



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 2AEB / pdb_00002aeb
Title : Crystal structure of human arginase I at 1.29 Å resolution and exploration of inhibition in immune response.
Authors : Di Costanzo, L.; Sabio, G.; Mora, A.; Rodriguez, P.C.; Ochoa, A.C.; Centeno, F.; Christianson, D.W.
Deposited on : 2005-07-21
Resolution : 1.29 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)
Xtrriage (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

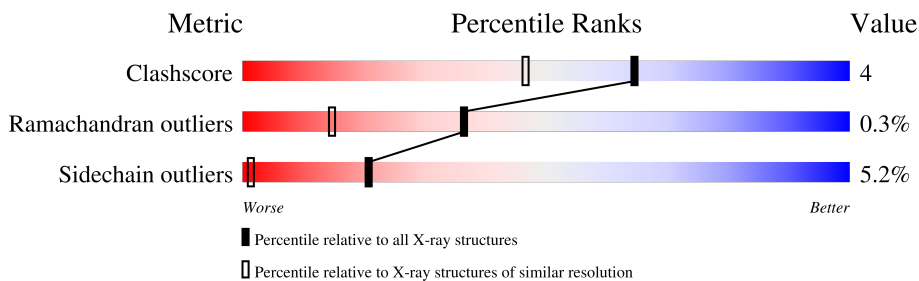
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.29 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	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)

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	322	76% 20% ...
1	B	322	75% 19% ...

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10011 atoms, of which 4851 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.

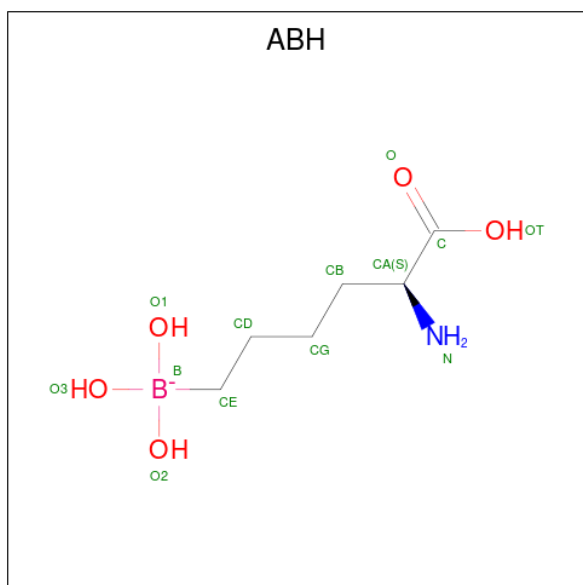
- Molecule 1 is a protein called Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	314	4827	1529	2431	408	453	6	0	2	0
1	B	309	4740	1495	2390	401	448	6	0	2	0

- 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 2(S)-AMINO-6-BORONOHEXANOIC ACID (CCD ID: ABH) (formula: C₆H₁₅BNO₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	B	C	H	N			O
3	A	1	28	1	6	15	1	5	0	0
3	B	1	28	1	6	15	1	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		
4	B	166	Total	O	0	0
			166	166		

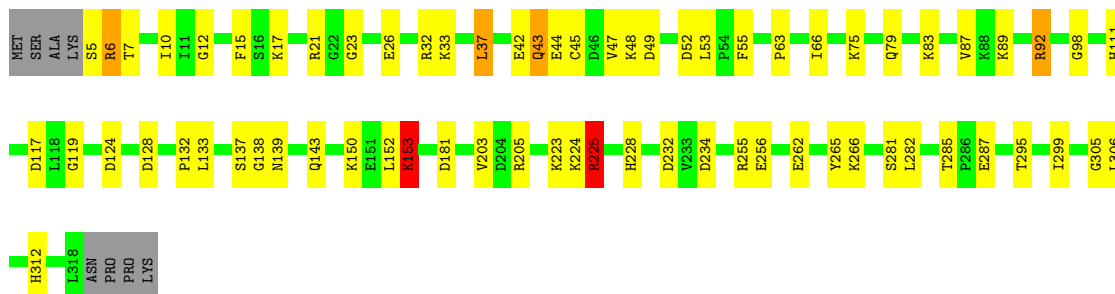
3 Residue-property plots

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.

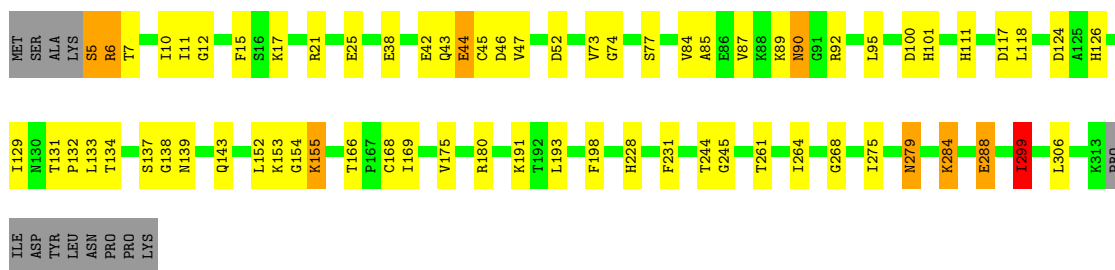
- Molecule 1: Arginase 1

Chain A: 



- Molecule 1: Arginase 1

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	91.42Å 91.42Å 69.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.29	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.29)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	(Not available) , 0.152	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10011	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	0.88	0/2455	1.81	64/3329 (1.9%)
1	B	0.84	1/2407 (0.0%)	1.73	48/3264 (1.5%)
All	All	0.86	1/4862 (0.0%)	1.78	112/6593 (1.7%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	HIS	CE1-NE2	-5.12	1.27	1.32

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ARG	CA-C-N	10.50	134.35	120.28
1	A	255	ARG	C-N-CA	10.50	134.35	120.28
1	A	6	ARG	CA-C-N	9.10	133.80	120.87
1	A	6	ARG	C-N-CA	9.10	133.80	120.87
1	A	132	PRO	CA-C-N	8.37	136.41	121.92
1	A	132	PRO	C-N-CA	8.37	136.41	121.92
1	A	228	HIS	ND1-CG-CD2	-8.23	97.87	106.10
1	A	312	HIS	CA-CB-CG	8.23	122.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	SER	CA-C-N	8.03	136.34	120.77
1	A	137	SER	C-N-CA	8.03	136.34	120.77
1	A	92	ARG	CD-NE-CZ	7.95	135.52	124.40
1	A	282	LEU	CA-C-N	-7.93	112.80	120.34
1	A	282	LEU	C-N-CA	-7.93	112.80	120.34
1	B	244	THR	CA-C-N	7.85	128.69	119.98
1	B	244	THR	C-N-CA	7.85	128.69	119.98
1	B	268	GLY	CA-C-N	7.84	134.53	122.29
1	B	268	GLY	C-N-CA	7.84	134.53	122.29
1	A	287	GLU	CA-C-O	-7.71	112.25	120.42
1	A	228	HIS	ND1-CE1-NE2	-7.47	100.93	108.40
1	B	129	ILE	CA-C-O	7.43	126.73	119.97
1	B	45	CYS	N-CA-C	7.41	121.92	109.76
1	B	166	THR	CA-C-O	-7.36	113.85	119.59
1	A	181	ASP	CA-CB-CG	7.36	119.96	112.60
1	B	47	VAL	CB-CA-C	-7.28	100.94	110.84
1	B	124	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	255	ARG	O-C-N	-7.12	114.68	122.09
1	A	124	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	279	ASN	O-C-N	7.03	127.72	121.32
1	A	205	ARG	CD-NE-CZ	7.02	134.23	124.40
1	B	138	GLY	CA-C-N	7.01	131.75	122.42
1	B	138	GLY	C-N-CA	7.01	131.75	122.42
1	B	6	ARG	CA-C-O	6.99	129.76	120.89
1	B	92	ARG	CD-NE-CZ	6.95	134.13	124.40
1	A	312	HIS	ND1-CG-CD2	-6.95	99.15	106.10
1	A	111	HIS	CB-CG-CD2	6.92	140.20	131.20
1	A	138	GLY	CA-C-N	6.76	131.41	122.42
1	A	138	GLY	C-N-CA	6.76	131.41	122.42
1	A	138	GLY	O-C-N	-6.65	114.73	122.31
1	A	6	ARG	CD-NE-CZ	6.64	133.70	124.40
1	A	111	HIS	ND1-CG-CD2	-6.61	99.49	106.10
1	B	6	ARG	O-C-N	-6.59	115.64	123.28
1	A	225	ARG	CD-NE-CZ	6.52	133.53	124.40
1	A	305	GLY	O-C-N	-6.47	115.04	122.42
1	A	111	HIS	ND1-CE1-NE2	-6.44	101.96	108.40
1	B	124	ASP	O-C-N	-6.43	116.74	123.56
1	B	73	VAL	O-C-N	-6.41	115.23	121.83
1	A	232	ASP	CA-CB-CG	6.37	118.97	112.60
1	B	228	HIS	ND1-CG-CD2	-6.35	99.75	106.10
1	B	138	GLY	O-C-N	-6.34	114.61	122.34
1	B	73	VAL	CA-C-O	6.33	127.56	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	CA-C-O	6.32	127.24	120.10
1	A	228	HIS	CG-ND1-CE1	6.18	119.80	109.30
1	A	53	LEU	O-C-N	6.14	127.42	121.28
1	A	132	PRO	O-C-N	-6.12	114.04	122.24
1	B	138	GLY	CA-C-O	6.09	127.50	119.58
1	B	288	GLU	CA-C-N	6.07	128.21	120.56
1	B	288	GLU	C-N-CA	6.07	128.21	120.56
1	A	21	ARG	O-C-N	-5.97	116.26	123.13
1	A	285	THR	O-C-N	-5.97	117.29	121.65
1	B	117	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	45	CYS	N-CA-C	5.93	119.38	109.95
1	A	63	PRO	CA-C-O	5.79	127.92	121.43
1	B	133	LEU	N-CA-C	5.79	120.35	113.28
1	A	265	TYR	O-C-N	5.79	128.11	122.09
1	B	100	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	124	ASP	O-C-N	-5.77	117.44	123.56
1	A	128	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	74	GLY	CA-C-O	5.72	126.64	120.75
1	B	245	GLY	O-C-N	-5.66	116.75	122.19
1	A	281	SER	O-C-N	-5.64	114.93	122.43
1	A	47	VAL	N-CA-C	5.62	115.95	107.80
1	B	139	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	B	21	ARG	O-C-N	-5.57	116.73	123.13
1	B	118	LEU	CA-C-O	5.55	127.44	121.55
1	B	299	ILE	CA-C-O	5.55	126.72	120.95
1	A	111	HIS	CG-ND1-CE1	5.54	118.71	109.30
1	A	55	PHE	CA-C-N	-5.50	112.67	122.07
1	A	55	PHE	C-N-CA	-5.50	112.67	122.07
1	B	11	ILE	O-C-N	-5.47	117.49	123.18
1	B	137	SER	CA-C-N	5.47	131.64	120.80
1	B	137	SER	C-N-CA	5.47	131.64	120.80
1	B	175	VAL	O-C-N	5.47	129.10	123.20
1	A	43	GLN	OE1-CD-NE2	5.46	128.06	122.60
1	B	43	GLN	O-C-N	-5.44	115.36	122.59
1	A	153[A]	LYS	N-CA-CB	5.36	117.90	109.69
1	A	153[B]	LYS	N-CA-CB	5.36	117.90	109.69
1	A	255	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	42	GLU	CA-C-N	5.34	131.75	121.54
1	A	42	GLU	C-N-CA	5.34	131.75	121.54
1	B	198	PHE	CA-C-O	-5.33	114.56	121.11
1	B	132	PRO	CA-C-N	5.31	131.94	122.06
1	B	132	PRO	C-N-CA	5.31	131.94	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	O-C-N	-5.30	116.73	121.87
1	A	133	LEU	O-C-N	-5.28	115.41	122.49
1	B	111	HIS	ND1-CG-CD2	-5.28	100.82	106.10
1	A	98	GLY	CA-C-N	5.23	131.12	121.70
1	A	98	GLY	C-N-CA	5.23	131.12	121.70
1	A	139	ASN	N-CA-CB	5.23	118.53	110.21
1	B	47	VAL	O-C-N	5.21	128.82	123.03
1	A	32	ARG	CA-C-O	-5.20	115.04	120.55
1	A	6	ARG	CG-CD-NE	5.17	123.36	112.00
1	B	180	ARG	CD-NE-CZ	5.14	131.60	124.40
1	B	25	GLU	CA-C-N	5.14	130.13	121.14
1	B	25	GLU	C-N-CA	5.14	130.13	121.14
1	A	89	LYS	O-C-N	-5.13	116.22	122.22
1	A	234	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	312	HIS	ND1-CE1-NE2	-5.11	103.29	108.40
1	A	256	GLU	N-CA-C	-5.10	105.72	111.28
1	A	312	HIS	CG-ND1-CE1	5.10	117.97	109.30
1	B	129	ILE	O-C-N	-5.09	116.54	122.09
1	B	10	ILE	CB-CA-C	-5.08	104.13	111.34
1	B	275	ILE	CA-C-O	-5.03	114.16	120.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	GLU	Peptide
1	B	44	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2396	2431	2450	16	0
1	B	2350	2390	2393	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	13	15	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	15	12	0	0
4	A	218	0	0	1	0
4	B	166	0	0	4	0
All	All	5160	4851	4867	38	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 (38) 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:38:GLU:O	1:B:42:GLU:HG3	1.84	0.78
1:A:66:ILE:HG22	4:A:2495:HOH:O	1.87	0.75
1:A:150:LYS:O	1:A:153[B]:LYS:HG3	1.88	0.73
1:A:79:GLN:O	1:A:83[A]:LYS:HG2	1.88	0.73
1:A:295:THR:O	1:A:299:ILE:HD13	1.91	0.70
1:A:117:ASP:O	1:A:225:ARG:HD3	1.96	0.65
1:B:153:LYS:HA	4:B:1528:HOH:O	2.00	0.62
1:B:84:VAL:O	1:B:87:VAL:HG22	1.99	0.61
1:A:262:GLU:O	1:A:266:LYS:HD3	2.00	0.61
1:A:48:LYS:HG3	1:A:92:ARG:NH2	2.17	0.60
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.40	0.56
1:B:7:THR:HG23	1:B:46:ASP:O	2.06	0.55
1:B:5:SER:O	1:B:6:ARG:HG2	2.08	0.54
1:A:119:GLY:N	1:A:225:ARG:HD2	2.24	0.53
1:B:154:GLY:C	1:B:155:LYS:HD3	2.34	0.53
1:B:155:LYS:HD3	1:B:155:LYS:N	2.24	0.52
1:B:90:ASN:N	1:B:90:ASN:HD22	2.08	0.52
1:A:48:LYS:HG3	1:A:92:ARG:CZ	2.41	0.51
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.45	0.51
1:B:231:PHE:CZ	1:B:299:ILE:HD12	2.46	0.51
1:B:264:ILE:HB	4:B:1427:HOH:O	2.12	0.50
1:B:85:ALA:O	1:B:89:LYS:HG3	2.12	0.49
1:A:37:LEU:HD11	1:A:49:ASP:OD2	2.12	0.49
1:B:168:CYS:HB2	4:B:1429:HOH:O	2.12	0.48
1:B:6:ARG:HB3	4:B:1455:HOH:O	2.14	0.47
1:B:279:ASN:HD22	1:B:279:ASN:C	2.25	0.45
1:B:5:SER:O	1:B:6:ARG:NH1	2.50	0.45
1:B:284:LYS:HE3	1:B:288:GLU:OE2	2.16	0.45
1:B:152:LEU:O	1:B:155:LYS:HB2	2.17	0.45
1:B:12:GLY:HA3	1:B:52:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:THR:OG1	1:B:134:THR:HG23	2.19	0.43
1:A:12:GLY:HA3	1:A:52:ASP:OD1	2.19	0.43
1:A:23:GLY:O	1:A:26:GLU:HG2	2.19	0.42
1:A:225:ARG:O	1:A:225:ARG:HG3	2.15	0.42
1:B:169:ILE:O	1:B:169:ILE:HG13	2.19	0.41
1:B:261:THR:HG21	1:B:299:ILE:HG23	2.02	0.41

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	314/322 (98%)	305 (97%)	8 (2%)	1 (0%)	36	15
1	B	309/322 (96%)	299 (97%)	9 (3%)	1 (0%)	36	15
All	All	623/644 (97%)	604 (97%)	17 (3%)	2 (0%)	36	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	A	143	GLN

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	265/270 (98%)	249 (94%)	16 (6%)	17	1
1	B	260/270 (96%)	248 (95%)	12 (5%)	24	2
All	All	525/540 (97%)	497 (95%)	28 (5%)	21	1

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	6	ARG
1	A	7	THR
1	A	10	ILE
1	A	33	LYS
1	A	37	LEU
1	A	43	GLN
1	A	75	LYS
1	A	87	VAL
1	A	152	LEU
1	A	153[A]	LYS
1	A	153[B]	LYS
1	A	223	LYS
1	A	224	LYS
1	A	225	ARG
1	A	306	LEU
1	B	5	SER
1	B	44	GLU
1	B	77	SER
1	B	90	ASN
1	B	95	LEU
1	B	101	HIS
1	B	155	LYS
1	B	191	LYS
1	B	193	LEU
1	B	284	LYS
1	B	299	ILE
1	B	306	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	69	ASN
1	A	143	GLN

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Mol	Chain	Res	Type
1	B	90	ASN
1	B	130	ASN
1	B	143	GLN
1	B	279	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	ABH	A	551	2	11,12,12	0.70	0	10,16,16	1.45	1 (10%)
3	ABH	B	552	2	11,12,12	1.19	0	10,16,16	1.14	1 (10%)

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	ABH	A	551	2	-	1/9/12/12	-
3	ABH	B	552	2	-	0/9/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	551	ABH	CG-CB-CA	2.82	122.33	113.22
3	B	552	ABH	O2-B-O1	-2.30	100.15	108.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	551	ABH	CG-CD-CE-B

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.