



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 01:20 AM EDT

PDB ID : 3LZB  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

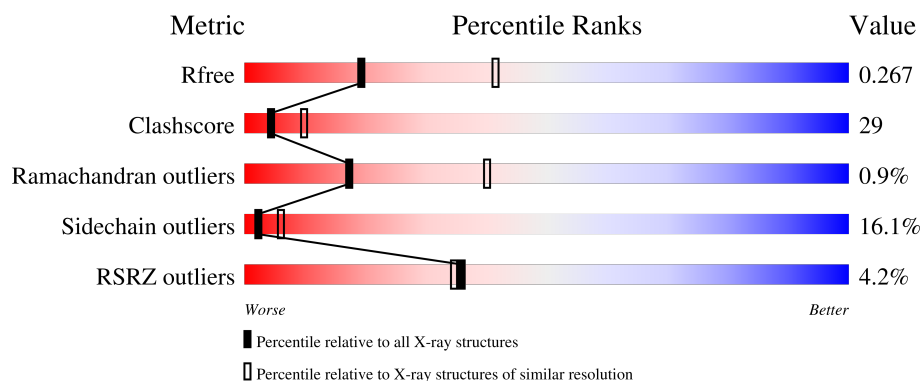
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>2%</div> <div> <div>46%</div> <div>28%</div> <div>7%</div> <div>19%</div> </div> </div>
1	B	327	<div> <div>%</div> <div> <div>46%</div> <div>28%</div> <div>6%</div> <div>19%</div> </div> </div>
1	C	327	<div> <div>5%</div> <div> <div>46%</div> <div>25%</div> <div>7%</div> <div>21%</div> </div> </div>
1	D	327	<div> <div>6%</div> <div> <div>43%</div> <div>28%</div> <div>9%</div> <div>20%</div> </div> </div>
1	E	327	<div> <div>..</div> <div>97%</div> </div>

*Continued on next page...*

*Continued from previous page...*

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.

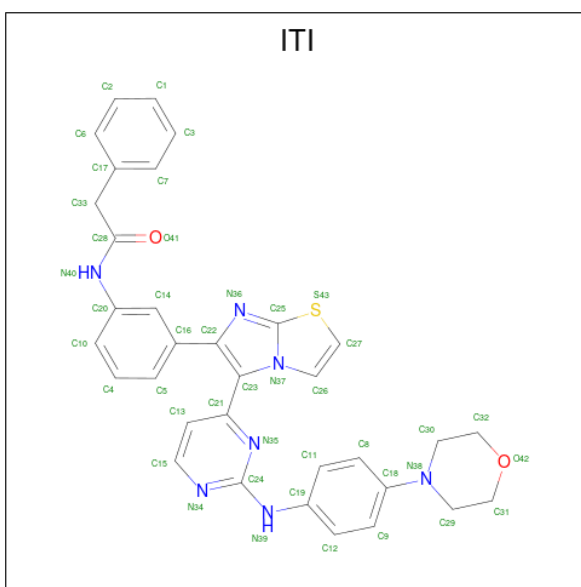
- Molecule 1 is a protein called Epidermal growth factor receptor.

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 (three-letter code: ITI) (formula: C<sub>33</sub>H<sub>29</sub>N<sub>7</sub>O<sub>2</sub>S).



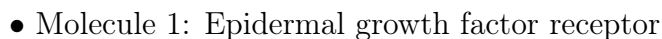
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			43	33	7	2	1		
2	B	1	Total	C	N	O	S	0	0
			43	33	7	2	1		
2	C	1	Total	C	N	O	S	0	0
			43	33	7	2	1		
2	D	1	Total	C	N	O	S	0	0
			43	33	7	2	1		

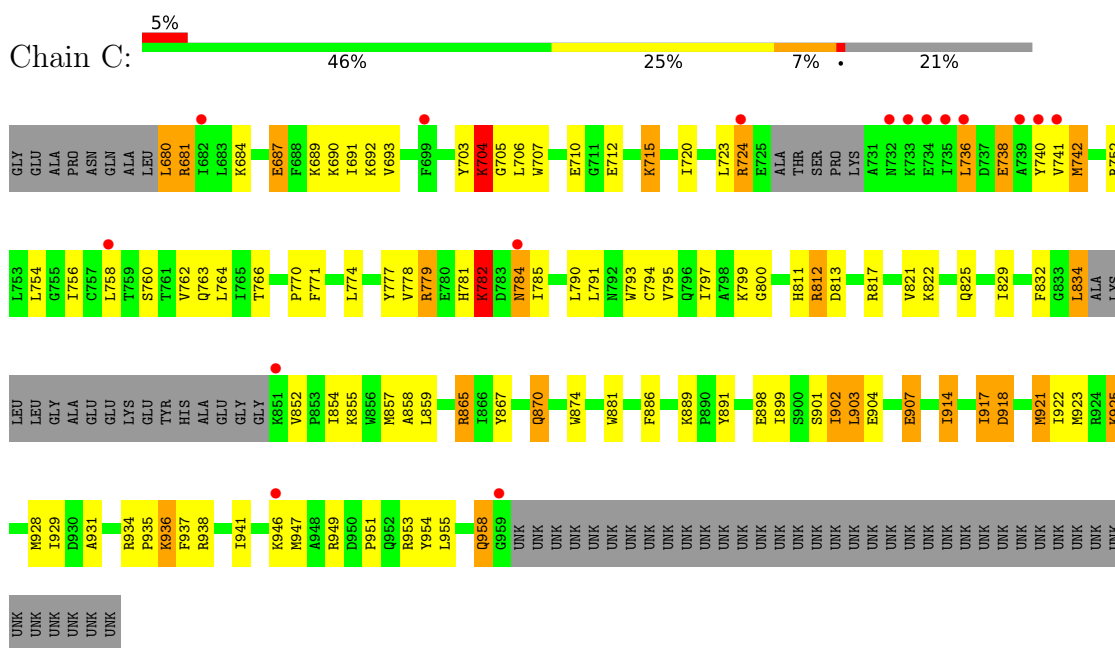
- Molecule 3 is water.

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		

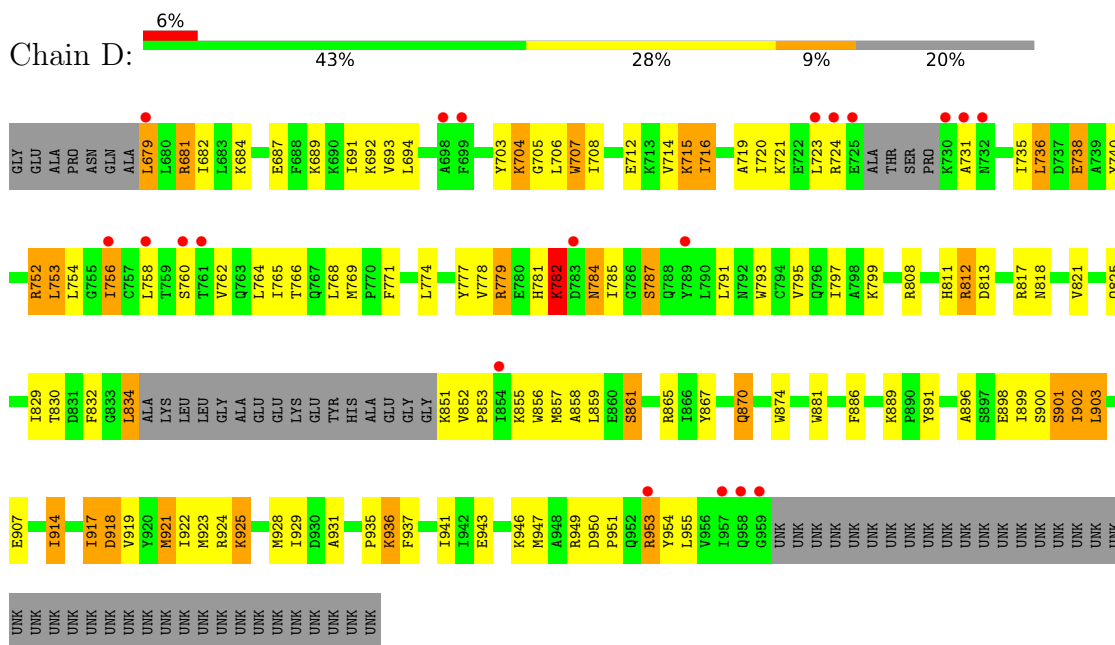


- Molecule 1: Epidermal growth factor receptor





- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor



VAL	PRO	PRO	ILE	LYS	TRP	MET	ALA	LEU	GLU	SER	SER	ILE	LEU	HIS	ARG	ILE	TYR	THR	HIS	GLN	SER	ASP	VAL	TRP	SER	TYR	GLY	VAL	THR	THR	TRP	GLU	LEU	GLU	MET	THR	THR	PHE	GLY	SER	LYS	PRO	TYR	ASP	GLY	ILE	PRO	ALA	SER	GLU	ILE	SER	LYS	GLU	ARG	GLU	LEU	PRO	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

[illegible]

- Molecule 1: Epidermal growth factor receptor

Chain F: .. 98%

GLY	GLU	ALA	PRO	ASN	GLN	ALA	LEU	LEU	ARG	ILE	LEU	LYS	GLU	THR	PHE	GLY	LYS	LYS	ILE	LYS	VAL	LEU	GLY	SER	GLY	ALA	PHE	GLY	THR	VAL	TYR	LYS	LYS	LEU	TRP	ILE	PRO	GLU	GLY	GLY	LYS	VAL	LYS	VAL	PRO	PRO	VAL	ALA	ALA	ILE	LYS	GLU	LEU	ARG	GLU	ALA	THR	SER	PRO	LYS	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN LYS GLU ILE ASP GLU ALA SER VAL ASP ASP ASN PRO HIS CYS ARG LEU LEU GLY ILE CYS LEU LEU ASP TYR ARG HIS LYS ASP ASN ILE GLY TYR GLN LEU

ASN	TRP	CYS	VAL	GLN	ILE	ALA	LYS	GLY	MET	ASN	TYR	LEU	GLU	ASP	ARG	ARG	LEU	ALA	ALA	ARG	ASN	VAL	VAL	VAL	LYS	THR	PRO	GLN	HIS	VAL	LYS	ILE	THR	ASP	PHE	GLY	LEU	ALA	LYS	LEU	LEU	GLY	ALA	GLU	GLU	LYS	GLU	TYR	HIS	ALA	GLU	GLY	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	PRO	PRO	ILE	LYS	TRP	MET	ALA	LEU	GLU	SER	SER	ILE	HIS	ARG	ILE	TYR	THR	HIS	GLN	SER	ASP	VAL	TRP	SER	TYR	GLY	VAL	THR	THR	TRP	LEU	LEU	NET	THR	THR	PHE	GLY	SER	SER	LYS	PRO	PRO	TYR	ASP	GLY	ILE	ILE	PRO	ALA	SER	SER	ILE	LEU	GLU	LYS	GLY	GLU	ARG	ARG	LEU	LEU	PRO	PRO	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible][illegible]

- Molecule 1: Epidermal growth factor receptor

Chain G:  98%

GLY	GLU	ALA	PRO	ASN	GLN	ALA	LEU	LEU	ARG	LEU	ILE	LYS	GLU	THR	GLU	PHE	LYS	LYS	ILE	LYS	VAL	LEU	GLY	SER	GLY	ALA	ALA	GLY	THR	VAL	TYR	LYS	GLY	LEU	TRP	ILE	PRO	GLU	GLY	LYS	VAL	ALA	ILE	LYS	GLU	LEU	ARG	GLU	ALA	THR	SER	PRO	LYS	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	LYS	GLU	ILE	LEU	ASP	GLU	ALA	ALA	VAL	MET	THR	SER	ASP	ASN	PRO	HIS	VAL	CYS	ARG	LEU	LEU	GLY	ILE	CYS	LEU	THR	THR	THR	VAL	GLN	LEU	ILE	ILE	THR	THR	LEU	LEU	MET	PRO	PRO	PHE	GLY	CYS	LEU	LEU	ASP	THR	VAL	ARG	GLU	HIS	LYS	ASP	ASN	ILE	GLY	SER	GLN	TYR	LEU	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN TRP CYS VAL GLN ILE ALA LYS GLY MET ASN TYR LEU GLU ASP ARG ARG LEU ALA HIS ASP ASP LEU ALA VAL VAL LYS THR PRO GLN GLN HIS VAL LYS ILE THR ASP ASP PHE GLY LEU LEU LYS GLY ALA GLU GLU LYS GLY TYR HIS ALA GLU GLY GLY CYS

VAL	PRO	LEU	LYS	TRP	MET	ALA	LEU	GLU	SER	ILE	HIS	ARG	ILE	TYR	THR	HIS	GLN	SER	ASP	VAL	TRP	SER	TYR	GLY	VAL	THR	TRP	GLU	LEU	MET	PHE	GLY	SER	LYS	PRO	TYR	THR	ASP	GLY	ILE	PRO	ALA	SER	GLU	LYS	LEU	LEU	PRO	VAL	THR	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

[illegible]

- Molecule 1: Epidermal growth factor receptor

Chain H:  97%

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.59Å 70.87Å 115.18Å 90.00° 109.36° 90.00°	Depositor
Resolution (Å)	44.17 – 2.70 44.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.17-2.70) 99.7 (44.16-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 91.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.70	0/2167	0.84	1/2935 (0.0%)
1	B	0.69	1/2163 (0.0%)	0.85	2/2930 (0.1%)
1	C	0.60	0/2123	0.75	1/2873 (0.0%)
1	D	0.55	0/2132	0.75	1/2886 (0.0%)
All	All	0.64	1/8585 (0.0%)	0.80	5/11624 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	750	VAL	CB-CG1	5.56	1.64	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	728	SER	C-N-CD	-14.71	88.23	120.60
1	A	728	SER	C-N-CD	-14.55	88.58	120.60
1	B	736	LEU	CA-CB-CG	5.62	128.21	115.30
1	C	704	LYS	N-CA-C	-5.17	97.03	111.00
1	D	704	LYS	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2120	0	2169	113	0
1	B	2116	0	2165	119	0
1	C	2078	0	2122	115	0
1	D	2087	0	2129	136	0
1	E	45	0	11	6	0
1	F	35	0	10	4	0
1	G	35	0	11	8	0
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	1	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	505	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 (505) 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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:947:MET:HE2	1:D:954:TYR:HB3	1.63	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:B:924:ARG:HH22	1:B:928:MET:HE1	1.48	0.78
1:D:834:LEU:HD21	2:D:1:ITI:H3	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: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:B:705:GLY:HA3	1:B:720:ILE:CD1	2.14	0.77
1:D:947:MET:HE3	1:D:954:TYR:CD2	2.19	0.77
1:A:715:LYS:H	1:A:715:LYS:HE2	1.48	0.76
1:A:812:ARG:HG3	1:A:812:ARG:HH11	1.51	0.75
1:B:924:ARG:NH2	1:B:928:MET:HE1	2.02	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:914:ILE:HG13	1:D:955:LEU:HD22	1.68	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: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: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: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:B:928:MET:HA	1:B:928:MET:CE	2.21	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
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
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:736:LEU:HD12	1:C:758:LEU:HD11	1.78	0.66
1:C:742:MET:CE	2:C:1:ITI:H2	2.26	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:A:881:TRP:CD1	1:A:923:MET:HE1	2.32	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:707:TRP:CD1	1:D:707:TRP:C	2.71	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: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:742:MET:HE1	2:C:1:ITI:H2	1.84	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
1:A:725:GLU:HG2	1:A:726:ALA:N	2.13	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
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:B:881:TRP:CD1	1:B:923:MET:HE1	2.39	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:881:TRP:HD1	1:A:923:MET:HE1	1.69	0.56
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
1:A:881:TRP:HB2	1:A:923:MET:HE3	1.87	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:C:881:TRP:CD1	1:C:923:MET:HE1	2.41	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: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
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:D:919:VAL:HG22	1:D:947:MET:CE	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:928:MET:HA	1:B:928:MET:HE2	1.90	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:D:881:TRP:CD1	1:D:923:MET:HE1	2.43	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: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:B:928:MET:HA	1:B:928:MET:HE3	1.91	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:947:MET:HE2	1:D:954:TYR:CB	2.38	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: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:679:LEU:N	1:D:679:LEU:HD12	2.28	0.48
1:C:917:ILE:HD12	1:C:921:MET:SD	2.53	0.48
1:D:707:TRP:HD1	1:D:707:TRP:C	2.11	0.48
1:D:832:PHE:CE2	2:D:1:ITI:H6	2.48	0.48
1:D:881:TRP:HB2	1:D:923:MET:HE3	1.96	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:742:MET:CE	2:C:1:ITI:C2	2.91	0.47
1:D:797:ILE:O	1:D:829:ILE:HD11	2.14	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
1:D:947:MET:CE	1:D:954:TYR:CD2	2.95	0.47
2:B:1:ITI:N35	2:B:1:ITI:H12	2.29	0.47
1:C:742:MET:HE2	2:C:1:ITI:H2	1.95	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:881:TRP:HB2	1:C:923:MET:HE3	1.97	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:881:TRP:HB2	1:B:923:MET:HE3	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: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: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
1:B:881:TRP:HD1	1:B:923:MET:CE	2.28	0.46
1:B:881:TRP:HD1	1:B:923:MET:HE1	1.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:881:TRP:CB	1:C:923:MET:HE1	2.46	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:881:TRP:HD1	1:C:923:MET:CE	2.29	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:D:881:TRP:CB	1:D:923:MET:HE1	2.47	0.45
1:D:881:TRP:HD1	1:D:923:MET:CE	2.30	0.45
1:B:911:GLN:HB2	1:B:920:TYR:CD2	2.51	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

*Continued on next page...*

*Continued from previous page...*

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: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: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
2:A:1:ITI:H30A	2:A:1:ITI:H9	1.52	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: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:919:VAL:CG2	1:D:947:MET:CE	2.96	0.43
1:A:782:LYS:HZ1	1:B:946:LYS:HD2	1.82	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: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
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:C:936:LYS:HE2	1:C:936:LYS:HB3	1.61	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:881:TRP:CB	1:B:923:MET:HE1	2.49	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:C:881:TRP:HD1	1:C:923:MET:HE1	1.83	0.42
1:C:881:TRP:HA	1:C:923:MET:HE1	2.01	0.42
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:881:TRP:HD1	1:A:923:MET:CE	2.31	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:921:MET:HG3	1:C:898:GLU:CD	2.40	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:881:TRP:CD1	1:C:923:MET:CE	3.02	0.42
1:B:881:TRP:CD1	1:B:923:MET:CE	3.02	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:742:MET:HE2	1:B:832:PHE:O	2.19	0.41
1:B:776:ASP:CB	3:B:99:HOH:O	2.67	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:SER:OG	1:B:951:PRO:CB	2.68	0.41
1:D:715:LYS:C	1:D:716:ILE:HD13	2.40	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
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: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:881:TRP:HA	1:D:923:MET:HE1	2.02	0.41
1:A:807:ARG:O	1:A:808:ARG:HB2	2.21	0.41
1:D:899:ILE:HG22	1:D:903:LEU:CD2	2.51	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: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:D:881:TRP:CD1	1:D:923:MET:CE	3.03	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: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
1:A:881:TRP:CD1	1:A:923:MET:CE	3.03	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%)	10	26
1	B	261/327 (80%)	247 (95%)	11 (4%)	3 (1%)	14	34
1	C	253/327 (77%)	243 (96%)	9 (4%)	1 (0%)	34	60
1	D	255/327 (78%)	240 (94%)	14 (6%)	1 (0%)	34	60
All	All	1030/1308 (79%)	975 (95%)	46 (4%)	9 (1%)	17	40

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%)	195 (84%)	38 (16%)	2	6
1	B	232/251 (92%)	199 (86%)	33 (14%)	3	8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	228/251 (91%)	191 (84%)	37 (16%)	2	6
1	D	228/251 (91%)	188 (82%)	40 (18%)	2	4
All	All	921/1004 (92%)	773 (84%)	148 (16%)	2	6

All (148) 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	752	ARG
1	A	760	SER
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	903	LEU
1	A	907	GLU
1	A	908	ARG
1	A	914	ILE
1	A	917	ILE
1	A	918	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	921	MET
1	A	925	LYS
1	A	936	LYS
1	A	953	ARG
1	B	679	LEU
1	B	681	ARG
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	736	LEU
1	B	738	GLU
1	B	752	ARG
1	B	760	SER
1	B	779	ARG
1	B	782	LYS
1	B	787	SER
1	B	812	ARG
1	B	825	GLN
1	B	851	LYS
1	B	865	ARG
1	B	870	GLN
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	752	ARG
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	825	GLN
1	C	834	LEU
1	C	865	ARG
1	C	870	GLN
1	C	889	LYS
1	C	901	SER
1	C	902	ILE
1	C	903	LEU
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
1	D	679	LEU
1	D	681	ARG
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	736	LEU
1	D	738	GLU
1	D	752	ARG
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	787	SER
1	D	812	ARG
1	D	825	GLN
1	D	834	LEU
1	D	851	LYS
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	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	953	ARG

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	784	ASN
1	D	802	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides 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	A	1	-	45,49,49	1.15	4 (8%)	53,68,68	1.70	13 (24%)
2	ITI	D	1	-	45,49,49	0.98	4 (8%)	53,68,68	1.23	3 (5%)
2	ITI	C	1	-	45,49,49	1.07	3 (6%)	53,68,68	1.57	8 (15%)
2	ITI	B	1	-	45,49,49	1.46	4 (8%)	53,68,68	1.63	10 (18%)

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	A	1	-	-	4/21/32/32	0/7/7/7
2	ITI	D	1	-	-	4/21/32/32	0/7/7/7
2	ITI	C	1	-	-	6/21/32/32	0/7/7/7
2	ITI	B	1	-	-	5/21/32/32	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	C16-C22	-6.99	1.41	1.49
2	B	1	ITI	C23-C21	-4.13	1.42	1.49
2	D	1	ITI	C16-C22	-3.91	1.44	1.49
2	A	1	ITI	C16-C22	-3.85	1.44	1.49
2	C	1	ITI	C16-C22	-3.66	1.44	1.49
2	C	1	ITI	C23-C21	-2.84	1.44	1.49
2	A	1	ITI	C23-C21	-2.81	1.44	1.49
2	C	1	ITI	C24-N39	2.67	1.41	1.36
2	D	1	ITI	C23-C21	-2.66	1.44	1.49
2	A	1	ITI	C30-N38	-2.43	1.42	1.46
2	B	1	ITI	C23-C22	-2.41	1.38	1.43
2	A	1	ITI	C23-C22	-2.22	1.38	1.43
2	D	1	ITI	C24-N39	2.09	1.40	1.36
2	B	1	ITI	C24-N39	2.02	1.40	1.36
2	D	1	ITI	C23-C22	-2.00	1.39	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ITI	C30-N38-C29	6.02	124.81	111.52
2	D	1	ITI	C30-N38-C29	5.23	123.06	111.52
2	C	1	ITI	C20-N40-C28	-4.91	118.90	127.50
2	A	1	ITI	C32-C30-N38	-4.47	101.77	110.02
2	A	1	ITI	C30-N38-C29	4.38	121.18	111.52
2	C	1	ITI	C30-N38-C29	4.22	120.84	111.52
2	A	1	ITI	C9-C18-N38	-4.19	115.60	121.38
2	A	1	ITI	C15-N34-C24	4.07	119.06	115.45
2	C	1	ITI	N34-C24-N35	-3.52	123.21	126.55
2	C	1	ITI	C15-N34-C24	3.38	118.45	115.45
2	B	1	ITI	C15-C13-C21	-3.23	114.17	117.22
2	B	1	ITI	C33-C28-N40	-3.17	108.21	114.77
2	B	1	ITI	C8-C18-N38	-3.04	117.19	121.38
2	A	1	ITI	C33-C28-N40	-2.98	108.61	114.77
2	B	1	ITI	O41-C28-N40	2.85	128.83	123.63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ITI	N34-C24-N35	-2.79	123.91	126.55
2	A	1	ITI	O41-C28-N40	2.79	128.71	123.63
2	B	1	ITI	C13-C21-N35	2.72	125.49	121.97
2	B	1	ITI	C5-C16-C14	2.71	121.99	118.16
2	C	1	ITI	C8-C18-N38	-2.59	117.80	121.38
2	C	1	ITI	C32-C30-N38	-2.49	105.43	110.02
2	A	1	ITI	C33-C17-C7	-2.47	117.35	120.89
2	B	1	ITI	N34-C24-N35	-2.45	124.23	126.55
2	D	1	ITI	N34-C24-N35	-2.40	124.28	126.55
2	A	1	ITI	C13-C15-N34	-2.37	121.02	123.96
2	B	1	ITI	C15-N34-C24	2.33	117.52	115.45
2	A	1	ITI	C20-N40-C28	-2.29	123.50	127.50
2	B	1	ITI	C22-N36-C25	-2.27	99.33	103.71
2	C	1	ITI	C31-C29-N38	-2.25	105.87	110.02
2	A	1	ITI	C12-C9-C18	-2.14	117.50	120.32
2	A	1	ITI	C13-C21-N35	2.13	124.73	121.97
2	D	1	ITI	C5-C16-C14	2.12	121.16	118.16
2	C	1	ITI	C23-C21-N35	2.08	119.17	115.62
2	A	1	ITI	C31-C29-N38	-2.06	106.23	110.02

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1	ITI	O41-C28-N40-C20

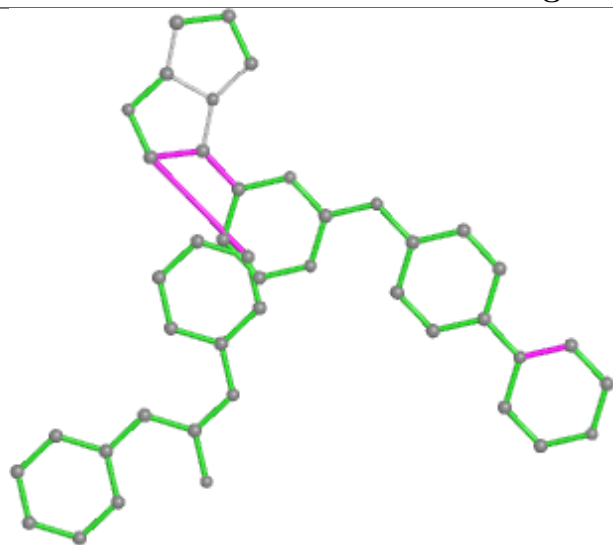
There are no ring outliers.

4 monomers are involved in 59 short contacts:

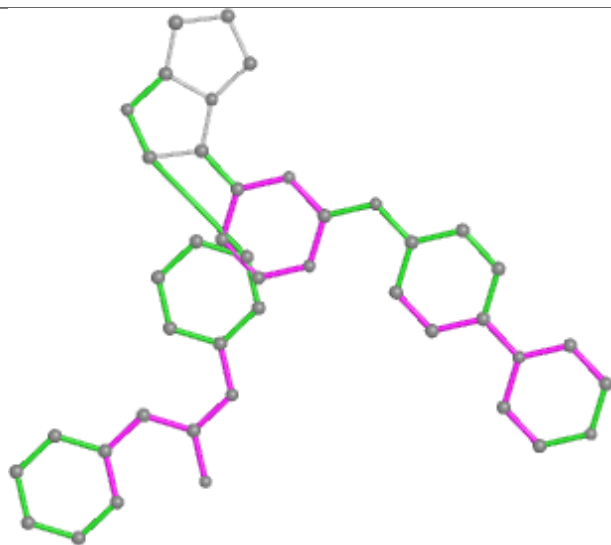
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ITI	16	0
2	D	1	ITI	19	0
2	C	1	ITI	13	0
2	B	1	ITI	11	0

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.

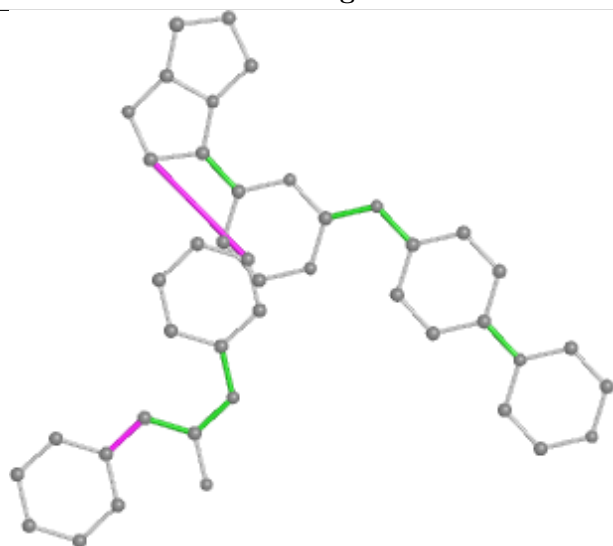
## Ligand ITI A 1



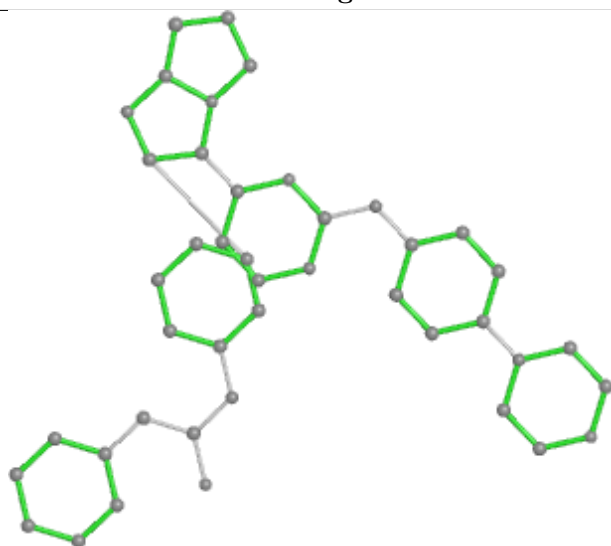
Bond lengths



Bond angles

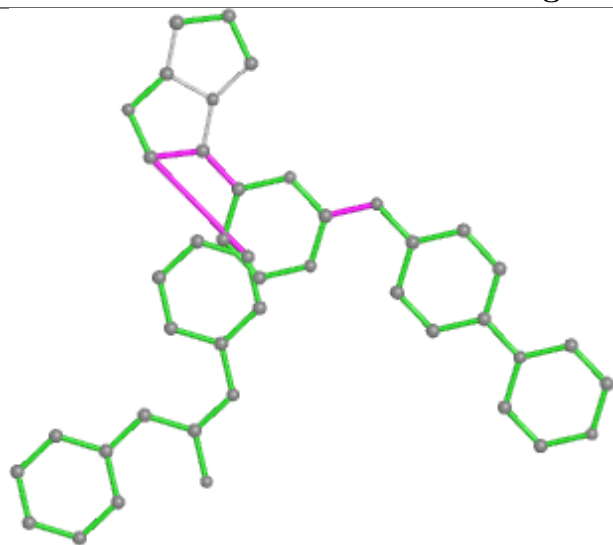


Torsions

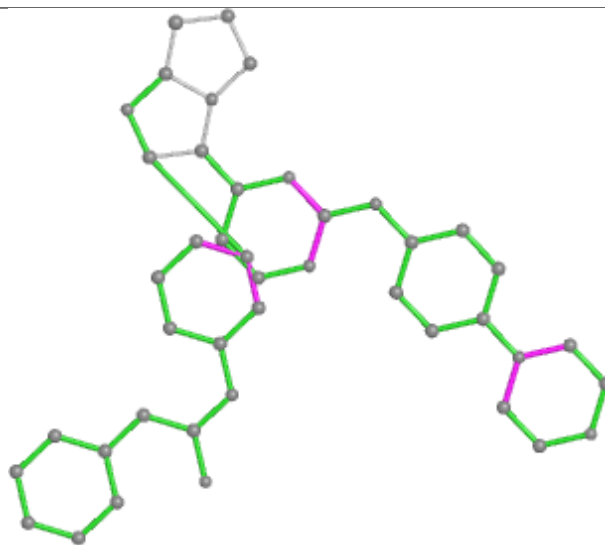


Rings

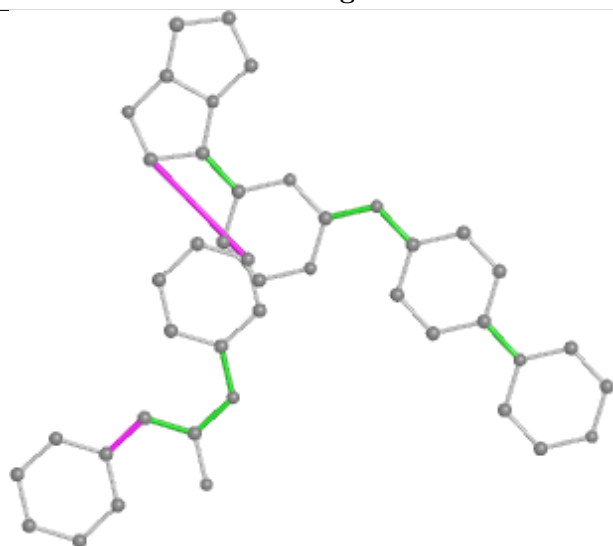
## Ligand ITI D 1



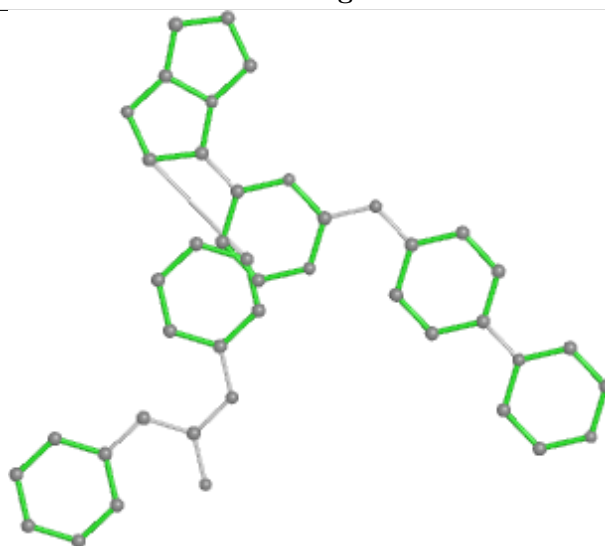
Bond lengths



Bond angles

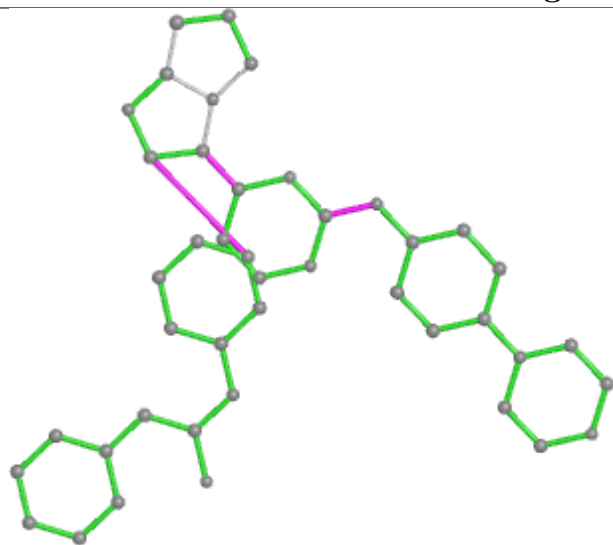


Torsions

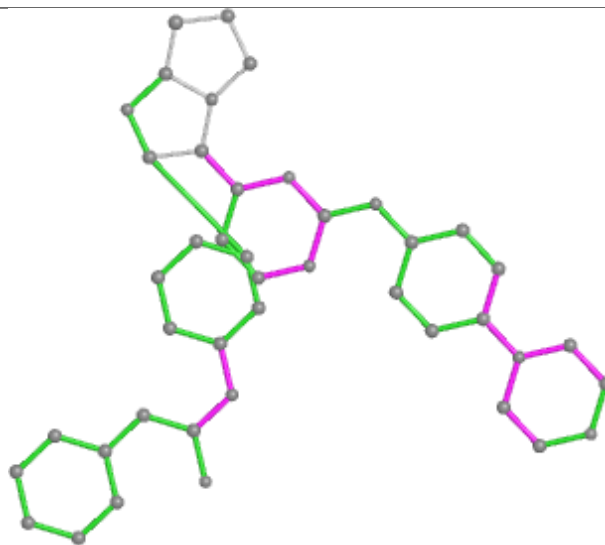


Rings

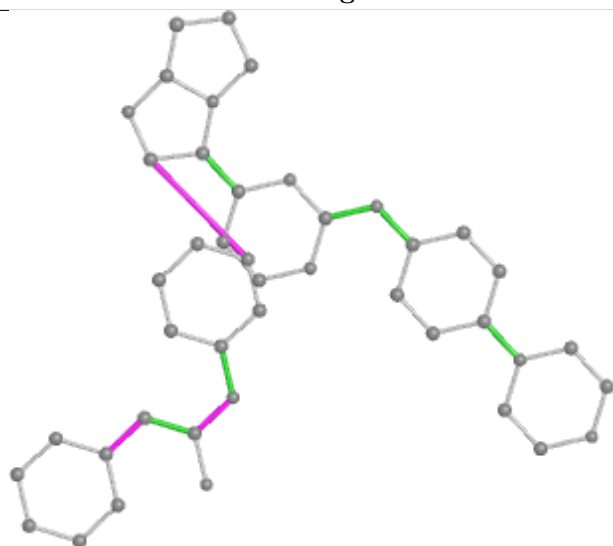
## Ligand ITI C 1



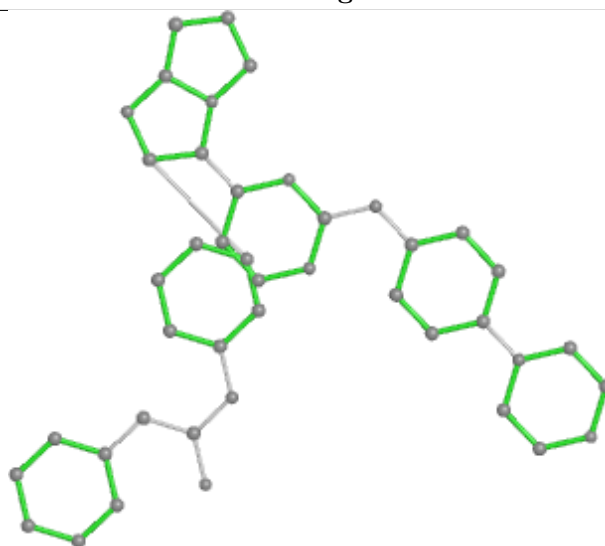
Bond lengths



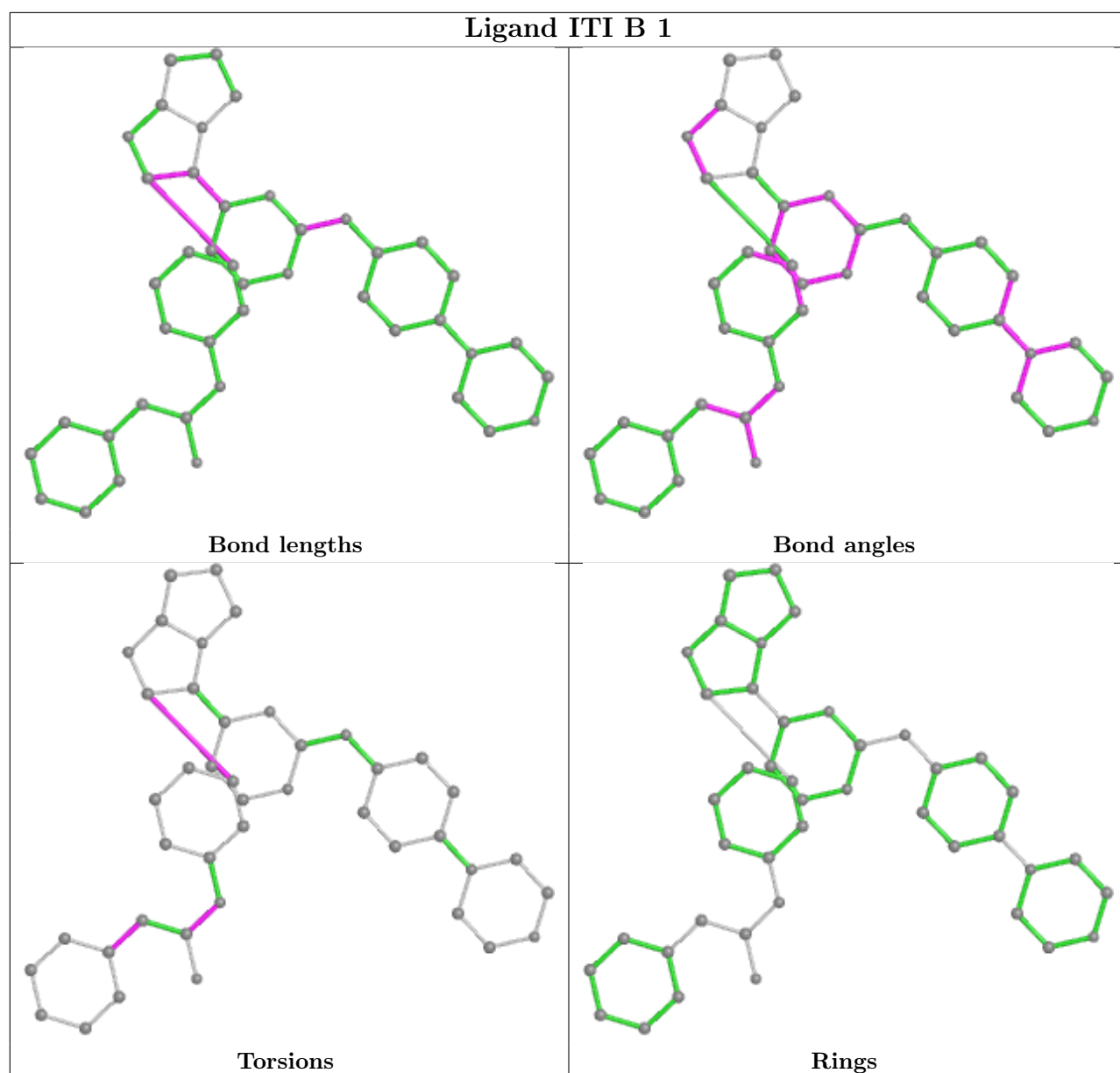
Bond angles



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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	265/327 (81%)	-0.03	6 (2%) 60 62	27, 47, 80, 117	0
1	B	265/327 (81%)	-0.11	2 (0%) 86 87	27, 45, 79, 112	0
1	C	259/327 (79%)	0.23	16 (6%) 20 19	39, 60, 93, 130	0
1	D	261/327 (79%)	0.36	20 (7%) 13 11	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%)	0.11	44 (4%) 36 35	27, 56, 92, 136	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	728	SER	6.3
1	B	727	THR	5.7
1	C	735	ILE	5.6
1	A	699	PHE	5.5
1	A	726	ALA	5.4
1	A	760	SER	5.4
1	D	957	ILE	5.0
1	D	730	LYS	4.7
1	D	698	ALA	4.4
1	D	758	LEU	4.0
1	D	731	ALA	4.0
1	D	699	PHE	3.9
1	C	758	LEU	3.9
1	A	725	GLU	3.9
1	C	959	GLY	3.8
1	C	736	LEU	3.6
1	C	734	GLU	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	784	ASN	3.4
1	D	760	SER	3.4
1	D	732	ASN	3.3
1	C	733	LYS	3.2
1	D	679	LEU	3.2
1	C	740	TYR	3.1
1	D	723	LEU	3.1
1	D	725	GLU	2.9
1	D	854	ILE	2.8
1	D	789	TYR	2.8
1	D	724	ARG	2.7
1	D	958	GLN	2.7
1	D	761	THR	2.7
1	C	741	VAL	2.6
1	C	724	ARG	2.5
1	C	699	PHE	2.5
1	D	959	GLY	2.4
1	C	946	LYS	2.4
1	D	756	ILE	2.4
1	C	739	ALA	2.3
1	C	732	ASN	2.3
1	A	727	THR	2.2
1	C	851	LYS	2.1
1	A	735	ILE	2.1
1	D	783	ASP	2.1
1	C	682	ILE	2.1
1	D	953	ARG	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

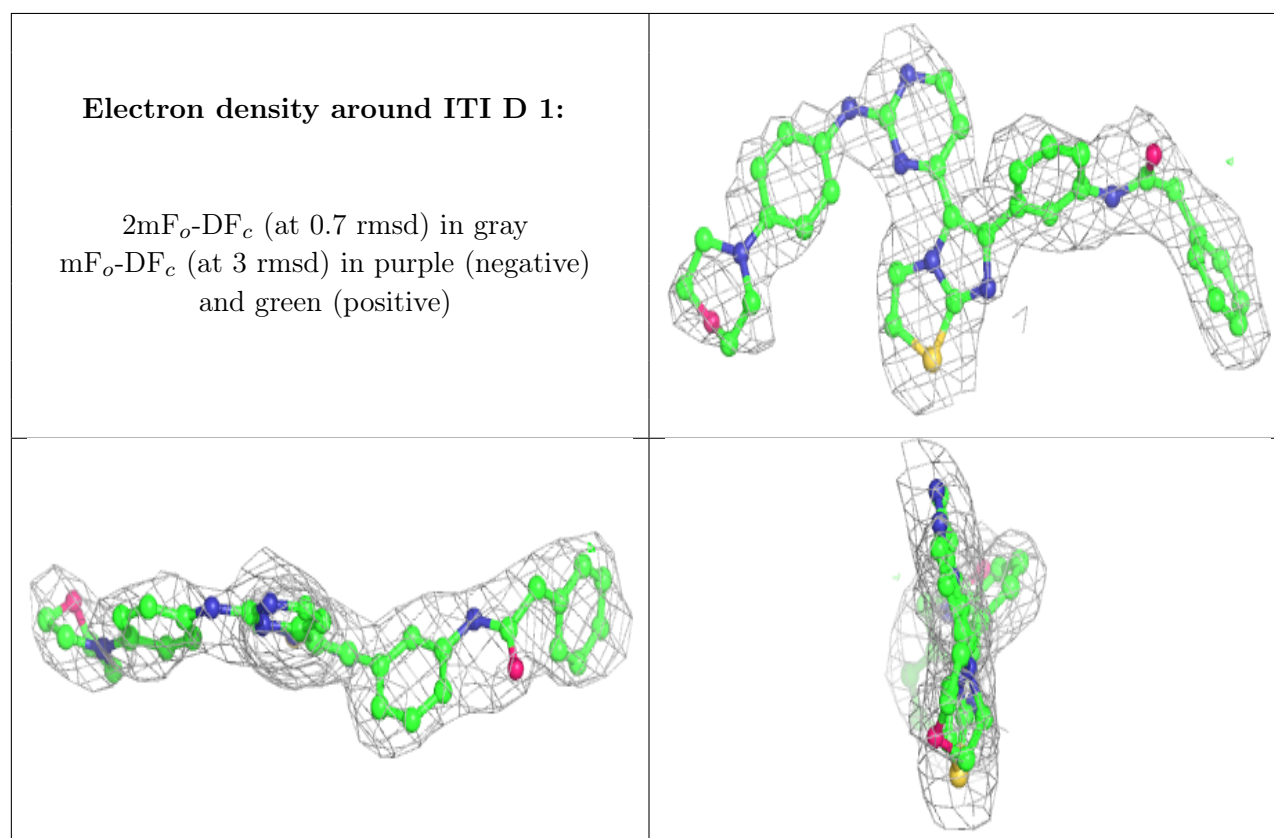
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

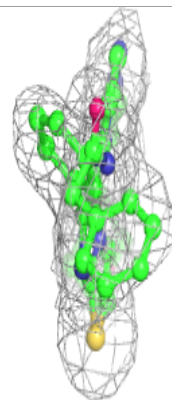
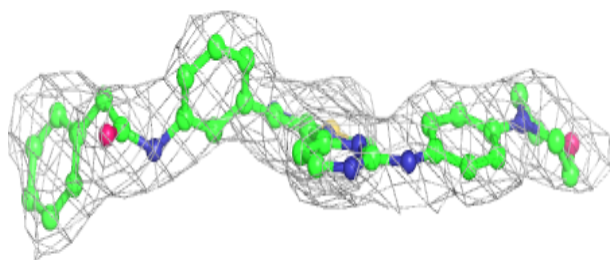
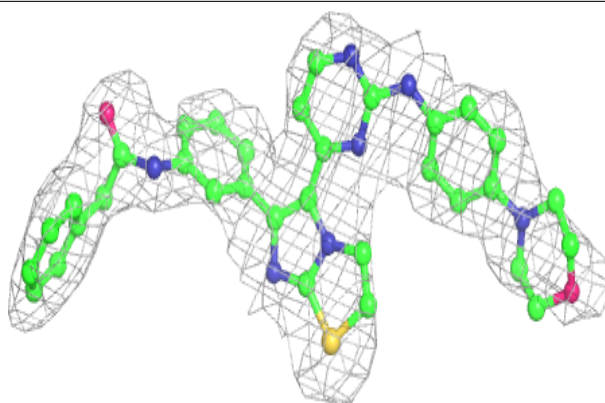
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ITI	D	1	43/43	0.94	0.18	14,57,195,300	0
2	ITI	C	1	43/43	0.96	0.15	23,56,210,300	0
2	ITI	A	1	43/43	0.97	0.16	11,36,81,106	0
2	ITI	B	1	43/43	0.98	0.14	6,33,79,236	0

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.

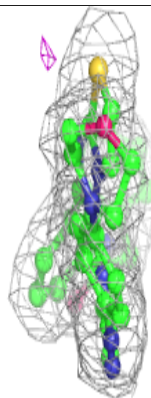
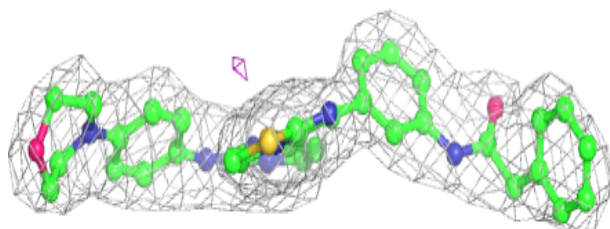
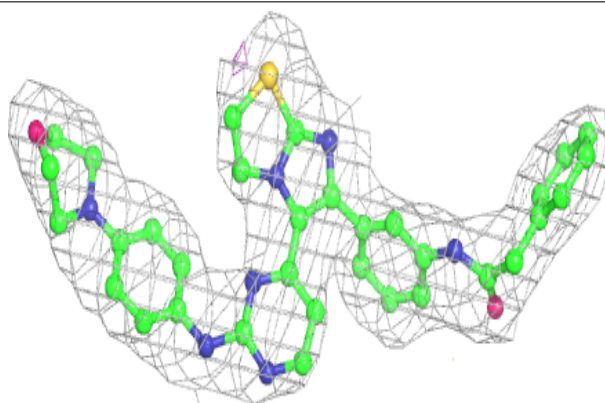


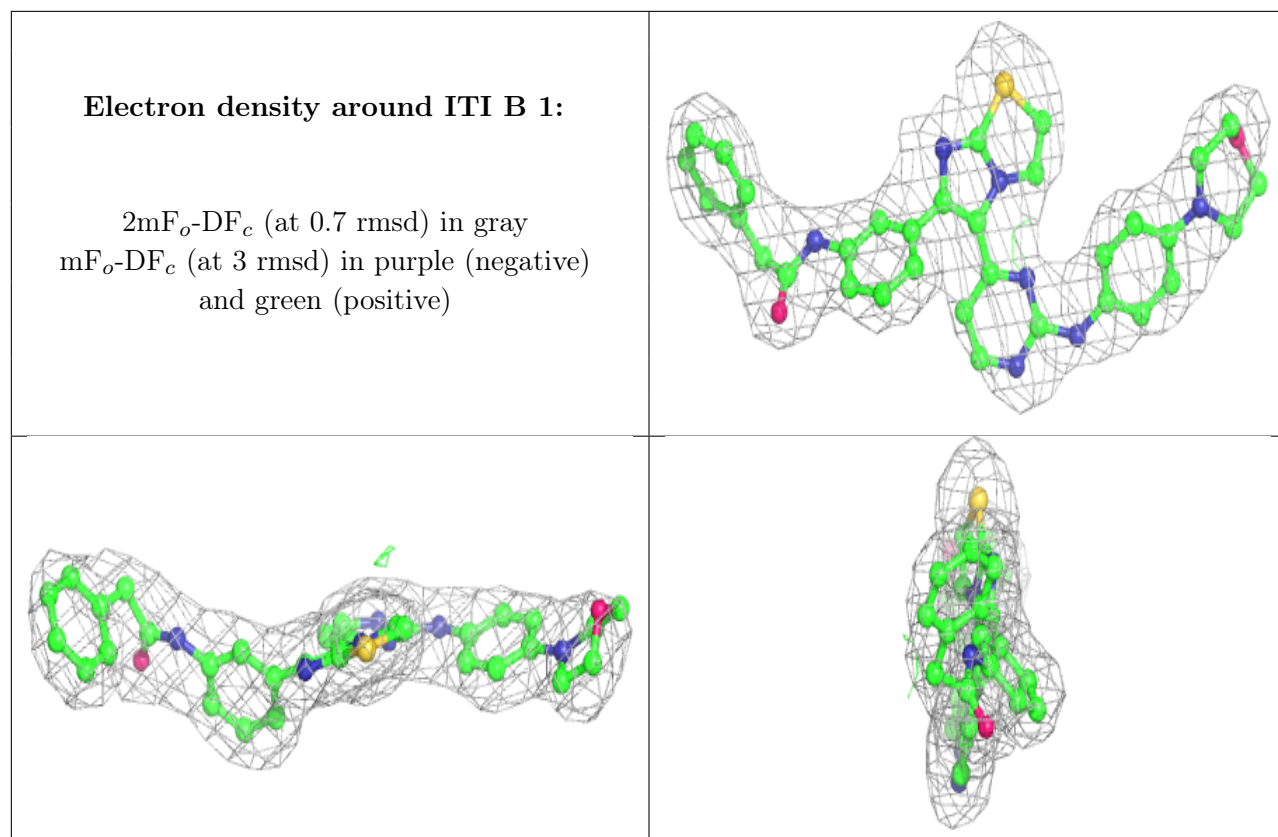
**Electron density around ITI C 1:**

$2mF_o-DF_c$  (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.