



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:43 PM UTC

PDB ID : 4AT1 / pdb_00004at1
Title : STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE T STATE OF ASPARTATE CARBAMOYLTRANSFERASE. CRYSTAL STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION
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Deposited on : 1990-04-26
Resolution : 2.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

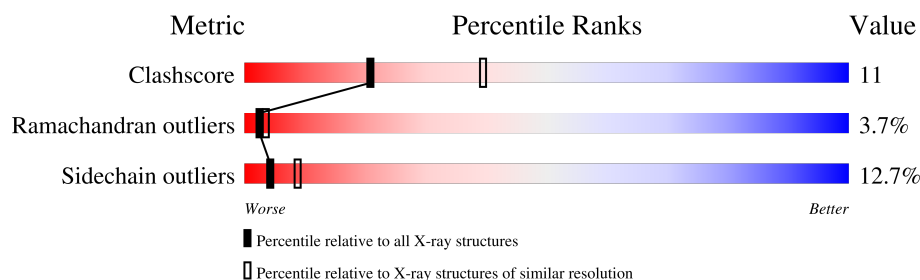
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	310	
1	C	310	
2	B	153	
2	D	153	

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
4	ATP	B	155	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7170 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 ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
C	60	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLU	GLN	conflict	UNP P0A786
C	196	GLU	GLN	conflict	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

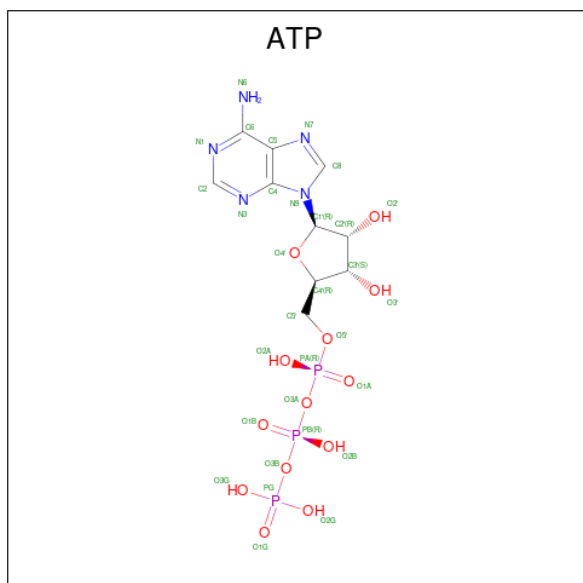
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



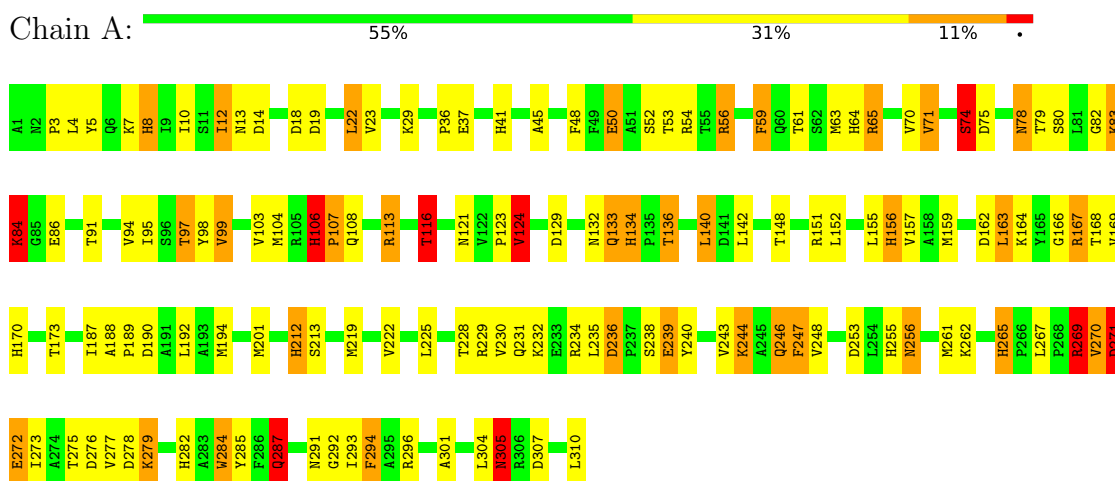
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

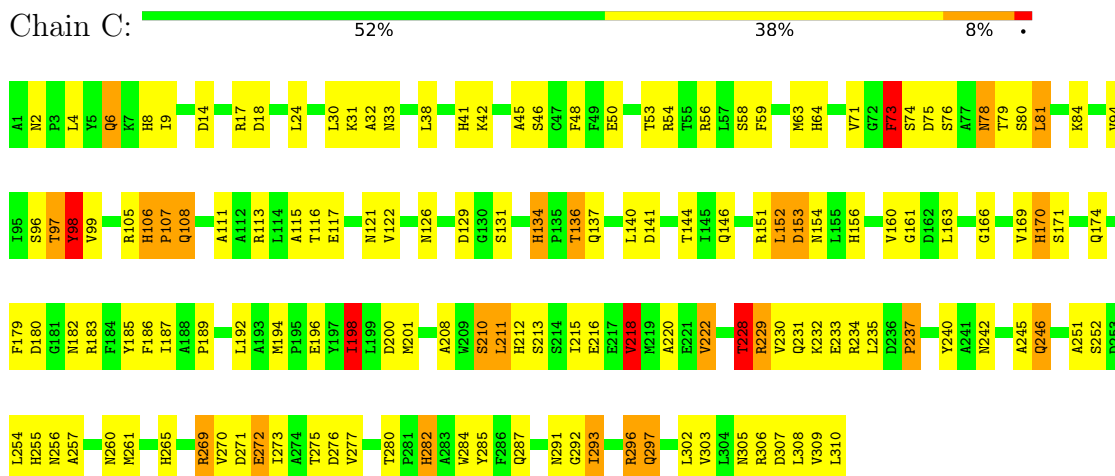
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

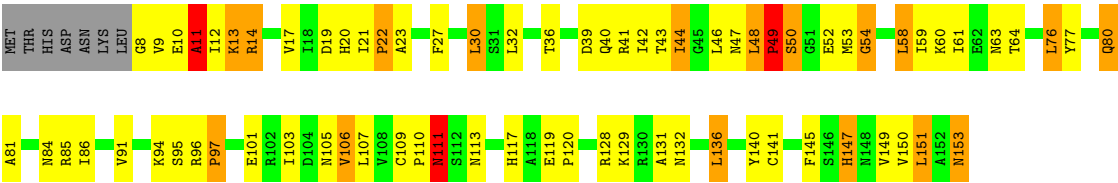


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN

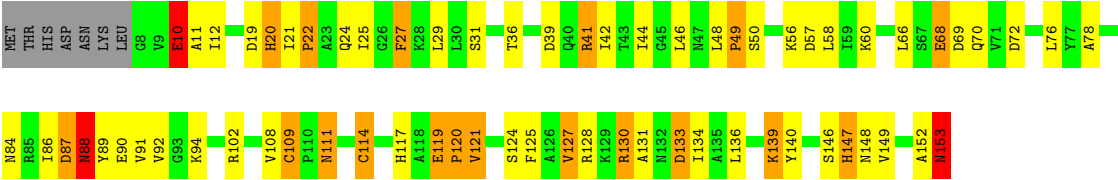


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.00Å 122.00Å 142.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: ZN, ATP

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	1.15	14/2461 (0.6%)	2.03	79/3339 (2.4%)
1	C	1.21	16/2461 (0.7%)	2.03	84/3339 (2.5%)
2	B	1.05	3/1155 (0.3%)	2.02	37/1561 (2.4%)
2	D	1.02	5/1155 (0.4%)	2.00	34/1561 (2.2%)
All	All	1.14	38/7232 (0.5%)	2.02	234/9800 (2.4%)

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	A	0	5
1	C	0	4
2	B	0	3
All	All	0	12

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	282	HIS	CD2-NE2	-7.61	1.29	1.37
1	A	124	VAL	CA-CB	7.53	1.64	1.54
1	A	156	HIS	CD2-NE2	-7.32	1.29	1.37
1	C	106	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.82	1.30	1.37
1	C	170	HIS	CD2-NE2	-6.80	1.30	1.37
2	B	20	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.70	1.30	1.37
2	D	147	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	170	HIS	CD2-NE2	-6.42	1.30	1.37
1	C	8	HIS	CD2-NE2	-6.42	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	HIS	CD2-NE2	-6.38	1.30	1.37
1	C	156	HIS	CD2-NE2	-6.32	1.30	1.37
2	D	117	HIS	CD2-NE2	-6.28	1.30	1.37
2	B	147	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	255	HIS	CD2-NE2	-6.24	1.30	1.37
1	C	134	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	265	HIS	CD2-NE2	-6.17	1.31	1.37
2	D	20	HIS	CD2-NE2	-6.14	1.31	1.37
1	C	41	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	282	HIS	CD2-NE2	-6.03	1.31	1.37
2	B	117	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	212	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	8	HIS	CD2-NE2	-5.89	1.31	1.37
1	C	64	HIS	CD2-NE2	-5.73	1.31	1.37
2	D	117	HIS	CG-ND1	-5.72	1.31	1.38
1	C	106	HIS	CG-ND1	-5.66	1.32	1.38
1	A	212	HIS	CD2-NE2	-5.65	1.31	1.37
1	C	8	HIS	CG-ND1	-5.57	1.32	1.38
2	D	111	ASN	CA-CB	-5.38	1.46	1.53
1	C	255	HIS	CD2-NE2	-5.38	1.31	1.37
1	C	75	ASP	N-CA	-5.36	1.43	1.46
1	A	156	HIS	CG-ND1	-5.35	1.32	1.38
1	A	106	HIS	CG-ND1	-5.25	1.32	1.38
1	C	265	HIS	CD2-NE2	-5.19	1.32	1.37
1	C	265	HIS	CG-ND1	-5.13	1.32	1.38
1	A	64	HIS	CD2-NE2	-5.12	1.32	1.37
1	C	134	HIS	CG-ND1	-5.00	1.32	1.38

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ASN	CA-CB-CG	13.44	126.04	112.60
2	B	11	ALA	N-CA-C	10.81	133.83	110.80
1	A	276	ASP	CA-CB-CG	10.77	123.36	112.60
1	A	18	ASP	CA-CB-CG	10.34	122.94	112.60
1	C	218	VAL	N-CA-CB	-10.02	100.40	112.33
2	D	153	ASN	CA-CB-CG	10.00	122.60	112.60
1	C	269	ARG	N-CA-C	-9.38	93.98	109.07
2	D	117	HIS	N-CA-C	9.13	121.32	111.36
1	A	71	VAL	O-C-N	-9.07	113.26	122.97
2	B	132	ASN	CA-CB-CG	8.92	121.52	112.60
1	C	242	ASN	OD1-CG-ND2	-8.73	113.87	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	THR	CA-CB-OG1	-8.66	96.60	109.60
1	C	75	ASP	N-CA-CB	-8.56	103.62	111.59
1	C	269	ARG	NE-CZ-NH2	8.53	126.87	119.20
2	D	10	GLU	N-CA-C	8.50	126.74	114.16
2	B	106	VAL	N-CA-CB	-8.33	98.08	112.08
2	B	105	ASN	N-CA-C	8.29	128.45	110.80
1	A	10	ILE	N-CA-C	8.21	118.87	111.81
2	D	133	ASP	CA-CB-CG	8.10	120.70	112.60
1	C	6	GLN	OE1-CD-NE2	-8.05	114.55	122.60
1	C	122	VAL	N-CA-C	-7.94	98.68	108.05
1	A	56	ARG	NE-CZ-NH1	-7.93	113.57	121.50
2	B	21	ILE	N-CA-C	-7.88	98.75	108.05
1	C	14	ASP	CA-CB-CG	7.86	120.46	112.60
2	D	114	CYS	N-CA-C	-7.84	98.68	110.28
1	C	136	THR	N-CA-CB	-7.84	98.56	110.16
1	C	8	HIS	CA-CB-CG	7.78	121.58	113.80
1	A	14	ASP	CA-CB-CG	7.77	120.37	112.60
1	C	287	GLN	OE1-CD-NE2	-7.76	114.84	122.60
2	D	19	ASP	CA-CB-CG	7.75	120.35	112.60
2	D	48	LEU	N-CA-C	-7.74	100.00	109.83
1	C	271	ASP	N-CA-C	7.71	122.36	112.34
1	A	271	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	54	ARG	NE-CZ-NH1	-7.65	113.85	121.50
1	A	86	GLU	N-CA-C	7.63	121.40	109.96
1	C	56	ARG	NE-CZ-NH1	-7.58	113.92	121.50
1	C	269	ARG	NE-CZ-NH1	-7.56	113.94	121.50
1	C	222	VAL	N-CA-CB	-7.49	100.22	110.56
1	A	136	THR	N-CA-C	7.44	120.45	111.82
1	A	75	ASP	CA-CB-CG	7.43	120.03	112.60
1	C	180	ASP	N-CA-C	7.42	121.51	110.52
1	A	162	ASP	CA-CB-CG	7.40	120.00	112.60
1	C	141	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	129	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	167	ARG	CA-CB-CG	7.25	128.59	114.10
2	B	52	GLU	O-C-N	7.23	131.91	123.02
1	C	273	ILE	N-CA-C	-7.22	97.21	107.75
1	C	117	GLU	CB-CG-CD	7.14	124.75	112.60
1	A	190	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	291	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	C	78	ASN	CA-CB-CG	6.99	119.59	112.60
1	A	64	HIS	CA-CB-CG	-6.96	106.84	113.80
1	C	121	ASN	N-CA-C	6.94	121.43	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	THR	CA-CB-OG1	-6.92	99.21	109.60
1	C	53	THR	CA-C-O	-6.89	113.59	120.82
2	B	153	ASN	OD1-CG-ND2	-6.86	115.74	122.60
1	C	154	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	A	256	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	74	SER	O-C-N	-6.67	116.26	123.26
1	C	97	THR	OG1-CB-CG2	-6.64	96.01	109.30
1	A	255	HIS	CA-CB-CG	6.64	120.44	113.80
1	A	294	PHE	CA-CB-CG	-6.63	107.17	113.80
1	A	157	VAL	N-CA-CB	-6.62	103.05	110.99
1	A	78	ASN	OD1-CG-ND2	-6.62	115.98	122.60
2	D	69	ASP	CA-CB-CG	6.61	119.21	112.60
1	C	94	VAL	CA-C-O	-6.61	113.64	120.71
1	C	222	VAL	CB-CA-C	6.60	120.26	111.21
1	C	32	ALA	N-CA-C	6.59	119.44	111.40
1	C	275	THR	CA-CB-OG1	-6.58	99.73	109.60
1	C	6	GLN	CG-CD-NE2	6.55	126.23	116.40
2	B	19	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	33	ASN	OD1-CG-ND2	-6.54	116.06	122.60
2	B	111	ASN	CA-CB-CG	6.53	119.13	112.60
1	A	229	ARG	CA-CB-CG	6.52	127.14	114.10
1	C	97	THR	N-CA-CB	-6.50	101.05	110.47
1	C	198	ILE	N-CA-C	-6.49	104.53	110.82
1	A	116	THR	CA-CB-CG2	6.42	121.42	110.50
1	C	137	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	A	56	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	A	99	VAL	N-CA-C	6.41	118.39	109.29
1	C	196	GLU	N-CA-C	6.39	119.06	111.33
2	B	20	HIS	CA-C-O	6.37	129.62	120.51
1	A	170	HIS	CA-CB-CG	6.36	120.16	113.80
1	C	71	VAL	O-C-N	-6.35	114.63	122.57
1	C	56	ARG	NE-CZ-NH2	6.35	124.92	119.20
2	D	121	VAL	N-CA-CB	-6.32	101.09	111.45
2	D	88	ASN	N-CA-C	-6.31	97.35	110.80
1	C	108	GLN	CA-CB-CG	-6.29	101.52	114.10
2	B	63	ASN	CA-CB-CG	6.27	118.87	112.60
1	C	220	ALA	N-CA-C	6.26	118.91	111.71
2	D	119	GLU	N-CA-C	6.25	119.77	110.39
2	D	119	GLU	CA-C-N	6.24	127.64	119.84
2	D	119	GLU	C-N-CA	6.24	127.64	119.84
1	A	287	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	C	75	ASP	CA-CB-CG	6.24	118.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ILE	CA-C-O	-6.22	115.14	119.19
2	D	84	ASN	N-CA-C	6.21	118.53	108.41
1	C	111	ALA	N-CA-C	6.21	117.71	111.07
1	A	50	GLU	N-CA-C	-6.16	100.16	109.95
1	A	113	ARG	CA-C-O	-6.15	113.97	120.55
1	C	200	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	305	ASN	CA-CB-CG	-6.14	106.46	112.60
1	C	81	LEU	N-CA-C	6.13	118.64	109.25
2	D	27	PHE	CA-CB-CG	-6.13	107.67	113.80
2	B	106	VAL	N-CA-C	6.13	118.90	112.83
1	C	306	ARG	N-CA-C	6.13	118.76	111.71
1	A	167	ARG	CB-CA-C	-6.11	100.60	110.74
2	B	39	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	307	ASP	CA-CB-CG	6.08	118.69	112.60
1	C	183	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	A	222	VAL	CA-C-O	6.01	127.82	120.84
1	C	117	GLU	CA-CB-CG	-6.01	102.08	114.10
2	D	78	ALA	CA-C-N	5.99	125.67	119.56
2	D	78	ALA	C-N-CA	5.99	125.67	119.56
1	A	239	GLU	O-C-N	5.99	128.56	122.09
2	B	132	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	A	86	GLU	CA-CB-CG	-5.97	102.15	114.10
2	D	148	ASN	CA-CB-CG	5.96	118.56	112.60
1	C	115	ALA	CA-C-N	5.95	128.53	120.38
1	C	115	ALA	C-N-CA	5.95	128.53	120.38
1	A	70	VAL	O-C-N	-5.94	117.08	123.14
2	D	109	CYS	CA-C-N	5.93	125.81	119.28
2	D	109	CYS	C-N-CA	5.93	125.81	119.28
1	A	136	THR	OG1-CB-CG2	5.93	121.17	109.30
1	C	2	ASN	CA-CB-CG	5.92	118.52	112.60
1	C	18	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	107	PRO	N-CA-C	5.91	121.30	114.03
1	C	126	ASN	CA-C-O	5.90	127.04	120.43
1	C	136	THR	CB-CA-C	5.89	120.86	110.85
2	B	40	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	C	107	PRO	N-CA-C	5.88	122.20	114.27
2	B	49	PRO	CA-C-N	5.83	132.68	121.54
2	B	49	PRO	C-N-CA	5.83	132.68	121.54
1	C	129	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	86	GLU	CA-C-O	5.79	127.46	120.81
1	A	244	LYS	N-CA-C	5.77	123.09	110.80
1	C	309	VAL	O-C-N	5.73	128.59	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	GLY	CA-C-N	5.72	128.96	120.95
2	B	54	GLY	C-N-CA	5.72	128.96	120.95
1	A	113	ARG	CG-CD-NE	5.72	124.57	112.00
2	B	47	ASN	CA-CB-CG	5.69	118.29	112.60
1	C	276	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	230	VAL	N-CA-C	-5.67	99.55	108.23
1	A	97	THR	OG1-CB-CG2	-5.65	98.00	109.30
2	B	13	LYS	N-CA-C	-5.63	100.01	109.07
2	D	153	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	A	113	ARG	CB-CG-CD	5.62	124.23	111.30
1	C	255	HIS	CA-CB-CG	5.60	119.40	113.80
1	C	42	LYS	CA-CB-CG	-5.60	102.90	114.10
2	B	23	ALA	N-CA-C	-5.58	98.92	110.80
1	C	182	ASN	OD1-CG-ND2	-5.58	117.02	122.60
2	D	87	ASP	N-CA-C	5.57	122.69	113.89
1	A	232	LYS	N-CA-C	5.57	122.66	110.80
1	A	278	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	126	ASN	CA-CB-CG	5.57	118.17	112.60
2	D	86	ILE	N-CA-C	-5.56	99.87	107.99
2	D	139	LYS	O-C-N	5.52	127.83	122.09
1	A	61	THR	N-CA-C	-5.51	105.17	111.07
1	C	218	VAL	CA-CB-CG2	-5.51	101.03	110.40
1	A	22	LEU	N-CA-C	-5.50	105.19	111.07
2	D	19	ASP	N-CA-CB	-5.49	101.37	111.37
1	C	210	SER	CA-CB-OG	5.49	122.08	111.10
1	A	82	GLY	N-CA-C	-5.49	100.18	113.18
1	A	134	HIS	CA-CB-CG	5.49	119.29	113.80
2	B	85	ARG	CB-CG-CD	-5.48	98.70	111.30
1	A	194	MET	CA-C-N	5.47	125.41	119.78
1	A	194	MET	C-N-CA	5.47	125.41	119.78
1	A	222	VAL	N-CA-C	5.47	116.86	108.71
2	D	92	VAL	CA-CB-CG2	-5.47	101.11	110.40
1	A	222	VAL	N-CA-CB	-5.46	102.12	110.86
1	A	277	VAL	N-CA-C	-5.45	105.06	111.00
1	C	6	GLN	N-CA-CB	-5.45	103.97	112.41
1	C	228	THR	N-CA-CB	-5.43	102.24	111.69
2	B	153	ASN	CA-CB-CG	5.42	118.02	112.60
2	D	92	VAL	CA-CB-CG1	5.42	119.61	110.40
1	A	56	ARG	N-CA-C	-5.40	105.03	111.03
1	C	218	VAL	N-CA-C	5.40	118.92	113.47
1	A	133	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	C	260	ASN	OD1-CG-ND2	-5.39	117.21	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ILE	CA-C-N	5.37	126.56	119.84
2	B	21	ILE	C-N-CA	5.37	126.56	119.84
1	A	56	ARG	CG-CD-NE	-5.37	100.18	112.00
1	C	78	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	222	VAL	CG1-CB-CG2	-5.37	98.99	110.80
2	B	64	THR	N-CA-C	-5.37	100.65	109.40
1	C	309	VAL	CA-C-O	5.34	125.54	120.31
1	C	218	VAL	CB-CA-C	5.34	116.39	110.62
2	B	52	GLU	CA-C-O	5.33	126.68	120.49
1	C	137	GLN	O-C-N	-5.33	115.71	122.27
1	A	247	PHE	CA-CB-CG	5.33	119.13	113.80
2	B	44	ILE	N-CA-C	-5.33	100.52	108.46
1	C	54	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	C	98	TYR	CB-CA-C	-5.33	99.82	110.42
1	A	164	LYS	N-CA-C	5.32	117.16	111.36
1	A	236	ASP	N-CA-C	-5.30	103.10	109.83
1	A	103	VAL	N-CA-C	-5.26	100.80	108.17
1	C	144	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	37	GLU	N-CA-C	-5.25	105.20	113.02
1	C	78	ASN	N-CA-C	5.24	121.95	110.80
1	C	297	GLN	OE1-CD-NE2	-5.23	117.37	122.60
2	B	97	PRO	N-CA-C	5.22	119.40	110.95
2	D	153	ASN	N-CA-C	5.20	125.56	111.00
2	D	121	VAL	CB-CA-C	5.20	119.71	110.71
2	D	152	ALA	CA-C-N	5.20	131.06	121.70
2	D	152	ALA	C-N-CA	5.20	131.06	121.70
1	A	269	ARG	N-CA-C	-5.19	102.09	110.14
1	C	208	ALA	O-C-N	-5.19	116.64	123.02
1	A	54	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	C	183	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	C	303	VAL	CA-CB-CG2	-5.16	101.63	110.40
1	A	104	MET	N-CA-C	5.14	117.73	108.48
1	A	228	THR	CA-CB-OG1	-5.13	101.91	109.60
2	B	80	GLN	CA-CB-CG	-5.11	103.87	114.10
1	A	113	ARG	N-CA-C	-5.11	105.17	111.40
1	C	284	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	A	304	LEU	N-CA-C	5.10	119.49	113.16
1	C	272	GLU	N-CA-C	5.09	119.21	112.89
1	A	279	LYS	N-CA-C	5.09	116.91	111.36
1	A	163	LEU	CD1-CG-CD2	-5.09	99.60	110.80
2	B	119	GLU	CA-C-N	5.09	126.20	119.84
2	B	119	GLU	C-N-CA	5.09	126.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	TYR	CA-CB-CG	5.08	123.05	113.90
1	C	134	HIS	CA-CB-CG	5.08	118.88	113.80
2	B	43	THR	CA-CB-OG1	-5.07	101.99	109.60
1	C	73	PHE	CA-C-O	-5.07	116.00	121.38
2	D	22	PRO	N-CA-C	5.07	122.92	112.47
2	D	72	ASP	N-CA-C	5.07	116.80	111.28
2	D	88	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	C	282	HIS	N-CA-C	-5.05	107.11	113.28
1	C	182	ASN	CB-CG-ND2	5.03	123.95	116.40
1	A	284	TRP	CE2-CD2-CE3	5.02	123.82	118.80
2	B	52	GLU	CA-C-N	5.01	131.12	121.54
2	B	52	GLU	C-N-CA	5.01	131.12	121.54
1	A	275	THR	CA-CB-CG2	5.01	119.02	110.50

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	HIS	Sidechain
1	A	156	HIS	Sidechain
1	A	294	PHE	Sidechain
1	A	5	TYR	Sidechain
1	A	59	PHE	Sidechain
2	B	140	TYR	Sidechain
2	B	48	LEU	Peptide
2	B	77	TYR	Sidechain
1	C	240	TYR	Sidechain
1	C	48	PHE	Sidechain
1	C	73	PHE	Sidechain
1	C	98	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	2415	0	2422	53	0
1	C	2415	0	2422	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1138	0	1154	36	0
2	D	1138	0	1154	34	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	31	0	10	10	0
4	D	31	0	12	8	0
All	All	7170	0	7174	159	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 (159) 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)
2:B:11:ALA:HA	4:B:155:ATP:N1	1.48	1.26
2:B:8:GLY:N	2:B:50:SER:HG	1.69	0.89
1:A:8:HIS:HD2	1:A:124:VAL:H	1.19	0.84
2:D:60:LYS:NZ	4:D:155:ATP:N3	2.25	0.84
2:D:11:ALA:HA	4:D:155:ATP:N1	1.94	0.82
1:A:136:THR:HB	1:A:296:ARG:NH2	1.96	0.81
1:A:136:THR:HB	1:A:296:ARG:HH21	1.47	0.77
1:A:94:VAL:O	1:A:97:THR:HG22	1.85	0.77
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.02	0.74
2:B:11:ALA:HA	4:B:155:ATP:C6	2.25	0.68
1:C:254:LEU:HD11	1:C:277:VAL:HG13	1.75	0.68
1:A:140:LEU:HD22	1:A:292:GLY:HA2	1.77	0.66
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.75	0.66
1:A:189:PRO:HG2	1:A:192:LEU:HB2	1.77	0.66
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.78	0.65
1:A:301:ALA:O	1:A:305:ASN:HB2	1.96	0.64
2:B:46:LEU:HD21	2:D:36:THR:HG22	1.80	0.64
1:A:4:LEU:HA	1:A:7:LYS:HD3	1.80	0.64
2:D:10:GLU:HA	4:D:155:ATP:O2'	1.97	0.64
1:A:48:PHE:O	1:A:74:SER:HA	1.98	0.64
2:B:11:ALA:HA	4:B:155:ATP:C2	2.31	0.63
1:C:151:ARG:HD2	1:C:153:ASP:O	1.98	0.63
2:D:124:SER:HB3	2:D:139:LYS:HB2	1.80	0.63
2:B:30:LEU:HD21	2:B:44:ILE:HD13	1.80	0.63
2:B:58:LEU:HD21	2:B:60:LYS:HE3	1.81	0.62
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.84	0.60
1:A:8:HIS:CD2	1:A:124:VAL:H	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:O	1:C:170:HIS:HE1	1.86	0.59
1:A:3:PRO:HG2	1:A:22:LEU:HD22	1.85	0.59
1:A:231:GLN:O	1:A:234:ARG:HG3	2.02	0.59
2:B:11:ALA:CA	4:B:155:ATP:N1	2.43	0.58
1:C:4:LEU:HD12	1:C:302:LEU:HD13	1.85	0.58
1:C:277:VAL:O	1:C:280:THR:HB	2.03	0.58
1:C:106:HIS:HD2	1:C:108:GLN:H	1.51	0.58
1:C:302:LEU:HD23	1:C:308:LEU:HD12	1.85	0.58
1:C:113:ARG:O	1:C:116:THR:HB	2.04	0.58
2:B:49:PRO:HA	2:B:54:GLY:O	2.03	0.57
1:C:254:LEU:HD13	1:C:280:THR:HG21	1.86	0.57
2:B:94:LYS:CE	4:B:155:ATP:O1B	2.52	0.57
2:D:11:ALA:HA	4:D:155:ATP:C2	2.39	0.57
2:B:91:VAL:HG21	4:B:155:ATP:O1A	2.04	0.57
2:B:111:ASN:ND2	2:B:141:CYS:SG	2.78	0.57
2:B:14:ARG:HA	2:B:86:ILE:O	2.05	0.56
2:B:81:ALA:O	2:B:97:PRO:HD2	2.06	0.56
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.88	0.56
2:D:127:VAL:HG22	2:D:134:ILE:HG21	1.87	0.55
1:C:280:THR:HG22	1:C:282:HIS:H	1.70	0.55
2:D:111:ASN:HB3	2:D:114:CYS:HB2	1.90	0.54
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.90	0.54
1:C:146:GLN:HB2	1:C:152:LEU:HD13	1.89	0.54
1:C:194:MET:HE3	1:C:198:ILE:HG21	1.89	0.54
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.43	0.54
1:A:132:ASN:OD1	1:A:133:GLN:HG2	2.08	0.53
2:B:136:LEU:HD22	2:B:147:HIS:HA	1.90	0.53
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.91	0.53
1:A:236:ASP:HB3	1:A:239:GLU:HB2	1.91	0.53
2:B:12:ILE:N	4:B:155:ATP:N1	2.57	0.52
1:A:59:PHE:HB3	1:A:63:MET:HE3	1.91	0.52
1:C:160:VAL:HG11	1:C:215:ILE:HD11	1.90	0.52
2:D:10:GLU:CA	4:D:155:ATP:O2'	2.57	0.51
1:A:8:HIS:CD2	1:A:123:PRO:HA	2.45	0.51
1:A:166:GLY:O	1:A:169:VAL:HG22	2.10	0.51
1:A:134:HIS:HB2	1:A:167:ARG:HD3	1.93	0.51
1:C:229:ARG:NH1	1:C:231:GLN:HA	2.26	0.51
1:A:48:PHE:HB3	1:A:50:GLU:O	2.11	0.51
1:A:113:ARG:O	1:A:116:THR:HB	2.11	0.51
1:C:232:LYS:CE	1:C:237:PRO:HA	2.41	0.50
2:D:94:LYS:NZ	4:D:155:ATP:O1A	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:LYS:HE3	4:B:155:ATP:O1B	2.11	0.50
1:C:38:LEU:HD21	1:C:308:LEU:HD21	1.93	0.50
1:C:136:THR:HG23	1:C:296:ARG:NH2	2.27	0.50
2:B:84:ASN:OD1	2:B:94:LYS:HG2	2.11	0.50
1:C:245:ALA:O	1:C:246:GLN:HB2	2.12	0.50
1:C:161:GLY:HA3	1:C:228:THR:HG22	1.94	0.50
2:D:146:SER:HB3	2:D:149:VAL:HG23	1.93	0.49
1:C:292:GLY:O	1:C:296:ARG:HB2	2.11	0.49
2:B:41:ARG:HE	2:D:49:PRO:HD3	1.78	0.49
1:C:31:LYS:NZ	1:C:291:ASN:HD21	2.11	0.49
1:C:174:GLN:HG2	1:C:201:MET:HE2	1.95	0.48
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.73	0.48
1:A:106:HIS:HD2	1:A:108:GLN:H	1.59	0.48
1:C:185:TYR:CD2	1:C:218:VAL:HG21	2.48	0.48
2:B:8:GLY:HA2	2:B:48:LEU:HD13	1.96	0.48
2:B:44:ILE:HD12	2:D:44:ILE:HG21	1.96	0.47
1:A:8:HIS:CD2	1:A:124:VAL:HG13	2.49	0.47
2:D:124:SER:HB3	2:D:139:LYS:HD2	1.95	0.47
1:A:78:ASN:HA	1:A:83:LYS:HD3	1.97	0.47
2:D:108:VAL:HB	2:D:153:ASN:HB2	1.97	0.47
2:B:80:GLN:HG2	2:B:96:ARG:NH1	2.29	0.47
1:A:219:MET:HB3	1:A:256:ASN:ND2	2.29	0.47
2:B:44:ILE:HB	2:D:44:ILE:HB	1.97	0.47
2:D:130:ARG:CZ	2:D:130:ARG:HA	2.44	0.47
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.98	0.46
1:A:219:MET:HG2	1:A:253:ASP:O	2.15	0.46
2:B:17:VAL:HG23	2:B:86:ILE:HD13	1.97	0.46
1:C:50:GLU:HA	1:C:76:SER:OG	2.15	0.46
1:A:108:GLN:HG2	2:B:113:ASN:OD1	2.16	0.46
1:A:270:VAL:HG13	1:A:271:ASP:N	2.31	0.46
2:D:12:ILE:N	4:D:155:ATP:N1	2.63	0.46
1:A:159:MET:HE3	1:A:173:THR:OG1	2.16	0.45
2:D:25:ILE:HG22	2:D:29:LEU:HG	1.98	0.45
2:B:76:LEU:HD23	2:B:103:ILE:HD11	1.98	0.45
1:C:254:LEU:CD2	1:C:261:MET:HE1	2.46	0.45
1:A:240:TYR:O	1:A:243:VAL:HG22	2.17	0.45
2:B:147:HIS:O	2:B:151:LEU:HB2	2.16	0.45
1:A:19:ASP:O	1:A:23:VAL:HG23	2.17	0.45
1:A:246:GLN:HB3	1:A:248:VAL:HG13	1.98	0.45
1:C:46:SER:HB2	1:C:63:MET:HE1	1.99	0.45
1:A:84:LYS:HD3	1:A:84:LYS:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLU:HB3	1:C:105:ARG:HG2	2.00	0.44
1:A:142:LEU:HD22	1:A:152:LEU:HD13	1.99	0.44
2:D:41:ARG:HH21	2:D:41:ARG:HB2	1.82	0.44
1:A:148:THR:HG21	1:A:262:LYS:HG3	1.99	0.44
1:C:152:LEU:HD23	1:C:179:PHE:CZ	2.52	0.44
1:A:270:VAL:HG13	1:A:271:ASP:H	1.82	0.44
2:D:128:ARG:CZ	2:D:130:ARG:HD2	2.47	0.44
2:D:127:VAL:HG23	2:D:136:LEU:CD2	2.48	0.44
2:B:107:LEU:HD22	2:B:150:VAL:HG12	2.00	0.43
2:D:66:LEU:HA	2:D:70:GLN:OE1	2.17	0.43
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.81	0.43
1:C:134:HIS:HD2	1:C:136:THR:HG22	1.84	0.43
1:A:29:LYS:HD3	1:A:310:LEU:HB2	1.99	0.43
1:A:91:THR:O	1:A:95:ILE:HG13	2.18	0.43
2:B:109:CYS:HA	2:B:110:PRO:HD2	1.89	0.43
2:B:12:ILE:HG12	4:B:155:ATP:C2	2.53	0.43
2:D:42:ILE:HG22	2:D:44:ILE:HG13	2.01	0.42
1:A:48:PHE:CE1	1:A:56:ARG:HG3	2.54	0.42
2:D:60:LYS:CE	4:D:155:ATP:C2	3.02	0.42
1:A:269:ARG:HG3	1:A:273:ILE:HB	2.00	0.42
1:A:36:PRO:HA	1:A:65:ARG:O	2.19	0.42
1:A:106:HIS:CD2	1:A:108:GLN:H	2.36	0.42
2:B:30:LEU:HD13	2:B:59:ILE:HD13	2.02	0.42
1:C:73:PHE:CE2	1:C:81:LEU:HD12	2.55	0.42
1:C:234:ARG:O	1:C:235:LEU:HD23	2.19	0.42
1:A:8:HIS:HD2	1:A:124:VAL:N	2.01	0.41
1:A:52:SER:O	1:A:56:ARG:HB2	2.20	0.41
1:C:257:ALA:CB	1:C:261:MET:HE3	2.50	0.41
2:D:119:GLU:HA	2:D:120:PRO:HD2	1.74	0.41
1:A:265:HIS:HE2	1:A:272:GLU:HG3	1.85	0.41
1:C:189:PRO:CG	1:C:192:LEU:HD12	2.50	0.41
1:A:113:ARG:HH21	1:A:113:ARG:HG2	1.85	0.41
1:A:45:ALA:HA	1:A:71:VAL:O	2.21	0.41
1:C:186:PHE:HB2	1:C:211:LEU:HD12	2.02	0.41
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.85	0.41
2:D:139:LYS:HD3	2:D:140:TYR:CZ	2.56	0.41
1:C:50:GLU:HA	1:C:76:SER:HG	1.84	0.41
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.85	0.41
2:D:20:HIS:HA	2:D:56:LYS:HD2	2.02	0.41
2:D:21:ILE:HB	2:D:57:ASP:HB2	2.02	0.41
1:C:293:ILE:O	1:C:297:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:PRO:HG2	2:B:145:PHE:CD2	2.57	0.40
2:B:94:LYS:HE2	4:B:155:ATP:O1B	2.21	0.40
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.78	0.40
2:D:127:VAL:HG22	2:D:134:ILE:CG2	2.49	0.40
1:A:151:ARG:O	1:A:155:LEU:HD11	2.21	0.40
1:C:50:GLU:HB2	1:C:107:PRO:HD3	2.04	0.40
1:C:251:ALA:HA	1:C:254:LEU:HD12	2.02	0.40
2:B:27:PHE:CE1	2:D:27:PHE:CE1	3.09	0.40
2:B:42:ILE:HG12	2:B:61:ILE:HG23	2.03	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	308/310 (99%)	283 (92%)	17 (6%)	8 (3%)	4	7
1	C	308/310 (99%)	283 (92%)	18 (6%)	7 (2%)	5	9
2	B	144/153 (94%)	121 (84%)	15 (10%)	8 (6%)	1	1
2	D	144/153 (94%)	124 (86%)	10 (7%)	10 (7%)	1	1
All	All	904/926 (98%)	811 (90%)	60 (7%)	33 (4%)	2	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
2	B	22	PRO
2	B	50	SER
2	B	53	MET
1	C	78	ASN
1	C	256	ASN

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Mol	Chain	Res	Type
2	D	68	GLU
2	D	131	ALA
1	A	83	LYS
1	A	270	VAL
2	B	131	ALA
1	C	80	SER
2	D	24	GLN
2	D	49	PRO
2	D	50	SER
2	D	89	TYR
1	A	244	LYS
1	A	246	GLN
2	B	11	ALA
1	C	246	GLN
1	C	270	VAL
2	D	120	PRO
1	A	84	LYS
1	A	271	ASP
2	B	14	ARG
2	D	88	ASN
2	D	91	VAL
2	B	120	PRO
1	C	131	SER
2	B	129	LYS
1	A	267	LEU
1	C	166	GLY
2	D	22	PRO

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	261/261 (100%)	234 (90%)	27 (10%)	7	15
1	C	261/261 (100%)	224 (86%)	37 (14%)	3	6
2	B	129/136 (95%)	110 (85%)	19 (15%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	129/136 (95%)	113 (88%)	16 (12%)	4	9
All	All	780/794 (98%)	681 (87%)	99 (13%)	4	9

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ASN
1	A	53	THR
1	A	65	ARG
1	A	74	SER
1	A	79	THR
1	A	84	LYS
1	A	116	THR
1	A	121	ASN
1	A	124	VAL
1	A	140	LEU
1	A	168	THR
1	A	201	MET
1	A	213	SER
1	A	225	LEU
1	A	230	VAL
1	A	235	LEU
1	A	238	SER
1	A	247	PHE
1	A	261	MET
1	A	269	ARG
1	A	272	GLU
1	A	279	LYS
1	A	285	TYR
1	A	287	GLN
1	A	293	ILE
1	A	305	ASN
2	B	9	VAL
2	B	10	GLU
2	B	13	LYS
2	B	22	PRO
2	B	30	LEU
2	B	32	LEU
2	B	36	THR
2	B	49	PRO
2	B	58	LEU

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Mol	Chain	Res	Type
2	B	76	LEU
2	B	95	SER
2	B	101	GLU
2	B	106	VAL
2	B	111	ASN
2	B	128	ARG
2	B	136	LEU
2	B	149	VAL
2	B	151	LEU
2	B	153	ASN
1	C	6	GLN
1	C	9	ILE
1	C	17	ARG
1	C	24	LEU
1	C	58	SER
1	C	59	PHE
1	C	74	SER
1	C	79	THR
1	C	84	LYS
1	C	96	SER
1	C	97	THR
1	C	98	TYR
1	C	140	LEU
1	C	152	LEU
1	C	153	ASP
1	C	169	VAL
1	C	171	SER
1	C	198	ILE
1	C	210	SER
1	C	211	LEU
1	C	213	SER
1	C	216	GLU
1	C	218	VAL
1	C	222	VAL
1	C	228	THR
1	C	229	ARG
1	C	233	GLU
1	C	237	PRO
1	C	252	SER
1	C	269	ARG
1	C	272	GLU
1	C	285	TYR

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Mol	Chain	Res	Type
1	C	293	ILE
1	C	296	ARG
1	C	305	ASN
1	C	307	ASP
1	C	310	LEU
2	D	10	GLU
2	D	31	SER
2	D	39	ASP
2	D	41	ARG
2	D	46	LEU
2	D	58	LEU
2	D	68	GLU
2	D	76	LEU
2	D	87	ASP
2	D	88	ASN
2	D	90	GLU
2	D	102	ARG
2	D	121	VAL
2	D	127	VAL
2	D	130	ARG
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	33	ASN
1	A	106	HIS
1	A	134	HIS
1	A	174	GLN
1	A	242	ASN
1	A	255	HIS
1	A	287	GLN
2	B	47	ASN
1	C	2	ASN
1	C	8	HIS
1	C	134	HIS
1	C	137	GLN
1	C	154	ASN
1	C	170	HIS
1	C	174	GLN
1	C	231	GLN

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Mol	Chain	Res	Type
1	C	256	ASN
1	C	282	HIS
1	C	291	ASN
2	D	20	HIS
2	D	40	GLN
2	D	63	ASN
2	D	147	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	ATP	D	155	-	32,33,33	3.50	14 (43%)	48,52,52	2.61	17 (35%)
4	ATP	B	155	-	32,33,33	3.31	13 (40%)	48,52,52	3.08	14 (29%)

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	ATP	D	155	-	-	5/22/38/38	0/3/3/3
4	ATP	B	155	-	-	6/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	155	ATP	PB-O3A	9.60	1.69	1.59
4	B	155	ATP	PB-O3A	9.40	1.69	1.59
4	D	155	ATP	PB-O3B	8.54	1.68	1.59
4	B	155	ATP	PB-O3B	8.08	1.68	1.59
4	B	155	ATP	C3'-C4'	-5.58	1.38	1.53
4	D	155	ATP	C3'-C4'	-5.57	1.38	1.53
4	D	155	ATP	C4-N3	-5.33	1.24	1.34
4	D	155	ATP	O4'-C4'	4.67	1.55	1.45
4	B	155	ATP	O4'-C4'	4.64	1.55	1.45
4	B	155	ATP	PG-O3G	-4.61	1.37	1.54
4	D	155	ATP	PG-O3G	-4.58	1.37	1.54
4	D	155	ATP	C2-N3	-4.51	1.25	1.33
4	B	155	ATP	PA-O3A	-4.48	1.54	1.59
4	D	155	ATP	PA-O3A	-4.39	1.54	1.59
4	B	155	ATP	O2'-C2'	4.39	1.53	1.43
4	D	155	ATP	O3'-C3'	4.32	1.53	1.43
4	B	155	ATP	O3'-C3'	4.27	1.53	1.43
4	D	155	ATP	O5'-C5'	3.36	1.57	1.44
4	B	155	ATP	O5'-C5'	3.35	1.57	1.44
4	B	155	ATP	PB-O1B	2.93	1.61	1.50
4	D	155	ATP	PB-O1B	2.86	1.60	1.50
4	B	155	ATP	PA-O5'	-2.81	1.48	1.59
4	D	155	ATP	PA-O5'	-2.79	1.48	1.59
4	D	155	ATP	PG-O2G	-2.64	1.45	1.54
4	B	155	ATP	PG-O2G	-2.61	1.45	1.54
4	B	155	ATP	O4'-C1'	2.33	1.47	1.42
4	D	155	ATP	O4'-C1'	2.32	1.47	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	155	ATP	O2'-C2'-C3'	-13.81	67.54	111.82
4	D	155	ATP	C2'-C3'-C4'	7.32	116.75	102.61
4	B	155	ATP	C2'-C3'-C4'	7.31	116.73	102.61
4	B	155	ATP	O3G-PG-O3B	6.67	127.02	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	155	ATP	O3G-PG-O3B	6.67	127.01	104.64
4	D	155	ATP	N3-C2-N1	-6.32	119.02	128.58
4	B	155	ATP	O2'-C2'-C1'	-5.77	90.23	110.10
4	D	155	ATP	C3'-C2'-C1'	-5.14	91.74	101.46
4	B	155	ATP	C3'-C2'-C1'	-5.13	91.76	101.46
4	D	155	ATP	C2-N3-C4	5.11	124.32	111.83
4	D	155	ATP	O4'-C1'-N9	-4.32	99.80	108.09
4	B	155	ATP	O4'-C1'-N9	-4.31	99.82	108.09
4	D	155	ATP	O2'-C2'-C1'	-3.71	97.32	110.10
4	D	155	ATP	N3-C4-N9	3.44	133.03	127.17
4	D	155	ATP	C5-C4-N3	-3.14	122.39	126.72
4	D	155	ATP	O4'-C4'-C3'	-3.12	98.97	105.15
4	B	155	ATP	O4'-C4'-C3'	-3.11	98.98	105.15
4	B	155	ATP	C2-N1-C6	2.71	123.17	118.73
4	B	155	ATP	O3A-PB-O1B	-2.66	102.69	110.70
4	D	155	ATP	O3A-PB-O1B	-2.65	102.74	110.70
4	D	155	ATP	C2-N1-C6	2.54	122.90	118.73
4	D	155	ATP	O3B-PG-O1G	-2.34	98.74	111.04
4	B	155	ATP	O3B-PG-O1G	-2.30	98.93	111.04
4	D	155	ATP	O2A-PA-O3A	-2.30	101.05	107.27
4	B	155	ATP	O2A-PA-O3A	-2.30	101.06	107.27
4	B	155	ATP	O2B-PB-O3B	2.23	113.31	107.27
4	D	155	ATP	O2B-PB-O3B	2.21	113.24	107.27
4	D	155	ATP	O3'-C3'-C4'	-2.05	105.20	111.08
4	B	155	ATP	O3'-C3'-C4'	-2.04	105.21	111.08
4	B	155	ATP	C2'-C1'-N9	-2.01	108.30	113.30
4	D	155	ATP	C2'-C1'-N9	-2.00	108.33	113.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	155	ATP	C5'-O5'-PA-O3A
4	D	155	ATP	C5'-O5'-PA-O3A
4	B	155	ATP	C3'-C4'-C5'-O5'
4	D	155	ATP	C3'-C4'-C5'-O5'
4	B	155	ATP	O4'-C4'-C5'-O5'
4	D	155	ATP	O4'-C4'-C5'-O5'
4	B	155	ATP	C5'-O5'-PA-O1A
4	B	155	ATP	PG-O3B-PB-O2B
4	B	155	ATP	PA-O3A-PB-O2B
4	D	155	ATP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	D	155	ATP	PA-O3A-PB-O2B

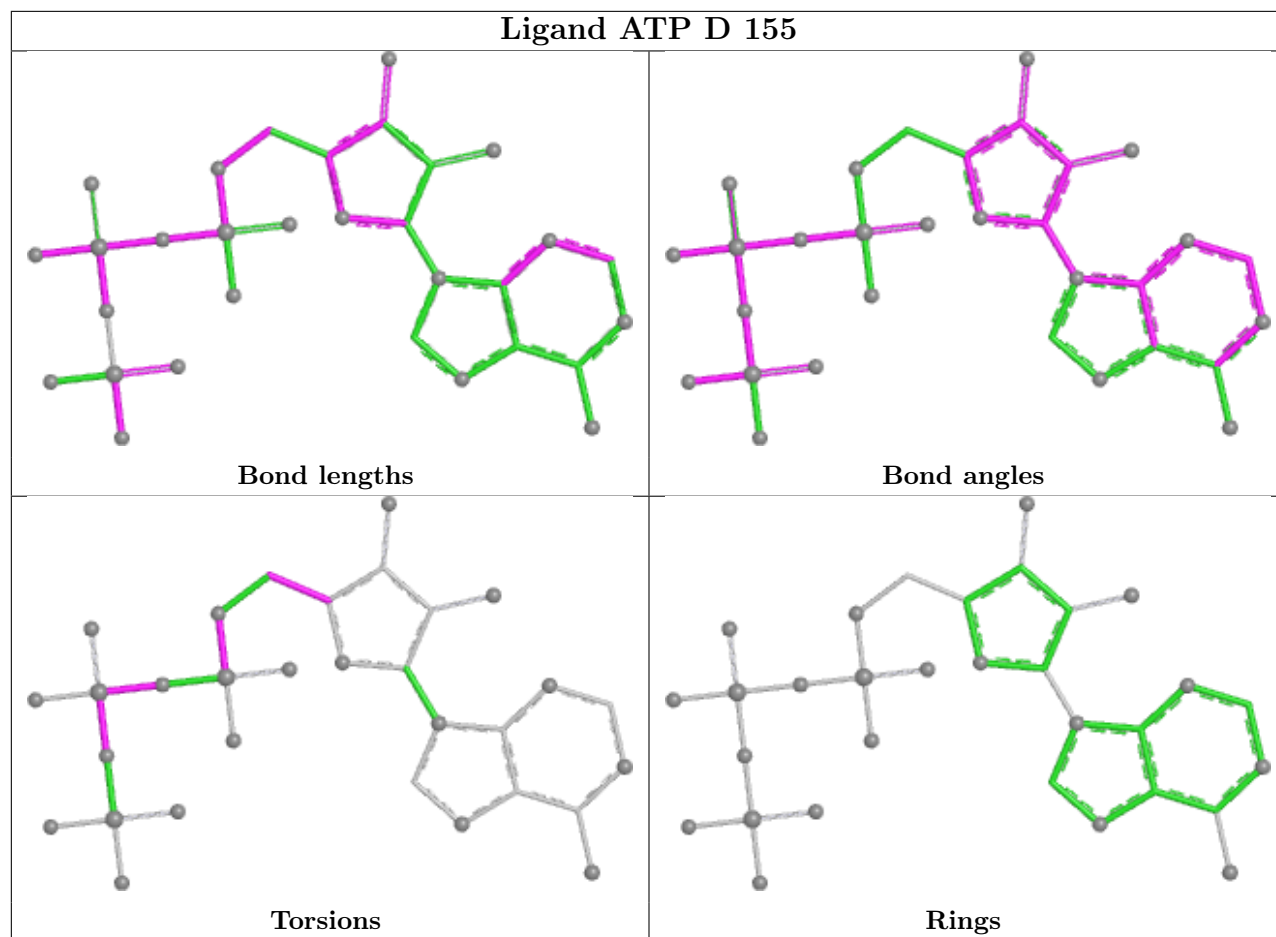
There are no ring outliers.

2 monomers are involved in 18 short contacts:

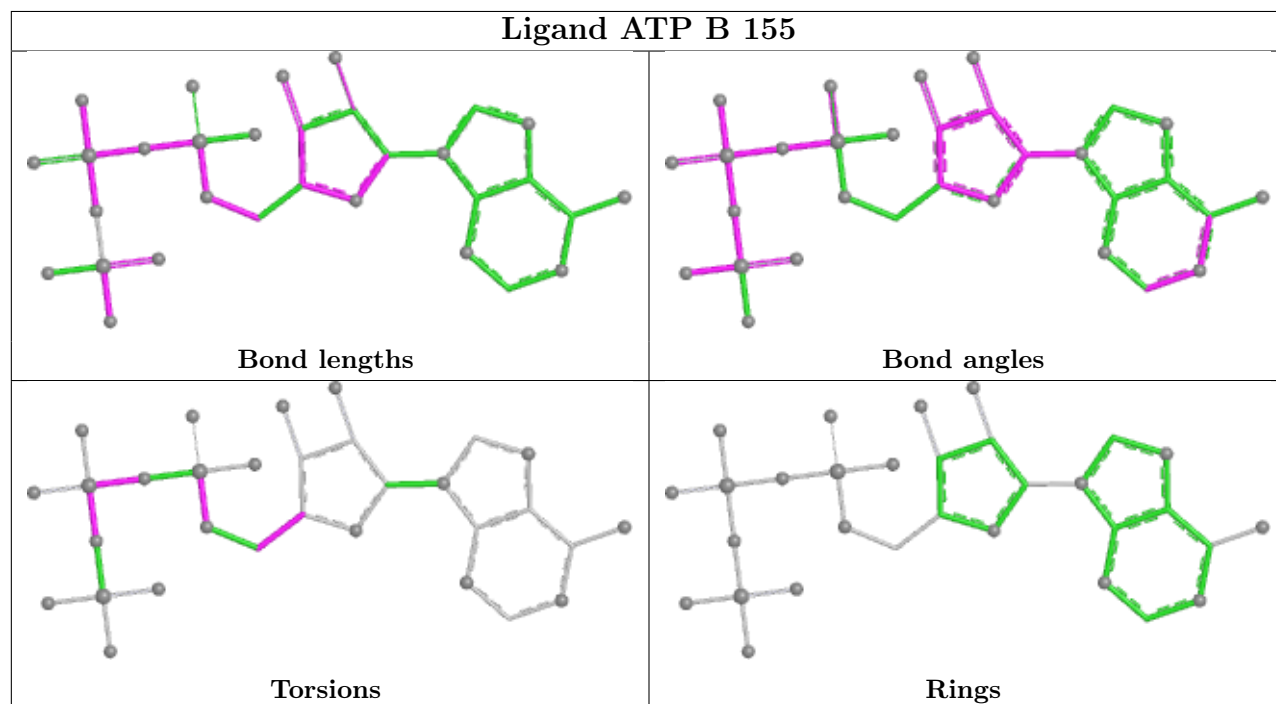
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	155	ATP	8	0
4	B	155	ATP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP D 155



Ligand ATP B 155



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.