



# Full wwPDB X-ray Structure Validation 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

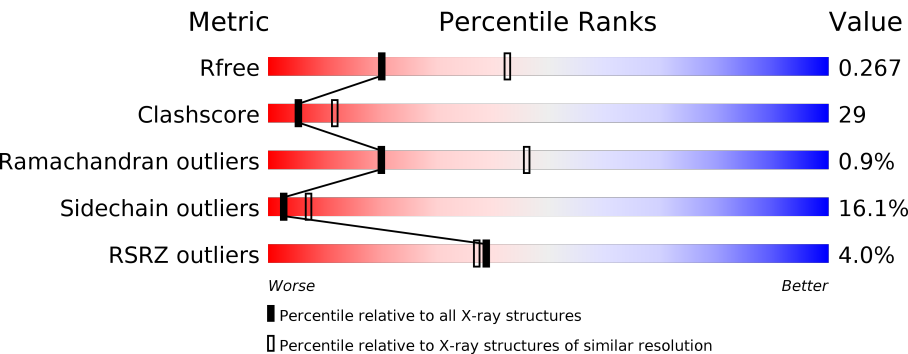
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance 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))
$R_{free}$	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  $\geq 3$ , 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><div></div><div>97%</div></div></div>
1	F	327	<div><div>..</div><div><div></div><div>98%</div></div></div>

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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.

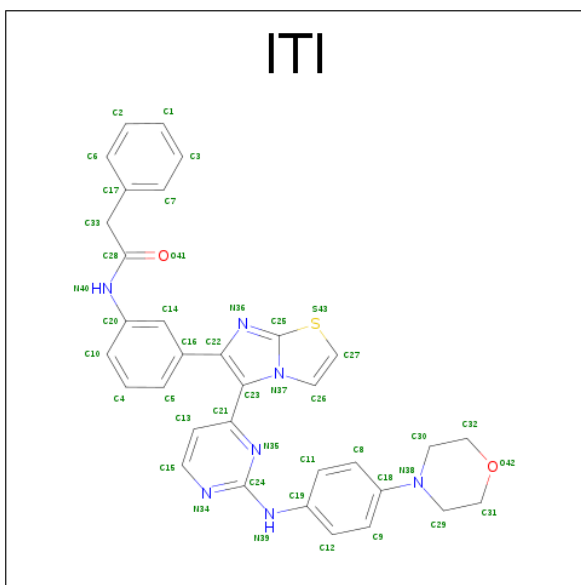
- Molecule 1 is a protein called Epidermal growth factor receptor.

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: 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		

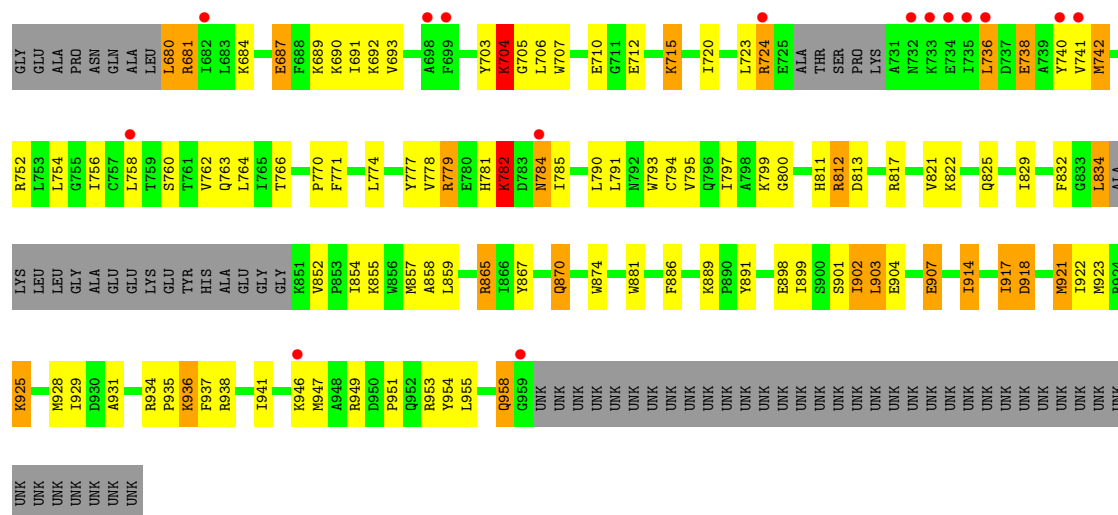
- Molecule 3 is water.

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		

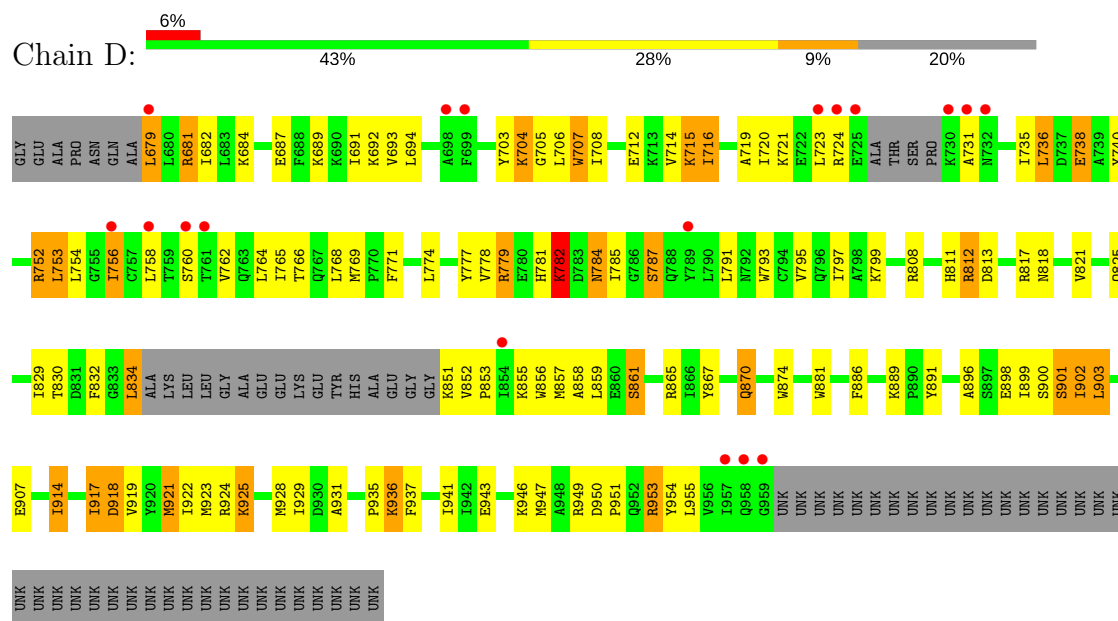
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- Molecule 1: Epidermal growth factor receptor

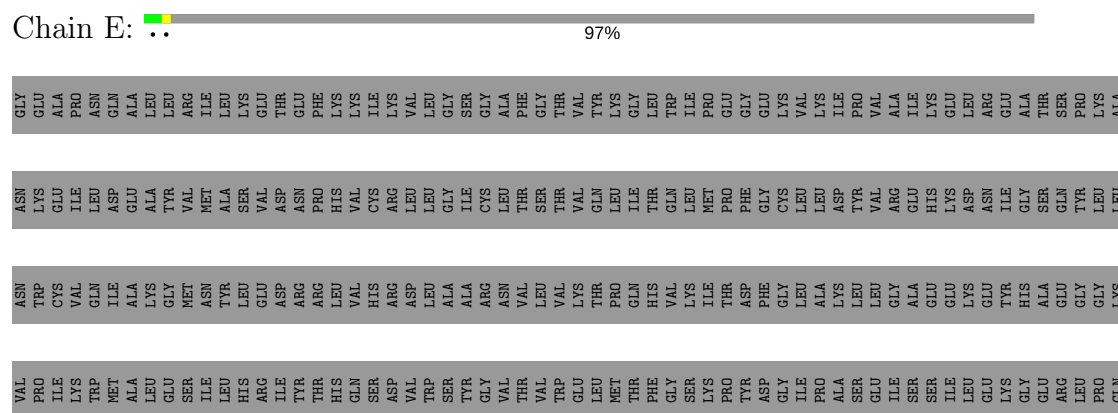




• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor









## 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 (5.26%)	DCC
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

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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:CE	1:D:715:LYS:H	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:N35	2:D:1:ITI:H12	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:HE2	1:A:715:LYS:H	1.48	0.76
1:A:812:ARG:HH11	1:A:812:ARG:HG3	1.51	0.75
1:B:924:ARG:NH2	1:B:928:MET:HE1	2.02	0.75

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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:O	1:A:715:LYS:HD2	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:H26	2:D:1:ITI:H12	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:N	1:D:715:LYS:HE3	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:707:TRP:HH2	1:H:8:UNK:CB	2.05	0.69
1:D:681:ARG:CZ	1:D:707:TRP:HZ3	2.06	0.69

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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:ND2	1:C:784:ASN:N	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:742:MET:CE	2:C:1:ITI:H2	2.26	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: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:C	1:D:707:TRP:CD1	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:HD12	1:A:679:LEU:N	2.15	0.62
1:A:784:ASN:H	1:A:784:ASN:ND2	1.96	0.62
1:A:947:MET:HG2	1:A:954:TYR:CG	2.34	0.62

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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
2:C:1:ITI:N35	2:C:1:ITI:H12	2.16	0.61
1:C:691:ILE:HG22	1:C:692:LYS:CG	2.25	0.61
2:A:1:ITI:N35	2:A:1:ITI:H11	2.16	0.61
1:A:723:LEU:HD12	1:A:762:VAL:CG1	2.30	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:N40	2:B:1:ITI:H6	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:CD	1:D:715:LYS:H	2.15	0.57
1:D:753:LEU:HD12	1:D:754:LEU:N	2.20	0.57

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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
2:D:1:ITI:H26	2:D:1:ITI:C12	2.36	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
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:CD	1:C:715:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:928:MET:HE2	1:B:928:MET:HA	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
2:B:1:ITI:H13	2:B:1:ITI:C16	2.38	0.53
1:B:679:LEU:O	1:B:752:ARG:NH2	2.41	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:CG	1:D:953:ARG:HH11	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:719:ALA:CB	2:B:1:ITI:C15	2.88	0.52
1:B:705:GLY:HA3	1:B:720:ILE:HD12	1.88	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

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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:HD22	1:C:784:ASN:N	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:C5	2:B:1:ITI:H13	2.41	0.49
2:A:1:ITI:O41	2:A:1:ITI:H10	2.12	0.49
2:C:1:ITI:H26	2:C:1:ITI:N35	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:NH1	1:A:812:ARG:HG3	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:C	1:D:707:TRP:HD1	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

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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:834:LEU:HD21	2:C:1:ITI:H6	1.96	0.47
1:C:742:MET:HE2	2:C:1:ITI:H2	1.95	0.47
2:A:1:ITI:C5	2:A:1:ITI:H13	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:D:681:ARG:NH1	1:D:707:TRP:CZ3	2.83	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:HG3	1:B:953:ARG:O	2.14	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:C26	2:C:1:ITI:N35	2.78	0.47
1:A:852:VAL:HA	1:A:853:PRO:HD3	1.65	0.46
2:C:1:ITI:H26	2:C:1:ITI:H12	1.97	0.46
1:C:724:ARG:NH1	1:D:808:ARG:HG3	2.30	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

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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:HB3	1:D:936:LYS:HE2	1.58	0.46
1:C:766:THR:CG2	2:C:1:ITI:O41	2.63	0.46
1:C:782:LYS:HB2	1:C:782:LYS:HE2	1.51	0.46
2:B:1:ITI:N35	2:B:1:ITI:C26	2.77	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
1:D:682:ILE:HD12	1:D:682:ILE:N	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:CG	1:D:953:ARG:NH1	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

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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: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:H9	2:A:1:ITI:H30A	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:HA	1:C:706:LEU:HD23	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
2:C:1:ITI:H30	2:C:1:ITI:H9	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:LYS:HB3	1:C:936:LYS:HE2	1.61	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:NH1	1:D:924:ARG:O	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:HA	1:C:923:MET:HE1	2.01	0.42
1:C:881:TRP:HD1	1:C:923:MET:HE1	1.83	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:HA	1:D:706:LEU:HD23	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:H8	2:B:1:ITI:H29A	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:NH1	1:B:924:ARG:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:MET:HE2	1:B:832:PHE:O	2.19	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:HB2	1:B:704:LYS:HE2	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:H9	2:D:1:ITI:H30	1.76	0.41
1:D:881:TRP:HA	1:D:923:MET:HE1	2.02	0.41
1:C:754:LEU:HD11	1:G:9:UNK:CB	2.50	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:766:THR:HG22	2:B:1:ITI:C10	2.51	0.41
1:B:704:LYS:HD3	1:B:768:LEU:HD21	2.02	0.41
1:A:691:ILE:HD13	1:A:706:LEU:CG	2.42	0.41
1:C:858:ALA:HA	1:C:874:TRP:CD2	2.55	0.41
1:D:719:ALA:HB2	1:D:768:LEU:HA	2.02	0.41
1:A:834:LEU:HD22	1:A:834:LEU:HA	1.86	0.41
1:C:917:ILE:O	1:C:921:MET:HB2	2.20	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:N	1:B:682:ILE:HD12	2.37	0.40
1:B:852:VAL:CG2	1:B:854:ILE:CD1	2.99	0.40
1:C:790:LEU:HD23	1:C:790:LEU:HA	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:A:881:TRP:CD1	1:A:923:MET:CE	3.03	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:861:SER:O	1:A:865:ARG:NE	2.49	0.40
1:A:782:LYS:NZ	1:B:946:LYS:CD	2.84	0.40
2:D:1:ITI:H29A	2:D:1:ITI:H8	1.78	0.40
1:D:720:ILE:CG1	1:D:765:ILE:HD12	2.51	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%)	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

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%)	3	7
1	B	232/251 (92%)	199 (86%)	33 (14%)	4	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

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

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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

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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

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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

Some 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

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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 carbohydrates 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	-	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

All (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
2	B	1	ITI	C23-C22	-2.31	1.38	1.43
2	A	1	ITI	C23-C22	-2.12	1.38	1.43
2	A	1	ITI	C24-N39	2.18	1.40	1.36
2	B	1	ITI	C24-N39	2.22	1.40	1.36
2	D	1	ITI	C24-N39	2.29	1.40	1.36
2	C	1	ITI	C24-N39	2.91	1.41	1.36

All (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
2	B	1	ITI	C8-C18-N38	-2.99	117.19	121.39
2	A	1	ITI	N34-C24-N35	-2.88	123.91	126.68
2	B	1	ITI	C33-C28-N40	-2.69	108.21	114.94
2	C	1	ITI	C8-C18-N38	-2.55	117.80	121.39
2	B	1	ITI	N34-C24-N35	-2.55	124.23	126.68
2	C	1	ITI	C32-C30-N38	-2.53	105.43	109.98
2	A	1	ITI	C33-C28-N40	-2.53	108.61	114.94
2	A	1	ITI	C13-C15-N34	-2.52	121.02	123.92
2	D	1	ITI	N34-C24-N35	-2.50	124.28	126.68
2	A	1	ITI	C33-C17-C7	-2.45	117.35	120.89
2	C	1	ITI	C31-C29-N38	-2.28	105.87	109.98
2	B	1	ITI	C22-N36-C25	-2.27	99.33	103.71
2	A	1	ITI	C20-N40-C28	-2.23	123.50	127.49
2	C	1	ITI	C19-N39-C24	-2.16	123.54	129.17
2	A	1	ITI	C12-C9-C18	-2.09	117.50	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ITI	C31-C29-N38	-2.08	106.23	109.98
2	A	1	ITI	C13-C21-N35	2.03	124.73	121.97
2	D	1	ITI	C5-C16-C14	2.32	121.16	118.16
2	B	1	ITI	C15-N34-C24	2.50	117.52	115.43
2	B	1	ITI	C13-C21-N35	2.59	125.49	121.97
2	A	1	ITI	O41-C28-N40	2.68	128.71	123.67
2	B	1	ITI	O41-C28-N40	2.74	128.83	123.67
2	B	1	ITI	C5-C16-C14	2.97	121.99	118.16
2	C	1	ITI	C15-N34-C24	3.62	118.45	115.43
2	A	1	ITI	C15-N34-C24	4.36	119.06	115.43
2	C	1	ITI	C30-N38-C29	4.37	120.84	111.57
2	A	1	ITI	C30-N38-C29	4.54	121.18	111.57
2	D	1	ITI	C30-N38-C29	5.42	123.06	111.57
2	B	1	ITI	C30-N38-C29	6.25	124.81	111.57

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

### 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%)	-0.06	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

All (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
1	A	760	SER	5.0
1	D	730	LYS	4.9
1	D	957	ILE	4.8
1	D	698	ALA	4.5
1	D	758	LEU	4.2
1	C	959	GLY	4.2
1	A	725	GLU	4.1
1	D	699	PHE	3.8
1	D	731	ALA	3.8
1	C	758	LEU	3.7
1	C	736	LEU	3.6
1	C	734	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	760	SER	3.4
1	C	733	LYS	3.2
1	D	679	LEU	3.2
1	C	740	TYR	3.1
1	D	732	ASN	3.1
1	D	723	LEU	3.1
1	C	784	ASN	3.1
1	D	789	TYR	3.0
1	D	725	GLU	2.9
1	D	854	ILE	2.8
1	D	756	ILE	2.6
1	D	724	ARG	2.6
1	D	958	GLN	2.6
1	C	699	PHE	2.6
1	C	741	VAL	2.5
1	D	959	GLY	2.5
1	D	761	THR	2.5
1	C	724	ARG	2.5
1	C	946	LYS	2.3
1	A	852	VAL	2.2
1	C	682	ILE	2.2
1	A	727	THR	2.1
1	C	732	ASN	2.1
1	A	735	ILE	2.1
1	C	698	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 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	LLDF	B-factors( $\text{\AA}^2$ )	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.