



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:10 PM UTC

PDB ID : 3M2K / pdb_00003m2k
Title : Crystal Structure of fluorescein-labeled Class A -beta lactamase PenP in complex with cefotaxime
Authors : Zhao, Y.X.; Leung, Y.C.; Wong, W.T.
Deposited on : 2010-03-07
Resolution : 3.50 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

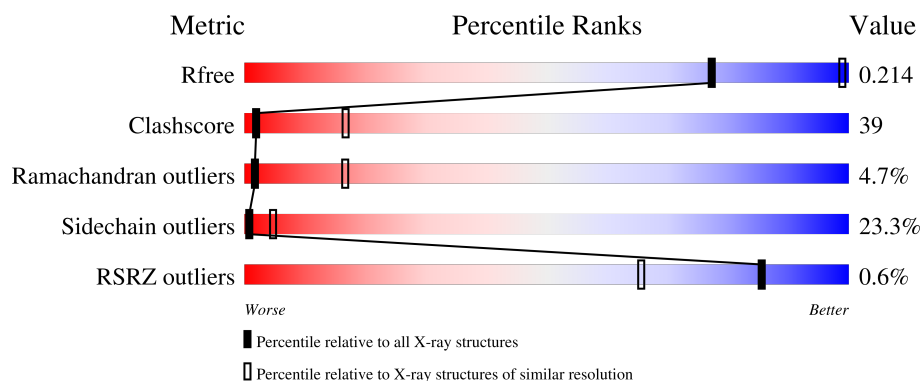
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	16% 39% 31% 9% 5%
1	B	257	18% 42% 29% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3964 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.

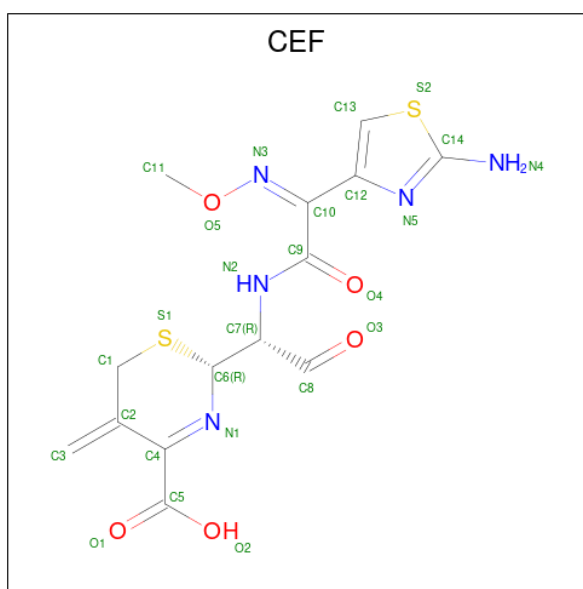
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1910	1197	330	380	3			
1	B	251	Total	C	N	O	S	0	0	0
			1963	1232	341	387	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	CYS	GLU	engineered mutation	UNP P00808
B	166	CYS	GLU	engineered mutation	UNP P00808

- Molecule 2 is CEFOTAXIME, C3' cleaved, open, bound form (CCD ID: CEF) (formula: C₁₄H₁₅N₅O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

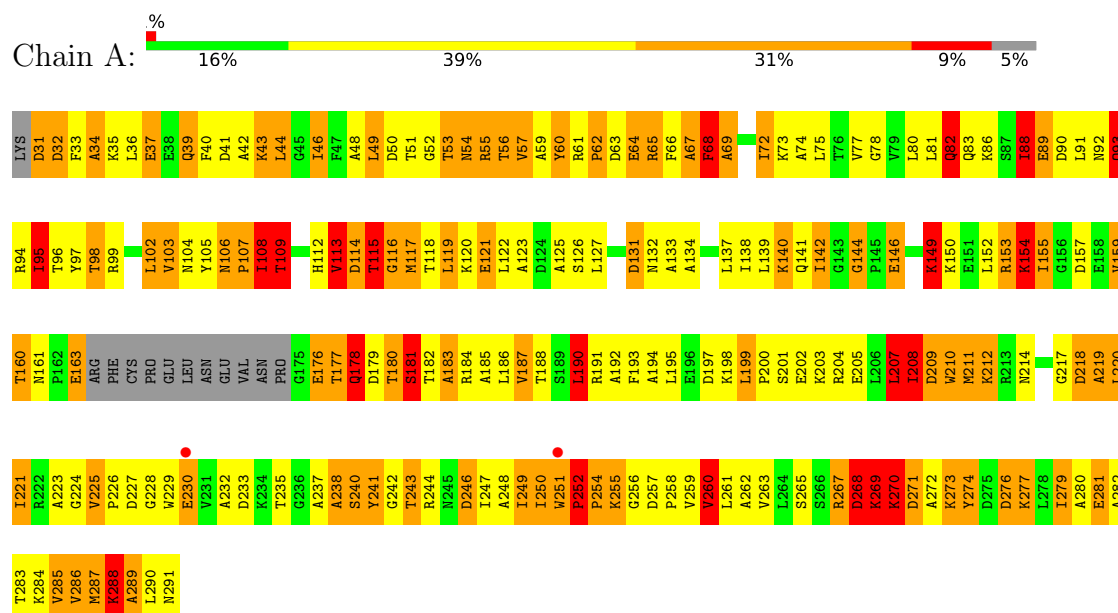
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	19	Total	O	0	0
			19	19		

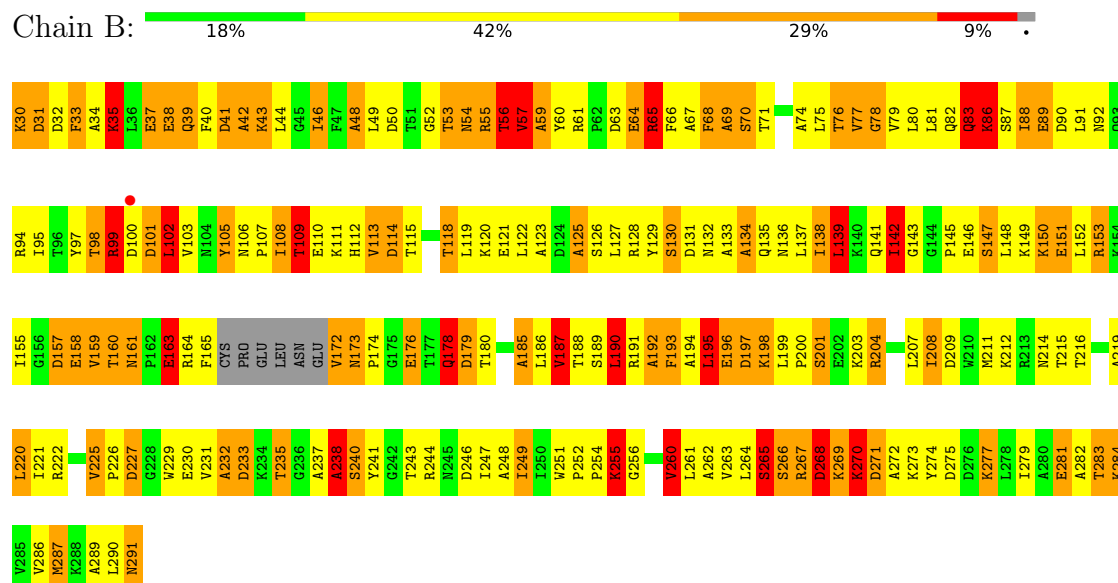
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.54Å 91.52Å 66.30Å 90.00° 104.22° 90.00°	Depositor
Resolution (Å)	40.23 – 3.50 40.23 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.23-3.50) 95.0 (40.23-3.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.236 0.181 , 0.214	Depositor DCC
R_{free} test set	308 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3964	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	2.85	145/1936 (7.5%)	2.32	106/2617 (4.1%)
1	B	2.57	127/1991 (6.4%)	2.20	86/2691 (3.2%)
All	All	2.71	272/3927 (6.9%)	2.26	192/5308 (3.6%)

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	9
1	B	0	10
All	All	0	19

All (272) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLN	C-N	17.03	1.57	1.33
1	A	61	ARG	C-O	14.72	1.31	1.23
1	A	74	ALA	CA-CB	-13.61	1.32	1.53
1	A	125	ALA	CA-CB	-12.53	1.32	1.53
1	A	181	SER	CA-C	-12.30	1.42	1.53
1	A	194	ALA	CA-CB	-11.94	1.33	1.53
1	B	125	ALA	CA-CB	-11.80	1.35	1.53
1	A	208	ILE	CA-CB	-11.48	1.38	1.54
1	A	126	SER	CA-C	-11.47	1.37	1.52
1	A	57	VAL	C-N	10.97	1.50	1.33
1	A	155	ILE	N-CA	10.95	1.57	1.46
1	A	180	THR	C-O	-10.65	1.10	1.23
1	B	208	ILE	N-CA	-10.57	1.34	1.46
1	B	55	ARG	N-CA	10.06	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	TYR	CA-C	9.95	1.64	1.52
1	A	86	LYS	C-O	9.77	1.36	1.23
1	A	183	ALA	CA-CB	-9.47	1.38	1.53
1	A	88	ILE	CA-CB	-9.25	1.43	1.54
1	B	31	ASP	CA-C	8.95	1.65	1.52
1	A	252	PRO	C-N	8.94	1.54	1.33
1	A	146	GLU	C-O	8.81	1.35	1.24
1	A	248	ALA	CA-CB	-8.78	1.38	1.53
1	B	138	ILE	CA-CB	-8.77	1.43	1.54
1	A	183	ALA	CA-C	-8.74	1.41	1.52
1	B	57	VAL	C-N	8.72	1.46	1.33
1	A	280	ALA	CA-CB	-8.64	1.39	1.53
1	B	113	VAL	CA-C	-8.57	1.40	1.52
1	A	117	MET	N-CA	8.55	1.56	1.46
1	B	160	THR	C-O	-8.42	1.13	1.23
1	A	201	SER	CA-C	8.32	1.64	1.52
1	A	180	THR	CA-C	-8.17	1.42	1.52
1	B	43	LYS	CA-C	8.15	1.63	1.52
1	A	257	ASP	C-O	8.08	1.34	1.23
1	B	214	ASN	N-CA	8.05	1.56	1.46
1	A	67	ALA	CA-CB	-8.04	1.40	1.53
1	A	131	ASP	N-CA	-8.03	1.36	1.46
1	A	31	ASP	N-CA	8.00	1.61	1.46
1	A	34	ALA	CA-CB	-7.98	1.40	1.53
1	B	248	ALA	CA-CB	-7.96	1.40	1.53
1	A	57	VAL	CA-CB	-7.91	1.44	1.54
1	A	286	VAL	CA-C	7.89	1.62	1.52
1	A	107	PRO	N-CA	-7.84	1.37	1.47
1	A	227	ASP	CA-C	7.80	1.62	1.52
1	B	176	GLU	N-CA	7.73	1.55	1.46
1	B	284	LYS	CA-C	7.73	1.63	1.52
1	A	46	ILE	CA-CB	-7.66	1.44	1.54
1	A	89	GLU	CD-OE2	7.61	1.39	1.25
1	B	41	ASP	C-O	7.60	1.34	1.23
1	A	240	SER	C-O	7.59	1.34	1.23
1	A	48	ALA	CA-C	-7.53	1.43	1.52
1	B	136	ASN	C-O	7.51	1.32	1.24
1	A	43	LYS	N-CA	-7.50	1.36	1.46
1	B	251	TRP	CA-CB	-7.49	1.41	1.52
1	A	235	THR	C-N	7.41	1.42	1.33
1	A	83	GLN	C-N	7.41	1.44	1.33
1	A	190	LEU	C-O	-7.38	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ASP	CB-CG	7.37	1.70	1.52
1	A	134	ALA	CA-CB	-7.30	1.42	1.53
1	B	88	ILE	CA-CB	-7.27	1.44	1.54
1	A	116	GLY	N-CA	7.23	1.51	1.45
1	A	88	ILE	N-CA	-7.19	1.38	1.46
1	B	262	ALA	CA-CB	-7.18	1.42	1.53
1	B	279	ILE	C-O	7.17	1.32	1.24
1	A	46	ILE	C-O	-7.15	1.16	1.24
1	A	69	ALA	CA-C	7.13	1.62	1.52
1	B	163	GLU	N-CA	7.07	1.55	1.45
1	A	279	ILE	N-CA	7.03	1.54	1.46
1	B	102	LEU	C-O	6.99	1.32	1.23
1	A	132	ASN	N-CA	6.98	1.55	1.46
1	B	176	GLU	CA-C	6.96	1.61	1.52
1	A	89	GLU	CA-CB	-6.92	1.41	1.53
1	B	233	ASP	C-O	-6.92	1.15	1.23
1	B	68	PHE	N-CA	6.91	1.55	1.46
1	A	235	THR	N-CA	-6.91	1.37	1.45
1	B	209	ASP	C-O	-6.89	1.16	1.24
1	A	274	TYR	N-CA	6.87	1.54	1.45
1	B	208	ILE	CA-CB	-6.82	1.46	1.54
1	A	68	PHE	N-CA	6.80	1.55	1.46
1	A	89	GLU	CD-OE1	6.79	1.38	1.25
1	A	248	ALA	CA-C	-6.74	1.44	1.52
1	A	41	ASP	C-O	6.74	1.32	1.23
1	B	128	ARG	CZ-NH2	-6.73	1.24	1.33
1	A	281	GLU	CD-OE2	6.71	1.38	1.25
1	B	70	SER	N-CA	6.71	1.54	1.46
1	A	126	SER	C-O	-6.69	1.15	1.24
1	B	114	ASP	CG-OD1	6.69	1.38	1.25
1	A	210	TRP	CA-CB	-6.69	1.42	1.53
1	B	41	ASP	CG-OD1	6.66	1.38	1.25
1	A	235	THR	C-O	6.64	1.32	1.23
1	A	205	GLU	CA-C	6.63	1.62	1.52
1	A	284	LYS	C-O	6.59	1.31	1.24
1	B	263	VAL	CA-CB	-6.58	1.45	1.54
1	B	185	ALA	CA-CB	-6.57	1.42	1.53
1	A	185	ALA	CA-CB	-6.56	1.42	1.53
1	A	221	ILE	N-CA	6.55	1.54	1.46
1	B	139	LEU	CA-CB	-6.53	1.42	1.53
1	B	112	HIS	N-CA	6.47	1.56	1.46
1	B	196	GLU	CA-C	6.46	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	ASP	CG-OD1	6.45	1.37	1.25
1	B	134	ALA	CA-C	6.44	1.61	1.52
1	A	193	PHE	N-CA	6.42	1.54	1.46
1	A	185	ALA	CA-C	-6.42	1.44	1.52
1	B	231	VAL	C-O	-6.41	1.17	1.24
1	A	56	THR	C-O	6.40	1.31	1.23
1	B	222	ARG	N-CA	6.39	1.54	1.46
1	A	88	ILE	CA-C	-6.38	1.45	1.52
1	A	176	GLU	C-O	6.38	1.31	1.24
1	B	112	HIS	C-O	6.37	1.30	1.23
1	B	267	ARG	CA-C	6.35	1.60	1.53
1	B	64	GLU	CG-CD	6.35	1.68	1.52
1	B	151	GLU	CA-C	-6.35	1.44	1.52
1	A	89	GLU	N-CA	-6.33	1.38	1.46
1	A	204	ARG	C-O	6.33	1.31	1.24
1	A	207	LEU	CA-C	-6.32	1.44	1.52
1	A	268	ASP	N-CA	-6.32	1.37	1.46
1	B	77	VAL	N-CA	6.32	1.54	1.46
1	B	114	ASP	C-O	6.28	1.31	1.23
1	B	284	LYS	N-CA	-6.28	1.38	1.46
1	A	123	ALA	N-CA	6.26	1.54	1.46
1	A	163	GLU	CG-CD	6.24	1.67	1.52
1	B	284	LYS	C-O	6.22	1.31	1.24
1	A	271	ASP	CA-C	6.20	1.61	1.52
1	B	212	LYS	C-O	-6.19	1.16	1.24
1	B	275	ASP	C-O	-6.19	1.17	1.24
1	B	55	ARG	NE-CZ	6.19	1.39	1.33
1	A	157	ASP	CA-C	-6.17	1.45	1.53
1	B	33	PHE	CA-C	-6.12	1.44	1.52
1	B	126	SER	C-O	-6.11	1.16	1.24
1	B	48	ALA	CA-C	-6.08	1.45	1.52
1	A	214	ASN	CA-C	-6.08	1.45	1.52
1	B	119	LEU	CA-C	-6.07	1.44	1.52
1	A	273	LYS	CA-C	-6.06	1.45	1.52
1	B	229	TRP	N-CA	6.05	1.53	1.46
1	A	185	ALA	C-O	-6.04	1.16	1.24
1	A	177	THR	N-CA	6.04	1.53	1.46
1	A	197	ASP	N-CA	-6.02	1.38	1.46
1	A	144	GLY	N-CA	6.02	1.52	1.44
1	B	219	ALA	N-CA	-6.01	1.38	1.46
1	A	238	ALA	C-N	6.01	1.41	1.33
1	B	256	GLY	N-CA	6.00	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	GLU	CA-CB	6.00	1.63	1.53
1	A	227	ASP	N-CA	5.99	1.53	1.46
1	B	287	MET	CG-SD	5.98	1.95	1.80
1	B	122	LEU	CA-C	-5.97	1.44	1.52
1	B	54	ASN	C-N	5.95	1.42	1.33
1	B	271	ASP	CG-OD2	5.95	1.36	1.25
1	B	63	ASP	CA-C	5.94	1.60	1.52
1	A	199	LEU	CA-C	5.92	1.60	1.52
1	B	260	VAL	CB-CG2	-5.91	1.33	1.52
1	A	150	LYS	CA-C	-5.90	1.44	1.52
1	B	160	THR	N-CA	5.89	1.53	1.46
1	B	240	SER	C-N	-5.89	1.25	1.33
1	B	89	GLU	CA-CB	5.88	1.62	1.53
1	A	188	THR	C-O	-5.86	1.16	1.24
1	A	97	TYR	C-O	5.85	1.31	1.23
1	B	231	VAL	CA-CB	-5.84	1.46	1.54
1	A	66	PHE	CA-C	-5.83	1.45	1.52
1	B	132	ASN	N-CA	-5.83	1.39	1.46
1	B	221	ILE	CB-CG2	-5.82	1.33	1.52
1	A	146	GLU	CA-C	5.82	1.60	1.52
1	A	268	ASP	CG-OD2	5.81	1.36	1.25
1	B	151	GLU	C-O	-5.81	1.16	1.24
1	A	267	ARG	CZ-NH1	5.80	1.40	1.32
1	A	146	GLU	N-CA	5.79	1.53	1.46
1	B	251	TRP	CA-C	-5.77	1.45	1.52
1	A	228	GLY	C-O	5.77	1.30	1.24
1	A	177	THR	CA-CB	5.75	1.63	1.53
1	B	164	ARG	CA-C	5.75	1.60	1.52
1	A	217	GLY	C-O	-5.74	1.16	1.23
1	B	120	LYS	N-CA	5.73	1.53	1.46
1	B	267	ARG	CD-NE	5.72	1.54	1.46
1	A	146	GLU	CB-CG	5.72	1.69	1.52
1	A	246	ASP	CG-OD2	5.71	1.36	1.25
1	A	160	THR	C-O	-5.71	1.17	1.23
1	A	44	LEU	CG-CD1	-5.70	1.33	1.52
1	B	178	GLN	CD-OE1	5.69	1.34	1.23
1	A	218	ASP	N-CA	-5.68	1.38	1.46
1	B	269	LYS	CA-C	5.68	1.60	1.52
1	A	153	ARG	CZ-NH1	5.67	1.40	1.32
1	B	40	PHE	C-O	5.66	1.31	1.24
1	B	157	ASP	C-O	5.66	1.30	1.23
1	A	131	ASP	CG-OD1	5.65	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	PRO	C-O	-5.65	1.16	1.24
1	B	249	ILE	N-CA	5.63	1.52	1.46
1	B	193	PHE	CE2-CZ	-5.63	1.21	1.38
1	A	153	ARG	NE-CZ	5.62	1.39	1.33
1	B	216	THR	CA-C	-5.62	1.45	1.52
1	B	63	ASP	N-CA	-5.61	1.39	1.46
1	A	181	SER	C-O	-5.61	1.17	1.24
1	A	62	PRO	N-CA	-5.60	1.39	1.47
1	B	76	THR	C-O	-5.57	1.17	1.24
1	A	279	ILE	CA-C	5.56	1.59	1.52
1	B	64	GLU	N-CA	-5.54	1.39	1.46
1	A	116	GLY	C-O	5.54	1.29	1.23
1	B	281	GLU	C-O	-5.53	1.17	1.24
1	A	93	GLN	CD-OE1	5.49	1.33	1.23
1	B	138	ILE	C-O	-5.49	1.18	1.24
1	B	86	LYS	C-N	5.48	1.40	1.33
1	B	194	ALA	C-O	-5.47	1.17	1.24
1	A	246	ASP	N-CA	-5.46	1.39	1.46
1	A	91	LEU	C-O	5.46	1.31	1.24
1	A	177	THR	C-O	5.46	1.31	1.23
1	A	95	ILE	C-O	5.46	1.30	1.24
1	A	90	ASP	CG-OD2	5.45	1.35	1.25
1	B	189	SER	CA-C	-5.45	1.46	1.52
1	A	178	GLN	C-O	-5.45	1.17	1.24
1	A	270	LYS	CG-CD	5.42	1.68	1.52
1	B	78	GLY	N-CA	-5.42	1.38	1.45
1	B	35	LYS	C-O	-5.41	1.17	1.24
1	A	256	GLY	N-CA	5.40	1.52	1.45
1	A	161	ASN	CA-CB	-5.40	1.47	1.53
1	B	109	THR	C-O	5.39	1.30	1.24
1	B	54	ASN	C-O	5.38	1.30	1.24
1	A	40	PHE	C-O	-5.36	1.16	1.24
1	B	230	GLU	CD-OE2	5.35	1.35	1.25
1	B	61	ARG	CZ-NH1	5.34	1.40	1.32
1	B	41	ASP	CG-OD2	5.33	1.35	1.25
1	A	49	LEU	CA-C	-5.32	1.46	1.52
1	A	286	VAL	C-O	5.32	1.30	1.24
1	B	34	ALA	CA-C	5.30	1.59	1.52
1	A	221	ILE	CA-CB	5.29	1.62	1.54
1	B	75	LEU	CA-C	-5.29	1.45	1.52
1	A	217	GLY	C-N	-5.28	1.25	1.33
1	B	283	THR	N-CA	5.27	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	LEU	C-O	-5.25	1.18	1.23
1	B	142	ILE	CA-C	-5.25	1.46	1.52
1	B	102	LEU	CA-C	5.23	1.59	1.52
1	A	205	GLU	N-CA	5.23	1.52	1.46
1	B	76	THR	CA-CB	-5.22	1.45	1.53
1	B	68	PHE	C-O	-5.21	1.17	1.24
1	B	145	PRO	C-O	5.20	1.30	1.24
1	B	215	THR	N-CA	5.20	1.52	1.46
1	B	251	TRP	C-N	5.19	1.39	1.33
1	A	93	GLN	CA-C	-5.18	1.46	1.52
1	B	187	VAL	CA-CB	5.18	1.60	1.54
1	A	40	PHE	CA-C	-5.17	1.46	1.52
1	B	138	ILE	N-CA	-5.17	1.40	1.46
1	B	43	LYS	C-O	5.16	1.29	1.24
1	B	197	ASP	N-CA	-5.16	1.38	1.46
1	A	221	ILE	CA-C	5.16	1.59	1.52
1	A	113	VAL	C-O	5.15	1.30	1.24
1	B	275	ASP	CA-C	-5.15	1.46	1.52
1	A	202	GLU	N-CA	-5.15	1.39	1.46
1	B	111	LYS	CA-C	-5.14	1.45	1.52
1	A	55	ARG	NE-CZ	5.12	1.38	1.33
1	B	176	GLU	CG-CD	5.12	1.64	1.52
1	A	141	GLN	C-O	-5.11	1.18	1.24
1	B	97	TYR	C-O	5.10	1.30	1.24
1	A	268	ASP	CG-OD1	5.10	1.35	1.25
1	B	255	LYS	C-O	-5.09	1.18	1.23
1	A	99	ARG	CD-NE	5.09	1.53	1.46
1	B	277	LYS	C-O	5.08	1.30	1.24
1	B	123	ALA	CA-CB	-5.08	1.45	1.53
1	A	224	GLY	C-N	-5.08	1.29	1.33
1	B	142	ILE	C-O	-5.08	1.18	1.24
1	A	277	LYS	C-O	-5.08	1.17	1.24
1	A	178	GLN	CA-C	-5.07	1.46	1.52
1	B	69	ALA	C-O	-5.07	1.19	1.24
1	B	141	GLN	C-O	-5.07	1.17	1.24
1	A	241	TYR	CG-CD2	5.06	1.50	1.39
1	A	99	ARG	NE-CZ	5.05	1.38	1.33
1	B	157	ASP	CA-C	5.04	1.59	1.53
1	A	268	ASP	C-O	5.04	1.30	1.24
1	A	56	THR	CB-CG2	5.04	1.69	1.52
1	B	132	ASN	CA-CB	-5.03	1.45	1.53
1	B	270	LYS	CA-C	-5.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	THR	CA-C	5.03	1.59	1.52
1	A	80	LEU	C-O	-5.02	1.18	1.24
1	B	235	THR	CA-C	5.02	1.58	1.52
1	A	60	TYR	CE2-CZ	5.02	1.50	1.38
1	A	149	LYS	CE-NZ	5.01	1.64	1.49
1	B	155	ILE	N-CA	5.01	1.52	1.46

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	PRO	O-C-N	-15.42	103.26	121.46
1	B	57	VAL	O-C-N	-12.47	109.82	122.92
1	B	83	GLN	O-C-N	-11.75	104.14	122.93
1	B	31	ASP	N-CA-C	-11.32	98.73	112.54
1	A	61	ARG	CA-C-N	-10.66	108.79	119.56
1	A	61	ARG	C-N-CA	-10.66	108.79	119.56
1	B	268	ASP	N-CA-C	10.52	133.20	110.80
1	A	57	VAL	CA-C-N	-10.40	105.88	122.73
1	A	57	VAL	C-N-CA	-10.40	105.88	122.73
1	A	141	GLN	N-CA-C	10.28	122.49	111.28
1	B	161	ASN	CA-C-N	-9.67	109.21	120.13
1	B	161	ASN	C-N-CA	-9.67	109.21	120.13
1	A	46	ILE	N-CA-C	9.65	122.26	108.17
1	A	257	ASP	N-CA-C	9.54	121.76	109.93
1	A	106	ASN	CA-C-N	-9.31	108.70	118.85
1	A	106	ASN	C-N-CA	-9.31	108.70	118.85
1	A	54	ASN	N-CA-C	8.93	123.83	113.38
1	A	183	ALA	N-CA-C	-8.88	100.19	111.02
1	B	252	PRO	CA-C-N	8.67	130.68	119.84
1	B	252	PRO	C-N-CA	8.67	130.68	119.84
1	A	204	ARG	N-CA-C	-8.62	101.97	111.36
1	A	181	SER	N-CA-CB	8.27	117.94	109.51
1	B	128	ARG	NE-CZ-NH2	-8.24	111.79	119.20
1	A	92	ASN	N-CA-C	8.21	122.72	112.87
1	A	61	ARG	CB-CA-C	-8.17	105.40	111.20
1	B	163	GLU	N-CA-C	8.12	125.41	114.12
1	B	204	ARG	N-CA-C	-7.85	102.81	111.36
1	B	108	ILE	CA-C-O	7.83	127.66	120.30
1	A	285	VAL	CB-CA-C	-7.77	102.03	111.97
1	B	136	ASN	N-CA-C	7.70	120.65	111.33
1	A	57	VAL	N-CA-C	7.61	118.85	107.75
1	A	150	LYS	N-CA-C	-7.57	103.84	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASN	N-CA-C	7.57	122.26	108.94
1	B	260	VAL	CB-CA-C	7.48	121.25	110.33
1	A	186	LEU	CA-C-N	-7.44	109.85	120.42
1	A	186	LEU	C-N-CA	-7.44	109.85	120.42
1	B	75	LEU	N-CA-C	-7.43	102.87	112.23
1	A	82	GLN	N-CA-C	-7.37	102.41	111.33
1	B	248	ALA	N-CA-C	7.13	119.01	108.60
1	A	212	LYS	CA-C-N	-7.12	107.95	121.54
1	A	212	LYS	C-N-CA	-7.12	107.95	121.54
1	A	277	LYS	N-CA-C	-7.12	104.34	113.16
1	A	142	ILE	O-C-N	7.10	128.48	122.09
1	B	42	ALA	N-CA-C	7.05	120.99	109.85
1	A	223	ALA	N-CA-C	7.00	121.27	112.87
1	A	181	SER	CA-C-O	-6.96	115.18	120.19
1	B	187	VAL	N-CA-CB	6.95	119.15	110.47
1	B	192	ALA	N-CA-C	-6.85	102.18	112.04
1	A	141	GLN	CA-C-N	-6.84	112.56	122.28
1	A	141	GLN	C-N-CA	-6.84	112.56	122.28
1	A	207	LEU	CA-C-N	-6.83	109.67	121.97
1	A	207	LEU	C-N-CA	-6.83	109.67	121.97
1	A	240	SER	CA-CB-OG	-6.76	97.58	111.10
1	B	138	ILE	N-CA-C	-6.67	104.35	110.82
1	A	65	ARG	NE-CZ-NH2	6.67	125.20	119.20
1	A	180	THR	CA-C-O	-6.67	114.04	121.51
1	B	128	ARG	NE-CZ-NH1	6.61	128.11	121.50
1	B	188	THR	O-C-N	6.61	129.13	122.12
1	A	33	PHE	N-CA-C	6.57	119.27	111.71
1	A	39	GLN	CA-C-N	-6.54	112.21	122.49
1	A	39	GLN	C-N-CA	-6.54	112.21	122.49
1	B	110	GLU	N-CA-C	-6.53	105.30	113.20
1	B	227	ASP	N-CA-C	6.51	119.20	110.35
1	B	55	ARG	N-CA-CB	6.46	119.72	109.51
1	B	105	TYR	N-CA-C	6.41	117.94	107.23
1	A	115	THR	CB-CA-C	-6.40	100.21	110.84
1	B	88	ILE	CB-CA-C	-6.40	101.89	112.26
1	A	108	ILE	CB-CA-C	-6.39	101.74	112.16
1	B	220	LEU	CD1-CG-CD2	-6.37	96.78	110.80
1	B	178	GLN	CB-CA-C	6.36	120.96	109.83
1	B	195	LEU	N-CA-CB	-6.35	99.75	110.49
1	A	250	ILE	N-CA-C	-6.35	99.05	108.45
1	B	197	ASP	CB-CA-C	-6.34	102.01	111.72
1	B	65	ARG	N-CA-C	6.33	119.64	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ILE	CA-C-N	-6.32	111.26	122.07
1	B	95	ILE	C-N-CA	-6.32	111.26	122.07
1	A	75	LEU	N-CA-C	-6.32	105.40	113.23
1	B	176	GLU	CA-C-N	-6.30	112.77	122.60
1	B	176	GLU	C-N-CA	-6.30	112.77	122.60
1	B	152	LEU	N-CA-C	-6.28	103.72	112.45
1	B	89	GLU	CA-C-N	6.28	133.53	121.54
1	B	89	GLU	C-N-CA	6.28	133.53	121.54
1	B	33	PHE	N-CA-C	-6.24	104.73	112.90
1	B	189	SER	N-CA-C	6.22	117.86	111.14
1	B	143	GLY	CA-C-O	-6.21	112.81	119.27
1	B	108	ILE	CB-CA-C	-6.17	105.38	111.30
1	A	204	ARG	NE-CZ-NH1	-6.13	115.37	121.50
1	A	122	LEU	CA-C-O	-6.11	113.94	120.42
1	B	161	ASN	CB-CA-C	-6.10	99.78	111.12
1	B	190	LEU	N-CA-C	6.05	118.37	111.11
1	A	211	MET	CG-SD-CE	6.03	114.17	100.90
1	A	202	GLU	N-CA-CB	-6.02	101.02	110.30
1	B	34	ALA	N-CA-C	-6.01	104.06	111.40
1	A	185	ALA	N-CA-C	-6.00	104.68	112.23
1	A	233	ASP	N-CA-C	6.00	118.29	109.24
1	A	204	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	48	ALA	N-CA-C	-5.96	100.08	109.50
1	A	83	GLN	O-C-N	-5.92	114.00	122.41
1	B	277	LYS	CA-CB-CG	5.92	125.94	114.10
1	B	240	SER	N-CA-C	-5.91	103.14	110.41
1	B	146	GLU	N-CA-C	-5.89	106.09	113.28
1	A	73	LYS	N-CA-C	-5.87	104.83	112.23
1	B	37	GLU	CA-C-O	-5.87	114.62	120.90
1	B	248	ALA	CA-C-O	-5.82	115.21	121.38
1	A	154	LYS	N-CA-C	5.81	123.18	110.80
1	A	69	ALA	O-C-N	-5.78	114.90	122.59
1	A	177	THR	N-CA-CB	5.77	119.04	110.49
1	A	217	GLY	N-CA-C	5.76	126.83	113.18
1	B	74	ALA	N-CA-C	5.72	117.52	111.28
1	B	55	ARG	CB-CA-C	-5.72	101.92	110.16
1	B	232	ALA	CA-C-O	-5.72	114.53	121.28
1	A	272	ALA	CA-C-N	-5.71	112.82	123.05
1	A	272	ALA	C-N-CA	-5.71	112.82	123.05
1	B	153	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	A	155	ILE	CA-C-N	5.70	130.81	122.10
1	A	155	ILE	C-N-CA	5.70	130.81	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ASP	O-C-N	-5.68	115.03	122.59
1	B	204	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	B	281	GLU	N-CA-C	5.67	117.27	111.14
1	A	280	ALA	CA-C-O	-5.67	114.41	120.42
1	A	285	VAL	N-CA-C	5.66	115.86	110.42
1	A	46	ILE	CA-C-N	5.65	131.82	122.33
1	A	46	ILE	C-N-CA	5.65	131.82	122.33
1	A	60	TYR	CB-CA-C	5.65	118.17	110.94
1	A	251	TRP	O-C-N	5.63	127.79	121.32
1	A	183	ALA	CA-C-O	-5.63	114.88	121.07
1	A	65	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	B	40	PHE	N-CA-CB	5.61	119.16	110.80
1	A	214	ASN	CA-C-O	-5.61	115.02	121.19
1	A	80	LEU	N-CA-C	-5.56	105.30	111.36
1	A	121	GLU	N-CA-C	5.55	118.05	111.33
1	A	127	LEU	CD1-CG-CD2	-5.55	98.59	110.80
1	B	226	PRO	CB-CA-C	-5.54	104.31	111.39
1	B	118	THR	N-CA-C	-5.51	103.43	110.53
1	A	187	VAL	N-CA-CB	5.49	118.81	110.58
1	A	225	VAL	N-CA-CB	-5.48	106.56	112.37
1	A	260	VAL	N-CA-CB	5.47	119.50	111.52
1	A	32	ASP	N-CA-C	5.44	117.91	111.33
1	A	126	SER	CB-CA-C	-5.41	99.35	110.38
1	B	130	SER	CB-CA-C	5.41	118.98	111.63
1	B	190	LEU	CA-C-N	-5.40	112.50	120.38
1	B	190	LEU	C-N-CA	-5.40	112.50	120.38
1	B	76	THR	N-CA-C	5.39	117.16	111.28
1	B	31	ASP	CB-CA-C	5.39	121.58	110.31
1	A	64	GLU	N-CA-CB	-5.38	101.65	110.52
1	B	98	THR	N-CA-C	5.36	118.01	109.65
1	B	123	ALA	N-CA-C	-5.36	104.86	111.40
1	A	276	ASP	N-CA-C	5.36	122.21	110.80
1	A	282	ALA	CA-C-O	5.35	126.91	120.92
1	A	160	THR	CA-C-N	-5.34	116.69	123.15
1	A	160	THR	C-N-CA	-5.34	116.69	123.15
1	B	225	VAL	CB-CA-C	5.34	121.08	111.36
1	A	201	SER	CA-CB-OG	-5.33	100.44	111.10
1	A	159	VAL	CB-CA-C	5.33	120.02	111.29
1	B	238	ALA	O-C-N	-5.32	118.62	123.41
1	A	109	THR	N-CA-CB	-5.30	101.76	110.40
1	B	77	VAL	N-CA-C	5.29	117.71	111.09
1	B	264	LEU	CD1-CG-CD2	-5.29	99.15	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ILE	CB-CA-C	-5.27	102.83	110.63
1	B	173	ASN	N-CA-CB	5.26	117.05	109.78
1	A	105	TYR	CB-CA-C	5.25	118.55	110.62
1	A	141	GLN	CB-CA-C	-5.24	102.08	110.79
1	A	252	PRO	C-N-CD	-5.23	103.57	125.00
1	A	283	THR	CA-C-O	-5.22	115.33	120.82
1	B	265	SER	N-CA-CB	-5.22	102.10	110.77
1	A	64	GLU	N-CA-C	-5.21	101.21	109.76
1	A	263	VAL	CA-C-N	-5.21	114.49	122.62
1	A	263	VAL	C-N-CA	-5.21	114.49	122.62
1	A	268	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	193	PHE	N-CA-CB	5.20	117.71	110.07
1	A	138	ILE	N-CA-C	-5.18	105.34	110.62
1	B	196	GLU	CA-C-N	-5.17	115.86	122.79
1	B	196	GLU	C-N-CA	-5.17	115.86	122.79
1	B	61	ARG	N-CA-C	5.14	121.18	109.81
1	A	198	LYS	CD-CE-NZ	5.14	128.35	111.90
1	A	98	THR	N-CA-CB	-5.13	103.27	111.43
1	A	108	ILE	CA-CB-CG1	5.13	119.13	110.40
1	A	219	ALA	N-CA-C	-5.12	107.08	113.38
1	B	179	ASP	N-CA-C	5.12	121.70	110.80
1	B	268	ASP	O-C-N	-5.12	115.79	122.59
1	B	32	ASP	N-CA-C	5.11	118.67	112.23
1	B	89	GLU	O-C-N	5.09	127.32	122.07
1	A	89	GLU	N-CA-C	5.08	117.71	111.82
1	A	269	LYS	CA-C-N	5.07	127.49	120.29
1	A	269	LYS	C-N-CA	5.07	127.49	120.29
1	B	71	THR	N-CA-C	-5.07	106.20	112.38
1	A	238	ALA	O-C-N	-5.05	116.89	122.75
1	A	197	ASP	N-CA-CB	-5.04	104.23	111.54
1	B	112	HIS	CA-C-N	-5.03	112.39	120.64
1	B	112	HIS	C-N-CA	-5.03	112.39	120.64
1	B	185	ALA	N-CA-C	-5.01	105.52	111.69
1	B	155	ILE	O-C-N	5.01	127.31	122.05

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLU	Peptide
1	A	238	ALA	Mainchain
1	A	252	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	267	ARG	Peptide
1	A	268	ASP	Peptide,Mainchain
1	A	288	LYS	Peptide
1	A	31	ASP	Peptide
1	A	57	VAL	Mainchain
1	B	163	GLU	Peptide
1	B	178	GLN	Peptide
1	B	238	ALA	Mainchain
1	B	255	LYS	Peptide
1	B	268	ASP	Peptide
1	B	56	THR	Peptide
1	B	57	VAL	Peptide,Mainchain
1	B	83	GLN	Mainchain
1	B	99	ARG	Peptide

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	1910	0	1928	152	3
1	B	1963	0	1985	151	3
2	A	26	0	0	1	0
2	B	26	0	0	0	0
3	A	20	0	0	1	0
3	B	19	0	0	2	0
All	All	3964	0	3913	304	3

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 39.

All (304) 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:251:TRP:CD1	1:A:258:PRO:HB3	1.47	1.49
1:A:176:GLU:HG2	1:A:178:GLN:NE2	1.35	1.35
1:A:251:TRP:NE1	1:A:258:PRO:HB3	1.49	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:O	1:B:86:LYS:CG	1.88	1.20
1:B:83:GLN:O	1:B:86:LYS:HG2	1.01	1.16
1:B:67:ALA:HB2	1:B:172:VAL:HG21	1.17	1.10
1:B:82:GLN:CA	1:B:199:LEU:HD21	1.83	1.07
1:A:208:ILE:CG2	1:A:209:ASP:N	2.12	1.07
1:A:35:LYS:O	1:A:39:GLN:HG3	1.54	1.07
1:A:269:LYS:O	1:A:269:LYS:HG3	1.52	1.06
1:B:163:GLU:OE2	1:B:178:GLN:HB2	1.55	1.05
1:A:109:THR:HG21	1:A:133:ALA:HB3	1.39	1.05
1:A:208:ILE:HG22	1:A:209:ASP:N	1.31	1.04
1:B:82:GLN:HA	1:B:199:LEU:HD21	1.39	1.03
1:A:251:TRP:CD1	1:A:258:PRO:CB	2.43	1.01
1:B:83:GLN:C	1:B:86:LYS:HG2	1.84	1.00
1:A:176:GLU:CG	1:A:178:GLN:NE2	2.24	1.00
1:A:115:THR:OG1	1:A:116:GLY:O	1.82	0.98
1:B:98:THR:OG1	1:B:100:ASP:OD2	1.81	0.98
1:A:207:LEU:O	1:A:208:ILE:C	1.97	0.98
1:B:67:ALA:CB	1:B:172:VAL:HG21	1.94	0.98
1:A:63:ASP:CG	1:A:184:ARG:HH21	1.74	0.96
1:A:176:GLU:CG	1:A:178:GLN:HE22	1.77	0.95
1:A:251:TRP:NE1	1:A:258:PRO:CB	2.29	0.95
1:A:207:LEU:O	1:A:208:ILE:O	1.84	0.95
1:B:83:GLN:C	1:B:86:LYS:CG	2.38	0.95
1:B:157:ASP:OD1	1:B:159:VAL:HG13	1.66	0.93
1:B:82:GLN:CB	1:B:199:LEU:HD21	1.99	0.93
1:A:149:LYS:HD3	1:A:153:ARG:NH2	1.84	0.93
1:B:83:GLN:HE22	1:B:142:ILE:HB	1.33	0.92
1:A:176:GLU:HG2	1:A:178:GLN:HE22	0.94	0.92
1:B:99:ARG:N	1:B:100:ASP:CB	2.33	0.92
1:A:103:VAL:HG23	1:A:104:ASN:H	1.32	0.92
1:A:252:PRO:HB2	1:A:255:LYS:HE2	1.53	0.91
1:A:208:ILE:HG22	1:A:209:ASP:H	1.13	0.90
1:B:35:LYS:O	1:B:39:GLN:HG3	1.72	0.90
1:B:82:GLN:HB2	1:B:199:LEU:HD21	1.52	0.90
1:B:83:GLN:NE2	1:B:142:ILE:HB	1.88	0.88
1:A:103:VAL:HG23	1:A:104:ASN:N	1.87	0.88
1:A:63:ASP:OD2	1:A:184:ARG:NH2	2.06	0.88
1:A:208:ILE:O	1:A:209:ASP:C	2.12	0.87
1:B:57:VAL:CG1	1:B:59:ALA:H	1.88	0.86
1:B:287:MET:O	1:B:291:ASN:HB2	1.76	0.85
1:A:115:THR:OG1	1:A:116:GLY:N	2.03	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLY:O	1:B:53:THR:CG2	2.25	0.84
1:B:82:GLN:HA	1:B:199:LEU:CD2	2.07	0.84
1:A:241:TYR:CE1	1:A:270:LYS:HB2	2.13	0.83
1:B:99:ARG:N	1:B:100:ASP:HB2	1.92	0.83
1:B:109:THR:HG21	1:B:133:ALA:HB3	1.57	0.83
1:A:37:GLU:CB	1:A:42:ALA:O	2.27	0.82
1:A:149:LYS:HD3	1:A:153:ARG:HH21	1.43	0.82
1:A:88:ILE:O	1:A:88:ILE:HG22	1.78	0.82
1:A:59:ALA:HB1	1:A:62:PRO:HG3	1.60	0.82
1:B:57:VAL:CG1	1:B:59:ALA:N	2.42	0.81
1:B:98:THR:CB	1:B:100:ASP:HB3	2.11	0.81
1:B:198:LYS:O	1:B:199:LEU:HG	1.81	0.80
1:B:193:PHE:HD1	1:B:199:LEU:HD12	1.46	0.79
1:A:208:ILE:O	1:A:211:MET:N	2.16	0.79
1:A:53:THR:HG21	1:A:55:ARG:HH22	1.47	0.78
1:A:277:LYS:HE3	1:A:281:GLU:OE2	1.83	0.78
1:B:99:ARG:HH11	1:B:99:ARG:HG2	1.49	0.78
1:B:98:THR:C	1:B:100:ASP:HB3	2.09	0.78
1:A:37:GLU:HB3	1:A:42:ALA:O	1.83	0.77
1:A:211:MET:HB3	1:A:232:ALA:HB1	1.67	0.77
1:B:99:ARG:N	1:B:100:ASP:HB3	2.00	0.77
1:A:178:GLN:O	1:A:178:GLN:HG2	1.85	0.77
1:B:57:VAL:HG12	1:B:59:ALA:H	1.49	0.76
1:B:57:VAL:HG12	1:B:59:ALA:N	1.98	0.76
1:B:88:ILE:HG22	1:B:88:ILE:O	1.83	0.76
1:A:255:LYS:O	1:A:255:LYS:CG	2.32	0.74
1:A:51:THR:OG1	1:A:258:PRO:O	2.04	0.74
1:B:78:GLY:O	1:B:199:LEU:HD11	1.86	0.74
1:A:285:VAL:O	1:A:289:ALA:CB	2.37	0.73
1:B:99:ARG:H	1:B:100:ASP:HB2	1.53	0.72
1:A:251:TRP:HE1	1:A:258:PRO:HB3	1.52	0.72
1:B:52:GLY:C	1:B:53:THR:HG23	2.15	0.72
1:B:98:THR:HG1	1:B:100:ASP:CG	1.98	0.72
1:A:212:LYS:HD3	1:A:230:GLU:OE1	1.89	0.71
1:B:56:THR:HG23	1:B:57:VAL:CA	2.19	0.71
1:B:99:ARG:HG2	1:B:99:ARG:NH1	2.03	0.71
1:A:251:TRP:HE1	1:A:258:PRO:CB	2.01	0.71
1:A:241:TYR:CZ	1:A:270:LYS:HB2	2.26	0.71
1:B:35:LYS:HZ3	1:B:35:LYS:HB2	1.56	0.70
1:B:88:ILE:O	1:B:88:ILE:CG2	2.37	0.70
1:B:82:GLN:HB2	1:B:199:LEU:CD2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:HB2	1:A:42:ALA:O	1.92	0.70
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.56	0.70
1:A:255:LYS:O	1:A:255:LYS:HG2	1.90	0.70
1:A:109:THR:HG21	1:A:133:ALA:CB	2.20	0.69
1:B:190:LEU:O	1:B:191:ARG:C	2.32	0.69
1:A:112:HIS:O	1:A:114:ASP:N	2.25	0.69
1:A:229:TRP:CZ3	1:A:252:PRO:HB3	2.28	0.69
1:A:251:TRP:HD1	1:A:258:PRO:HB3	1.51	0.68
1:B:190:LEU:HD13	1:B:249:ILE:HD11	1.75	0.68
1:B:52:GLY:O	1:B:53:THR:HG22	1.94	0.68
1:B:159:VAL:HG11	1:B:185:ALA:CB	2.23	0.68
1:A:249:ILE:HG21	1:A:251:TRP:CZ2	2.29	0.68
1:A:112:HIS:O	1:A:113:VAL:C	2.36	0.67
1:A:252:PRO:O	1:A:255:LYS:N	2.27	0.67
1:A:94:ARG:HA	1:A:118:THR:HG22	1.74	0.67
1:A:252:PRO:C	1:A:255:LYS:H	2.02	0.67
1:A:181:SER:OG	1:A:182:THR:N	2.08	0.67
1:B:131:ASP:HB3	1:B:134:ALA:HB3	1.76	0.67
1:B:56:THR:HG23	1:B:57:VAL:N	2.09	0.67
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.77	0.66
1:B:52:GLY:O	1:B:53:THR:HG23	1.94	0.66
1:B:192:ALA:HA	1:B:196:GLU:HB2	1.75	0.66
1:A:118:THR:O	1:A:121:GLU:N	2.28	0.66
1:B:193:PHE:CD1	1:B:199:LEU:HD12	2.29	0.66
1:A:208:ILE:O	1:A:210:TRP:N	2.29	0.66
1:B:261:LEU:HD13	1:B:286:VAL:HG11	1.76	0.66
1:A:252:PRO:C	1:A:255:LYS:N	2.53	0.66
1:B:244:ARG:O	1:B:265:SER:HB3	1.95	0.66
1:B:67:ALA:HB2	1:B:172:VAL:CG2	2.11	0.65
1:A:241:TYR:HD2	1:A:269:LYS:H	1.44	0.65
1:A:285:VAL:O	1:A:289:ALA:HB2	1.95	0.65
1:B:98:THR:OG1	1:B:100:ASP:HB3	1.97	0.65
1:A:288:LYS:O	1:A:290:LEU:N	2.30	0.65
1:A:269:LYS:O	1:A:269:LYS:CG	2.30	0.64
1:B:57:VAL:HG13	1:B:59:ALA:H	1.61	0.64
1:A:277:LYS:O	1:A:277:LYS:HG3	1.97	0.64
1:A:50:ASP:HA	1:A:259:VAL:HG22	1.80	0.64
1:A:252:PRO:O	1:A:254:PRO:C	2.37	0.64
1:B:244:ARG:HD3	1:B:274:TYR:CE1	2.33	0.63
1:A:286:VAL:O	1:A:289:ALA:HB3	1.99	0.63
1:A:53:THR:HG21	1:A:55:ARG:NH2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:HA	1:A:180:THR:HA	1.81	0.62
1:B:220:LEU:HD12	1:B:220:LEU:N	2.14	0.62
1:B:52:GLY:C	1:B:53:THR:CG2	2.72	0.62
1:B:98:THR:OG1	1:B:100:ASP:CG	2.41	0.62
1:A:106:ASN:O	1:A:107:PRO:C	2.39	0.61
1:A:88:ILE:O	1:A:88:ILE:CG2	2.48	0.61
1:B:159:VAL:HG11	1:B:185:ALA:HB1	1.81	0.61
1:B:159:VAL:HG22	1:B:160:THR:N	2.16	0.61
1:B:87:SER:O	1:B:90:ASP:HB2	2.01	0.60
1:B:153:ARG:NH1	1:B:157:ASP:O	2.32	0.60
1:A:288:LYS:C	1:A:290:LEU:N	2.59	0.60
1:B:211:MET:HB2	1:B:232:ALA:HB1	1.84	0.60
1:B:244:ARG:HD3	1:B:274:TYR:CD1	2.36	0.60
1:B:35:LYS:HB2	1:B:35:LYS:NZ	2.16	0.60
1:A:32:ASP:O	1:A:35:LYS:HB3	2.00	0.60
1:A:237:ALA:HB2	1:A:244:ARG:HH11	1.65	0.59
1:B:163:GLU:OE2	1:B:178:GLN:CB	2.41	0.59
1:A:190:LEU:HD21	1:A:211:MET:HE1	1.84	0.59
1:A:191:ARG:O	1:A:192:ALA:C	2.44	0.59
1:A:49:LEU:O	1:A:259:VAL:HG13	2.03	0.58
1:B:56:THR:HG23	1:B:57:VAL:C	2.27	0.58
1:A:285:VAL:O	1:A:289:ALA:HB3	2.03	0.58
1:B:281:GLU:O	1:B:282:ALA:C	2.46	0.57
1:A:139:LEU:HD22	1:A:144:GLY:HA2	1.85	0.57
1:B:99:ARG:HH11	1:B:99:ARG:CG	2.18	0.57
1:A:220:LEU:N	1:A:220:LEU:HD12	2.19	0.57
1:B:89:GLU:O	1:B:92:ASN:HB2	2.05	0.57
1:B:98:THR:CB	1:B:100:ASP:OD2	2.53	0.57
1:B:98:THR:HB	1:B:100:ASP:CB	2.36	0.56
1:B:200:PRO:HD2	1:B:203:LYS:HD2	1.86	0.56
1:B:98:THR:CB	1:B:100:ASP:CB	2.82	0.56
1:A:51:THR:O	1:A:53:THR:N	2.39	0.56
1:A:237:ALA:HB2	1:A:244:ARG:NH1	2.21	0.56
1:B:79:VAL:HG21	1:B:148:LEU:HD12	1.86	0.56
1:B:289:ALA:O	1:B:290:LEU:C	2.47	0.55
1:B:44:LEU:HG	1:B:46:ILE:CD1	2.36	0.55
1:B:68:PHE:O	1:B:69:ALA:HB3	2.05	0.55
1:A:251:TRP:HE1	1:A:258:PRO:HG3	1.71	0.55
1:A:51:THR:O	1:A:52:GLY:C	2.49	0.54
1:A:102:LEU:HD11	1:A:109:THR:HG23	1.90	0.54
1:A:240:SER:O	1:A:241:TYR:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:CG2	1:A:251:TRP:CZ2	2.90	0.54
1:B:159:VAL:HG11	1:B:185:ALA:HB2	1.90	0.54
1:B:108:ILE:HD11	1:B:129:TYR:CD1	2.42	0.54
1:B:235:THR:HG22	1:B:246:ASP:OD1	2.07	0.54
1:A:251:TRP:HE1	1:A:258:PRO:CG	2.20	0.54
1:A:72:ILE:HG13	1:A:72:ILE:O	2.08	0.53
1:A:152:LEU:O	1:A:153:ARG:C	2.49	0.53
1:B:100:ASP:O	1:B:101:ASP:CB	2.56	0.53
1:B:98:THR:HB	1:B:100:ASP:HB3	1.91	0.53
1:A:211:MET:CB	1:A:232:ALA:HB1	2.36	0.53
1:B:98:THR:OG1	1:B:100:ASP:CB	2.57	0.53
1:A:243:THR:HA	1:A:265:SER:O	2.09	0.53
1:A:269:LYS:NZ	1:A:271:ASP:OD1	2.25	0.53
1:B:270:LYS:O	1:B:270:LYS:HG3	2.09	0.53
1:A:226:PRO:HG2	1:A:229:TRP:CD1	2.44	0.53
1:B:106:ASN:HB3	1:B:109:THR:HG22	1.91	0.53
1:A:108:ILE:O	1:A:108:ILE:HG22	2.07	0.52
1:A:219:ALA:HB3	1:A:220:LEU:HD12	1.90	0.52
1:B:35:LYS:NZ	1:B:35:LYS:CB	2.72	0.52
1:B:186:LEU:O	1:B:187:VAL:C	2.50	0.52
1:B:159:VAL:CG1	1:B:185:ALA:HB1	2.40	0.52
1:A:95:ILE:HD11	1:A:119:LEU:HG	1.90	0.52
1:A:288:LYS:O	1:A:289:ALA:C	2.53	0.51
1:A:149:LYS:HD3	1:A:153:ARG:CZ	2.41	0.51
1:B:57:VAL:HG13	1:B:59:ALA:N	2.22	0.51
1:A:68:PHE:O	1:A:69:ALA:C	2.49	0.51
2:A:1:CEF:C3	2:A:1:CEF:O1	2.59	0.51
1:A:182:THR:O	1:A:183:ALA:C	2.53	0.51
1:B:211:MET:CB	1:B:232:ALA:HB1	2.41	0.50
1:B:94:ARG:HD3	1:B:115:THR:O	2.12	0.50
1:B:30:LYS:HA	1:B:33:PHE:HB2	1.92	0.50
1:A:221:ILE:HG13	1:A:246:ASP:OD2	2.12	0.49
1:B:77:VAL:HG23	3:B:294:HOH:O	2.11	0.49
1:A:229:TRP:CH2	1:A:252:PRO:HB3	2.47	0.49
1:A:112:HIS:C	1:A:114:ASP:N	2.68	0.49
1:B:42:ALA:HB2	1:B:267:ARG:HG2	1.94	0.49
1:B:99:ARG:O	1:B:102:LEU:HB2	2.13	0.49
1:B:100:ASP:O	1:B:101:ASP:OD2	2.30	0.49
1:B:100:ASP:O	1:B:101:ASP:CG	2.56	0.49
1:B:190:LEU:HG	1:B:247:ILE:HD12	1.93	0.49
1:A:261:LEU:HD12	1:A:262:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:O	1:B:265:SER:HA	2.13	0.49
1:A:88:ILE:HG22	3:A:296:HOH:O	2.12	0.49
1:B:99:ARG:H	1:B:100:ASP:CB	2.13	0.49
1:B:283:THR:O	1:B:284:LYS:C	2.54	0.49
1:A:259:VAL:HG12	1:A:260:VAL:N	2.26	0.48
1:A:286:VAL:C	1:A:289:ALA:HB3	2.38	0.48
1:A:200:PRO:HG2	1:A:203:LYS:HD2	1.95	0.48
1:A:46:ILE:O	1:A:60:TYR:N	2.39	0.48
1:A:269:LYS:HE2	1:A:270:LYS:N	2.28	0.48
1:A:288:LYS:C	1:A:290:LEU:H	2.21	0.48
1:B:207:LEU:O	1:B:208:ILE:C	2.54	0.48
1:A:220:LEU:N	1:A:220:LEU:CD1	2.77	0.48
1:A:103:VAL:CG2	1:A:104:ASN:N	2.61	0.47
1:A:240:SER:C	1:A:242:GLY:H	2.21	0.47
1:B:41:ASP:HB3	1:B:267:ARG:HH21	1.79	0.47
1:A:247:ILE:HG22	1:A:262:ALA:CB	2.45	0.47
1:A:240:SER:C	1:A:242:GLY:N	2.70	0.47
1:B:48:ALA:HB2	1:B:261:LEU:HD13	1.97	0.47
1:B:150:LYS:O	1:B:150:LYS:HG3	2.14	0.47
1:A:59:ALA:HB1	1:A:62:PRO:CG	2.38	0.47
1:A:81:LEU:O	1:A:82:GLN:C	2.58	0.46
1:A:268:ASP:CA	1:A:269:LYS:HB3	2.45	0.46
1:B:98:THR:CA	1:B:100:ASP:HB3	2.44	0.46
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.35	0.46
1:B:118:THR:N	1:B:121:GLU:OE1	2.44	0.46
1:B:37:GLU:OE1	1:B:60:TYR:OH	2.29	0.46
1:A:287:MET:O	1:A:290:LEU:HB2	2.16	0.46
1:A:178:GLN:O	1:A:178:GLN:CG	2.59	0.46
1:B:83:GLN:O	1:B:83:GLN:HG3	2.15	0.46
1:B:282:ALA:O	1:B:286:VAL:HG23	2.16	0.46
1:B:173:ASN:HB2	1:B:176:GLU:OE2	2.16	0.46
1:B:191:ARG:O	1:B:195:LEU:HB2	2.17	0.45
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.59	0.45
1:B:125:ALA:O	1:B:129:TYR:HB2	2.16	0.45
1:B:66:PHE:O	1:B:67:ALA:C	2.59	0.45
1:A:93:GLN:HE21	1:A:93:GLN:HB3	1.52	0.45
1:A:119:LEU:O	1:A:120:LYS:C	2.59	0.45
1:B:35:LYS:HZ3	1:B:35:LYS:CB	2.23	0.45
1:A:43:LYS:O	1:A:265:SER:HA	2.17	0.44
1:A:160:THR:HA	1:A:181:SER:HB2	1.99	0.44
1:A:209:ASP:O	1:A:210:TRP:C	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASP:OD1	1:B:50:ASP:C	2.56	0.44
1:B:201:SER:HA	1:B:204:ARG:NH1	2.32	0.44
1:A:107:PRO:HD2	1:A:131:ASP:CG	2.43	0.44
1:A:287:MET:O	1:A:291:ASN:N	2.49	0.44
1:A:63:ASP:OD1	1:A:184:ARG:NH2	2.46	0.44
1:B:118:THR:OG1	1:B:121:GLU:HG3	2.17	0.44
1:B:77:VAL:HG12	1:B:81:LEU:HG	1.99	0.44
1:B:49:LEU:HD21	1:B:191:ARG:NH1	2.32	0.44
1:B:211:MET:HG2	3:B:3:HOH:O	2.16	0.44
1:A:259:VAL:CG1	1:A:260:VAL:N	2.81	0.44
1:A:274:TYR:CD1	1:A:274:TYR:C	2.95	0.44
1:B:56:THR:CG2	1:B:57:VAL:N	2.73	0.44
1:A:200:PRO:HD2	1:A:203:LYS:HD2	1.99	0.44
1:B:81:LEU:HA	1:B:81:LEU:HD23	1.61	0.43
1:B:38:GLU:HB3	1:B:39:GLN:H	1.56	0.43
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.77	0.43
1:A:183:ALA:O	1:A:184:ARG:C	2.59	0.43
1:B:65:ARG:NH1	1:B:180:THR:OG1	2.51	0.43
1:B:66:PHE:CD2	1:B:266:SER:HB3	2.53	0.43
1:A:37:GLU:OE1	1:A:60:TYR:OH	2.30	0.43
1:B:187:VAL:HB	1:B:260:VAL:HG22	2.00	0.43
1:B:142:ILE:O	1:B:142:ILE:HG13	2.19	0.43
1:A:65:ARG:HH11	1:A:65:ARG:HD3	1.61	0.43
1:A:219:ALA:C	1:A:220:LEU:HD12	2.44	0.43
1:B:82:GLN:HB2	1:B:199:LEU:CG	2.49	0.43
1:A:94:ARG:CA	1:A:118:THR:HG22	2.44	0.42
1:B:66:PHE:CE2	1:B:266:SER:HB3	2.54	0.42
1:A:60:TYR:C	1:A:60:TYR:CD2	2.97	0.42
1:A:117:MET:HB3	1:A:117:MET:HE2	1.78	0.42
1:B:79:VAL:HG21	1:B:148:LEU:CD1	2.48	0.42
1:B:80:LEU:HD13	1:B:138:ILE:HG23	2.02	0.42
1:B:267:ARG:NH1	1:B:272:ALA:HB1	2.34	0.42
1:A:176:GLU:CD	1:A:178:GLN:NE2	2.78	0.42
1:A:103:VAL:CG2	1:A:104:ASN:H	2.09	0.42
1:A:78:GLY:O	1:A:199:LEU:HD21	2.20	0.42
1:A:94:ARG:HB2	1:A:118:THR:HG22	2.00	0.42
1:B:77:VAL:O	1:B:81:LEU:HG	2.19	0.42
1:B:238:ALA:C	1:B:240:SER:O	2.57	0.42
1:A:106:ASN:CB	1:A:109:THR:HG22	2.49	0.41
1:A:230:GLU:O	1:A:250:ILE:HA	2.21	0.41
1:B:108:ILE:HD11	1:B:129:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:HD3	1:B:158:GLU:HA	2.01	0.41
1:B:90:ASP:C	1:B:92:ASN:H	2.28	0.41
1:B:241:TYR:CZ	1:B:270:LYS:HB2	2.56	0.41
1:B:190:LEU:C	1:B:192:ALA:N	2.77	0.41
1:A:34:ALA:HA	1:A:37:GLU:HG3	2.03	0.41
1:A:118:THR:O	1:A:119:LEU:C	2.63	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.80	0.41
1:B:99:ARG:CA	1:B:100:ASP:HB2	2.51	0.41
1:B:147:SER:O	1:B:151:GLU:HG2	2.21	0.41
1:A:43:LYS:HB3	1:A:43:LYS:HE3	1.85	0.40
1:B:76:THR:CB	1:B:135:GLN:HE22	2.33	0.40
1:A:50:ASP:O	1:A:54:ASN:N	2.53	0.40
1:B:105:TYR:CE2	1:B:107:PRO:HG3	2.56	0.40
1:B:237:ALA:HA	1:B:243:THR:O	2.22	0.40

All (3) 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:A:140:LYS:NZ	1:B:271:ASP:OD1[2_444]	1.45	0.75
1:A:140:LYS:NZ	1:B:271:ASP:CG[2_444]	1.59	0.61
1:A:140:LYS:NZ	1:B:271:ASP:OD2[2_444]	1.69	0.51

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	241/257 (94%)	207 (86%)	22 (9%)	12 (5%)	1	15
1	B	247/257 (96%)	209 (85%)	27 (11%)	11 (4%)	2	17
All	All	488/514 (95%)	416 (85%)	49 (10%)	23 (5%)	2	17

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ILE
1	A	254	PRO
1	A	269	LYS
1	A	289	ALA
1	B	38	GLU
1	B	39	GLN
1	B	54	ASN
1	B	86	LYS
1	B	91	LEU
1	A	179	ASP
1	A	207	LEU
1	A	276	ASP
1	B	101	ASP
1	B	179	ASP
1	B	268	ASP
1	A	114	ASP
1	A	154	LYS
1	A	209	ASP
1	A	252	PRO
1	B	53	THR
1	B	59	ALA
1	B	103	VAL
1	A	103	VAL

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	205/217 (94%)	154 (75%)	51 (25%)	0	4
1	B	211/217 (97%)	165 (78%)	46 (22%)	1	6
All	All	416/434 (96%)	319 (77%)	97 (23%)	1	5

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	37	GLU
1	A	44	LEU
1	A	56	THR
1	A	64	GLU
1	A	68	PHE
1	A	72	ILE
1	A	77	VAL
1	A	82	GLN
1	A	88	ILE
1	A	89	GLU
1	A	93	GLN
1	A	95	ILE
1	A	96	THR
1	A	98	THR
1	A	102	LEU
1	A	108	ILE
1	A	109	THR
1	A	113	VAL
1	A	115	THR
1	A	119	LEU
1	A	137	LEU
1	A	140	LYS
1	A	142	ILE
1	A	146	GLU
1	A	149	LYS
1	A	154	LYS
1	A	155	ILE
1	A	159	VAL
1	A	163	GLU
1	A	177	THR
1	A	178	GLN
1	A	181	SER
1	A	187	VAL
1	A	190	LEU
1	A	195	LEU
1	A	208	ILE
1	A	218	ASP
1	A	220	LEU
1	A	225	VAL
1	A	243	THR
1	A	249	ILE
1	A	255	LYS

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Mol	Chain	Res	Type
1	A	260	VAL
1	A	268	ASP
1	A	269	LYS
1	A	270	LYS
1	A	273	LYS
1	A	279	ILE
1	A	287	MET
1	A	288	LYS
1	B	30	LYS
1	B	31	ASP
1	B	35	LYS
1	B	55	ARG
1	B	56	THR
1	B	64	GLU
1	B	65	ARG
1	B	70	SER
1	B	99	ARG
1	B	102	LEU
1	B	109	THR
1	B	113	VAL
1	B	114	ASP
1	B	130	SER
1	B	137	LEU
1	B	139	LEU
1	B	142	ILE
1	B	147	SER
1	B	149	LYS
1	B	150	LYS
1	B	158	GLU
1	B	159	VAL
1	B	161	ASN
1	B	163	GLU
1	B	165	PHE
1	B	172	VAL
1	B	174	PRO
1	B	187	VAL
1	B	190	LEU
1	B	195	LEU
1	B	197	ASP
1	B	198	LYS
1	B	201	SER
1	B	225	VAL

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Mol	Chain	Res	Type
1	B	227	ASP
1	B	233	ASP
1	B	255	LYS
1	B	260	VAL
1	B	265	SER
1	B	266	SER
1	B	268	ASP
1	B	269	LYS
1	B	270	LYS
1	B	273	LYS
1	B	277	LYS
1	B	291	ASN

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	82	GLN
1	A	93	GLN
1	A	106	ASN
1	A	141	GLN
1	A	161	ASN
1	A	178	GLN
1	B	82	GLN
1	B	83	GLN
1	B	173	ASN
1	B	214	ASN
1	B	245	ASN

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

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	CEF	B	1	1	24,27,27	3.35	8 (33%)	25,37,37	6.30	17 (68%)
2	CEF	A	1	1	24,27,27	4.07	15 (62%)	25,37,37	7.07	13 (52%)

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	CEF	B	1	1	-	8/18/38/38	0/1/2/2
2	CEF	A	1	1	-	5/18/38/38	0/1/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CEF	C1-C2	-10.53	1.36	1.50
2	B	1	CEF	C13-C12	9.90	1.54	1.36
2	A	1	CEF	C4-N1	8.76	1.36	1.28
2	B	1	CEF	C1-C2	-7.43	1.40	1.50
2	A	1	CEF	C1-S1	-6.41	1.69	1.82
2	B	1	CEF	C12-N5	-6.00	1.25	1.38
2	A	1	CEF	C13-C12	5.49	1.46	1.36
2	A	1	CEF	C14-S2	5.40	1.82	1.74
2	B	1	CEF	C1-S1	-4.92	1.72	1.82
2	A	1	CEF	O5-N3	-4.50	1.30	1.40
2	B	1	CEF	C14-S2	-3.91	1.69	1.74
2	A	1	CEF	C4-C5	-3.39	1.41	1.48
2	A	1	CEF	C13-S2	3.37	1.80	1.71
2	A	1	CEF	C3-C2	3.26	1.39	1.32
2	A	1	CEF	C4-C2	-3.23	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CEF	O4-C9	-3.04	1.17	1.23
2	A	1	CEF	C14-N5	3.01	1.36	1.31
2	B	1	CEF	C14-N5	-2.81	1.27	1.31
2	A	1	CEF	C10-C9	-2.53	1.43	1.48
2	A	1	CEF	C14-N4	2.49	1.39	1.34
2	B	1	CEF	C13-S2	2.24	1.77	1.71
2	A	1	CEF	O1-C5	2.14	1.27	1.22
2	B	1	CEF	O1-C5	2.09	1.27	1.22

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	CEF	C6-N1-C4	22.10	135.62	116.33
2	B	1	CEF	C11-O5-N3	18.94	131.43	108.32
2	A	1	CEF	C13-S2-C14	17.92	96.56	88.84
2	B	1	CEF	C6-N1-C4	13.08	127.74	116.33
2	B	1	CEF	C12-C13-S2	-11.56	96.89	110.24
2	B	1	CEF	C8-C7-N2	-9.29	95.15	109.80
2	A	1	CEF	S2-C14-N5	-9.27	107.23	114.54
2	A	1	CEF	C12-C13-S2	-9.16	99.66	110.24
2	A	1	CEF	S2-C14-N4	8.34	130.68	120.99
2	A	1	CEF	C1-S1-C6	7.48	108.06	94.36
2	B	1	CEF	C2-C1-S1	7.45	126.99	111.65
2	B	1	CEF	C13-S2-C14	7.38	92.02	88.84
2	A	1	CEF	C2-C1-S1	6.97	126.01	111.65
2	A	1	CEF	C11-O5-N3	5.52	115.05	108.32
2	B	1	CEF	O5-N3-C10	5.24	131.21	111.65
2	B	1	CEF	C1-S1-C6	4.99	103.51	94.36
2	B	1	CEF	S2-C14-N4	4.33	126.03	120.99
2	A	1	CEF	O2-C5-O1	-3.64	115.24	123.90
2	A	1	CEF	C13-C12-N5	3.46	120.19	115.43
2	B	1	CEF	C10-C9-N2	3.16	119.25	114.27
2	A	1	CEF	C7-N2-C9	3.06	128.02	121.97
2	B	1	CEF	S2-C14-N5	-2.96	112.21	114.54
2	B	1	CEF	O2-C5-O1	-2.57	117.78	123.90
2	B	1	CEF	C7-N2-C9	2.55	127.00	121.97
2	B	1	CEF	C13-C12-N5	-2.44	112.07	115.43
2	B	1	CEF	O3-C8-C7	-2.41	118.50	124.86
2	A	1	CEF	C13-C12-C10	-2.29	121.60	125.69
2	B	1	CEF	O2-C5-C4	2.28	122.05	116.02
2	A	1	CEF	O4-C9-C10	-2.07	118.27	121.60
2	B	1	CEF	N4-C14-N5	-2.06	121.66	124.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	CEF	C8-C7-N2-C9
2	B	1	CEF	N1-C4-C5-O2
2	B	1	CEF	C9-C10-C12-C13
2	B	1	CEF	C9-C10-C12-N5
2	B	1	CEF	N3-C10-C12-C13
2	B	1	CEF	N3-C10-C12-N5
2	B	1	CEF	C10-N3-O5-C11
2	B	1	CEF	C2-C4-C5-O1
2	A	1	CEF	C6-C7-N2-C9
2	A	1	CEF	C2-C4-C5-O1
2	A	1	CEF	N3-C10-C9-O4
2	B	1	CEF	N3-C10-C9-O4
2	A	1	CEF	N1-C4-C5-O2

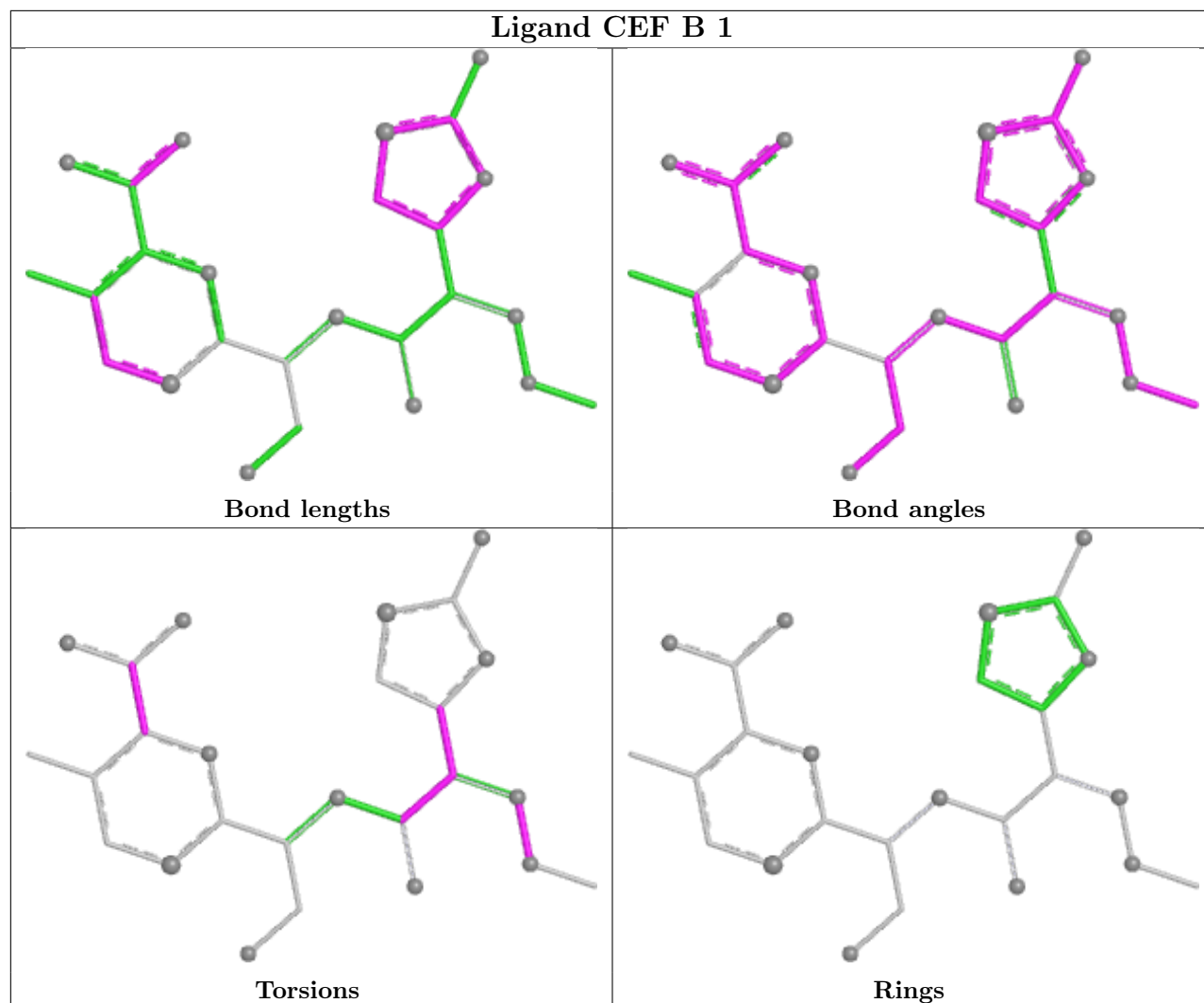
There are no ring outliers.

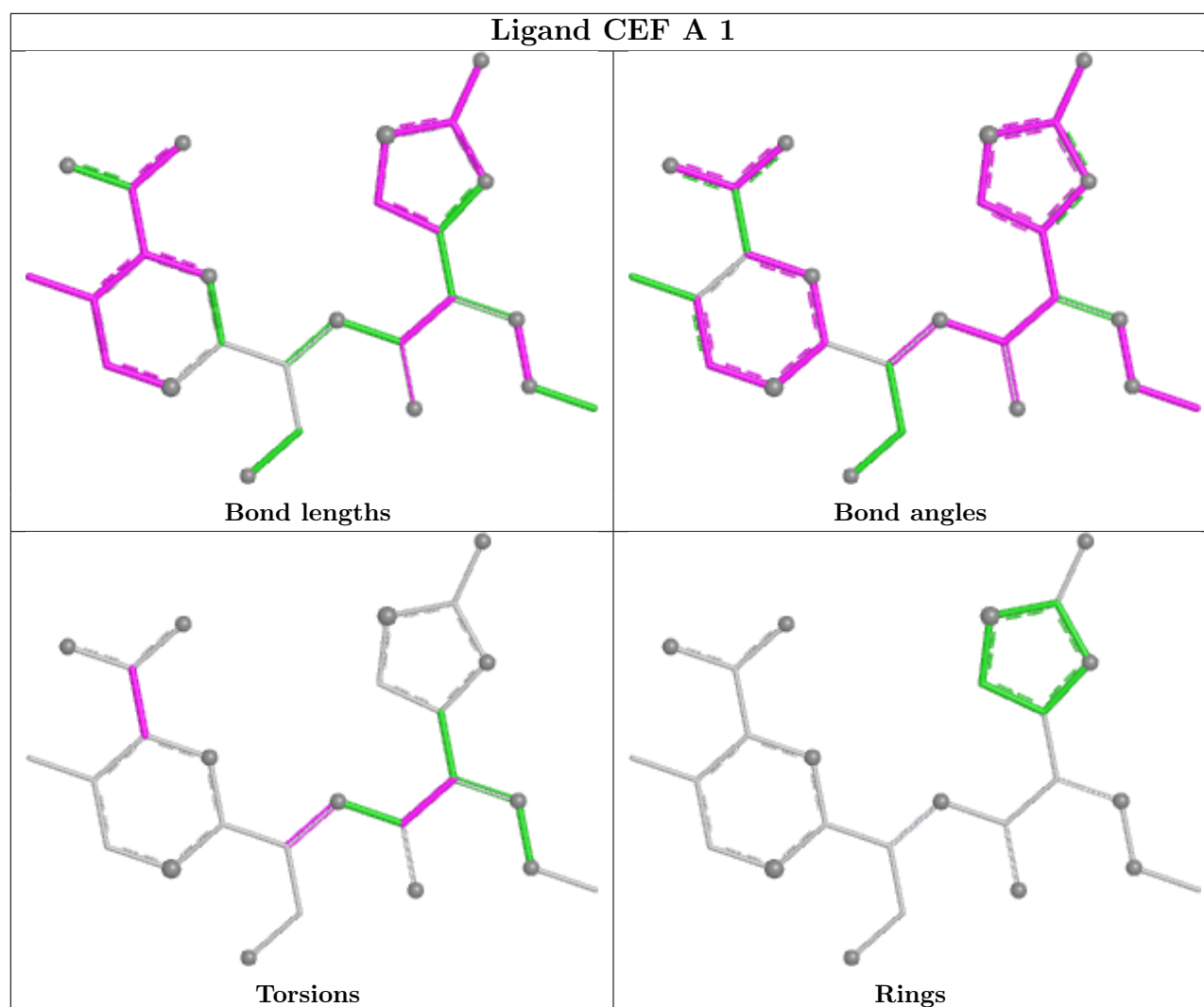
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	CEF	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.

Ligand CEF B 1





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	245/257 (95%)	-0.36	2 (0%)	82 60	7, 13, 19, 34	0
1	B	251/257 (97%)	-0.38	1 (0%)	88 72	7, 13, 19, 44	0
All	All	496/514 (96%)	-0.37	3 (0%)	85 65	7, 13, 19, 44	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	ASP	5.2
1	A	230	GLU	2.2
1	A	251	TRP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

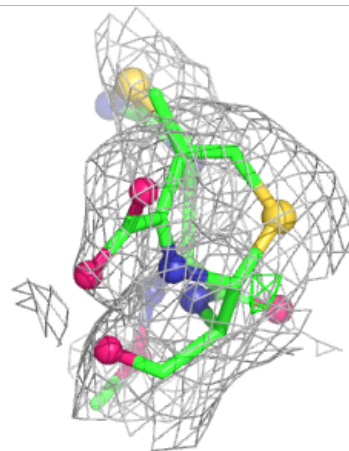
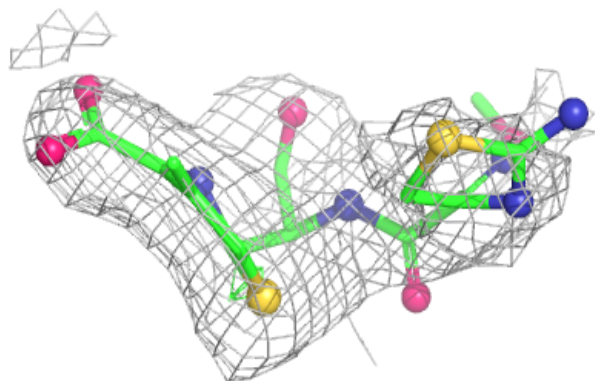
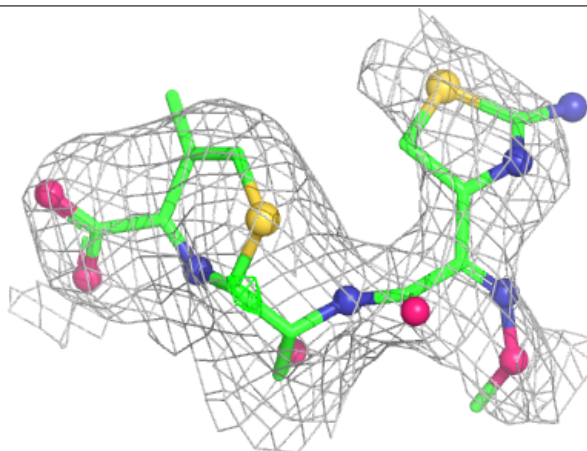
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

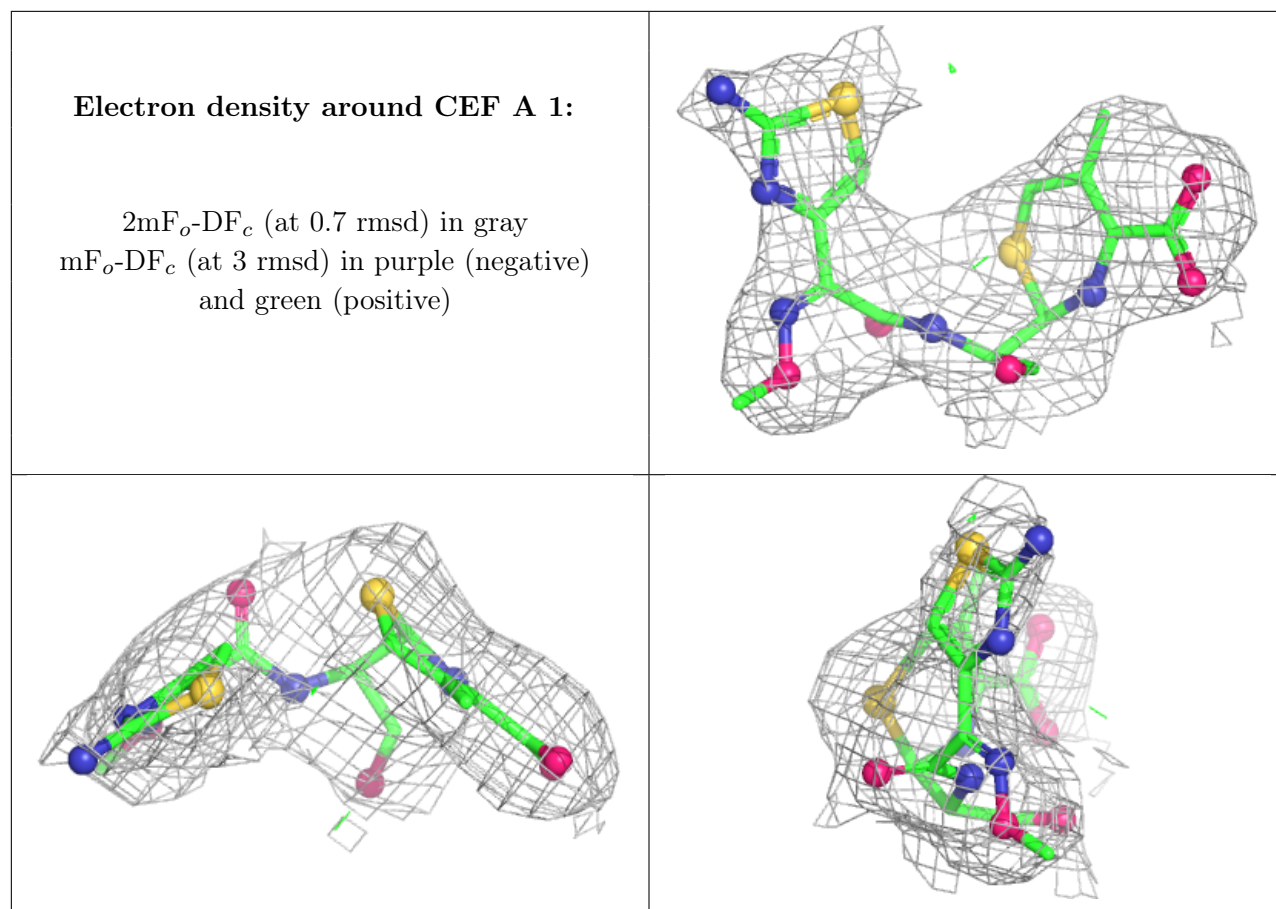
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	CEF	B	1	26/26	0.90	0.14	32,44,75,78	0
2	CEF	A	1	26/26	0.95	0.08	11,16,35,45	0

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 CEF B 1:

$2mF_o-DF_c$ (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.