



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 10:36 PM EDT

PDB ID : 3M2K  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

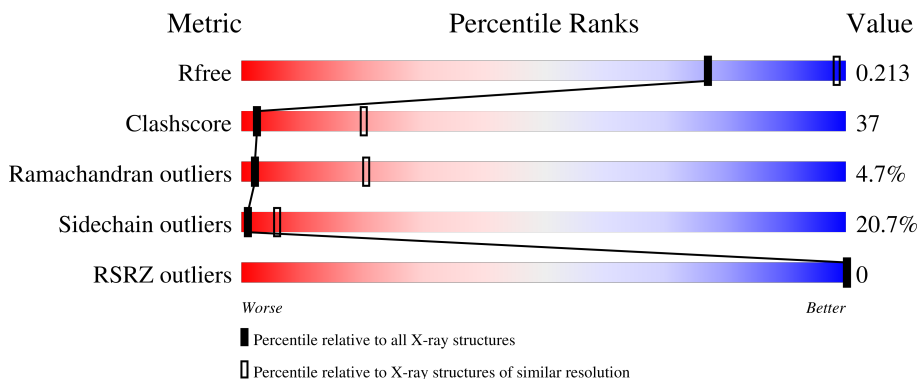
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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  $\geq 3$ , 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	 27% 40% 23% 5%
1	B	257	 33% 37% 22% 6%



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

- Molecule 3 is water.

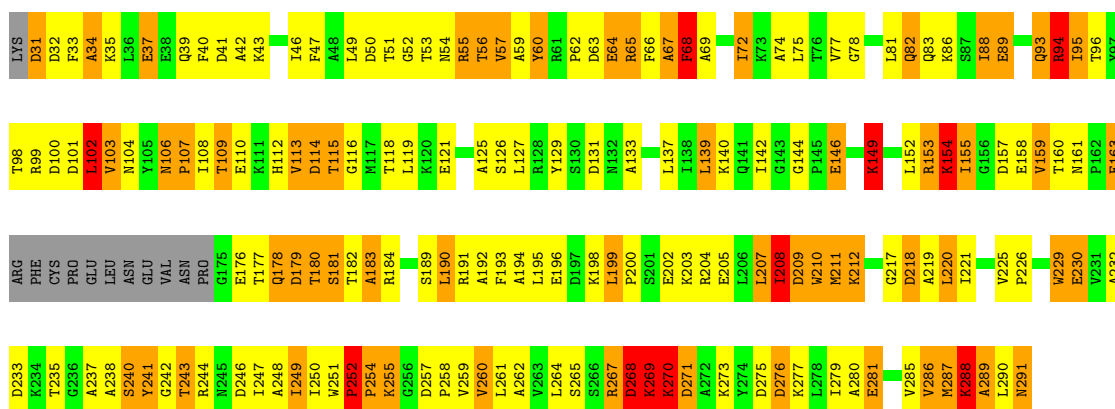
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	19	Total	O	0	0
			19	19		

### 3 Residue-property plots [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.

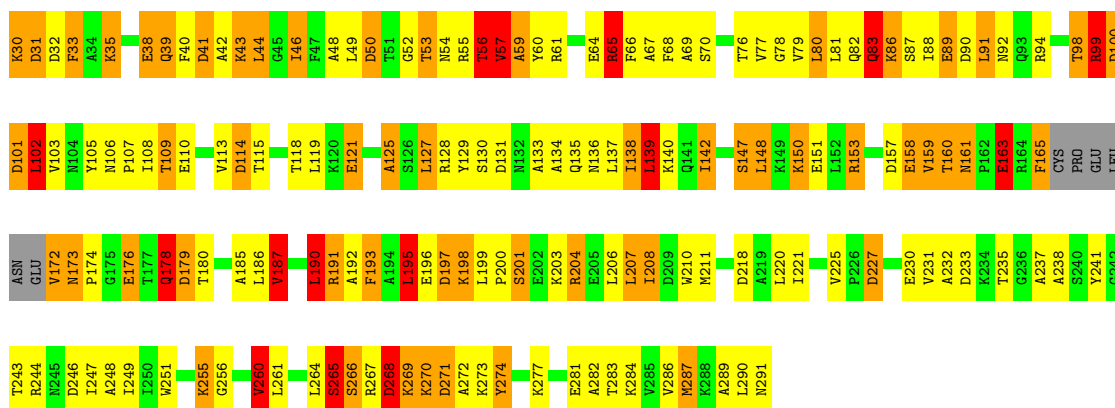
#### • Molecule 1: Beta-lactamase

Chain A: 



#### • Molecule 1: Beta-lactamase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.54Å 91.52Å 66.30Å 90.00° 104.22° 90.00°	Depositor
Resolution (Å)	40.23 – 3.50 52.60 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.23-3.50) 95.0 (52.60-3.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.236 0.181 , 0.213	Depositor DCC
$R_{free}$ test set	308 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtrriage
Anisotropy	0.216	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 24.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	2.31	80/1936 (4.1%)	1.89	43/2617 (1.6%)
1	B	2.05	49/1991 (2.5%)	1.87	53/2691 (2.0%)
All	All	2.18	129/3927 (3.3%)	1.88	96/5308 (1.8%)

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 (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	GLU	CD-OE2	12.87	1.39	1.25
1	A	89	GLU	CD-OE1	11.46	1.38	1.25
1	A	281	GLU	CD-OE2	11.32	1.38	1.25
1	A	252	PRO	C-N	10.79	1.54	1.34
1	B	64	GLU	CG-CD	10.65	1.68	1.51
1	A	163	GLU	CG-CD	10.47	1.67	1.51
1	B	83	GLN	C-N	10.21	1.57	1.34
1	A	74	ALA	CA-CB	-9.70	1.32	1.52
1	B	260	VAL	CB-CG2	-9.43	1.33	1.52
1	A	125	ALA	CA-CB	-9.37	1.32	1.52
1	A	146	GLU	CB-CG	9.19	1.69	1.52
1	A	60	TYR	CE2-CZ	9.04	1.50	1.38
1	B	230	GLU	CD-OE2	8.97	1.35	1.25
1	A	271	ASP	CB-CG	8.91	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	ALA	CA-CB	-8.82	1.33	1.52
1	B	176	GLU	CG-CD	8.60	1.64	1.51
1	A	241	TYR	CG-CD2	8.33	1.50	1.39
1	B	125	ALA	CA-CB	-8.31	1.35	1.52
1	A	196	GLU	CD-OE1	8.23	1.34	1.25
1	B	193	PHE	CE2-CZ	-8.20	1.21	1.37
1	B	64	GLU	CD-OE1	7.93	1.34	1.25
1	A	159	VAL	CB-CG2	-7.84	1.36	1.52
1	A	281	GLU	CG-CD	7.78	1.63	1.51
1	A	31	ASP	N-CA	7.55	1.61	1.46
1	A	60	TYR	CG-CD2	7.44	1.48	1.39
1	B	89	GLU	CD-OE2	7.32	1.33	1.25
1	A	146	GLU	CG-CD	7.29	1.62	1.51
1	A	110	GLU	CD-OE1	7.18	1.33	1.25
1	A	57	VAL	C-N	7.17	1.50	1.34
1	A	129	TYR	CG-CD2	-7.14	1.29	1.39
1	A	196	GLU	CD-OE2	7.12	1.33	1.25
1	B	230	GLU	CG-CD	7.01	1.62	1.51
1	A	281	GLU	CD-OE1	6.97	1.33	1.25
1	A	180	THR	C-O	-6.97	1.10	1.23
1	A	208	ILE	CA-CB	-6.96	1.38	1.54
1	A	225	VAL	CB-CG2	-6.91	1.38	1.52
1	A	60	TYR	CD1-CE1	6.90	1.49	1.39
1	A	86	LYS	C-O	6.75	1.36	1.23
1	B	64	GLU	CD-OE2	6.74	1.33	1.25
1	B	230	GLU	CD-OE1	6.70	1.33	1.25
1	A	68	PHE	CE2-CZ	6.67	1.50	1.37
1	A	183	ALA	CA-CB	-6.63	1.38	1.52
1	A	248	ALA	CA-CB	-6.59	1.38	1.52
1	B	89	GLU	CG-CD	6.54	1.61	1.51
1	A	64	GLU	CB-CG	-6.50	1.39	1.52
1	A	163	GLU	CD-OE2	6.50	1.32	1.25
1	B	55	ARG	N-CA	6.44	1.59	1.46
1	B	128	ARG	CZ-NH2	-6.42	1.24	1.33
1	A	193	PHE	CE2-CZ	-6.38	1.25	1.37
1	A	196	GLU	CG-CD	6.32	1.61	1.51
1	B	221	ILE	CB-CG2	-6.29	1.33	1.52
1	A	146	GLU	C-O	6.18	1.35	1.23
1	A	47	PHE	CD2-CE2	6.16	1.51	1.39
1	B	121	GLU	CD-OE1	6.16	1.32	1.25
1	A	64	GLU	CG-CD	6.15	1.61	1.51
1	A	280	ALA	CA-CB	-6.14	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	LYS	CE-NZ	6.14	1.64	1.49
1	A	126	SER	CA-C	-6.13	1.37	1.52
1	A	189	SER	CB-OG	6.12	1.50	1.42
1	A	212	LYS	CE-NZ	6.10	1.64	1.49
1	B	40	PHE	CD1-CE1	6.09	1.51	1.39
1	B	208	ILE	N-CA	-6.07	1.34	1.46
1	B	89	GLU	CB-CG	6.05	1.63	1.52
1	B	176	GLU	CD-OE1	6.04	1.32	1.25
1	A	267	ARG	CZ-NH1	6.01	1.40	1.33
1	B	269	LYS	CE-NZ	6.01	1.64	1.49
1	B	210	TRP	CZ3-CH2	-6.00	1.30	1.40
1	A	33	PHE	CD1-CE1	-5.99	1.27	1.39
1	A	233	ASP	CB-CG	5.98	1.64	1.51
1	B	231	VAL	CB-CG1	-5.96	1.40	1.52
1	B	41	ASP	C-O	5.95	1.34	1.23
1	A	205	GLU	CG-CD	5.93	1.60	1.51
1	A	153	ARG	CZ-NH1	5.88	1.40	1.33
1	A	270	LYS	CE-NZ	5.86	1.63	1.49
1	A	110	GLU	CG-CD	5.82	1.60	1.51
1	A	240	SER	C-O	5.81	1.34	1.23
1	B	248	ALA	CA-CB	-5.79	1.40	1.52
1	A	205	GLU	CD-OE2	5.76	1.31	1.25
1	B	251	TRP	CA-CB	-5.76	1.41	1.53
1	A	107	PRO	N-CA	-5.75	1.37	1.47
1	A	257	ASP	C-O	5.74	1.34	1.23
1	A	34	ALA	CA-CB	-5.73	1.40	1.52
1	A	67	ALA	CA-CB	-5.67	1.40	1.52
1	B	187	VAL	CB-CG2	-5.67	1.41	1.52
1	B	287	MET	CG-SD	5.60	1.95	1.81
1	B	165	PHE	CG-CD1	5.56	1.47	1.38
1	A	66	PHE	CD2-CE2	-5.55	1.28	1.39
1	A	89	GLU	CA-CB	-5.53	1.41	1.53
1	B	114	ASP	CG-OD1	5.53	1.38	1.25
1	B	61	ARG	CZ-NH1	5.52	1.40	1.33
1	A	155	ILE	N-CA	5.51	1.57	1.46
1	B	41	ASP	CG-OD1	5.50	1.38	1.25
1	B	33	PHE	CE2-CZ	-5.48	1.26	1.37
1	A	291	ASN	CB-CG	5.48	1.63	1.51
1	A	235	THR	C-N	5.44	1.42	1.33
1	B	271	ASP	CB-CG	5.44	1.63	1.51
1	A	158	GLU	CD-OE2	5.43	1.31	1.25
1	A	110	GLU	CD-OE2	5.42	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	TRP	CZ3-CH2	-5.41	1.31	1.40
1	A	47	PHE	CE2-CZ	-5.39	1.27	1.37
1	A	77	VAL	CB-CG2	-5.38	1.41	1.52
1	B	110	GLU	CD-OE1	5.37	1.31	1.25
1	B	256	GLY	N-CA	5.35	1.54	1.46
1	A	99	ARG	CG-CD	5.33	1.65	1.51
1	B	179	ASP	CG-OD1	5.33	1.37	1.25
1	B	193	PHE	CB-CG	-5.32	1.42	1.51
1	B	165	PHE	CE2-CZ	5.31	1.47	1.37
1	A	55	ARG	CZ-NH2	5.30	1.40	1.33
1	A	158	GLU	CD-OE1	5.29	1.31	1.25
1	A	33	PHE	CE2-CZ	-5.27	1.27	1.37
1	B	55	ARG	NE-CZ	5.24	1.39	1.33
1	A	154	LYS	CE-NZ	5.18	1.62	1.49
1	A	131	ASP	N-CA	-5.17	1.36	1.46
1	B	60	TYR	CZ-OH	5.16	1.46	1.37
1	B	57	VAL	C-N	5.15	1.46	1.34
1	B	138	ILE	CA-CB	-5.12	1.43	1.54
1	A	56	THR	CB-CG2	5.10	1.69	1.52
1	A	210	TRP	CA-CB	-5.06	1.42	1.53
1	A	229	TRP	CZ3-CH2	5.06	1.48	1.40
1	B	136	ASN	C-O	5.06	1.32	1.23
1	A	275	ASP	CB-CG	5.05	1.62	1.51
1	B	274	TYR	CG-CD2	5.04	1.45	1.39
1	A	41	ASP	C-O	5.03	1.32	1.23
1	B	178	GLN	CG-CD	5.03	1.62	1.51
1	A	40	PHE	CE2-CZ	-5.02	1.27	1.37
1	B	61	ARG	CZ-NH2	5.02	1.39	1.33
1	A	57	VAL	CA-CB	-5.02	1.44	1.54
1	B	160	THR	C-O	-5.01	1.13	1.23
1	A	153	ARG	CZ-NH2	5.00	1.39	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ARG	NE-CZ-NH2	-17.02	111.79	120.30
1	B	128	ARG	NE-CZ-NH1	15.62	128.11	120.30
1	B	41	ASP	CB-CG-OD2	-12.51	107.04	118.30
1	B	153	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	B	65	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	B	83	GLN	O-C-N	-11.60	104.14	122.70
1	A	204	ARG	NE-CZ-NH1	-9.86	115.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH2	9.80	125.20	120.30
1	A	252	PRO	O-C-N	-9.39	103.26	121.10
1	A	267	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	179	ASP	CB-CG-OD2	8.98	126.38	118.30
1	A	65	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	211	MET	CG-SD-CE	8.73	114.17	100.20
1	A	275	ASP	CB-CG-OD1	8.73	126.16	118.30
1	B	195	LEU	CB-CG-CD2	8.57	125.57	111.00
1	A	204	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	B	268	ASP	N-CA-C	8.22	133.20	111.00
1	B	218	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	B	57	VAL	O-C-N	-8.05	109.82	122.70
1	B	197	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	204	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	199	LEU	CB-CG-CD2	7.90	124.43	111.00
1	A	252	PRO	C-N-CD	-7.74	103.57	120.60
1	B	264	LEU	CB-CG-CD2	7.31	123.42	111.00
1	B	264	LEU	CA-CB-CG	7.30	132.09	115.30
1	A	198	LYS	CD-CE-NZ	7.24	128.35	111.70
1	A	89	GLU	OE1-CD-OE2	7.18	131.92	123.30
1	A	101	ASP	CB-CG-OD2	-7.07	111.93	118.30
1	B	179	ASP	CB-CG-OD1	7.05	124.65	118.30
1	B	218	ASP	CB-CG-OD2	7.03	124.62	118.30
1	B	197	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	276	ASP	CB-CG-OD1	-7.01	111.99	118.30
1	A	94	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	B	43	LYS	CD-CE-NZ	6.87	127.49	111.70
1	A	159	VAL	CG1-CB-CG2	-6.77	100.06	110.90
1	A	102	LEU	CB-CG-CD2	6.64	122.28	111.00
1	A	218	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	B	102	LEU	CB-CG-CD1	6.55	122.13	111.00
1	A	267	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	B	207	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	190	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	139	LEU	CB-CG-CD1	-6.37	100.18	111.00
1	A	57	VAL	C-N-CA	-6.33	105.88	121.70
1	A	218	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	157	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	55	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	286	VAL	CG1-CB-CG2	-6.21	100.96	110.90
1	B	50	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	B	206	LEU	CB-CG-CD2	6.08	121.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	LEU	CB-CG-CD2	6.04	121.27	111.00
1	B	80	LEU	CB-CG-CD1	5.85	120.95	111.00
1	B	148	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	264	LEU	CB-CG-CD2	5.78	120.83	111.00
1	B	140	LYS	CD-CE-NZ	5.78	124.99	111.70
1	B	55	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	179	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	277	LYS	CA-CB-CG	5.70	125.94	113.40
1	B	114	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	99	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	127	LEU	CA-CB-CG	5.66	128.33	115.30
1	B	44	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	99	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	126	SER	CB-CA-C	-5.66	99.35	110.10
1	B	265	SER	N-CA-CB	-5.60	102.10	110.50
1	B	31	ASP	CB-CA-C	5.59	121.58	110.40
1	B	268	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	75	LEU	CB-CG-CD1	-5.53	101.59	111.00
1	B	55	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	A	212	LYS	C-N-CA	-5.50	107.95	121.70
1	A	106	ASN	C-N-CD	5.50	139.94	128.40
1	A	217	GLY	N-CA-C	5.49	126.83	113.10
1	B	227	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	83	GLN	O-C-N	-5.44	114.00	122.70
1	A	94	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	191	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	139	LEU	CA-CB-CG	-5.38	102.93	115.30
1	B	163	GLU	N-CA-C	5.34	125.41	111.00
1	B	113	VAL	CA-CB-CG1	-5.32	102.92	110.90
1	B	195	LEU	N-CA-CB	-5.32	99.75	110.40
1	A	202	GLU	N-CA-CB	-5.32	101.02	110.60
1	B	161	ASN	CB-CA-C	-5.31	99.78	110.40
1	B	46	ILE	CG1-CB-CG2	-5.30	99.75	111.40
1	B	178	GLN	CB-CA-C	5.28	120.96	110.40
1	B	173	ASN	C-N-CD	-5.27	109.00	120.60
1	B	260	VAL	CB-CA-C	5.18	121.25	111.40
1	B	119	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	100	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	158	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	B	225	VAL	CB-CA-C	5.09	121.08	111.40
1	B	98	THR	CA-CB-CG2	-5.09	105.28	112.40
1	A	60	TYR	CB-CG-CD2	5.07	124.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ARG	N-CA-CB	5.07	119.72	110.60
1	B	127	LEU	CB-CG-CD1	5.06	119.59	111.00
1	A	240	SER	CA-CB-OG	-5.04	97.58	111.20
1	A	270	LYS	CD-CE-NZ	-5.04	100.12	111.70
1	B	91	LEU	CB-CG-CD1	-5.02	102.47	111.00

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
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 [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	1910	0	1928	142	3
1	B	1963	0	1985	146	3
2	A	26	0	0	1	0
2	B	26	0	0	0	0
3	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	0	2	0
All	All	3964	0	3913	289	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 37.

All (289) 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
1:A:208:ILE:HG22	1:A:209:ASP:N	1.31	1.24
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: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: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:B:67:ALA:CB	1:B:172:VAL:HG21	1.94	0.98
1:B:83:GLN:C	1:B:86:LYS:HG2	1.84	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:A:207:LEU:O	1:A:208:ILE:C	1.97	0.94
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:63:ASP:CG	1:A:184:ARG:HH21	1.74	0.92
1:A:103:VAL:HG23	1:A:104:ASN:H	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:GLN:C	1:B:86:LYS:CG	2.38	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: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
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:208:ILE:O	1:A:209:ASP:C	2.12	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: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:181:SER:OG	1:A:182:THR:N	2.08	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:C	1:B:100:ASP:HB3	2.09	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:A:212:LYS:HD3	1:A:230:GLU:OE1	1.89	0.71
1:B:88:ILE:O	1:B:88:ILE:CG2	2.37	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:82:GLN:HB2	1:B:199:LEU:CD2	2.21	0.70
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: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:252:PRO:O	1:A:255:LYS:N	2.27	0.67
1:B:52:GLY:C	1:B:53:THR:HG23	2.15	0.67
1:A:94:ARG:HA	1:A:118:THR:HG22	1.74	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: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:B:190:LEU:O	1:B:191:ARG:C	2.32	0.65
1:A:269:LYS:O	1:A:269:LYS:CG	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:112:HIS:O	1:A:113:VAL:C	2.36	0.63
1:B:35:LYS:HZ3	1:B:35:LYS:HB2	1.64	0.63
1:A:252:PRO:C	1:A:255:LYS:H	2.02	0.62
1:A:53:THR:HG21	1:A:55:ARG:NH2	2.15	0.62
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: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:A:252:PRO:C	1:A:255:LYS:N	2.53	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:B:35:LYS:HB2	1:B:35:LYS:NZ	2.16	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:A:106:ASN:O	1:A:107:PRO:C	2.39	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:252:PRO:O	1:A:254:PRO:C	2.37	0.59
1:A:49:LEU:O	1:A:259:VAL:HG13	2.03	0.58
1:A:285:VAL:O	1:A:289:ALA:HB3	2.03	0.58
1:A:139:LEU:HD22	1:A:144:GLY:HA2	1.85	0.57
1:B:52:GLY:C	1:B:53:THR:CG2	2.72	0.57
1:B:98:THR:OG1	1:B:100:ASP:CG	2.41	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:98:THR:HG1	1:B:100:ASP:CG	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:C	1:A:290:LEU:N	2.59	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: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
1:A:249:ILE:CG2	1:A:251:TRP:CZ2	2.90	0.54
1:A:191:ARG:O	1:A:192:ALA:C	2.44	0.54
1:B:56:THR:HG23	1:B:57:VAL:C	2.27	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: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:108:ILE:O	1:A:108:ILE:HG22	2.07	0.53
1:A:243:THR:HA	1:A:265:SER:O	2.09	0.53
1:B:270:LYS:O	1:B:270:LYS:HG3	2.09	0.53
1:B:281:GLU:O	1:B:282:ALA:C	2.46	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: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: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:149:LYS:HD3	1:A:153:ARG:CZ	2.41	0.51
1:B:56:THR:CG2	1:B:57:VAL:N	2.73	0.51
1:B:57:VAL:HG13	1:B:59:ALA:N	2.22	0.51
2:A:1:CEF:C3	2:A:1:CEF:O1	2.59	0.51
1:B:289:ALA:O	1:B:290:LEU:C	2.47	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:A:51:THR:O	1:A:52:GLY:C	2.49	0.50
1:A:152:LEU:O	1:A:153:ARG:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:186:LEU:O	1:B:187:VAL:C	2.50	0.49
1:A:259:VAL:HG12	1:A:260:VAL:N	2.26	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: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: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: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:288:LYS:O	1:A:289:ALA:C	2.53	0.47
1:A:68:PHE:O	1:A:69:ALA:C	2.49	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: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:A:182:THR:O	1:A:183:ALA:C	2.53	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:A:93:GLN:HE21	1:A:93:GLN:HB3	1.52	0.45
1:A:112:HIS:C	1:A:114:ASP:N	2.68	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:B:201:SER:HA	1:B:204:ARG:NH1	2.32	0.44
1:A:287:MET:O	1:A:291:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASP:O	1:B:101:ASP:CG	2.56	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:B:283:THR:O	1:B:284:LYS:C	2.54	0.44
1:A:240:SER:C	1:A:242:GLY:H	2.21	0.44
1:A:286:VAL:C	1:A:289:ALA:HB3	2.38	0.44
1:B:207:LEU:O	1:B:208:ILE:C	2.54	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: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:A:288:LYS:C	1:A:290:LEU:H	2.21	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: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: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:240:SER:C	1:A:242:GLY:N	2.70	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:81:LEU:O	1:A:82:GLN:C	2.58	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: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
1:A:269:LYS:NZ	1:A:271:ASP:OD1	2.25	0.41
1:B:153:ARG:HD3	1:B:158:GLU:HA	2.01	0.41
1:A:209:ASP:O	1:A:210:TRP:C	2.57	0.41
1:B:241:TYR:CZ	1:B:270:LYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HA	1:A:37:GLU:HG3	2.03	0.41
1:B:50:ASP:C	1:B:50:ASP:OD1	2.56	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:66:PHE:O	1:B:67:ALA:C	2.59	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 [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	241/257 (94%)	207 (86%)	22 (9%)	12 (5%)	2	19
1	B	247/257 (96%)	209 (85%)	27 (11%)	11 (4%)	2	21
All	All	488/514 (95%)	416 (85%)	49 (10%)	23 (5%)	2	20

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	205/217 (94%)	160 (78%)	45 (22%)	<b>1</b> <b>5</b>
1	B	211/217 (97%)	170 (81%)	41 (19%)	<b>1</b> <b>7</b>
All	All	416/434 (96%)	330 (79%)	86 (21%)	<b>1</b> <b>6</b>

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	56	THR
1	A	64	GLU
1	A	68	PHE
1	A	72	ILE
1	A	82	GLN
1	A	88	ILE
1	A	89	GLU
1	A	93	GLN
1	A	94	ARG
1	A	95	ILE
1	A	96	THR
1	A	98	THR
1	A	102	LEU
1	A	109	THR
1	A	113	VAL
1	A	115	THR
1	A	137	LEU
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	161	ASN
1	A	163	GLU
1	A	177	THR
1	A	178	GLN
1	A	181	SER
1	A	190	LEU
1	A	195	LEU
1	A	208	ILE
1	A	218	ASP
1	A	220	LEU
1	A	243	THR
1	A	249	ILE
1	A	255	LYS
1	A	260	VAL
1	A	268	ASP
1	A	269	LYS
1	A	270	LYS
1	A	273	LYS
1	A	279	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	287	MET
1	A	288	LYS
1	B	30	LYS
1	B	31	ASP
1	B	32	ASP
1	B	35	LYS
1	B	56	THR
1	B	65	ARG
1	B	70	SER
1	B	99	ARG
1	B	100	ASP
1	B	102	LEU
1	B	109	THR
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	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	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

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Mol	Chain	Res	Type
1	B	273	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	93	GLN
1	A	178	GLN
1	B	83	GLN
1	B	173	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 monosaccharides 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	CEF	A	1	1	19,27,27	3.00	9 (47%)	14,37,37	4.55	7 (50%)
2	CEF	B	1	1	19,27,27	2.04	3 (15%)	14,37,37	8.38	10 (71%)

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	A	1	1	-	4/14/38/38	0/1/2/2
2	CEF	B	1	1	-	4/14/38/38	0/1/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	CEF	C13-S2	6.11	1.80	1.70
2	A	1	CEF	C1-S1	-5.74	1.69	1.82
2	A	1	CEF	O5-N3	-4.49	1.30	1.40
2	B	1	CEF	C1-S1	-4.41	1.72	1.82
2	B	1	CEF	C13-S2	4.33	1.77	1.70
2	B	1	CEF	C12-N5	-3.82	1.25	1.37
2	A	1	CEF	C10-C9	-3.48	1.43	1.50
2	A	1	CEF	C4-N1	3.44	1.36	1.28
2	A	1	CEF	C4-C5	-3.30	1.41	1.48
2	A	1	CEF	C4-C2	-3.17	1.36	1.46
2	A	1	CEF	C3-C2	3.08	1.39	1.32
2	A	1	CEF	O4-C9	-3.05	1.17	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	CEF	C11-O5-N3	19.82	131.43	108.40
2	B	1	CEF	O5-N3-C10	18.10	131.21	111.28
2	B	1	CEF	C12-C13-S2	-12.14	96.89	111.79
2	A	1	CEF	C12-C13-S2	-9.88	99.66	111.79
2	B	1	CEF	C2-C1-S1	7.45	126.99	111.65
2	A	1	CEF	C2-C1-S1	6.97	126.01	111.65
2	A	1	CEF	C1-S1-C6	6.93	108.06	94.47
2	A	1	CEF	C11-O5-N3	5.73	115.05	108.40
2	A	1	CEF	O5-N3-C10	4.81	116.57	111.28
2	B	1	CEF	C1-S1-C6	4.61	103.51	94.47
2	A	1	CEF	C7-N2-C9	3.69	128.02	122.26
2	A	1	CEF	O2-C5-O1	-3.66	115.24	123.61
2	B	1	CEF	C7-N2-C9	3.03	127.00	122.26
2	B	1	CEF	C10-C9-N2	2.93	119.25	114.38
2	B	1	CEF	O2-C5-O1	-2.55	117.78	123.61
2	B	1	CEF	O3-C8-C7	-2.27	118.50	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	CEF	O2-C5-C4	2.26	122.05	116.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

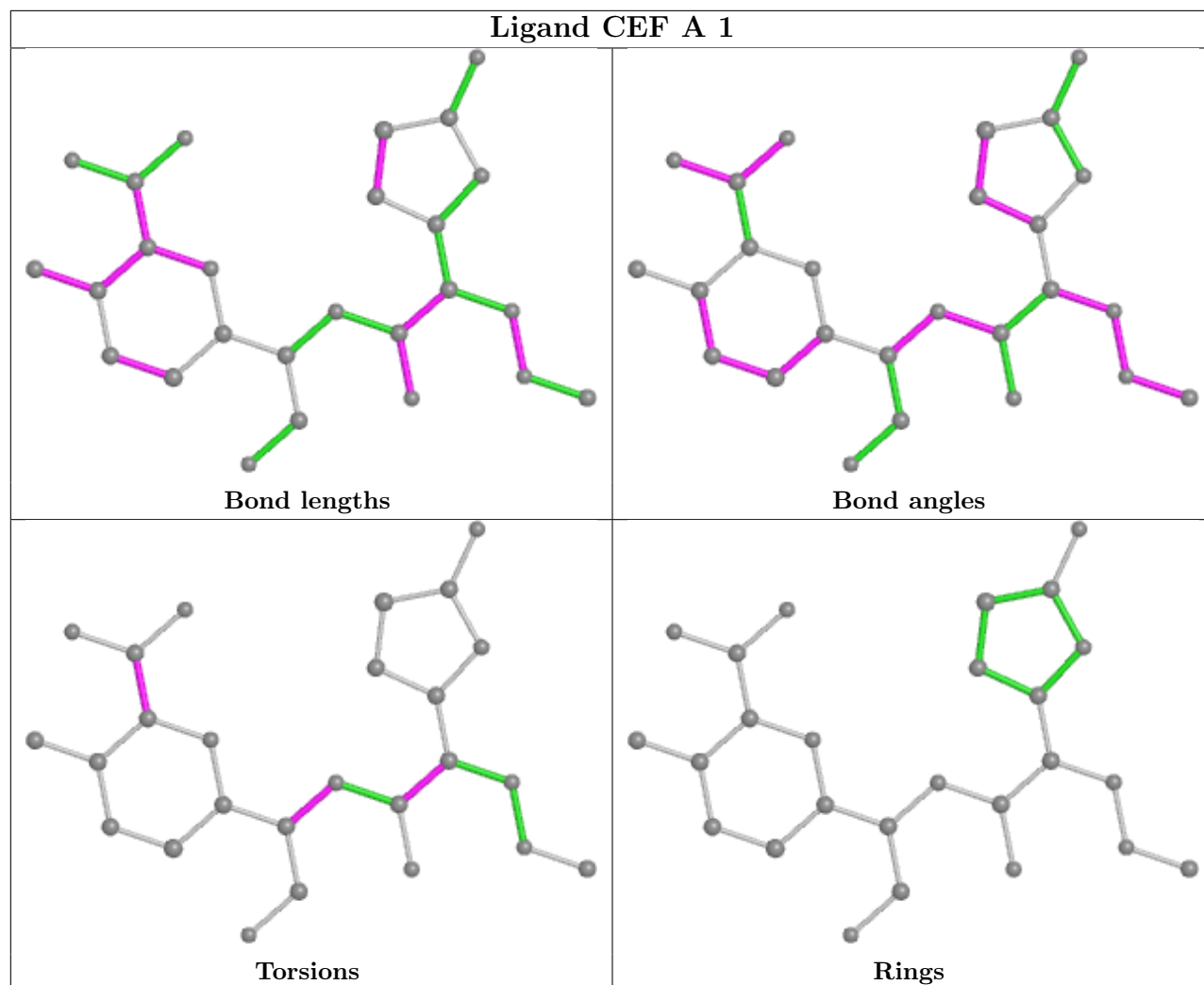
Mol	Chain	Res	Type	Atoms
2	A	1	CEF	C8-C7-N2-C9
2	B	1	CEF	N1-C4-C5-O2
2	B	1	CEF	C10-N3-O5-C11
2	B	1	CEF	C2-C4-C5-O1
2	A	1	CEF	C6-C7-N2-C9
2	A	1	CEF	C2-C4-C5-O1
2	A	1	CEF	N3-C10-C9-O4
2	B	1	CEF	N3-C10-C9-O4

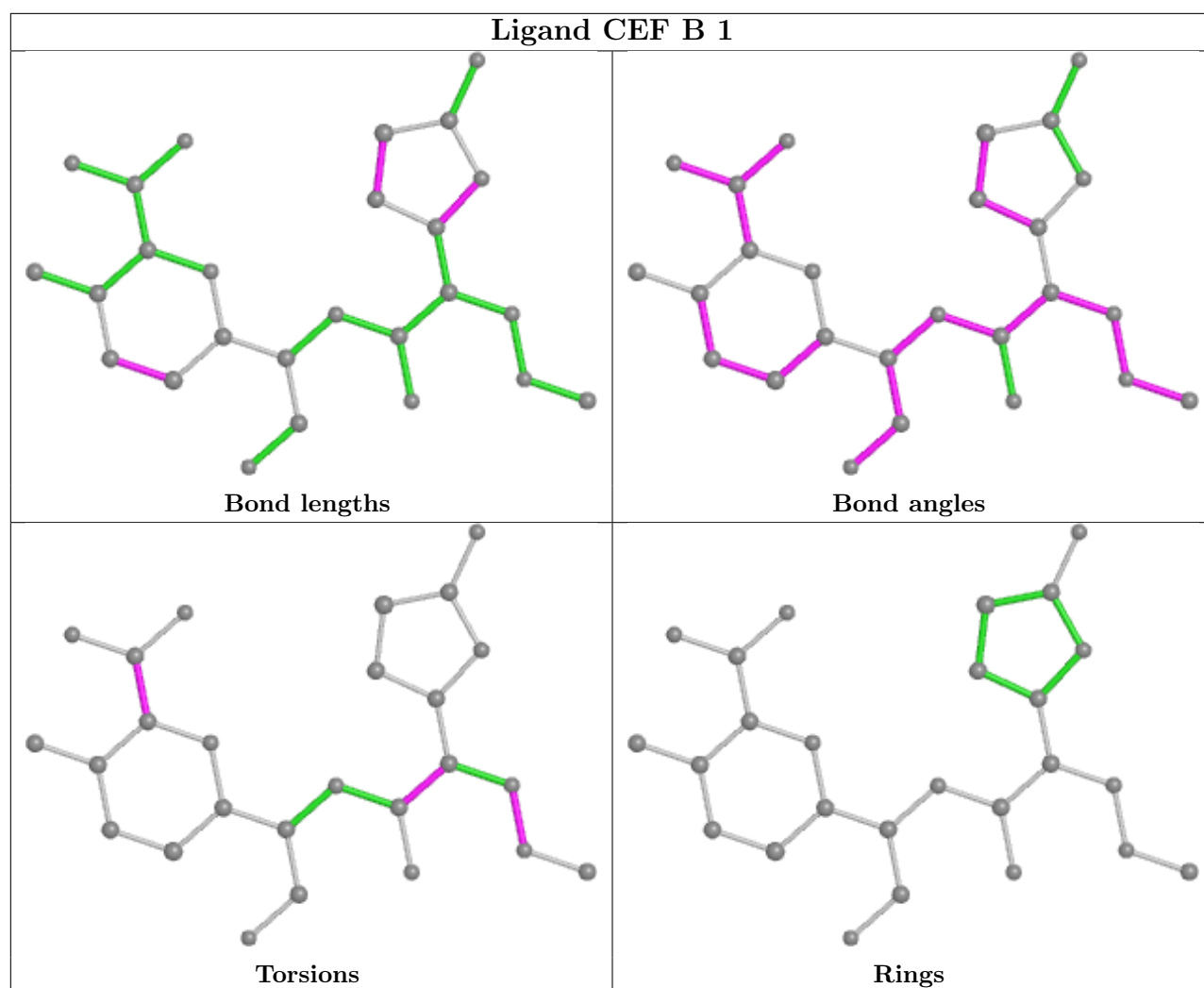
There are no ring outliers.

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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	245/257 (95%)	-0.60	0 100 100	7, 13, 19, 34	0
1	B	251/257 (97%)	-0.60	0 100 100	7, 13, 19, 44	0
All	All	496/514 (96%)	-0.60	0 100 100	7, 13, 19, 44	0

There are no RSRZ outliers to report.

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

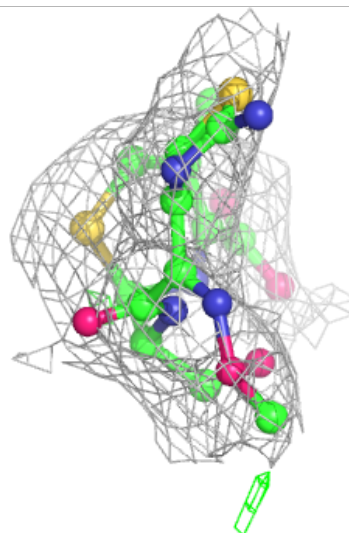
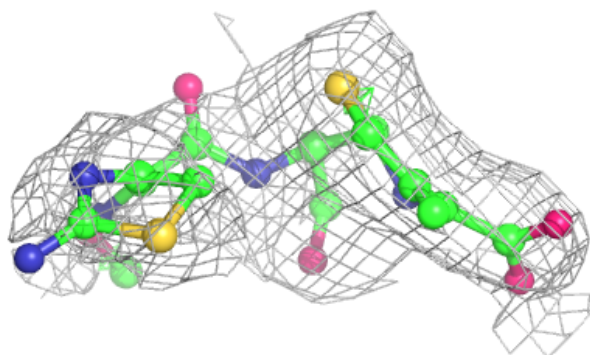
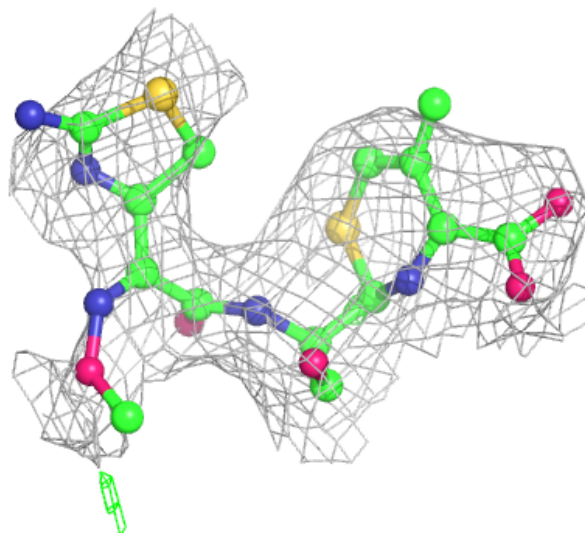
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

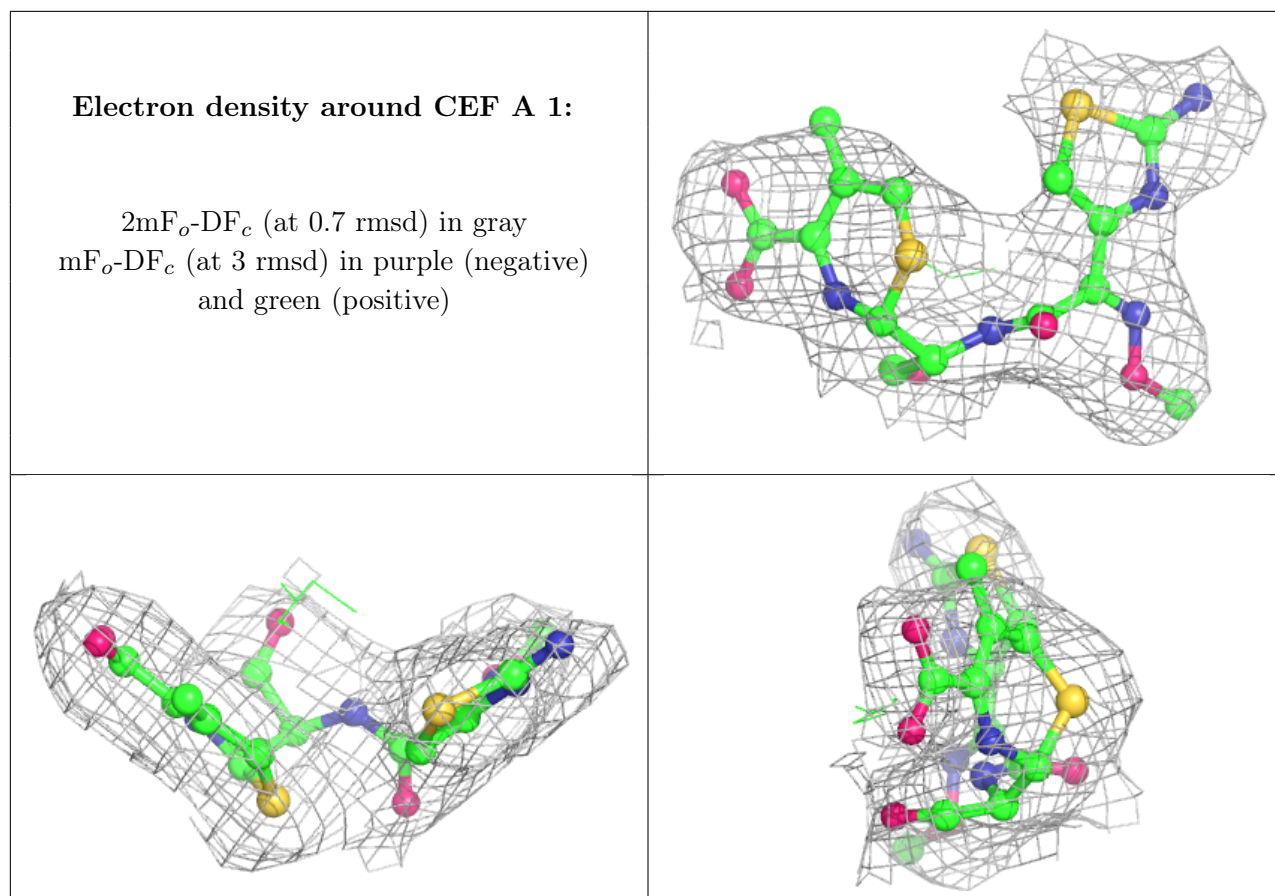
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CEF	B	1	26/26	0.93	0.23	32,44,75,78	0
2	CEF	A	1	26/26	0.95	0.15	11,16,35,45	0

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.