



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:16 PM UTC

PDB ID : 3LZB / pdb_00003lzb
Title : EGFR kinase domain complexed with an imidazo[2,1-b]thiazole inhibitor
Authors : Swinger, K.K.
Deposited on : 2010-03-01
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

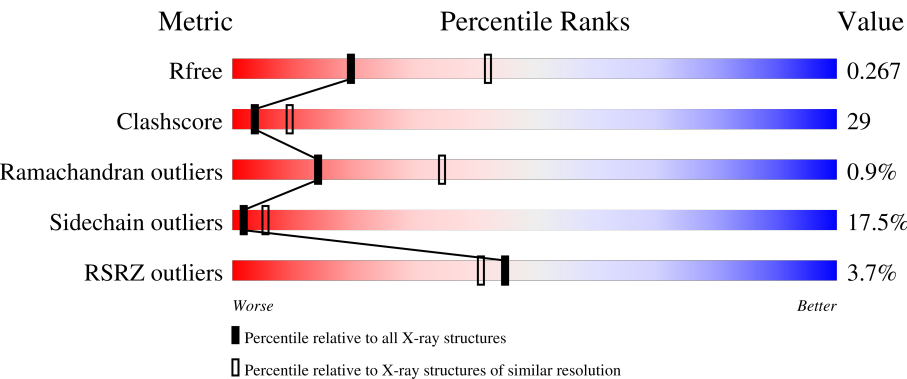
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	327	3% 43%28%8%19%
1	B	327	2% 43%30%7%19%
1	C	327	3% 46%23%9%21%
1	D	327	4% 40%29%9%20%
1	E	327	97%

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Mol	Chain	Length	Quality of chain
1	F	327	 98%
1	G	327	 98%
1	H	327	 97%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8885 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.

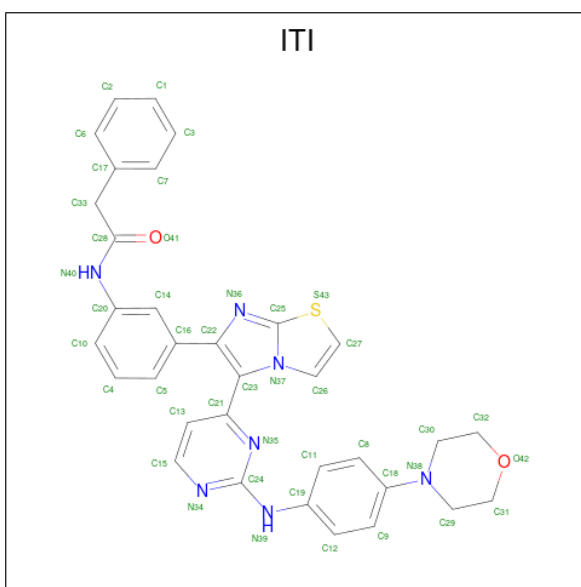
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2120	1370	360	375	15			
1	B	265	Total	C	N	O	S	0	0	0
			2116	1368	360	373	15			
1	C	259	Total	C	N	O	S	0	0	0
			2078	1343	354	366	15			
1	D	261	Total	C	N	O	S	0	0	0
			2087	1350	355	367	15			
1	E	9	Total	C	N	O		0	0	0
			45	27	9	9				
1	F	7	Total	C	N	O		0	0	0
			35	21	7	7				
1	G	7	Total	C	N	O		0	0	0
			35	21	7	7				
1	H	9	Total	C	N	O		0	0	0
			45	27	9	9				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	924	ARG	VAL	engineered mutation	UNP P00533
B	924	ARG	VAL	engineered mutation	UNP P00533
C	924	ARG	VAL	engineered mutation	UNP P00533
D	924	ARG	VAL	engineered mutation	UNP P00533
E	-29	ARG	VAL	engineered mutation	UNP P00533
F	-28	ARG	VAL	engineered mutation	UNP P00533
G	-30	ARG	VAL	engineered mutation	UNP P00533
H	-31	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is N-[3-(5-{2-[(4-morpholin-4-ylphenyl)amino]pyrimidin-4-yl}imidazo[2,1-b][1,3]thiazol-6-yl)phenyl]-2-phenylacetamide (CCD ID: ITI) (formula: C₃₃H₂₉N₇O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			43	33	7	2	1		
2	B	1	Total	C	N	O	S	0	0
			43	33	7	2	1		
2	C	1	Total	C	N	O	S	0	0
			43	33	7	2	1		
2	D	1	Total	C	N	O	S	0	0
			43	33	7	2	1		

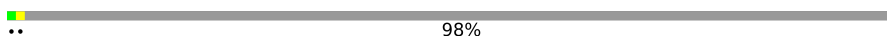
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	45	Total	O	0	0
			45	45		
3	C	35	Total	O	0	0
			35	35		
3	D	21	Total	O	0	0
			21	21		
3	E	3	Total	O	0	0
			3	3		
3	F	4	Total	O	0	0
			4	4		
3	G	2	Total	O	0	0
			2	2		
3	H	2	Total	O	0	0
			2	2		

GLY	GLU	ALA	PRO	ASN	GLN	ALA	LEU	LEU	ARG	ILE	LEU	LYS	GLU	THR	GLU	PHE	LYS	ILE	LYS	VAL	LEU	GLY	SER	GLY	ALA	PHE	GLY	THR	VAL	TYR	LYS	GLY	LEU	TRP	ILE	PRO	GLU	GLY	LYS	VAL	LYS	ILE	PRO	ILE	VAL	ALA	ALA	ILE	LYS	GLU	LEU	ARG	GLU	ALA	THR	SER	PRO	SER	LYS	ALA
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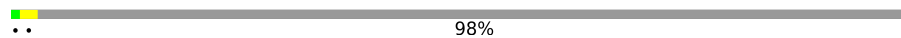
	UNK	PRO	VAL	ASN	ASN
UNK	PRO	PRO	PRO	TRP	CYS
UNK	ILE	ILE	LYS	VAL	GLY
UNK	CYS	THR	TRP	LEU	GLN
UNK	ILE	MET	MET	ILE	ASP
UNK	ASP	ALA	ALA	ALA	GLU
UNK	VAL	VAL	LEU	LYS	ALA
UNK	TYR	TYR	GLU	GLY	TYR
UNK	MET	SER	SER	MET	VAL
UNK	ILE	ILE	ILE	ASN	MET
UNK	MET	MET	LEU	TYR	ALA
UNK	ARG	ARG	HIS	LEU	SER
UNK	CYS	LYS	ILE	ASP	VAL
UNK	TRP	TRP	TYR	ARG	ASN
UNK	MET	THR	THR	ARG	PRO
UNK	ILE	GLN	GLN	LEU	HIS
UNK	ASP	ALA	SER	HIS	VAL
UNK	ALA	ASP	ASP	VAL	CYS
UNK	SER	SER	VAL	ASP	LEU
UNK	ARG	TRP	LEU	LEU	LEU
UNK	PRO	SER	SER	ALA	GLY
UNK	LYS	TYR	TYR	ALA	ILE
PHE	ARG	VAL	VAL	ARG	CYS
GLU	GLU	THR	THR	ASN	LEU
LEU	LEU	VAL	VAL	VAL	THR
ILE	ILE	TRP	TRP	VAL	THR
ILE	ILE	GLU	GLU	LYS	VAL
PHE	PHE	MET	MET	PRO	LEU
SER	SER	THR	THR	GLN	ILE
LYS	LYS	PHE	PHE	HIS	THR
MET	MET	GLY	GLY	VAL	GLN
ALA	ALA	SER	SER	LYS	LEU
ARG	ARG	ILE	LYS	ILE	MET
PRO	PRO	ASP	PRO	THR	PRO
GLN	GLN	TYR	TYR	ASP	PHE
ARG	ARG	GLY	GLY	PHE	GLY
TYR	TYR	ILE	ILE	GLY	CYS
LEU	LEU	PRO	PRO	LEU	LEU
ILE	ILE	VAL	ALA	LYS	ASP
ILE	ILE	SER	SER	LEU	TYR
GLN	GLN	GLU	GLU	LEU	VAL
GLY	GLY	ILE	ILE	GLY	ARG
X7	X7	SER	SER	ALA	GLU
X10	X10	SER	ILE	GLU	HIS
X15	X15	LEU	LYS	LYS	ASN
UNK	UNK	LYS	GLU	ASN	ILE
UNK	UNK	GLY	GLY	TYR	GLY
UNK	UNK	GLU	ALA	SER	SER
UNK	UNK	ARG	ARG	GLN	GLN
UNK	UNK	LEU	LEU	GLY	TYR
UNK	UNK	PRO	GLN	GLY	LEU
UNK	UNK	CTR	CTR	LYS	LYS

- Molecule 1: Epidermal growth factor receptor

Chain F:  [illegible]

- Molecule 1: Epidermal growth factor receptor

Chain G: ..



UNK	UNK	PRO	VAL	ASN	ASN	GLY
UNK	UNK	PRO	PRO	TRP	LYS	GLU
UNK	UNK	ILE	ILE	CYS	GLY	ALA
UNK	UNK	CYS	LYS	VAL	ILE	PRO
UNK	UNK	THR	TRP	GLN	LEU	ASN
UNK	UNK	ILE	MET	ILE	ASP	GLN
UNK	UNK	ASP	ALA	ALA	GLU	ALA
UNK	UNK	VAL	LEU	LYS	ALA	LEU
UNK	UNK	TYP	GLU	GLY	TYP	LEU
UNK	UNK	MET	SER	MET	VAL	ARG
UNK	UNK	ILE	ILE	ASN	MET	ILE
UNK	UNK	MET	LEU	TYP	ALA	LEU
UNK	UNK	ARG	HIS	LEU	SER	LYS
UNK	UNK	CYS	ARG	GLU	VAL	GLU
UNK	UNK	CYS	ILE	ASP	ASP	THR
UNK	UNK	TRP	TRP	ARG	ASN	GLU
UNK	UNK	MET	THR	ARG	PRO	PHE
UNK	UNK	ILE	HIS	LEU	HIS	LYS
UNK	UNK	ASP	GLN	VAL	VAL	ILE
UNK	UNK	ALA	SER	HIS	CYS	ILE
UNK	UNK	ASP	ASP	ARG	ARG	LYS
UNK	UNK	SER	VAL	ASP	LEU	VAL
UNK	UNK	ARG	TRP	LEU	LEU	LEU
UNK	UNK	PRO	SER	ALA	GLY	GLY
UNK	UNK	LYS	TYP	ALA	ILE	SER
UNK	UNK	PHE	GLY	ARG	CYS	GLY
UNK	UNK	ARG	VAL	ASN	LEU	ALA
UNK	UNK	GLU	THR	VAL	THR	PHE
UNK	UNK	LEU	VAL	LEU	SER	GLY
UNK	UNK	ILE	TRP	VAL	THR	THR
UNK	UNK	ILE	GLU	LYS	VAL	VAL
UNK	UNK	GLU	LEU	THR	GLN	TYP
UNK	UNK	PHE	MET	PRO	LEU	LYS
UNK	UNK	SER	THR	THR	ILE	GLY
UNK	UNK	LYS	PHE	HIS	THR	LEU
UNK	UNK	MET	GLY	VAL	GLN	TRP
UNK	UNK	ALA	SER	LYS	LEU	ILE
UNK	UNK	ARG	LYS	ILE	MET	ILE
UNK	UNK	ASP	PRO	THR	PRO	GLU
UNK	UNK	GLN	ASP	ASP	PHE	GLY
UNK	UNK	PRO	GLY	PHE	GLY	GLY
UNK	UNK	ARG	GLY	GLY	CYS	LYS
UNK	UNK	TYP	ILE	LEU	LEU	VAL
UNK	UNK	LEU	PRO	ALA	LEU	LYS
UNK	UNK	VAL	ALA	LYS	ASP	ILE
UNK	UNK	ILE	SER	LEU	TYP	VAL
UNK	UNK	GLN	GLU	LEU	VAL	VAL
UNK	UNK	GLY	ILE	GLY	ARG	ALA
UNK	UNK	X6	SER	ALA	GLU	ILE
UNK	UNK	X7	SER	GLU	HIS	LYS
UNK	UNK	X8	ILE	GLU	LYS	GLU
UNK	UNK	X9	LEU	LYS	ASP	LEU
UNK	UNK	X10	GLU	GLU	ASN	ARG
UNK	UNK	X11	LYS	TYP	ILE	GLU
UNK	UNK	X12	GLY	HIS	GLY	ALA
UNK	UNK	UNK	GLU	ALA	SER	THR
UNK	UNK	UNK	ARG	GLY	GLN	SER
UNK	UNK	UNK	LEU	GLY	TYP	PRO
UNK	UNK	UNK	PRO	GLY	LYS	LYS
UNK	UNK	UNK	GLN	LYS	LEU	ALA

Chain H: 97%

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.59Å 70.87Å 115.18Å 90.00° 109.36° 90.00°	Depositor
Resolution (Å)	44.17 – 2.70 44.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.17-2.70) 99.8 (44.17-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.69Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.204 , 0.257 0.208 , 0.267	Depositor DCC
R_{free} test set	1801 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8885	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3626e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ITI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	0/2167	1.21	24/2935 (0.8%)
1	B	0.85	0/2163	1.20	17/2930 (0.6%)
1	C	0.74	1/2123 (0.0%)	1.13	17/2873 (0.6%)
1	D	0.68	0/2132	1.13	22/2886 (0.8%)
All	All	0.79	1/8585 (0.0%)	1.17	80/11624 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	928	MET	SD-CE	5.37	1.93	1.79

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	SER	CA-C-N	14.31	137.72	119.84
1	A	728	SER	C-N-CA	14.31	137.72	119.84
1	B	728	SER	CA-C-N	12.72	135.75	119.84
1	B	728	SER	C-N-CA	12.72	135.75	119.84
1	D	831	ASP	N-CA-C	9.54	124.45	112.24
1	B	728	SER	C-N-CD	-8.97	88.23	125.00
1	A	728	SER	C-N-CD	-8.88	88.58	125.00
1	B	760	SER	N-CA-C	-8.44	102.03	111.14
1	D	760	SER	N-CA-C	-8.19	102.30	111.14
1	A	760	SER	N-CA-C	-7.95	102.55	111.14
1	A	716	ILE	N-CA-C	7.90	115.74	107.76
1	C	760	SER	N-CA-C	-7.68	102.84	111.14
1	C	704	LYS	N-CA-C	-7.49	97.03	109.46
1	C	852	VAL	N-CA-C	7.49	115.32	107.76
1	C	771	PHE	N-CA-C	7.46	123.41	113.72
1	D	704	LYS	N-CA-C	-7.35	97.26	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	LYS	N-CA-C	-7.32	97.66	109.96
1	B	771	PHE	N-CA-C	7.12	122.97	113.72
1	B	773	CYS	N-CA-C	7.00	119.77	110.53
1	B	899	ILE	N-CA-C	6.99	117.10	110.53
1	D	773	CYS	N-CA-C	6.97	120.33	110.50
1	D	903	LEU	N-CA-C	-6.93	103.81	111.36
1	C	716	ILE	N-CA-C	6.90	114.73	107.76
1	B	704	LYS	N-CA-C	-6.88	98.04	109.46
1	B	716	ILE	N-CA-C	6.83	115.42	107.77
1	C	773	CYS	N-CA-C	6.30	119.38	110.50
1	A	691	ILE	CB-CA-C	6.28	116.64	111.05
1	C	785	ILE	CA-C-N	6.26	126.28	120.34
1	C	785	ILE	C-N-CA	6.26	126.28	120.34
1	A	852	VAL	N-CA-C	6.20	114.03	107.76
1	B	852	VAL	N-CA-C	6.05	113.87	107.76
1	C	899	ILE	N-CA-C	5.94	116.68	110.62
1	B	730	LYS	N-CA-C	5.93	119.14	109.59
1	A	773	CYS	N-CA-C	5.87	118.78	110.50
1	B	907	GLU	N-CA-C	5.84	119.77	109.96
1	D	899	ILE	N-CA-C	5.84	115.96	110.30
1	C	861	SER	N-CA-C	-5.78	105.06	111.36
1	A	950	ASP	CA-C-N	5.78	125.91	119.32
1	A	950	ASP	C-N-CA	5.78	125.91	119.32
1	C	782	LYS	CA-C-N	-5.73	113.65	122.60
1	C	782	LYS	C-N-CA	-5.73	113.65	122.60
1	D	950	ASP	CA-C-N	5.73	126.11	119.47
1	D	950	ASP	C-N-CA	5.73	126.11	119.47
1	A	771	PHE	N-CA-C	5.71	122.05	114.12
1	A	899	ILE	N-CA-C	5.71	116.48	110.72
1	D	716	ILE	N-CA-C	5.67	113.67	107.60
1	D	771	PHE	N-CA-C	5.64	122.07	113.61
1	A	861	SER	N-CA-C	-5.55	104.87	111.69
1	B	861	SER	N-CA-C	-5.53	105.33	111.36
1	C	831	ASP	N-CA-C	5.51	119.18	111.74
1	C	852	VAL	CA-C-N	5.49	126.70	119.84
1	C	852	VAL	C-N-CA	5.49	126.70	119.84
1	D	916	THR	N-CA-C	-5.48	103.67	110.41
1	D	710	GLU	N-CA-C	5.41	118.01	109.96
1	A	852	VAL	CA-C-N	5.38	126.57	119.84
1	A	852	VAL	C-N-CA	5.38	126.57	119.84
1	A	690	LYS	N-CA-C	-5.37	102.92	110.50
1	A	732	ASN	N-CA-C	5.30	117.05	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	785	ILE	CA-C-N	5.29	125.37	120.34
1	D	785	ILE	C-N-CA	5.29	125.37	120.34
1	C	732	ASN	N-CA-C	5.29	117.04	111.28
1	A	782	LYS	CA-C-N	-5.28	114.36	122.60
1	A	782	LYS	C-N-CA	-5.28	114.36	122.60
1	D	822	LYS	N-CA-C	-5.27	103.50	111.56
1	A	903	LEU	N-CA-C	-5.25	105.20	111.03
1	C	903	LEU	N-CA-C	-5.23	105.49	111.14
1	D	934	ARG	CA-C-N	-5.22	114.86	120.03
1	D	934	ARG	C-N-CA	-5.22	114.86	120.03
1	B	732	ASN	N-CA-C	5.19	116.94	111.28
1	A	852	VAL	CB-CA-C	5.16	116.23	110.71
1	D	889	LYS	CA-C-N	-5.15	114.61	119.76
1	D	889	LYS	C-N-CA	-5.15	114.61	119.76
1	B	831	ASP	N-CA-C	5.14	118.53	111.54
1	A	823	THR	N-CA-C	-5.14	98.45	109.81
1	A	793	TRP	N-CA-C	-5.11	105.89	111.82
1	D	861	SER	N-CA-C	-5.11	105.62	111.14
1	D	782	LYS	CA-C-N	-5.10	114.64	122.60
1	D	782	LYS	C-N-CA	-5.10	114.64	122.60
1	B	852	VAL	CA-C-N	5.06	126.16	119.84
1	B	852	VAL	C-N-CA	5.06	126.16	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2120	0	2169	113	0
1	B	2116	0	2165	118	0
1	C	2078	0	2122	113	0
1	D	2087	0	2129	141	0
1	E	45	0	11	6	0
1	F	35	0	10	4	0
1	G	35	0	11	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	45	0	11	6	0
2	A	43	0	29	16	0
2	B	43	0	29	11	0
2	C	43	0	29	13	0
2	D	43	0	29	19	0
3	A	40	0	0	2	0
3	B	45	0	0	8	0
3	C	35	0	0	2	0
3	D	21	0	0	0	0
3	E	3	0	0	1	0
3	F	4	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
All	All	8885	0	8744	507	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (507) 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:D:715:LYS:HE3	1:D:715:LYS:H	1.23	1.00
1:C:691:ILE:HG22	1:C:692:LYS:HG2	1.41	1.00
1:D:691:ILE:HG22	1:D:692:LYS:HG2	1.41	0.99
1:B:736:LEU:HD13	1:B:758:LEU:HD11	1.43	0.99
1:C:715:LYS:HE2	1:C:715:LYS:H	1.28	0.98
1:D:753:LEU:HD21	1:D:764:LEU:HD22	1.42	0.98
1:B:725:GLU:HG2	1:B:726:ALA:H	1.27	0.97
1:C:925:LYS:HD2	1:C:935:PRO:HD3	1.44	0.97
1:B:691:ILE:HG22	1:B:692:LYS:HG2	1.46	0.97
1:A:925:LYS:HD2	1:A:935:PRO:HD3	1.46	0.96
1:B:925:LYS:HD2	1:B:935:PRO:HD3	1.46	0.96
1:D:925:LYS:HD2	1:D:935:PRO:HD3	1.47	0.94
1:B:928:MET:HE2	1:B:928:MET:HA	1.50	0.93
1:A:725:GLU:HG2	1:A:726:ALA:H	1.34	0.92
1:C:947:MET:HG2	1:C:954:TYR:CG	2.03	0.92
1:C:742:MET:HE2	2:C:1:ITI:H2	1.49	0.92
1:D:914:ILE:HG13	1:D:955:LEU:CD2	2.00	0.91
1:C:706:LEU:HD22	1:C:715:LYS:HB2	1.51	0.90
1:A:693:VAL:HG11	1:B:806:ASP:HB3	1.54	0.89
1:D:925:LYS:CD	1:D:935:PRO:HD3	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:LYS:HG2	1:A:891:TYR:HD1	1.39	0.86
1:C:855:LYS:HG2	1:C:891:TYR:HD1	1.40	0.86
1:C:925:LYS:CD	1:C:935:PRO:HD3	2.06	0.86
1:A:925:LYS:CD	1:A:935:PRO:HD3	2.06	0.85
1:D:855:LYS:HG2	1:D:891:TYR:HD1	1.39	0.85
1:B:925:LYS:CD	1:B:935:PRO:HD3	2.07	0.83
1:B:855:LYS:HG2	1:B:891:TYR:HD1	1.42	0.83
1:D:681:ARG:NH2	1:D:707:TRP:HZ3	1.77	0.83
1:A:699:PHE:CG	1:A:834:LEU:HD12	2.13	0.83
1:D:715:LYS:HD2	1:D:715:LYS:O	1.80	0.82
1:D:715:LYS:H	1:D:715:LYS:CE	1.92	0.81
1:A:691:ILE:HD13	1:A:706:LEU:HG	1.60	0.81
1:A:939:GLU:O	1:A:943:GLU:HG3	1.79	0.81
1:B:921:MET:HG3	1:C:898:GLU:HG2	1.63	0.81
1:C:715:LYS:HD2	1:C:715:LYS:O	1.81	0.80
1:B:729:PRO:HA	3:B:23:HOH:O	1.80	0.80
1:D:834:LEU:HD23	2:D:1:ITI:H1	1.63	0.80
1:B:948:ALA:O	1:B:951:PRO:HD3	1.81	0.80
1:A:736:LEU:HD23	1:A:740:TYR:CE1	2.17	0.79
2:D:1:ITI:H12	2:D:1:ITI:N35	1.97	0.79
1:C:681:ARG:NH2	1:G:12:UNK:HA	1.98	0.79
1:D:947:MET:HE2	1:D:954:TYR:HB3	1.64	0.78
1:D:834:LEU:HD21	2:D:1:ITI:H3	1.63	0.78
1:D:919:VAL:HG22	1:D:947:MET:HE1	1.63	0.78
1:C:715:LYS:H	1:C:715:LYS:CE	1.96	0.78
1:D:787:SER:OG	1:D:951:PRO:HB2	1.82	0.78
1:B:921:MET:HG3	1:C:898:GLU:CG	2.13	0.78
1:B:881:TRP:HD1	1:B:923:MET:HE1	1.48	0.78
1:D:684:LYS:H	1:D:687:GLU:HG3	1.49	0.78
1:C:705:GLY:HA3	1:C:720:ILE:CD1	2.14	0.77
1:A:691:ILE:HG22	1:A:692:LYS:HG2	1.67	0.77
1:A:787:SER:HB2	1:A:951:PRO:HB2	1.67	0.77
1:D:705:GLY:HA3	1:D:720:ILE:CD1	2.14	0.77
1:C:881:TRP:HD1	1:C:923:MET:HE1	1.49	0.77
1:B:705:GLY:HA3	1:B:720:ILE:CD1	2.14	0.77
1:B:881:TRP:CD1	1:B:923:MET:HE1	2.21	0.76
1:D:919:VAL:CG2	1:D:947:MET:HE1	2.16	0.76
1:A:715:LYS:H	1:A:715:LYS:HE2	1.48	0.76
1:C:881:TRP:CD1	1:C:923:MET:HE1	2.21	0.75
1:A:812:ARG:HG3	1:A:812:ARG:HH11	1.51	0.75
1:D:914:ILE:HG13	1:D:955:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:TRP:HD1	1:A:923:MET:HE1	1.51	0.75
1:C:723:LEU:HB2	1:C:762:VAL:CG1	2.17	0.75
1:E:15:UNK:HA	3:E:68:HOH:O	1.87	0.75
1:A:736:LEU:HD12	1:A:758:LEU:HD11	1.68	0.74
1:A:699:PHE:CD1	1:A:834:LEU:HD12	2.22	0.74
1:B:793:TRP:O	1:B:797:ILE:HG13	1.87	0.74
1:C:742:MET:HE2	2:C:1:ITI:C2	2.17	0.74
1:A:881:TRP:CD1	1:A:923:MET:HE1	2.22	0.74
1:D:881:TRP:HD1	1:D:923:MET:HE1	1.51	0.74
1:A:769:MET:HB3	3:A:257:HOH:O	1.86	0.73
1:C:756:ILE:HG13	1:C:764:LEU:HD23	1.68	0.73
1:A:723:LEU:HB2	1:A:762:VAL:CG1	2.18	0.73
1:D:723:LEU:HB2	1:D:762:VAL:CG1	2.19	0.73
1:D:855:LYS:HG2	1:D:891:TYR:CD1	2.24	0.73
1:D:881:TRP:CD1	1:D:923:MET:HE1	2.23	0.73
1:A:793:TRP:O	1:A:797:ILE:HG13	1.89	0.72
1:A:784:ASN:N	1:A:784:ASN:ND2	2.36	0.72
1:B:924:ARG:HH22	1:B:928:MET:HE1	1.52	0.72
1:A:681:ARG:NH1	1:F:13:UNK:CB	2.53	0.72
1:A:855:LYS:HG2	1:A:891:TYR:CD1	2.24	0.72
1:D:795:VAL:O	1:D:799:LYS:HG3	1.89	0.72
1:D:707:TRP:HD1	1:D:708:ILE:N	1.87	0.71
1:C:793:TRP:O	1:C:797:ILE:HG13	1.90	0.71
1:A:715:LYS:HD2	1:A:715:LYS:O	1.89	0.71
1:D:793:TRP:O	1:D:797:ILE:HG13	1.90	0.71
1:A:705:GLY:HA3	1:A:720:ILE:CD1	2.19	0.71
1:B:928:MET:HA	1:B:928:MET:CE	2.21	0.71
2:D:1:ITI:H12	2:D:1:ITI:H26	1.72	0.71
1:B:723:LEU:HB2	1:B:762:VAL:CG1	2.21	0.71
1:D:784:ASN:N	1:D:784:ASN:ND2	2.39	0.70
1:C:693:VAL:HG22	1:C:703:TYR:CE2	2.27	0.70
1:B:855:LYS:HG2	1:B:891:TYR:CD1	2.27	0.70
1:G:9:UNK:HA	1:G:12:UNK:C	2.22	0.70
1:B:921:MET:CG	1:C:898:GLU:HG2	2.21	0.70
1:A:693:VAL:HG22	1:A:703:TYR:CE2	2.26	0.69
1:A:715:LYS:HE2	1:A:715:LYS:N	2.07	0.69
1:A:736:LEU:CD1	1:A:758:LEU:HD11	2.21	0.69
1:D:694:LEU:O	2:D:1:ITI:H30A	1.92	0.69
1:A:795:VAL:O	1:A:799:LYS:HG3	1.91	0.69
1:C:795:VAL:O	1:C:799:LYS:HG3	1.91	0.69
1:B:795:VAL:O	1:B:799:LYS:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:LYS:HE3	1:D:715:LYS:N	2.05	0.69
1:C:936:LYS:HE3	3:C:198:HOH:O	1.93	0.69
1:D:707:TRP:CD1	1:D:707:TRP:C	2.71	0.69
1:D:715:LYS:O	1:D:716:ILE:HD13	1.93	0.69
1:D:681:ARG:CZ	1:D:707:TRP:HZ3	2.06	0.69
1:D:707:TRP:HH2	1:H:8:UNK:CB	2.05	0.69
1:C:855:LYS:HG2	1:C:891:TYR:CD1	2.25	0.68
1:D:898:GLU:O	1:D:902:ILE:HG23	1.94	0.68
1:D:947:MET:HE2	1:D:954:TYR:CB	2.23	0.68
1:C:723:LEU:HB2	1:C:762:VAL:HG13	1.76	0.68
1:C:784:ASN:N	1:C:784:ASN:ND2	2.42	0.67
1:D:693:VAL:HG22	1:D:703:TYR:CE2	2.29	0.67
1:A:769:MET:O	2:A:1:ITI:H12	1.95	0.67
1:A:779:ARG:O	1:A:782:LYS:HG2	1.94	0.67
1:D:881:TRP:HB2	1:D:923:MET:HE3	1.77	0.67
1:A:881:TRP:HB2	1:A:923:MET:HE3	1.77	0.66
1:D:707:TRP:CH2	1:H:8:UNK:CB	2.78	0.66
1:C:898:GLU:O	1:C:902:ILE:HG23	1.96	0.66
1:B:953:ARG:HG2	1:B:954:TYR:CE1	2.30	0.66
1:C:881:TRP:HB2	1:C:923:MET:HE3	1.78	0.66
1:C:736:LEU:HD12	1:C:758:LEU:HD11	1.78	0.66
1:C:899:ILE:HG22	1:C:903:LEU:CD2	2.26	0.66
1:A:898:GLU:O	1:A:902:ILE:HG23	1.96	0.65
1:C:958:GLN:HA	1:C:958:GLN:OE1	1.95	0.65
1:D:723:LEU:HB2	1:D:762:VAL:HG13	1.78	0.65
1:A:715:LYS:H	1:A:715:LYS:CE	2.10	0.65
1:A:723:LEU:HB2	1:A:762:VAL:HG13	1.78	0.65
1:B:924:ARG:HH22	1:B:928:MET:CE	2.09	0.65
1:C:715:LYS:HE2	1:C:715:LYS:N	2.07	0.65
1:F:8:UNK:O	1:F:12:UNK:N	2.29	0.65
1:B:795:VAL:HG12	1:B:799:LYS:HE3	1.77	0.65
1:D:795:VAL:HG12	1:D:799:LYS:HE3	1.79	0.64
1:A:795:VAL:HG12	1:A:799:LYS:HE3	1.79	0.64
1:D:787:SER:HG	1:D:951:PRO:HB2	1.63	0.64
1:A:723:LEU:HD12	1:A:762:VAL:HG11	1.80	0.64
1:A:721:LYS:HE3	2:A:1:ITI:N36	2.13	0.63
1:B:723:LEU:HD12	1:B:762:VAL:HG11	1.79	0.63
1:B:736:LEU:HD13	1:B:758:LEU:CD1	2.23	0.63
1:D:947:MET:HE2	1:D:954:TYR:CG	2.32	0.63
1:B:895:PRO:HA	3:B:229:HOH:O	1.99	0.63
1:B:917:ILE:HD12	1:C:898:GLU:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:GLY:HA3	1:D:720:ILE:HD11	1.80	0.63
1:B:779:ARG:O	1:B:782:LYS:HE2	1.99	0.62
1:C:947:MET:HG2	1:C:954:TYR:CD1	2.34	0.62
1:B:723:LEU:HD12	1:B:762:VAL:CG1	2.29	0.62
1:A:902:ILE:HD12	1:A:907:GLU:HG2	1.82	0.62
1:B:681:ARG:CD	1:E:10:UNK:CB	2.78	0.62
1:A:679:LEU:N	1:A:679:LEU:HD12	2.15	0.62
1:A:784:ASN:ND2	1:A:784:ASN:H	1.96	0.62
1:A:947:MET:HG2	1:A:954:TYR:CG	2.34	0.62
1:C:742:MET:CE	2:C:1:ITI:H2	2.26	0.62
1:B:881:TRP:HB2	1:B:923:MET:HE3	1.81	0.61
1:C:684:LYS:H	1:C:687:GLU:HG3	1.65	0.61
1:D:779:ARG:O	1:D:782:LYS:HE2	2.00	0.61
1:B:705:GLY:HA3	1:B:720:ILE:HD11	1.81	0.61
1:B:693:VAL:HG22	1:B:703:TYR:CE2	2.34	0.61
1:B:725:GLU:HG2	1:B:726:ALA:N	2.08	0.61
1:C:705:GLY:HA3	1:C:720:ILE:HD11	1.83	0.61
1:B:723:LEU:HB2	1:B:762:VAL:HG13	1.82	0.61
1:C:691:ILE:HG22	1:C:692:LYS:CG	2.25	0.61
2:C:1:ITI:H12	2:C:1:ITI:N35	2.16	0.61
1:A:723:LEU:HD12	1:A:762:VAL:CG1	2.30	0.61
2:A:1:ITI:N35	2:A:1:ITI:H11	2.16	0.61
1:B:811:HIS:O	1:B:812:ARG:HB2	2.01	0.61
1:D:896:ALA:HA	1:D:899:ILE:HG12	1.83	0.60
1:D:684:LYS:O	1:D:687:GLU:HG3	2.01	0.60
1:D:705:GLY:HA3	1:D:720:ILE:HD12	1.83	0.60
1:B:924:ARG:NH2	1:B:928:MET:HE1	2.17	0.60
1:C:779:ARG:O	1:C:782:LYS:HE2	2.01	0.60
1:A:784:ASN:N	1:A:784:ASN:HD22	2.00	0.60
1:D:818:ASN:O	1:D:830:THR:HG22	2.01	0.60
1:A:948:ALA:O	1:A:951:PRO:HD3	2.02	0.60
1:A:811:HIS:O	1:A:812:ARG:HB2	2.02	0.60
1:B:736:LEU:CD1	1:B:758:LEU:HD11	2.25	0.59
1:A:693:VAL:CG1	1:B:806:ASP:HB3	2.32	0.59
1:C:736:LEU:HD23	1:C:740:TYR:CE1	2.38	0.58
1:D:834:LEU:HD23	2:D:1:ITI:C1	2.33	0.58
2:B:1:ITI:H6	2:B:1:ITI:N40	2.18	0.58
1:B:943:GLU:O	1:B:947:MET:HG3	2.04	0.58
1:D:684:LYS:N	1:D:687:GLU:HG3	2.18	0.58
1:D:784:ASN:ND2	1:D:784:ASN:H	2.02	0.58
1:D:721:LYS:HE3	2:D:1:ITI:N36	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:SER:N	1:B:729:PRO:HD3	2.19	0.57
1:B:781:HIS:O	1:B:785:ILE:HG13	2.04	0.57
1:A:881:TRP:HB2	1:A:923:MET:CE	2.34	0.57
1:A:690:LYS:HD3	1:A:703:TYR:CD1	2.40	0.57
1:C:723:LEU:HD12	1:C:762:VAL:HG11	1.86	0.57
1:D:723:LEU:HD12	1:D:762:VAL:HG11	1.86	0.57
1:B:691:ILE:HG22	1:B:692:LYS:CG	2.28	0.57
1:D:715:LYS:H	1:D:715:LYS:CD	2.15	0.57
1:D:753:LEU:HD12	1:D:754:LEU:N	2.20	0.57
1:C:795:VAL:HG12	1:C:799:LYS:HE3	1.87	0.57
1:C:791:LEU:HD12	1:C:951:PRO:HB3	1.86	0.57
1:D:679:LEU:O	1:D:752:ARG:NH2	2.38	0.57
1:D:766:THR:HG23	2:D:1:ITI:H10	1.87	0.56
1:C:771:PHE:HB2	1:C:821:VAL:O	2.04	0.56
1:A:684:LYS:O	1:A:687:GLU:HG3	2.06	0.56
1:A:795:VAL:CG1	1:A:799:LYS:HE3	2.35	0.56
2:A:1:ITI:C16	2:A:1:ITI:H13	2.35	0.56
1:D:731:ALA:O	1:D:735:ILE:HD12	2.06	0.56
1:D:735:ILE:O	1:D:738:GLU:HB2	2.05	0.56
2:D:1:ITI:H26	2:D:1:ITI:C12	2.36	0.56
1:A:705:GLY:HA3	1:A:720:ILE:HD11	1.87	0.56
1:D:881:TRP:HB2	1:D:923:MET:CE	2.36	0.56
1:B:881:TRP:HB2	1:B:923:MET:CE	2.36	0.56
1:C:832:PHE:CE2	2:C:1:ITI:H3	2.41	0.56
1:C:899:ILE:HG22	1:C:903:LEU:HD22	1.87	0.56
1:D:691:ILE:HG22	1:D:692:LYS:CG	2.26	0.56
1:D:834:LEU:HD21	2:D:1:ITI:C3	2.35	0.56
1:B:787:SER:OG	1:B:951:PRO:HB2	2.05	0.56
1:C:705:GLY:HA3	1:C:720:ILE:HD12	1.88	0.56
1:B:795:VAL:CG1	1:B:799:LYS:HE3	2.36	0.55
1:C:881:TRP:HB2	1:C:923:MET:CE	2.36	0.55
1:D:795:VAL:CG1	1:D:799:LYS:HE3	2.36	0.55
1:D:953:ARG:NH1	1:D:953:ARG:HG3	2.21	0.55
1:D:781:HIS:O	1:D:785:ILE:HG13	2.06	0.55
1:D:925:LYS:HD3	1:D:935:PRO:HD3	1.87	0.55
1:C:736:LEU:HD23	1:C:740:TYR:HE1	1.70	0.55
1:D:723:LEU:HD12	1:D:762:VAL:CG1	2.36	0.55
1:A:725:GLU:HG2	1:A:726:ALA:N	2.13	0.55
1:A:721:LYS:CE	2:A:1:ITI:N36	2.70	0.55
1:A:782:LYS:NZ	1:B:946:LYS:HD2	2.22	0.54
1:D:691:ILE:CG2	1:D:692:LYS:HE2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:THR:HG23	1:A:954:TYR:O	2.07	0.54
1:C:723:LEU:HD12	1:C:762:VAL:CG1	2.37	0.54
1:C:715:LYS:H	1:C:715:LYS:CD	2.20	0.54
1:G:8:UNK:O	1:G:12:UNK:O	2.25	0.54
1:B:899:ILE:O	1:B:903:LEU:HD22	2.08	0.54
1:C:684:LYS:O	1:C:687:GLU:HG3	2.07	0.54
1:C:766:THR:HG21	2:C:1:ITI:O41	2.08	0.54
1:A:946:LYS:HA	1:A:949:ARG:NH1	2.23	0.54
1:B:679:LEU:O	1:B:752:ARG:NH2	2.41	0.53
2:B:1:ITI:C16	2:B:1:ITI:H13	2.38	0.53
1:B:681:ARG:CZ	1:E:10:UNK:CB	2.86	0.53
1:B:683:LEU:HD23	1:B:687:GLU:OE1	2.08	0.53
1:C:691:ILE:CG2	1:C:692:LYS:HE2	2.37	0.53
1:D:953:ARG:HH11	1:D:953:ARG:CG	2.21	0.53
1:A:925:LYS:HD3	1:A:935:PRO:HD3	1.90	0.53
1:C:918:ASP:O	1:C:922:ILE:HG13	2.08	0.53
1:A:736:LEU:HD23	1:A:740:TYR:HE1	1.70	0.53
1:C:781:HIS:O	1:C:785:ILE:HG13	2.07	0.53
1:D:919:VAL:HG22	1:D:947:MET:CE	2.37	0.53
1:D:707:TRP:HD1	1:D:707:TRP:C	2.11	0.53
1:D:784:ASN:N	1:D:784:ASN:HD22	2.06	0.53
1:D:681:ARG:NH2	1:D:707:TRP:CZ3	2.68	0.53
1:B:899:ILE:HG22	1:B:903:LEU:CD2	2.38	0.53
2:D:1:ITI:H10	2:D:1:ITI:O41	2.08	0.53
1:A:725:GLU:CG	1:A:726:ALA:H	2.12	0.52
1:A:859:LEU:HD21	1:A:904:GLU:HG3	1.91	0.52
1:C:946:LYS:HA	1:C:949:ARG:NH1	2.25	0.52
1:D:943:GLU:O	1:D:947:MET:HG3	2.08	0.52
1:C:680:LEU:HD23	1:C:740:TYR:CE2	2.44	0.52
1:B:787:SER:HB3	3:B:39:HOH:O	2.09	0.52
1:D:834:LEU:CD2	2:D:1:ITI:H1	2.37	0.52
1:B:691:ILE:CG2	1:B:692:LYS:HE2	2.39	0.52
1:B:859:LEU:HD21	1:B:904:GLU:HG3	1.90	0.52
1:C:859:LEU:HD23	1:C:929:ILE:HD12	1.90	0.52
1:A:728:SER:N	1:A:729:PRO:HD3	2.24	0.52
1:B:899:ILE:HG22	1:B:903:LEU:HD22	1.92	0.52
1:A:918:ASP:O	1:A:922:ILE:HG13	2.09	0.52
1:B:705:GLY:HA3	1:B:720:ILE:HD12	1.88	0.52
1:B:719:ALA:CB	2:B:1:ITI:C15	2.88	0.52
1:D:791:LEU:CD1	1:D:955:LEU:HD12	2.40	0.52
1:C:738:GLU:O	1:C:741:VAL:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:918:ASP:O	1:D:922:ILE:HG13	2.09	0.51
1:D:681:ARG:CZ	1:H:8:UNK:CB	2.88	0.51
1:A:705:GLY:HA3	1:A:720:ILE:HD12	1.92	0.51
1:B:870:GLN:HG3	1:B:931:ALA:O	2.11	0.51
1:B:946:LYS:HA	1:B:949:ARG:NH1	2.25	0.51
1:C:925:LYS:HD2	1:C:935:PRO:CD	2.30	0.51
1:D:870:GLN:HG3	1:D:931:ALA:O	2.11	0.51
1:B:681:ARG:HD3	1:E:10:UNK:CB	2.41	0.51
1:C:914:ILE:HG13	1:C:955:LEU:HD22	1.91	0.51
1:A:870:GLN:HG3	1:A:931:ALA:O	2.11	0.50
1:B:936:LYS:HE3	3:B:999:HOH:O	2.10	0.50
1:B:738:GLU:O	1:B:742:MET:HG3	2.10	0.50
1:B:953:ARG:HG2	1:B:954:TYR:CZ	2.45	0.50
1:C:870:GLN:HG3	1:C:931:ALA:O	2.12	0.50
1:D:946:LYS:HA	1:D:949:ARG:NH1	2.26	0.50
1:D:681:ARG:CZ	1:D:707:TRP:CZ3	2.92	0.50
1:B:859:LEU:HD23	1:B:929:ILE:HD12	1.94	0.50
1:B:925:LYS:O	1:B:928:MET:HG2	2.12	0.50
1:D:777:TYR:O	1:D:781:HIS:HD2	1.95	0.50
1:C:784:ASN:N	1:C:784:ASN:HD22	2.09	0.50
1:A:917:ILE:HD12	1:A:921:MET:SD	2.52	0.50
1:C:800:GLY:HA3	1:C:829:ILE:HD12	1.94	0.50
1:C:777:TYR:O	1:C:781:HIS:HD2	1.94	0.49
1:C:928:MET:HB2	1:C:934:ARG:HG3	1.92	0.49
1:A:679:LEU:O	1:A:752:ARG:NH2	2.46	0.49
1:D:947:MET:CE	1:D:954:TYR:CD2	2.95	0.49
1:A:859:LEU:HD23	1:A:929:ILE:HD12	1.94	0.49
2:B:1:ITI:H13	2:B:1:ITI:C5	2.41	0.49
2:A:1:ITI:H10	2:A:1:ITI:O41	2.12	0.49
2:C:1:ITI:N35	2:C:1:ITI:H26	2.27	0.49
2:A:1:ITI:N35	2:A:1:ITI:C11	2.73	0.49
1:C:855:LYS:HE2	1:C:899:ILE:HD11	1.94	0.49
1:D:707:TRP:CD1	1:D:708:ILE:N	2.74	0.49
1:A:812:ARG:HG3	1:A:812:ARG:NH1	2.26	0.49
1:C:795:VAL:CG1	1:C:799:LYS:HE3	2.43	0.49
1:B:937:PHE:O	1:B:941:ILE:HG13	2.14	0.48
1:D:681:ARG:NE	1:H:8:UNK:CB	2.76	0.48
1:B:909:LEU:N	3:B:42:HOH:O	2.29	0.48
1:D:681:ARG:NH2	1:H:8:UNK:CB	2.77	0.48
1:D:919:VAL:HG23	1:D:947:MET:HE1	1.95	0.48
1:D:679:LEU:N	1:D:679:LEU:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:917:ILE:HD12	1:C:921:MET:SD	2.53	0.48
1:D:832:PHE:CE2	2:D:1:ITI:H6	2.48	0.48
1:A:736:LEU:CD1	1:A:758:LEU:CD1	2.91	0.48
1:D:917:ILE:HD12	1:D:921:MET:SD	2.54	0.48
1:B:774:LEU:O	1:B:778:VAL:HG13	2.14	0.48
1:C:859:LEU:HD21	1:C:904:GLU:HG3	1.95	0.48
1:A:770:PRO:HD2	3:A:257:HOH:O	2.13	0.48
1:G:6:UNK:C	1:G:10:UNK:CB	2.91	0.48
1:D:797:ILE:O	1:D:829:ILE:HD11	2.14	0.47
1:A:925:LYS:HA	1:A:928:MET:HE3	1.94	0.47
1:A:937:PHE:O	1:A:941:ILE:HG13	2.14	0.47
1:B:777:TYR:O	1:B:781:HIS:HD2	1.97	0.47
1:C:784:ASN:ND2	1:C:784:ASN:H	2.07	0.47
2:B:1:ITI:N35	2:B:1:ITI:H12	2.29	0.47
1:C:834:LEU:HD21	2:C:1:ITI:H6	1.96	0.47
2:A:1:ITI:H13	2:A:1:ITI:C5	2.44	0.47
1:C:902:ILE:O	1:C:907:GLU:HB2	2.14	0.47
1:A:693:VAL:HG21	1:B:807:ARG:HD2	1.95	0.47
1:A:714:VAL:HA	1:A:715:LYS:HE2	1.96	0.47
1:B:953:ARG:O	1:B:953:ARG:HG3	2.14	0.47
1:D:681:ARG:NH1	1:D:707:TRP:CZ3	2.83	0.47
1:D:715:LYS:HD2	1:D:715:LYS:C	2.39	0.47
1:D:811:HIS:O	1:D:812:ARG:HB2	2.13	0.47
1:B:918:ASP:O	1:B:922:ILE:HG13	2.15	0.47
1:B:921:MET:HG3	1:C:898:GLU:CD	2.40	0.47
1:C:899:ILE:O	1:C:903:LEU:HD22	2.15	0.47
1:C:925:LYS:HD3	1:C:935:PRO:HD3	1.93	0.47
1:D:782:LYS:O	1:D:886:PHE:CD1	2.67	0.47
1:A:719:ALA:CB	2:A:1:ITI:C15	2.93	0.47
1:B:791:LEU:HG	1:B:955:LEU:CD1	2.45	0.47
1:B:828:LYS:NZ	3:B:181:HOH:O	2.47	0.47
1:B:917:ILE:O	1:B:921:MET:HB2	2.15	0.47
1:C:782:LYS:O	1:C:886:PHE:CD1	2.68	0.47
1:A:782:LYS:O	1:A:886:PHE:CD1	2.68	0.47
1:B:766:THR:HG22	2:B:1:ITI:C4	2.45	0.47
2:C:1:ITI:N35	2:C:1:ITI:C26	2.78	0.47
1:A:852:VAL:HA	1:A:853:PRO:HD3	1.65	0.46
1:C:724:ARG:NH1	1:D:808:ARG:HG3	2.30	0.46
2:C:1:ITI:H12	2:C:1:ITI:H26	1.97	0.46
1:D:950:ASP:OD2	1:D:953:ARG:HD2	2.15	0.46
1:A:812:ARG:HH11	1:A:812:ARG:CG	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:LYS:C	1:D:716:ILE:HD13	2.40	0.46
1:D:859:LEU:HD23	1:D:929:ILE:HD12	1.97	0.46
1:A:727:THR:O	1:A:728:SER:OG	2.29	0.46
1:D:736:LEU:CD2	1:D:740:TYR:CE1	2.98	0.46
1:D:812:ARG:NH1	1:D:867:TYR:HB2	2.31	0.46
1:D:936:LYS:HE2	1:D:936:LYS:HB3	1.58	0.46
1:C:766:THR:CG2	2:C:1:ITI:O41	2.63	0.46
1:C:782:LYS:HE2	1:C:782:LYS:HB2	1.51	0.46
1:B:681:ARG:NH1	1:E:10:UNK:CB	2.79	0.46
1:B:742:MET:CE	2:B:1:ITI:H1	2.46	0.46
2:B:1:ITI:N35	2:B:1:ITI:C26	2.77	0.46
1:C:689:LYS:NZ	3:C:251:HOH:O	2.47	0.46
1:D:682:ILE:N	1:D:682:ILE:HD12	2.31	0.46
1:C:707:TRP:CD1	1:G:12:UNK:CB	2.98	0.46
1:A:791:LEU:O	1:A:795:VAL:HG23	2.15	0.46
1:C:865:ARG:HD3	1:C:865:ARG:HA	1.40	0.46
1:A:766:THR:HG22	2:A:1:ITI:C4	2.45	0.45
1:B:681:ARG:NE	1:E:10:UNK:CB	2.79	0.45
1:B:791:LEU:HG	1:B:955:LEU:HD12	1.96	0.45
1:C:680:LEU:O	1:C:680:LEU:HG	2.14	0.45
1:C:812:ARG:NH1	1:C:867:TYR:HB2	2.31	0.45
1:B:830:THR:OG1	1:B:831:ASP:N	2.49	0.45
1:B:779:ARG:HD3	1:B:887:GLY:HA3	1.98	0.45
1:B:813:ASP:OD1	1:B:817:ARG:NH2	2.50	0.45
1:A:747:ASN:HB3	1:A:750:VAL:HG23	1.98	0.45
1:C:742:MET:CE	2:C:1:ITI:C2	2.91	0.45
1:D:953:ARG:NH1	1:D:953:ARG:CG	2.78	0.45
1:B:690:LYS:NZ	1:B:763:GLN:OE1	2.50	0.45
1:B:776:ASP:HB2	3:B:99:HOH:O	2.17	0.45
1:B:807:ARG:O	1:B:808:ARG:HB2	2.17	0.45
1:B:911:GLN:HB2	1:B:920:TYR:CD2	2.51	0.45
1:B:924:ARG:NH2	1:B:928:MET:CE	2.78	0.45
1:A:772:GLY:HA2	2:A:1:ITI:H26	1.97	0.45
1:A:774:LEU:O	1:A:778:VAL:HG13	2.16	0.45
1:A:813:ASP:OD1	1:A:817:ARG:NH2	2.50	0.45
2:B:1:ITI:N35	2:B:1:ITI:H26	2.32	0.45
1:C:736:LEU:CD1	1:C:758:LEU:HD11	2.45	0.45
1:A:715:LYS:N	1:A:715:LYS:CD	2.80	0.45
1:A:925:LYS:HD2	1:A:935:PRO:CD	2.32	0.45
1:C:681:ARG:NH2	1:G:12:UNK:CA	2.75	0.45
1:C:724:ARG:HH11	1:D:808:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:ASP:OD1	1:C:817:ARG:NH2	2.49	0.45
1:D:937:PHE:O	1:D:941:ILE:HG13	2.17	0.45
1:B:725:GLU:CG	1:B:726:ALA:H	2.06	0.45
1:B:782:LYS:O	1:B:886:PHE:CD1	2.70	0.45
1:A:917:ILE:O	1:A:921:MET:HB2	2.18	0.44
1:C:690:LYS:NZ	1:C:763:GLN:OE1	2.50	0.44
1:D:693:VAL:HG22	1:D:703:TYR:HE2	1.80	0.44
1:D:813:ASP:OD1	1:D:817:ARG:NH2	2.50	0.44
1:D:947:MET:HE3	1:D:954:TYR:CD2	2.52	0.44
1:B:865:ARG:HA	1:B:865:ARG:HD3	1.41	0.44
1:D:681:ARG:HH22	1:D:707:TRP:HZ3	1.61	0.44
1:A:781:HIS:O	1:A:785:ILE:HG13	2.18	0.44
1:B:781:HIS:HB2	1:B:785:ILE:HD11	2.00	0.44
1:B:925:LYS:HD2	1:B:935:PRO:CD	2.32	0.44
1:D:690:LYS:C	1:D:691:ILE:HD12	2.42	0.44
1:A:720:ILE:CG1	1:A:765:ILE:HD12	2.47	0.44
1:C:925:LYS:O	1:C:928:MET:HG2	2.18	0.44
1:C:937:PHE:O	1:C:941:ILE:HG13	2.18	0.44
1:D:753:LEU:HD12	1:D:753:LEU:C	2.42	0.44
2:A:1:ITI:H30A	2:A:1:ITI:H9	1.52	0.44
1:D:947:MET:HE2	1:D:954:TYR:CD2	2.52	0.44
1:A:716:ILE:HA	1:A:717:PRO:HD3	1.88	0.44
1:A:865:ARG:HA	1:A:865:ARG:HD3	1.41	0.44
1:A:946:LYS:HA	1:A:949:ARG:CZ	2.48	0.44
1:C:690:LYS:C	1:C:691:ILE:HD12	2.42	0.44
1:C:706:LEU:HD23	1:C:706:LEU:HA	1.65	0.44
1:D:834:LEU:CD2	2:D:1:ITI:C1	2.94	0.44
1:F:8:UNK:O	1:F:11:UNK:N	2.51	0.44
1:C:946:LYS:HA	1:C:949:ARG:CZ	2.48	0.43
1:D:782:LYS:HE2	1:D:782:LYS:HB2	1.52	0.43
1:D:925:LYS:HD2	1:D:935:PRO:CD	2.33	0.43
1:A:715:LYS:H	1:A:715:LYS:CD	2.31	0.43
1:A:919:VAL:HG22	1:A:947:MET:HE2	1.99	0.43
1:B:925:LYS:HD3	1:B:935:PRO:HD3	1.93	0.43
1:D:858:ALA:HA	1:D:874:TRP:CD2	2.53	0.43
1:F:8:UNK:C	1:F:12:UNK:CB	2.96	0.43
1:A:721:LYS:HB2	2:A:1:ITI:C5	2.49	0.43
1:A:811:HIS:CD2	1:A:832:PHE:HB3	2.54	0.43
1:A:781:HIS:HB2	1:A:785:ILE:HD11	1.99	0.43
1:B:812:ARG:NH1	1:B:867:TYR:HB2	2.33	0.43
1:C:774:LEU:O	1:C:778:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:LYS:H	1:D:687:GLU:CG	2.26	0.43
1:D:736:LEU:HD23	1:D:740:TYR:CE1	2.54	0.43
1:D:853:PRO:HB2	1:D:856:TRP:HB2	1.99	0.43
1:B:948:ALA:C	1:B:951:PRO:HD3	2.44	0.43
1:C:936:LYS:HE2	1:C:936:LYS:HB3	1.61	0.43
2:C:1:ITI:H9	2:C:1:ITI:H30	1.87	0.43
1:A:691:ILE:CD1	1:A:706:LEU:HG	2.41	0.43
1:A:756:ILE:HG13	1:A:764:LEU:HD23	2.01	0.43
1:D:771:PHE:HB3	1:D:821:VAL:HB	2.01	0.43
1:D:914:ILE:HG13	1:D:955:LEU:HD23	1.92	0.43
1:D:924:ARG:O	1:D:924:ARG:NH1	2.52	0.43
1:A:859:LEU:HD23	1:A:929:ILE:CD1	2.49	0.43
1:D:834:LEU:CD2	2:D:1:ITI:C3	2.97	0.43
1:D:834:LEU:CD2	2:D:1:ITI:H3	2.43	0.43
1:B:720:ILE:CG1	1:B:765:ILE:HD12	2.49	0.43
1:C:947:MET:HG2	1:C:954:TYR:CD2	2.52	0.43
1:H:9:UNK:O	1:H:13:UNK:N	2.52	0.43
1:D:946:LYS:HA	1:D:949:ARG:CZ	2.49	0.42
1:A:858:ALA:HA	1:A:874:TRP:CD2	2.53	0.42
1:A:779:ARG:HD3	1:A:887:GLY:HA3	2.02	0.42
1:D:706:LEU:HD23	1:D:706:LEU:HA	1.64	0.42
1:D:769:MET:O	2:D:1:ITI:N39	2.36	0.42
1:B:936:LYS:HB3	1:B:936:LYS:HE2	1.59	0.42
1:C:680:LEU:HD23	1:C:740:TYR:CD2	2.54	0.42
1:D:917:ILE:O	1:D:921:MET:HB2	2.19	0.42
2:B:1:ITI:H29A	2:B:1:ITI:H8	1.59	0.42
1:C:770:PRO:HG2	1:C:771:PHE:CD2	2.54	0.42
1:A:693:VAL:HG22	1:A:703:TYR:HE2	1.78	0.42
1:B:946:LYS:HA	1:B:949:ARG:CZ	2.49	0.42
1:B:858:ALA:HA	1:B:874:TRP:CD2	2.54	0.42
1:B:924:ARG:O	1:B:924:ARG:NH1	2.52	0.42
1:C:756:ILE:HA	1:C:763:GLN:O	2.19	0.42
1:D:900:SER:OG	1:D:901:SER:N	2.52	0.42
1:C:852:VAL:CG2	1:C:854:ILE:CD1	2.98	0.42
1:D:774:LEU:O	1:D:778:VAL:HG13	2.19	0.42
1:D:953:ARG:HG3	1:D:953:ARG:HH11	1.80	0.42
1:A:719:ALA:HB2	1:A:768:LEU:HA	2.02	0.41
1:B:776:ASP:CB	3:B:99:HOH:O	2.67	0.41
1:B:787:SER:OG	1:B:951:PRO:CB	2.68	0.41
1:D:791:LEU:O	1:D:795:VAL:HG23	2.19	0.41
1:B:853:PRO:HB2	1:B:856:TRP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:735:ILE:O	1:D:738:GLU:N	2.51	0.41
1:B:947:MET:HB3	1:B:954:TYR:CD1	2.56	0.41
1:D:852:VAL:HG23	1:D:857:MET:SD	2.61	0.41
1:B:704:LYS:HE2	1:B:704:LYS:HB2	1.80	0.41
1:B:742:MET:HE2	1:B:832:PHE:O	2.20	0.41
1:C:704:LYS:HE2	1:C:704:LYS:HB2	1.86	0.41
1:C:791:LEU:O	1:C:794:CYS:HB2	2.21	0.41
2:D:1:ITI:H30	2:D:1:ITI:H9	1.76	0.41
1:C:754:LEU:HD11	1:G:9:UNK:CB	2.50	0.41
1:D:899:ILE:HG22	1:D:903:LEU:CD2	2.51	0.41
1:A:807:ARG:O	1:A:808:ARG:HB2	2.21	0.41
1:B:704:LYS:HD3	1:B:768:LEU:HD21	2.02	0.41
1:B:766:THR:HG22	2:B:1:ITI:C10	2.51	0.41
1:A:691:ILE:HD13	1:A:706:LEU:CG	2.42	0.41
1:A:782:LYS:HZ1	1:B:946:LYS:HD2	1.84	0.41
1:A:834:LEU:HD22	1:A:834:LEU:HA	1.86	0.41
1:C:858:ALA:HA	1:C:874:TRP:CD2	2.55	0.41
1:C:917:ILE:O	1:C:921:MET:HB2	2.20	0.41
1:D:719:ALA:HB2	1:D:768:LEU:HA	2.02	0.41
1:D:756:ILE:HD11	1:D:758:LEU:HD21	2.03	0.41
1:C:811:HIS:O	1:C:812:ARG:HB2	2.20	0.41
1:B:682:ILE:HD12	1:B:682:ILE:N	2.37	0.40
1:B:690:LYS:C	1:B:691:ILE:HD12	2.45	0.40
1:B:852:VAL:CG2	1:B:854:ILE:CD1	2.99	0.40
1:C:790:LEU:HA	1:C:790:LEU:HD23	1.82	0.40
1:D:857:MET:HB3	1:D:861:SER:HB3	2.03	0.40
2:A:1:ITI:C5	2:A:1:ITI:C13	2.99	0.40
1:C:852:VAL:HG23	1:C:857:MET:SD	2.61	0.40
1:D:899:ILE:CG2	1:D:903:LEU:CD2	3.00	0.40
2:A:1:ITI:C16	2:A:1:ITI:C13	2.98	0.40
1:G:8:UNK:O	1:G:12:UNK:C	2.69	0.40
1:A:721:LYS:NZ	2:A:1:ITI:N36	2.69	0.40
1:A:782:LYS:NZ	1:B:946:LYS:CD	2.84	0.40
1:A:861:SER:O	1:A:865:ARG:NE	2.49	0.40
1:D:720:ILE:CG1	1:D:765:ILE:HD12	2.51	0.40
2:D:1:ITI:H8	2:D:1:ITI:H29A	1.78	0.40

There are no symmetry-related clashes.

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	261/327 (80%)	245 (94%)	12 (5%)	4 (2%)	8	22
1	B	261/327 (80%)	247 (95%)	11 (4%)	3 (1%)	11	29
1	C	253/327 (77%)	243 (96%)	9 (4%)	1 (0%)	30	54
1	D	255/327 (78%)	240 (94%)	14 (6%)	1 (0%)	30	54
All	All	1030/1308 (79%)	975 (95%)	46 (4%)	9 (1%)	14	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	728	SER
1	A	729	PRO
1	B	728	SER
1	B	729	PRO
1	B	784	ASN
1	A	812	ARG
1	A	782	LYS
1	C	782	LYS
1	D	782	LYS

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	233/251 (93%)	194 (83%)	39 (17%)	2	6
1	B	232/251 (92%)	192 (83%)	40 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	228/251 (91%)	189 (83%)	39 (17%)	2	6
1	D	228/251 (91%)	185 (81%)	43 (19%)	1	4
All	All	921/1004 (92%)	760 (82%)	161 (18%)	2	5

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	679	LEU
1	A	687	GLU
1	A	689	LYS
1	A	690	LYS
1	A	691	ILE
1	A	704	LYS
1	A	710	GLU
1	A	712	GLU
1	A	715	LYS
1	A	727	THR
1	A	730	LYS
1	A	736	LEU
1	A	738	GLU
1	A	742	MET
1	A	760	SER
1	A	778	VAL
1	A	779	ARG
1	A	782	LYS
1	A	784	ASN
1	A	787	SER
1	A	822	LYS
1	A	825	GLN
1	A	834	LEU
1	A	851	LYS
1	A	852	VAL
1	A	865	ARG
1	A	870	GLN
1	A	901	SER
1	A	902	ILE
1	A	903	LEU
1	A	907	GLU
1	A	908	ARG
1	A	914	ILE
1	A	917	ILE

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Mol	Chain	Res	Type
1	A	918	ASP
1	A	921	MET
1	A	925	LYS
1	A	936	LYS
1	A	952	GLN
1	B	679	LEU
1	B	689	LYS
1	B	704	LYS
1	B	710	GLU
1	B	712	GLU
1	B	724	ARG
1	B	727	THR
1	B	730	LYS
1	B	736	LEU
1	B	738	GLU
1	B	756	ILE
1	B	760	SER
1	B	778	VAL
1	B	779	ARG
1	B	782	LYS
1	B	787	SER
1	B	812	ARG
1	B	822	LYS
1	B	825	GLN
1	B	829	ILE
1	B	831	ASP
1	B	851	LYS
1	B	852	VAL
1	B	865	ARG
1	B	870	GLN
1	B	889	LYS
1	B	900	SER
1	B	901	SER
1	B	902	ILE
1	B	903	LEU
1	B	914	ILE
1	B	917	ILE
1	B	918	ASP
1	B	921	MET
1	B	925	LYS
1	B	928	MET
1	B	936	LYS

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Mol	Chain	Res	Type
1	B	938	ARG
1	B	946	LYS
1	B	953	ARG
1	C	680	LEU
1	C	681	ARG
1	C	687	GLU
1	C	689	LYS
1	C	704	LYS
1	C	710	GLU
1	C	712	GLU
1	C	715	LYS
1	C	724	ARG
1	C	736	LEU
1	C	738	GLU
1	C	742	MET
1	C	756	ILE
1	C	760	SER
1	C	779	ARG
1	C	782	LYS
1	C	784	ASN
1	C	812	ARG
1	C	822	LYS
1	C	834	LEU
1	C	852	VAL
1	C	865	ARG
1	C	870	GLN
1	C	889	LYS
1	C	899	ILE
1	C	901	SER
1	C	902	ILE
1	C	903	LEU
1	C	904	GLU
1	C	907	GLU
1	C	914	ILE
1	C	917	ILE
1	C	918	ASP
1	C	921	MET
1	C	925	LYS
1	C	936	LYS
1	C	938	ARG
1	C	953	ARG
1	C	958	GLN

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Mol	Chain	Res	Type
1	D	679	LEU
1	D	681	ARG
1	D	687	GLU
1	D	689	LYS
1	D	704	LYS
1	D	707	TRP
1	D	712	GLU
1	D	714	VAL
1	D	715	LYS
1	D	716	ILE
1	D	724	ARG
1	D	730	LYS
1	D	736	LEU
1	D	738	GLU
1	D	741	VAL
1	D	753	LEU
1	D	756	ILE
1	D	760	SER
1	D	779	ARG
1	D	782	LYS
1	D	784	ASN
1	D	812	ARG
1	D	834	LEU
1	D	851	LYS
1	D	852	VAL
1	D	861	SER
1	D	865	ARG
1	D	870	GLN
1	D	889	LYS
1	D	901	SER
1	D	902	ILE
1	D	903	LEU
1	D	904	GLU
1	D	907	GLU
1	D	914	ILE
1	D	917	ILE
1	D	918	ASP
1	D	921	MET
1	D	925	LYS
1	D	928	MET
1	D	936	LYS
1	D	938	ARG

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Mol	Chain	Res	Type
1	D	953	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	784	ASN
1	A	802	ASN
1	B	749	HIS
1	B	781	HIS
1	C	749	HIS
1	C	781	HIS
1	C	784	ASN
1	C	802	ASN
1	D	749	HIS
1	D	781	HIS
1	D	784	ASN
1	D	802	ASN
1	D	869	HIS

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 ⓘ

4 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	ITI	B	1	-	49,49,49	1.43	3 (6%)	65,68,68	1.94	18 (27%)
2	ITI	A	1	-	49,49,49	1.16	4 (8%)	65,68,68	1.91	15 (23%)
2	ITI	D	1	-	49,49,49	0.94	4 (8%)	65,68,68	1.32	6 (9%)
2	ITI	C	1	-	49,49,49	1.10	4 (8%)	65,68,68	1.73	16 (24%)

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	ITI	B	1	-	-	7/24/32/32	0/7/7/7
2	ITI	A	1	-	-	6/24/32/32	0/7/7/7
2	ITI	D	1	-	-	6/24/32/32	0/7/7/7
2	ITI	C	1	-	-	8/24/32/32	0/7/7/7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ITI	C21-C23	-5.98	1.42	1.48
2	B	1	ITI	C16-C22	-4.72	1.41	1.48
2	C	1	ITI	C21-C23	-3.80	1.44	1.48
2	A	1	ITI	C21-C23	-3.75	1.44	1.48
2	B	1	ITI	C23-N37	-3.67	1.35	1.39
2	D	1	ITI	C21-C23	-3.49	1.44	1.48
2	A	1	ITI	C23-N37	-3.22	1.36	1.39
2	C	1	ITI	C23-N37	-2.87	1.36	1.39
2	C	1	ITI	C24-N39	2.60	1.41	1.36
2	D	1	ITI	C23-N37	-2.37	1.36	1.39
2	D	1	ITI	C16-C22	-2.36	1.44	1.48
2	A	1	ITI	C16-C22	-2.31	1.44	1.48
2	A	1	ITI	C30-N38	-2.24	1.42	1.46
2	C	1	ITI	C16-C22	-2.17	1.44	1.48
2	D	1	ITI	C24-N39	2.04	1.40	1.36

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ITI	C16-C22-C23	-6.06	122.87	130.15
2	B	1	ITI	C30-N38-C29	5.89	124.81	111.57
2	B	1	ITI	C16-C22-C23	-5.83	123.15	130.15
2	D	1	ITI	C30-N38-C29	5.11	123.06	111.57
2	C	1	ITI	C20-N40-C28	-4.87	118.90	127.52
2	B	1	ITI	C15-C13-C21	-4.61	114.17	117.02
2	A	1	ITI	C15-N34-C24	4.36	119.06	115.42
2	A	1	ITI	C32-C30-N38	-4.31	101.77	109.93
2	A	1	ITI	C30-N38-C29	4.27	121.18	111.57
2	B	1	ITI	C23-C22-N36	4.21	114.14	110.09
2	A	1	ITI	C16-C22-N36	4.21	125.75	119.53
2	A	1	ITI	C9-C18-N38	-4.17	115.60	121.39
2	C	1	ITI	C30-N38-C29	4.12	120.84	111.57
2	C	1	ITI	C15-N34-C24	3.63	118.45	115.42
2	B	1	ITI	C27-C26-N37	-3.60	108.65	112.19
2	B	1	ITI	C33-C28-N40	-3.48	108.21	114.73
2	C	1	ITI	C16-C22-C23	-3.38	126.09	130.15
2	C	1	ITI	N34-C24-N35	-3.32	123.21	126.42
2	C	1	ITI	S43-C25-N37	-3.30	107.90	110.55
2	A	1	ITI	C33-C28-N40	-3.27	108.61	114.73
2	B	1	ITI	C26-N37-C25	3.17	118.74	113.59
2	C	1	ITI	C26-N37-C25	3.13	118.67	113.59
2	C	1	ITI	C27-C26-N37	-3.04	109.20	112.19
2	C	1	ITI	C23-C21-N35	3.03	119.17	115.57
2	B	1	ITI	C8-C18-N38	-3.02	117.19	121.39
2	A	1	ITI	C27-C26-N37	-3.01	109.23	112.19
2	B	1	ITI	O41-C28-N40	2.89	128.83	123.64
2	A	1	ITI	O41-C28-N40	2.83	128.71	123.64
2	A	1	ITI	N34-C24-N35	-2.60	123.91	126.42
2	C	1	ITI	C8-C18-N38	-2.58	117.80	121.39
2	D	1	ITI	C23-C22-N36	2.58	112.58	110.09
2	B	1	ITI	N37-C25-N36	2.52	117.01	113.23
2	B	1	ITI	C15-N34-C24	2.51	117.52	115.42
2	A	1	ITI	C26-N37-C25	2.45	117.56	113.59
2	A	1	ITI	C13-C15-N34	-2.41	121.02	123.97
2	A	1	ITI	C33-C17-C7	-2.41	117.35	120.89
2	C	1	ITI	C32-C30-N38	-2.38	105.43	109.93
2	D	1	ITI	C15-C13-C21	-2.38	115.55	117.02
2	B	1	ITI	C5-C16-C14	2.37	121.99	119.25
2	C	1	ITI	C23-C22-N36	2.33	112.33	110.09
2	B	1	ITI	C25-N36-C22	-2.29	99.33	106.28
2	A	1	ITI	C20-N40-C28	-2.27	123.50	127.52
2	B	1	ITI	N34-C24-N35	-2.27	124.23	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	ITI	C26-N37-C23	-2.22	134.82	139.91
2	D	1	ITI	N34-C24-N35	-2.22	124.28	126.42
2	A	1	ITI	C12-C9-C18	-2.21	117.50	120.30
2	B	1	ITI	C13-C21-N35	2.21	125.49	122.92
2	D	1	ITI	C27-C26-N37	-2.20	110.03	112.19
2	C	1	ITI	C13-C21-C23	-2.17	117.58	121.26
2	C	1	ITI	C19-N39-C24	-2.17	123.54	129.38
2	C	1	ITI	C31-C29-N38	-2.14	105.87	109.93
2	B	1	ITI	C16-C22-N36	2.14	122.69	119.53
2	B	1	ITI	S43-C25-N37	-2.09	108.87	110.55
2	D	1	ITI	C4-C5-C16	-2.03	118.37	120.36
2	B	1	ITI	O42-C32-C30	-2.02	107.41	111.77

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	ITI	C33-C28-N40-C20
2	C	1	ITI	O41-C28-N40-C20
2	C	1	ITI	C6-C17-C33-C28
2	C	1	ITI	C7-C17-C33-C28
2	A	1	ITI	C14-C16-C22-C23
2	A	1	ITI	C14-C16-C22-N36
2	A	1	ITI	C6-C17-C33-C28
2	A	1	ITI	C7-C17-C33-C28
2	B	1	ITI	C6-C17-C33-C28
2	D	1	ITI	C7-C17-C33-C28
2	B	1	ITI	C7-C17-C33-C28
2	D	1	ITI	C6-C17-C33-C28
2	C	1	ITI	C14-C16-C22-N36
2	D	1	ITI	C5-C16-C22-C23
2	C	1	ITI	C5-C16-C22-N36
2	C	1	ITI	C5-C16-C22-C23
2	A	1	ITI	C5-C16-C22-C23
2	C	1	ITI	C14-C16-C22-C23
2	D	1	ITI	C5-C16-C22-N36
2	D	1	ITI	C14-C16-C22-C23
2	B	1	ITI	C5-C16-C22-C23
2	D	1	ITI	C14-C16-C22-N36
2	B	1	ITI	C5-C16-C22-N36
2	B	1	ITI	C14-C16-C22-C23
2	B	1	ITI	O41-C28-N40-C20

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Mol	Chain	Res	Type	Atoms
2	B	1	ITI	C14-C16-C22-N36
2	A	1	ITI	C5-C16-C22-N36

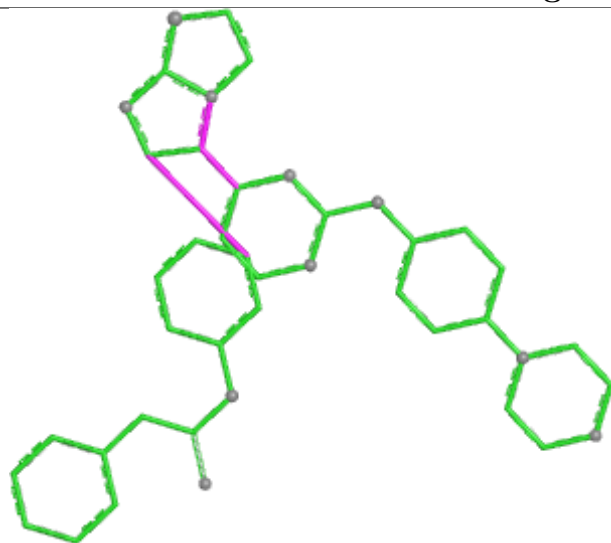
There are no ring outliers.

4 monomers are involved in 59 short contacts:

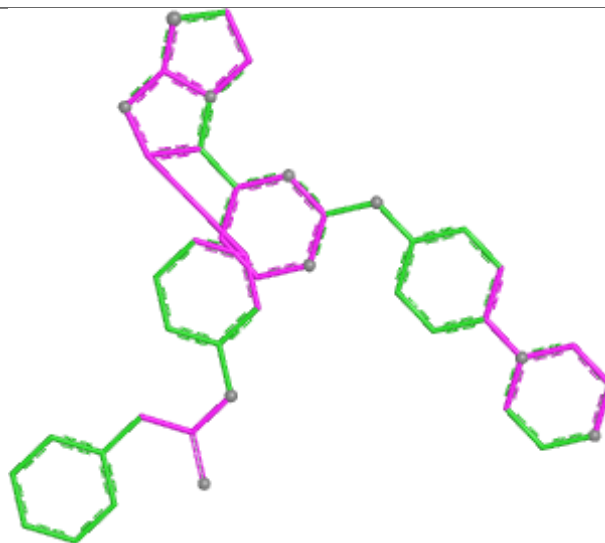
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	ITI	11	0
2	A	1	ITI	16	0
2	D	1	ITI	19	0
2	C	1	ITI	13	0

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.

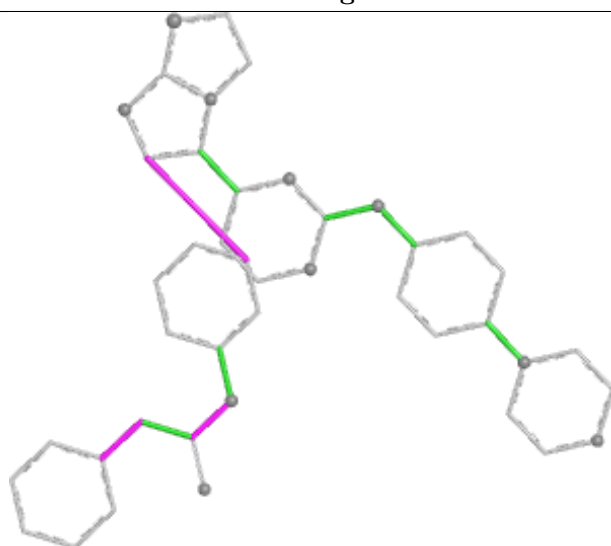
Ligand ITI B 1



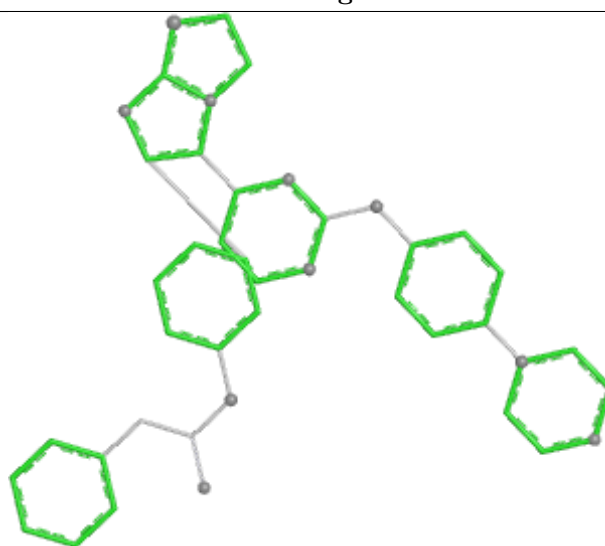
Bond lengths



Bond angles

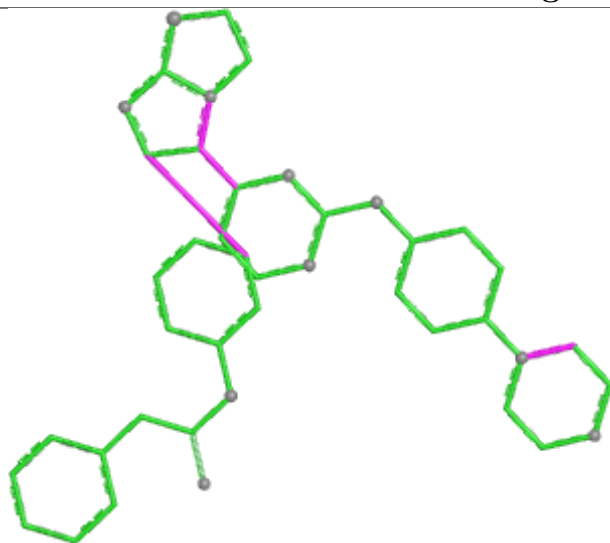


Torsions

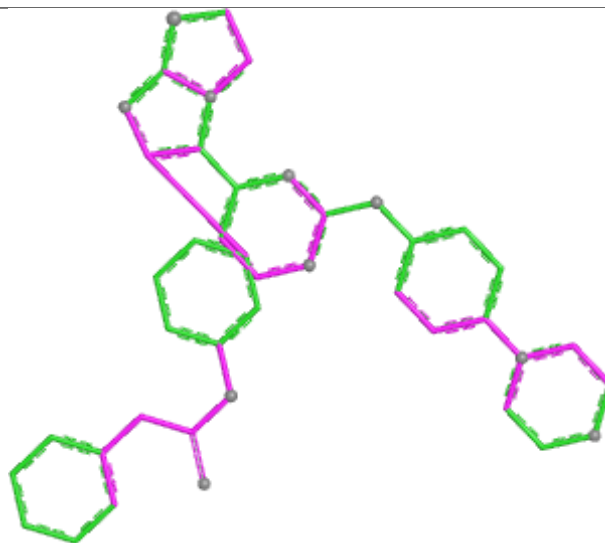


Rings

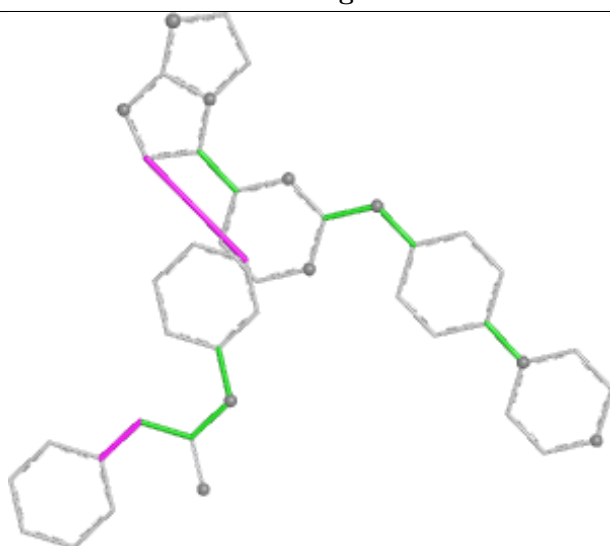
Ligand ITI A 1



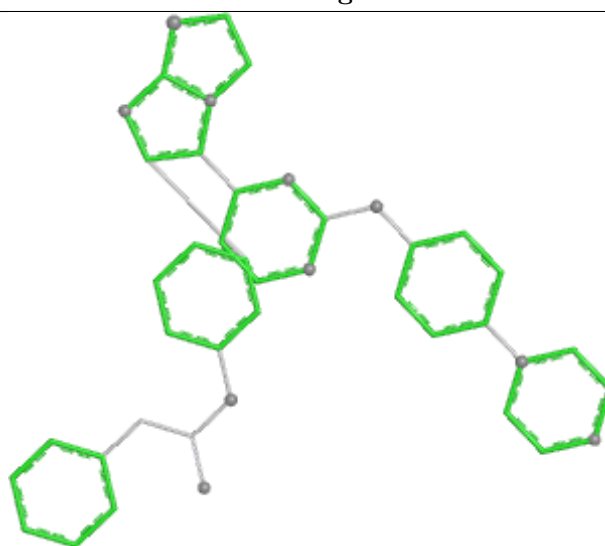
Bond lengths



Bond angles

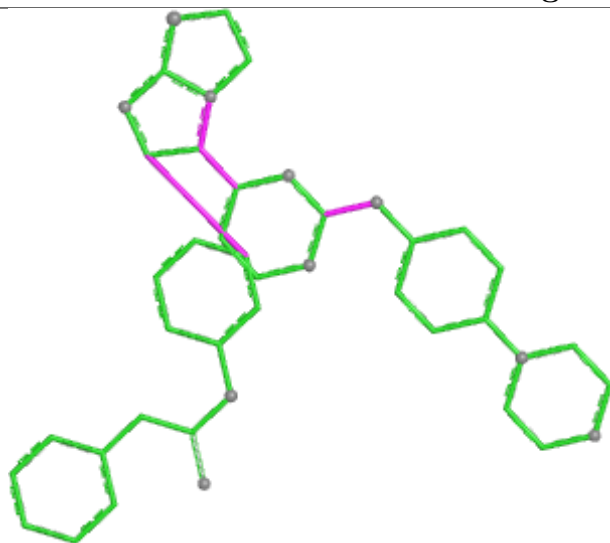


Torsions

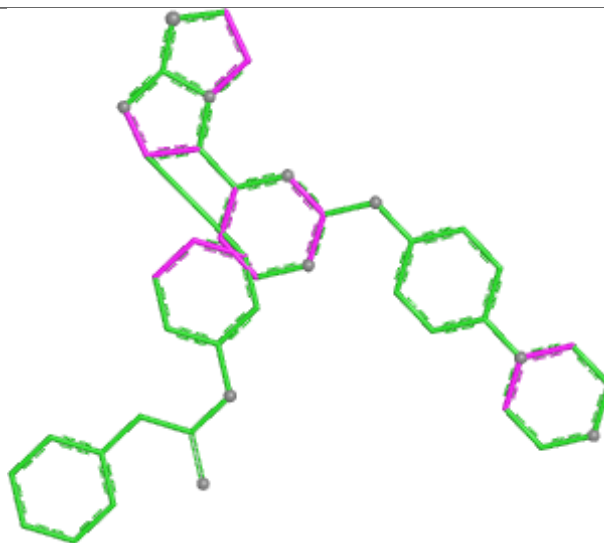


Rings

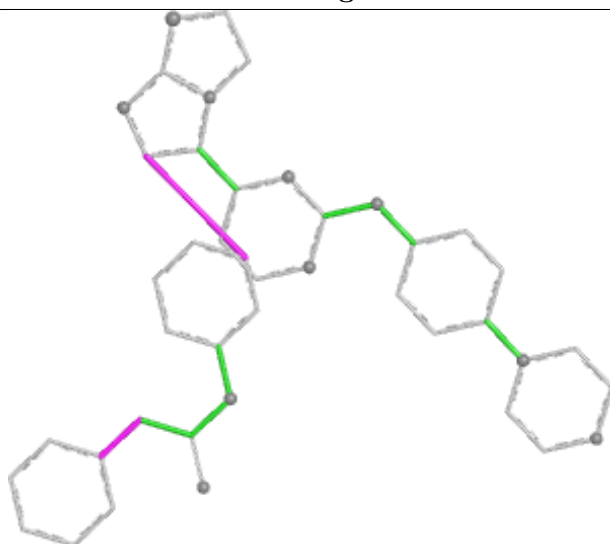
Ligand ITI D 1



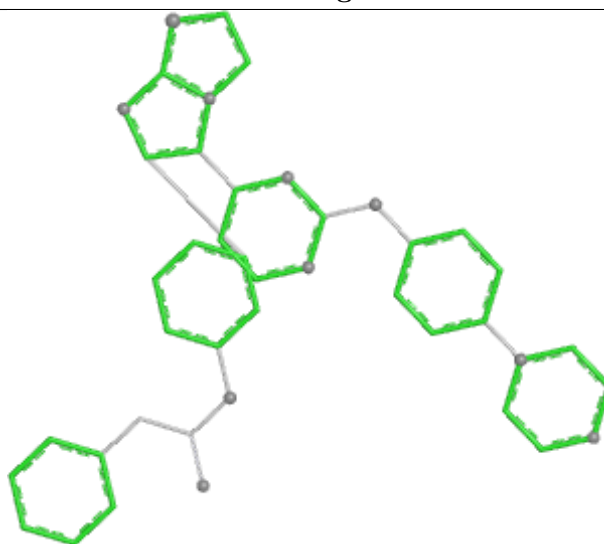
Bond lengths



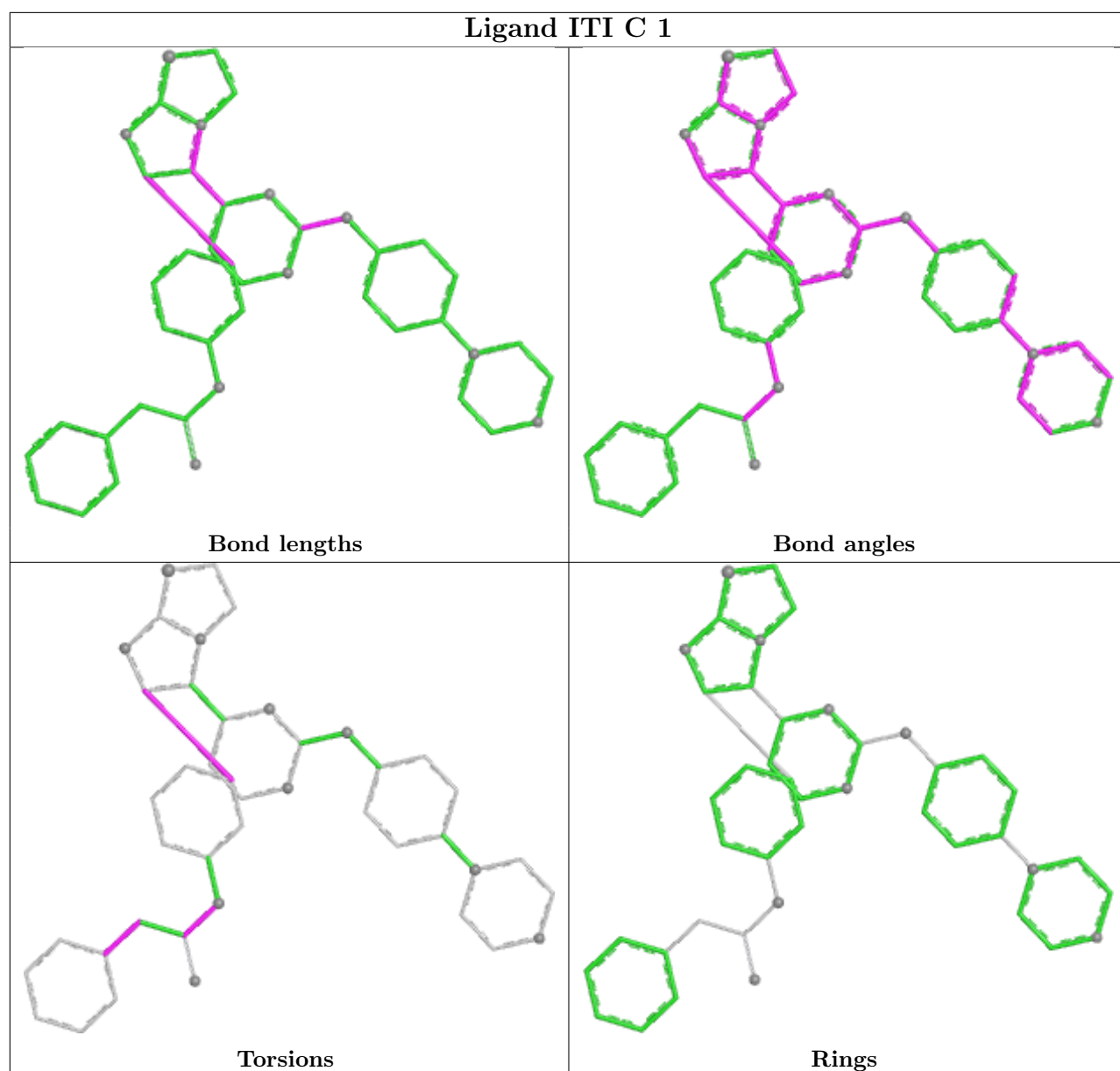
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/327 (81%)	0.14	10 (3%) 44 40	27, 47, 80, 117	0
1	B	265/327 (81%)	0.08	7 (2%) 57 54	27, 45, 79, 112	0
1	C	259/327 (79%)	0.42	9 (3%) 47 43	39, 60, 93, 130	0
1	D	261/327 (79%)	0.59	13 (4%) 34 30	41, 64, 97, 136	0
1	E	0/327	-	-	-	-
1	F	0/327	-	-	-	-
1	G	0/327	-	-	-	-
1	H	0/327	-	-	-	-
All	All	1050/2616 (40%)	0.30	39 (3%) 45 41	27, 56, 92, 136	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	PHE	4.8
1	C	959	GLY	3.8
1	D	957	ILE	3.5
1	A	959	GLY	3.5
1	A	729	PRO	3.3
1	C	731	ALA	3.2
1	D	698	ALA	3.1
1	B	959	GLY	3.1
1	D	699	PHE	3.1
1	C	724	ARG	3.0
1	C	699	PHE	2.8
1	D	731	ALA	2.8
1	D	789	TYR	2.7
1	C	725	GLU	2.7
1	D	696	SER	2.6
1	B	729	PRO	2.6
1	D	758	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	681	ARG	2.6
1	A	782	LYS	2.5
1	D	723	LEU	2.5
1	C	698	ALA	2.4
1	A	760	SER	2.4
1	D	891	TYR	2.3
1	B	786	GLY	2.3
1	D	854	ILE	2.3
1	A	892	ASP	2.3
1	C	733	LYS	2.2
1	B	824	PRO	2.2
1	D	680	LEU	2.2
1	B	728	SER	2.2
1	A	726	ALA	2.2
1	B	726	ALA	2.1
1	B	724	ARG	2.1
1	A	727	THR	2.1
1	C	761	THR	2.1
1	A	784	ASN	2.1
1	A	725	GLU	2.0
1	D	679	LEU	2.0
1	C	785	ILE	2.0

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.

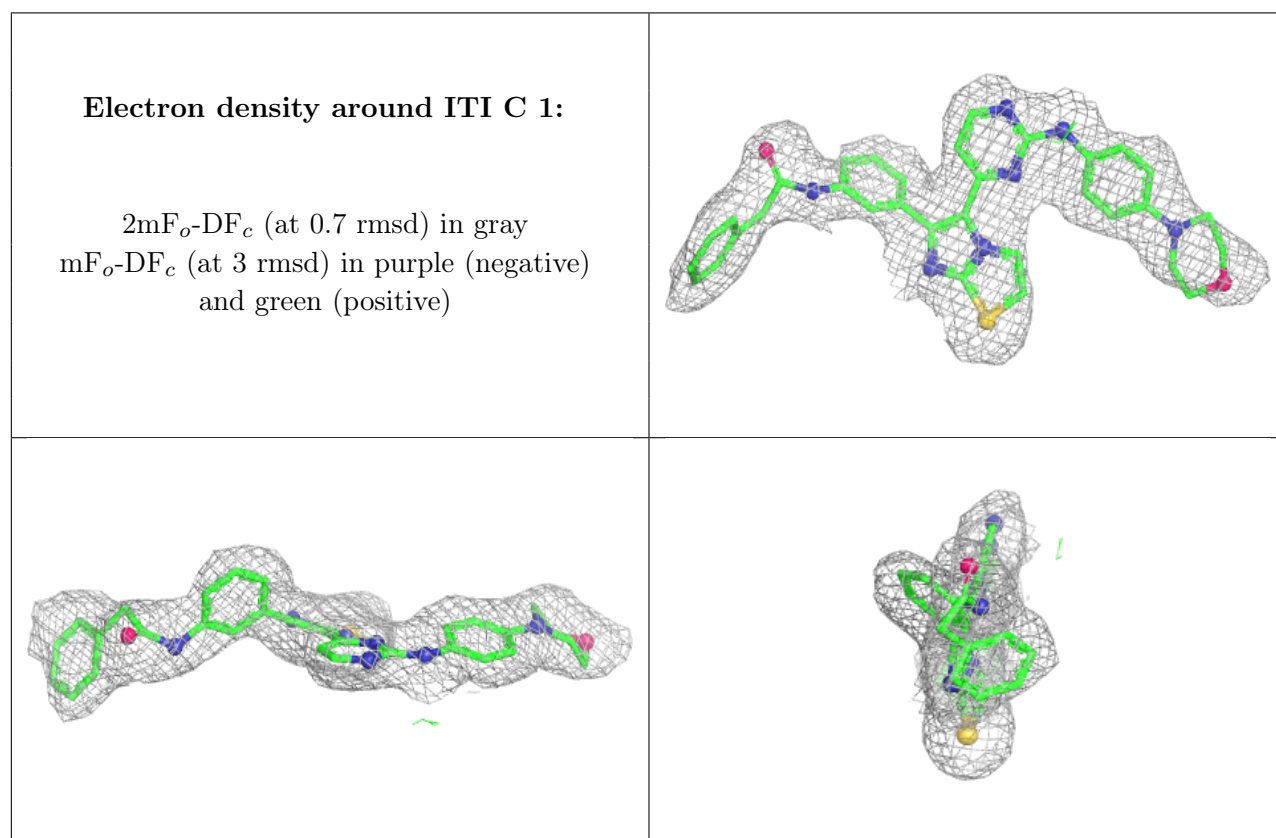
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ITI	C	1	43/43	0.94	0.14	23,56,210,300	0

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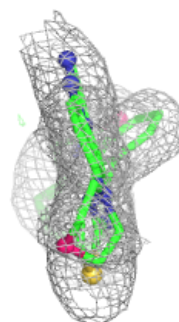
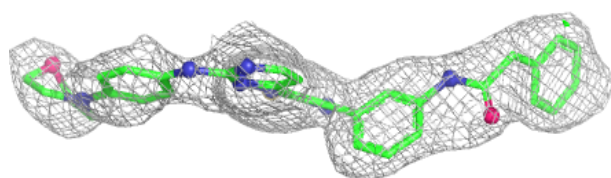
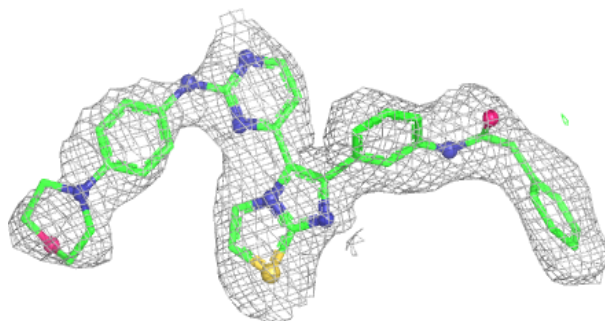
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ITI	D	1	43/43	0.94	0.12	14,57,195,300	0
2	ITI	A	1	43/43	0.97	0.07	11,36,81,106	0
2	ITI	B	1	43/43	0.98	0.07	6,33,79,236	0

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.

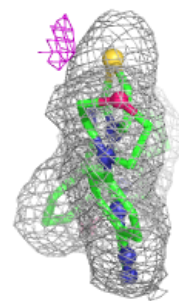
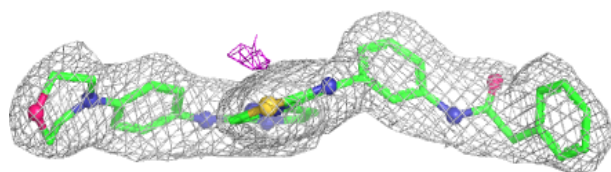
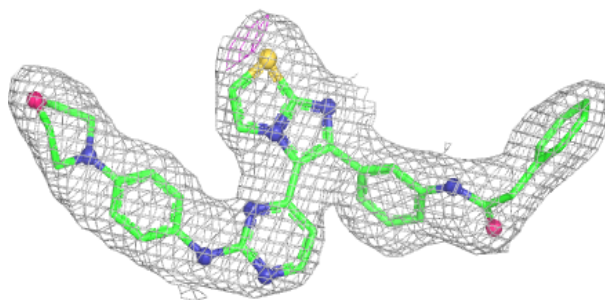


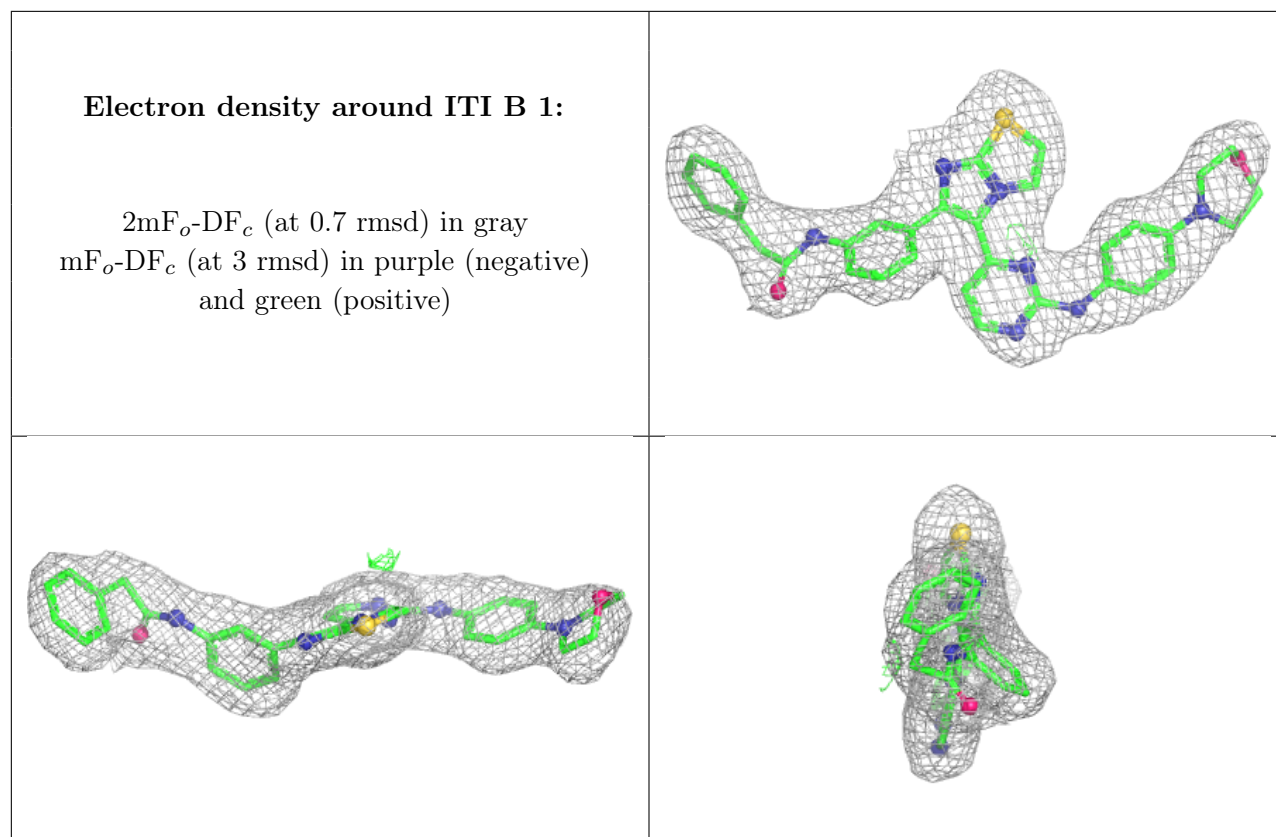
Electron density around ITI D 1:

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

**Electron density around ITI A 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.