9207:HOH:O	1.96	0.66
1:A:281:SER:OG	1:B:192:THR:HG23	1.96	0.65
1:B:15:PHE:HB2	1:B:55:PHE:CE2	2.33	0.64
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.32	0.64
1:B:210:LYS:HD2	1:B:214:GLU:HG3	1.79	0.64
1:A:246:THR:HG23	4:A:9231:HOH:O	1.97	0.64
1:A:222:ARG:HG2	1:A:223:LYS:HZ3	1.62	0.64
1:B:152:LEU:O	1:B:155:LYS:HB2	1.99	0.63
1:A:35:GLY:O	1:A:39:LYS:HG3	1.99	0.62
1:B:240:PHE:CD1	1:B:254:TYR:HB2	2.36	0.61
1:B:70:PRO:HB2	1:B:160:PRO:O	2.01	0.60
1:A:224:LYS:N	1:A:224:LYS:HD2	2.15	0.60
1:A:53:LEU:HD22	1:A:83:LYS:HE3	1.83	0.60
1:B:258:LEU:HD23	1:B:299:ILE:HD12	1.83	0.59
1:B:266:LYS:HD3	4:B:9174:HOH:O	2.02	0.59
1:A:9:GLY:HA3	1:A:87:VAL:CG1	2.34	0.58
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.84	0.57
1:A:66:ILE:HG12	1:A:66:ILE:O	2.03	0.57
1:B:66:ILE:HG13	1:B:66:ILE:O	2.05	0.57
1:A:53:LEU:CD2	1:A:83:LYS:HG3	2.35	0.57
1:B:243:ALA:HB3	1:B:292:THR:HG21	1.87	0.57
1:A:100:ASP:O	1:A:103:LEU:HD12	2.06	0.56
1:A:319:ASN:HD22	1:A:319:ASN:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HD3	1:B:200:MET:HG3	1.89	0.55
1:B:29:THR:CG2	1:B:33:LYS:HD2	2.36	0.54
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.89	0.54
1:B:53:LEU:HD11	1:B:83:LYS:HG3	1.90	0.53
1:B:73:VAL:HG11	1:B:140:LEU:HD13	1.89	0.53
1:A:258:LEU:O	1:A:262:GLU:HG3	2.08	0.53
1:B:7:THR:HG22	1:B:92:ARG:HD3	1.91	0.53
1:B:168:CYS:SG	1:B:169:ILE:HD13	2.49	0.53
1:B:29:THR:O	1:B:33:LYS:HG3	2.08	0.52
1:B:79:GLN:O	1:B:83:LYS:HG2	2.09	0.52
1:B:53:LEU:HD21	1:B:83:LYS:HG3	1.92	0.52
1:A:150:LYS:O	1:A:153:LYS:HB2	2.10	0.52
1:B:30:VAL:HG21	1:B:280:PRO:HG2	1.92	0.51
1:A:265:TYR:CE2	1:A:305:GLY:HA2	2.46	0.51
1:A:319:ASN:H	1:A:319:ASN:ND2	2.09	0.51
1:A:155:LYS:HA	1:A:155:LYS:HE3	1.93	0.51
1:B:224:LYS:CG	1:B:269:LEU:HD11	2.39	0.51
1:A:10:ILE:HD13	1:A:47:VAL:HG13	1.93	0.51
1:A:35:GLY:HA2	1:A:38:GLU:OE1	2.11	0.51
1:A:118:LEU:HD13	1:A:228:HIS:HB2	1.92	0.51
1:A:222:ARG:HG2	1:A:223:LYS:NZ	2.26	0.50
1:B:64:PHE:O	1:B:67:VAL:HB	2.11	0.50
1:A:32:ARG:HH11	1:A:32:ARG:HG3	1.76	0.50
1:B:220:LEU:O	1:B:221:GLY:O	2.30	0.50
1:A:210:LYS:O	1:A:214:GLU:HG3	2.11	0.50
1:A:79:GLN:O	1:A:83:LYS:HG2	2.12	0.49
1:A:53:LEU:CD2	1:A:83:LYS:HE3	2.43	0.49
1:B:111:HIS:CE1	1:B:271:SER:HB3	2.48	0.49
1:A:224:LYS:HD2	1:A:224:LYS:H	1.78	0.48
1:A:101:HIS:CE1	1:A:232:ASP:HB2	2.48	0.48
1:A:289:VAL:O	1:A:293:VAL:HG23	2.13	0.48
1:B:15:PHE:O	1:B:99:GLY:HA2	2.13	0.48
1:A:191:LYS:HE3	1:A:197:TYR:OH	2.13	0.48
1:B:242:PRO:HD2	1:B:292:THR:OG1	2.14	0.48
1:B:133:LEU:HD12	4:B:9200:HOH:O	2.15	0.47
1:A:312:HIS:HB2	1:A:317:TYR:CE2	2.49	0.47
1:B:16:SER:HB2	1:B:24:VAL:HG12	1.96	0.47
1:B:53:LEU:HD11	1:B:80:LEU:HA	1.96	0.47
1:B:75:LYS:O	1:B:79:GLN:HB2	2.14	0.47
1:B:53:LEU:HD21	1:B:83:LYS:CD	2.45	0.47
1:B:240:PHE:CE1	1:B:254:TYR:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:O	1:A:65:GLN:HB2	2.14	0.47
1:A:229:LEU:HD22	1:A:264:ILE:HD13	1.96	0.46
1:A:222:ARG:O	1:A:223:LYS:HB3	2.15	0.46
1:B:16:SER:OG	1:B:17:LYS:NZ	2.48	0.46
1:A:7:THR:HG23	1:A:46:ASP:CG	2.41	0.46
1:A:7:THR:CG2	1:A:92:ARG:HH11	2.28	0.46
1:A:229:LEU:HD23	1:A:273:LEU:CD1	2.45	0.46
1:B:236:LEU:HD23	1:B:252:LEU:HB2	1.98	0.46
1:A:246:THR:N	4:A:9231:HOH:O	2.49	0.45
1:B:153:LYS:HE2	1:B:153:LYS:C	2.42	0.45
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.59	0.45
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.85	0.45
1:B:180:ARG:CZ	1:B:251:GLY:HA2	2.47	0.45
1:B:32:ARG:NH1	1:B:52:ASP:OD1	2.50	0.45
1:B:88:LYS:O	1:B:91:GLY:N	2.49	0.45
1:A:23:GLY:O	1:A:26:GLU:HG2	2.17	0.44
1:B:11:ILE:HD11	1:B:87:VAL:HG11	1.98	0.44
1:B:115:HIS:HB3	1:B:226:PRO:HG2	1.99	0.44
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.99	0.44
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.53	0.44
1:A:133:LEU:HD11	1:A:157:PRO:HG3	2.00	0.44
1:B:120:VAL:O	1:B:174:ILE:HA	2.18	0.44
1:B:210:LYS:HD3	1:B:210:LYS:HA	1.69	0.44
1:B:88:LYS:HD2	1:B:88:LYS:HA	1.67	0.44
1:B:7:THR:HG23	1:B:46:ASP:HB3	2.00	0.44
1:B:62:SER:O	1:B:71:ARG:NH1	2.49	0.44
1:B:155:LYS:HA	1:B:155:LYS:HD2	1.49	0.44
1:A:53:LEU:HD11	1:A:83:LYS:HG3	1.98	0.44
1:B:254:TYR:CE2	1:B:258:LEU:HD11	2.53	0.44
1:B:17:LYS:NZ	4:B:9033:HOH:O	2.50	0.44
1:B:7:THR:HG23	1:B:46:ASP:CG	2.43	0.43
1:B:46:ASP:OD1	1:B:48:LYS:NZ	2.48	0.43
1:B:130:ASN:O	1:B:143:GLN:HG2	2.17	0.43
1:A:230:SER:HA	1:A:274:ASP:HB2	2.01	0.43
1:B:256:GLU:O	1:B:260:ILE:HG13	2.18	0.43
1:A:62:SER:HA	4:A:9182:HOH:O	2.19	0.43
1:A:15:PHE:HB3	1:A:103:LEU:HD11	2.00	0.43
1:A:128:ASP:HB3	1:A:144:PRO:HD2	2.00	0.43
1:B:148:LEU:HB3	1:B:169:ILE:CD1	2.42	0.43
1:B:83:LYS:O	1:B:86:GLU:HB3	2.19	0.43
1:A:37:LEU:HD23	1:A:37:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ALA:HB1	1:A:279:ASN:O	2.19	0.42
1:A:315:ILE:HG23	1:A:316:ASP:N	2.34	0.42
1:B:265:TYR:CD2	1:B:305:GLY:HA2	2.55	0.42
1:A:151:GLU:CD	1:A:171:ALA:H	2.27	0.41
1:B:74:GLY:HA2	1:B:162:PHE:CE2	2.55	0.41
1:B:42:GLU:O	1:B:43:GLN:O	2.39	0.41
1:A:15:PHE:O	1:A:99:GLY:HA2	2.20	0.41
1:B:58:ILE:HA	1:B:59:PRO:HD2	1.81	0.41
1:B:265:TYR:CE2	1:B:305:GLY:HA2	2.55	0.41
1:A:131:THR:O	1:A:135:THR:N	2.52	0.41
1:A:265:TYR:CD2	1:A:305:GLY:HA2	2.55	0.41
1:B:53:LEU:HA	1:B:54:PRO:HD3	1.85	0.41
1:B:131:THR:HG22	1:B:146:SER:HB2	2.02	0.41
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.93	0.41
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.92	0.40
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.84	0.40
1:B:313:LYS:O	1:B:315:ILE:N	2.54	0.40
1:A:83:LYS:O	1:A:87:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	312/322 (97%)	296 (95%)	15 (5%)	1 (0%)	36	29
1	B	311/322 (97%)	292 (94%)	14 (4%)	5 (2%)	7	2
All	All	623/644 (97%)	588 (94%)	29 (5%)	6 (1%)	12	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	GLN
1	B	221	GLY
1	B	222	ARG
1	B	143	GLN
1	B	54	PRO
1	A	143	GLN

5.3.2 Protein sidechains ⓘ

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	263/270 (97%)	230 (88%)	33 (12%)	4	1
1	B	262/270 (97%)	223 (85%)	39 (15%)	3	1
All	All	525/540 (97%)	453 (86%)	72 (14%)	3	1

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	17	LYS
1	A	25	GLU
1	A	26	GLU
1	A	32	ARG
1	A	33	LYS
1	A	37	LEU
1	A	43	GLN
1	A	44	GLU
1	A	58	ILE
1	A	66	ILE
1	A	75	LYS
1	A	89	LYS
1	A	95	LEU
1	A	101	HIS
1	A	118	LEU
1	A	127	THR
1	A	152	LEU

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Mol	Chain	Res	Type
1	A	153	LYS
1	A	155	LYS
1	A	166	THR
1	A	170	SER
1	A	172	LYS
1	A	174	ILE
1	A	191	LYS
1	A	210	LYS
1	A	223	LYS
1	A	224	LYS
1	A	225	ARG
1	A	299	ILE
1	A	306	LEU
1	A	313	LYS
1	A	315	ILE
1	B	6	ARG
1	B	17	LYS
1	B	21	ARG
1	B	25	GLU
1	B	33	LYS
1	B	37	LEU
1	B	42	GLU
1	B	43	GLN
1	B	44	GLU
1	B	48	LYS
1	B	65	GLN
1	B	66	ILE
1	B	77	SER
1	B	86	GLU
1	B	87	VAL
1	B	95	LEU
1	B	101	HIS
1	B	108	ILE
1	B	109	SER
1	B	136	THR
1	B	149	LEU
1	B	152	LEU
1	B	153	LYS
1	B	155	LYS
1	B	169	ILE
1	B	172	LYS
1	B	174	ILE

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Mol	Chain	Res	Type
1	B	210	LYS
1	B	223	LYS
1	B	224	LYS
1	B	225	ARG
1	B	230	SER
1	B	266	LYS
1	B	281	SER
1	B	284	LYS
1	B	299	ILE
1	B	306	LEU
1	B	313	LYS
1	B	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	69	ASN
1	A	79	GLN
1	A	130	ASN
1	A	143	GLN
1	A	319	ASN

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, 4 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$
3	2AI	B	5000	-	5,6,6	1.61	1 (20%)	6,7,7	4.05	4 (66%)
3	2AI	A	5001	-	5,6,6	1.52	1 (20%)	6,7,7	3.76	4 (66%)

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
3	2AI	B	5000	-	-	-	0/1/1/1
3	2AI	A	5001	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5000	2AI	CE1-NT	3.08	1.41	1.34
3	A	5001	2AI	CE1-NT	2.89	1.40	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5000	2AI	CD2-NE2-CE1	6.33	111.22	103.31
3	B	5000	2AI	ND1-CE1-NE2	-5.80	107.09	112.36
3	A	5001	2AI	CD2-NE2-CE1	5.75	110.49	103.31
3	A	5001	2AI	ND1-CE1-NE2	-5.07	107.76	112.36
3	A	5001	2AI	NT-CE1-ND1	4.24	128.96	122.68
3	B	5000	2AI	NT-CE1-ND1	3.54	127.92	122.68
3	B	5000	2AI	CG-CD2-NE2	-3.13	104.84	109.87
3	A	5001	2AI	CG-CD2-NE2	-2.66	105.60	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5001	2AI	1	0

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/322 (97%)	-1.67	0 100 100	14, 24, 42, 66	0
1	B	313/322 (97%)	-1.60	0 100 100	13, 29, 51, 74	0
All	All	627/644 (97%)	-1.64	0 100 100	13, 26, 46, 74	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	2AI	A	5001	6/6	0.99	0.03	31,43,44,74	0
2	MN	A	3315	1/1	1.00	0.01	18,18,18,18	0
2	MN	B	4314	1/1	1.00	0.01	21,21,21,21	0
2	MN	B	4315	1/1	1.00	0.01	27,27,27,27	0
2	MN	A	3314	1/1	1.00	0.00	20,20,20,20	0
3	2AI	B	5000	6/6	1.00	0.03	28,35,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.