Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:00 PM EDT

PDB ID	:	1FR6
Title	:	REFINED CRYSTAL STRUCTURE OF BETA-LACTAMASE FROM CITROBACTER FREUNDII INDICATES A MECHANISM FOR BETA-LACTAM HYDROLYSIS
Authors	:	Oefner, C.; D'Arcy, A.; Daly, J.J.; Winkler, F.K.
Deposited on	:	2000-09-07
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

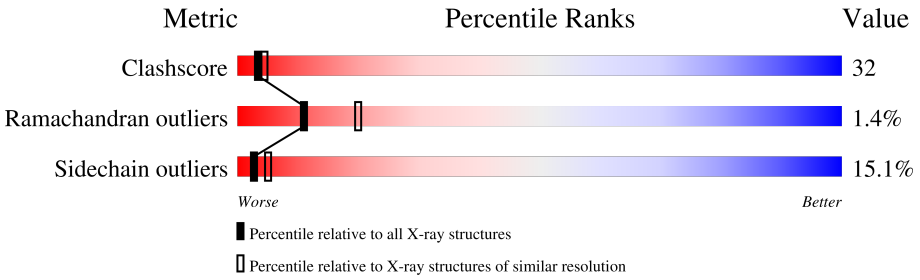
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	39% 45% 13% •
1	B	361	39% 44% 14% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AZR	B	362	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6038 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.

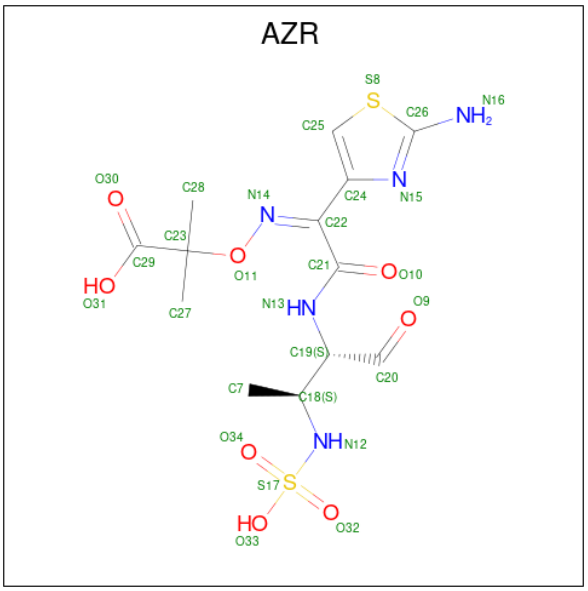
- Molecule 1 is a protein called BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2806	1801	479	517	9	0	0	0
1	B	361	2806	1801	479	517	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	SER	THR	SEE REMARK 999	UNP Q46041
A	176	LYS	THR	SEE REMARK 999	UNP Q46041
A	180	HIS	GLN	SEE REMARK 999	UNP Q46041
A	228	ILE	VAL	SEE REMARK 999	UNP Q46041
A	253	GLU	LYS	SEE REMARK 999	UNP Q46041
A	278	VAL	LEU	SEE REMARK 999	UNP Q46041
A	285	SER	ASN	SEE REMARK 999	UNP Q46041
A	348	VAL	ALA	SEE REMARK 999	UNP Q46041
B	175	SER	THR	SEE REMARK 999	UNP Q46041
B	176	LYS	THR	SEE REMARK 999	UNP Q46041
B	180	HIS	GLN	SEE REMARK 999	UNP Q46041
B	228	ILE	VAL	SEE REMARK 999	UNP Q46041
B	253	GLU	LYS	SEE REMARK 999	UNP Q46041
B	278	VAL	LEU	SEE REMARK 999	UNP Q46041
B	285	SER	ASN	SEE REMARK 999	UNP Q46041
B	348	VAL	ALA	SEE REMARK 999	UNP Q46041

- Molecule 2 is 2-({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-oxo-2-{[(2S,3S)-1-oxo-3-(sulfoamino) butan-2-yl]amino}ethylidene]amino}oxy)-2-methylpropanoic acid (three-letter code: AZR) (formula: $C_{13}H_{19}N_5O_8S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	28	13	5	8	2	0	0
			Total	C	N	O	S		
2	B	1	28	13	5	8	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	189	189	189	0	0
			Total	O		
3	B	181	181	181	0	0

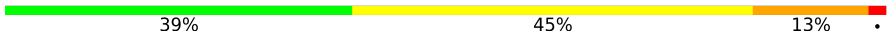
3 Residue-property plots (i)

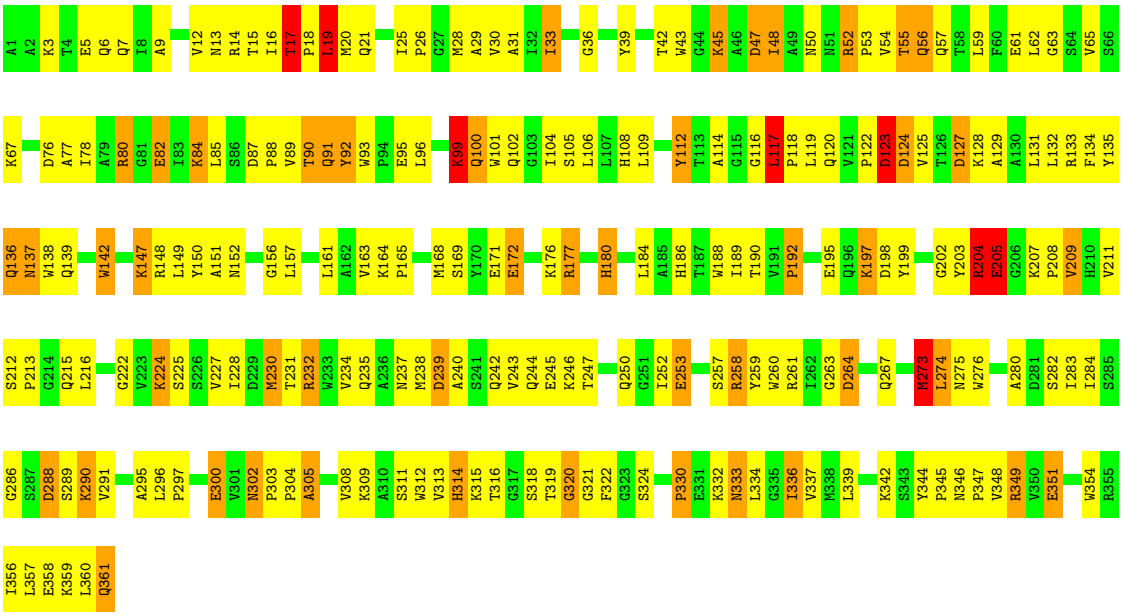
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: BETA-LACTAMASE

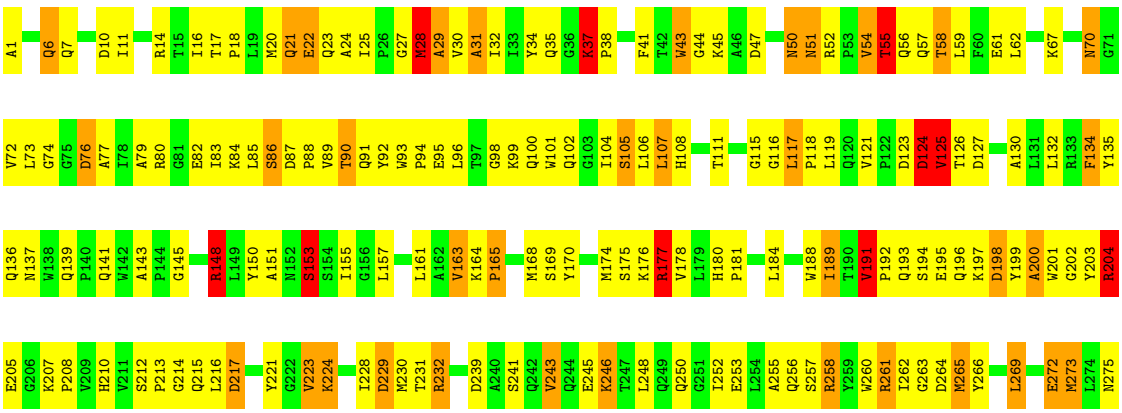
Chain A:





• Molecule 1: BETA-LACTAMASE

Chain B:



K279
A280
D281
S282
I283
I284
S285
G286
S287
D288
S289
K290
V291
A292
L293
A294
A295
L296
N302
P303
P304
A305
K309
H314
K315
S318
T319
G320
G321
F322
Y325
V326
A327
F328
L334
G335
I336
V337
N341
Y344
P345
V348
R349
V350
E351
A352
A353
W354
R355
I356
L357
E358
K359
L360
Q361

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.07Å 84.63Å 89.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6038	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.18	3/2881 (0.1%)	1.92	66/3925 (1.7%)
1	B	1.23	3/2881 (0.1%)	1.91	80/3925 (2.0%)
All	All	1.20	6/5762 (0.1%)	1.91	146/7850 (1.9%)

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	B	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	SER	CB-OG	7.83	1.52	1.42
1	A	105	SER	CB-OG	7.58	1.52	1.42
1	B	105	SER	CB-OG	5.96	1.50	1.42
1	B	241	SER	CB-OG	5.76	1.49	1.42
1	A	14	ARG	CD-NE	-5.71	1.36	1.46
1	B	188	TRP	CA-CB	5.41	1.65	1.53

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	ARG	CD-NE-CZ	32.96	169.75	123.60
1	B	349	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	A	14	ARG	NE-CZ-NH1	15.06	127.83	120.30
1	A	264	ASP	CB-CG-OD1	13.26	130.24	118.30
1	B	258	ARG	NE-CZ-NH2	-11.86	114.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	B	349	ARG	CD-NE-CZ	-10.76	108.53	123.60
1	B	10	ASP	CB-CG-OD2	-10.76	108.61	118.30
1	B	148	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	B	349	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	A	133	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	205	GLU	CA-CB-CG	9.80	134.95	113.40
1	A	204	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	B	264	ASP	CA-CB-CG	9.56	134.43	113.40
1	B	198	ASP	CB-CG-OD1	9.56	126.90	118.30
1	B	148	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	A	232	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	264	ASP	CA-CB-CG	8.55	132.22	113.40
1	B	44	GLY	N-CA-C	8.13	133.44	113.10
1	B	355	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	184	LEU	CB-CA-C	7.82	125.06	110.20
1	B	29	ALA	CB-CA-C	7.81	121.82	110.10
1	A	351	GLU	CA-CB-CG	7.80	130.57	113.40
1	A	39	TYR	CA-CB-CG	7.72	128.08	113.40
1	B	232	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	A	177	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	B	22	GLU	CA-CB-CG	7.69	130.31	113.40
1	B	258	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	322	PHE	CA-CB-CG	7.46	131.81	113.90
1	A	65	VAL	CB-CA-C	7.39	125.45	111.40
1	A	205	GLU	N-CA-CB	7.30	123.74	110.60
1	B	117	LEU	CA-CB-CG	7.25	131.96	115.30
1	A	117	LEU	CB-CA-C	7.15	123.79	110.20
1	A	258	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	B	230	MET	CA-CB-CG	-6.86	101.63	113.30
1	B	10	ASP	CA-CB-CG	-6.80	98.44	113.40
1	A	100	GLN	CA-CB-CG	6.79	128.33	113.40
1	A	6	GLN	CA-CB-CG	6.78	128.32	113.40
1	B	145	GLY	N-CA-C	6.75	129.99	113.10
1	A	47	ASP	CB-CG-OD2	6.74	124.37	118.30
1	B	153	SER	C-N-CA	6.74	138.55	121.70
1	B	31	ALA	N-CA-CB	6.74	119.53	110.10
1	A	349	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	177	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	172	GLU	CA-CB-CG	6.63	127.99	113.40
1	A	80	ARG	CD-NE-CZ	-6.63	114.32	123.60
1	A	177	ARG	CG-CD-NE	6.62	125.69	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	355	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	204	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	37	LYS	CB-CA-C	-6.51	97.38	110.40
1	B	52	ARG	CD-NE-CZ	-6.50	114.50	123.60
1	B	153	SER	CA-CB-OG	6.49	128.73	111.20
1	B	243	VAL	CB-CA-C	6.47	123.69	111.40
1	A	92	TYR	CA-CB-CG	-6.46	101.12	113.40
1	B	87	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	125	VAL	N-CA-C	-6.44	93.62	111.00
1	A	186	HIS	CA-CB-CG	-6.43	102.66	113.60
1	A	177	ARG	CD-NE-CZ	6.39	132.55	123.60
1	B	351	GLU	CG-CD-OE1	6.36	131.02	118.30
1	B	124	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	190	THR	N-CA-CB	6.33	122.32	110.30
1	B	28	MET	CA-CB-CG	6.31	124.02	113.30
1	A	349	ARG	CA-CB-CG	6.26	127.18	113.40
1	A	82	GLU	CA-CB-CG	6.25	127.15	113.40
1	A	5	GLU	CA-CB-CG	6.24	127.14	113.40
1	A	14	ARG	NH1-CZ-NH2	-6.24	112.53	119.40
1	B	264	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	209	VAL	N-CA-CB	-6.22	97.81	111.50
1	B	224	LYS	N-CA-CB	6.13	121.63	110.60
1	B	273	MET	N-CA-CB	-6.11	99.61	110.60
1	A	257	SER	O-C-N	6.09	132.44	122.70
1	B	70	ASN	CB-CA-C	6.08	122.56	110.40
1	A	133	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	90	THR	CA-CB-CG2	6.07	120.89	112.40
1	B	269	LEU	CB-CA-C	6.05	121.69	110.20
1	A	17	THR	CA-CB-CG2	6.03	120.85	112.40
1	A	120	GLN	CG-CD-OE1	-6.01	109.58	121.60
1	B	285	SER	CB-CA-C	-6.00	98.70	110.10
1	A	106	LEU	CB-CA-C	5.99	121.57	110.20
1	B	56	GLN	CB-CG-CD	5.97	127.13	111.60
1	B	55	THR	N-CA-CB	-5.96	98.97	110.30
1	A	305	ALA	CB-CA-C	5.88	118.92	110.10
1	B	232	ARG	CD-NE-CZ	-5.86	115.39	123.60
1	A	5	GLU	N-CA-CB	5.79	121.03	110.60
1	A	197	LYS	CA-CB-CG	5.79	126.15	113.40
1	B	72	VAL	CA-CB-CG1	5.77	119.56	110.90
1	B	351	GLU	CA-CB-CG	5.73	126.01	113.40
1	A	198	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	217	ASP	CB-CA-C	5.71	121.81	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	TRP	CA-CB-CG	-5.70	102.88	113.70
1	A	117	LEU	N-CA-C	-5.68	95.67	111.00
1	B	239	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	204	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	272	GLU	CG-CD-OE2	-5.65	107.00	118.30
1	B	351	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	B	6	GLN	CA-CB-CG	5.60	125.72	113.40
1	A	288	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	62	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	325	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	A	300	GLU	CB-CA-C	-5.52	99.36	110.40
1	B	106	LEU	CB-CA-C	5.51	120.67	110.20
1	A	123	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	82	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	B	295	ALA	N-CA-CB	5.50	117.80	110.10
1	B	10	ASP	OD1-CG-OD2	5.50	133.74	123.30
1	A	258	ARG	N-CA-CB	-5.49	100.71	110.60
1	B	54	VAL	CA-CB-CG2	5.47	119.10	110.90
1	B	191	VAL	CB-CA-C	5.47	121.78	111.40
1	B	117	LEU	N-CA-C	-5.46	96.27	111.00
1	B	229	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	B	309	LYS	CB-CA-C	-5.41	99.58	110.40
1	B	223	VAL	CB-CA-C	5.39	121.64	111.40
1	A	112	TYR	CB-CG-CD1	5.39	124.23	121.00
1	A	124	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	171	GLU	CG-CD-OE1	5.34	128.98	118.30
1	A	92	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	147	LYS	CA-CB-CG	5.34	125.14	113.40
1	A	282	SER	N-CA-CB	5.33	118.50	110.50
1	B	82	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	B	117	LEU	CB-CA-C	5.33	120.32	110.20
1	B	121	VAL	N-CA-C	-5.31	96.67	111.00
1	B	189	ILE	N-CA-C	-5.28	96.73	111.00
1	A	273	MET	CA-CB-CG	5.27	122.25	113.30
1	A	222	GLY	N-CA-C	5.26	126.26	113.10
1	B	116	GLY	N-CA-C	5.21	126.13	113.10
1	A	9	ALA	CB-CA-C	5.20	117.91	110.10
1	B	143	ALA	N-CA-CB	-5.20	102.82	110.10
1	B	305	ALA	N-CA-CB	5.20	117.39	110.10
1	A	257	SER	N-CA-CB	5.17	118.26	110.50
1	A	275	ASN	CB-CA-C	5.17	120.75	110.40
1	B	328	PHE	N-CA-CB	5.17	119.90	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	ASP	CA-CB-CG	5.17	124.77	113.40
1	B	96	LEU	CB-CA-C	5.14	119.97	110.20
1	A	80	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	50	ASN	C-N-CA	5.13	134.53	121.70
1	B	76	ASP	CB-CA-C	5.13	120.65	110.40
1	B	229	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	230	MET	CG-SD-CE	5.12	108.38	100.20
1	A	19	LEU	CB-CA-C	5.11	119.90	110.20
1	A	163	VAL	CA-CB-CG1	5.09	118.53	110.90
1	B	153	SER	O-C-N	-5.07	114.59	122.70
1	B	153	SER	N-CA-CB	-5.05	102.92	110.50
1	B	293	LEU	N-CA-CB	-5.03	100.35	110.40
1	B	28	MET	CB-CA-C	5.02	120.45	110.40
1	A	180	HIS	CA-CB-CG	-5.02	105.07	113.60
1	A	259	TYR	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	148	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	204	ARG	Sidechain
1	B	261	ARG	Sidechain
1	B	80	ARG	Sidechain

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	2806	0	2795	194	3
1	B	2806	0	2795	185	6
2	A	28	0	17	5	0
2	B	28	0	17	9	0
3	A	189	0	0	27	2
3	B	181	0	0	14	1
All	All	6038	0	5624	367	6

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 32.

All (367) 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:227:VAL:HG23	1:A:339:LEU:HD12	1.38	1.02
1:A:25:ILE:HD13	1:A:28:MET:HE1	1.45	0.97
1:B:258:ARG:NH1	1:B:275:ASN:HD21	1.62	0.95
1:B:55:THR:H	1:B:58:THR:CG2	1.80	0.95
1:B:73:LEU:HD22	1:B:174:MET:HE2	1.46	0.94
3:A:551:HOH:O	1:B:214:GLY:HA2	1.68	0.92
1:A:55:THR:HG22	1:A:57:GLN:H	1.32	0.92
1:A:361:GLN:O	3:A:508:HOH:O	1.88	0.91
1:B:258:ARG:HH12	1:B:275:ASN:ND2	1.69	0.89
1:B:17:THR:HB	1:B:18:PRO:HD3	1.55	0.88
1:B:258:ARG:HH12	1:B:275:ASN:HD21	0.89	0.85
1:A:344:TYR:HB2	1:A:345:PRO:HD2	1.58	0.84
1:A:42:THR:HB	1:A:54:VAL:HG12	1.61	0.81
1:A:232:ARG:HD3	3:A:372:HOH:O	1.81	0.80
1:A:128:LYS:HB2	3:A:478:HOH:O	1.80	0.80
1:A:45:LYS:HA	1:A:53:PRO:HA	1.64	0.79
1:B:118:PRO:O	1:B:153:SER:HB2	1.80	0.79
1:B:345:PRO:HB2	1:B:348:VAL:HG23	1.64	0.79
1:A:230:MET:O	1:A:234:VAL:HG23	1.82	0.79
1:A:308:VAL:HG12	3:A:382:HOH:O	1.82	0.78
1:B:54:VAL:HA	1:B:58:THR:HG21	1.64	0.78
1:B:191:VAL:HG22	1:B:196:GLN:NE2	1.99	0.77
1:A:80:ARG:HG2	1:A:247:THR:HG21	1.67	0.76
1:A:345:PRO:HG2	1:A:348:VAL:HG21	1.68	0.75
1:A:123:ASP:HB2	2:B:362:AZR:C27	2.16	0.75
1:A:231:THR:O	1:A:235:GLN:HG3	1.87	0.74
1:B:61:GLU:OE2	1:B:199:TYR:OH	2.06	0.73
1:A:142:TRP:CE2	1:A:147:LYS:HD2	2.23	0.73
1:B:255:ALA:HA	1:B:269:LEU:HB2	1.69	0.73
1:B:47:ASP:OD1	1:B:50:ASN:HB2	1.89	0.72
1:A:260:TRP:CE3	1:A:300:GLU:HA	2.24	0.72
1:A:290:LYS:HE3	1:B:139:GLN:HE22	1.54	0.72
1:A:19:LEU:HD23	1:A:20:MET:N	2.03	0.72
1:B:55:THR:HG22	1:B:57:GLN:H	1.55	0.71
1:B:256:GLN:HG3	3:B:397:HOH:O	1.90	0.71
1:A:20:MET:HG2	1:A:28:MET:HE3	1.73	0.70
1:A:192:PRO:HB2	1:A:195:GLU:HG2	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:MET:HE3	1:B:272:GLU:HG2	1.74	0.69
1:B:345:PRO:HB2	1:B:348:VAL:CG2	2.22	0.69
1:B:202:GLY:O	1:B:208:PRO:HA	1.93	0.68
1:B:192:PRO:HA	3:B:413:HOH:O	1.93	0.67
1:B:246:LYS:HE3	1:B:250:GLN:OE1	1.93	0.67
2:A:362:AZR:H27B	1:B:123:ASP:HB2	1.77	0.67
1:A:7:GLN:NE2	3:A:497:HOH:O	2.28	0.66
1:A:142:TRP:CZ2	1:A:147:LYS:HD2	2.31	0.66
1:A:123:ASP:HB2	2:B:362:AZR:H27B	1.77	0.66
1:B:163:VAL:HG21	1:B:170:TYR:HA	1.75	0.66
1:A:33:ILE:O	1:A:334:LEU:HA	1.95	0.66
1:B:17:THR:CB	1:B:18:PRO:HD3	2.25	0.66
1:B:55:THR:H	1:B:58:THR:HG21	1.61	0.66
1:A:168:MET:HE3	1:A:176:LYS:HD2	1.78	0.66
1:A:319:THR:OG1	1:A:322:PHE:HB2	1.95	0.65
1:B:258:ARG:HH22	1:B:275:ASN:ND2	1.95	0.65
1:B:265:MET:CE	1:B:272:GLU:HG2	2.27	0.65
1:A:30:VAL:HA	1:A:337:VAL:O	1.97	0.65
1:B:7:GLN:O	1:B:11:ILE:HG13	1.97	0.65
1:B:191:VAL:HG22	1:B:196:GLN:HE22	1.59	0.65
1:A:304:PRO:HG3	3:A:464:HOH:O	1.96	0.65
1:A:92:TYR:HB2	1:A:161:LEU:HD13	1.79	0.65
1:B:284:ILE:O	1:B:287:SER:HB2	1.96	0.64
1:A:47:ASP:OD1	1:A:50:ASN:HB2	1.98	0.64
1:B:125:VAL:HG22	1:B:130:ALA:HB1	1.79	0.64
1:B:318:SER:CB	2:B:362:AZR:H28B	2.27	0.64
1:B:318:SER:HB2	2:B:362:AZR:H28B	1.79	0.64
1:B:258:ARG:HH22	1:B:275:ASN:HD22	1.45	0.64
1:A:288:ASP:OD2	1:A:290:LYS:HG2	1.97	0.63
1:B:177:ARG:O	1:B:181:PRO:HG2	1.99	0.63
1:A:189:ILE:O	1:A:224:LYS:NZ	2.32	0.63
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.64	0.62
1:A:319:THR:O	1:A:320:GLY:C	2.37	0.62
1:A:84:LYS:HB2	1:A:87:ASP:OD2	1.99	0.62
1:B:302:ASN:HD22	1:B:303:PRO:HA	1.63	0.62
1:A:204:ARG:HG3	1:B:213:PRO:HB2	1.82	0.62
1:A:164:LYS:HB2	1:A:165:PRO:HD3	1.82	0.61
1:A:315:LYS:HG3	1:A:316:THR:N	2.14	0.61
1:A:359:LYS:HE3	3:A:534:HOH:O	1.99	0.61
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.65	0.61
1:A:127:ASP:OD1	1:A:129:ALA:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASN:HD22	1:B:303:PRO:CA	2.13	0.61
1:A:99:LYS:HD2	1:A:102:GLN:OE1	2.00	0.60
1:B:284:ILE:HD13	1:B:351:GLU:HG3	1.83	0.60
1:A:239:ASP:O	1:A:242:GLN:HG2	2.01	0.60
1:A:82:GLU:OE1	1:A:177:ARG:NH2	2.30	0.60
1:A:12:VAL:HG12	1:A:43:TRP:HH2	1.66	0.60
1:B:203:TYR:HA	1:B:207:LYS:O	2.02	0.59
1:B:27:GLY:HA3	1:B:54:VAL:HG21	1.83	0.59
1:A:55:THR:HG22	1:A:57:GLN:N	2.11	0.59
1:A:276:TRP:HH2	1:A:361:GLN:NE2	2.00	0.59
1:B:88:PRO:HD2	1:B:91:GLN:NE2	2.17	0.59
1:B:34:TYR:O	1:B:37:LYS:HB2	2.02	0.59
1:A:147:LYS:HD3	1:A:295:ALA:HB1	1.85	0.59
1:B:55:THR:O	1:B:58:THR:HG23	2.03	0.59
1:A:55:THR:CG2	1:A:57:GLN:H	2.12	0.59
1:A:205:GLU:N	3:A:454:HOH:O	2.34	0.59
1:B:279:LYS:HB3	1:B:282:SER:HG	1.67	0.59
1:B:180:HIS:HB2	1:B:181:PRO:HD3	1.85	0.59
1:B:1:ALA:HA	3:B:380:HOH:O	2.02	0.59
1:A:20:MET:HA	1:A:25:ILE:HD12	1.85	0.58
1:B:104:ILE:HA	1:B:108:HIS:ND1	2.19	0.58
1:B:23:GLN:O	1:B:24:ALA:HB3	2.04	0.58
1:B:20:MET:CG	1:B:28:MET:HE3	2.34	0.58
1:A:101:TRP:CZ3	1:A:104:ILE:HG21	2.38	0.58
1:B:132:LEU:HD11	1:B:136:GLN:HE21	1.68	0.58
1:B:221:TYR:HE2	3:B:539:HOH:O	1.87	0.58
1:A:26:PRO:HB3	1:A:48:ILE:HD11	1.85	0.57
1:A:91:GLN:HG2	1:A:92:TYR:CE2	2.37	0.57
1:A:344:TYR:CZ	1:A:349:ARG:HG3	2.39	0.57
1:A:100:GLN:NE2	1:A:138:TRP:O	2.31	0.57
1:B:45:LYS:HE3	1:B:51:ASN:HB2	1.87	0.57
1:A:19:LEU:HD23	1:A:19:LEU:C	2.25	0.56
1:B:38:PRO:HB3	1:B:231:THR:HG21	1.86	0.56
1:A:168:MET:CE	1:A:176:LYS:HD2	2.35	0.56
1:A:45:LYS:HB2	1:A:52:ARG:O	2.06	0.56
1:B:55:THR:H	1:B:58:THR:HG22	1.67	0.56
1:B:88:PRO:HD2	1:B:91:GLN:HE21	1.71	0.56
1:A:137:ASN:HB3	1:B:290:LYS:NZ	2.20	0.56
1:B:200:ALA:O	1:B:210:HIS:HE1	1.88	0.55
1:A:227:VAL:HG23	1:A:339:LEU:CD1	2.26	0.55
1:A:273:MET:HG3	3:A:368:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:PRO:O	1:B:348:VAL:HB	2.07	0.54
1:A:302:ASN:HA	1:A:303:PRO:C	2.26	0.54
1:B:148:ARG:HD2	1:B:262:ILE:CD1	2.38	0.54
1:A:308:VAL:CG1	3:A:382:HOH:O	2.50	0.54
1:B:318:SER:HB2	2:B:362:AZR:C28	2.37	0.54
1:B:215:GLN:O	1:B:216:LEU:HB2	2.06	0.54
1:A:33:ILE:HG22	1:A:36:GLY:HA2	1.89	0.54
1:A:122:PRO:O	1:A:125:VAL:HB	2.08	0.54
1:A:148:ARG:HD3	3:A:428:HOH:O	2.08	0.54
1:A:118:PRO:O	1:A:151:ALA:HB1	2.07	0.54
1:A:252:ILE:HG23	3:A:544:HOH:O	2.08	0.54
1:B:14:ARG:NH1	3:B:427:HOH:O	2.41	0.54
1:A:227:VAL:CG2	1:A:339:LEU:HD12	2.26	0.53
1:B:17:THR:HB	1:B:18:PRO:CD	2.33	0.53
1:A:312:TRP:CH2	1:A:357:LEU:HD12	2.43	0.53
1:A:17:THR:HG22	1:A:18:PRO:HD3	1.90	0.53
1:A:56:GLN:O	1:A:228:ILE:HG12	2.09	0.53
1:B:344:TYR:N	1:B:344:TYR:CD2	2.75	0.53
1:A:205:GLU:HG2	1:B:213:PRO:HB3	1.91	0.53
1:A:204:ARG:NH1	1:B:213:PRO:O	2.42	0.53
1:B:70:ASN:HB2	1:B:170:TYR:OH	2.08	0.53
1:A:207:LYS:HG2	1:A:208:PRO:HD2	1.89	0.53
1:A:344:TYR:HB2	1:A:345:PRO:CD	2.34	0.53
1:A:50:ASN:O	1:A:52:ARG:HG2	2.09	0.53
1:B:104:ILE:HG23	1:B:108:HIS:HB2	1.90	0.53
2:A:362:AZR:O31	1:B:123:ASP:HB2	2.08	0.52
1:A:345:PRO:HB2	1:A:348:VAL:HG23	1.91	0.52
1:B:204:ARG:HG3	1:B:204:ARG:HH11	1.73	0.52
1:A:202:GLY:O	1:A:209:VAL:HG12	2.10	0.52
1:B:31:ALA:O	1:B:336:ILE:HA	2.09	0.52
1:B:127:ASP:HA	3:B:470:HOH:O	2.09	0.52
1:B:287:SER:OG	1:B:350:VAL:HG21	2.08	0.52
1:B:288:ASP:OD2	1:B:290:LYS:HB3	2.10	0.52
1:B:302:ASN:HD22	1:B:303:PRO:N	2.08	0.52
1:A:117:LEU:HD23	1:A:118:PRO:HD2	1.92	0.52
1:A:152:ASN:ND2	2:A:362:AZR:O10	2.40	0.52
1:B:20:MET:HG2	1:B:28:MET:HE3	1.91	0.52
1:A:89:VAL:HG23	1:A:104:ILE:O	2.10	0.52
1:A:213:PRO:HG3	1:B:207:LYS:HD2	1.92	0.51
1:A:13:ASN:ND2	3:A:384:HOH:O	2.44	0.51
1:B:59:LEU:HB2	1:B:199:TYR:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:NZ	1:A:150:TYR:OH	2.40	0.51
1:B:86:SER:HB2	3:B:541:HOH:O	2.10	0.51
1:B:164:LYS:O	1:B:165:PRO:C	2.48	0.51
1:B:261:ARG:HD2	1:B:266:TYR:CE2	2.46	0.51
1:A:88:PRO:HB2	1:A:90:THR:HG23	1.93	0.51
1:B:58:THR:HB	3:B:442:HOH:O	2.11	0.51
1:A:290:LYS:CE	1:B:139:GLN:HE22	2.23	0.51
1:B:30:VAL:HA	1:B:337:VAL:O	2.11	0.51
1:B:67:LYS:NZ	1:B:150:TYR:OH	2.43	0.51
1:B:212:SER:OG	1:B:213:PRO:HD2	2.10	0.51
1:A:28:MET:O	1:A:54:VAL:HG11	2.11	0.51
1:A:356:ILE:O	1:A:359:LYS:HB2	2.09	0.51
1:B:350:VAL:O	1:B:353:ALA:HB3	2.10	0.51
1:A:192:PRO:HB2	1:A:195:GLU:CG	2.40	0.51
1:B:17:THR:CB	1:B:18:PRO:CD	2.89	0.51
1:A:55:THR:HB	3:A:446:HOH:O	2.11	0.50
1:B:327:ALA:O	1:B:335:GLY:HA2	2.10	0.50
1:A:137:ASN:HB3	1:B:290:LYS:HZ2	1.77	0.50
1:A:204:ARG:HG2	1:A:204:ARG:NH1	2.26	0.50
1:B:125:VAL:HG21	1:B:134:PHE:HB2	1.93	0.50
1:A:354:TRP:NE1	1:A:358:GLU:OE1	2.44	0.50
1:A:168:MET:CE	1:A:172:GLU:HG2	2.41	0.50
1:B:132:LEU:O	1:B:136:GLN:HG3	2.11	0.50
1:A:238:MET:SD	1:A:333:ASN:HA	2.52	0.50
1:A:89:VAL:HG21	1:A:104:ILE:HG22	1.94	0.50
1:A:213:PRO:HB2	1:B:205:GLU:HG3	1.94	0.50
1:B:123:ASP:O	1:B:126:THR:HG22	2.12	0.50
1:A:3:LYS:HZ2	1:A:360:LEU:HD23	1.77	0.49
1:A:116:GLY:N	3:A:381:HOH:O	2.17	0.49
1:A:148:ARG:NH2	1:A:267:GLN:OE1	2.43	0.49
1:A:31:ALA:O	1:A:336:ILE:HA	2.12	0.49
1:B:67:LYS:NZ	1:B:150:TYR:CZ	2.79	0.49
1:B:85:LEU:HB3	1:B:107:LEU:HB2	1.94	0.49
1:A:104:ILE:HA	1:A:108:HIS:ND1	2.27	0.49
1:A:274:LEU:HD13	1:A:283:ILE:HG21	1.94	0.49
1:A:119:LEU:HA	1:A:151:ALA:HA	1.94	0.49
1:B:132:LEU:HG	1:B:136:GLN:NE2	2.27	0.49
1:A:320:GLY:H	2:A:362:AZR:HN1A	1.59	0.49
1:B:18:PRO:O	1:B:21:GLN:HB3	2.13	0.49
1:B:118:PRO:O	1:B:151:ALA:HB1	2.13	0.49
1:B:258:ARG:NH1	1:B:275:ASN:ND2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASP:O	1:B:79:ALA:HB3	2.12	0.48
1:B:281:ASP:O	1:B:285:SER:HB2	2.12	0.48
1:A:261:ARG:HD3	3:A:392:HOH:O	2.13	0.48
1:B:55:THR:CG2	1:B:57:GLN:H	2.25	0.48
1:B:100:GLN:N	1:B:100:GLN:OE1	2.46	0.48
1:A:244:GLN:HG3	1:A:245:GLU:OE2	2.13	0.48
1:A:212:SER:HB3	1:A:213:PRO:HD2	1.96	0.48
1:B:148:ARG:HD2	1:B:262:ILE:HD11	1.95	0.48
1:B:358:GLU:HA	1:B:361:GLN:HE21	1.77	0.48
1:A:346:ASN:CB	1:A:347:PRO:HD3	2.43	0.48
1:A:274:LEU:O	1:A:311:SER:HA	2.13	0.48
1:B:99:LYS:HE3	3:B:509:HOH:O	2.13	0.48
1:A:33:ILE:HD11	1:A:231:THR:HG23	1.96	0.47
1:A:204:ARG:CZ	3:A:551:HOH:O	2.61	0.47
1:A:260:TRP:CE3	1:A:300:GLU:CA	2.95	0.47
1:B:258:ARG:NH2	1:B:275:ASN:ND2	2.61	0.47
1:A:127:ASP:OD1	1:A:129:ALA:HB3	2.15	0.47
1:A:77:ALA:HB2	3:A:401:HOH:O	2.13	0.47
1:B:184:LEU:HD23	1:B:232:ARG:HD2	1.96	0.47
1:A:63:GLY:HA2	1:A:319:THR:HG23	1.97	0.47
1:B:314:HIS:C	1:B:314:HIS:CD2	2.87	0.47
1:A:139:GLN:HA	3:A:449:HOH:O	2.14	0.47
1:B:111:THR:HG21	1:B:260:TRP:CD1	2.49	0.47
1:B:261:ARG:NE	1:B:263:GLY:O	2.48	0.47
1:A:156:GLY:C	1:A:216:LEU:HD13	2.34	0.47
1:A:63:GLY:CA	1:A:319:THR:HG23	2.45	0.47
1:B:37:LYS:NZ	3:B:380:HOH:O	2.29	0.47
1:A:203:TYR:HA	1:A:207:LYS:O	2.15	0.46
1:A:132:LEU:O	1:A:136:GLN:N	2.43	0.46
1:A:3:LYS:NZ	1:A:360:LEU:HD23	2.31	0.46
1:A:108:HIS:HB3	1:A:114:ALA:HA	1.97	0.46
1:A:258:ARG:HD3	3:A:455:HOH:O	2.16	0.46
1:B:29:ALA:HA	1:B:41:PHE:O	2.15	0.46
1:B:217:ASP:HB2	3:B:539:HOH:O	2.15	0.46
1:B:83:ILE:HG23	1:B:165:PRO:HG2	1.97	0.46
1:A:47:ASP:HB3	1:A:52:ARG:HG3	1.98	0.46
1:A:245:GLU:HG3	3:A:509:HOH:O	2.15	0.46
1:B:85:LEU:O	1:B:105:SER:HB2	2.15	0.46
1:A:29:ALA:HB1	1:A:227:VAL:HG21	1.97	0.46
1:A:205:GLU:HG2	1:B:213:PRO:CB	2.46	0.46
2:B:362:AZR:N13	2:B:362:AZR:O11	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:CG2	1:A:57:GLN:HB2	2.46	0.45
1:A:25:ILE:HG21	1:A:28:MET:CE	2.47	0.45
1:B:279:LYS:HB3	1:B:282:SER:OG	2.16	0.45
1:A:321:GLY:O	1:A:342:LYS:N	2.49	0.45
1:B:14:ARG:O	1:B:18:PRO:HG2	2.16	0.45
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.69	0.45
1:A:123:ASP:N	2:B:362:AZR:H27	2.30	0.45
1:B:105:SER:N	1:B:108:HIS:ND1	2.51	0.45
1:B:150:TYR:OH	1:B:315:LYS:NZ	2.43	0.45
1:B:201:TRP:O	1:B:341:ASN:ND2	2.50	0.45
1:B:289:SER:HA	1:B:292:ALA:HB3	1.99	0.45
1:A:61:GLU:CD	1:A:211:VAL:HG12	2.37	0.45
1:A:296:LEU:CD2	1:A:297:PRO:HD2	2.47	0.45
1:B:32:ILE:HD13	1:B:336:ILE:HG13	1.98	0.45
1:B:302:ASN:HD22	1:B:302:ASN:C	2.20	0.45
1:A:26:PRO:CB	1:A:48:ILE:HD11	2.47	0.45
1:A:62:LEU:HD11	1:A:225:SER:HB3	1.99	0.45
1:A:169:SER:HB2	3:A:418:HOH:O	2.15	0.45
1:A:274:LEU:HD13	1:A:283:ILE:CG2	2.47	0.45
1:B:132:LEU:HD11	1:B:136:GLN:NE2	2.31	0.45
1:B:189:ILE:HG13	1:B:223:VAL:HG22	1.98	0.45
1:A:296:LEU:HD23	1:A:297:PRO:HD2	1.98	0.44
1:A:168:MET:HE3	1:A:172:GLU:HG2	1.98	0.44
1:A:280:ALA:HB2	1:A:354:TRP:CE2	2.53	0.44
1:A:345:PRO:HA	1:B:124:ASP:OD2	2.17	0.44
1:B:38:PRO:CB	1:B:231:THR:HG21	2.47	0.44
1:B:92:TYR:CB	1:B:161:LEU:HD22	2.47	0.44
1:B:295:ALA:O	1:B:296:LEU:HD23	2.17	0.44
1:A:63:GLY:HA2	1:A:319:THR:CG2	2.47	0.44
1:A:284:ILE:HD13	1:A:351:GLU:HG3	1.99	0.44
1:A:93:TRP:O	1:A:96:LEU:HB3	2.18	0.44
1:B:20:MET:O	1:B:24:ALA:N	2.51	0.44
1:A:253:GLU:HG3	3:A:380:HOH:O	2.16	0.44
1:A:78:ILE:HD11	1:A:85:LEU:HG	2.00	0.44
1:A:245:GLU:OE2	1:A:245:GLU:N	2.51	0.44
1:A:361:GLN:OXT	1:A:361:GLN:HG2	2.17	0.44
1:B:88:PRO:CD	1:B:91:GLN:NE2	2.80	0.44
1:A:36:GLY:CA	1:A:333:ASN:HD22	2.30	0.44
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.76	0.44
1:B:351:GLU:O	1:B:355:ARG:HG3	2.18	0.44
1:A:3:LYS:NZ	1:A:359:LYS:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:CB	1:A:165:PRO:HD3	2.48	0.43
1:B:119:LEU:O	1:B:119:LEU:HG	2.16	0.43
1:A:13:ASN:O	1:A:17:THR:HB	2.18	0.43
1:A:149:LEU:O	1:A:150:TYR:C	2.57	0.43
1:A:250:GLN:HG2	3:A:541:HOH:O	2.17	0.43
1:B:93:TRP:HB2	1:B:161:LEU:HD21	1.99	0.43
1:B:349:ARG:HH11	1:B:349:ARG:HD2	1.20	0.43
1:A:80:ARG:HH11	1:A:80:ARG:HD3	1.48	0.43
1:B:89:VAL:HG13	1:B:161:LEU:CD1	2.48	0.43
1:B:344:TYR:HB2	1:B:345:PRO:CD	2.48	0.43
1:A:45:LYS:HB3	1:A:45:LYS:HE2	1.62	0.43
1:B:168:MET:CE	1:B:176:LYS:HD2	2.49	0.43
1:B:258:ARG:CZ	1:B:275:ASN:HD21	2.27	0.43
1:A:240:ALA:O	1:A:243:VAL:HB	2.19	0.43
1:A:290:LYS:HD3	3:A:409:HOH:O	2.19	0.43
1:A:101:TRP:HZ3	1:A:104:ILE:HG21	1.83	0.43
1:A:205:GLU:CG	1:B:213:PRO:HB3	2.49	0.43
1:B:132:LEU:CG	1:B:136:GLN:NE2	2.82	0.43
1:B:314:HIS:HD2	1:B:314:HIS:O	2.02	0.43
1:A:313:VAL:O	1:A:314:HIS:HB3	2.19	0.42
1:B:262:ILE:O	1:B:262:ILE:HG22	2.18	0.42
1:B:90:THR:HG23	3:B:537:HOH:O	2.18	0.42
1:B:6:GLN:HE21	1:B:6:GLN:HB3	1.50	0.42
1:B:191:VAL:HG23	1:B:195:GLU:HB2	2.01	0.42
1:A:303:PRO:HA	1:A:304:PRO:HD3	1.89	0.42
1:B:14:ARG:HG2	1:B:14:ARG:NH1	2.33	0.42
1:A:96:LEU:HG	1:A:96:LEU:O	2.19	0.42
1:A:258:ARG:HB2	1:A:305:ALA:HB3	2.00	0.42
1:B:176:LYS:O	1:B:181:PRO:HD3	2.19	0.42
1:A:31:ALA:HB2	1:A:227:VAL:HG13	2.02	0.42
1:B:16:ILE:HG21	1:B:43:TRP:CH2	2.55	0.42
1:B:92:TYR:O	1:B:94:PRO:HD3	2.19	0.42
1:B:95:GLU:O	1:B:136:GLN:NE2	2.53	0.42
1:B:229:ASP:O	1:B:232:ARG:HB2	2.20	0.42
1:B:293:LEU:HA	1:B:293:LEU:HD12	1.72	0.42
1:A:25:ILE:HA	1:A:26:PRO:HD3	1.71	0.42
1:B:124:ASP:O	1:B:126:THR:HG23	2.20	0.42
1:B:344:TYR:CZ	1:B:349:ARG:HG3	2.55	0.42
1:B:357:LEU:HD12	1:B:357:LEU:HA	1.93	0.42
1:A:122:PRO:O	1:A:124:ASP:N	2.53	0.42
1:A:188:TRP:CZ3	1:A:192:PRO:HG2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:O	1:A:209:VAL:HG13	2.19	0.42
1:B:25:ILE:HD13	1:B:28:MET:HE2	2.01	0.42
1:B:302:ASN:C	1:B:302:ASN:ND2	2.72	0.42
1:B:67:LYS:HE2	1:B:155:ILE:HG21	2.02	0.42
1:A:118:PRO:CG	1:A:134:PHE:HZ	2.32	0.41
1:A:127:ASP:OD1	1:A:127:ASP:C	2.58	0.41
1:B:164:LYS:HB2	1:B:165:PRO:HD3	2.02	0.41
1:B:117:LEU:HA	1:B:118:PRO:HD3	1.85	0.41
1:B:221:TYR:CE2	2:B:362:AZR:S8	3.13	0.41
1:A:109:LEU:HD21	1:A:157:LEU:HD23	2.03	0.41
1:A:122:PRO:C	1:A:124:ASP:H	2.23	0.41
1:A:224:LYS:HD3	1:A:224:LYS:N	2.35	0.41
1:A:238:MET:HG2	1:A:330:PRO:HA	2.01	0.41
1:B:174:MET:SD	1:B:178:VAL:HG21	2.61	0.41
1:A:29:ALA:HB1	1:A:227:VAL:CG2	2.50	0.41
1:B:177:ARG:O	1:B:248:LEU:HD22	2.21	0.41
1:B:318:SER:HB3	2:B:362:AZR:H28B	2.01	0.41
1:B:320:GLY:HA3	3:B:391:HOH:O	2.20	0.41
1:A:117:LEU:HD21	1:A:135:TYR:CE1	2.55	0.41
1:A:318:SER:HA	1:A:322:PHE:O	2.21	0.41
1:A:131:LEU:HD22	1:A:215:GLN:HB3	2.02	0.41
1:A:332:LYS:HA	1:A:332:LYS:HD2	1.83	0.41
2:A:362:AZR:H27B	1:B:123:ASP:CB	2.49	0.41
1:B:27:GLY:HA3	1:B:54:VAL:CG2	2.47	0.41
1:A:33:ILE:HD12	1:A:235:GLN:HG2	2.03	0.41
1:A:45:LYS:CB	1:A:52:ARG:O	2.69	0.41
1:A:89:VAL:CG2	1:A:104:ILE:HG22	2.51	0.41
1:B:89:VAL:HG13	1:B:161:LEU:HD11	2.02	0.41
1:B:115:GLY:HA2	3:B:384:HOH:O	2.21	0.41
1:A:204:ARG:CG	1:B:213:PRO:HB2	2.48	0.40
1:A:246:LYS:HA	1:A:246:LYS:HD2	1.88	0.40
1:A:284:ILE:HD13	1:A:351:GLU:HB2	2.02	0.40
1:B:25:ILE:HG21	1:B:28:MET:HE2	2.04	0.40
1:B:58:THR:HA	1:B:198:ASP:O	2.22	0.40
1:B:104:ILE:HG23	1:B:108:HIS:CB	2.51	0.40
1:A:59:LEU:HB2	1:A:199:TYR:HA	2.04	0.40
1:B:74:GLY:O	1:B:77:ALA:HB3	2.21	0.40
1:B:168:MET:HE3	1:B:168:MET:HB3	1.69	0.40
1:A:345:PRO:O	1:A:348:VAL:HB	2.20	0.40
1:A:237:ASN:ND2	3:A:544:HOH:O	2.41	0.40
1:A:286:GLY:HA2	1:A:291:VAL:HG11	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:OH	1:B:216:LEU:CD1	2.70	0.40
1:B:252:ILE:O	1:B:255:ALA:HB3	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE2	3:B:542:HOH:O[2_664]	1.73	0.47
1:A:180:HIS:NE2	1:B:1:ALA:CA[2_664]	1.74	0.46
1:A:180:HIS:NE2	1:B:1:ALA:CB[2_664]	1.81	0.39
1:B:355:ARG:NH1	3:A:549:HOH:O[4_555]	1.92	0.28
1:A:180:HIS:CD2	1:B:1:ALA:CB[2_664]	2.02	0.18
1:B:14:ARG:CD	3:A:547:HOH:O[4_555]	2.09	0.11

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	359/361 (99%)	323 (90%)	30 (8%)	6 (2%)	9 16
1	B	359/361 (99%)	327 (91%)	28 (8%)	4 (1%)	14 26
All	All	718/722 (99%)	650 (90%)	58 (8%)	10 (1%)	11 20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	B	98	GLY
1	B	102	GLN
1	A	263	GLY
1	A	320	GLY
1	B	200	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	LYS
1	A	239	ASP
1	A	48	ILE
1	B	165	PRO

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	292/292 (100%)	252 (86%)	40 (14%)	3 7
1	B	292/292 (100%)	244 (84%)	48 (16%)	2 4
All	All	584/584 (100%)	496 (85%)	88 (15%)	3 5

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	16	ILE
1	A	17	THR
1	A	19	LEU
1	A	21	GLN
1	A	33	ILE
1	A	45	LYS
1	A	52	ARG
1	A	55	THR
1	A	56	GLN
1	A	76	ASP
1	A	84	LYS
1	A	90	THR
1	A	91	GLN
1	A	95	GLU
1	A	99	LYS
1	A	112	TYR
1	A	117	LEU
1	A	127	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	136	GLN
1	A	137	ASN
1	A	142	TRP
1	A	192	PRO
1	A	197	LYS
1	A	204	ARG
1	A	205	GLU
1	A	224	LYS
1	A	253	GLU
1	A	264	ASP
1	A	273	MET
1	A	274	LEU
1	A	289	SER
1	A	290	LYS
1	A	302	ASN
1	A	309	LYS
1	A	314	HIS
1	A	330	PRO
1	A	333	ASN
1	A	336	ILE
1	A	361	GLN
1	B	21	GLN
1	B	28	MET
1	B	35	GLN
1	B	37	LYS
1	B	43	TRP
1	B	51	ASN
1	B	55	THR
1	B	58	THR
1	B	84	LYS
1	B	86	SER
1	B	107	LEU
1	B	124	ASP
1	B	125	VAL
1	B	134	PHE
1	B	137	ASN
1	B	141	GLN
1	B	153	SER
1	B	163	VAL
1	B	169	SER
1	B	175	SER
1	B	177	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	191	VAL
1	B	193	GLN
1	B	194	SER
1	B	197	LYS
1	B	204	ARG
1	B	224	LYS
1	B	228	ILE
1	B	243	VAL
1	B	245	GLU
1	B	246	LYS
1	B	253	GLU
1	B	257	SER
1	B	265	MET
1	B	273	MET
1	B	282	SER
1	B	287	SER
1	B	290	LYS
1	B	293	LEU
1	B	302	ASN
1	B	309	LYS
1	B	314	HIS
1	B	315	LYS
1	B	319	THR
1	B	334	LEU
1	B	344	TYR
1	B	357	LEU
1	B	359	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	91	GLN
1	A	102	GLN
1	A	237	ASN
1	A	256	GLN
1	A	302	ASN
1	A	333	ASN
1	A	361	GLN
1	B	6	GLN
1	B	50	ASN
1	B	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	GLN
1	B	137	ASN
1	B	139	GLN
1	B	141	GLN
1	B	193	GLN
1	B	196	GLN
1	B	210	HIS
1	B	244	GLN
1	B	275	ASN
1	B	302	ASN
1	B	346	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	AZR	B	362	1	23,28,28	3.95	8 (34%)	22,41,41	2.49	9 (40%)
2	AZR	A	362	1	23,28,28	4.68	4 (17%)	22,41,41	3.49	14 (63%)

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	AZR	B	362	1	-	9/28/35/35	0/1/1/1
2	AZR	A	362	1	-	15/28/35/35	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	362	AZR	O34-S17	14.95	1.59	1.42
2	B	362	AZR	O34-S17	14.26	1.58	1.42
2	A	362	AZR	O32-S17	14.17	1.58	1.42
2	B	362	AZR	O32-S17	9.03	1.52	1.42
2	A	362	AZR	S17-N12	6.86	1.68	1.59
2	B	362	AZR	S17-N12	5.91	1.67	1.59
2	A	362	AZR	C19-C18	-3.32	1.50	1.54
2	B	362	AZR	O11-C23	-2.80	1.41	1.46
2	B	362	AZR	C19-N13	2.53	1.50	1.46
2	B	362	AZR	O11-N14	-2.11	1.38	1.42
2	B	362	AZR	C18-N12	2.06	1.49	1.47
2	B	362	AZR	C22-N14	2.02	1.32	1.29

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	362	AZR	O10-C21-C22	9.34	131.12	120.35
2	B	362	AZR	C23-O11-N14	8.03	117.47	110.33
2	A	362	AZR	O11-N14-C22	5.42	120.30	111.87
2	A	362	AZR	O32-S17-O34	-5.32	107.59	120.16
2	A	362	AZR	C23-O11-N14	4.34	114.19	110.33
2	B	362	AZR	C28-C23-C27	-3.85	101.75	110.75
2	A	362	AZR	O31-C29-C23	3.69	125.13	113.99
2	A	362	AZR	O11-C23-C29	-3.48	104.10	109.67
2	A	362	AZR	C24-C25-S8	-3.41	107.60	111.79
2	A	362	AZR	O32-S17-N12	-3.39	102.69	108.87
2	A	362	AZR	O31-C29-O30	-3.24	113.52	123.82
2	A	362	AZR	C22-C21-N13	-3.02	109.37	114.38
2	A	362	AZR	C7-C18-N12	2.94	115.57	110.45
2	A	362	AZR	C28-C23-C27	-2.84	104.11	110.75
2	B	362	AZR	O32-S17-O34	-2.81	113.51	120.16
2	B	362	AZR	O32-S17-N12	2.44	113.32	108.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	362	AZR	C19-N13-C21	2.40	126.00	122.26
2	B	362	AZR	O34-S17-N12	-2.29	104.69	108.87
2	A	362	AZR	N16-C26-N15	2.19	126.02	123.19
2	B	362	AZR	O10-C21-C22	-2.07	117.97	120.35
2	B	362	AZR	C22-C21-N13	2.05	117.78	114.38
2	A	362	AZR	O10-C21-N13	-2.03	119.52	123.08
2	B	362	AZR	O31-C29-O30	-2.01	117.43	123.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	362	AZR	C22-N14-O11-C23
2	A	362	AZR	C27-C23-O11-N14
2	A	362	AZR	C28-C23-O11-N14
2	A	362	AZR	C18-N12-S17-O33
2	A	362	AZR	C18-N12-S17-O34
2	B	362	AZR	C27-C23-O11-N14
2	B	362	AZR	C28-C23-O11-N14
2	B	362	AZR	O11-C23-C29-O30
2	B	362	AZR	O11-C23-C29-O31
2	A	362	AZR	C24-C22-N14-O11
2	B	362	AZR	C24-C22-N14-O11
2	A	362	AZR	C28-C23-C29-O30
2	A	362	AZR	C18-N12-S17-O32
2	B	362	AZR	C21-C22-N14-O11
2	A	362	AZR	O10-C21-C22-N14
2	A	362	AZR	N13-C21-C22-N14
2	A	362	AZR	O11-C23-C29-O30
2	A	362	AZR	O11-C23-C29-O31
2	A	362	AZR	C28-C23-C29-O31
2	B	362	AZR	C18-N12-S17-O34
2	A	362	AZR	C7-C18-C19-C20
2	B	362	AZR	O10-C21-C22-C24
2	A	362	AZR	N12-C18-C19-N13
2	B	362	AZR	N12-C18-C19-N13

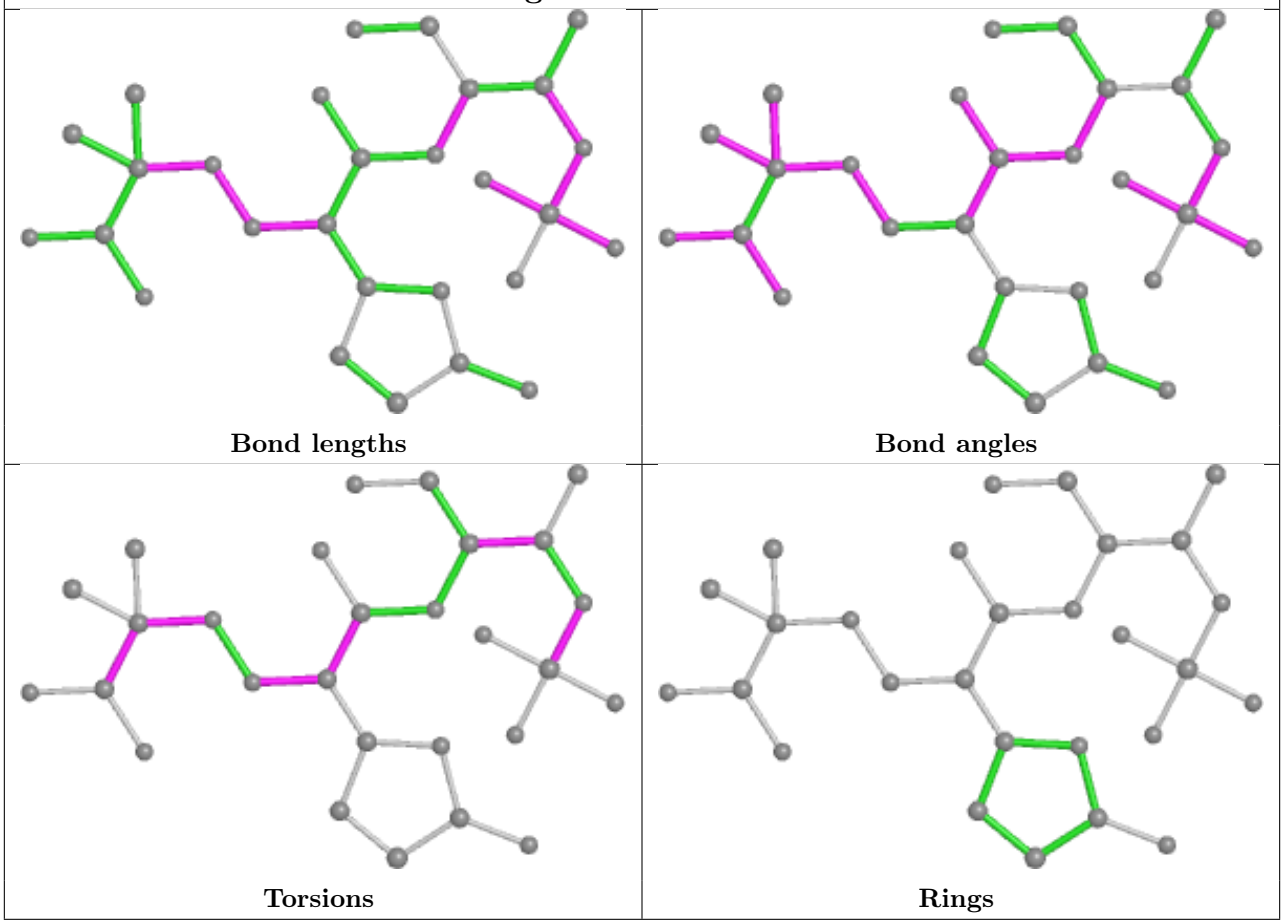
There are no ring outliers.

2 monomers are involved in 14 short contacts:

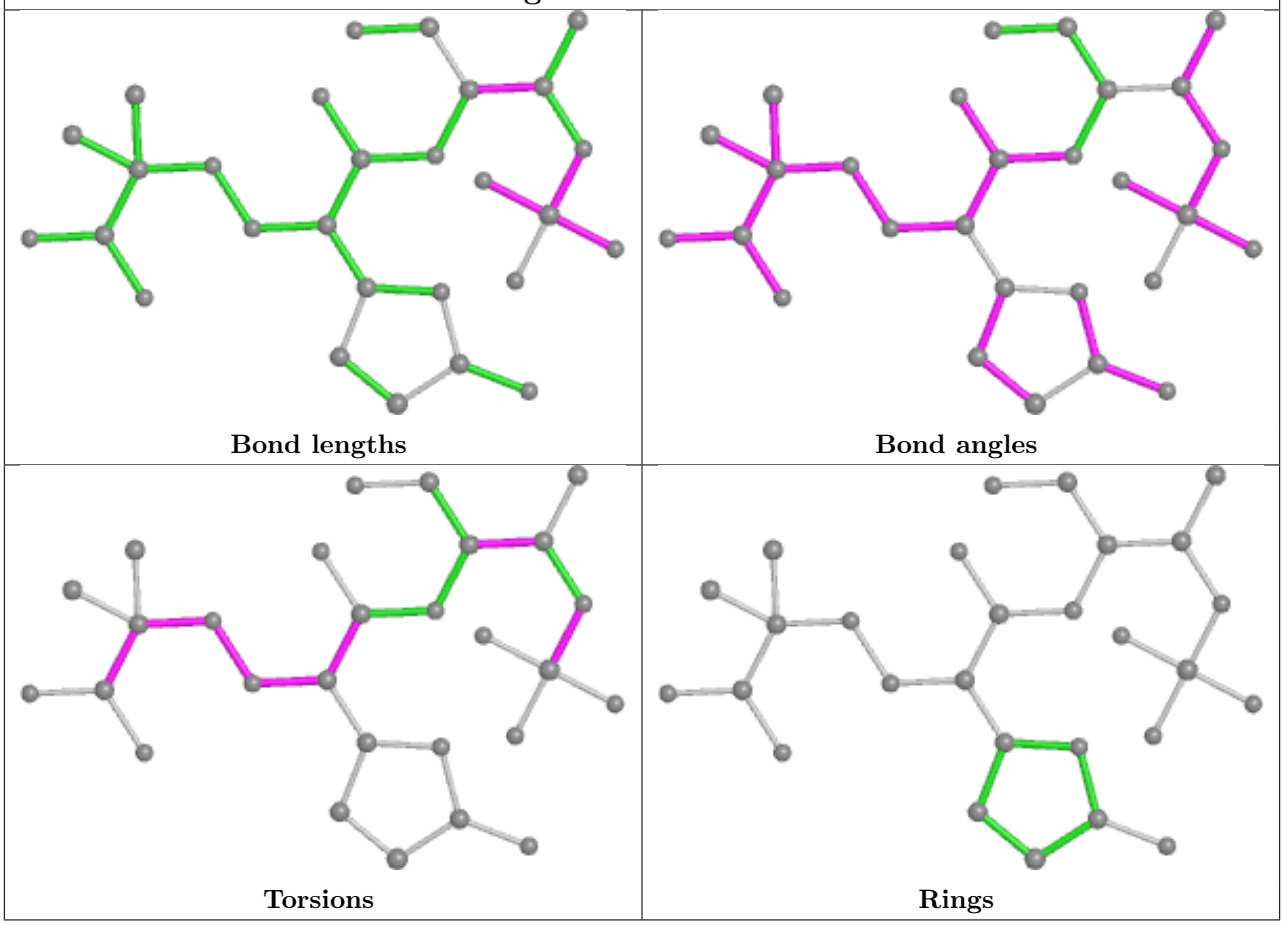
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	362	AZR	9	0
2	A	362	AZR	5	0

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 then 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 AZR B 362



Ligand AZR A 362



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.