



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:41 AM UTC

PDB ID : 9DC6 / pdb_00009dc6
Title : Structure of J-PKAc chimera in complex with Aplithianine e1
Authors : Martinez Fiesco, J.A.; Zhang, P.
Deposited on : 2024-08-25
Resolution : 2.70 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

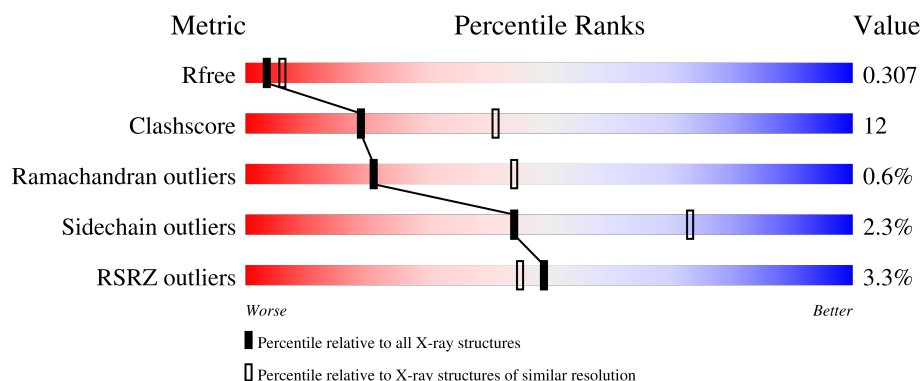
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	405	 77% 22% .
1	B	405	 68% 30% .
2	I	20	 70% 30%
2	J	20	 80% 10% 5% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7058 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	P	S	0	0	0
			3356	2162	571	613	2	8			
1	B	405	Total	C	N	O	P	S	0	0	0
			3356	2162	571	613	2	8			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P17612
A	2	LYS	-	expression tag	UNP P17612
A	3	ASP	-	expression tag	UNP P17612
A	4	TYR	-	expression tag	UNP P17612
A	5	TYR	-	expression tag	UNP P17612
A	6	GLN	-	expression tag	UNP P17612
A	7	THR	-	expression tag	UNP P17612
A	8	LEU	-	expression tag	UNP P17612
A	9	GLY	-	expression tag	UNP P17612
A	10	LEU	-	expression tag	UNP P17612
A	11	ALA	-	expression tag	UNP P17612
A	12	ARG	-	expression tag	UNP P17612
A	13	GLY	-	expression tag	UNP P17612
A	14	ALA	-	expression tag	UNP P17612
A	15	SER	-	expression tag	UNP P17612
A	16	ASP	-	expression tag	UNP P17612
A	17	GLU	-	expression tag	UNP P17612
A	18	GLU	-	expression tag	UNP P17612
A	19	ILE	-	expression tag	UNP P17612
A	20	LYS	-	expression tag	UNP P17612
A	21	ARG	-	expression tag	UNP P17612
A	22	ALA	-	expression tag	UNP P17612
A	23	TYR	-	expression tag	UNP P17612
A	24	ARG	-	expression tag	UNP P17612
A	25	ARG	-	expression tag	UNP P17612

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLN	-	expression tag	UNP P17612
A	27	ALA	-	expression tag	UNP P17612
A	28	LEU	-	expression tag	UNP P17612
A	29	ARG	-	expression tag	UNP P17612
A	30	TYR	-	expression tag	UNP P17612
A	31	HIS	-	expression tag	UNP P17612
A	32	PRO	-	expression tag	UNP P17612
A	33	ASP	-	expression tag	UNP P17612
A	34	LYS	-	expression tag	UNP P17612
A	35	ASN	-	expression tag	UNP P17612
A	36	LYS	-	expression tag	UNP P17612
A	37	GLU	-	expression tag	UNP P17612
A	38	PRO	-	expression tag	UNP P17612
A	39	GLY	-	expression tag	UNP P17612
A	40	ALA	-	expression tag	UNP P17612
A	41	GLU	-	expression tag	UNP P17612
A	42	GLU	-	expression tag	UNP P17612
A	43	LYS	-	expression tag	UNP P17612
A	44	PHE	-	expression tag	UNP P17612
A	45	LYS	-	expression tag	UNP P17612
A	46	GLU	-	expression tag	UNP P17612
A	47	ILE	-	expression tag	UNP P17612
A	48	ALA	-	expression tag	UNP P17612
A	49	GLU	-	expression tag	UNP P17612
A	50	ALA	-	expression tag	UNP P17612
A	51	TYR	-	expression tag	UNP P17612
A	52	ASP	-	expression tag	UNP P17612
A	53	VAL	-	expression tag	UNP P17612
A	54	LEU	-	expression tag	UNP P17612
A	55	SER	-	expression tag	UNP P17612
A	56	ASP	-	expression tag	UNP P17612
A	57	PRO	-	expression tag	UNP P17612
A	58	ARG	-	expression tag	UNP P17612
A	59	LYS	-	expression tag	UNP P17612
A	60	ARG	-	expression tag	UNP P17612
A	61	GLU	-	expression tag	UNP P17612
A	62	ILE	-	expression tag	UNP P17612
A	63	PHE	-	expression tag	UNP P17612
A	64	ASP	-	expression tag	UNP P17612
A	65	ARG	-	expression tag	UNP P17612
A	66	TYR	-	expression tag	UNP P17612
A	67	GLY	-	expression tag	UNP P17612

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLU	-	expression tag	UNP P17612
A	69	GLU	-	expression tag	UNP P17612
B	1	GLY	-	expression tag	UNP P17612
B	2	LYS	-	expression tag	UNP P17612
B	3	ASP	-	expression tag	UNP P17612
B	4	TYR	-	expression tag	UNP P17612
B	5	TYR	-	expression tag	UNP P17612
B	6	GLN	-	expression tag	UNP P17612
B	7	THR	-	expression tag	UNP P17612
B	8	LEU	-	expression tag	UNP P17612
B	9	GLY	-	expression tag	UNP P17612
B	10	LEU	-	expression tag	UNP P17612
B	11	ALA	-	expression tag	UNP P17612
B	12	ARG	-	expression tag	UNP P17612
B	13	GLY	-	expression tag	UNP P17612
B	14	ALA	-	expression tag	UNP P17612
B	15	SER	-	expression tag	UNP P17612
B	16	ASP	-	expression tag	UNP P17612
B	17	GLU	-	expression tag	UNP P17612
B	18	GLU	-	expression tag	UNP P17612
B	19	ILE	-	expression tag	UNP P17612
B	20	LYS	-	expression tag	UNP P17612
B	21	ARG	-	expression tag	UNP P17612
B	22	ALA	-	expression tag	UNP P17612
B	23	TYR	-	expression tag	UNP P17612
B	24	ARG	-	expression tag	UNP P17612
B	25	ARG	-	expression tag	UNP P17612
B	26	GLN	-	expression tag	UNP P17612
B	27	ALA	-	expression tag	UNP P17612
B	28	LEU	-	expression tag	UNP P17612
B	29	ARG	-	expression tag	UNP P17612
B	30	TYR	-	expression tag	UNP P17612
B	31	HIS	-	expression tag	UNP P17612
B	32	PRO	-	expression tag	UNP P17612
B	33	ASP	-	expression tag	UNP P17612
B	34	LYS	-	expression tag	UNP P17612
B	35	ASN	-	expression tag	UNP P17612
B	36	LYS	-	expression tag	UNP P17612
B	37	GLU	-	expression tag	UNP P17612
B	38	PRO	-	expression tag	UNP P17612
B	39	GLY	-	expression tag	UNP P17612
B	40	ALA	-	expression tag	UNP P17612

Continued on next page...

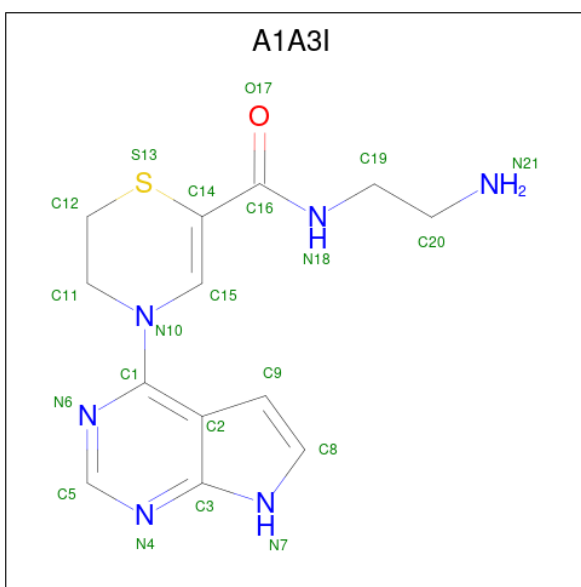
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	GLU	-	expression tag	UNP P17612
B	42	GLU	-	expression tag	UNP P17612
B	43	LYS	-	expression tag	UNP P17612
B	44	PHE	-	expression tag	UNP P17612
B	45	LYS	-	expression tag	UNP P17612
B	46	GLU	-	expression tag	UNP P17612
B	47	ILE	-	expression tag	UNP P17612
B	48	ALA	-	expression tag	UNP P17612
B	49	GLU	-	expression tag	UNP P17612
B	50	ALA	-	expression tag	UNP P17612
B	51	TYR	-	expression tag	UNP P17612
B	52	ASP	-	expression tag	UNP P17612
B	53	VAL	-	expression tag	UNP P17612
B	54	LEU	-	expression tag	UNP P17612
B	55	SER	-	expression tag	UNP P17612
B	56	ASP	-	expression tag	UNP P17612
B	57	PRO	-	expression tag	UNP P17612
B	58	ARG	-	expression tag	UNP P17612
B	59	LYS	-	expression tag	UNP P17612
B	60	ARG	-	expression tag	UNP P17612
B	61	GLU	-	expression tag	UNP P17612
B	62	ILE	-	expression tag	UNP P17612
B	63	PHE	-	expression tag	UNP P17612
B	64	ASP	-	expression tag	UNP P17612
B	65	ARG	-	expression tag	UNP P17612
B	66	TYR	-	expression tag	UNP P17612
B	67	GLY	-	expression tag	UNP P17612
B	68	GLU	-	expression tag	UNP P17612
B	69	GLU	-	expression tag	UNP P17612

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			156	94	32	30			
2	J	19	Total	C	N	O	0	0	0
			148	90	31	27			

- Molecule 3 is N-(2-aminoethyl)-4-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)-3,4-dihydro-2H-1,4-thiazine-6-carboxamide (CCD ID: A1A3I) (formula: C₁₃H₁₆N₆OS) (labeled as "Ligand of Interest" by depositor).

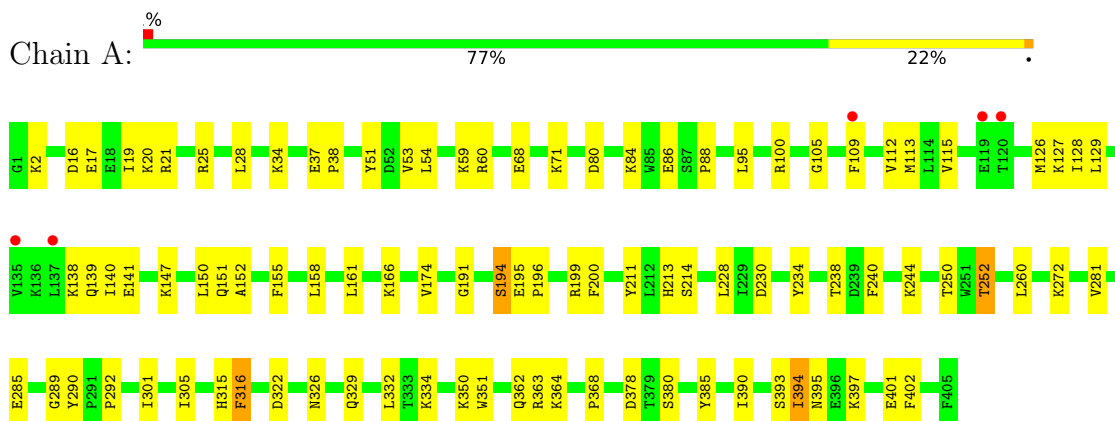


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			21	13	6	1	1		
3	B	1	Total	C	N	O	S	0	0
			21	13	6	1	1		

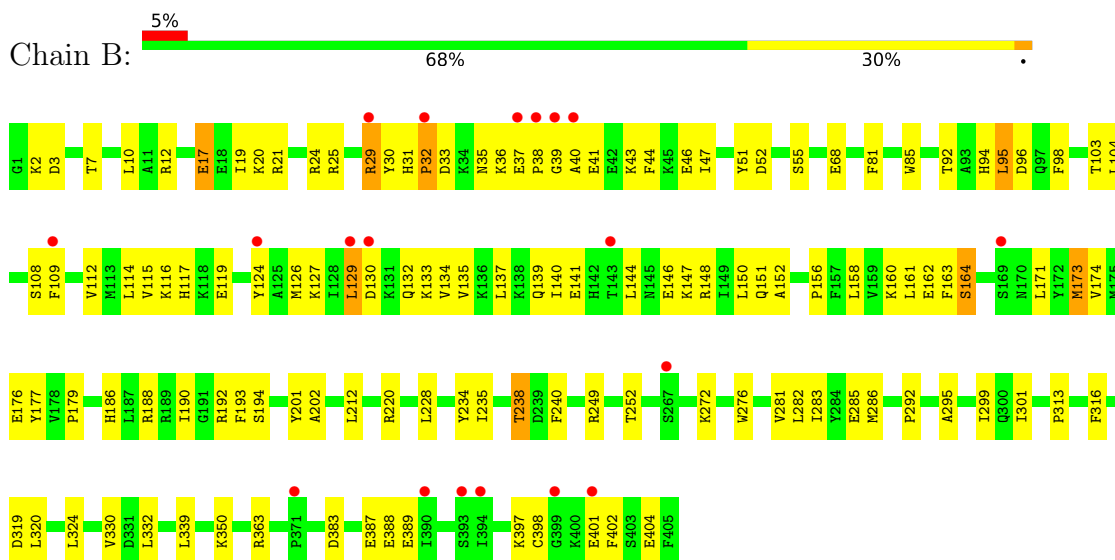
3 Residue-property plots [i](#)

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.

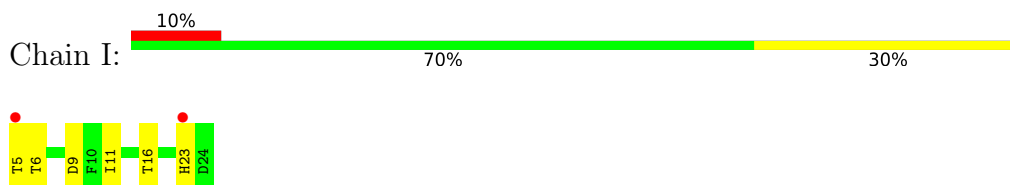
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha




- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 2: cAMP-dependent protein kinase inhibitor alpha



- Molecule 2: cAMP-dependent protein kinase inhibitor alpha

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.76Å 124.93Å 129.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.73 – 2.70 41.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.73-2.70) 99.6 (41.73-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.232 , 0.311 0.229 , 0.307	Depositor DCC
R_{free} test set	2010 reflections (7.23%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7058	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, A1A3I, SEP

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	0.39	0/3418	0.58	0/4598
1	B	0.42	0/3418	0.64	1/4598 (0.0%)
2	I	0.37	0/158	0.54	0/212
2	J	0.42	0/150	0.59	0/201
All	All	0.41	0/7144	0.61	1/9609 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	MET	CB-CG-SD	-6.07	94.50	112.70

There are no chirality outliers.

There are no planarity outliers.

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	3356	0	3321	69	0
1	B	3356	0	3321	90	1
2	I	156	0	146	6	0
2	J	148	0	142	2	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7058	0	6930	165	1

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 12.

All (165) 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:290:TYR:HH	2:I:5:THR:N	1.44	1.16
1:B:135:VAL:HG21	1:B:397:LYS:HE2	1.46	0.93
1:B:109:PHE:HA	1:B:139:GLN:HE22	1.36	0.90
1:B:37:GLU:H	1:B:41:GLU:HG2	1.39	0.84
2:I:6:THR:HB	2:I:9:ASP:HB2	1.60	0.83
1:A:140:ILE:HD12	1:A:141:GLU:N	1.93	0.82
1:B:115:VAL:HG11	1:B:126:MET:HE2	1.61	0.81
1:A:322:ASP:O	1:A:326:ASN:ND2	2.16	0.77
1:B:104:LEU:HD21	1:B:114:LEU:HB2	1.71	0.73
1:B:202:ALA:HB2	1:B:283:ILE:HD11	1.70	0.73
1:A:250:THR:OG1	1:A:252:TPO:O2P	2.07	0.72
1:A:21:ARG:HH22	1:A:25:ARG:HD3	1.53	0.71
1:B:37:GLU:O	1:B:39:GLY:N	2.23	0.71
1:B:130:ASP:HB3	1:B:171:LEU:H	1.56	0.71
1:A:290:TYR:OH	2:I:5:THR:N	2.20	0.70
1:B:132:GLN:HA	1:B:397:LYS:HD3	1.72	0.70
1:A:158:LEU:HD22	1:A:240:PHE:HZ	1.57	0.70
1:B:36:LYS:H	1:B:41:GLU:HG3	1.59	0.68
1:B:146:GLU:HG2	1:B:173:MET:HE1	1.75	0.67
1:B:85:TRP:O	1:B:148:ARG:NH1	2.27	0.67
1:A:281:VAL:HG13	1:A:292:PRO:HD2	1.76	0.66
1:A:140:ILE:HD12	1:A:141:GLU:H	1.61	0.66
1:A:362:GLN:HB2	1:A:364:LYS:HD3	1.78	0.65
1:B:85:TRP:CZ3	1:B:148:ARG:HG2	2.31	0.64
1:B:130:ASP:HB3	1:B:171:LEU:N	2.12	0.63
1:A:21:ARG:NH2	1:A:25:ARG:HD3	2.13	0.63
1:B:117:HIS:HB2	1:B:124:TYR:HE2	1.62	0.63
1:B:7:THR:HG21	1:B:46:GLU:HG3	1.81	0.62
1:B:158:LEU:HD22	1:B:240:PHE:HZ	1.64	0.62
1:B:2:LYS:HD3	1:B:3:ASP:N	2.15	0.61
1:A:19:ILE:HD11	1:A:60:ARG:HH21	1.65	0.60
1:B:192:ARG:NH1	1:B:193:PHE:O	2.33	0.60
1:A:315:HIS:O	1:A:316:PHE:HB2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HG22	1:A:402:PHE:CZ	2.37	0.60
1:A:126:MET:HG3	1:A:174:VAL:HG22	1.82	0.60
1:B:103:THR:N	1:B:387:GLU:OE2	2.35	0.60
1:B:163:PHE:HD2	1:B:174:VAL:HG11	1.67	0.59
1:B:135:VAL:CG2	1:B:397:LYS:HE2	2.26	0.59
1:A:115:VAL:HG11	1:A:126:MET:HE2	1.84	0.59
1:B:17:GLU:CD	1:B:21:ARG:HE	2.12	0.58
1:A:200:PHE:CD1	1:A:368:PRO:HD2	2.40	0.57
1:B:112:VAL:HG22	1:B:127:LYS:HG3	1.87	0.57
1:B:31:HIS:HB3	1:B:32:PRO:HD3	1.86	0.57
1:B:135:VAL:HA	1:B:140:ILE:HD11	1.86	0.56
1:A:228:LEU:HD13	1:A:238:THR:HG21	1.88	0.56
1:A:20:LYS:HD2	1:A:51:TYR:HE1	1.70	0.55
1:A:199:ARG:HD3	1:A:351:TRP:O	2.06	0.55
1:A:17:GLU:OE1	1:A:17:GLU:N	2.34	0.55
1:A:21:ARG:NH2	1:A:25:ARG:HH11	2.06	0.54
1:A:16:ASP:O	1:A:20:LYS:HD3	2.08	0.54
1:B:299:ILE:H	1:B:299:ILE:HD12	1.73	0.54
1:A:393:SER:HB3	1:A:397:LYS:HE2	1.89	0.54
1:B:108:SER:O	1:B:133:LYS:NZ	2.40	0.53
1:B:29:ARG:HG3	1:B:30:TYR:CD1	2.44	0.53
1:B:7:THR:HG22	1:B:47:ILE:HG22	1.90	0.53
2:I:6:THR:HB	2:I:9:ASP:CB	2.37	0.53
1:A:378:ASP:OD2	1:A:380:SER:OG	2.20	0.53
1:B:388:GLU:HG2	1:B:389:GLU:H	1.73	0.53
1:A:53:VAL:HG13	1:A:59:LYS:HG3	1.91	0.52
1:B:36:LYS:HA	1:B:36:LYS:HE2	1.91	0.52
1:B:228:LEU:HD12	1:B:238:THR:HG21	1.91	0.52
1:B:130:ASP:HA	1:B:134:VAL:HG21	1.91	0.52
1:A:166:LYS:NZ	1:A:402:PHE:O	2.35	0.52
1:B:404:GLU:OE2	1:B:404:GLU:N	2.30	0.52
1:B:20:LYS:O	1:B:24:ARG:HG3	2.10	0.52
1:B:140:ILE:HG23	1:B:402:PHE:HE1	1.74	0.52
1:B:129:LEU:O	1:B:134:VAL:HG21	2.10	0.51
1:B:281:VAL:HG13	1:B:292:PRO:HD2	1.93	0.51
1:A:28:LEU:HD23	1:A:28:LEU:O	2.10	0.51
1:A:230:ASP:OD2	1:A:363:ARG:NH2	2.44	0.51
1:B:160:LYS:HE2	1:B:176:GLU:OE1	2.11	0.50
1:B:144:LEU:HD11	1:B:401:GLU:O	2.11	0.50
1:A:194:SEP:OG	1:A:196:PRO:HD2	2.11	0.50
1:B:51:TYR:CE1	1:B:55:SER:HB3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE3	1:A:128:ILE:HD13	1.93	0.50
1:B:30:TYR:HB2	1:B:44:PHE:HB3	1.94	0.49
1:A:37:GLU:HG2	1:A:38:PRO:HD2	1.95	0.49
1:A:155:PHE:CE1	1:A:211:TYR:HB2	2.47	0.49
1:A:115:VAL:HG11	1:A:126:MET:CE	2.43	0.49
1:A:394:ILE:HD12	1:A:395:ASN:N	2.28	0.49
1:B:282:LEU:O	1:B:286:MET:HG3	2.13	0.49
1:B:117:HIS:HD2	1:B:119:GLU:H	1.61	0.49
1:B:141:GLU:H	1:B:141:GLU:CD	2.20	0.49
1:B:163:PHE:H	1:B:174:VAL:HG13	1.78	0.49
1:A:139:GLN:HA	1:A:139:GLN:OE1	2.12	0.48
1:B:30:TYR:CZ	1:B:43:LYS:HG2	2.49	0.48
1:B:162:GLU:OE2	1:B:162:GLU:HA	2.13	0.48
1:B:2:LYS:HD3	1:B:2:LYS:C	2.38	0.48
1:B:201:TYR:HB3	1:B:235:ILE:HD11	1.95	0.48
1:A:161:LEU:HD12	1:A:174:VAL:O	2.14	0.48
1:B:94:HIS:O	1:B:95:LEU:HB3	2.14	0.48
1:B:135:VAL:HG13	1:B:140:ILE:HD11	1.95	0.48
1:B:160:LYS:HE3	1:B:176:GLU:HB2	1.96	0.47
1:A:113:MET:HE3	1:A:113:MET:HB2	1.79	0.47
1:A:401:GLU:H	1:A:401:GLU:CD	2.21	0.47
1:A:113:MET:HE1	1:A:390:ILE:HD11	1.96	0.47
1:A:17:GLU:H	1:A:17:GLU:CD	2.23	0.46
1:B:313:PRO:HD2	1:B:316:PHE:CD2	2.51	0.46
1:A:329:GLN:HG2	1:A:334:LYS:HB3	1.96	0.46
1:B:147:LYS:HG3	1:B:148:ARG:N	2.25	0.46
1:B:31:HIS:C	1:B:31:HIS:CD2	2.94	0.46
1:B:36:LYS:N	1:B:41:GLU:HG3	2.28	0.46
1:A:350:LYS:HD2	1:A:350:LYS:H	1.80	0.46
1:A:109:PHE:CD1	1:A:127:LYS:HE3	2.51	0.46
1:B:94:HIS:ND1	1:B:96:ASP:HB2	2.31	0.46
1:A:19:ILE:HD13	1:A:54:LEU:HB3	1.98	0.45
1:A:362:GLN:CB	1:A:364:LYS:HD3	2.46	0.45
1:B:295:ALA:HB3	1:B:301:ILE:HG13	1.98	0.45
1:B:234:TYR:CE2	1:B:363:ARG:HG2	2.51	0.45
1:B:44:PHE:HA	1:B:47:ILE:CG1	2.47	0.45
1:B:81:PHE:HD1	1:B:152:ALA:O	2.00	0.45
1:A:112:VAL:HA	1:A:126:MET:O	2.17	0.45
1:B:7:THR:HA	1:B:43:LYS:HZ1	1.82	0.44
1:B:164:SER:O	1:B:164:SER:OG	2.35	0.44
2:I:11:ILE:HA	2:I:16:THR:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:C	1:A:88:PRO:HD3	2.42	0.44
1:B:272:LYS:NZ	1:B:276:TRP:HE1	2.14	0.44
1:B:202:ALA:CB	1:B:283:ILE:HD11	2.45	0.44
1:B:272:LYS:HZ2	1:B:276:TRP:HE1	1.65	0.44
1:B:30:TYR:CB	1:B:44:PHE:HB3	2.47	0.44
1:B:21:ARG:HB3	1:B:25:ARG:HH12	1.82	0.44
1:A:109:PHE:HB2	1:A:129:LEU:HD23	1.98	0.44
1:B:151:GLN:HB3	1:B:161:LEU:HD23	1.99	0.44
1:A:34:LYS:HA	1:A:34:LYS:HD2	1.75	0.43
1:A:244:LYS:NZ	1:A:252:TPO:O2P	2.51	0.43
1:B:158:LEU:HD22	1:B:240:PHE:CZ	2.50	0.43
1:B:85:TRP:CE3	1:B:148:ARG:HG2	2.53	0.43
1:B:188:ARG:NH2	1:B:285:GLU:OE2	2.51	0.43
1:B:319:ASP:OD1	1:B:350:LYS:HE3	2.18	0.43
1:A:105:GLY:HA2	1:A:385:TYR:CZ	2.53	0.43
1:A:394:ILE:HD12	1:A:395:ASN:HB2	1.99	0.43
1:B:10:LEU:HD13	1:B:19:ILE:HG13	2.00	0.43
1:A:150:LEU:HG	1:A:161:LEU:HB2	2.01	0.43
1:B:12:ARG:NH2	1:B:68:GLU:OE2	2.52	0.42
1:A:195:GLU:HB2	1:A:196:PRO:HD3	2.00	0.42
1:A:200:PHE:HZ	1:A:234:TYR:CZ	2.37	0.42
1:B:320:LEU:O	1:B:324:LEU:HG	2.20	0.42
1:A:211:TYR:O	1:A:214:SER:OG	2.30	0.42
1:A:394:ILE:H	1:A:394:ILE:HG13	1.60	0.42
1:B:158:LEU:HD11	1:B:212:LEU:HD21	2.02	0.42
1:A:80:ASP:O	1:A:84:LYS:HG3	2.20	0.41
1:A:95:LEU:HD11	1:A:100:ARG:HH11	1.85	0.41
1:B:94:HIS:CE1	1:B:96:ASP:HB2	2.55	0.41
2:J:11:ILE:HA	2:J:16:THR:HG21	2.01	0.41
1:A:213:HIS:CE1	1:A:272:LYS:HB2	2.55	0.41
1:B:117:HIS:CD2	1:B:119:GLU:HB3	2.56	0.41
2:I:5:THR:O	2:I:6:THR:OG1	2.30	0.41
2:J:15:ARG:HE	2:J:15:ARG:HB3	1.68	0.41
1:A:128:ILE:HD12	1:A:128:ILE:N	2.34	0.41
1:A:147:LYS:O	1:A:151:GLN:HG3	2.21	0.41
1:A:191:GLY:O	1:A:289:GLY:HA3	2.20	0.41
1:A:260:LEU:HA	1:A:260:LEU:HD23	1.78	0.41
1:A:285:GLU:HA	1:A:290:TYR:O	2.21	0.41
1:B:186:HIS:O	1:B:190:ILE:HG13	2.21	0.41
1:A:68:GLU:OE1	1:A:71:LYS:HD3	2.20	0.40
1:B:397:LYS:HE3	1:B:398:CYS:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HB2	1:A:138:LYS:HE3	1.68	0.40
1:B:92:THR:HB	1:B:163:PHE:HB3	2.02	0.40
1:B:156:PRO:HB3	1:B:363:ARG:NH2	2.36	0.40
1:B:33:ASP:C	1:B:35:ASN:H	2.29	0.40
1:B:98:PHE:HA	1:B:116:LYS:O	2.21	0.40
1:B:150:LEU:HG	1:B:161:LEU:HB2	2.03	0.40
1:B:177:TYR:CE2	1:B:179:PRO:HB3	2.57	0.40
1:B:188:ARG:HA	1:B:188:ARG:HD3	1.96	0.40
1:A:301:ILE:HG22	1:A:305:ILE:HD11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:OD1	1:B:249:ARG:NH1[4_555]	2.18	0.02

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	401/405 (99%)	380 (95%)	19 (5%)	2 (0%)	24	48
1	B	401/405 (99%)	370 (92%)	28 (7%)	3 (1%)	18	41
2	I	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
2	J	17/20 (85%)	15 (88%)	2 (12%)	0	100	100
All	All	837/850 (98%)	782 (93%)	50 (6%)	5 (1%)	21	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	316	PHE
1	B	95	LEU
1	A	152	ALA
1	B	40	ALA

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	352/352 (100%)	349 (99%)	3 (1%)	70	87
1	B	352/352 (100%)	340 (97%)	12 (3%)	32	62
2	I	15/15 (100%)	14 (93%)	1 (7%)	15	36
2	J	14/15 (93%)	13 (93%)	1 (7%)	13	33
All	All	733/734 (100%)	716 (98%)	17 (2%)	44	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	332	LEU
1	A	394	ILE
1	B	17	GLU
1	B	29	ARG
1	B	32	PRO
1	B	129	LEU
1	B	137	LEU
1	B	164	SER
1	B	220	ARG
1	B	238	THR
1	B	330	VAL
1	B	332	LEU
1	B	339	LEU
1	B	383	ASP
2	I	23	HIS
2	J	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	122	ASN
1	A	151	GLN
1	A	170	ASN
1	A	329	GLN
1	B	6	GLN
1	B	31	HIS
1	B	90	GLN
1	B	117	HIS
1	B	139	GLN
1	B	341	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	SEP	B	194	1	8,9,10	1.81	2 (25%)	7,12,14	2.82	2 (28%)
1	TPO	B	252	1	8,10,11	2.36	1 (12%)	10,14,16	1.60	3 (30%)
1	TPO	A	252	1	8,10,11	2.18	1 (12%)	10,14,16	1.07	1 (10%)
1	SEP	A	194	1	8,9,10	1.66	1 (12%)	7,12,14	1.63	1 (14%)

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
1	SEP	B	194	1	-	4/6/8/10	-
1	TPO	B	252	1	-	2/9/11/13	-
1	TPO	A	252	1	-	5/9/11/13	-
1	SEP	A	194	1	-	2/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	TPO	P-OG1	6.37	1.70	1.59
1	A	252	TPO	P-OG1	5.84	1.69	1.59
1	B	194	SEP	P-O1P	3.80	1.62	1.50
1	A	194	SEP	P-O1P	3.68	1.61	1.50
1	B	194	SEP	P-O3P	2.17	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	SEP	OG-CB-CA	6.87	114.83	108.14
1	A	194	SEP	OG-CB-CA	4.02	112.06	108.14
1	B	252	TPO	OG1-P-O1P	-3.14	98.12	109.33
1	B	194	SEP	OG-P-O1P	2.49	113.17	106.44
1	B	252	TPO	P-OG1-CB	-2.34	116.97	123.33
1	B	252	TPO	O3P-P-O1P	2.13	119.14	110.83
1	A	252	TPO	O-C-CA	-2.01	119.60	124.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	194	SEP	C-CA-CB-OG
1	A	252	TPO	N-CA-CB-CG2
1	A	252	TPO	N-CA-CB-OG1
1	A	252	TPO	C-CA-CB-CG2
1	A	252	TPO	O-C-CA-CB
1	B	194	SEP	CB-OG-P-O2P
1	B	194	SEP	CB-OG-P-O3P
1	A	252	TPO	CG2-CB-OG1-P
1	A	194	SEP	N-CA-CB-OG
1	B	194	SEP	N-CA-CB-OG
1	B	252	TPO	CB-OG1-P-O1P
1	B	194	SEP	CA-CB-OG-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	252	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	252	TPO	2	0
1	A	194	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	A1A3I	B	501	-	22,23,23	0.49	0	19,31,31	1.42	3 (15%)
3	A1A3I	A	501	-	22,23,23	0.48	0	19,31,31	1.18	2 (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	A1A3I	B	501	-	-	3/8/22/22	0/3/3/3
3	A1A3I	A	501	-	-	2/8/22/22	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	A1A3I	C3-N7-C8	4.56	110.74	108.11
3	A	501	A1A3I	C3-N7-C8	3.65	110.22	108.11
3	B	501	A1A3I	C2-C3-N7	-2.42	106.95	108.33
3	A	501	A1A3I	C5-N6-C1	2.13	117.05	111.83
3	B	501	A1A3I	C5-N6-C1	2.00	116.72	111.83

There are no chirality outliers.

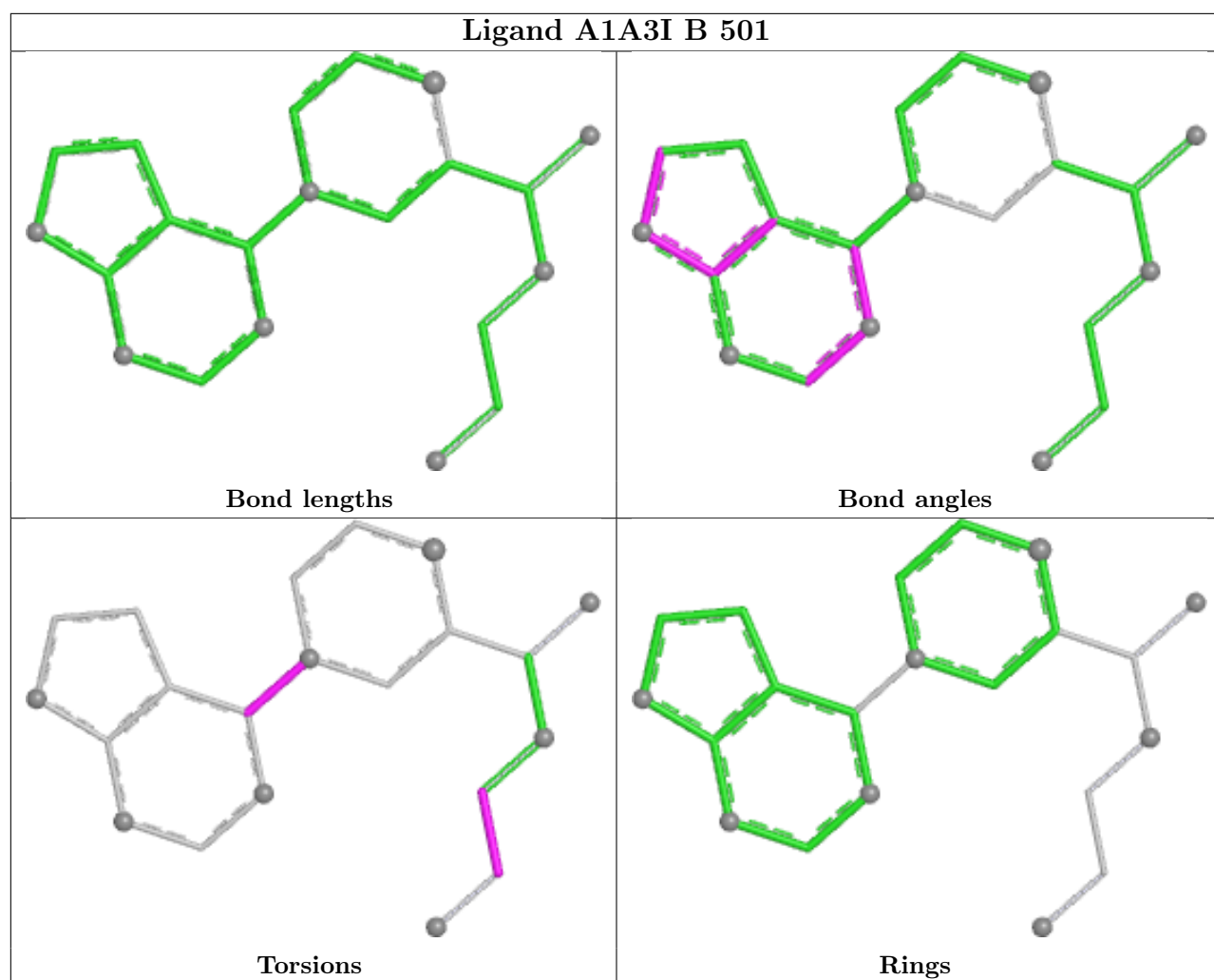
All (5) torsion outliers are listed below:

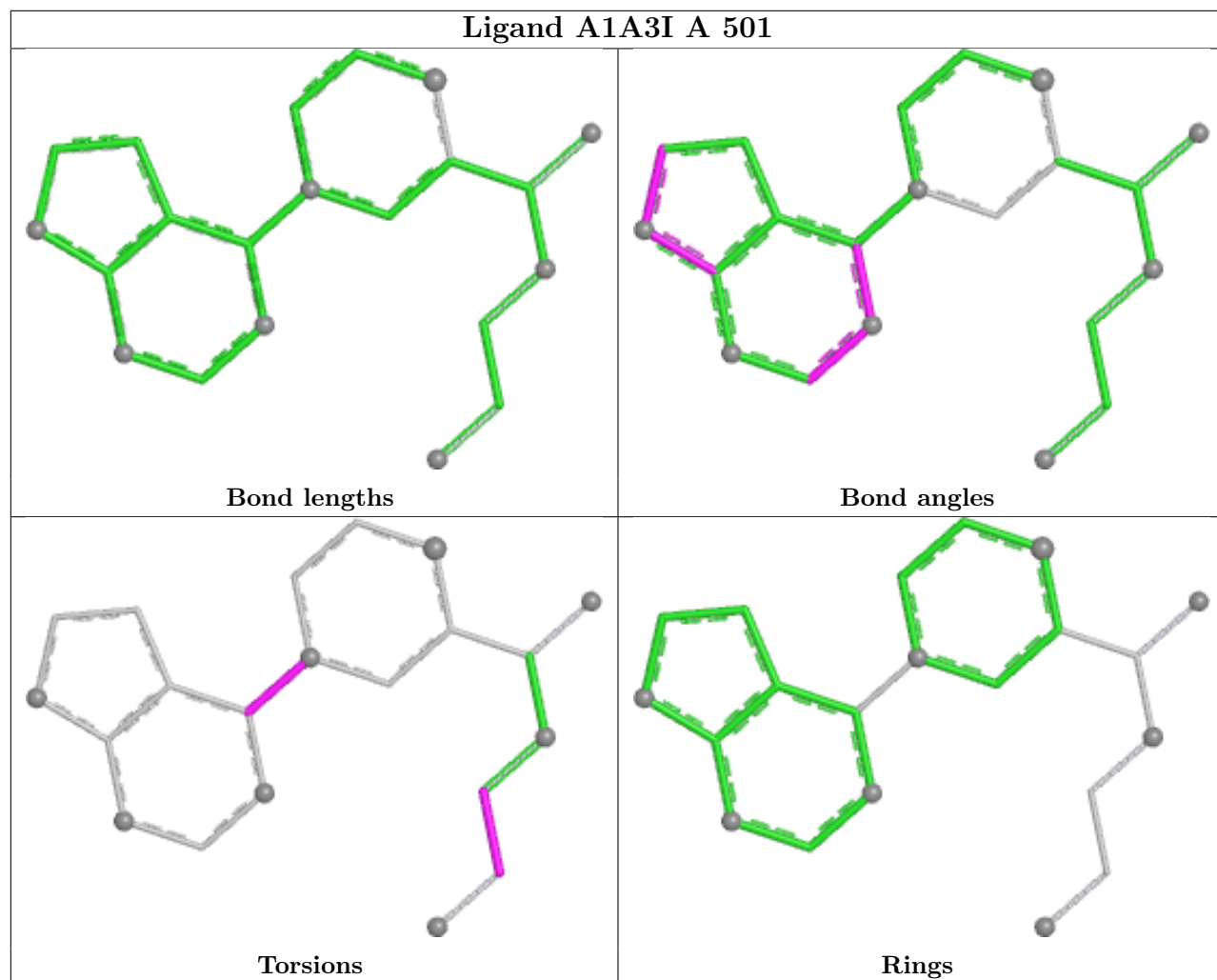
Mol	Chain	Res	Type	Atoms
3	A	501	A1A3I	C2-C1-N10-C15
3	A	501	A1A3I	N18-C19-C20-N21
3	B	501	A1A3I	C2-C1-N10-C15
3	B	501	A1A3I	N18-C19-C20-N21
3	B	501	A1A3I	N6-C1-N10-C15

There are no ring outliers.

No monomer is involved in short contacts.

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.





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

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	403/405 (99%)	0.11	5 (1%) 76 75	35, 73, 101, 154	0
1	B	403/405 (99%)	0.22	19 (4%) 36 33	39, 74, 131, 191	0
2	I	20/20 (100%)	0.11	2 (10%) 12 10	48, 58, 107, 144	0
2	J	19/20 (95%)	0.34	2 (10%) 11 9	47, 66, 103, 124	0
All	All	845/850 (99%)	0.17	28 (3%) 49 45	35, 73, 120, 191	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	LEU	4.8
1	B	39	GLY	4.1
1	B	109	PHE	3.8
1	A	109	PHE	3.6
1	B	38	PRO	3.1
1	A	135	VAL	3.0
1	B	32	PRO	3.0
1	B	130	ASP	2.9
1	B	401	GLU	2.9
1	A	120	THR	2.8
1	B	394	ILE	2.7
1	B	393	SER	2.7
1	A	137	LEU	2.6
2	I	5	THR	2.5
2	J	23	HIS	2.4
1	B	371	PRO	2.4
1	B	40	ALA	2.4
1	B	399	GLY	2.3
2	J	5	THR	2.3
1	B	29	ARG	2.3
2	I	23	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	143	THR	2.2
1	B	37	GLU	2.2
1	B	169	SER	2.2
1	B	267	SER	2.1
1	B	124	TYR	2.1
1	A	119	GLU	2.0
1	B	390	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	194	10/11	0.80	0.11	90,105,125,128	0
1	SEP	B	194	10/11	0.84	0.09	63,78,95,96	0
1	TPO	A	252	11/12	0.86	0.10	65,70,83,88	0
1	TPO	B	252	11/12	0.97	0.05	46,49,55,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

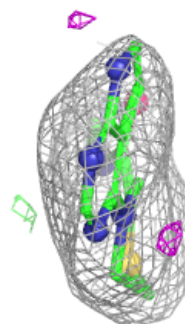
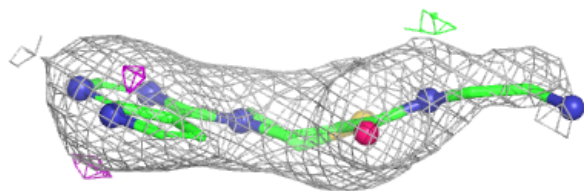
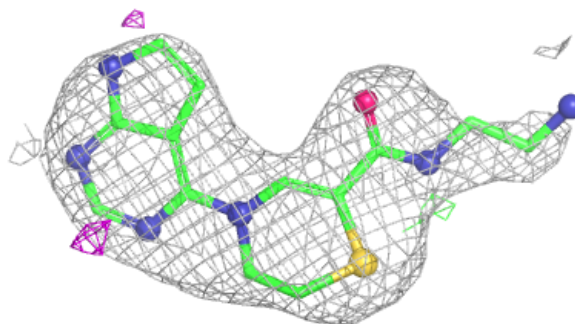
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1A3I	B	501	21/21	0.90	0.11	70,76,84,89	0
3	A1A3I	A	501	21/21	0.94	0.09	55,64,67,69	0

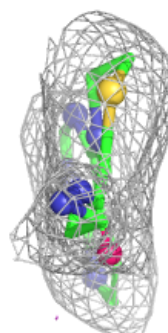
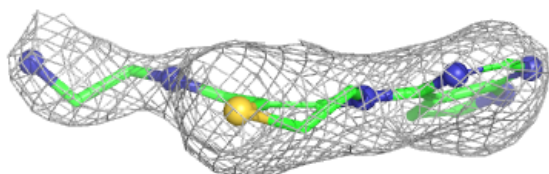
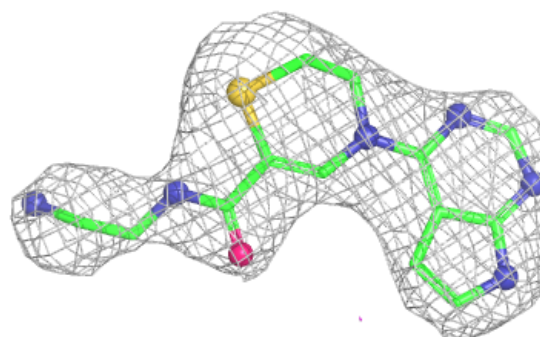
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1A3I B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around A1A3I A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.