



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:06 PM UTC

PDB ID : 3MFW / pdb_00003mfw
Title : Crystal structure of human arginase I in complex with L-2-aminohistidine and sulphate
Authors : Di Costanzo, L.; Christianson, D.W.
Deposited on : 2010-04-04
Resolution : 1.47 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

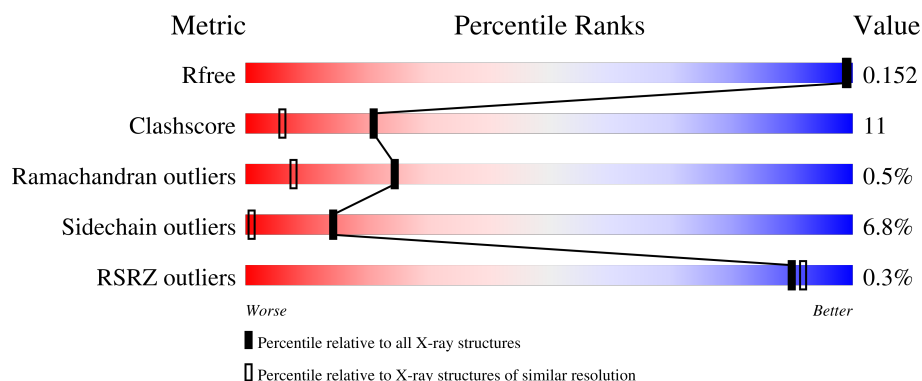
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	 75% 19% . .
1	B	322	 67% 24% 6% . .

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
2	SO4	A	551	-	-	X	-
2	SO4	B	552	-	-	X	-

2 Entry composition [i](#)

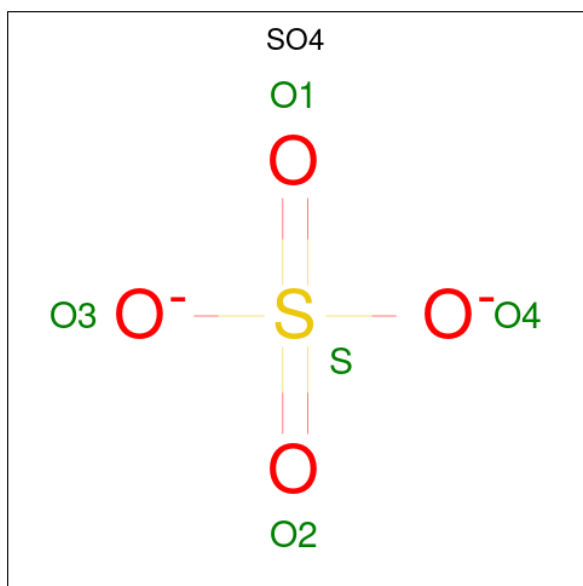
There are 5 unique types of molecules in this entry. The entry contains 5279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

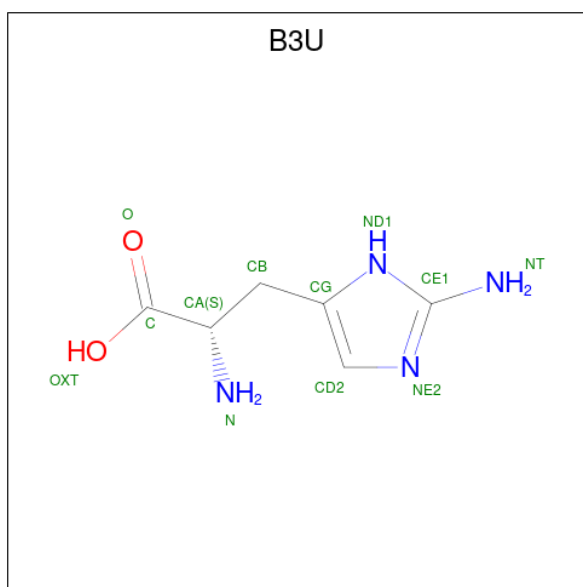
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2395	1526	408	455	6			
1	B	314	Total	C	N	O	S	0	0	0
			2387	1522	406	453	6			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-amino-L-histidine (CCD ID: B3U) (formula: C₆H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

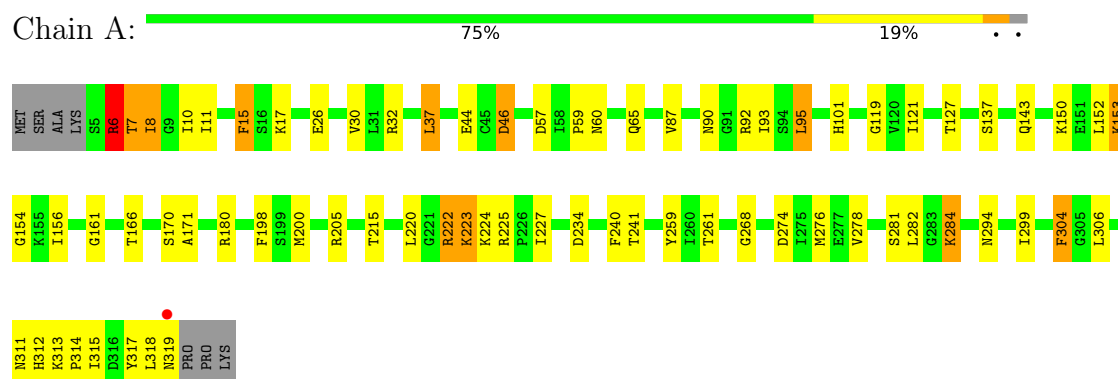
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	0
			265	265		
5	B	194	Total	O	0	0
			194	194		

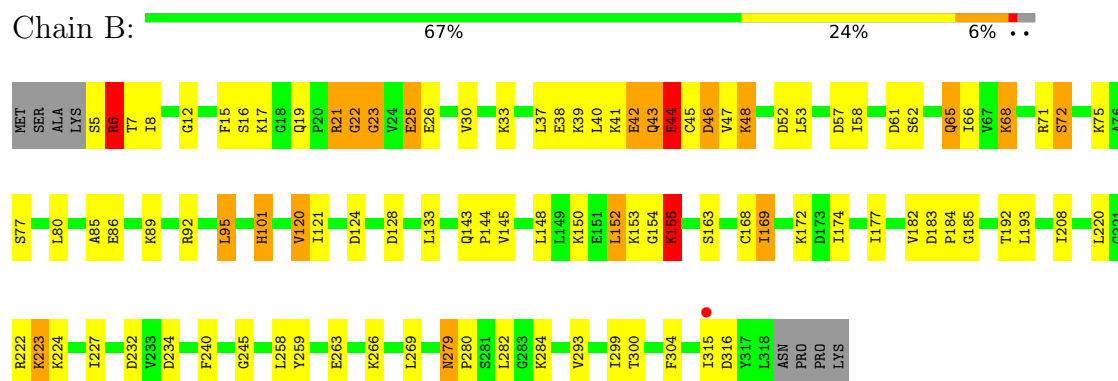
3 Residue-property plots

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	90.34Å 90.34Å 69.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.47 50.00 – 1.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.47) 96.8 (50.00-1.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.47Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.149 , 0.162 0.137 , 0.152	Depositor DCC
R_{free} test set	5389 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.305 for -h,-k,l 0.097 for h,-h-k,-l 0.096 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5279	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: B3U, SO4, 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	0.75	2/2445 (0.1%)	1.73	38/3318 (1.1%)
1	B	0.72	0/2437	1.76	43/3307 (1.3%)
All	All	0.73	2/4882 (0.0%)	1.75	81/6625 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	PHE	N-CA	-5.37	1.39	1.46
1	A	318	LEU	C-N	5.06	1.40	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LEU	CA-C-N	17.61	153.41	121.70
1	A	318	LEU	C-N-CA	17.61	153.41	121.70
1	A	6	ARG	CA-C-N	8.17	132.47	120.87
1	A	6	ARG	C-N-CA	8.17	132.47	120.87
1	B	22	GLY	O-C-N	-7.47	114.32	122.24
1	A	205	ARG	CD-NE-CZ	7.42	134.79	124.40
1	B	6	ARG	CD-NE-CZ	7.05	134.26	124.40
1	B	240	PHE	CA-CB-CG	-6.98	106.82	113.80
1	B	19	GLN	OE1-CD-NE2	6.92	129.52	122.60
1	B	21	ARG	CA-C-O	6.82	128.06	120.43
1	B	23	GLY	N-CA-C	6.79	122.14	114.67
1	B	234	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	279	ASN	O-C-N	6.67	127.39	121.32
1	B	121	ILE	O-C-N	6.58	130.80	123.10
1	B	182	VAL	CA-C-O	-6.54	113.55	120.48
1	B	47	VAL	N-CA-C	6.53	117.04	107.37
1	B	168	CYS	CA-C-N	-6.49	112.36	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	CYS	C-N-CA	-6.49	112.36	122.69
1	A	304	PHE	CA-CB-CG	-6.45	107.36	113.80
1	A	154	GLY	N-CA-C	-6.35	106.36	113.79
1	B	155	LYS	CA-C-N	-6.32	115.65	122.85
1	B	155	LYS	C-N-CA	-6.32	115.65	122.85
1	A	282	LEU	CA-C-N	-6.30	113.88	120.31
1	A	282	LEU	C-N-CA	-6.30	113.88	120.31
1	B	22	GLY	N-CA-C	6.24	121.41	113.24
1	A	156	ILE	O-C-N	6.20	126.62	120.92
1	B	124	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	154	GLY	N-CA-C	-5.98	107.18	113.58
1	B	19	GLN	CA-C-O	-5.98	115.51	120.71
1	A	171	ALA	CA-C-O	-5.96	113.53	120.20
1	B	234	ASP	CA-C-N	-5.92	112.70	120.22
1	B	234	ASP	C-N-CA	-5.92	112.70	120.22
1	A	234	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	93	ILE	O-C-N	5.82	129.27	122.81
1	B	154	GLY	CA-C-O	5.80	124.76	119.83
1	B	185	GLY	CA-C-O	5.80	126.73	120.75
1	A	241	THR	O-C-N	-5.79	115.78	121.17
1	A	278	VAL	CA-C-O	-5.79	113.95	120.95
1	A	65	GLN	CA-C-N	-5.76	114.11	122.69
1	A	65	GLN	C-N-CA	-5.76	114.11	122.69
1	A	240	PHE	CA-CB-CG	-5.74	108.06	113.80
1	B	145	VAL	O-C-N	-5.72	115.33	121.80
1	B	300	THR	CA-C-O	-5.67	114.87	120.82
1	A	121	ILE	O-C-N	5.61	129.07	123.18
1	A	60	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	B	44	GLU	CA-C-N	-5.57	114.15	122.39
1	B	44	GLU	C-N-CA	-5.57	114.15	122.39
1	B	95	LEU	CA-C-O	-5.56	114.36	120.70
1	A	57	ASP	CA-CB-CG	-5.55	107.05	112.60
1	A	278	VAL	O-C-N	5.53	129.02	122.66
1	B	47	VAL	CB-CA-C	-5.51	103.53	111.19
1	A	119	GLY	CA-C-N	-5.47	116.41	123.19
1	A	119	GLY	C-N-CA	-5.47	116.41	123.19
1	B	6	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	B	304	PHE	CA-CB-CG	-5.43	108.36	113.80
1	A	215	THR	CA-C-O	5.37	126.45	120.82
1	B	208	ILE	CA-C-N	-5.34	114.12	119.94
1	B	208	ILE	C-N-CA	-5.34	114.12	119.94
1	A	166	THR	CA-C-O	-5.33	114.43	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	311	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	170	SER	O-C-N	5.22	128.93	123.03
1	A	30	VAL	CA-C-N	-5.21	112.89	120.29
1	A	30	VAL	C-N-CA	-5.21	112.89	120.29
1	A	294	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	B	269	LEU	CA-C-N	-5.18	113.51	120.82
1	B	269	LEU	C-N-CA	-5.18	113.51	120.82
1	A	46	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	46	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	284	LYS	CA-C-N	5.16	131.31	122.38
1	A	284	LYS	C-N-CA	5.16	131.31	122.38
1	B	21	ARG	O-C-N	-5.14	117.22	123.13
1	B	72	SER	O-C-N	5.13	128.00	122.15
1	B	259	TYR	CA-C-O	5.13	125.98	120.70
1	A	259	TYR	CA-CB-CG	-5.12	104.68	113.90
1	B	177	ILE	O-C-N	5.09	128.70	123.20
1	B	120	VAL	CA-C-O	-5.07	115.06	120.39
1	A	161	GLY	CA-C-N	-5.02	114.60	122.49
1	A	161	GLY	C-N-CA	-5.02	114.60	122.49
1	B	71	ARG	CA-C-N	-5.00	113.19	120.29
1	B	71	ARG	C-N-CA	-5.00	113.19	120.29

There are no chirality outliers.

There are no planarity outliers.

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	2395	0	2438	41	0
1	B	2387	0	2432	61	0
2	A	5	0	0	3	0
2	B	5	0	0	3	0
3	A	12	0	9	4	0
3	B	12	0	9	4	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	265	0	0	9	0
5	B	194	0	0	8	0
All	All	5279	0	4888	107	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 11.

All (107) 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:32:ARG:HD3	5:A:534:HOH:O	1.84	0.77
1:B:155:LYS:HG3	5:B:414:HOH:O	1.86	0.75
1:B:39:LYS:HA	1:B:42:GLU:OE1	1.87	0.74
1:B:23:GLY:O	1:B:26:GLU:HG2	1.89	0.72
1:A:90:ASN:HB3	1:A:92:ARG:NH1	2.08	0.69
1:A:7:THR:HG22	5:A:398:HOH:O	1.92	0.68
1:B:22:GLY:O	1:B:25:GLU:HG3	1.92	0.68
1:B:315:ILE:HD12	1:B:316:ASP:H	1.59	0.68
1:B:16:SER:HB3	1:B:25:GLU:HG2	1.77	0.67
1:A:224:LYS:HE3	5:A:329:HOH:O	1.93	0.67
1:B:220:LEU:HD11	1:B:227:ILE:HD11	1.79	0.65
1:B:7:THR:HG22	1:B:92:ARG:HG2	1.79	0.65
1:B:172:LYS:HE2	5:B:345:HOH:O	1.96	0.64
1:B:8:ILE:HD12	1:B:45:CYS:HB3	1.79	0.64
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.32	0.64
1:A:90:ASN:HB3	1:A:92:ARG:HH11	1.64	0.63
1:B:223:LYS:HD2	5:B:427:HOH:O	1.99	0.62
1:B:152:LEU:HD13	1:B:193:LEU:HD11	1.83	0.60
1:B:62:SER:HB3	5:B:388:HOH:O	1.99	0.60
1:B:169:ILE:HA	5:B:367:HOH:O	2.01	0.60
1:B:40:LEU:O	1:B:45:CYS:HB2	2.01	0.60
1:A:222:ARG:HG2	1:A:223:LYS:HE3	1.84	0.60
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.83	0.60
1:B:85:ALA:O	1:B:89:LYS:HE2	2.02	0.59
1:B:58:ILE:HD12	1:B:72:SER:HA	1.84	0.58
1:B:101:HIS:HB2	2:B:552:SO4:O3	2.02	0.58
1:A:11:ILE:HD11	1:A:87:VAL:HG21	1.85	0.58
1:B:44:GLU:OE2	1:B:44:GLU:O	2.21	0.58
1:A:150:LYS:O	1:A:153:LYS:HG3	2.04	0.56
1:B:7:THR:CG2	1:B:92:ARG:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:CD1	1:B:193:LEU:HD11	2.35	0.56
1:B:65:GLN:HE22	1:B:133:LEU:CD2	2.20	0.55
1:B:48:LYS:HG2	1:B:92:ARG:HE	1.72	0.55
3:B:601:B3U:HB	5:B:381:HOH:O	2.06	0.55
1:B:37:LEU:HB3	1:B:41:LYS:HZ1	1.72	0.54
1:A:7:THR:CG2	1:A:92:ARG:HG2	2.38	0.54
1:B:258:LEU:HD23	1:B:299:ILE:HD13	1.89	0.54
1:B:53:LEU:HD11	1:B:80:LEU:HA	1.89	0.52
1:B:150:LYS:O	1:B:153:LYS:HG2	2.10	0.52
1:A:314:PRO:C	1:A:315:ILE:HD12	2.36	0.51
1:A:222:ARG:HG2	1:A:223:LYS:CE	2.41	0.50
1:A:223:LYS:HD2	5:A:460:HOH:O	2.11	0.50
1:A:222:ARG:HG2	1:A:223:LYS:HG3	1.93	0.50
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.94	0.50
1:B:30:VAL:HG21	1:B:280:PRO:CG	2.42	0.49
1:A:101:HIS:HB2	2:A:551:SO4:O3	2.12	0.49
1:A:222:ARG:HG2	1:A:223:LYS:CD	2.42	0.49
1:B:30:VAL:CG1	1:B:293:VAL:HG21	2.43	0.49
1:B:58:ILE:HD12	1:B:72:SER:CA	2.43	0.48
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.49	0.48
2:A:551:SO4:O1	3:A:600:B3U:NT	2.46	0.48
1:B:26:GLU:HB2	1:B:280:PRO:HG2	1.95	0.48
1:B:263:GLU:OE2	1:B:266:LYS:NZ	2.47	0.48
1:A:10:ILE:HD12	1:A:95:LEU:HD13	1.96	0.48
1:A:7:THR:C	1:A:8:ILE:HD13	2.39	0.47
1:B:184:PRO:HD2	5:B:364:HOH:O	2.14	0.47
2:B:552:SO4:O2	3:B:601:B3U:NE2	2.48	0.47
1:B:43:GLN:HB2	1:B:44:GLU:H	1.46	0.47
1:B:21:ARG:NH2	1:B:245:GLY:O	2.48	0.47
2:A:551:SO4:O2	3:A:600:B3U:NE2	2.47	0.46
1:A:26:GLU:HA	1:A:26:GLU:OE1	2.15	0.46
1:B:315:ILE:HD12	1:B:316:ASP:N	2.28	0.46
1:A:32:ARG:HH11	1:A:32:ARG:HG3	1.79	0.46
1:B:12:GLY:HA3	1:B:52:ASP:OD1	2.16	0.46
1:A:8:ILE:HD12	1:A:304:PHE:CE1	2.51	0.45
1:A:312:HIS:HB2	1:A:317:TYR:CE2	2.52	0.45
1:B:279:ASN:CG	1:B:282:LEU:HG	2.41	0.45
1:A:317:TYR:C	1:A:319:ASN:H	2.23	0.45
1:B:68:LYS:NZ	5:B:408:HOH:O	2.49	0.45
2:B:552:SO4:O1	3:B:601:B3U:NT	2.49	0.45
1:B:183:ASP:OD2	3:B:601:B3U:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:NH2	1:A:268:GLY:O	2.50	0.45
1:B:46:ASP:OD1	1:B:48:LYS:NZ	2.44	0.45
1:A:59:PRO:HD2	5:A:511:HOH:O	2.17	0.45
1:B:26:GLU:O	1:B:30:VAL:HG23	2.16	0.44
1:B:223:LYS:HD2	1:B:223:LYS:H	1.82	0.44
1:A:150:LYS:NZ	5:A:448:HOH:O	2.50	0.44
1:B:6:ARG:HD3	1:B:6:ARG:HA	1.27	0.44
1:B:65:GLN:HB3	1:B:66:ILE:H	1.68	0.43
1:A:37:LEU:HD23	1:A:37:LEU:N	2.32	0.43
1:A:7:THR:HG23	1:A:46:ASP:CG	2.43	0.43
1:A:281:SER:HB3	1:B:192:THR:HG23	2.01	0.43
1:B:120:VAL:O	1:B:174:ILE:HA	2.19	0.43
1:B:155:LYS:HA	1:B:155:LYS:HD2	1.73	0.43
1:A:315:ILE:HD12	1:A:315:ILE:N	2.34	0.43
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.62	0.43
1:A:7:THR:HB	1:A:92:ARG:HG2	2.01	0.42
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.54	0.42
1:A:223:LYS:HD2	1:A:223:LYS:N	2.34	0.42
1:B:38:GLU:OE2	1:B:38:GLU:N	2.49	0.42
1:A:137:SER:HA	1:B:222:ARG:HH22	1.84	0.42
1:A:92:ARG:NH1	5:A:479:HOH:O	2.48	0.42
1:B:39:LYS:HA	1:B:42:GLU:CD	2.45	0.42
3:A:600:B3U:HB	5:A:581:HOH:O	2.20	0.41
1:B:223:LYS:HD2	1:B:223:LYS:N	2.34	0.41
1:B:152:LEU:HA	1:B:152:LEU:HD12	1.78	0.41
1:A:274:ASP:HB3	1:A:276:MET:SD	2.61	0.41
1:A:313:LYS:HB3	1:A:314:PRO:HD2	2.01	0.41
1:B:86:GLU:HA	1:B:89:LYS:HE3	2.02	0.41
1:B:148:LEU:O	1:B:169:ILE:HD13	2.21	0.41
1:A:180:ARG:HD3	1:A:200:MET:HG3	2.02	0.41
3:A:600:B3U:HD2	5:A:354:HOH:O	2.20	0.41
1:A:220:LEU:HD21	1:A:227:ILE:HD11	2.02	0.40
1:B:30:VAL:HG11	1:B:293:VAL:HG21	2.04	0.40
1:A:222:ARG:CG	1:A:223:LYS:HG3	2.50	0.40
1:B:30:VAL:HG12	1:B:293:VAL:HG21	2.03	0.40
1:B:61:ASP:OD2	1:B:72:SER:N	2.52	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	313/322 (97%)	301 (96%)	11 (4%)	1 (0%)	36	17
1	B	312/322 (97%)	298 (96%)	12 (4%)	2 (1%)	21	6
All	All	625/644 (97%)	599 (96%)	23 (4%)	3 (0%)	24	8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ARG
1	A	143	GLN
1	B	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	264/270 (98%)	250 (95%)	14 (5%)	20	2
1	B	263/270 (97%)	241 (92%)	22 (8%)	10	0
All	All	527/540 (98%)	491 (93%)	36 (7%)	14	1

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

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	THR
1	A	8	ILE

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Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	GLU
1	A	95	LEU
1	A	127	THR
1	A	152	LEU
1	A	153	LYS
1	A	222	ARG
1	A	223	LYS
1	A	225	ARG
1	A	284	LYS
1	A	306	LEU
1	B	5	SER
1	B	6	ARG
1	B	25	GLU
1	B	33	LYS
1	B	42	GLU
1	B	43	GLN
1	B	44	GLU
1	B	48	LYS
1	B	57	ASP
1	B	65	GLN
1	B	68	LYS
1	B	75	LYS
1	B	77	SER
1	B	95	LEU
1	B	101	HIS
1	B	152	LEU
1	B	155	LYS
1	B	163	SER
1	B	169	ILE
1	B	223	LYS
1	B	224	LYS
1	B	284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	90	ASN
1	A	319	ASN
1	B	65	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	SO4	B	552	4	4,4,4	0.76	0	6,6,6	0.98	0
2	SO4	A	551	4	4,4,4	0.96	0	6,6,6	0.92	0
3	B3U	A	600	-	10,12,12	1.54	3 (30%)	8,16,16	2.05	2 (25%)
3	B3U	B	601	-	10,12,12	1.60	2 (20%)	8,16,16	2.26	2 (25%)

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	B3U	A	600	-	-	2/8/8/8	0/1/1/1
3	B3U	B	601	-	-	2/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	B3U	CE1-NT	3.90	1.43	1.34
3	A	600	B3U	CE1-NT	3.63	1.42	1.34
3	A	600	B3U	OXT-C	-2.13	1.23	1.30
3	B	601	B3U	OXT-C	-2.09	1.24	1.30
3	A	600	B3U	CE1-ND1	-2.03	1.32	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	B3U	ND1-CE1-NE2	-5.01	107.81	112.36
3	A	600	B3U	ND1-CE1-NE2	-4.68	108.11	112.36
3	B	601	B3U	CA-CB-CG	2.96	118.14	113.23
3	A	600	B3U	CG-CD2-NE2	-2.27	105.69	109.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	B3U	CA-CB-CG-ND1
3	B	601	B3U	CA-CB-CG-ND1
3	A	600	B3U	CA-CB-CG-CD2
3	B	601	B3U	CA-CB-CG-CD2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	552	SO4	3	0
2	A	551	SO4	3	0
3	A	600	B3U	4	0
3	B	601	B3U	4	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	315/322 (97%)	-1.03	1 (0%) 90 92	13, 20, 38, 76	1 (0%)
1	B	314/322 (97%)	-0.78	1 (0%) 90 92	16, 26, 49, 75	1 (0%)
All	All	629/644 (97%)	-0.91	2 (0%) 90 92	13, 23, 47, 76	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	ILE	2.3
1	A	319	ASN	2.1

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
2	SO4	A	551	5/5	0.98	0.08	24,26,34,34	0
2	SO4	B	552	5/5	0.98	0.08	29,31,44,51	0
3	B3U	A	600	12/12	0.99	0.04	24,29,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	B3U	B	601	12/12	0.99	0.04	29,37,46,49	0
4	MN	A	5362	1/1	1.00	0.06	20,20,20,20	0
4	MN	A	5363	1/1	1.00	0.07	19,19,19,19	0
4	MN	B	6362	1/1	1.00	0.05	25,25,25,25	0
4	MN	B	6363	1/1	1.00	0.08	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.