



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:00 am GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

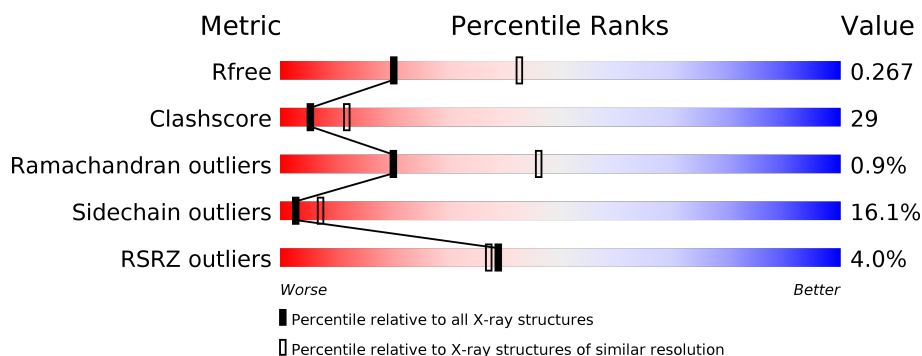
1 Overall quality at a glance

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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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></div> <div>46%</div> <div>28%</div> <div>7%</div> <div>19%</div> </div> </div>
1	B	327	<div> <div>%</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></div> <div>46%</div> <div>25%</div> <div>7%</div> <div>21%</div> </div> </div>
1	D	327	<div> <div>6%</div> <div> <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>
1	F	327	<div> <div>..</div> <div>98%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	UNP P00533
B	924	ARG	VAL	ENGINEERED	UNP P00533
C	924	ARG	VAL	ENGINEERED	UNP P00533
D	924	ARG	VAL	ENGINEERED	UNP P00533
E	-29	ARG	VAL	ENGINEERED	UNP P00533
F	-28	ARG	VAL	ENGINEERED	UNP P00533
G	-30	ARG	VAL	ENGINEERED	UNP P00533
H	-31	ARG	VAL	ENGINEERED	UNP P00533

- Molecule 2 is N-[3-(5-{2-[(4-MORPHOLIN-4-YLPHENYL)AMINO]PYRIMIDIN-4-YL}IMI DAZO[2,1-B][1,3]THIAZOL-6-YL)PHENYL]-2-PHENYLACETAMIDE (three-letter code: ITI) (formula: C₃₃H₂₉N₇O₂S).



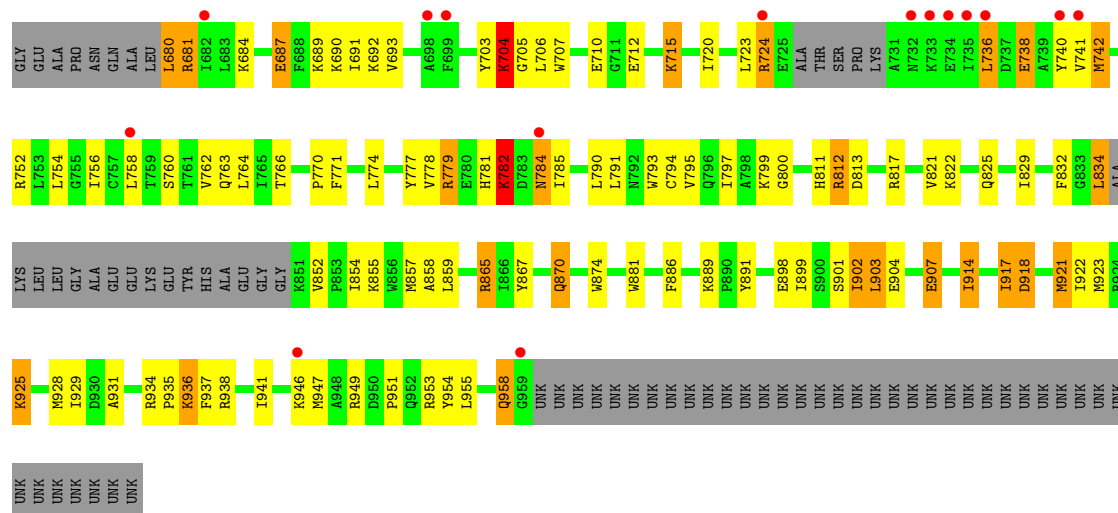
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 7	O 2	S 1	0	0
2	B	1	Total 43	C 33	N 7	O 2	S 1	0	0
2	C	1	Total 43	C 33	N 7	O 2	S 1	0	0
2	D	1	Total 43	C 33	N 7	O 2	S 1	0	0

- Molecule 3 is water.

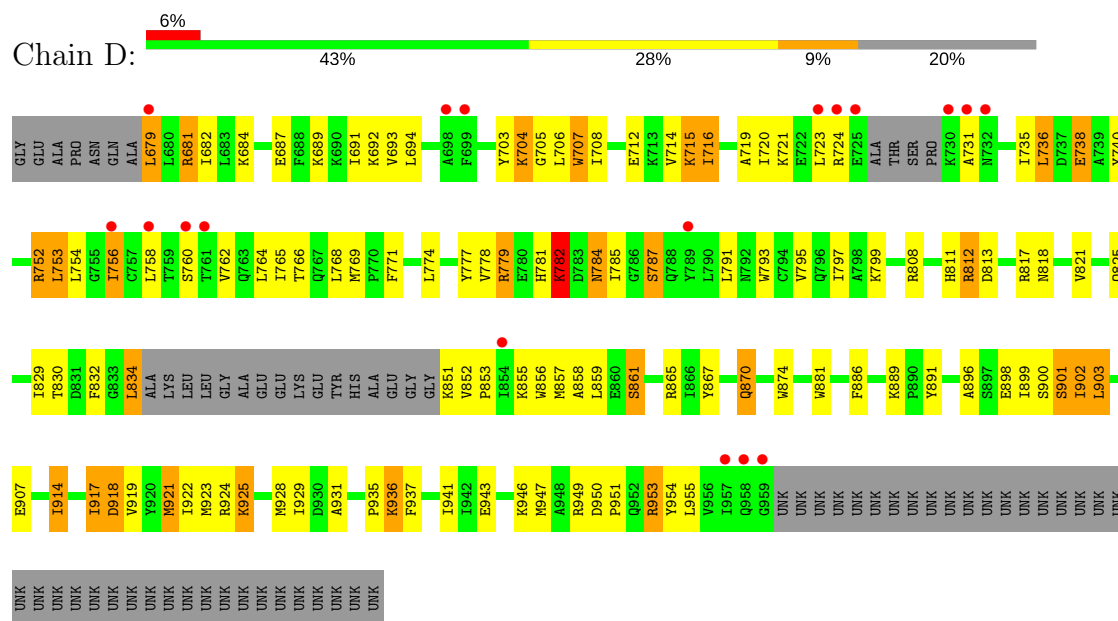
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0
3	B	45	Total O 45 45	0	0
3	C	35	Total O 35 35	0	0
3	D	21	Total O 21 21	0	0
3	E	3	Total O 3 3	0	0
3	F	4	Total O 4 4	0	0
3	G	2	Total O 2 2	0	0
3	H	2	Total O 2 2	0	0

- Molecule 1: Epidermal growth factor receptor

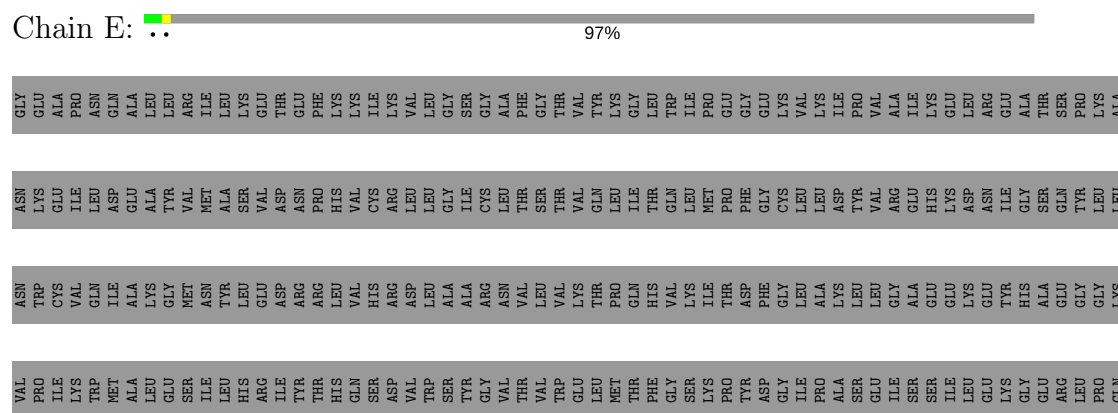




• Molecule 1: Epidermal growth factor receptor

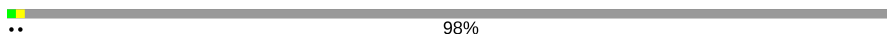


• Molecule 1: Epidermal growth factor receptor



[illegible]

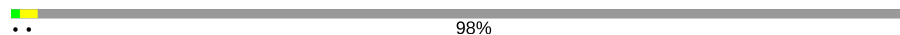
- Molecule 1: Epidermal growth factor receptor

Chain F: 

UNK	UNK	PRO	VAL	ASN	TRP	GLY	ASN	GLY
UNK	UNK	PRO	PRO	ASN	TRP	GLU	LYS	GLU
UNK	UNK	ILE	ILE	CYS	CYS	ALA	LYS	ALA
UNK	UNK	CYS	LYS	VAL	GLN	ILE	ILE	PRO
UNK	UNK	THR	TRP	TRP	VAL	ASN	ASP	GLN
UNK	UNK	ILE	MET	ILE	ILE	ALA	GLU	ALA
UNK	UNK	ASP	ALA	ALA	LYS	TYR	ALA	LEU
UNK	UNK	VAL	LEU	GLY	GLY	TYR	VAL	LEU
UNK	UNK	TYR	GLU	MET	MET	VAL	ARG	ARG
UNK	UNK	MET	ILE	ASN	ASN	MET	ILE	ILE
UNK	UNK	ILE	ILE	ASN	TYR	ALA	ALA	LEU
UNK	UNK	MET	LEU	LEU	LEU	SER	LYS	LYS
UNK	UNK	ARG	HIS	LEU	GLU	VAL	VAL	GLU
UNK	UNK	LYS	ARG	GLU	ASP	VAL	VAL	THR
UNK	UNK	CYS	ILE	ASP	ASP	ARG	ARG	GLU
UNK	UNK	TRP	TYR	ARG	ARG	ASN	ASN	GLU
UNK	UNK	MET	THR	ARG	THR	PRO	PRO	PHE
UNK	UNK	ILE	HIS	LEU	VAL	HIS	VAL	LYS
UNK	UNK	ASP	GLN	VAL	VAL	CYS	VAL	LYS
UNK	UNK	ALA	SER	HIS	ARG	ILE	CYS	ILE
UNK	UNK	ASP	ASP	ARG	VAL	LEU	ARG	LYS
UNK	UNK	SER	VAL	ASP	ASP	LEU	VAL	VAL
UNK	UNK	ARG	TRP	LEU	LEU	LEU	VAL	LEU
UNK	UNK	PRO	SER	ALA	ALA	GLY	GLY	GLY
UNK	UNK	LYS	TYR	ALA	ALA	ILE	ILE	SER
UNK	UNK	PHE	GLY	ARG	ARG	CYS	CYS	GLY
UNK	UNK	ARG	VAL	ASN	VAL	LEU	LEU	ALA
UNK	UNK	GLU	THR	VAL	VAL	THR	THR	PHE
UNK	UNK	LEU	VAL	LEU	LEU	SER	SER	GLY
UNK	UNK	ILE	TRP	VAL	VAL	THR	THR	THR
UNK	UNK	ILE	GLU	LYS	LYS	VAL	VAL	VAL
UNK	UNK	GLU	LEU	THR	THR	GLN	GLN	TYR
UNK	UNK	PHE	MET	PRO	PRO	LEU	ILE	LYS
UNK	UNK	SER	THR	GLN	GLN	ILE	ILE	GLY
UNK	UNK	LYS	PHE	HIS	HIS	THR	THR	LEU
UNK	UNK	MET	GLY	VAL	VAL	GLN	GLN	TRP
UNK	UNK	ALA	SER	LYS	LYS	LEU	LEU	ILE
UNK	UNK	ARG	LYS	ILE	ILE	MET	MET	PRO
UNK	UNK	ASP	PRO	THR	THR	PRO	PHE	GLU
UNK	UNK	PRO	THR	ASP	PHE	GLY	GLY	GLY
UNK	UNK	GLN	ASP	GLY	GLY	CYS	CYS	LYS
UNK	UNK	ARG	GLY	LEU	LEU	LEU	VAL	VAL
UNK	UNK	TYR	ILE	ILE	ALA	LEU	LYS	LYS
UNK	UNK	LEU	PRO	LYS	ALA	LEU	ASP	ILE
UNK	UNK	VAL	ALA	LYS	LEU	TYR	PRO	PRO
UNK	UNK	ILE	SER	LEU	LEU	VAL	VAL	VAL
UNK	UNK	GLN	GLU	GLY	GLY	ARG	ALA	ALA
UNK	UNK	GLY	ILE	GLY	ALA	GLU	ILE	ILE
UNK	UNK	X8	SER	ALA	ALA	GLU	GLU	GLY
UNK	UNK	X11	SER	ALA	ALA	HIS	LYS	LYS
UNK	UNK	X12	ILE	GLU	GLU	GLU	GLU	GLU
UNK	UNK	X13	GLU	LYS	LYS	ASP	ASN	ARG
UNK	UNK	X14	GLU	LYS	TYR	ILE	ILE	GLU
UNK	UNK	UNK	GLY	HIS	HIS	GLY	GLY	ALA
UNK	UNK	UNK	GLU	ALA	ALA	SER	GLN	THR
UNK	UNK	UNK	ARG	GLY	GLY	THR	PRO	SER
UNK	UNK	UNK	LEU	GLY	GLY	TYR	LYS	THR
UNK	UNK	UNK	PRO	GLN	GLY	LEU	LEU	ALA

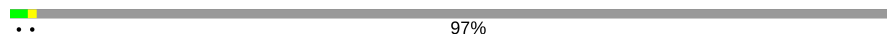
- Molecule 1: Epidermal growth factor receptor

Chain G:



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

- Molecule 1: Epidermal growth factor receptor

Chain H: ..



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 44.16 – 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
$\langle I/\sigma(I) \rangle$ 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 (5.26%)	DCC
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 , 91.0	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 [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.

The worst 5 of 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

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%)	12	30
1	B	261/327 (80%)	247 (95%)	11 (4%)	3 (1%)	17	40
1	C	253/327 (77%)	243 (96%)	9 (4%)	1 (0%)	38	66
1	D	255/327 (78%)	240 (94%)	14 (6%)	1 (0%)	38	66
All	All	1030/1308 (79%)	975 (95%)	46 (4%)	9 (1%)	20	46

5 of 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

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%)	3	7
1	B	232/251 (92%)	199 (86%)	33 (14%)	4	9
1	C	228/251 (91%)	191 (84%)	37 (16%)	3	7
1	D	228/251 (91%)	188 (82%)	40 (18%)	2	5
All	All	921/1004 (92%)	773 (84%)	148 (16%)	3	7

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	925	LYS
1	C	742	MET
1	D	901	SER
1	B	936	LYS
1	C	704	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	44,49,49	1.10	4 (9%)	51,68,68	1.75	13 (25%)
2	ITI	B	1	-	44,49,49	1.39	3 (6%)	51,68,68	1.67	10 (19%)
2	ITI	C	1	-	44,49,49	1.02	2 (4%)	51,68,68	1.58	8 (15%)
2	ITI	D	1	-	44,49,49	0.93	2 (4%)	51,68,68	1.28	3 (5%)

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	-	-	0/21/32/32	0/7/7/7
2	ITI	B	1	-	-	0/21/32/32	0/7/7/7
2	ITI	C	1	-	-	1/21/32/32	0/7/7/7
2	ITI	D	1	-	-	0/21/32/32	0/7/7/7

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ITI	C16-C22	-7.40	1.41	1.49
2	D	1	ITI	C16-C22	-4.10	1.44	1.49
2	A	1	ITI	C16-C22	-4.04	1.44	1.49
2	C	1	ITI	C16-C22	-3.84	1.44	1.49
2	A	1	ITI	C30-N38	-2.50	1.42	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	ITI	C20-N40-C28	-4.80	118.90	127.49
2	A	1	ITI	C32-C30-N38	-4.56	101.77	109.98
2	A	1	ITI	C9-C18-N38	-4.12	115.60	121.39
2	C	1	ITI	N34-C24-N35	-3.60	123.21	126.68
2	B	1	ITI	C15-C13-C21	-3.49	114.17	117.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	ITI	C33-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	B	1	ITI	11	0
2	C	1	ITI	13	0
2	D	1	ITI	19	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/327 (81%)	-0.06	7 (2%) 56 56	27, 47, 80, 117	0
1	B	265/327 (81%)	-0.14	2 (0%) 86 86	27, 45, 79, 112	0
1	C	259/327 (79%)	0.20	15 (5%) 24 22	39, 60, 93, 130	0
1	D	261/327 (79%)	0.32	18 (6%) 18 16	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%)	0.08	42 (4%) 39 37	27, 56, 92, 136	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	728	SER	6.0
1	A	699	PHE	5.5
1	C	735	ILE	5.4
1	B	727	THR	5.3
1	A	726	ALA	5.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ITI	D	1	43/43	0.94	0.18	0.26	14,57,195,300	0
2	ITI	A	1	43/43	0.97	0.15	-0.46	11,36,81,106	0
2	ITI	C	1	43/43	0.96	0.15	-0.83	23,56,210,300	0
2	ITI	B	1	43/43	0.98	0.14	-0.93	6,33,79,236	0

6.5 Other polymers [i](#)

There are no such residues in this entry.