



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:46 AM UTC

PDB ID : 1HAK / pdb_00001hak
Title : CRYSTAL STRUCTURE OF RECOMBINANT HUMAN PLACENTAL ANNEXIN V COMPLEXED WITH K-201 AS A CALCIUM CHANNEL ACTIVITY INHIBITOR
Authors : Ago, H.; Inagaki, E.; Miyano, M.
Deposited on : 1997-12-10
Resolution : 3.00 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)	:	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

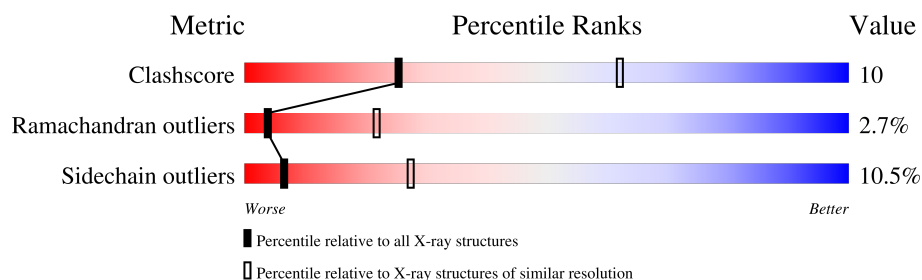
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	320	 42% 39% 17% ..
1	B	320	 46% 41% 11% ..

2 Entry composition [i](#)

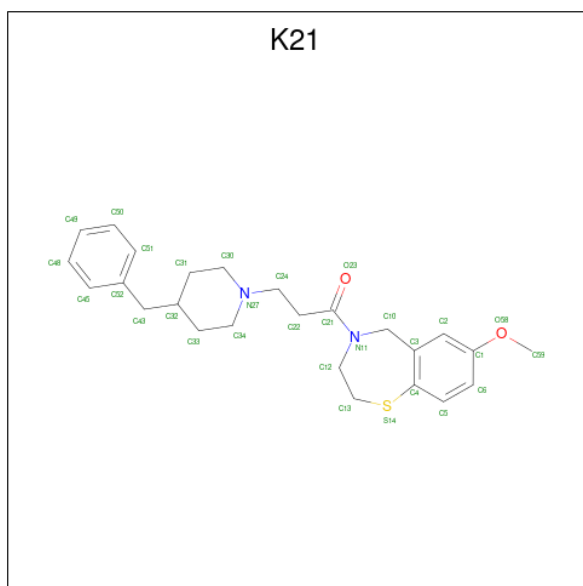
There are 3 unique types of molecules in this entry. The entry contains 5195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	318	Total	C	N	O	S	0	0	0
			2513	1582	422	501	8			
1	A	318	Total	C	N	O	S	0	0	0
			2513	1582	422	501	8			

- Molecule 2 is 4-[3-{1-(4-BENZYL)PIPERODINYL}PROPIONYL]-7-METHOXY-2,3,4,5-TETRAHYDRO-1,4-BENZOTHAZEPINE (CCD ID: K21) (formula: C₂₅H₃₂N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			30	25	2	2	1		
2	A	1	Total	C	N	O	S	0	0
			30	25	2	2	1		

- Molecule 3 is water.

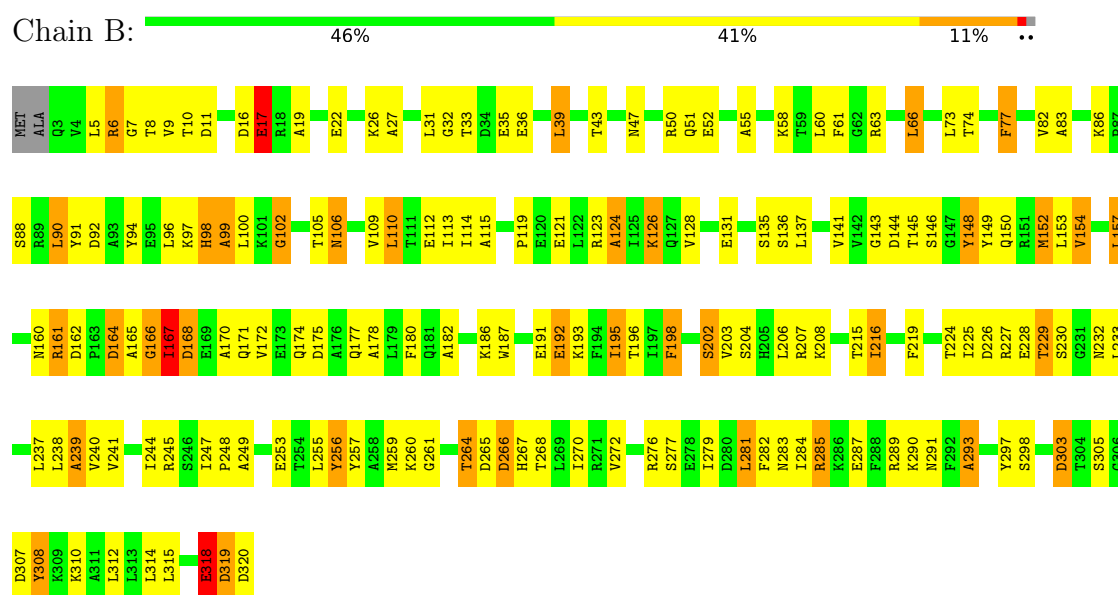
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	59	Total	O	0	0
			59	59		
3	A	50	Total	O	0	0
			50	50		

3 Residue-property plots

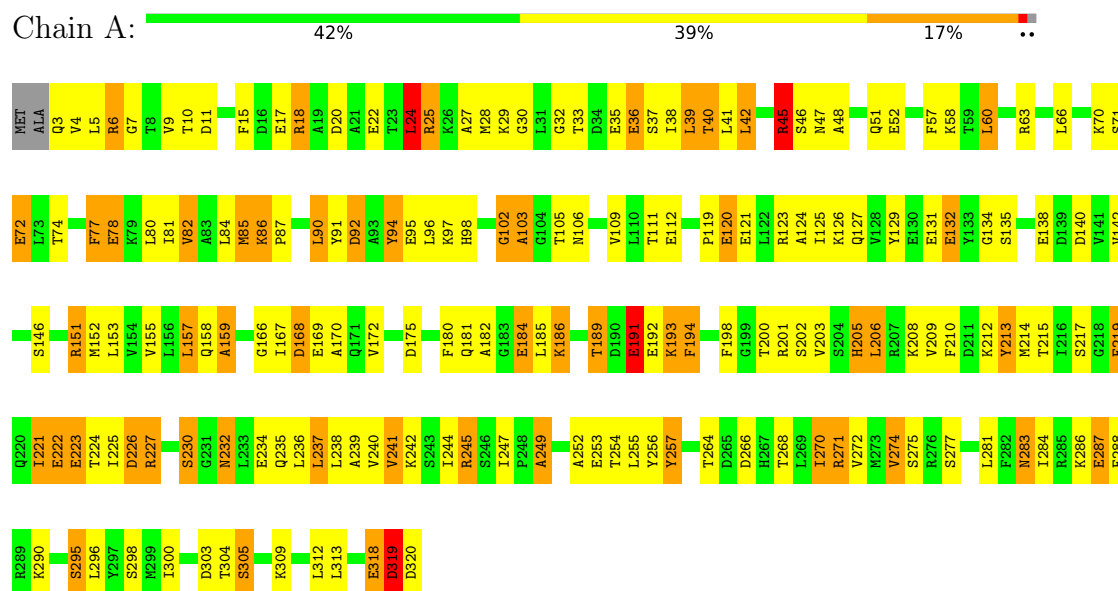
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ANNEXIN V



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	99.30 Å 99.30 Å 130.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	97.4 (20.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5195	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K21

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	1.14	1/2547 (0.0%)	2.20	150/3427 (4.4%)
1	B	1.16	4/2547 (0.2%)	2.18	129/3427 (3.8%)
All	All	1.15	5/5094 (0.1%)	2.19	279/6854 (4.1%)

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	8
1	B	0	10
All	All	0	18

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	HIS	ND1-CE1	5.94	1.38	1.32
1	A	320	ASP	C-OXT	5.80	1.35	1.23
1	B	247	ILE	CA-C	5.47	1.57	1.52
1	B	267	HIS	CG-CD2	5.20	1.41	1.35
1	B	98	HIS	CE1-NE2	5.04	1.37	1.32

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASN	CA-CB-CG	-12.48	100.12	112.60
1	B	319	ASP	N-CA-C	10.87	124.28	111.02
1	B	293	ALA	N-CA-C	10.10	124.99	112.47
1	A	319	ASP	N-CA-C	10.08	121.98	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	N-CA-C	10.07	120.93	110.36
1	B	167	ILE	N-CA-C	9.96	123.47	108.23
1	B	227	ARG	N-CA-C	9.94	125.21	112.89
1	B	241	VAL	N-CA-C	9.05	119.64	110.23
1	A	103	ALA	N-CA-C	8.74	123.50	113.01
1	A	27	ALA	CA-C-N	-8.55	109.21	122.37
1	A	27	ALA	C-N-CA	-8.55	109.21	122.37
1	B	141	VAL	N-CA-C	8.53	118.61	110.42
1	B	60	LEU	N-CA-C	8.12	120.22	111.36
1	B	22	GLU	N-CA-C	8.02	119.81	111.14
1	B	121	GLU	N-CA-C	8.02	119.80	111.14
1	B	47	ASN	N-CA-C	8.01	121.03	111.33
1	A	219	PHE	N-CA-C	7.89	122.32	109.85
1	B	255	LEU	N-CA-C	7.82	119.80	111.28
1	A	18	ARG	N-CA-C	7.80	122.90	113.23
1	A	158	GLN	N-CA-C	7.78	122.34	113.01
1	A	198	PHE	N-CA-C	7.77	119.39	111.07
1	B	203	VAL	N-CA-C	7.77	118.52	110.36
1	A	3	GLN	CA-C-N	-7.72	112.70	122.43
1	A	3	GLN	C-N-CA	-7.72	112.70	122.43
1	A	142	VAL	N-CA-C	7.71	117.83	110.42
1	B	230	SER	N-CA-C	7.65	127.09	110.80
1	B	206	LEU	N-CA-C	7.56	120.47	111.33
1	B	164	ASP	N-CA-C	7.30	119.99	108.67
1	A	140	ASP	N-CA-C	7.24	118.86	110.97
1	B	186	LYS	N-CA-C	7.23	121.38	111.54
1	B	170	ALA	N-CA-C	7.22	118.79	111.07
1	B	230	SER	CA-C-N	-7.11	112.90	120.43
1	B	230	SER	C-N-CA	-7.11	112.90	120.43
1	A	35	GLU	N-CA-C	7.10	119.63	111.11
1	A	66	LEU	N-CA-C	7.10	119.62	111.11
1	B	272	VAL	N-CA-C	7.06	117.06	110.42
1	B	106	ASN	N-CA-C	7.06	125.83	110.80
1	B	253	GLU	N-CA-C	7.04	119.60	111.02
1	A	60	LEU	N-CA-C	6.98	118.97	111.36
1	A	112	GLU	N-CA-C	6.98	119.53	111.02
1	B	182	ALA	N-CA-C	6.97	120.89	112.38
1	A	80	LEU	N-CA-C	6.97	118.53	111.07
1	B	249	ALA	N-CA-C	6.96	118.87	111.28
1	A	318	GLU	N-CA-C	6.96	125.62	110.80
1	A	318	GLU	CA-C-N	-6.95	111.94	122.23
1	A	318	GLU	C-N-CA	-6.95	111.94	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ILE	N-CA-C	6.95	120.69	112.35
1	B	305	SER	N-CA-C	6.91	120.23	109.52
1	B	281	LEU	N-CA-C	6.90	119.67	111.33
1	A	51	GLN	N-CA-C	6.87	118.77	111.28
1	A	274	VAL	N-CA-C	6.87	116.87	110.42
1	A	58	LYS	N-CA-C	6.83	118.80	111.36
1	A	74	THR	N-CA-C	6.82	120.09	109.52
1	A	105	THR	N-CA-C	6.81	118.87	109.54
1	B	290	LYS	N-CA-C	6.81	118.39	110.97
1	A	205	HIS	N-CA-C	6.78	118.36	110.97
1	B	291	ASN	N-CA-C	6.70	121.29	113.18
1	B	227	ARG	CA-C-N	-6.70	111.52	120.63
1	B	227	ARG	C-N-CA	-6.70	111.52	120.63
1	B	74	THR	N-CA-C	6.67	118.66	109.18
1	A	309	LYS	N-CA-C	6.64	118.18	111.07
1	A	313	LEU	CA-C-N	-6.64	110.86	120.29
1	A	313	LEU	C-N-CA	-6.64	110.86	120.29
1	B	98	HIS	CA-CB-CG	-6.64	107.16	113.80
1	A	172	VAL	N-CA-C	6.63	117.13	110.23
1	B	146	SER	N-CA-C	6.60	119.46	109.23
1	B	165	ALA	N-CA-C	6.60	118.16	108.86
1	A	170	ALA	N-CA-C	6.58	119.00	111.11
1	B	219	PHE	N-CA-C	6.57	120.23	109.72
1	A	298	SER	N-CA-C	6.57	121.00	113.19
1	A	268	THR	N-CA-C	6.56	118.09	111.07
1	A	242	LYS	N-CA-C	6.55	118.08	111.07
1	A	40	THR	N-CA-C	6.51	118.46	111.36
1	B	227	ARG	CA-CB-CG	6.49	127.08	114.10
1	B	225	ILE	N-CA-C	6.48	118.14	106.61
1	A	186	LYS	N-CA-C	6.47	120.49	112.47
1	B	66	LEU	N-CA-C	6.47	118.33	111.28
1	B	266	ASP	N-CA-C	6.45	118.39	111.36
1	A	131	GLU	CB-CA-C	-6.45	100.75	110.88
1	B	177	GLN	N-CA-C	6.45	118.85	111.11
1	B	154	VAL	N-CA-C	6.42	117.17	110.62
1	A	192	GLU	N-CA-C	6.42	119.09	111.71
1	B	180	PHE	N-CA-C	6.41	117.95	110.97
1	A	90	LEU	CA-C-N	-6.40	112.11	120.44
1	A	90	LEU	C-N-CA	-6.40	112.11	120.44
1	A	275	SER	N-CA-C	6.38	118.77	111.11
1	B	88	SER	N-CA-C	6.37	120.31	112.54
1	B	245	ARG	N-CA-C	6.37	118.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ALA	N-CA-C	6.37	119.52	111.69
1	A	208	LYS	N-CA-C	6.36	118.29	111.36
1	B	261	GLY	N-CA-C	6.35	120.16	112.48
1	B	157	LEU	N-CA-C	6.34	120.62	113.01
1	A	277	SER	N-CA-C	6.34	120.12	112.38
1	A	151	ARG	CD-NE-CZ	-6.34	115.52	124.40
1	B	277	SER	N-CA-C	6.33	118.99	111.33
1	A	213	TYR	N-CA-C	6.32	118.73	111.02
1	B	247	ILE	N-CA-C	6.32	119.93	112.35
1	A	36	GLU	N-CA-C	6.31	120.58	113.01
1	A	175	ASP	N-CA-C	6.31	117.82	111.07
1	B	171	GLN	N-CA-C	6.30	119.13	111.82
1	B	233	LEU	N-CA-C	6.30	117.84	110.97
1	A	281	LEU	N-CA-C	6.29	118.13	111.28
1	B	58	LYS	N-CA-C	6.27	117.78	111.07
1	A	11	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	43	THR	CA-C-N	-6.25	112.22	122.54
1	B	43	THR	C-N-CA	-6.25	112.22	122.54
1	A	48	ALA	N-CA-C	6.24	119.73	111.75
1	B	11	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	52	GLU	N-CA-C	6.23	118.87	111.33
1	A	192	GLU	CA-C-N	-6.20	110.14	120.68
1	A	192	GLU	C-N-CA	-6.20	110.14	120.68
1	A	9	VAL	N-CA-C	6.19	117.22	108.36
1	A	97	LYS	N-CA-C	6.18	118.52	111.11
1	B	238	LEU	N-CA-C	6.16	118.07	111.36
1	A	200	THR	CA-C-N	-6.15	111.29	120.94
1	A	200	THR	C-N-CA	-6.15	111.29	120.94
1	B	285	ARG	N-CA-C	6.14	117.77	111.14
1	A	206	LEU	N-CA-C	6.13	118.76	111.71
1	B	148	TYR	N-CA-C	6.11	118.73	111.71
1	A	15	PHE	CA-C-N	-6.09	114.13	123.14
1	A	15	PHE	C-N-CA	-6.09	114.13	123.14
1	A	189	THR	N-CA-C	6.08	116.27	108.24
1	A	182	ALA	N-CA-C	6.07	118.86	111.82
1	A	146	SER	N-CA-C	6.05	117.98	108.96
1	A	245	ARG	N-CA-C	6.02	117.92	111.36
1	A	200	THR	N-CA-C	6.02	121.68	113.97
1	A	272	VAL	N-CA-C	6.02	116.19	110.53
1	A	305	SER	N-CA-C	6.01	119.00	109.81
1	A	271	ARG	N-CA-C	5.99	118.30	111.11
1	A	320	ASP	N-CA-C	5.99	127.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ASP	N-CA-C	5.99	119.33	112.57
1	B	257	TYR	N-CA-C	5.96	119.65	112.38
1	B	143	GLY	CA-C-N	-5.96	113.74	122.86
1	B	143	GLY	C-N-CA	-5.96	113.74	122.86
1	B	99	ALA	N-CA-C	5.93	117.54	111.14
1	B	109	VAL	N-CA-C	5.93	116.14	110.74
1	B	270	ILE	N-CA-C	5.93	116.05	110.30
1	A	232	ASN	N-CA-C	5.92	123.40	110.80
1	B	110	LEU	N-CA-C	5.88	118.16	111.11
1	B	83	ALA	N-CA-C	5.87	117.68	111.28
1	B	202	SER	N-CA-C	5.86	119.19	110.52
1	B	226	ASP	N-CA-C	5.86	118.95	110.28
1	B	145	THR	CA-C-N	-5.86	112.62	122.29
1	B	145	THR	C-N-CA	-5.86	112.62	122.29
1	A	309	LYS	CA-C-N	-5.86	111.84	120.28
1	A	309	LYS	C-N-CA	-5.86	111.84	120.28
1	A	138	GLU	N-CA-C	5.85	117.34	110.97
1	A	20	ASP	N-CA-C	5.84	117.65	111.28
1	A	159	ALA	N-CA-C	5.84	123.24	110.80
1	A	39	LEU	N-CA-CB	-5.82	100.66	110.49
1	A	254	THR	N-CA-C	5.82	117.70	111.36
1	B	215	THR	CA-C-N	-5.81	113.12	120.56
1	B	215	THR	C-N-CA	-5.81	113.12	120.56
1	A	45	ARG	N-CA-C	5.79	118.68	109.24
1	A	290	LYS	CA-C-N	-5.79	113.51	122.49
1	A	290	LYS	C-N-CA	-5.79	113.51	122.49
1	B	265	ASP	N-CA-C	5.79	118.71	107.71
1	A	290	LYS	N-CA-C	5.79	120.06	112.89
1	B	195	ILE	N-CA-C	5.78	116.43	110.36
1	B	207	ARG	N-CA-C	5.78	117.26	111.07
1	A	102	GLY	N-CA-C	5.78	126.88	113.18
1	A	224	THR	CA-C-N	-5.77	115.61	123.12
1	A	224	THR	C-N-CA	-5.77	115.61	123.12
1	B	114	ILE	N-CA-C	5.77	115.96	110.42
1	B	27	ALA	N-CA-C	5.76	117.24	111.07
1	A	209	VAL	N-CA-C	5.76	116.50	110.62
1	B	264	THR	N-CA-C	5.75	123.06	110.80
1	A	24	LEU	N-CA-C	5.75	118.50	111.82
1	A	270	ILE	N-CA-C	5.75	115.93	110.53
1	B	77	PHE	N-CA-C	5.74	117.23	110.97
1	B	51	GLN	N-CA-C	5.74	118.00	111.11
1	B	145	THR	N-CA-C	5.74	116.95	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLU	CA-C-O	5.73	126.43	119.38
1	B	98	HIS	N-CA-C	5.73	118.26	111.33
1	B	166	GLY	CA-C-N	-5.71	115.23	122.37
1	B	166	GLY	C-N-CA	-5.71	115.23	122.37
1	A	222	GLU	N-CA-C	5.71	118.24	111.33
1	B	224	THR	N-CA-C	5.69	119.33	112.38
1	B	9	VAL	N-CA-C	5.69	116.30	107.99
1	B	136	SER	N-CA-C	5.69	118.91	109.46
1	A	131	GLU	N-CA-C	5.69	117.16	111.07
1	B	172	VAL	N-CA-C	5.68	116.33	110.36
1	B	126	LYS	N-CA-C	5.68	117.92	111.11
1	B	135	SER	CA-C-N	-5.67	114.19	122.19
1	B	135	SER	C-N-CA	-5.67	114.19	122.19
1	B	298	SER	N-CA-C	5.66	117.90	111.11
1	A	226	ASP	N-CA-C	5.66	118.88	108.58
1	B	115	ALA	N-CA-C	5.66	118.38	111.82
1	A	252	ALA	N-CA-C	5.64	117.43	111.28
1	A	70	LYS	N-CA-C	5.64	120.22	113.23
1	A	255	LEU	N-CA-C	5.63	117.11	110.97
1	B	6	ARG	N-CA-C	5.61	117.05	108.52
1	A	168	ASP	N-CA-C	5.61	118.55	108.17
1	A	106	ASN	N-CA-C	5.61	122.75	110.80
1	B	91	TYR	N-CA-C	5.60	118.11	111.33
1	A	241	VAL	N-CA-C	5.60	116.24	110.36
1	B	152	MET	N-CA-C	5.59	117.45	111.36
1	A	123	ARG	N-CA-C	5.58	117.81	111.11
1	A	155	VAL	N-CA-C	5.58	116.22	110.36
1	B	112	GLU	N-CA-C	5.58	117.16	111.14
1	A	235	GLN	N-CA-C	5.57	117.35	111.28
1	A	283	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	A	90	LEU	N-CA-C	5.56	120.13	113.23
1	A	227	ARG	N-CA-C	5.56	122.64	110.80
1	A	180	PHE	N-CA-C	5.55	117.00	111.07
1	B	82	VAL	N-CA-C	5.53	116.92	110.62
1	A	193	LYS	N-CA-C	5.49	119.15	112.23
1	A	86	LYS	CA-C-O	5.48	123.86	119.59
1	B	307	ASP	N-CA-C	5.46	118.41	111.69
1	B	215	THR	N-CA-C	5.46	119.79	113.18
1	B	123	ARG	N-CA-C	5.46	117.66	111.11
1	B	268	THR	N-CA-C	5.43	117.00	111.14
1	B	52	GLU	N-CA-C	5.42	118.11	111.82
1	A	42	LEU	N-CA-C	5.42	119.38	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLU	N-CA-C	5.41	118.10	111.82
1	A	132	GLU	N-CA-C	5.39	119.11	112.54
1	B	315	LEU	CB-CA-C	-5.37	102.22	110.81
1	A	221	ILE	CA-C-O	5.36	126.62	121.05
1	B	175	ASP	N-CA-C	5.35	117.19	111.36
1	A	46	SER	N-CA-C	5.34	117.97	110.23
1	A	7	GLY	CA-C-N	-5.33	113.78	122.26
1	A	7	GLY	C-N-CA	-5.33	113.78	122.26
1	A	109	VAL	N-CA-C	5.33	116.11	110.72
1	A	82	VAL	N-CA-C	5.33	119.56	111.89
1	A	166	GLY	CA-C-N	-5.32	115.72	122.43
1	A	166	GLY	C-N-CA	-5.32	115.72	122.43
1	A	124	ALA	N-CA-C	5.32	117.16	111.36
1	B	192	GLU	N-CA-C	5.31	122.10	110.80
1	A	184	GLU	CA-C-O	5.30	126.09	120.10
1	B	55	ALA	N-CA-C	5.29	116.86	111.14
1	B	303	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	25	ARG	CA-C-N	-5.28	112.15	120.60
1	A	25	ARG	C-N-CA	-5.28	112.15	120.60
1	B	239	ALA	N-CA-C	5.28	116.72	110.97
1	A	71	SER	CA-C-N	-5.27	112.84	122.38
1	A	71	SER	C-N-CA	-5.27	112.84	122.38
1	A	94	TYR	N-CA-C	5.26	116.69	111.07
1	B	229	THR	N-CA-C	5.25	116.69	111.07
1	A	126	LYS	N-CA-C	5.25	120.03	111.37
1	B	308	TYR	N-CA-CB	-5.24	101.23	109.78
1	B	310	LYS	N-CA-C	5.24	116.68	110.97
1	B	216	ILE	N-CA-C	5.24	115.45	110.53
1	A	225	ILE	N-CA-C	5.23	115.39	107.80
1	A	191	GLU	N-CA-C	5.23	121.94	110.80
1	B	7	GLY	N-CA-C	5.21	120.06	112.60
1	B	100	LEU	CA-C-N	-5.21	114.11	122.08
1	B	100	LEU	C-N-CA	-5.21	114.11	122.08
1	A	266	ASP	N-CA-C	5.17	117.59	111.33
1	B	113	ILE	N-CA-C	5.17	115.32	110.30
1	A	303	ASP	CA-C-N	-5.17	113.34	122.74
1	A	303	ASP	C-N-CA	-5.17	113.34	122.74
1	A	169	GLU	N-CA-C	5.14	119.85	111.37
1	B	244	ILE	CA-C-N	-5.13	113.40	120.28
1	B	244	ILE	C-N-CA	-5.13	113.40	120.28
1	A	92	ASP	N-CA-C	5.13	117.26	111.11
1	A	70	LYS	CA-C-N	-5.13	112.64	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	LYS	C-N-CA	-5.13	112.64	121.66
1	A	135	SER	CA-C-N	-5.13	114.09	121.42
1	A	135	SER	C-N-CA	-5.13	114.09	121.42
1	A	230	SER	CA-C-N	-5.12	116.03	121.45
1	A	230	SER	C-N-CA	-5.12	116.03	121.45
1	A	167	ILE	N-CA-C	5.11	115.70	107.73
1	B	19	ALA	N-CA-C	5.10	116.65	111.14
1	B	131	GLU	CA-C-O	5.10	125.95	120.55
1	B	92	ASP	N-CA-C	5.09	116.91	111.36
1	B	259	MET	N-CA-C	5.08	120.48	113.97
1	A	215	THR	N-CA-C	5.06	119.31	113.18
1	B	318	GLU	N-CA-C	5.05	121.57	110.80
1	A	239	ALA	N-CA-C	5.05	116.78	111.28
1	B	102	GLY	N-CA-C	5.04	125.12	113.18
1	B	124	ALA	N-CA-C	5.02	116.44	111.07
1	B	178	ALA	N-CA-C	5.02	117.65	111.82
1	A	77	PHE	N-CA-C	5.02	117.13	111.11
1	B	174	GLN	CB-CA-C	-5.01	103.01	110.88
1	A	194	PHE	N-CA-C	5.01	117.63	111.82
1	A	212	LYS	N-CA-C	5.01	121.47	110.80
1	A	304	THR	CA-C-N	-5.01	114.06	123.03
1	A	304	THR	C-N-CA	-5.01	114.06	123.03
1	A	152	MET	N-CA-C	5.00	117.38	111.33

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	256	TYR	Sidechain
1	A	257	TYR	Sidechain
1	A	30	GLY	Peptide
1	A	319	ASP	Peptide
1	A	45	ARG	Sidechain
1	A	94	TYR	Sidechain
1	B	105	THR	Peptide
1	B	148	TYR	Sidechain
1	B	161	ARG	Sidechain
1	B	191	GLU	Peptide
1	B	198	PHE	Sidechain
1	B	204	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	276	ARG	Sidechain
1	B	293	ALA	Peptide
1	B	297	TYR	Sidechain
1	B	50	ARG	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	2513	0	2514	55	0
1	B	2513	0	2514	39	0
2	A	30	0	32	1	0
2	B	30	0	32	9	0
3	A	50	0	0	0	0
3	B	59	0	0	1	0
All	All	5195	0	5092	98	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 10.

All (98) 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:57:PHE:HE1	1:A:63:ARG:HB2	1.49	0.77
1:A:191:GLU:HA	1:A:194:PHE:CE2	2.23	0.73
1:A:6:ARG:H	1:A:283:ASN:HD21	1.40	0.68
1:A:41:LEU:HG	1:A:45:ARG:HH11	1.63	0.63
1:A:253:GLU:HG3	1:A:257:TYR:HE1	1.64	0.62
1:A:90:LEU:HD21	1:A:132:GLU:HG3	1.81	0.62
1:B:198:PHE:HB3	1:B:240:VAL:HG11	1.82	0.61
1:B:164:ASP:HB3	1:A:6:ARG:HG2	1.83	0.61
1:A:253:GLU:HG3	1:A:257:TYR:CE1	2.35	0.61
1:B:161:ARG:HD3	2:B:901:K21:H6	1.84	0.60
1:B:126:LYS:HG2	1:B:137:LEU:HD23	1.85	0.58
1:B:86:LYS:NZ	1:B:90:LEU:HB3	2.20	0.57
1:A:253:GLU:O	1:A:257:TYR:HD1	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HG	1:A:300:ILE:HD11	1.89	0.55
1:A:153:LEU:O	1:A:157:LEU:HB2	2.05	0.55
1:B:119:PRO:HD3	2:B:901:K21:C5	2.37	0.55
1:A:98:HIS:O	1:A:103:ALA:HB2	2.06	0.55
1:A:201:ARG:HB3	1:A:205:HIS:HD2	1.72	0.55
1:B:152:MET:HE3	1:B:195:ILE:HA	1.87	0.55
1:B:61:PHE:HB3	1:B:63:ARG:HG3	1.89	0.55
1:A:249:ALA:HB2	1:A:287:GLU:HG2	1.89	0.55
1:B:96:LEU:HD22	1:B:110:LEU:HD23	1.89	0.54
1:A:284:ILE:O	1:A:288:PHE:HB2	2.08	0.54
1:B:86:LYS:HE3	1:B:94:TYR:CD1	2.42	0.54
1:A:230:SER:OG	1:A:234:GLU:HB2	2.07	0.54
1:B:97:LYS:HE3	1:B:98:HIS:CD2	2.43	0.53
1:A:39:LEU:HD23	1:A:40:THR:HG23	1.90	0.53
1:A:18:ARG:HB2	1:A:60:LEU:HD21	1.91	0.53
1:A:57:PHE:CE1	1:A:63:ARG:HB2	2.39	0.52
1:B:149:TYR:CZ	1:B:153:LEU:HD11	2.43	0.52
1:A:191:GLU:HA	1:A:194:PHE:CZ	2.45	0.52
1:A:6:ARG:H	1:A:283:ASN:ND2	2.06	0.51
1:A:39:LEU:HD12	1:A:77:PHE:CE1	2.45	0.51
1:A:202:SER:O	1:A:205:HIS:HB3	2.10	0.51
1:B:153:LEU:O	1:B:157:LEU:HB2	2.11	0.51
1:B:35:GLU:O	1:B:39:LEU:HB2	2.11	0.50
1:B:285:ARG:NH2	1:B:319:ASP:HB2	2.26	0.50
1:B:279:ILE:HG21	2:B:901:K21:C49	2.40	0.50
1:A:181:GLN:O	1:A:185:LEU:HD13	2.12	0.50
1:A:78:GLU:O	1:A:82:VAL:HG23	2.12	0.50
2:B:901:K21:C24	2:B:901:K21:H101	2.42	0.49
1:B:162:ASP:O	1:B:202:SER:HB3	2.12	0.49
1:A:25:ARG:NH2	1:A:29:LYS:HD3	2.27	0.49
2:B:901:K21:H101	2:B:901:K21:H341	1.95	0.49
1:B:167:ILE:HD13	1:B:208:LYS:HG3	1.95	0.49
1:B:289:ARG:HD2	1:B:320:ASP:C	2.38	0.49
1:A:24:LEU:HD21	1:A:41:LEU:HD22	1.95	0.49
1:B:73:LEU:HD22	1:B:77:PHE:HE2	1.77	0.49
1:B:150:GLN:O	1:B:154:VAL:HG23	2.13	0.48
1:A:121:GLU:O	1:A:125:ILE:HG13	2.13	0.48
1:B:99:ALA:HB1	1:B:106:ASN:HB3	1.95	0.48
1:A:111:THR:HG23	1:A:236:LEU:HA	1.96	0.47
1:A:91:TYR:OH	1:A:271:ARG:HA	2.13	0.47
1:A:210:PHE:CZ	1:A:241:VAL:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:K21:H101	2:B:901:K21:C34	2.44	0.47
2:B:901:K21:C34	2:B:901:K21:C10	2.93	0.47
1:A:81:ILE:HA	1:A:84:LEU:HD12	1.95	0.47
1:A:85:MET:HE3	1:A:85:MET:HB3	1.82	0.47
1:A:95:GLU:HG2	1:A:271:ARG:HD3	1.97	0.47
1:A:25:ARG:HH22	1:A:63:ARG:HH11	1.62	0.46
1:A:28:MET:HB2	1:A:72:GLU:HG3	1.97	0.46
1:B:256:TYR:HE1	1:B:260:LYS:HD2	1.79	0.46
1:A:119:PRO:HD3	2:A:901:K21:C5	2.45	0.46
1:B:152:MET:HE1	1:B:198:PHE:HB2	1.98	0.45
1:B:283:ASN:O	1:B:287:GLU:HB2	2.16	0.45
1:A:129:TYR:C	1:A:129:TYR:CD1	2.94	0.45
1:A:42:LEU:HD12	1:A:81:ILE:HG13	1.99	0.45
1:B:73:LEU:HD22	1:B:77:PHE:CE2	2.53	0.44
1:B:266:ASP:HB3	1:B:308:TYR:OH	2.17	0.44
1:A:86:LYS:HA	1:A:87:PRO:HD3	1.74	0.44
1:B:8:THR:OG1	1:B:281:LEU:HD23	2.18	0.44
1:A:240:VAL:O	1:A:244:ILE:HG12	2.18	0.44
1:A:286:LYS:HB3	1:A:286:LYS:HE2	1.83	0.44
1:B:16:ASP:O	1:B:17:GLU:C	2.60	0.44
1:A:32:GLY:O	1:A:72:GLU:HB3	2.18	0.43
1:A:201:ARG:HB3	1:A:205:HIS:CD2	2.52	0.43
1:B:256:TYR:CD1	1:B:256:TYR:C	2.97	0.43
1:A:270:ILE:O	1:A:274:VAL:HG23	2.18	0.43
1:A:25:ARG:CZ	1:A:29:LYS:HD3	2.49	0.43
1:B:248:PRO:HA	1:B:284:ILE:HG12	2.00	0.42
1:A:234:GLU:O	1:A:238:LEU:HB2	2.19	0.42
1:B:6:ARG:H	1:B:283:ASN:ND2	2.16	0.42
2:B:901:K21:C10	2:B:901:K21:H342	2.50	0.42
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.82	0.42
1:A:222:GLU:H	1:A:222:GLU:HG3	1.67	0.42
1:A:237:LEU:O	1:A:241:VAL:HG23	2.20	0.42
1:A:18:ARG:O	1:A:22:GLU:HG2	2.20	0.41
1:B:161:ARG:HD3	2:B:901:K21:C6	2.48	0.41
1:A:295:SER:O	1:A:296:LEU:C	2.63	0.41
1:B:124:ALA:O	1:B:128:VAL:HG23	2.21	0.41
1:B:289:ARG:HH11	1:B:320:ASP:HA	1.86	0.41
1:B:282:PHE:CD1	1:B:282:PHE:C	2.99	0.41
1:B:36:GLU:HB2	3:B:932:HOH:O	2.21	0.41
1:A:201:ARG:HB2	1:A:206:LEU:HG	2.02	0.41
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TYR:O	1:A:214:MET:C	2.64	0.40
1:A:219:PHE:HB2	1:A:223:GLU:HG3	2.03	0.40
1:B:239:ALA:O	1:B:240:VAL:C	2.64	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	316/320 (99%)	268 (85%)	40 (13%)	8 (2%)	4	23
1	B	316/320 (99%)	271 (86%)	36 (11%)	9 (3%)	4	21
All	All	632/640 (99%)	539 (85%)	76 (12%)	17 (3%)	4	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	ASP
1	B	192	GLU
1	B	232	ASN
1	B	318	GLU
1	A	191	GLU
1	A	232	ASN
1	B	32	GLY
1	B	166	GLY
1	B	187	TRP
1	A	102	GLY
1	A	159	ALA
1	B	102	GLY
1	A	134	GLY
1	A	227	ARG
1	B	17	GLU

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Mol	Chain	Res	Type
1	A	47	ASN
1	A	38	ILE

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	271/272 (100%)	238 (88%)	33 (12%)	5	21
1	B	271/272 (100%)	247 (91%)	24 (9%)	9	34
All	All	542/544 (100%)	485 (90%)	57 (10%)	6	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	LEU
1	B	10	THR
1	B	17	GLU
1	B	26	LYS
1	B	31	LEU
1	B	33	THR
1	B	39	LEU
1	B	90	LEU
1	B	144	ASP
1	B	160	ASN
1	B	167	ILE
1	B	168	ASP
1	B	193	LYS
1	B	196	THR
1	B	216	ILE
1	B	228	GLU
1	B	229	THR
1	B	237	LEU
1	B	256	TYR
1	B	264	THR
1	B	303	ASP

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Mol	Chain	Res	Type
1	B	312	LEU
1	B	314	LEU
1	B	318	GLU
1	A	4	VAL
1	A	5	LEU
1	A	6	ARG
1	A	10	THR
1	A	17	GLU
1	A	24	LEU
1	A	33	THR
1	A	36	GLU
1	A	37	SER
1	A	72	GLU
1	A	78	GLU
1	A	85	MET
1	A	92	ASP
1	A	96	LEU
1	A	120	GLU
1	A	127	GLN
1	A	157	LEU
1	A	168	ASP
1	A	184	GLU
1	A	186	LYS
1	A	189	THR
1	A	193	LYS
1	A	217	SER
1	A	221	ILE
1	A	223	GLU
1	A	226	ASP
1	A	237	LEU
1	A	264	THR
1	A	295	SER
1	A	305	SER
1	A	312	LEU
1	A	318	GLU
1	A	319	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	B	181	GLN

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Mol	Chain	Res	Type
1	B	283	ASN
1	B	291	ASN
1	A	51	GLN
1	A	160	ASN
1	A	177	GLN
1	A	205	HIS
1	A	220	GLN
1	A	283	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](#)

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$
2	K21	B	901	-	32,33,33	1.25	3 (9%)	40,44,44	2.42	9 (22%)
2	K21	A	901	-	32,33,33	1.29	3 (9%)	40,44,44	1.62	7 (17%)

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
2	K21	B	901	-	-	6/13/35/35	1/3/4/4
2	K21	A	901	-	-	4/13/35/35	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	K21	C4-S14	4.26	1.81	1.77
2	A	901	K21	C4-S14	3.54	1.81	1.77
2	A	901	K21	C22-C21	3.35	1.58	1.51
2	A	901	K21	C21-N11	3.14	1.41	1.35
2	B	901	K21	C22-C21	2.41	1.56	1.51
2	B	901	K21	C24-C22	2.01	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	K21	C13-S14-C4	-7.70	91.81	102.71
2	B	901	K21	C24-C22-C21	7.62	121.98	111.22
2	B	901	K21	C10-N11-C12	6.91	121.33	113.92
2	A	901	K21	C13-S14-C4	-5.37	95.11	102.71
2	A	901	K21	C24-C22-C21	3.41	116.04	111.22
2	A	901	K21	C24-N27-C30	3.31	120.05	111.24
2	B	901	K21	C3-C10-N11	3.28	119.61	112.75
2	B	901	K21	C33-C34-N27	3.23	116.31	111.08
2	A	901	K21	C24-N27-C34	3.17	119.69	111.24
2	B	901	K21	C2-C3-C4	2.97	120.98	118.17
2	A	901	K21	C12-C13-S14	2.65	117.36	114.26
2	A	901	K21	C10-N11-C12	2.61	116.71	113.92
2	B	901	K21	C52-C43-C32	-2.33	110.17	114.45
2	B	901	K21	C5-C4-S14	2.33	123.47	116.89
2	B	901	K21	C22-C24-N27	2.22	122.12	113.12
2	A	901	K21	C33-C34-N27	-2.05	107.76	111.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	K21	C21-C22-C24-N27
2	B	901	K21	C31-C32-C43-C52

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Mol	Chain	Res	Type	Atoms
2	B	901	K21	C33-C32-C43-C52
2	A	901	K21	C21-C22-C24-N27
2	A	901	K21	C22-C24-N27-C34
2	A	901	K21	C22-C24-N27-C30
2	B	901	K21	O23-C21-C22-C24
2	B	901	K21	N11-C21-C22-C24
2	B	901	K21	O23-C21-N11-C10
2	A	901	K21	O23-C21-C22-C24

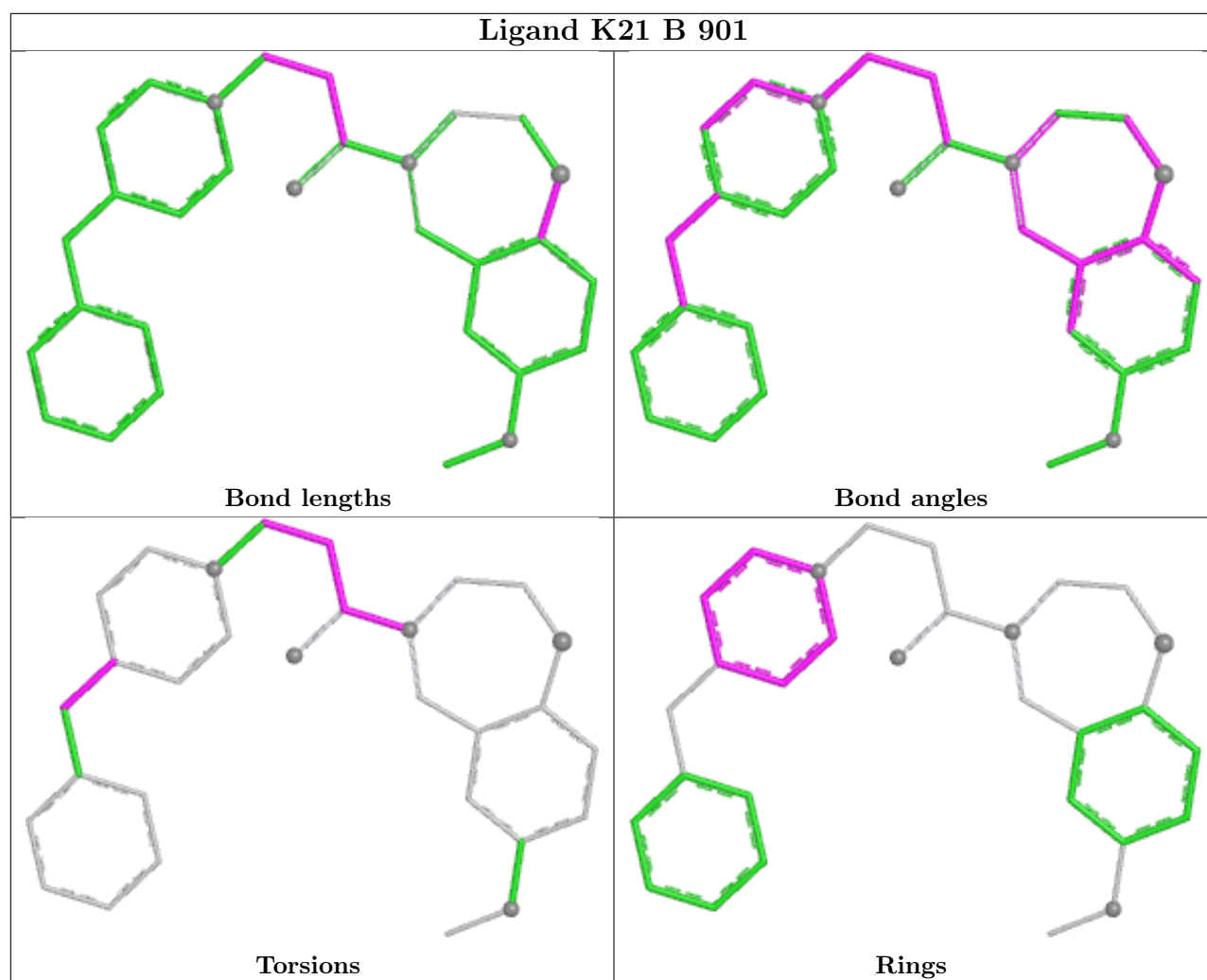
All (1) ring outliers are listed below:

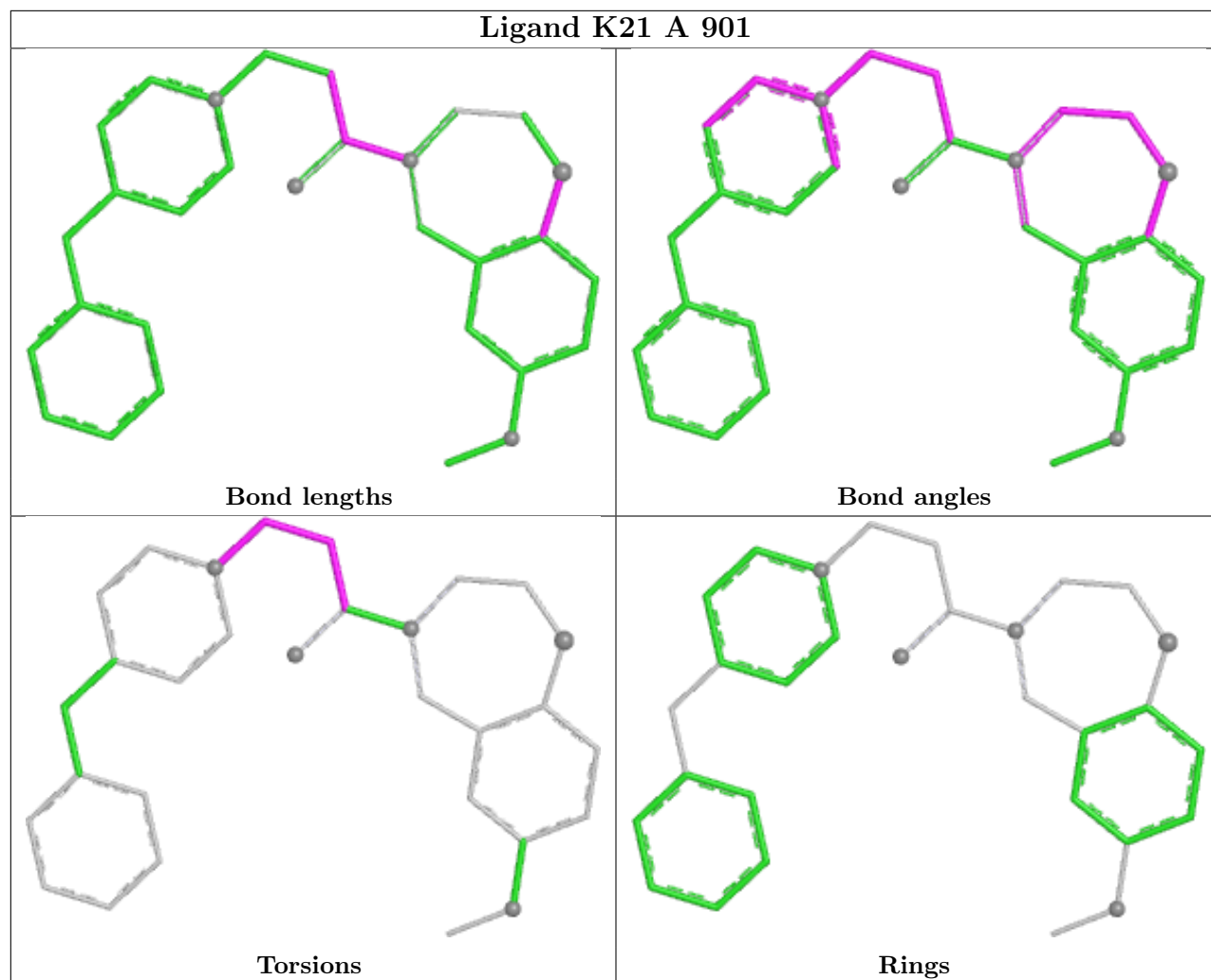
Mol	Chain	Res	Type	Atoms
2	B	901	K21	C30-C31-C32-C33-C34-N27

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	K21	9	0
2	A	901	K21	1	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.





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.