



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:44 PM GMT

PDB ID : 4A97  
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with zopiclone  
Authors : Spurny, R.; Brams, M.; Ulens, C.  
Deposited on : 2011-11-24  
Resolution : 3.34 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

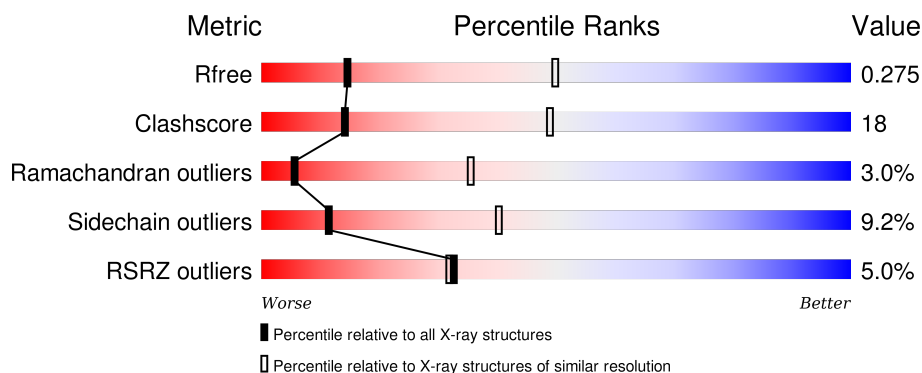
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.34 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))
$R_{free}$	91344	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	307	<div> <div>4%</div> <div>60% 35% 5% •</div> </div>
1	B	307	<div> <div>3%</div> <div>54% 40% 6% •</div> </div>
1	C	307	<div> <div>5%</div> <div>56% 37% 6% •</div> </div>
1	D	307	<div> <div>3%</div> <div>56% 37% 7% •</div> </div>
1	E	307	<div> <div>2%</div> <div>56% 39% 5% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZPC	A	1318	-	-	X	X
2	ZPC	D	1318	-	-	X	-
2	ZPC	F	1318	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25290 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 CYS-LOOP LIGAND-GATED ION CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

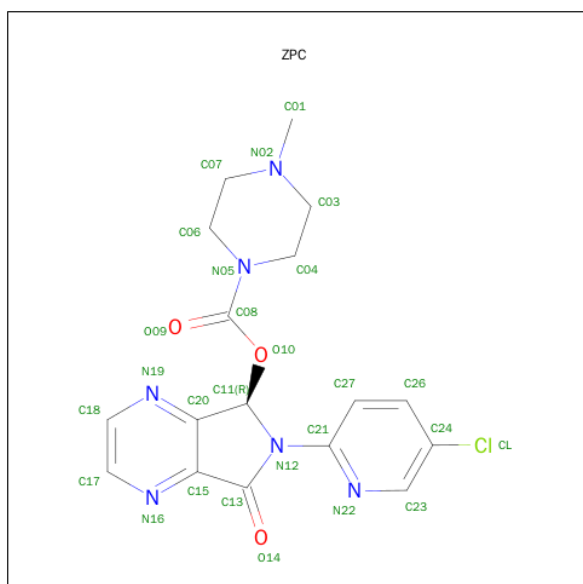
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	INSERTION	UNP P0C7B7
A	289	ASN	MET	CONFLICT	UNP P0C7B7
B	164	GLY	-	INSERTION	UNP P0C7B7
B	289	ASN	MET	CONFLICT	UNP P0C7B7
C	164	GLY	-	INSERTION	UNP P0C7B7
C	289	ASN	MET	CONFLICT	UNP P0C7B7
D	164	GLY	-	INSERTION	UNP P0C7B7
D	289	ASN	MET	CONFLICT	UNP P0C7B7
E	164	GLY	-	INSERTION	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	CONFLICT	UNP P0C7B7
F	164	GLY	-	INSERTION	UNP P0C7B7
F	289	ASN	MET	CONFLICT	UNP P0C7B7
G	164	GLY	-	INSERTION	UNP P0C7B7
G	289	ASN	MET	CONFLICT	UNP P0C7B7
H	164	GLY	-	INSERTION	UNP P0C7B7
H	289	ASN	MET	CONFLICT	UNP P0C7B7
I	164	GLY	-	INSERTION	UNP P0C7B7
I	289	ASN	MET	CONFLICT	UNP P0C7B7
J	164	GLY	-	INSERTION	UNP P0C7B7
J	289	ASN	MET	CONFLICT	UNP P0C7B7

- Molecule 2 is (5R)-6-(5-CHLOROPYRIDIN-2-YL)-7-OXO-6,7-DIHYDRO-5H-PYRROLO[3,4-B]PYRAZIN-5-YL 4-METHYLPIPERAZINE-1-CARBOXYLATE (three-letter code: ZPC) (formula: C<sub>17</sub>H<sub>17</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	B	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	C	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	D	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	E	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		

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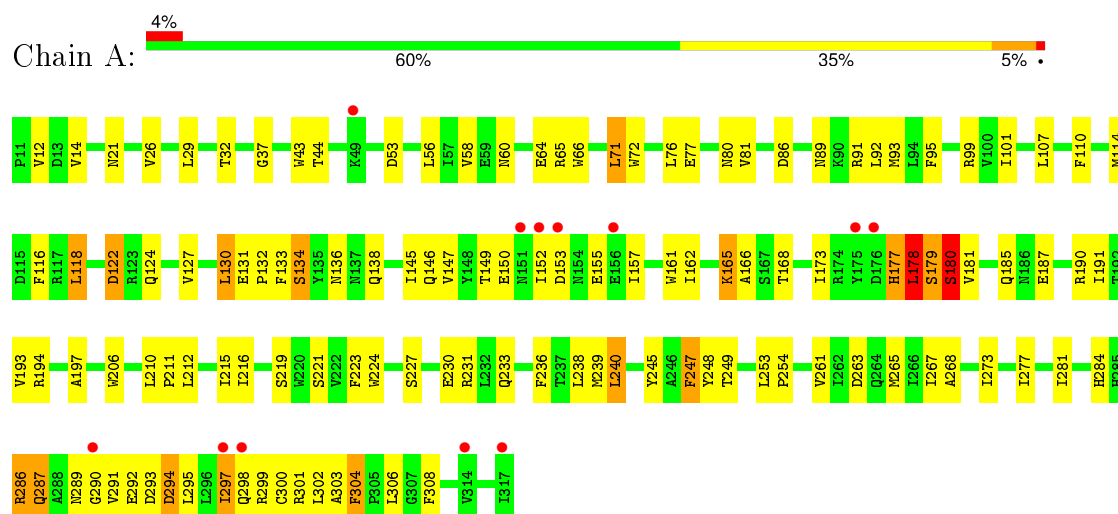
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	G	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	H	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	I	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	J	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		

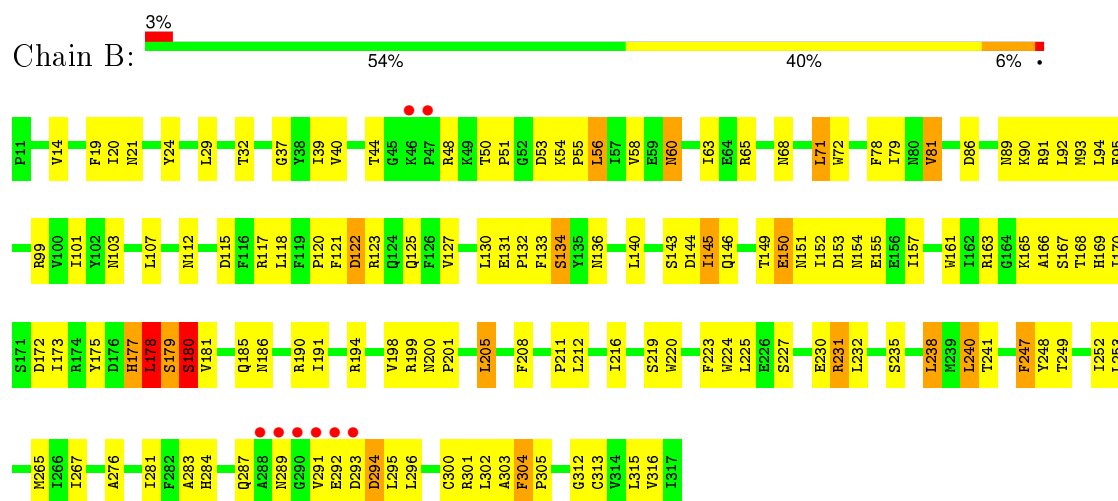
### 3 Residue-property plots

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

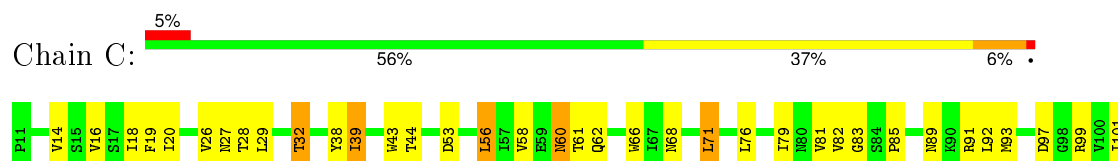
#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

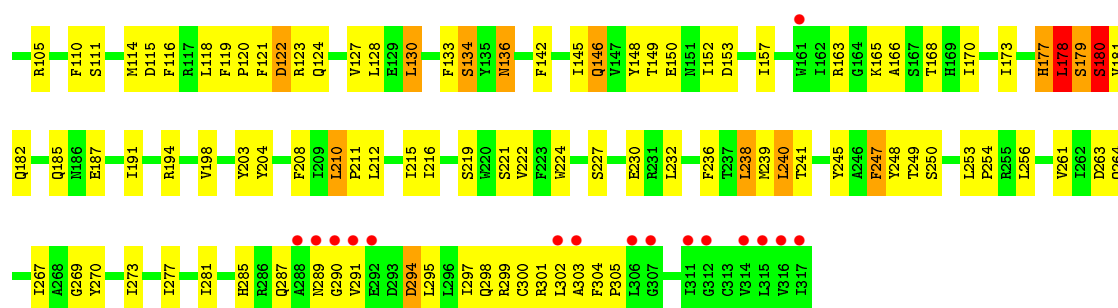


#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

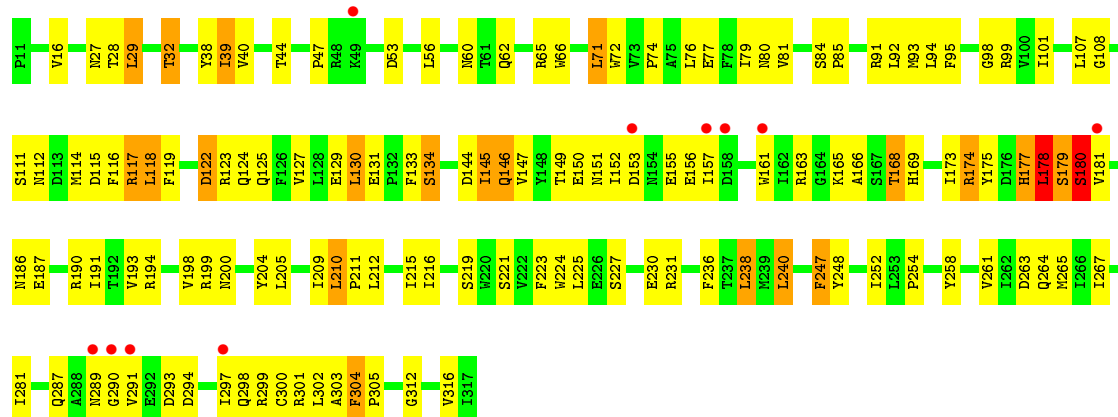


#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

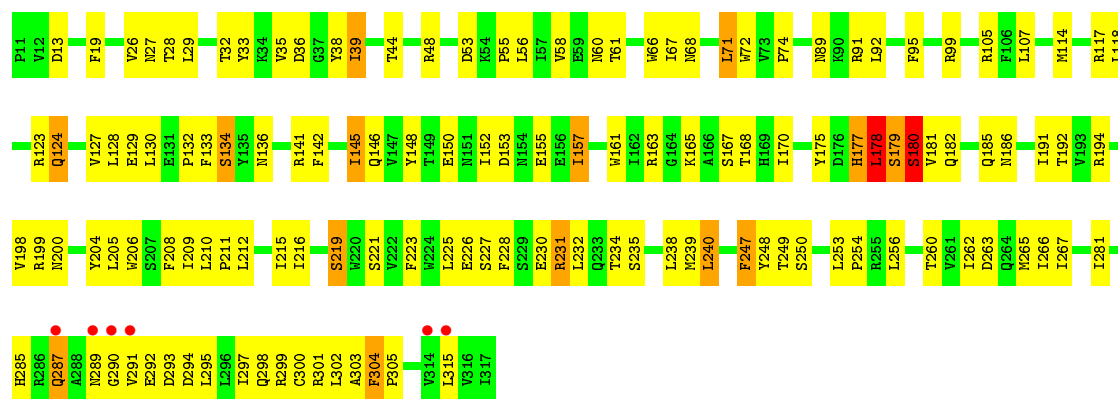




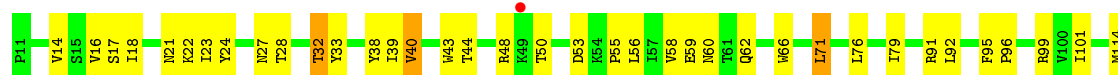
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

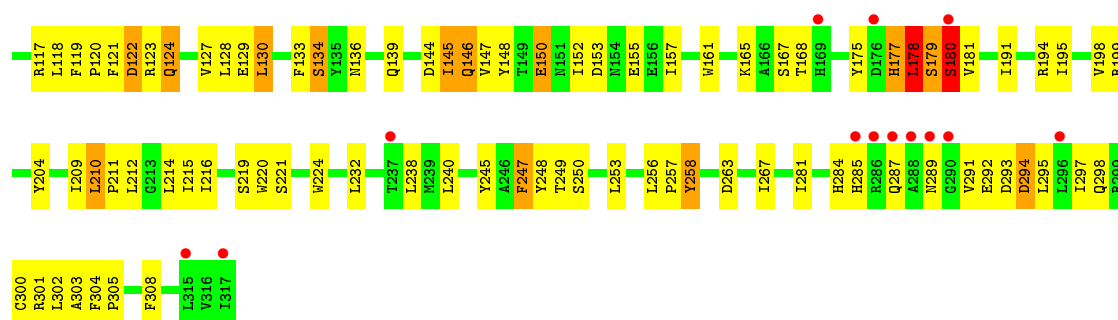


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

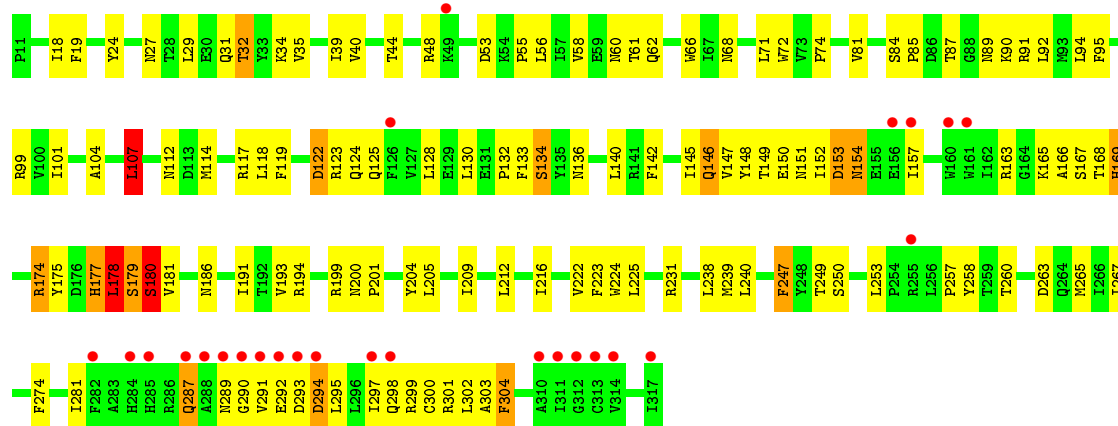


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

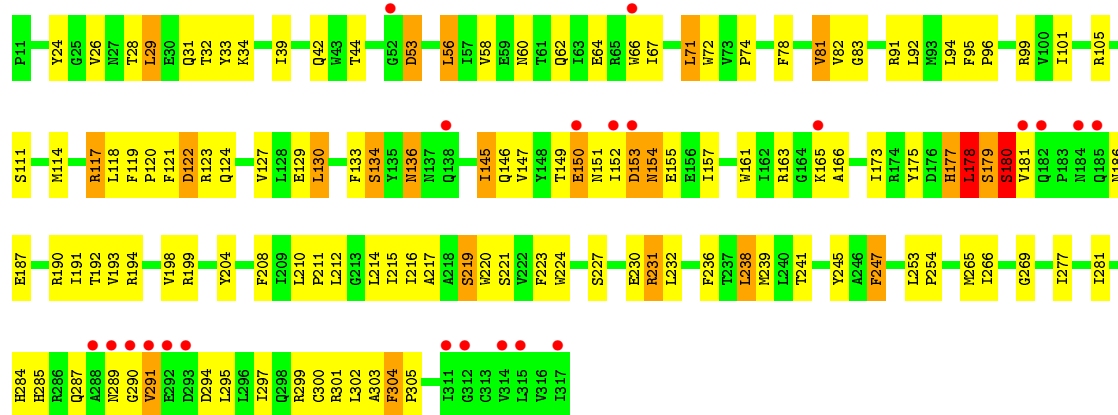




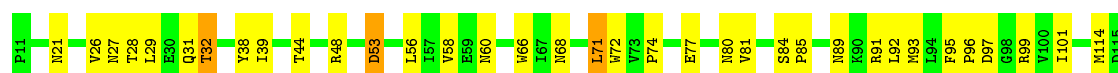
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

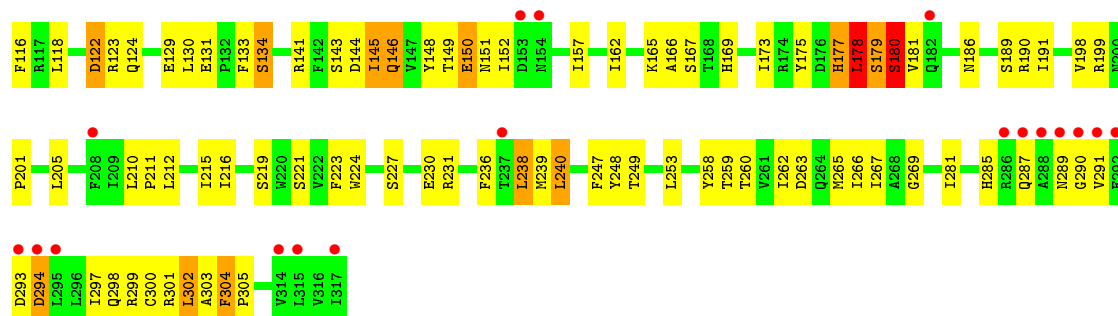


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

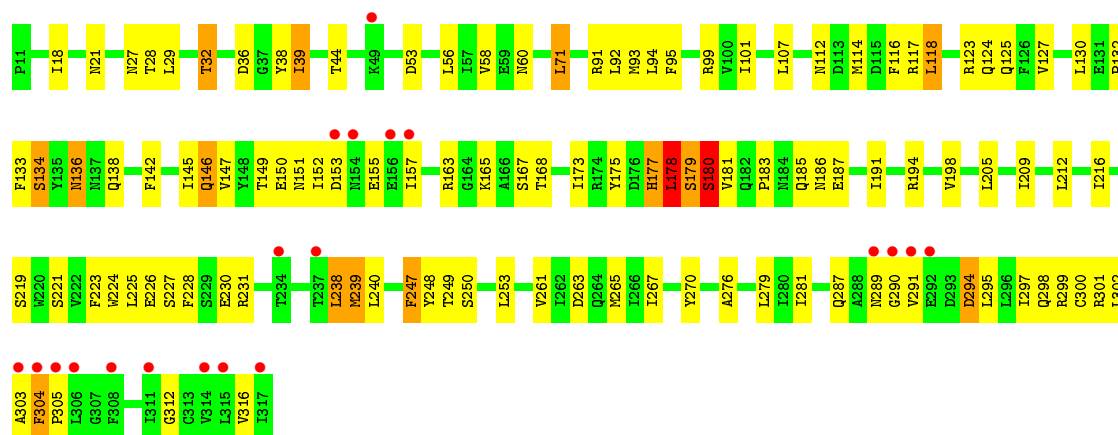


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL





• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.40 Å   266.83 Å   110.76 Å 90.00°   109.20°   90.00°	Depositor
Resolution (Å)	43.47 – 3.34 43.43 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.47-3.34) 99.3 (43.43-3.34)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.32 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, $R_{free}$	0.205   ,   0.259 0.226   ,   0.275	Depositor DCC
$R_{free}$ test set	4131 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.2	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 78.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 82845 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	25290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.57	0/2570	0.81	3/3503 (0.1%)
1	B	0.67	0/2570	0.92	2/3503 (0.1%)
1	C	0.64	0/2570	0.84	0/3503
1	D	0.67	0/2570	0.91	4/3503 (0.1%)
1	E	0.61	0/2570	0.83	4/3503 (0.1%)
1	F	0.57	0/2570	0.82	1/3503 (0.0%)
1	G	0.66	0/2570	0.90	2/3503 (0.1%)
1	H	0.60	0/2570	0.82	1/3503 (0.0%)
1	I	0.64	0/2570	0.84	1/3503 (0.0%)
1	J	0.59	0/2570	0.80	1/3503 (0.0%)
All	All	0.62	0/25700	0.85	19/35030 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
All	All	0	21

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	LEU	CA-CB-CG	8.47	134.79	115.30
1	J	39	ILE	CB-CA-C	-7.01	97.58	111.60
1	D	199	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	240	LEU	CA-CB-CG	6.34	129.88	115.30
1	E	199	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	E	240	LEU	CA-CB-CG	5.91	128.90	115.30
1	F	128	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	G	107	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	I	205	LEU	CA-CB-CG	-5.56	102.51	115.30
1	D	174	ARG	C-N-CA	5.53	135.53	121.70
1	G	107	LEU	CB-CG-CD1	5.52	120.38	111.00
1	A	76	LEU	CA-CB-CG	5.40	127.73	115.30
1	E	315	LEU	CA-CB-CG	5.38	127.66	115.30
1	D	117	ARG	CB-CG-CD	-5.30	97.81	111.60
1	H	117	ARG	CG-CD-NE	5.29	122.91	111.80
1	D	39	ILE	CG1-CB-CG2	-5.27	99.80	111.40
1	E	39	ILE	CB-CA-C	-5.18	101.25	111.60
1	A	210	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	205	LEU	CA-CB-CG	-5.16	103.43	115.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	HIS	Peptide
1	A	178	LEU	Peptide
1	B	177	HIS	Peptide
1	B	178	LEU	Peptide
1	C	177	HIS	Peptide
1	C	178	LEU	Peptide
1	D	174	ARG	Peptide
1	D	177	HIS	Peptide
1	D	178	LEU	Peptide
1	E	177	HIS	Peptide
1	E	178	LEU	Peptide
1	F	177	HIS	Peptide
1	F	178	LEU	Peptide
1	G	177	HIS	Peptide
1	G	178	LEU	Peptide
1	H	177	HIS	Peptide
1	H	178	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	I	177	HIS	Peptide
1	I	178	LEU	Peptide
1	J	177	HIS	Peptide
1	J	178	LEU	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2502	0	2469	107	0
1	B	2502	0	2469	118	0
1	C	2502	0	2469	114	0
1	D	2502	0	2469	105	0
1	E	2502	0	2469	108	0
1	F	2502	0	2469	96	0
1	G	2502	0	2469	96	0
1	H	2502	0	2469	102	0
1	I	2502	0	2469	93	0
1	J	2502	0	2469	86	0
2	A	27	0	17	9	0
2	B	27	0	17	3	0
2	C	27	0	17	8	0
2	D	27	0	17	12	0
2	E	27	0	17	7	0
2	F	27	0	17	11	0
2	G	27	0	17	6	0
2	H	27	0	17	7	0
2	I	27	0	17	8	0
2	J	27	0	17	4	0
All	All	25290	0	24860	911	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 18.

All (911) 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:J:133:PHE:O	2:J:1318:ZPC:H03A	1.56	1.05
1:H:150:GLU:OE2	2:I:1318:ZPC:H17	1.58	1.01
1:E:13:ASP:OD1	1:E:141:ARG:NH1	1.94	0.99
1:C:91:ARG:NH2	2:D:1318:ZPC:H23	1.79	0.98
1:F:133:PHE:O	2:F:1318:ZPC:H07	1.66	0.96
1:E:155:GLU:OE2	1:E:163:ARG:NH2	2.02	0.92
1:I:91:ARG:NH2	1:I:93:MET:SD	2.43	0.92
1:C:91:ARG:HH22	2:D:1318:ZPC:H23	1.29	0.90
1:H:175:TYR:O	1:H:186:ASN:ND2	2.06	0.88
1:E:161:TRP:HB3	1:E:163:ARG:HH21	1.40	0.87
1:C:249:THR:HG23	1:C:253:LEU:HD22	1.55	0.86
1:E:294:ASP:HB2	1:E:297:ILE:HG22	1.58	0.85
1:E:293:ASP:O	1:E:298:GLN:NE2	2.10	0.84
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.58	0.83
1:F:59:GLU:OE2	1:G:134:SER:OG	1.95	0.83
1:J:44:THR:HA	1:J:99:ARG:HA	1.61	0.82
1:J:294:ASP:HB2	1:J:297:ILE:HG22	1.62	0.81
1:E:132:PRO:O	2:E:1318:ZPC:H01A	1.80	0.81
1:F:133:PHE:O	2:F:1318:ZPC:C07	2.28	0.81
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.63	0.81
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.45	0.81
1:A:133:PHE:O	2:A:1318:ZPC:H07	1.80	0.80
1:C:123:ARG:HD2	1:C:198:VAL:HG22	1.64	0.79
1:C:133:PHE:O	2:C:1318:ZPC:H07	1.82	0.79
1:I:123:ARG:HD2	1:I:198:VAL:HG22	1.65	0.79
1:I:293:ASP:O	1:I:298:GLN:NE2	2.16	0.78
1:H:224:TRP:CH2	1:H:301:ARG:HB3	2.19	0.78
1:B:123:ARG:HD2	1:B:198:VAL:HG22	1.67	0.77
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.67	0.77
1:B:167:SER:HB3	1:B:194:ARG:HB2	1.65	0.76
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.19	0.76
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.67	0.76
1:F:66:TRP:HB3	1:F:71:LEU:HD12	1.68	0.76
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.68	0.75
1:C:91:ARG:HH22	2:D:1318:ZPC:C23	2.00	0.75
1:C:178:LEU:HD12	1:C:180:SER:HB3	1.68	0.75
1:F:177:HIS:O	1:F:179:SER:N	2.20	0.75
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.67	0.74
1:A:224:TRP:CH2	1:A:301:ARG:HB3	2.23	0.73
1:J:249:THR:HG23	1:J:253:LEU:HD22	1.71	0.72
1:B:122:ASP:N	1:B:122:ASP:OD1	2.22	0.72
1:I:77:GLU:OE1	2:I:1318:ZPC:H01	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:MET:HB3	1:D:101:ILE:HB	1.72	0.71
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.73	0.71
1:C:122:ASP:N	1:C:122:ASP:OD1	2.22	0.71
1:A:127:VAL:HG22	1:A:194:ARG:HG2	1.74	0.70
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.74	0.69
1:B:175:TYR:O	1:B:186:ASN:ND2	2.25	0.69
1:F:212:LEU:O	1:F:216:ILE:HG12	1.92	0.69
1:I:95:PHE:HB2	1:I:99:ARG:HG2	1.74	0.69
1:E:161:TRP:HB3	1:E:163:ARG:NH2	2.08	0.69
1:I:44:THR:HA	1:I:99:ARG:HA	1.73	0.69
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.74	0.69
1:C:212:LEU:O	1:C:216:ILE:HG12	1.93	0.69
1:G:178:LEU:HD12	1:G:180:SER:HB3	1.72	0.69
1:H:181:VAL:HG11	2:H:1318:ZPC:CL	2.30	0.68
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.76	0.68
1:H:44:THR:HA	1:H:99:ARG:HA	1.75	0.68
1:I:216:ILE:O	1:I:219:SER:HB3	1.93	0.68
1:A:93:MET:HB3	1:A:101:ILE:HB	1.75	0.68
1:G:44:THR:HA	1:G:99:ARG:HA	1.73	0.68
1:F:133:PHE:CD1	2:F:1318:ZPC:H07A	2.29	0.68
1:B:208:PHE:HE2	1:B:249:THR:HA	1.59	0.68
1:F:150:GLU:OE2	2:G:1318:ZPC:H17	1.94	0.68
1:E:177:HIS:O	1:E:179:SER:N	2.27	0.68
1:H:101:ILE:HD13	2:I:1318:ZPC:CL	2.31	0.68
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.75	0.68
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.75	0.67
1:D:212:LEU:O	1:D:216:ILE:HG12	1.94	0.67
1:A:287:GLN:HA	1:A:292:GLU:OE1	1.95	0.67
1:F:150:GLU:OE2	2:G:1318:ZPC:C17	2.42	0.67
1:J:177:HIS:O	1:J:179:SER:N	2.27	0.67
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.58	0.67
1:B:212:LEU:O	1:B:216:ILE:HG12	1.93	0.67
1:B:40:VAL:HG11	2:C:1318:ZPC:H26	1.75	0.67
1:A:294:ASP:O	1:A:298:GLN:HG2	1.94	0.67
1:F:91:ARG:HH22	2:G:1318:ZPC:H23	1.60	0.67
1:B:40:VAL:HG21	2:C:1318:ZPC:H27	1.77	0.66
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.77	0.66
1:D:145:ILE:HD12	1:D:191:ILE:HG21	1.78	0.66
1:D:216:ILE:O	1:D:219:SER:HB3	1.96	0.66
1:J:178:LEU:HD12	1:J:180:SER:HB3	1.78	0.66
1:G:301:ARG:HH12	1:H:285:HIS:CE1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:TYR:O	1:D:186:ASN:ND2	2.28	0.65
1:I:179:SER:O	1:I:181:VAL:N	2.29	0.65
1:G:225:LEU:HD21	1:H:232:LEU:HD22	1.78	0.65
1:J:167:SER:HB3	1:J:194:ARG:HB2	1.78	0.65
1:D:179:SER:O	1:D:181:VAL:N	2.30	0.65
1:B:103:ASN:ND2	2:C:1318:ZPC:H06A	2.11	0.65
1:H:284:HIS:CE1	1:H:291:VAL:HG13	2.31	0.65
1:D:144:ASP:OD1	1:D:146:GLN:NE2	2.29	0.65
1:D:123:ARG:HD2	1:D:198:VAL:HG22	1.77	0.65
1:A:289:ASN:OD1	1:A:290:GLY:N	2.26	0.65
1:A:179:SER:O	1:A:181:VAL:N	2.30	0.65
1:D:173:ILE:O	1:D:187:GLU:HA	1.95	0.65
1:B:65:ARG:HD2	1:C:68:ASN:ND2	2.12	0.64
1:B:149:THR:O	1:B:151:ASN:N	2.26	0.64
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.79	0.64
1:F:133:PHE:HA	2:F:1318:ZPC:C01	2.28	0.64
1:E:216:ILE:O	1:E:219:SER:HB3	1.96	0.64
1:G:289:ASN:OD1	1:G:290:GLY:N	2.28	0.64
1:H:179:SER:O	1:H:181:VAL:N	2.31	0.64
1:D:76:LEU:HB3	1:D:130:LEU:HD21	1.78	0.64
1:F:133:PHE:HA	2:F:1318:ZPC:H01	1.80	0.64
1:G:295:LEU:HA	1:G:298:GLN:OE1	1.97	0.64
1:E:178:LEU:HD12	1:E:180:SER:HB3	1.78	0.64
1:I:212:LEU:O	1:I:216:ILE:HG12	1.98	0.64
1:F:284:HIS:HE1	1:J:226:GLU:OE2	1.80	0.64
1:F:294:ASP:HB2	1:F:297:ILE:HG22	1.79	0.63
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.34	0.63
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.81	0.63
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.80	0.63
1:E:27:ASN:HB3	1:E:32:THR:HB	1.81	0.63
1:C:179:SER:O	1:C:181:VAL:N	2.32	0.63
1:A:223:PHE:HE2	1:A:304:PHE:CE1	2.17	0.63
1:G:157:ILE:HD11	1:H:117:ARG:HE	1.64	0.63
1:D:161:TRP:HB3	1:D:163:ARG:HH21	1.62	0.63
1:C:136:ASN:HD22	1:C:136:ASN:H	1.46	0.62
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.81	0.62
1:E:181:VAL:HG11	2:E:1318:ZPC:CL	2.36	0.62
1:D:81:VAL:HG21	1:D:85:PRO:HG3	1.82	0.62
1:B:284:HIS:NE2	1:B:291:VAL:HG13	2.13	0.62
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.81	0.62
1:E:289:ASN:OD1	1:E:290:GLY:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ASP:HB2	1:E:297:ILE:CG2	2.29	0.62
1:F:175:TYR:CE2	2:F:1318:ZPC:H04A	2.35	0.62
1:F:293:ASP:O	1:F:298:GLN:NE2	2.33	0.62
1:B:143:SER:OG	1:B:144:ASP:N	2.33	0.61
1:H:66:TRP:HB3	1:H:71:LEU:HD12	1.81	0.61
1:H:123:ARG:HD2	1:H:198:VAL:HG22	1.81	0.61
1:D:177:HIS:O	1:D:179:SER:N	2.33	0.61
1:G:179:SER:O	1:G:181:VAL:N	2.34	0.61
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.83	0.61
1:F:123:ARG:HD2	1:F:198:VAL:HG22	1.82	0.61
1:E:223:PHE:HE2	1:E:304:PHE:CE1	2.19	0.61
1:C:58:VAL:HB	1:C:92:LEU:HB2	1.81	0.61
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.15	0.61
1:E:263:ASP:O	1:E:267:ILE:HG12	2.00	0.61
1:F:167:SER:HB3	1:F:194:ARG:HB2	1.81	0.60
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.83	0.60
1:D:145:ILE:HD12	1:D:191:ILE:CG2	2.31	0.60
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.84	0.60
1:D:133:PHE:O	2:D:1318:ZPC:H07	2.01	0.60
1:I:294:ASP:HB2	1:I:297:ILE:HG22	1.83	0.60
1:C:177:HIS:O	1:C:179:SER:N	2.35	0.60
1:D:122:ASP:N	1:D:122:ASP:OD1	2.33	0.60
1:A:65:ARG:HD2	1:B:68:ASN:ND2	2.15	0.60
1:E:175:TYR:O	1:E:186:ASN:ND2	2.35	0.60
1:F:91:ARG:HB2	1:G:133:PHE:HE2	1.66	0.60
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.82	0.60
1:I:212:LEU:CD1	1:I:265:MET:HB3	2.31	0.60
1:H:129:GLU:HG2	1:H:192:THR:HG23	1.84	0.60
1:H:177:HIS:O	1:H:179:SER:N	2.35	0.60
1:H:216:ILE:O	1:H:219:SER:HB3	2.01	0.59
1:D:147:VAL:HG21	1:D:193:VAL:HG13	1.84	0.59
1:E:44:THR:HA	1:E:99:ARG:HA	1.85	0.59
1:B:55:PRO:HG3	1:C:182:GLN:HE21	1.67	0.59
1:E:227:SER:HB3	1:E:230:GLU:HG3	1.83	0.59
2:F:1318:ZPC:H23	1:J:91:ARG:HH22	1.66	0.59
1:C:211:PRO:O	1:C:215:ILE:HG12	2.03	0.59
1:D:178:LEU:HD12	1:D:180:SER:HB3	1.85	0.59
1:A:249:THR:O	1:A:253:LEU:HB2	2.03	0.59
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.85	0.59
1:G:101:ILE:HD13	2:H:1318:ZPC:CL	2.40	0.59
1:I:175:TYR:O	1:I:186:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:O	1:B:181:VAL:N	2.36	0.59
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.85	0.59
1:E:179:SER:O	1:E:182:GLN:N	2.36	0.59
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.20	0.59
1:D:211:PRO:O	1:D:215:ILE:HG12	2.03	0.59
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.85	0.59
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.83	0.59
1:F:114:MET:HE3	1:F:124:GLN:HG2	1.84	0.59
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.85	0.59
1:F:145:ILE:HD12	1:F:191:ILE:HG21	1.84	0.58
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.38	0.58
1:C:101:ILE:HD13	2:D:1318:ZPC:CL	2.40	0.58
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.32	0.58
1:G:122:ASP:N	1:G:122:ASP:OD1	2.37	0.58
1:G:48:ARG:HB2	1:G:48:ARG:NH1	2.18	0.58
1:D:71:LEU:HD11	1:D:94:LEU:HD21	1.86	0.58
1:D:221:SER:HB2	1:E:281:ILE:HD11	1.84	0.58
1:A:95:PHE:HB2	1:A:99:ARG:HG2	1.86	0.58
1:A:268:ALA:HB1	1:A:308:PHE:HE1	1.69	0.58
1:F:44:THR:HA	1:F:99:ARG:HA	1.85	0.58
1:F:224:TRP:CH2	1:F:301:ARG:HB3	2.39	0.58
1:F:179:SER:O	1:F:181:VAL:N	2.37	0.58
1:H:150:GLU:OE2	2:I:1318:ZPC:C17	2.45	0.58
1:A:177:HIS:O	1:A:179:SER:N	2.36	0.58
1:J:114:MET:HE2	1:J:124:GLN:HG2	1.85	0.58
1:H:91:ARG:HD2	1:I:134:SER:HB3	1.86	0.58
1:F:22:LYS:HE3	1:F:24:TYR:CG	2.39	0.57
1:H:28:THR:HG21	1:H:254:PRO:HB2	1.85	0.57
1:I:91:ARG:HB2	1:J:133:PHE:CE2	2.33	0.57
1:B:19:PHE:CE2	2:C:1318:ZPC:C15	2.87	0.57
1:I:58:VAL:HB	1:I:92:LEU:HB2	1.86	0.57
1:B:216:ILE:O	1:B:219:SER:HB3	2.04	0.57
1:A:122:ASP:N	1:A:122:ASP:OD1	2.34	0.57
1:F:263:ASP:O	1:F:267:ILE:HG12	2.03	0.57
1:F:33:TYR:OH	1:F:127:VAL:N	2.37	0.57
1:H:212:LEU:HD11	1:H:265:MET:HB3	1.87	0.57
1:H:31:GLN:HG2	1:H:114:MET:HB2	1.86	0.57
1:A:299:ARG:HA	1:A:301:ARG:HG3	1.86	0.57
1:A:178:LEU:HD12	1:A:180:SER:HB3	1.86	0.57
1:H:212:LEU:O	1:H:216:ILE:HG12	2.05	0.57
1:J:263:ASP:O	1:J:267:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HA	1:A:298:GLN:OE1	2.05	0.57
1:C:216:ILE:O	1:C:219:SER:HB3	2.05	0.57
1:A:289:ASN:OD1	1:A:292:GLU:N	2.38	0.57
1:C:136:ASN:HD22	1:C:136:ASN:N	2.03	0.57
1:F:136:ASN:ND2	1:F:139:GLN:OE1	2.38	0.57
1:I:219:SER:HA	1:I:238:LEU:HD21	1.87	0.56
1:I:173:ILE:HD13	1:I:190:ARG:HB3	1.85	0.56
1:I:294:ASP:HB2	1:I:297:ILE:CG2	2.35	0.56
1:G:223:PHE:HE2	1:G:304:PHE:CE1	2.22	0.56
1:E:262:ILE:O	1:E:266:ILE:HG12	2.05	0.56
1:I:145:ILE:HD12	1:I:191:ILE:CG2	2.35	0.56
1:E:123:ARG:HD2	1:E:198:VAL:HG22	1.86	0.56
1:B:103:ASN:HD21	2:C:1318:ZPC:H06A	1.69	0.56
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.87	0.56
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.88	0.56
1:A:284:HIS:HE1	1:E:226:GLU:OE2	1.89	0.56
1:E:145:ILE:HG21	1:E:191:ILE:HG12	1.87	0.56
1:E:28:THR:HB	1:E:256:LEU:HD21	1.87	0.56
1:C:145:ILE:HG23	1:C:168:THR:HG21	1.86	0.56
1:E:227:SER:OG	1:E:228:PHE:N	2.39	0.56
1:A:14:VAL:HG22	1:A:43:TRP:HB3	1.88	0.56
1:C:91:ARG:CD	1:D:134:SER:HB3	2.36	0.55
1:A:212:LEU:O	1:A:216:ILE:HG12	2.06	0.55
1:B:248:TYR:HA	1:C:247:PHE:CE1	2.42	0.55
1:I:150:GLU:OE2	2:J:1318:ZPC:H17	2.06	0.55
1:B:91:ARG:HB2	1:C:133:PHE:HE2	1.70	0.55
1:G:224:TRP:CH2	1:G:301:ARG:HB3	2.41	0.55
1:E:19:PHE:CD1	1:E:148:TYR:HB2	2.41	0.55
1:B:20:ILE:HB	1:B:149:THR:HG22	1.87	0.55
1:H:219:SER:HA	1:H:238:LEU:HD21	1.88	0.55
1:D:147:VAL:HG21	1:D:193:VAL:CG1	2.36	0.55
1:C:145:ILE:HD12	1:C:191:ILE:HG21	1.88	0.55
1:C:19:PHE:CE1	1:C:148:TYR:CD2	2.95	0.55
1:B:150:GLU:OE1	2:C:1318:ZPC:H17	2.06	0.55
1:E:227:SER:O	1:E:231:ARG:HD3	2.07	0.55
1:B:177:HIS:O	1:B:179:SER:N	2.40	0.55
1:F:216:ILE:O	1:F:219:SER:HB3	2.07	0.55
1:C:44:THR:HA	1:C:99:ARG:HA	1.88	0.55
1:J:145:ILE:HD12	1:J:191:ILE:HG21	1.89	0.55
1:G:212:LEU:O	1:G:216:ILE:HG12	2.06	0.55
1:C:241:THR:HA	1:D:240:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:ILE:HD13	2:J:1318:ZPC:CL	2.43	0.55
1:F:91:ARG:NH2	2:G:1318:ZPC:H23	2.22	0.55
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.87	0.55
1:F:178:LEU:HD12	1:F:180:SER:HB3	1.87	0.55
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.89	0.55
1:C:105:ARG:HD3	1:D:77:GLU:OE2	2.06	0.55
1:C:294:ASP:HB2	1:C:297:ILE:CG2	2.37	0.55
1:E:133:PHE:HA	2:E:1318:ZPC:C01	2.36	0.55
1:A:133:PHE:HA	2:A:1318:ZPC:C01	2.37	0.55
1:A:58:VAL:HB	1:A:92:LEU:HB2	1.88	0.55
1:C:301:ARG:O	1:C:305:PRO:HG2	2.07	0.54
1:B:249:THR:HG23	1:B:253:LEU:HD22	1.89	0.54
1:A:133:PHE:CD1	2:A:1318:ZPC:H07A	2.42	0.54
1:F:27:ASN:HB3	1:F:32:THR:HB	1.88	0.54
1:D:79:ILE:N	1:D:129:GLU:O	2.37	0.54
1:C:81:VAL:HG12	1:C:83:GLY:O	2.07	0.54
1:D:223:PHE:HE2	1:D:304:PHE:CE1	2.26	0.54
1:J:127:VAL:HG22	1:J:194:ARG:HG2	1.88	0.54
1:A:216:ILE:O	1:A:219:SER:HB3	2.07	0.54
1:G:62:GLN:O	1:G:66:TRP:HD1	1.91	0.54
1:H:122:ASP:OD1	1:H:122:ASP:N	2.40	0.54
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.72	0.54
1:B:224:TRP:CH2	1:B:301:ARG:HB3	2.42	0.54
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.90	0.54
1:J:136:ASN:H	1:J:136:ASN:HD22	1.56	0.54
1:D:289:ASN:OD1	1:D:290:GLY:N	2.40	0.54
1:E:133:PHE:O	2:E:1318:ZPC:N02	2.40	0.54
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.73	0.54
1:D:293:ASP:O	1:D:298:GLN:NE2	2.41	0.54
1:B:172:ASP:HB2	1:I:141:ARG:NH2	2.22	0.54
1:E:294:ASP:O	1:E:298:GLN:HG2	2.08	0.54
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.26	0.53
1:G:294:ASP:O	1:G:298:GLN:HG2	2.07	0.53
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.88	0.53
1:F:133:PHE:O	2:F:1318:ZPC:N02	2.42	0.53
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.25	0.53
1:J:175:TYR:O	1:J:186:ASN:ND2	2.40	0.53
1:D:294:ASP:HB2	1:D:297:ILE:CG2	2.38	0.53
1:I:212:LEU:HD12	1:I:265:MET:HB3	1.90	0.53
1:J:138:GLN:OE1	1:J:185:GLN:HB3	2.07	0.53
1:C:119:PHE:CE2	1:C:254:PRO:HG3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:SER:O	1:F:40:VAL:HG23	2.09	0.53
1:B:145:ILE:HG22	1:B:170:ILE:HD11	1.91	0.53
1:D:156:GLU:HA	1:D:200:ASN:ND2	2.24	0.53
1:E:212:LEU:HD11	1:E:265:MET:HB3	1.90	0.53
1:B:55:PRO:HB3	1:B:95:PHE:CE1	2.43	0.53
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.91	0.53
1:E:299:ARG:HA	1:E:301:ARG:HG3	1.89	0.53
1:D:44:THR:HA	1:D:99:ARG:HA	1.90	0.53
1:F:204:TYR:O	1:F:209:ILE:HG12	2.09	0.53
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.27	0.53
1:H:122:ASP:OD2	1:H:199:ARG:NH2	2.41	0.53
1:B:145:ILE:HD12	1:B:191:ILE:HG21	1.90	0.53
1:C:203:TYR:HB2	1:D:258:TYR:HA	1.91	0.53
1:F:295:LEU:HA	1:F:298:GLN:NE2	2.24	0.52
1:G:119:PHE:HA	1:G:122:ASP:OD1	2.09	0.52
1:I:260:THR:N	1:I:263:ASP:OD2	2.27	0.52
1:B:283:ALA:O	1:B:293:ASP:HA	2.09	0.52
1:G:40:VAL:HG11	2:H:1318:ZPC:H26	1.91	0.52
1:B:212:LEU:HD12	1:B:265:MET:HB3	1.91	0.52
1:J:178:LEU:HD12	1:J:180:SER:CB	2.38	0.52
1:H:212:LEU:HD12	1:H:265:MET:SD	2.49	0.52
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.75	0.52
1:B:78:PHE:HB3	1:B:81:VAL:HB	1.91	0.52
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.90	0.52
1:J:93:MET:HB3	1:J:101:ILE:HB	1.92	0.52
1:A:133:PHE:HA	2:A:1318:ZPC:H01A	1.92	0.52
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.90	0.52
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.92	0.52
1:I:133:PHE:CE1	2:I:1318:ZPC:H07A	2.44	0.52
1:H:178:LEU:HD12	1:H:180:SER:HB3	1.91	0.52
1:G:224:TRP:CZ3	1:G:301:ARG:HB3	2.45	0.52
1:G:177:HIS:O	1:G:179:SER:N	2.42	0.52
1:B:248:TYR:CD1	1:C:247:PHE:HA	2.45	0.52
1:A:295:LEU:O	1:A:299:ARG:NE	2.42	0.52
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.44	0.52
1:D:65:ARG:HD2	1:E:68:ASN:ND2	2.24	0.52
1:G:224:TRP:HD1	1:H:285:HIS:CD2	2.27	0.52
1:B:95:PHE:HE2	1:B:101:ILE:HD12	1.75	0.52
1:D:178:LEU:HD12	1:D:180:SER:CB	2.39	0.52
1:A:212:LEU:HD23	1:A:245:TYR:CD1	2.45	0.52
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:ASP:O	1:H:96:PRO:HG3	2.10	0.52
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.92	0.52
1:J:132:PRO:HD3	1:J:142:PHE:CE2	2.45	0.52
1:B:91:ARG:HD2	1:C:134:SER:CB	2.40	0.52
1:E:145:ILE:HG23	1:E:168:THR:CG2	2.40	0.52
1:C:89:ASN:HB2	1:D:133:PHE:CE1	2.44	0.51
1:E:33:TYR:OH	1:E:127:VAL:N	2.38	0.51
1:H:26:VAL:CG1	1:H:114:MET:HE1	2.40	0.51
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.40	0.51
1:D:263:ASP:O	1:D:267:ILE:HG12	2.10	0.51
1:A:114:MET:HE2	1:A:116:PHE:CZ	2.44	0.51
1:H:119:PHE:HA	1:H:122:ASP:OD1	2.11	0.51
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.75	0.51
1:F:145:ILE:HG23	1:F:168:THR:HG21	1.91	0.51
1:E:145:ILE:HD12	1:E:191:ILE:HG21	1.92	0.51
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.92	0.51
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.92	0.51
1:E:179:SER:OG	1:E:180:SER:N	2.44	0.51
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.93	0.51
1:B:178:LEU:HD12	1:B:180:SER:HB3	1.92	0.51
1:D:27:ASN:HB3	1:D:32:THR:HB	1.91	0.51
1:H:211:PRO:O	1:H:215:ILE:HG12	2.09	0.51
1:C:93:MET:HB3	1:C:101:ILE:HB	1.93	0.51
1:D:133:PHE:CE1	2:D:1318:ZPC:H07A	2.46	0.51
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.45	0.51
1:H:42:GLN:HG3	1:H:101:ILE:HG12	1.91	0.51
1:A:249:THR:HG23	1:A:253:LEU:HD22	1.92	0.51
1:I:249:THR:HG23	1:I:253:LEU:HD22	1.92	0.51
1:F:144:ASP:OD2	1:F:146:GLN:NE2	2.39	0.51
1:F:122:ASP:N	1:F:122:ASP:OD1	2.32	0.51
1:I:177:HIS:O	1:I:179:SER:N	2.42	0.51
2:A:1318:ZPC:H23	1:E:91:ARG:HH22	1.76	0.51
1:B:131:GLU:OE2	2:B:1318:ZPC:H01B	2.10	0.51
1:C:224:TRP:CH2	1:C:301:ARG:HB3	2.46	0.51
1:B:145:ILE:HG23	1:B:168:THR:HG21	1.91	0.51
1:J:219:SER:HA	1:J:238:LEU:HD11	1.93	0.51
1:E:249:THR:HG23	1:E:253:LEU:HD22	1.93	0.51
1:I:133:PHE:O	2:I:1318:ZPC:H03A	2.11	0.51
1:A:294:ASP:HB2	1:A:297:ILE:HG22	1.92	0.51
1:H:212:LEU:HD21	1:H:266:ILE:HD13	1.93	0.51
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:223:PHE:HE2	1:I:304:PHE:CE1	2.29	0.51
1:F:250:SER:OG	1:J:248:TYR:HE1	1.94	0.51
1:A:150:GLU:OE2	2:B:1318:ZPC:H17	2.10	0.50
1:E:210:LEU:HB3	1:E:211:PRO:CD	2.42	0.50
1:C:18:ILE:HD13	1:C:39:ILE:HG23	1.93	0.50
1:I:289:ASN:OD1	1:I:290:GLY:N	2.43	0.50
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.45	0.50
1:D:219:SER:HA	1:D:238:LEU:HD21	1.93	0.50
1:H:212:LEU:HD23	1:H:245:TYR:CD1	2.47	0.50
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.28	0.50
1:D:302:LEU:C	1:D:305:PRO:HD2	2.32	0.50
1:D:149:THR:C	1:D:151:ASN:H	2.15	0.50
1:G:107:LEU:HD23	1:H:83:GLY:N	2.27	0.50
1:A:145:ILE:HG23	1:A:168:THR:HG21	1.94	0.50
1:H:224:TRP:HD1	1:I:285:HIS:ND1	2.10	0.50
1:C:208:PHE:O	1:C:245:TYR:OH	2.29	0.50
1:H:223:PHE:HE2	1:H:304:PHE:CE1	2.30	0.50
2:F:1318:ZPC:H23	1:J:91:ARG:NH2	2.25	0.50
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.94	0.50
1:G:204:TYR:O	1:G:209:ILE:HG12	2.11	0.50
1:A:145:ILE:HD12	1:A:191:ILE:HG21	1.94	0.50
1:F:95:PHE:HE2	1:F:101:ILE:HD12	1.77	0.50
1:G:132:PRO:O	2:G:1318:ZPC:H01A	2.11	0.50
1:B:103:ASN:HD21	2:C:1318:ZPC:C06	2.25	0.50
1:B:91:ARG:NH2	1:B:93:MET:SD	2.83	0.50
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.94	0.50
1:C:123:ARG:CD	1:C:198:VAL:HG22	2.37	0.50
1:J:212:LEU:O	1:J:216:ILE:HG12	2.12	0.50
1:J:155:GLU:OE2	1:J:163:ARG:NH1	2.44	0.50
1:F:133:PHE:CE1	2:F:1318:ZPC:H07A	2.46	0.50
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.93	0.50
1:A:253:LEU:HG	1:A:254:PRO:HD2	1.94	0.50
1:B:145:ILE:HG21	1:B:191:ILE:HG12	1.94	0.50
2:A:1318:ZPC:H06	1:E:38:TYR:CE2	2.47	0.49
1:A:212:LEU:HD11	1:A:265:MET:HB3	1.94	0.49
1:G:145:ILE:HD12	1:G:191:ILE:HG21	1.94	0.49
1:J:149:THR:O	1:J:151:ASN:N	2.44	0.49
1:A:77:GLU:OE2	1:E:105:ARG:HD3	2.12	0.49
1:E:33:TYR:OH	1:E:127:VAL:O	2.27	0.49
1:H:26:VAL:HG13	1:H:114:MET:HE1	1.94	0.49
1:I:27:ASN:HB3	1:I:32:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:GLN:HG3	1:G:148:TYR:OH	2.12	0.49
1:D:133:PHE:O	2:D:1318:ZPC:C07	2.61	0.49
1:E:225:LEU:HD22	1:E:230:GLU:HB3	1.94	0.49
1:D:264:GLN:HA	1:D:267:ILE:HG12	1.95	0.49
1:F:157:ILE:HD11	1:G:117:ARG:HE	1.77	0.49
1:G:149:THR:C	1:G:151:ASN:H	2.16	0.49
1:A:44:THR:HA	1:A:99:ARG:HA	1.95	0.49
1:J:149:THR:C	1:J:151:ASN:H	2.16	0.49
1:C:210:LEU:HB3	1:C:211:PRO:CD	2.42	0.49
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.48	0.49
1:G:212:LEU:HD12	1:G:265:MET:SD	2.53	0.49
1:D:156:GLU:HA	1:D:200:ASN:HD21	1.78	0.49
1:F:146:GLN:HG3	1:F:148:TYR:OH	2.11	0.49
1:E:204:TYR:O	1:E:208:PHE:HB2	2.12	0.49
1:I:97:ASP:OD1	1:I:99:ARG:HD3	2.13	0.49
1:C:38:TYR:CE2	2:D:1318:ZPC:H06	2.48	0.49
1:I:224:TRP:CZ3	1:I:301:ARG:HB3	2.46	0.49
1:J:71:LEU:HD11	1:J:94:LEU:HD21	1.94	0.49
1:F:220:TRP:CE3	1:F:305:PRO:HB3	2.47	0.49
1:I:146:GLN:HG3	1:I:148:TYR:OH	2.13	0.49
1:F:122:ASP:CG	1:F:199:ARG:HE	2.15	0.49
1:C:173:ILE:O	1:C:187:GLU:HA	2.12	0.49
1:F:58:VAL:HB	1:F:92:LEU:HB2	1.93	0.49
1:I:131:GLU:OE1	1:I:190:ARG:NH2	2.44	0.49
1:J:173:ILE:O	1:J:187:GLU:HA	2.13	0.49
1:F:232:LEU:HD22	1:J:225:LEU:HD21	1.94	0.49
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.95	0.49
1:A:247:PHE:CE1	1:E:248:TYR:HA	2.48	0.48
1:B:21:ASN:ND2	1:B:37:GLY:HA2	2.28	0.48
1:A:118:LEU:HA	1:A:261:VAL:HG23	1.93	0.48
1:E:179:SER:O	1:E:181:VAL:N	2.45	0.48
1:D:145:ILE:HG23	1:D:168:THR:HG21	1.94	0.48
1:A:284:HIS:CE1	1:E:226:GLU:OE2	2.67	0.48
1:D:248:TYR:HE1	1:E:250:SER:OG	1.97	0.48
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.96	0.48
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.48	0.48
1:B:136:ASN:ND2	1:B:185:GLN:HB2	2.28	0.48
1:C:142:PHE:HB3	1:C:170:ILE:HD13	1.95	0.48
1:I:302:LEU:C	1:I:305:PRO:HD2	2.33	0.48
1:D:131:GLU:OE1	1:D:190:ARG:NE	2.45	0.48
1:D:28:THR:HG21	1:D:254:PRO:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TRP:CZ3	1:A:301:ARG:HB3	2.48	0.48
1:D:76:LEU:HB3	1:D:130:LEU:CD2	2.43	0.48
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.95	0.48
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.44	0.48
1:E:232:LEU:O	1:E:235:SER:OG	2.26	0.48
1:A:145:ILE:HG23	1:A:168:THR:CG2	2.44	0.48
1:B:24:TYR:OH	1:B:107:LEU:HD21	2.14	0.48
1:A:66:TRP:O	1:A:71:LEU:HB2	2.13	0.48
1:A:236:PHE:CD2	1:E:234:THR:HG21	2.47	0.48
1:A:133:PHE:CE1	1:E:89:ASN:HB2	2.49	0.48
1:G:205:LEU:HA	1:G:209:ILE:CG1	2.44	0.48
1:G:249:THR:HG23	1:G:253:LEU:HD22	1.96	0.48
1:B:14:VAL:HG21	1:B:140:LEU:HD21	1.95	0.48
1:E:114:MET:HE2	1:E:124:GLN:HG2	1.96	0.48
1:J:18:ILE:HB	1:J:147:VAL:HG22	1.95	0.48
1:C:163:ARG:HD3	1:C:163:ARG:HA	1.58	0.48
1:I:212:LEU:HD11	1:I:265:MET:HB3	1.95	0.48
1:J:228:PHE:HA	1:J:231:ARG:NH1	2.29	0.48
1:D:248:TYR:O	1:D:252:ILE:HG12	2.14	0.48
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.95	0.48
1:E:72:TRP:CH2	1:E:74:PRO:HG3	2.49	0.48
1:H:105:ARG:HD3	1:I:77:GLU:OE2	2.13	0.47
1:F:294:ASP:O	1:F:298:GLN:HG2	2.14	0.47
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.95	0.47
1:E:129:GLU:HG2	1:E:192:THR:HG23	1.95	0.47
1:I:53:ASP:O	1:I:96:PRO:HG3	2.14	0.47
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.95	0.47
1:A:149:THR:OG1	1:A:165:LYS:HE2	2.14	0.47
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.97	0.47
1:G:112:ASN:ND2	1:G:125:GLN:O	2.46	0.47
1:A:91:ARG:HH22	2:B:1318:ZPC:H23	1.78	0.47
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.96	0.47
1:G:122:ASP:OD2	1:G:199:ARG:NH2	2.47	0.47
1:H:253:LEU:HG	1:H:254:PRO:HD2	1.96	0.47
1:A:80:ASN:ND2	1:A:110:PHE:HB3	2.28	0.47
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.95	0.47
1:J:136:ASN:HB2	1:J:187:GLU:O	2.15	0.47
1:A:286:ARG:HD3	1:A:286:ARG:HA	1.61	0.47
1:H:91:ARG:NH2	2:I:1318:ZPC:H23	2.28	0.47
1:B:131:GLU:OE1	1:B:190:ARG:NH2	2.46	0.47
1:A:212:LEU:HD23	1:A:245:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASP:O	1:B:295:LEU:N	2.47	0.47
1:H:227:SER:HB3	1:H:230:GLU:CG	2.44	0.47
1:E:285:HIS:O	1:E:287:GLN:NE2	2.43	0.47
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.96	0.47
1:C:157:ILE:HD13	1:C:157:ILE:HA	1.70	0.47
1:C:263:ASP:O	1:C:267:ILE:HG12	2.14	0.47
1:F:48:ARG:NH1	1:F:48:ARG:HB2	2.30	0.47
1:I:294:ASP:O	1:I:298:GLN:HG2	2.14	0.47
1:H:95:PHE:HB2	1:H:99:ARG:HG2	1.97	0.47
1:C:110:PHE:CE2	1:C:128:LEU:HG	2.49	0.47
1:F:22:LYS:HG2	1:F:24:TYR:CD1	2.50	0.47
1:E:211:PRO:O	1:E:215:ILE:HG12	2.14	0.47
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.50	0.47
1:D:47:PRO:HA	1:D:98:GLY:HA2	1.95	0.47
1:E:48:ARG:HB2	1:E:48:ARG:NH1	2.30	0.47
1:H:82:VAL:HG23	1:H:111:SER:HB2	1.97	0.47
1:E:133:PHE:HA	2:E:1318:ZPC:H01	1.95	0.47
1:H:232:LEU:HD23	1:H:236:PHE:HE2	1.79	0.47
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.80	0.47
1:B:132:PRO:HG3	1:B:140:LEU:HD22	1.97	0.47
1:B:313:CYS:HA	1:B:316:VAL:HG23	1.97	0.47
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.96	0.47
1:G:289:ASN:CG	1:G:292:GLU:HB2	2.36	0.47
1:H:241:THR:HA	1:I:240:LEU:HD23	1.97	0.47
1:I:48:ARG:HB2	1:I:48:ARG:NH1	2.29	0.47
1:F:91:ARG:HB2	1:G:133:PHE:CE2	2.48	0.46
1:A:81:VAL:O	1:E:105:ARG:NH2	2.48	0.46
1:F:224:TRP:CZ2	1:F:301:ARG:HB3	2.51	0.46
1:C:145:ILE:HG23	1:C:168:THR:CG2	2.45	0.46
1:E:299:ARG:C	1:E:301:ARG:H	2.18	0.46
1:D:125:GLN:NE2	1:D:194:ARG:HD3	2.30	0.46
1:A:157:ILE:HD11	1:B:117:ARG:HE	1.79	0.46
1:H:145:ILE:HG21	1:H:191:ILE:HG12	1.97	0.46
1:C:178:LEU:HD12	1:C:180:SER:CB	2.41	0.46
1:D:294:ASP:O	1:D:298:GLN:HG2	2.15	0.46
1:E:253:LEU:HG	1:E:254:PRO:HD2	1.97	0.46
1:E:136:ASN:ND2	1:E:185:GLN:HB2	2.29	0.46
1:G:287:GLN:HB3	1:G:292:GLU:HB3	1.98	0.46
1:A:26:VAL:HG13	1:A:114:MET:HE1	1.98	0.46
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.61	0.46
1:I:212:LEU:HD12	1:I:265:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:GLU:OE2	1:F:161:TRP:HB3	2.16	0.46
1:B:225:LEU:HD12	1:B:231:ARG:HA	1.97	0.46
1:J:224:TRP:CH2	1:J:301:ARG:HB3	2.51	0.46
1:G:132:PRO:HD3	1:G:142:PHE:CE2	2.51	0.46
1:E:178:LEU:HD13	1:E:178:LEU:HA	1.86	0.46
1:I:145:ILE:HD12	1:I:191:ILE:HG23	1.98	0.46
1:B:72:TRP:CZ2	1:B:140:LEU:HD12	2.50	0.46
1:D:157:ILE:HD11	1:E:117:ARG:NE	2.31	0.46
1:J:58:VAL:HB	1:J:92:LEU:HB2	1.98	0.46
1:H:78:PHE:HB3	1:H:81:VAL:HB	1.97	0.46
1:D:95:PHE:HE1	1:D:101:ILE:HD12	1.81	0.46
1:H:155:GLU:OE2	1:H:161:TRP:HB3	2.16	0.46
1:B:91:ARG:HB2	1:C:133:PHE:CE2	2.50	0.46
1:I:145:ILE:HD12	1:I:191:ILE:HG21	1.97	0.46
1:I:66:TRP:O	1:I:71:LEU:HB2	2.15	0.46
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.97	0.46
1:I:221:SER:HB2	1:J:281:ILE:HD11	1.96	0.46
1:A:267:ILE:HD12	1:E:206:TRP:O	2.16	0.46
1:H:72:TRP:CZ2	1:H:74:PRO:HB3	2.51	0.46
1:E:26:VAL:HG22	1:E:33:TYR:HB3	1.98	0.45
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.98	0.45
1:B:225:LEU:HD21	1:C:232:LEU:HD22	1.98	0.45
1:D:107:LEU:HD12	1:D:108:GLY:N	2.31	0.45
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.34	0.45
1:D:80:ASN:ND2	1:D:111:SER:O	2.29	0.45
1:I:143:SER:OG	1:I:144:ASP:N	2.49	0.45
1:G:27:ASN:HB3	1:G:32:THR:HB	1.98	0.45
1:B:289:ASN:OD1	1:B:292:GLU:HB2	2.16	0.45
1:D:133:PHE:CD1	2:D:1318:ZPC:H07A	2.51	0.45
1:B:54:LYS:HB3	1:B:55:PRO:HD2	1.99	0.45
1:B:145:ILE:HG23	1:B:168:THR:CG2	2.46	0.45
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.97	0.45
1:I:215:ILE:HD13	1:J:239:MET:CE	2.46	0.45
1:B:58:VAL:HB	1:B:92:LEU:HB2	1.98	0.45
1:C:227:SER:HB3	1:C:230:GLU:CG	2.45	0.45
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.97	0.45
1:H:295:LEU:O	1:H:299:ARG:HB2	2.16	0.45
1:G:87:THR:HG21	1:G:90:LYS:HE3	1.98	0.45
1:H:179:SER:OG	1:H:180:SER:N	2.49	0.45
1:E:304:PHE:CD1	1:E:304:PHE:C	2.90	0.45
1:H:216:ILE:HD12	1:H:269:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:LEU:HD12	1:G:265:MET:HB3	1.99	0.45
1:D:112:ASN:ND2	1:D:125:GLN:O	2.49	0.45
1:I:199:ARG:O	1:I:201:PRO:HD3	2.16	0.45
1:F:289:ASN:OD1	1:F:292:GLU:HB2	2.17	0.45
1:F:28:THR:HB	1:F:256:LEU:HD21	1.98	0.45
1:E:304:PHE:HD1	1:E:304:PHE:C	2.18	0.45
1:I:211:PRO:HB3	1:J:270:TYR:CD2	2.52	0.45
1:F:210:LEU:HB3	1:F:211:PRO:CD	2.47	0.45
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.52	0.45
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.76	0.45
1:C:295:LEU:HA	1:C:298:GLN:OE1	2.16	0.45
1:D:181:VAL:HG11	2:D:1318:ZPC:CL	2.53	0.45
1:I:253:LEU:HD21	1:I:262:ILE:CD1	2.46	0.45
1:B:312:GLY:O	1:B:315:LEU:HB2	2.17	0.45
1:C:27:ASN:HB3	1:C:32:THR:HB	1.98	0.45
1:F:16:VAL:O	1:F:145:ILE:HA	2.16	0.45
1:J:295:LEU:O	1:J:299:ARG:HB2	2.16	0.45
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.65	0.45
1:J:276:ALA:HB2	1:J:304:PHE:HZ	1.80	0.45
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.74	0.45
1:C:212:LEU:HB2	1:C:245:TYR:HH	1.82	0.45
1:G:89:ASN:HB2	1:H:133:PHE:CE1	2.51	0.45
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.52	0.45
1:C:146:GLN:HG3	1:C:148:TYR:OH	2.16	0.45
1:A:114:MET:HE2	1:A:116:PHE:HZ	1.82	0.45
1:F:55:PRO:HB3	1:F:95:PHE:CD1	2.52	0.45
1:J:227:SER:O	1:J:231:ARG:HD3	2.17	0.45
1:J:228:PHE:HA	1:J:231:ARG:HH11	1.82	0.45
1:D:157:ILE:HA	1:D:157:ILE:HD13	1.76	0.45
1:I:21:ASN:HD21	1:I:38:TYR:HE1	1.64	0.45
1:I:31:GLN:HG2	1:I:114:MET:HB2	1.98	0.45
1:H:33:TYR:OH	1:H:127:VAL:N	2.39	0.45
1:D:62:GLN:NE2	1:E:67:ILE:HG22	2.32	0.45
1:A:162:ILE:HD13	1:A:197:ALA:HB2	1.98	0.45
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.46	0.45
1:B:252:ILE:HG13	1:C:250:SER:HB3	1.99	0.45
1:C:179:SER:OG	1:C:180:SER:N	2.50	0.44
1:A:236:PHE:HZ	1:E:221:SER:OG	2.00	0.44
1:F:248:TYR:HE1	1:G:250:SER:OG	2.00	0.44
1:C:20:ILE:HB	1:C:149:THR:HG22	1.98	0.44
1:B:131:GLU:OE1	1:B:190:ARG:NE	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:VAL:HG21	2:H:1318:ZPC:CL	2.54	0.44
1:J:114:MET:CE	1:J:124:GLN:HG2	2.46	0.44
1:I:149:THR:O	1:I:151:ASN:N	2.47	0.44
1:A:132:PRO:O	2:A:1318:ZPC:H01A	2.17	0.44
1:G:40:VAL:HG21	2:H:1318:ZPC:H27	1.98	0.44
1:J:179:SER:O	1:J:181:VAL:N	2.50	0.44
1:D:66:TRP:HB3	1:D:71:LEU:HD12	1.98	0.44
1:I:80:ASN:OD1	1:I:129:GLU:N	2.50	0.44
1:G:24:TYR:CE2	1:G:34:LYS:HD2	2.53	0.44
1:H:24:TYR:CE2	1:H:34:LYS:HD2	2.52	0.44
1:J:294:ASP:HB2	1:J:297:ILE:CG2	2.41	0.44
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.76	0.44
1:G:260:THR:HG23	1:G:263:ASP:OD2	2.18	0.44
1:B:63:ILE:HD12	1:B:90:LYS:HB3	1.98	0.44
1:A:86:ASP:HB3	1:A:107:LEU:HB3	1.99	0.44
1:C:273:ILE:O	1:C:277:ILE:HG12	2.18	0.44
1:B:50:THR:HB	1:B:56:LEU:HB2	1.99	0.44
1:E:301:ARG:O	1:E:305:PRO:HG2	2.18	0.44
1:C:295:LEU:O	1:C:299:ARG:HB2	2.17	0.44
1:F:76:LEU:HB3	1:F:130:LEU:HD21	2.00	0.44
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.67	0.44
1:J:133:PHE:HA	2:J:1318:ZPC:H01A	1.99	0.44
1:A:77:GLU:OE1	2:A:1318:ZPC:H01	2.17	0.44
1:F:294:ASP:HB2	1:F:297:ILE:CG2	2.45	0.44
1:G:168:THR:HG22	1:G:169:HIS:N	2.32	0.44
1:F:119:PHE:CG	1:F:120:PRO:HA	2.53	0.44
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.98	0.44
1:E:289:ASN:OD1	1:E:292:GLU:N	2.51	0.44
1:B:120:PRO:HD2	1:B:121:PHE:CE2	2.52	0.44
1:C:249:THR:O	1:C:253:LEU:HB2	2.18	0.44
1:C:227:SER:HB3	1:C:230:GLU:HG3	2.00	0.44
1:J:112:ASN:ND2	1:J:125:GLN:O	2.51	0.44
1:E:142:PHE:HB3	1:E:170:ILE:HD13	2.00	0.44
1:J:177:HIS:C	1:J:179:SER:H	2.21	0.44
1:A:248:TYR:HA	1:B:247:PHE:CE1	2.52	0.44
1:D:224:TRP:CH2	1:D:301:ARG:HB3	2.51	0.44
1:I:210:LEU:HB3	1:I:211:PRO:CD	2.47	0.44
1:B:51:PRO:HD2	1:B:56:LEU:HG	2.00	0.44
1:C:120:PRO:HD2	1:C:121:PHE:CE2	2.53	0.44
1:A:211:PRO:O	1:A:215:ILE:HG12	2.17	0.44
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:ARG:HB3	1:G:174:ARG:HH11	1.82	0.44
1:G:147:VAL:HG21	1:G:193:VAL:HG13	1.99	0.44
1:I:212:LEU:HD21	1:I:266:ILE:HD13	2.00	0.43
1:G:89:ASN:O	1:G:104:ALA:HA	2.17	0.43
1:B:95:PHE:HB2	1:B:99:ARG:HG2	1.99	0.43
1:C:248:TYR:HA	1:D:247:PHE:CE1	2.53	0.43
1:A:147:VAL:HG21	1:A:193:VAL:HG13	2.00	0.43
1:H:56:LEU:HD12	1:H:94:LEU:HD12	1.99	0.43
1:B:241:THR:HA	1:C:240:LEU:HD23	1.99	0.43
1:A:223:PHE:CE2	1:A:304:PHE:CE1	3.02	0.43
1:A:236:PHE:CD2	1:E:234:THR:CG2	3.01	0.43
1:B:155:GLU:OE2	1:B:161:TRP:HB3	2.18	0.43
1:I:95:PHE:HE2	1:I:101:ILE:HD12	1.83	0.43
1:J:95:PHE:HB2	1:J:99:ARG:HG2	1.99	0.43
1:C:221:SER:OG	1:D:236:PHE:HZ	2.01	0.43
1:B:157:ILE:HD11	1:C:115:ASP:OD2	2.18	0.43
1:C:28:THR:HG22	1:C:116:PHE:CE2	2.53	0.43
1:J:223:PHE:HE2	1:J:304:PHE:CE1	2.36	0.43
1:G:263:ASP:O	1:G:267:ILE:HG12	2.17	0.43
1:C:212:LEU:HD23	1:C:245:TYR:CD1	2.54	0.43
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.75	0.43
1:H:26:VAL:HG22	1:H:33:TYR:HB3	2.01	0.43
1:A:131:GLU:OE1	1:A:190:ARG:NH2	2.39	0.43
1:D:149:THR:O	1:D:151:ASN:N	2.45	0.43
1:A:155:GLU:OE2	1:A:161:TRP:HB3	2.18	0.43
1:E:58:VAL:HB	1:E:92:LEU:HB2	1.99	0.43
1:B:220:TRP:CE3	1:B:305:PRO:HB3	2.53	0.43
1:A:173:ILE:HD13	1:A:190:ARG:CB	2.49	0.43
1:J:301:ARG:O	1:J:305:PRO:HG2	2.18	0.43
1:F:211:PRO:O	1:F:215:ILE:HG12	2.19	0.43
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.53	0.43
1:I:178:LEU:HD12	1:I:180:SER:HB3	2.00	0.43
1:H:136:ASN:HD22	1:H:136:ASN:H	1.66	0.43
1:I:89:ASN:HB2	1:J:133:PHE:CD1	2.54	0.43
1:D:38:TYR:CE2	2:E:1318:ZPC:H06A	2.54	0.43
1:H:173:ILE:O	1:H:187:GLU:HA	2.19	0.43
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.61	0.43
1:B:223:PHE:HE2	1:B:304:PHE:CE1	2.36	0.43
1:I:181:VAL:HG11	2:I:1318:ZPC:CL	2.56	0.43
1:C:219:SER:HA	1:C:238:LEU:HD21	1.99	0.43
1:A:177:HIS:CE1	1:E:148:TYR:CD1	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:VAL:C	1:C:128:LEU:HD12	2.39	0.43
1:H:149:THR:C	1:H:151:ASN:H	2.20	0.43
1:B:211:PRO:HB3	1:C:270:TYR:CD2	2.53	0.43
1:A:227:SER:HB3	1:A:230:GLU:HG3	2.00	0.43
1:C:150:GLU:OE1	2:D:1318:ZPC:H17	2.19	0.43
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.82	0.43
1:B:125:GLN:NE2	1:B:194:ARG:HD3	2.33	0.43
1:J:279:LEU:HD13	1:J:300:CYS:SG	2.59	0.43
1:A:89:ASN:HB2	1:B:133:PHE:CE1	2.54	0.43
1:D:119:PHE:HA	1:D:122:ASP:OD1	2.19	0.43
1:H:227:SER:HB3	1:H:230:GLU:HG3	2.01	0.43
1:H:136:ASN:N	1:H:136:ASN:HD22	2.16	0.43
1:C:76:LEU:HB3	1:C:130:LEU:HD21	2.00	0.43
1:A:273:ILE:O	1:A:277:ILE:HG12	2.19	0.43
1:D:312:GLY:O	1:D:316:VAL:HG23	2.18	0.43
1:H:130:LEU:HA	1:H:130:LEU:HD23	1.90	0.43
1:I:162:ILE:HA	1:I:162:ILE:HD13	1.82	0.43
1:B:238:LEU:HD13	1:C:236:PHE:CD2	2.54	0.42
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.36	0.42
1:H:294:ASP:HB2	1:H:297:ILE:CG2	2.48	0.42
1:B:145:ILE:O	1:B:168:THR:HG21	2.19	0.42
1:G:249:THR:O	1:G:253:LEU:HB2	2.19	0.42
1:F:79:ILE:N	1:F:129:GLU:O	2.44	0.42
1:J:118:LEU:HA	1:J:261:VAL:HG23	2.01	0.42
1:J:157:ILE:HA	1:J:157:ILE:HD13	1.80	0.42
1:B:212:LEU:HD11	1:B:265:MET:HB3	2.00	0.42
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.80	0.42
1:C:145:ILE:HG12	1:C:146:GLN:N	2.32	0.42
1:C:81:VAL:HG11	1:C:85:PRO:HG3	2.00	0.42
1:D:301:ARG:O	1:D:305:PRO:HG2	2.19	0.42
1:E:117:ARG:O	1:E:260:THR:HA	2.19	0.42
1:C:28:THR:HB	1:C:256:LEU:CD2	2.49	0.42
1:A:277:ILE:O	1:A:281:ILE:HD12	2.20	0.42
1:D:117:ARG:HD3	1:D:117:ARG:HH11	1.70	0.42
1:J:28:THR:HG22	1:J:116:PHE:CZ	2.54	0.42
1:F:216:ILE:HG21	1:F:308:PHE:CZ	2.54	0.42
1:G:84:SER:HA	1:G:85:PRO:HD3	1.70	0.42
1:A:145:ILE:HG21	1:A:191:ILE:HG12	2.01	0.42
2:G:1318:ZPC:C08	2:G:1318:ZPC:N22	2.83	0.42
1:A:293:ASP:O	1:A:295:LEU:N	2.52	0.42
1:F:212:LEU:HD23	1:F:245:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:LEU:HB3	1:D:211:PRO:CD	2.49	0.42
1:G:66:TRP:HB3	1:G:71:LEU:HD12	2.02	0.42
1:G:71:LEU:HD11	1:G:94:LEU:HD21	2.01	0.42
1:I:260:THR:O	1:I:263:ASP:HB2	2.19	0.42
1:A:173:ILE:O	1:A:187:GLU:HA	2.18	0.42
1:J:304:PHE:C	1:J:304:PHE:CD1	2.92	0.42
1:D:114:MET:HE2	1:D:116:PHE:CZ	2.54	0.42
1:E:157:ILE:HD13	1:E:157:ILE:HA	1.89	0.42
1:H:302:LEU:C	1:H:305:PRO:HD2	2.40	0.42
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.43	0.42
1:A:133:PHE:CE2	1:E:91:ARG:HB2	2.54	0.42
1:I:92:LEU:HA	1:I:92:LEU:HD23	1.85	0.42
1:I:114:MET:HB3	1:I:116:PHE:CE2	2.53	0.42
1:F:18:ILE:O	1:F:147:VAL:HA	2.20	0.42
1:D:84:SER:HA	1:D:85:PRO:HD3	1.78	0.42
1:F:157:ILE:HA	1:F:157:ILE:HD13	1.82	0.42
1:C:26:VAL:HG13	1:C:114:MET:HE1	2.02	0.42
1:A:21:ASN:ND2	1:A:37:GLY:HA2	2.34	0.42
1:I:157:ILE:HD11	1:J:117:ARG:HE	1.85	0.42
1:B:200:ASN:HA	1:B:201:PRO:HD3	1.84	0.42
1:G:289:ASN:OD1	1:G:292:GLU:HB2	2.19	0.42
1:A:212:LEU:HD12	1:A:265:MET:SD	2.60	0.42
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.49	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.74	0.42
1:I:263:ASP:O	1:I:267:ILE:HG12	2.20	0.42
1:B:232:LEU:O	1:B:235:SER:OG	2.35	0.42
1:J:27:ASN:HB3	1:J:32:THR:HB	2.02	0.42
1:H:300:CYS:HB2	1:H:303:ALA:HB3	2.02	0.42
1:F:284:HIS:CE1	1:J:226:GLU:OE2	2.65	0.42
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.40	0.42
1:B:63:ILE:CD1	1:B:90:LYS:HB3	2.50	0.42
1:H:64:GLU:HA	1:H:67:ILE:HD12	2.01	0.42
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.78	0.42
1:J:289:ASN:OD1	1:J:290:GLY:N	2.48	0.42
1:D:40:VAL:HG11	2:E:1318:ZPC:C26	2.50	0.42
1:B:112:ASN:ND2	1:B:125:GLN:O	2.53	0.42
1:C:212:LEU:HD23	1:C:245:TYR:CE1	2.55	0.42
1:I:216:ILE:HD12	1:I:269:GLY:HA2	2.02	0.42
1:A:157:ILE:HD12	1:B:115:ASP:HA	2.01	0.42
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.55	0.42
1:C:289:ASN:OD1	1:C:290:GLY:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:TRP:O	1:B:267:ILE:HD12	2.20	0.42
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.74	0.42
1:C:145:ILE:HG21	1:C:191:ILE:HG23	2.02	0.42
1:D:227:SER:HB3	1:D:230:GLU:CG	2.49	0.42
1:H:221:SER:OG	1:I:236:PHE:HZ	2.02	0.42
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.55	0.42
1:F:23:ILE:HD11	1:F:195:ILE:HD13	2.02	0.42
1:H:147:VAL:HG21	1:H:193:VAL:HG13	2.02	0.42
1:H:277:ILE:O	1:H:281:ILE:HD12	2.19	0.42
1:H:289:ASN:OD1	1:H:290:GLY:N	2.52	0.42
1:F:214:LEU:HD22	1:G:274:PHE:CG	2.55	0.42
1:H:204:TYR:O	1:H:208:PHE:HB2	2.20	0.42
1:B:163:ARG:HA	1:B:163:ARG:HD3	1.70	0.42
1:A:138:GLN:OE1	1:A:185:GLN:HB3	2.20	0.42
2:A:1318:ZPC:C23	1:E:91:ARG:HH22	2.33	0.41
1:G:19:PHE:CE2	2:H:1318:ZPC:C15	3.03	0.41
1:A:303:ALA:O	1:A:306:LEU:HG	2.20	0.41
1:I:26:VAL:CG1	1:I:114:MET:HE1	2.51	0.41
1:B:276:ALA:HB2	1:B:304:PHE:HZ	1.85	0.41
1:E:55:PRO:HB3	1:E:95:PHE:CD2	2.55	0.41
1:G:163:ARG:HD3	1:G:163:ARG:HA	1.68	0.41
1:B:89:ASN:HB2	1:C:133:PHE:CE1	2.55	0.41
1:F:120:PRO:HD2	1:F:121:PHE:CE2	2.55	0.41
1:B:223:PHE:CE2	1:B:304:PHE:CE1	3.09	0.41
1:D:72:TRP:CH2	1:D:74:PRO:HG3	2.55	0.41
1:G:72:TRP:CZ2	1:G:74:PRO:HB3	2.55	0.41
1:B:60:ASN:OD1	1:B:89:ASN:HA	2.19	0.41
1:G:205:LEU:HA	1:G:209:ILE:HG12	2.01	0.41
1:B:44:THR:HA	1:B:99:ARG:HA	2.01	0.41
1:D:299:ARG:C	1:D:301:ARG:H	2.23	0.41
1:I:178:LEU:HD13	1:I:178:LEU:HA	1.84	0.41
1:F:281:ILE:HD11	1:J:221:SER:HB2	2.01	0.41
1:H:120:PRO:HD2	1:H:121:PHE:CE2	2.55	0.41
1:F:257:PRO:HD2	1:F:258:TYR:CE1	2.54	0.41
1:E:225:LEU:HD13	1:E:230:GLU:O	2.20	0.41
1:I:247:PHE:CD2	1:J:247:PHE:CE2	3.07	0.41
1:F:178:LEU:HD12	1:F:180:SER:CB	2.48	0.41
1:G:175:TYR:O	1:G:186:ASN:ND2	2.40	0.41
1:J:183:PRO:C	1:J:185:GLN:H	2.23	0.41
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.01	0.41
1:A:12:VAL:HG11	1:A:72:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASN:HB2	1:C:61:THR:H	1.57	0.41
1:J:294:ASP:O	1:J:298:GLN:HG2	2.21	0.41
1:E:178:LEU:HD12	1:E:180:SER:CB	2.48	0.41
1:B:127:VAL:HG22	1:B:194:ARG:HG2	2.02	0.41
1:G:18:ILE:CD1	1:G:39:ILE:HG12	2.42	0.41
1:E:295:LEU:O	1:E:299:ARG:HB2	2.20	0.41
1:I:248:TYR:HE1	1:J:250:SER:OG	2.03	0.41
1:A:294:ASP:HB3	1:A:297:ILE:H	1.86	0.41
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.39	0.41
1:C:97:ASP:OD1	1:C:99:ARG:HD3	2.20	0.41
1:B:86:ASP:N	1:B:107:LEU:O	2.49	0.41
1:J:227:SER:HB3	1:J:230:GLU:HG3	2.02	0.41
1:F:285:HIS:CD2	1:J:224:TRP:HD1	2.39	0.41
1:A:263:ASP:O	1:A:267:ILE:HG12	2.20	0.41
1:G:153:ASP:HB3	1:G:154:ASN:OD1	2.20	0.41
1:F:14:VAL:HG22	1:F:43:TRP:HB3	2.02	0.41
1:A:64:GLU:CG	1:E:61:THR:HG21	2.50	0.41
1:G:40:VAL:HG11	2:H:1318:ZPC:C26	2.51	0.41
1:D:16:VAL:O	1:D:145:ILE:HA	2.21	0.41
1:A:216:ILE:HD12	1:A:216:ILE:HG23	1.78	0.41
1:C:232:LEU:HD11	1:C:281:ILE:HD11	2.01	0.41
1:B:71:LEU:HD11	1:B:94:LEU:HD21	2.02	0.41
1:C:261:VAL:HA	1:C:264:GLN:NE2	2.35	0.41
1:F:133:PHE:CD1	2:F:1318:ZPC:H01	2.55	0.41
1:F:66:TRP:O	1:F:71:LEU:HB2	2.21	0.41
1:B:122:ASP:OD2	1:B:199:ARG:NH2	2.45	0.41
1:C:136:ASN:OD1	1:C:185:GLN:HB2	2.21	0.41
1:C:62:GLN:O	1:C:66:TRP:HD1	2.02	0.41
1:A:247:PHE:CG	1:B:247:PHE:CE2	3.08	0.41
1:J:212:LEU:CD1	1:J:265:MET:HB3	2.50	0.41
1:G:58:VAL:HB	1:G:92:LEU:HB2	2.02	0.41
1:H:29:LEU:HA	1:H:29:LEU:HD23	1.76	0.41
1:B:48:ARG:NH1	1:B:48:ARG:HB2	2.36	0.41
1:C:82:VAL:HG23	1:C:111:SER:HB2	2.02	0.41
1:B:294:ASP:O	1:B:296:LEU:N	2.54	0.41
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.91	0.41
1:J:249:THR:O	1:J:253:LEU:HB2	2.21	0.41
1:G:297:ILE:HD13	1:G:297:ILE:HG21	1.89	0.41
1:B:219:SER:HA	1:B:238:LEU:HD21	2.03	0.41
1:H:232:LEU:CD2	1:H:236:PHE:HE2	2.34	0.41
1:D:62:GLN:OE1	1:D:65:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.77	0.41
1:D:39:ILE:HG21	1:D:39:ILE:HD13	1.82	0.41
1:C:216:ILE:HD12	1:C:269:GLY:HA2	2.03	0.40
1:G:178:LEU:HA	1:G:178:LEU:HD13	1.90	0.40
1:E:228:PHE:HA	1:E:231:ARG:NH1	2.37	0.40
1:I:131:GLU:OE2	1:I:175:TYR:HE2	2.05	0.40
1:C:16:VAL:O	1:C:145:ILE:HA	2.21	0.40
1:C:19:PHE:CE1	1:C:148:TYR:HD2	2.38	0.40
1:I:259:THR:HA	1:I:263:ASP:OD2	2.20	0.40
1:G:61:THR:HG21	1:H:64:GLU:HG3	2.02	0.40
1:I:84:SER:HA	1:I:85:PRO:HD3	1.78	0.40
1:G:31:GLN:HG2	1:G:114:MET:HB2	2.03	0.40
1:I:122:ASP:N	1:I:122:ASP:OD1	2.53	0.40
1:C:204:TYR:O	1:C:208:PHE:HB2	2.21	0.40
1:B:224:TRP:HD1	1:C:285:HIS:CD2	2.39	0.40
1:B:227:SER:HB3	1:B:230:GLU:CG	2.51	0.40
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.65	0.40
1:F:50:THR:HG23	1:F:96:PRO:HB3	2.03	0.40
1:G:35:VAL:HG21	1:G:128:LEU:HD11	2.03	0.40
1:D:118:LEU:HA	1:D:261:VAL:HG23	2.03	0.40
1:J:312:GLY:O	1:J:316:VAL:HG23	2.21	0.40
1:H:214:LEU:HD23	1:H:214:LEU:HA	1.86	0.40
1:H:231:ARG:HH11	1:H:231:ARG:HD3	1.73	0.40
1:B:249:THR:CG2	1:B:253:LEU:HD22	2.50	0.40
1:J:145:ILE:HG12	1:J:146:GLN:N	2.35	0.40
1:A:66:TRP:HB3	1:A:71:LEU:HD12	2.04	0.40
1:C:76:LEU:HB3	1:C:130:LEU:CD2	2.51	0.40
1:H:153:ASP:HB3	1:H:154:ASN:OD1	2.21	0.40
1:G:55:PRO:HB3	1:G:95:PHE:CD1	2.56	0.40
1:F:133:PHE:CE2	1:J:91:ARG:HB2	2.54	0.40
1:G:132:PRO:HG3	1:G:140:LEU:HD22	2.02	0.40
1:C:177:HIS:C	1:C:179:SER:H	2.24	0.40
1:I:238:LEU:HD12	1:I:238:LEU:HA	1.69	0.40
1:D:212:LEU:HD12	1:D:265:MET:HB3	2.04	0.40
1:G:205:LEU:HD23	1:G:205:LEU:HA	1.92	0.40
1:I:299:ARG:HA	1:I:301:ARG:HG3	2.04	0.40
1:A:233:GLN:O	1:A:236:PHE:HB2	2.20	0.40
1:J:304:PHE:HD1	1:J:304:PHE:C	2.24	0.40
1:G:200:ASN:HA	1:G:201:PRO:HD3	1.96	0.40
1:C:56:LEU:HA	1:C:56:LEU:HD22	1.80	0.40
1:D:133:PHE:O	2:D:1318:ZPC:N02	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.56	0.40
1:A:179:SER:OG	1:A:180:SER:N	2.54	0.40
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.38	0.40
1:D:204:TYR:O	1:D:209:ILE:HG12	2.22	0.40
1:C:114:MET:HE2	1:C:116:PHE:HZ	1.87	0.40
1:A:227:SER:HB3	1:A:230:GLU:CG	2.52	0.40
1:E:35:VAL:HG21	1:E:128:LEU:HD11	2.03	0.40
1:F:117:ARG:HD3	1:F:117:ARG:HH11	1.73	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	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	5	35
1	B	305/307 (99%)	274 (90%)	21 (7%)	10 (3%)	5	33
1	C	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	5	35
1	D	305/307 (99%)	274 (90%)	22 (7%)	9 (3%)	5	35
1	E	305/307 (99%)	275 (90%)	21 (7%)	9 (3%)	5	35
1	F	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	5	35
1	G	305/307 (99%)	278 (91%)	17 (6%)	10 (3%)	5	33
1	H	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	5	35
1	I	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	5	35
1	J	305/307 (99%)	271 (89%)	25 (8%)	9 (3%)	5	35
All	All	3050/3070 (99%)	2754 (90%)	204 (7%)	92 (3%)	5	35

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	178	LEU
1	A	179	SER
1	A	180	SER
1	B	60	ASN
1	B	166	ALA
1	B	178	LEU
1	B	179	SER
1	B	180	SER
1	C	166	ALA
1	C	178	LEU
1	C	179	SER
1	C	180	SER
1	D	60	ASN
1	D	166	ALA
1	D	178	LEU
1	D	179	SER
1	D	180	SER
1	E	60	ASN
1	E	178	LEU
1	E	179	SER
1	E	180	SER
1	F	60	ASN
1	F	178	LEU
1	F	179	SER
1	F	180	SER
1	G	60	ASN
1	G	166	ALA
1	G	178	LEU
1	G	179	SER
1	G	180	SER
1	H	60	ASN
1	H	166	ALA
1	H	178	LEU
1	H	179	SER
1	H	180	SER
1	I	60	ASN
1	I	166	ALA
1	I	178	LEU
1	I	179	SER
1	I	180	SER
1	J	60	ASN
1	J	178	LEU

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Mol	Chain	Res	Type
1	J	179	SER
1	J	180	SER
1	A	53	ASP
1	B	53	ASP
1	B	152	ILE
1	C	53	ASP
1	C	152	ILE
1	D	152	ILE
1	E	53	ASP
1	E	152	ILE
1	F	53	ASP
1	F	152	ILE
1	G	53	ASP
1	G	152	ILE
1	G	294	ASP
1	H	53	ASP
1	H	153	ASP
1	I	152	ILE
1	J	53	ASP
1	J	152	ILE
1	A	152	ILE
1	A	153	ASP
1	A	294	ASP
1	B	150	GLU
1	B	153	ASP
1	B	294	ASP
1	C	294	ASP
1	D	53	ASP
1	D	150	GLU
1	D	153	ASP
1	E	153	ASP
1	F	294	ASP
1	G	153	ASP
1	H	150	GLU
1	I	53	ASP
1	I	150	GLU
1	J	153	ASP
1	C	153	ASP
1	E	200	ASN
1	F	150	GLU
1	F	153	ASP
1	J	150	GLU

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Mol	Chain	Res	Type
1	J	294	ASP
1	A	166	ALA
1	C	60	ASN
1	G	150	GLU
1	H	152	ILE
1	I	294	ASP
1	E	150	GLU

### 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	274/275 (100%)	249 (91%)	25 (9%)	12	41
1	B	274/275 (100%)	250 (91%)	24 (9%)	12	43
1	C	274/275 (100%)	248 (90%)	26 (10%)	11	38
1	D	274/275 (100%)	250 (91%)	24 (9%)	12	43
1	E	274/275 (100%)	250 (91%)	24 (9%)	12	43
1	F	274/275 (100%)	250 (91%)	24 (9%)	12	43
1	G	274/275 (100%)	245 (89%)	29 (11%)	8	33
1	H	274/275 (100%)	248 (90%)	26 (10%)	11	38
1	I	274/275 (100%)	245 (89%)	29 (11%)	8	33
1	J	274/275 (100%)	253 (92%)	21 (8%)	16	51
All	All	2740/2750 (100%)	2488 (91%)	252 (9%)	11	40

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	THR
1	A	56	LEU
1	A	71	LEU
1	A	118	LEU
1	A	122	ASP

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	130	LEU
1	A	134	SER
1	A	136	ASN
1	A	146	GLN
1	A	165	LYS
1	A	178	LEU
1	A	180	SER
1	A	231	ARG
1	A	238	LEU
1	A	239	MET
1	A	240	LEU
1	A	247	PHE
1	A	286	ARG
1	A	287	GLN
1	A	291	VAL
1	A	297	ILE
1	A	302	LEU
1	A	304	PHE
1	B	29	LEU
1	B	32	THR
1	B	39	ILE
1	B	56	LEU
1	B	71	LEU
1	B	81	VAL
1	B	118	LEU
1	B	122	ASP
1	B	130	LEU
1	B	134	SER
1	B	145	ILE
1	B	146	GLN
1	B	154	ASN
1	B	165	LYS
1	B	169	HIS
1	B	178	LEU
1	B	180	SER
1	B	231	ARG
1	B	238	LEU
1	B	240	LEU
1	B	247	PHE
1	B	287	GLN
1	B	302	LEU

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Mol	Chain	Res	Type
1	B	304	PHE
1	C	29	LEU
1	C	32	THR
1	C	39	ILE
1	C	56	LEU
1	C	71	LEU
1	C	79	ILE
1	C	118	LEU
1	C	122	ASP
1	C	124	GLN
1	C	130	LEU
1	C	134	SER
1	C	136	ASN
1	C	146	GLN
1	C	165	LYS
1	C	178	LEU
1	C	180	SER
1	C	210	LEU
1	C	222	VAL
1	C	238	LEU
1	C	239	MET
1	C	240	LEU
1	C	247	PHE
1	C	287	GLN
1	C	291	VAL
1	C	302	LEU
1	C	304	PHE
1	D	29	LEU
1	D	32	THR
1	D	56	LEU
1	D	71	LEU
1	D	118	LEU
1	D	122	ASP
1	D	124	GLN
1	D	130	LEU
1	D	134	SER
1	D	145	ILE
1	D	146	GLN
1	D	165	LYS
1	D	168	THR
1	D	169	HIS
1	D	178	LEU

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Mol	Chain	Res	Type
1	D	180	SER
1	D	210	LEU
1	D	231	ARG
1	D	238	LEU
1	D	240	LEU
1	D	247	PHE
1	D	287	GLN
1	D	291	VAL
1	D	304	PHE
1	E	29	LEU
1	E	39	ILE
1	E	56	LEU
1	E	71	LEU
1	E	118	LEU
1	E	124	GLN
1	E	130	LEU
1	E	134	SER
1	E	145	ILE
1	E	146	GLN
1	E	157	ILE
1	E	165	LYS
1	E	178	LEU
1	E	180	SER
1	E	219	SER
1	E	231	ARG
1	E	238	LEU
1	E	239	MET
1	E	240	LEU
1	E	247	PHE
1	E	287	GLN
1	E	291	VAL
1	E	302	LEU
1	E	304	PHE
1	F	32	THR
1	F	39	ILE
1	F	40	VAL
1	F	56	LEU
1	F	71	LEU
1	F	118	LEU
1	F	122	ASP
1	F	124	GLN
1	F	130	LEU

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Mol	Chain	Res	Type
1	F	134	SER
1	F	145	ILE
1	F	146	GLN
1	F	165	LYS
1	F	178	LEU
1	F	180	SER
1	F	210	LEU
1	F	238	LEU
1	F	240	LEU
1	F	247	PHE
1	F	258	TYR
1	F	287	GLN
1	F	291	VAL
1	F	302	LEU
1	F	304	PHE
1	G	29	LEU
1	G	32	THR
1	G	56	LEU
1	G	107	LEU
1	G	118	LEU
1	G	122	ASP
1	G	123	ARG
1	G	124	GLN
1	G	130	LEU
1	G	134	SER
1	G	136	ASN
1	G	146	GLN
1	G	154	ASN
1	G	165	LYS
1	G	169	HIS
1	G	174	ARG
1	G	178	LEU
1	G	180	SER
1	G	222	VAL
1	G	231	ARG
1	G	238	LEU
1	G	239	MET
1	G	240	LEU
1	G	247	PHE
1	G	287	GLN
1	G	291	VAL
1	G	293	ASP

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Mol	Chain	Res	Type
1	G	302	LEU
1	G	304	PHE
1	H	29	LEU
1	H	32	THR
1	H	39	ILE
1	H	56	LEU
1	H	71	LEU
1	H	81	VAL
1	H	118	LEU
1	H	122	ASP
1	H	124	GLN
1	H	130	LEU
1	H	134	SER
1	H	136	ASN
1	H	145	ILE
1	H	146	GLN
1	H	154	ASN
1	H	165	LYS
1	H	178	LEU
1	H	180	SER
1	H	219	SER
1	H	231	ARG
1	H	238	LEU
1	H	239	MET
1	H	247	PHE
1	H	287	GLN
1	H	291	VAL
1	H	304	PHE
1	I	28	THR
1	I	29	LEU
1	I	32	THR
1	I	39	ILE
1	I	56	LEU
1	I	71	LEU
1	I	81	VAL
1	I	118	LEU
1	I	122	ASP
1	I	124	GLN
1	I	130	LEU
1	I	134	SER
1	I	145	ILE
1	I	146	GLN

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Mol	Chain	Res	Type
1	I	165	LYS
1	I	167	SER
1	I	169	HIS
1	I	178	LEU
1	I	180	SER
1	I	189	SER
1	I	231	ARG
1	I	238	LEU
1	I	239	MET
1	I	240	LEU
1	I	258	TYR
1	I	287	GLN
1	I	291	VAL
1	I	302	LEU
1	I	304	PHE
1	J	29	LEU
1	J	32	THR
1	J	39	ILE
1	J	56	LEU
1	J	71	LEU
1	J	118	LEU
1	J	130	LEU
1	J	134	SER
1	J	136	ASN
1	J	146	GLN
1	J	165	LYS
1	J	178	LEU
1	J	180	SER
1	J	238	LEU
1	J	239	MET
1	J	240	LEU
1	J	247	PHE
1	J	287	GLN
1	J	291	VAL
1	J	302	LEU
1	J	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	182	GLN

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Mol	Chain	Res	Type
1	B	103	ASN
1	B	125	GLN
1	B	182	GLN
1	C	68	ASN
1	C	136	ASN
1	C	139	GLN
1	C	182	GLN
1	C	233	GLN
1	C	284	HIS
1	C	285	HIS
1	D	182	GLN
1	D	264	GLN
1	D	298	GLN
1	E	284	HIS
1	F	103	ASN
1	F	264	GLN
1	F	284	HIS
1	F	285	HIS
1	F	298	GLN
1	G	136	ASN
1	G	185	GLN
1	G	264	GLN
1	H	103	ASN
1	H	136	ASN
1	H	285	HIS
1	I	298	GLN
1	J	124	GLN
1	J	284	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

10 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	ZPC	A	1318	-	29,30,30	2.76	9 (31%)	34,43,43	4.51	22 (64%)
2	ZPC	B	1318	-	29,30,30	2.97	10 (34%)	34,43,43	4.34	20 (58%)
2	ZPC	C	1318	-	29,30,30	2.67	11 (37%)	34,43,43	5.82	22 (64%)
2	ZPC	D	1318	-	29,30,30	2.78	9 (31%)	34,43,43	4.67	19 (55%)
2	ZPC	E	1318	-	29,30,30	2.72	9 (31%)	34,43,43	4.66	25 (73%)
2	ZPC	F	1318	-	29,30,30	2.77	10 (34%)	34,43,43	5.08	25 (73%)
2	ZPC	G	1318	-	29,30,30	2.83	9 (31%)	34,43,43	4.70	24 (70%)
2	ZPC	H	1318	-	29,30,30	2.85	11 (37%)	34,43,43	4.10	20 (58%)
2	ZPC	I	1318	-	29,30,30	2.68	8 (27%)	34,43,43	3.73	20 (58%)
2	ZPC	J	1318	-	29,30,30	2.30	9 (31%)	34,43,43	4.22	20 (58%)

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	ZPC	A	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	B	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	C	1318	-	-	2/12/38/38	0/4/4/4
2	ZPC	D	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	E	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	F	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	G	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	H	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	I	1318	-	-	0/12/38/38	0/4/4/4
2	ZPC	J	1318	-	-	0/12/38/38	0/4/4/4

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1318	ZPC	C06-N05	-4.82	1.38	1.47
2	E	1318	ZPC	C06-N05	-4.73	1.38	1.47
2	I	1318	ZPC	C06-N05	-4.69	1.38	1.47
2	J	1318	ZPC	C06-N05	-4.33	1.39	1.47
2	B	1318	ZPC	C06-N05	-4.17	1.39	1.47
2	A	1318	ZPC	C06-N05	-3.94	1.40	1.47
2	D	1318	ZPC	C06-N05	-3.87	1.40	1.47
2	G	1318	ZPC	C06-N05	-3.70	1.40	1.47
2	H	1318	ZPC	C06-N05	-3.68	1.40	1.47
2	C	1318	ZPC	C06-N05	-3.64	1.40	1.47
2	E	1318	ZPC	C18-N19	-2.29	1.29	1.34
2	C	1318	ZPC	C20-C11	2.01	1.53	1.51
2	H	1318	ZPC	O10-C11	2.04	1.47	1.43
2	C	1318	ZPC	C18-C17	2.05	1.43	1.38
2	B	1318	ZPC	C18-C17	2.08	1.44	1.38
2	A	1318	ZPC	O10-C11	2.15	1.47	1.43
2	J	1318	ZPC	C26-C24	2.17	1.42	1.38
2	J	1318	ZPC	C18-C17	2.19	1.44	1.38
2	E	1318	ZPC	C26-C24	2.19	1.42	1.38
2	H	1318	ZPC	C18-C17	2.25	1.44	1.38
2	D	1318	ZPC	C26-C24	2.26	1.42	1.38
2	F	1318	ZPC	C18-C17	2.28	1.44	1.38
2	A	1318	ZPC	C26-C24	2.42	1.42	1.38
2	F	1318	ZPC	C26-C24	2.46	1.42	1.38
2	F	1318	ZPC	C20-C11	2.50	1.53	1.51
2	J	1318	ZPC	O10-C08	2.53	1.39	1.34
2	H	1318	ZPC	C26-C24	2.55	1.43	1.38
2	C	1318	ZPC	C21-N22	2.58	1.39	1.34
2	J	1318	ZPC	C27-C26	2.62	1.43	1.38
2	I	1318	ZPC	C26-C24	2.64	1.43	1.38
2	B	1318	ZPC	C27-C26	2.78	1.43	1.38
2	D	1318	ZPC	C20-C11	2.85	1.53	1.51
2	D	1318	ZPC	C27-C26	2.87	1.43	1.38
2	H	1318	ZPC	C20-C11	2.89	1.53	1.51
2	J	1318	ZPC	C13-N12	3.02	1.44	1.38
2	A	1318	ZPC	C27-C26	3.05	1.44	1.38
2	I	1318	ZPC	O10-C08	3.05	1.40	1.34
2	H	1318	ZPC	C27-C26	3.09	1.44	1.38
2	C	1318	ZPC	C13-N12	3.16	1.45	1.38
2	I	1318	ZPC	C27-C26	3.20	1.44	1.38
2	B	1318	ZPC	C26-C24	3.24	1.44	1.38
2	D	1318	ZPC	O10-C08	3.27	1.41	1.34
2	C	1318	ZPC	C26-C24	3.33	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1318	ZPC	C27-C26	3.37	1.44	1.38
2	H	1318	ZPC	C13-N12	3.40	1.45	1.38
2	C	1318	ZPC	C27-C26	3.41	1.44	1.38
2	G	1318	ZPC	C26-C24	3.45	1.44	1.38
2	G	1318	ZPC	O10-C08	3.46	1.41	1.34
2	E	1318	ZPC	O10-C08	3.48	1.41	1.34
2	E	1318	ZPC	C27-C26	3.49	1.45	1.38
2	B	1318	ZPC	O10-C08	3.62	1.41	1.34
2	G	1318	ZPC	C27-C26	3.65	1.45	1.38
2	F	1318	ZPC	O10-C08	3.69	1.42	1.34
2	H	1318	ZPC	O10-C08	3.74	1.42	1.34
2	G	1318	ZPC	C13-N12	3.82	1.46	1.38
2	E	1318	ZPC	C20-N19	3.87	1.38	1.34
2	C	1318	ZPC	C20-N19	4.00	1.38	1.34
2	A	1318	ZPC	C20-N19	4.00	1.38	1.34
2	C	1318	ZPC	O10-C08	4.07	1.42	1.34
2	A	1318	ZPC	O10-C08	4.08	1.42	1.34
2	I	1318	ZPC	C13-N12	4.30	1.47	1.38
2	I	1318	ZPC	C20-N19	4.55	1.39	1.34
2	F	1318	ZPC	C13-N12	4.58	1.48	1.38
2	I	1318	ZPC	C08-N05	4.62	1.44	1.35
2	F	1318	ZPC	C20-N19	4.67	1.39	1.34
2	G	1318	ZPC	C20-C11	4.70	1.55	1.51
2	E	1318	ZPC	C13-N12	4.71	1.48	1.38
2	D	1318	ZPC	C13-N12	4.73	1.48	1.38
2	D	1318	ZPC	C20-N19	4.89	1.39	1.34
2	G	1318	ZPC	C20-N19	5.05	1.39	1.34
2	B	1318	ZPC	C20-C11	5.11	1.55	1.51
2	H	1318	ZPC	C08-N05	5.19	1.45	1.35
2	D	1318	ZPC	C08-N05	5.23	1.45	1.35
2	B	1318	ZPC	C08-N05	5.28	1.45	1.35
2	A	1318	ZPC	C13-N12	5.29	1.49	1.38
2	B	1318	ZPC	C13-N12	5.33	1.49	1.38
2	J	1318	ZPC	C20-N19	5.42	1.40	1.34
2	E	1318	ZPC	C08-N05	5.50	1.45	1.35
2	B	1318	ZPC	C20-N19	5.59	1.40	1.34
2	H	1318	ZPC	C20-N19	5.59	1.40	1.34
2	A	1318	ZPC	C08-N05	5.69	1.46	1.35
2	J	1318	ZPC	C21-N12	5.72	1.47	1.42
2	J	1318	ZPC	C08-N05	5.86	1.46	1.35
2	F	1318	ZPC	C08-N05	6.07	1.46	1.35
2	G	1318	ZPC	C08-N05	6.33	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1318	ZPC	C08-N05	6.34	1.47	1.35
2	C	1318	ZPC	C21-N12	7.62	1.49	1.42
2	G	1318	ZPC	C21-N12	7.89	1.49	1.42
2	F	1318	ZPC	C21-N12	8.00	1.49	1.42
2	E	1318	ZPC	C21-N12	8.48	1.49	1.42
2	B	1318	ZPC	C21-N12	8.65	1.50	1.42
2	A	1318	ZPC	C21-N12	8.96	1.50	1.42
2	I	1318	ZPC	C21-N12	9.12	1.50	1.42
2	D	1318	ZPC	C21-N12	9.35	1.50	1.42
2	H	1318	ZPC	C21-N12	9.81	1.51	1.42

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1318	ZPC	C04-N05-C08	-9.14	96.09	121.81
2	C	1318	ZPC	C04-N05-C08	-8.79	97.08	121.81
2	C	1318	ZPC	C04-C03-N02	-8.60	101.71	110.79
2	H	1318	ZPC	C04-N05-C08	-8.52	97.84	121.81
2	J	1318	ZPC	C04-N05-C08	-8.41	98.13	121.81
2	E	1318	ZPC	C04-N05-C08	-7.95	99.45	121.81
2	C	1318	ZPC	O09-C08-N05	-7.73	109.61	124.32
2	A	1318	ZPC	C04-N05-C08	-7.70	100.13	121.81
2	I	1318	ZPC	C04-N05-C08	-7.67	100.22	121.81
2	B	1318	ZPC	C04-N05-C08	-7.40	100.98	121.81
2	F	1318	ZPC	C04-C03-N02	-7.18	103.20	110.79
2	D	1318	ZPC	C04-N05-C08	-7.00	102.11	121.81
2	H	1318	ZPC	O09-C08-N05	-6.29	112.36	124.32
2	G	1318	ZPC	C04-N05-C08	-6.11	104.62	121.81
2	C	1318	ZPC	O10-C08-O09	-5.88	112.61	124.69
2	A	1318	ZPC	O09-C08-N05	-5.82	113.25	124.32
2	B	1318	ZPC	O09-C08-N05	-5.78	113.32	124.32
2	C	1318	ZPC	C24-C23-N22	-5.72	115.22	122.32
2	D	1318	ZPC	O09-C08-N05	-5.60	113.66	124.32
2	B	1318	ZPC	C24-C23-N22	-5.24	115.80	122.32
2	E	1318	ZPC	O09-C08-N05	-5.20	114.42	124.32
2	F	1318	ZPC	O09-C08-N05	-4.58	115.60	124.32
2	G	1318	ZPC	O10-C08-O09	-4.50	115.46	124.69
2	F	1318	ZPC	C27-C21-N22	-4.34	115.16	123.17
2	G	1318	ZPC	O09-C08-N05	-4.23	116.27	124.32
2	D	1318	ZPC	C27-C21-N22	-4.01	115.77	123.17
2	F	1318	ZPC	O10-C08-O09	-3.97	116.55	124.69
2	G	1318	ZPC	C23-C24-CL	-3.92	111.80	120.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1318	ZPC	C24-C23-N22	-3.92	117.45	122.32
2	B	1318	ZPC	O14-C13-C15	-3.83	110.83	128.68
2	J	1318	ZPC	O10-C08-O09	-3.71	117.08	124.69
2	C	1318	ZPC	C15-C20-N19	-3.69	118.25	124.00
2	G	1318	ZPC	C24-C23-N22	-3.63	117.81	122.32
2	A	1318	ZPC	O14-C13-C15	-3.57	112.02	128.68
2	G	1318	ZPC	O14-C13-C15	-3.56	112.10	128.68
2	F	1318	ZPC	O14-C13-C15	-3.52	112.28	128.68
2	C	1318	ZPC	C27-C21-N12	-3.52	119.71	122.21
2	D	1318	ZPC	O14-C13-C15	-3.42	112.74	128.68
2	I	1318	ZPC	C27-C21-N22	-3.36	116.97	123.17
2	E	1318	ZPC	O14-C13-C15	-3.35	113.04	128.68
2	B	1318	ZPC	C15-C20-N19	-3.25	118.93	124.00
2	E	1318	ZPC	C23-C24-CL	-3.24	113.23	120.02
2	G	1318	ZPC	C15-C20-N19	-3.22	118.97	124.00
2	A	1318	ZPC	C24-C23-N22	-3.22	118.32	122.32
2	A	1318	ZPC	C27-C21-N22	-3.19	117.30	123.17
2	E	1318	ZPC	O10-C08-O09	-3.18	118.17	124.69
2	E	1318	ZPC	C27-C21-N22	-3.18	117.31	123.17
2	B	1318	ZPC	C23-C24-CL	-3.14	113.43	120.02
2	H	1318	ZPC	C24-C23-N22	-3.14	118.42	122.32
2	B	1318	ZPC	O10-C08-O09	-3.13	118.26	124.69
2	E	1318	ZPC	C17-C18-N19	-3.07	118.44	122.25
2	J	1318	ZPC	O09-C08-N05	-3.07	118.48	124.32
2	H	1318	ZPC	C27-C21-N22	-3.06	117.52	123.17
2	J	1318	ZPC	C27-C21-N22	-3.03	117.58	123.17
2	C	1318	ZPC	O14-C13-C15	-3.01	114.65	128.68
2	E	1318	ZPC	C24-C23-N22	-2.99	118.61	122.32
2	A	1318	ZPC	O10-C08-O09	-2.98	118.57	124.69
2	I	1318	ZPC	O09-C08-N05	-2.94	118.73	124.32
2	F	1318	ZPC	C24-C23-N22	-2.91	118.70	122.32
2	J	1318	ZPC	C24-C23-N22	-2.90	118.72	122.32
2	F	1318	ZPC	C26-C24-C23	-2.82	117.50	119.46
2	I	1318	ZPC	O14-C13-C15	-2.80	115.65	128.68
2	G	1318	ZPC	C27-C21-N22	-2.76	118.07	123.17
2	C	1318	ZPC	C27-C21-N22	-2.72	118.15	123.17
2	H	1318	ZPC	O10-C08-O09	-2.67	119.20	124.69
2	E	1318	ZPC	C17-N16-C15	-2.63	112.08	116.88
2	J	1318	ZPC	O14-C13-C15	-2.61	116.52	128.68
2	F	1318	ZPC	C17-N16-C15	-2.56	112.20	116.88
2	B	1318	ZPC	C27-C21-N22	-2.55	118.46	123.17
2	A	1318	ZPC	C23-C24-CL	-2.47	114.84	120.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1318	ZPC	C17-N16-C15	-2.45	112.41	116.88
2	H	1318	ZPC	O14-C13-C15	-2.45	117.28	128.68
2	I	1318	ZPC	C23-C24-CL	-2.38	115.04	120.02
2	D	1318	ZPC	C15-C20-N19	-2.30	120.41	124.00
2	D	1318	ZPC	O10-C08-O09	-2.28	120.00	124.69
2	B	1318	ZPC	C17-C18-N19	-2.26	119.45	122.25
2	J	1318	ZPC	C17-C18-N19	-2.24	119.48	122.25
2	H	1318	ZPC	C07-C06-N05	-2.24	105.40	110.49
2	A	1318	ZPC	C15-C20-N19	-2.20	120.57	124.00
2	I	1318	ZPC	C07-C06-N05	-2.17	105.56	110.49
2	A	1318	ZPC	C17-N16-C15	-2.16	112.94	116.88
2	D	1318	ZPC	C17-N16-C15	-2.15	112.95	116.88
2	I	1318	ZPC	C24-C23-N22	-2.13	119.67	122.32
2	G	1318	ZPC	N22-C21-N12	-2.10	112.31	114.31
2	B	1318	ZPC	C17-N16-C15	-2.07	113.11	116.88
2	F	1318	ZPC	C23-C24-CL	-2.04	115.75	120.02
2	F	1318	ZPC	C15-C20-N19	-2.03	120.83	124.00
2	E	1318	ZPC	C20-C15-C13	2.02	113.10	108.51
2	H	1318	ZPC	C04-C03-N02	2.10	113.00	110.79
2	A	1318	ZPC	C21-N12-C11	2.11	120.63	118.44
2	G	1318	ZPC	C06-N05-C08	2.15	127.85	121.81
2	E	1318	ZPC	C06-N05-C08	2.19	127.97	121.81
2	D	1318	ZPC	C26-C27-C21	2.21	120.71	117.57
2	I	1318	ZPC	C26-C27-C21	2.21	120.71	117.57
2	F	1318	ZPC	C20-C15-N16	2.26	125.73	123.46
2	H	1318	ZPC	N22-C21-N12	2.36	116.56	114.31
2	A	1318	ZPC	C06-N05-C08	2.36	128.46	121.81
2	C	1318	ZPC	C20-C15-N16	2.44	125.91	123.46
2	I	1318	ZPC	C06-N05-C04	2.46	117.12	112.56
2	C	1318	ZPC	C21-N12-C11	2.46	120.99	118.44
2	B	1318	ZPC	C18-C17-N16	2.47	125.31	122.25
2	A	1318	ZPC	C06-N05-C04	2.56	117.30	112.56
2	J	1318	ZPC	C27-C21-N12	2.56	124.02	122.21
2	A	1318	ZPC	C07-N02-C03	2.64	112.99	109.53
2	F	1318	ZPC	C06-N05-C08	2.64	129.24	121.81
2	I	1318	ZPC	C27-C21-N12	2.71	124.13	122.21
2	C	1318	ZPC	C27-C26-C24	2.76	122.30	119.23
2	J	1318	ZPC	C26-C24-CL	2.88	124.08	119.35
2	F	1318	ZPC	C01-N02-C03	2.88	115.12	110.63
2	E	1318	ZPC	C04-C03-N02	2.95	113.91	110.79
2	H	1318	ZPC	C26-C24-CL	2.97	124.22	119.35
2	H	1318	ZPC	C06-N05-C08	3.03	130.32	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1318	ZPC	C03-C04-N05	3.04	117.41	110.49
2	G	1318	ZPC	C20-C15-N16	3.09	126.56	123.46
2	J	1318	ZPC	C07-N02-C03	3.13	113.64	109.53
2	C	1318	ZPC	C01-N02-C03	3.14	115.52	110.63
2	G	1318	ZPC	C04-C03-N02	3.16	114.12	110.79
2	E	1318	ZPC	N22-C21-N12	3.23	117.39	114.31
2	I	1318	ZPC	C26-C24-CL	3.24	124.66	119.35
2	B	1318	ZPC	C26-C24-CL	3.25	124.68	119.35
2	D	1318	ZPC	C03-C04-N05	3.45	118.34	110.49
2	B	1318	ZPC	C26-C24-C23	3.49	121.88	119.46
2	J	1318	ZPC	C04-C03-N02	3.51	114.49	110.79
2	A	1318	ZPC	C26-C24-CL	3.51	125.11	119.35
2	F	1318	ZPC	C21-N12-C11	3.76	122.33	118.44
2	H	1318	ZPC	C06-C07-N02	3.90	114.90	110.79
2	I	1318	ZPC	C23-N22-C21	3.92	125.18	117.70
2	J	1318	ZPC	C03-C04-N05	3.95	119.48	110.49
2	E	1318	ZPC	C21-N12-C11	3.96	122.54	118.44
2	H	1318	ZPC	C01-N02-C03	3.97	116.82	110.63
2	J	1318	ZPC	C01-N02-C03	3.98	116.83	110.63
2	F	1318	ZPC	C27-C21-N12	4.14	125.14	122.21
2	E	1318	ZPC	C26-C24-CL	4.16	126.16	119.35
2	E	1318	ZPC	C23-N22-C21	4.17	125.65	117.70
2	B	1318	ZPC	N22-C21-N12	4.25	118.36	114.31
2	J	1318	ZPC	N22-C21-N12	4.26	118.38	114.31
2	H	1318	ZPC	C23-N22-C21	4.30	125.90	117.70
2	G	1318	ZPC	C01-N02-C03	4.32	117.37	110.63
2	E	1318	ZPC	C27-C21-N12	4.35	125.30	122.21
2	J	1318	ZPC	C23-N22-C21	4.38	126.05	117.70
2	H	1318	ZPC	C03-C04-N05	4.39	120.47	110.49
2	D	1318	ZPC	C06-N05-C08	4.43	134.28	121.81
2	A	1318	ZPC	C23-N22-C21	4.45	126.19	117.70
2	E	1318	ZPC	C18-C17-N16	4.46	127.79	122.25
2	F	1318	ZPC	C26-C24-CL	4.51	126.75	119.35
2	C	1318	ZPC	C03-C04-N05	4.52	120.77	110.49
2	I	1318	ZPC	C07-N02-C03	4.56	115.51	109.53
2	C	1318	ZPC	C06-N05-C08	4.56	134.64	121.81
2	B	1318	ZPC	C03-C04-N05	4.56	120.87	110.49
2	E	1318	ZPC	C01-N02-C03	4.65	117.87	110.63
2	I	1318	ZPC	C03-C04-N05	4.66	121.09	110.49
2	I	1318	ZPC	N22-C21-N12	4.78	118.87	114.31
2	H	1318	ZPC	O14-C13-N12	4.97	137.12	126.03
2	H	1318	ZPC	C27-C21-N12	4.99	125.75	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1318	ZPC	C23-N22-C21	5.00	127.24	117.70
2	G	1318	ZPC	C06-C07-N02	5.03	116.11	110.79
2	D	1318	ZPC	C23-N22-C21	5.04	127.31	117.70
2	E	1318	ZPC	C01-N02-C07	5.07	118.53	110.63
2	G	1318	ZPC	C23-N22-C21	5.08	127.38	117.70
2	D	1318	ZPC	C07-N02-C03	5.16	116.30	109.53
2	E	1318	ZPC	C07-N02-C03	5.24	116.41	109.53
2	E	1318	ZPC	C03-C04-N05	5.28	122.50	110.49
2	F	1318	ZPC	C07-N02-C03	5.31	116.50	109.53
2	J	1318	ZPC	O14-C13-N12	5.33	137.91	126.03
2	H	1318	ZPC	C07-N02-C03	5.37	116.58	109.53
2	C	1318	ZPC	C23-N22-C21	5.49	128.16	117.70
2	G	1318	ZPC	C26-C24-CL	5.55	128.45	119.35
2	J	1318	ZPC	C06-C07-N02	5.58	116.68	110.79
2	F	1318	ZPC	N22-C21-N12	5.58	119.63	114.31
2	G	1318	ZPC	C07-N02-C03	5.61	116.89	109.53
2	A	1318	ZPC	N22-C21-N12	5.73	119.77	114.31
2	F	1318	ZPC	C23-N22-C21	5.79	128.74	117.70
2	I	1318	ZPC	O14-C13-N12	5.80	138.96	126.03
2	G	1318	ZPC	C01-N02-C07	5.84	119.73	110.63
2	G	1318	ZPC	C03-C04-N05	6.00	124.14	110.49
2	A	1318	ZPC	C03-C04-N05	6.01	124.15	110.49
2	H	1318	ZPC	C01-N02-C07	6.02	120.01	110.63
2	E	1318	ZPC	C06-C07-N02	6.05	117.18	110.79
2	C	1318	ZPC	O14-C13-N12	6.07	139.57	126.03
2	A	1318	ZPC	C01-N02-C03	6.19	120.28	110.63
2	A	1318	ZPC	C01-N02-C07	6.27	120.40	110.63
2	C	1318	ZPC	C07-N02-C03	6.40	117.93	109.53
2	B	1318	ZPC	C01-N02-C03	6.66	121.01	110.63
2	D	1318	ZPC	O14-C13-N12	6.75	141.09	126.03
2	I	1318	ZPC	C01-N02-C03	6.77	121.18	110.63
2	G	1318	ZPC	O14-C13-N12	6.78	141.16	126.03
2	D	1318	ZPC	C01-N02-C07	6.88	121.36	110.63
2	I	1318	ZPC	C21-N12-C11	6.96	125.64	118.44
2	F	1318	ZPC	O14-C13-N12	7.09	141.84	126.03
2	D	1318	ZPC	C06-C07-N02	7.10	118.28	110.79
2	J	1318	ZPC	C21-N12-C11	7.15	125.84	118.44
2	A	1318	ZPC	C06-C07-N02	7.27	118.47	110.79
2	G	1318	ZPC	C21-N12-C11	7.38	126.08	118.44
2	I	1318	ZPC	C01-N02-C07	7.49	122.31	110.63
2	D	1318	ZPC	C21-N12-C11	7.52	126.22	118.44
2	B	1318	ZPC	C01-N02-C07	7.66	122.57	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1318	ZPC	O10-C08-N05	7.73	118.62	111.25
2	E	1318	ZPC	O14-C13-N12	7.74	143.29	126.03
2	C	1318	ZPC	N22-C21-N12	7.83	121.78	114.31
2	J	1318	ZPC	C01-N02-C07	7.91	122.96	110.63
2	F	1318	ZPC	C01-N02-C07	7.92	122.98	110.63
2	F	1318	ZPC	C06-C07-N02	8.06	119.30	110.79
2	A	1318	ZPC	O14-C13-N12	8.06	144.01	126.03
2	B	1318	ZPC	O14-C13-N12	8.28	144.49	126.03
2	D	1318	ZPC	N22-C21-N12	8.41	122.33	114.31
2	C	1318	ZPC	C01-N02-C07	9.62	125.63	110.63
2	G	1318	ZPC	C27-C21-N12	10.08	129.36	122.21
2	C	1318	ZPC	C06-C07-N02	11.75	123.20	110.79
2	G	1318	ZPC	O10-C08-N05	13.01	123.66	111.25
2	B	1318	ZPC	O10-C08-N05	13.21	123.86	111.25
2	J	1318	ZPC	O10-C08-N05	13.59	124.22	111.25
2	H	1318	ZPC	O10-C08-N05	13.81	124.43	111.25
2	A	1318	ZPC	O10-C08-N05	14.36	124.96	111.25
2	D	1318	ZPC	O10-C08-N05	14.97	125.53	111.25
2	E	1318	ZPC	O10-C08-N05	15.91	126.43	111.25
2	F	1318	ZPC	O10-C08-N05	16.81	127.29	111.25
2	C	1318	ZPC	O10-C08-N05	18.63	129.03	111.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1318	ZPC	N22-C21-N12-C13
2	C	1318	ZPC	C27-C21-N12-C13

There are no ring outliers.

10 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1318	ZPC	9	0
2	B	1318	ZPC	3	0
2	C	1318	ZPC	8	0
2	D	1318	ZPC	12	0
2	E	1318	ZPC	7	0
2	F	1318	ZPC	11	0
2	G	1318	ZPC	6	0
2	H	1318	ZPC	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1318	ZPC	8	0
2	J	1318	ZPC	4	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	307/307 (100%)	-0.00	12 (3%)	43	42	74, 118, 187, 217	0
1	B	307/307 (100%)	0.01	8 (2%)	59	59	71, 108, 171, 263	0
1	C	307/307 (100%)	0.07	16 (5%)	31	30	71, 107, 186, 232	0
1	D	307/307 (100%)	-0.04	10 (3%)	50	49	74, 104, 186, 263	0
1	E	307/307 (100%)	-0.06	6 (1%)	68	67	73, 113, 188, 233	0
1	F	307/307 (100%)	-0.01	14 (4%)	36	35	78, 118, 190, 276	0
1	G	307/307 (100%)	0.02	26 (8%)	13	13	75, 108, 171, 236	0
1	H	307/307 (100%)	0.15	22 (7%)	18	18	75, 111, 187, 279	0
1	I	307/307 (100%)	-0.02	18 (5%)	26	25	76, 106, 192, 274	0
1	J	307/307 (100%)	-0.02	20 (6%)	22	22	77, 115, 203, 261	0
All	All	3070/3070 (100%)	0.01	152 (4%)	32	32	71, 111, 189, 279	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	GLY	11.4
1	C	317	ILE	9.6
1	B	289	ASN	9.5
1	B	290	GLY	9.5
1	H	289	ASN	9.3
1	G	290	GLY	8.8
1	B	291	VAL	8.6
1	C	289	ASN	7.8
1	C	314	VAL	7.6
1	C	291	VAL	7.0
1	F	317	ILE	7.0
1	H	291	VAL	6.8
1	C	290	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
1	I	291	VAL	6.2
1	J	153	ASP	6.2
1	C	315	LEU	6.0
1	I	290	GLY	5.9
1	D	291	VAL	5.6
1	E	291	VAL	5.6
1	F	287	GLN	5.6
1	I	289	ASN	5.5
1	H	150	GLU	5.4
1	H	290	GLY	5.4
1	F	288	ALA	5.1
1	G	314	VAL	5.0
1	J	290	GLY	5.0
1	G	285	HIS	4.9
1	J	308	PHE	4.9
1	C	311	ILE	4.9
1	J	291	VAL	4.7
1	F	285	HIS	4.7
1	D	153	ASP	4.5
1	H	293	ASP	4.4
1	D	157	ILE	4.4
1	A	153	ASP	4.3
1	H	153	ASP	4.3
1	A	314	VAL	4.3
1	H	315	LEU	4.2
1	J	304	PHE	4.2
1	H	314	VAL	4.1
1	A	176	ASP	4.0
1	C	288	ALA	3.9
1	E	289	ASN	3.8
1	G	287	GLN	3.8
1	J	303	ALA	3.8
1	I	292	GLU	3.7
1	H	165	LYS	3.7
1	H	311	ILE	3.7
1	C	316	VAL	3.6
1	I	314	VAL	3.6
1	J	289	ASN	3.6
1	F	49	LYS	3.5
1	G	291	VAL	3.5
1	H	288	ALA	3.5
1	B	293	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	286	ARG	3.5
1	H	312	GLY	3.4
1	A	290	GLY	3.4
1	G	293	ASP	3.4
1	F	290	GLY	3.4
1	H	182	GLN	3.3
1	G	297	ILE	3.3
1	I	288	ALA	3.3
1	J	306	LEU	3.2
1	H	138	GLN	3.2
1	J	156	GLU	3.2
1	D	49	LYS	3.1
1	H	292	GLU	3.1
1	B	292	GLU	3.1
1	A	317	ILE	3.1
1	F	315	LEU	3.0
1	C	312	GLY	3.0
1	J	314	VAL	3.0
1	A	156	GLU	3.0
1	I	153	ASP	3.0
1	G	156	GLU	3.0
1	G	126	PHE	2.9
1	G	161	TRP	2.9
1	I	237	THR	2.9
1	H	66	TRP	2.9
1	B	288	ALA	2.9
1	I	315	LEU	2.9
1	I	154	ASN	2.8
1	E	315	LEU	2.7
1	I	287	GLN	2.7
1	A	151	ASN	2.7
1	F	289	ASN	2.7
1	J	237	THR	2.7
1	G	311	ILE	2.7
1	I	294	ASP	2.7
1	J	305	PRO	2.7
1	J	317	ILE	2.6
1	J	49	LYS	2.6
1	F	180	SER	2.6
1	G	298	GLN	2.6
1	F	296	LEU	2.6
1	J	311	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	160	TRP	2.5
1	G	313	CYS	2.5
1	I	317	ILE	2.5
1	H	181	VAL	2.5
1	G	288	ALA	2.5
1	C	303	ALA	2.5
1	A	175	TYR	2.5
1	G	49	LYS	2.5
1	G	255	ARG	2.5
1	J	157	ILE	2.5
1	C	306	LEU	2.4
1	A	297	ILE	2.4
1	J	315	LEU	2.4
1	D	290	GLY	2.4
1	D	289	ASN	2.4
1	A	298	GLN	2.4
1	H	184	ASN	2.4
1	G	289	ASN	2.3
1	G	292	GLU	2.3
1	F	237	THR	2.3
1	J	154	ASN	2.3
1	C	161	TRP	2.3
1	G	312	GLY	2.3
1	A	49	LYS	2.3
1	I	208	PHE	2.3
1	E	287	GLN	2.3
1	I	286	ARG	2.3
1	D	297	ILE	2.3
1	C	302	LEU	2.3
1	B	46	LYS	2.3
1	H	317	ILE	2.3
1	A	152	ILE	2.2
1	F	176	ASP	2.2
1	E	314	VAL	2.2
1	G	284	HIS	2.2
1	B	47	PRO	2.2
1	J	292	GLU	2.1
1	G	310	ALA	2.1
1	G	157	ILE	2.1
1	I	182	GLN	2.1
1	G	317	ILE	2.1
1	J	234	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	294	ASP	2.1
1	I	295	LEU	2.1
1	D	158	ASP	2.1
1	H	185	GLN	2.1
1	C	292	GLU	2.1
1	H	52	GLY	2.1
1	G	282	PHE	2.1
1	D	181	VAL	2.1
1	H	152	ILE	2.0
1	I	293	ASP	2.0
1	F	169	HIS	2.0
1	C	307	GLY	2.0
1	D	161	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 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(Å <sup>2</sup> )	Q<0.9
2	ZPC	A	1318	27/27	0.87	0.45	1.46	73,96,144,160	0
2	ZPC	D	1318	27/27	0.87	0.29	0.54	49,74,112,136	0
2	ZPC	C	1318	27/27	0.93	0.25	0.39	29,69,126,170	0
2	ZPC	H	1318	27/27	0.88	0.25	0.33	52,91,138,212	0
2	ZPC	E	1318	27/27	0.94	0.20	-0.07	54,79,132,152	0
2	ZPC	G	1318	27/27	0.93	0.18	-0.17	55,91,123,138	0
2	ZPC	I	1318	27/27	0.89	0.22	-0.17	51,84,125,167	0
2	ZPC	B	1318	27/27	0.91	0.17	-0.40	55,84,115,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZPC	J	1318	27/27	0.94	0.17	-0.62	30,62,129,167	0
2	ZPC	F	1318	27/27	0.95	0.17	-0.71	33,81,133,160	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.