



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2016 – 03:50 PM EDT

PDB ID : 5LG3  
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with chlorpromazine  
Authors : Nys, M.; Wijckmans, E.; Farinha, A.; Brams, M.; Spurny, R.; Ulens, C.  
Deposited on : 2016-07-05  
Resolution : 3.57 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:

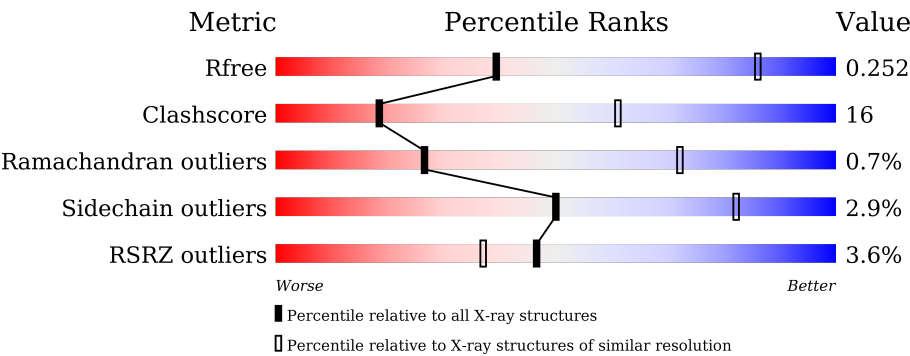
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

# 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 3.57 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	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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><div></div><div>67%</div><div>32%</div><div>.</div></div></div>
1	B	307	<div><div>4%</div><div><div></div><div>67%</div><div>32%</div><div>.</div></div></div>
1	C	307	<div><div>4%</div><div><div></div><div>66%</div><div>32%</div><div>.</div></div></div>
1	D	307	<div><div>3%</div><div><div></div><div>63%</div><div>35%</div><div>.</div></div></div>
1	E	307	<div><div>2%</div><div><div></div><div>68%</div><div>30%</div><div>.</div></div></div>
1	F	307	<div><div>5%</div><div><div></div><div>67%</div><div>32%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	307	 4% 63% 36%
1	H	307	 4% 67% 32%
1	I	307	 2% 68% 31%
1	J	307	 5% 67% 31%

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	Z80	A	401	-	-	-	X
2	Z80	B	401	-	-	-	X
2	Z80	C	401	-	-	-	X
2	Z80	D	401	-	-	-	X
2	Z80	G	401	-	-	X	X
2	Z80	H	401	-	-	-	X

## 2 Entry composition

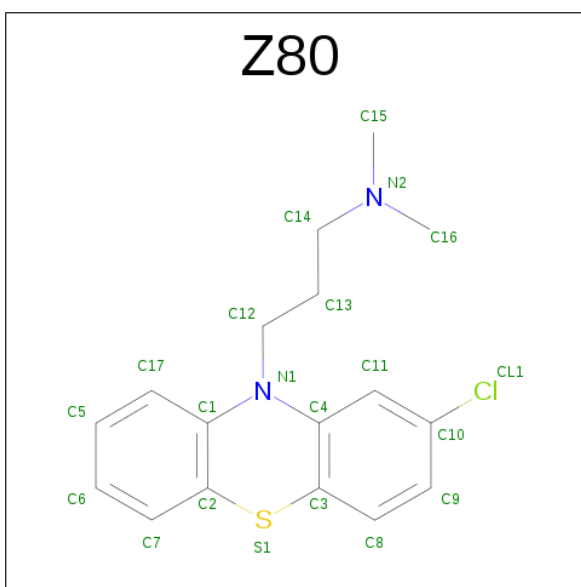
There are 2 unique types of molecules in this entry. The entry contains 25255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gamma-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2504	1633	415	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2501	1631	416	448	6			
1	J	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			

- Molecule 2 is 3-(2-chloro-10H-phenothiazin-10-yl)-N,N-dimethylpropan-1-amine (three-letter code: Z80) (formula: C<sub>17</sub>H<sub>19</sub>ClN<sub>2</sub>S).

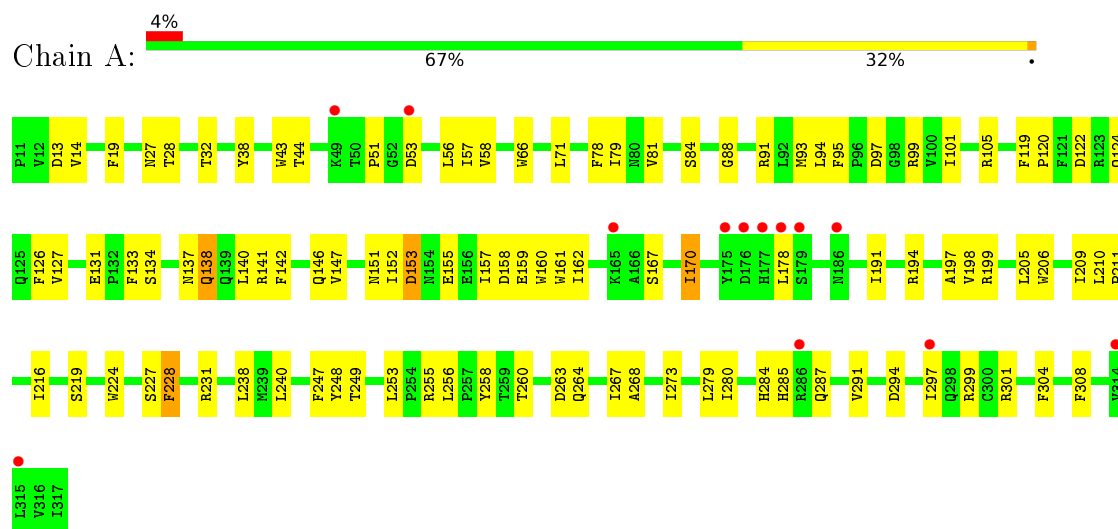


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	B	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	C	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	D	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	E	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	F	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	G	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	H	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	I	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	J	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		

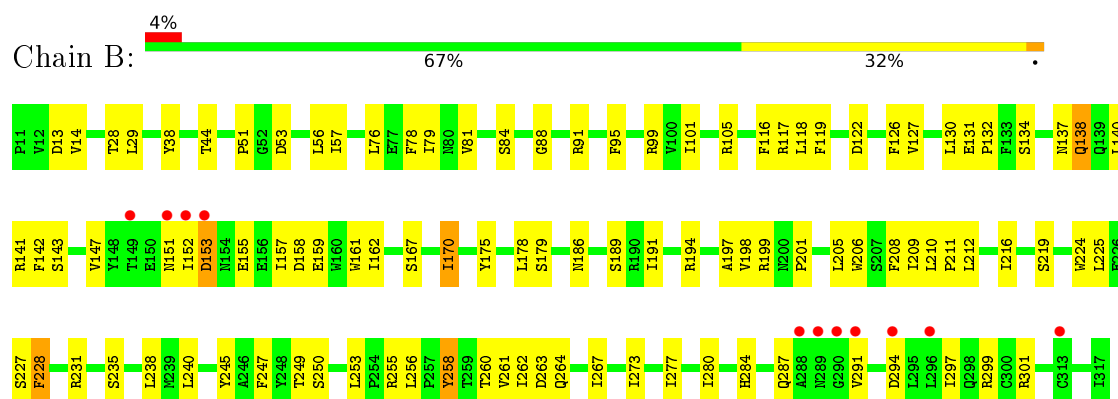
### 3 Residue-property plots

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.

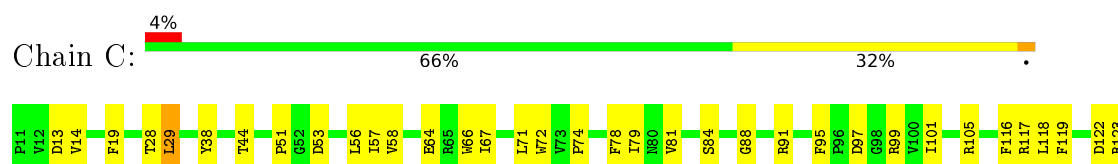
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

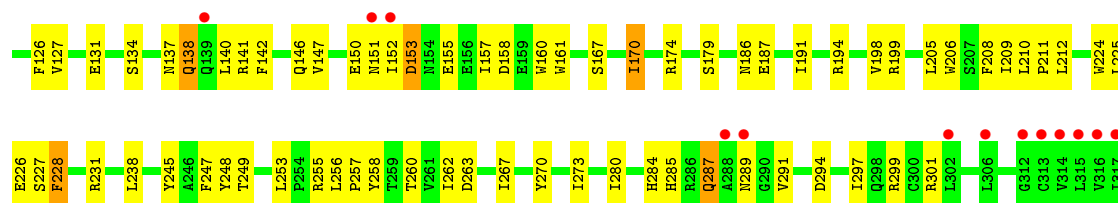


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

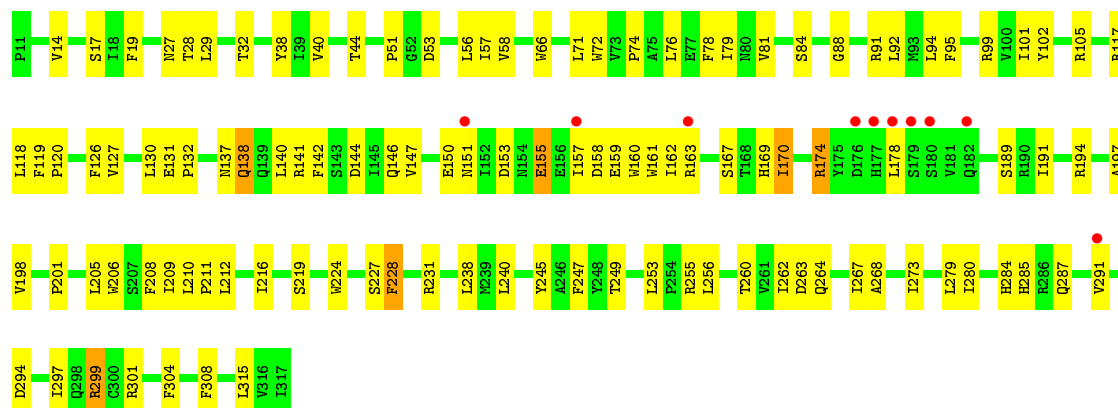


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

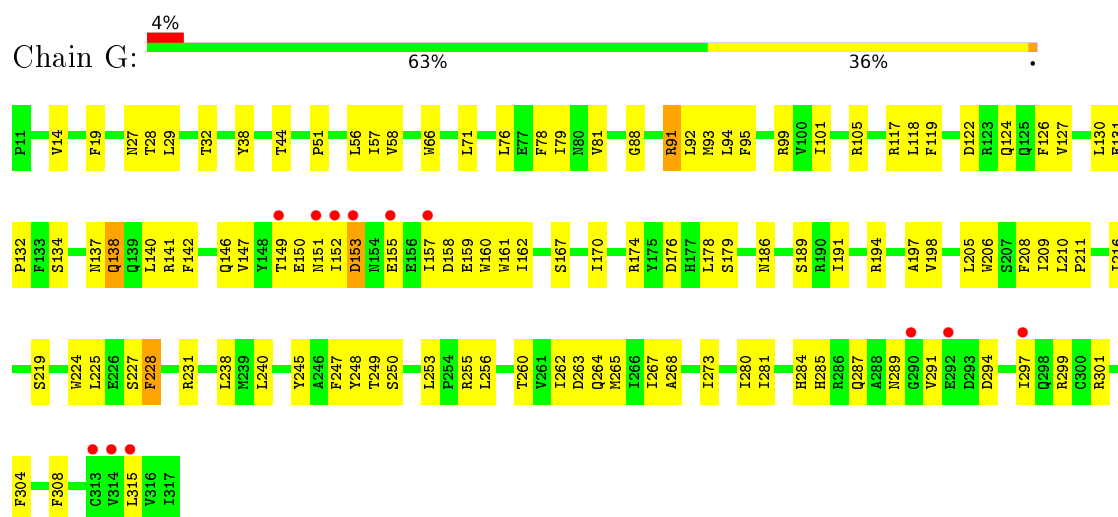




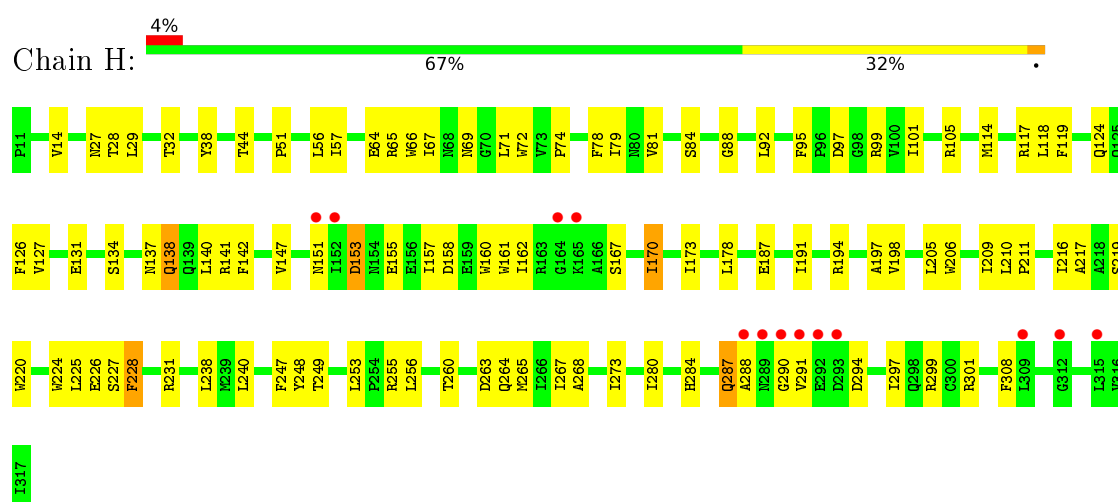
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



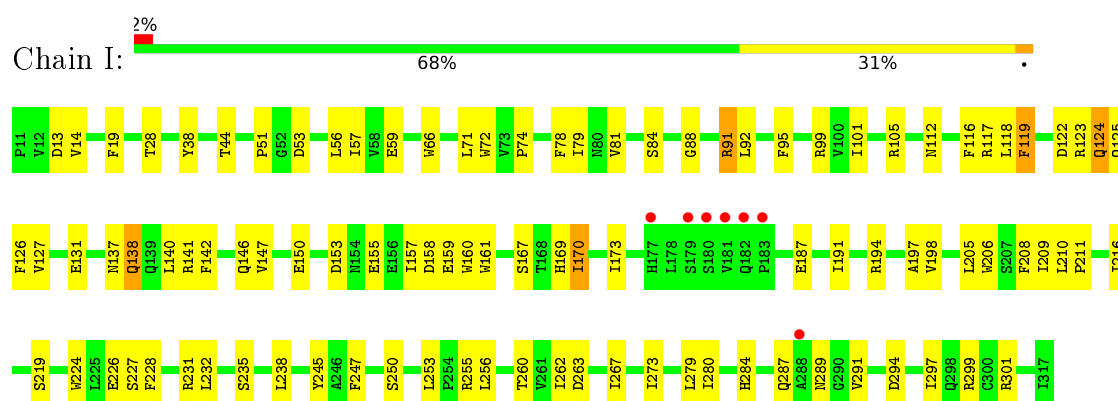
## • Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



## • Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



## • Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



## • Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.20Å 266.65Å 111.04Å 90.00° 107.71° 90.00°	Depositor
Resolution (Å)	44.75 – 3.57 44.75 – 3.57	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.75-3.57) 97.6 (44.75-3.57)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.220 , 0.253 0.218 , 0.252	Depositor DCC
$R_{free}$ test set	3409 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	92.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 71.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	25255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z80

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	0.29	0/2571	0.53	0/3503
1	B	0.30	0/2573	0.53	0/3507
1	C	0.29	0/2573	0.54	0/3507
1	D	0.35	0/2573	0.57	3/3507 (0.1%)
1	E	0.31	0/2573	0.53	0/3507
1	F	0.32	0/2573	0.53	0/3507
1	G	0.32	0/2573	0.56	2/3507 (0.1%)
1	H	0.31	0/2573	0.54	0/3507
1	I	0.27	0/2569	0.52	0/3502
1	J	0.33	0/2573	0.56	0/3507
All	All	0.31	0/25724	0.54	5/35061 (0.0%)

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	1
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
All	All	0	16

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	174	ARG	CG-CD-NE	5.96	124.31	111.80
1	G	174	ARG	CG-CD-NE	5.28	122.89	111.80
1	G	315	LEU	CA-CB-CG	5.27	127.43	115.30
1	D	155	GLU	CA-CB-CG	-5.23	101.89	113.40
1	D	315	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASN	Peptide
1	B	137	ASN	Peptide
1	C	118	LEU	Peptide
1	C	137	ASN	Peptide
1	D	118	LEU	Peptide
1	D	137	ASN	Peptide
1	E	137	ASN	Peptide
1	F	137	ASN	Peptide
1	G	118	LEU	Peptide
1	G	137	ASN	Peptide
1	H	118	LEU	Peptide
1	H	137	ASN	Peptide
1	I	118	LEU	Peptide
1	I	137	ASN	Peptide
1	J	118	LEU	Peptide
1	J	137	ASN	Peptide

## 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	2504	0	2475	92	0
1	B	2505	0	2478	84	0
1	C	2505	0	2478	82	0
1	D	2505	0	2478	85	0
1	E	2505	0	2478	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2505	0	2478	84	0
1	G	2505	0	2478	90	0
1	H	2505	0	2478	82	1
1	I	2501	0	2474	76	0
1	J	2505	0	2478	97	0
2	A	21	0	19	7	0
2	B	21	0	19	6	0
2	C	21	0	19	5	0
2	D	21	0	19	4	0
2	E	21	0	19	7	0
2	F	21	0	19	8	0
2	G	21	0	19	9	0
2	H	21	0	19	6	0
2	I	21	0	19	3	0
2	J	21	0	19	7	0
All	All	25255	0	24963	779	1

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 16.

All (779) 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:H:155:GLU:HG3	1:H:161:TRP:CD1	1.99	0.97
1:I:122:ASP:HB3	1:I:124:GLN:NE2	1.81	0.95
1:D:155:GLU:HG3	1:D:161:TRP:CD1	2.02	0.94
1:E:155:GLU:HG3	1:E:161:TRP:CD1	2.02	0.93
1:J:155:GLU:HG3	1:J:161:TRP:CD1	2.05	0.91
1:B:170:ILE:HG12	1:B:191:ILE:HG12	1.55	0.89
1:A:155:GLU:HG3	1:A:161:TRP:CD1	2.12	0.85
1:I:44:THR:HA	1:I:99:ARG:HA	1.59	0.85
1:D:170:ILE:HG12	1:D:191:ILE:HG12	1.60	0.84
1:C:155:GLU:HG3	1:C:161:TRP:CD1	2.13	0.84
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.58	0.84
1:I:122:ASP:HB3	1:I:124:GLN:HE22	1.40	0.83
1:F:231:ARG:HB3	1:F:280:ILE:HD13	1.61	0.83
1:G:155:GLU:HG3	1:G:161:TRP:CD1	2.14	0.83
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.60	0.83
1:A:44:THR:HA	1:A:99:ARG:HA	1.61	0.83
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.59	0.82
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:THR:HA	1:C:99:ARG:HA	1.62	0.82
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.63	0.80
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.62	0.80
1:H:44:THR:HA	1:H:99:ARG:HA	1.62	0.80
1:C:167:SER:HB2	1:C:194:ARG:HG3	1.63	0.80
1:J:154:ASN:O	1:J:156:GLU:N	2.15	0.80
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.63	0.79
1:E:155:GLU:HB3	2:E:401:Z80:H15	1.65	0.79
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.64	0.79
1:J:44:THR:HA	1:J:99:ARG:HA	1.65	0.78
1:G:44:THR:HA	1:G:99:ARG:HA	1.64	0.78
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.65	0.77
1:F:44:THR:HA	1:F:99:ARG:HA	1.66	0.76
1:H:287:GLN:NE2	1:H:290:GLY:O	2.18	0.76
1:H:155:GLU:HG3	1:H:161:TRP:HD1	1.48	0.76
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.66	0.76
1:G:287:GLN:OE1	1:G:289:ASN:O	2.03	0.76
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.68	0.75
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.69	0.74
1:H:170:ILE:HG12	1:H:191:ILE:HG12	1.69	0.74
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.69	0.74
1:I:170:ILE:HG12	1:I:191:ILE:HG12	1.68	0.74
1:C:170:ILE:HG12	1:C:191:ILE:HG12	1.69	0.73
1:C:249:THR:HG23	1:C:253:LEU:HD22	1.71	0.73
1:E:44:THR:HA	1:E:99:ARG:HA	1.70	0.73
1:B:44:THR:HA	1:B:99:ARG:HA	1.69	0.73
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.70	0.73
1:C:147:VAL:HG13	2:C:401:Z80:H4	1.71	0.72
1:F:155:GLU:HB3	2:F:401:Z80:H12	1.71	0.72
1:H:167:SER:HB2	1:H:194:ARG:HG3	1.71	0.72
1:I:155:GLU:HA	1:I:158:ASP:HB2	1.71	0.72
1:E:167:SER:HB2	1:E:194:ARG:HG3	1.71	0.72
1:A:170:ILE:HG12	1:A:191:ILE:HG12	1.70	0.72
1:G:240:LEU:HD12	1:H:240:LEU:HD11	1.70	0.72
1:D:44:THR:HA	1:D:99:ARG:HA	1.72	0.72
1:E:170:ILE:HG12	1:E:191:ILE:HG12	1.72	0.71
1:J:170:ILE:HG12	1:J:191:ILE:HG12	1.72	0.71
1:E:299:ARG:HA	1:E:301:ARG:HG3	1.72	0.71
1:E:155:GLU:HG3	1:E:161:TRP:HD1	1.53	0.71
1:B:88:GLY:HA2	1:C:84:SER:HB3	1.71	0.71
1:A:240:LEU:HD12	1:B:240:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.71	0.70
1:I:126:PHE:CZ	2:I:401:Z80:H2	2.26	0.70
1:D:155:GLU:HG3	1:D:161:TRP:HD1	1.53	0.70
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.74	0.70
1:G:249:THR:HG23	1:G:253:LEU:HD22	1.75	0.69
1:F:240:LEU:HD11	1:J:240:LEU:HD12	1.74	0.69
1:D:126:PHE:CZ	2:D:401:Z80:H2	2.28	0.69
1:D:155:GLU:HA	1:D:158:ASP:HB2	1.74	0.68
1:G:155:GLU:HA	1:G:158:ASP:HB2	1.74	0.68
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.75	0.68
1:F:299:ARG:HA	1:F:301:ARG:HG3	1.74	0.68
1:G:147:VAL:HG13	2:G:401:Z80:H4	1.75	0.68
1:B:147:VAL:HG13	2:B:401:Z80:H4	1.74	0.68
1:A:127:VAL:HG22	1:A:194:ARG:HB3	1.74	0.68
1:C:155:GLU:HA	1:C:158:ASP:HB2	1.75	0.68
1:F:151:ASN:HD22	2:F:401:Z80:H15	1.57	0.68
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.74	0.68
1:C:126:PHE:CZ	2:C:401:Z80:H2	2.29	0.68
1:F:127:VAL:HG22	1:F:194:ARG:HB3	1.75	0.67
1:H:249:THR:HG23	1:H:253:LEU:HD22	1.74	0.67
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.77	0.67
1:D:51:PRO:HD2	1:D:56:LEU:HD23	1.76	0.67
1:J:155:GLU:HG3	1:J:161:TRP:HD1	1.58	0.67
1:A:155:GLU:HA	1:A:158:ASP:HB2	1.76	0.67
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.76	0.67
1:F:79:ILE:HD11	1:F:131:GLU:HB3	1.77	0.67
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.77	0.67
1:G:105:ARG:NH2	1:H:81:VAL:O	2.27	0.67
1:D:240:LEU:HD12	1:E:240:LEU:HD11	1.76	0.67
1:J:287:GLN:N	1:J:287:GLN:OE1	2.27	0.67
1:A:51:PRO:HD2	1:A:56:LEU:HD23	1.77	0.67
1:F:170:ILE:HG12	1:F:191:ILE:HG12	1.75	0.66
1:B:51:PRO:HD2	1:B:56:LEU:HD23	1.77	0.66
1:C:174:ARG:HH11	1:C:187:GLU:HG3	1.60	0.66
1:E:127:VAL:HG22	1:E:194:ARG:HB3	1.78	0.66
1:H:299:ARG:HA	1:H:301:ARG:HG3	1.78	0.66
1:J:51:PRO:HD2	1:J:56:LEU:HD23	1.78	0.66
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.78	0.66
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.61	0.66
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.78	0.65
1:J:155:GLU:HA	1:J:158:ASP:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HA	1:A:301:ARG:HG3	1.79	0.65
1:H:127:VAL:HG22	1:H:194:ARG:HB3	1.79	0.65
1:J:151:ASN:HA	1:J:152:ILE:O	1.96	0.65
1:F:152:ILE:HA	1:F:155:GLU:OE2	1.97	0.64
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.78	0.64
1:G:51:PRO:HD2	1:G:56:LEU:HD23	1.79	0.64
1:D:249:THR:HG23	1:D:253:LEU:HD22	1.78	0.64
1:E:51:PRO:HD2	1:E:56:LEU:HD23	1.79	0.64
1:H:151:ASN:HD22	2:H:401:Z80:H15	1.62	0.64
1:A:249:THR:HG23	1:A:253:LEU:HD22	1.78	0.64
1:C:152:ILE:HA	1:C:155:GLU:OE2	1.97	0.64
1:F:155:GLU:HA	1:F:158:ASP:HB2	1.78	0.64
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.79	0.64
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.78	0.64
1:J:14:VAL:O	1:J:141:ARG:N	2.29	0.64
1:J:127:VAL:HG22	1:J:194:ARG:HB3	1.80	0.64
1:B:155:GLU:HA	1:B:158:ASP:HB2	1.79	0.63
1:C:127:VAL:HG22	1:C:194:ARG:HB3	1.80	0.63
1:H:155:GLU:HA	1:H:158:ASP:HB2	1.81	0.63
1:H:284:HIS:CE1	1:H:291:VAL:HG13	2.33	0.63
1:G:88:GLY:HA2	1:H:84:SER:HB3	1.80	0.63
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.81	0.63
1:J:249:THR:HG23	1:J:253:LEU:HD22	1.79	0.63
1:C:155:GLU:HG3	1:C:161:TRP:NE1	2.14	0.63
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.14	0.63
1:F:133:PHE:CE2	1:J:91:ARG:HG2	2.34	0.62
1:B:151:ASN:HD22	2:B:401:Z80:H15	1.64	0.62
1:C:299:ARG:HA	1:C:301:ARG:HG3	1.81	0.62
1:C:38:TYR:CZ	1:C:105:ARG:HD2	2.34	0.62
1:E:224:TRP:NE1	1:E:301:ARG:HB3	2.14	0.62
1:B:284:HIS:CE1	1:B:291:VAL:HG13	2.35	0.62
1:G:127:VAL:HG22	1:G:194:ARG:HB3	1.79	0.62
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.82	0.62
1:F:133:PHE:HE2	1:J:91:ARG:HG2	1.65	0.62
1:J:238:LEU:HB3	1:J:273:ILE:HD13	1.81	0.62
1:D:151:ASN:ND2	1:D:155:GLU:OE2	2.33	0.62
1:G:155:GLU:HG3	1:G:161:TRP:HD1	1.64	0.61
1:H:161:TRP:O	1:H:198:VAL:N	2.33	0.61
1:G:151:ASN:HD22	2:G:401:Z80:H15	1.65	0.61
1:F:51:PRO:HD2	1:F:56:LEU:HD23	1.82	0.61
1:H:238:LEU:HB3	1:H:273:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:HB3	1:E:88:GLY:HA2	1.82	0.61
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.16	0.60
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.36	0.60
1:A:105:ARG:NH2	1:B:81:VAL:O	2.34	0.60
1:B:126:PHE:CZ	2:B:401:Z80:H2	2.36	0.60
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.84	0.60
1:H:51:PRO:HD2	1:H:56:LEU:HD23	1.82	0.60
1:J:66:TRP:HE3	1:J:71:LEU:HD12	1.66	0.59
1:G:161:TRP:O	1:G:198:VAL:N	2.32	0.59
1:I:284:HIS:CE1	1:I:291:VAL:HG13	2.37	0.59
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.82	0.59
1:F:84:SER:HB3	1:J:88:GLY:HA2	1.83	0.59
1:E:227:SER:OG	1:E:228:PHE:N	2.35	0.59
1:G:155:GLU:HB3	2:G:401:Z80:H12	1.84	0.59
1:J:38:TYR:CZ	1:J:105:ARG:HD2	2.37	0.59
1:F:161:TRP:O	1:F:198:VAL:N	2.36	0.59
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.83	0.59
1:G:161:TRP:HB2	1:G:198:VAL:HB	1.84	0.59
1:H:38:TYR:CZ	1:H:105:ARG:HD2	2.37	0.59
1:J:284:HIS:CE1	1:J:291:VAL:HG13	2.37	0.59
1:I:227:SER:OG	1:I:228:PHE:N	2.36	0.59
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.85	0.59
1:A:155:GLU:OE1	2:A:401:Z80:H12	2.03	0.59
1:B:161:TRP:HB2	1:B:198:VAL:HB	1.83	0.59
1:E:155:GLU:HA	1:E:158:ASP:HB2	1.83	0.59
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.85	0.59
1:C:153:ASP:H	1:C:155:GLU:CD	2.06	0.59
1:C:238:LEU:HB3	1:C:273:ILE:HD13	1.84	0.59
1:E:227:SER:O	1:E:231:ARG:HD3	2.03	0.59
1:B:127:VAL:HG22	1:B:194:ARG:HB3	1.85	0.58
1:C:227:SER:OG	1:C:228:PHE:N	2.36	0.58
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.85	0.58
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.18	0.58
1:A:227:SER:O	1:A:231:ARG:HD3	2.02	0.58
1:H:224:TRP:NE1	1:H:301:ARG:HB3	2.17	0.58
1:I:279:LEU:HD22	1:I:297:ILE:HD11	1.85	0.58
1:B:253:LEU:HD21	1:B:262:ILE:HD12	1.84	0.58
1:D:147:VAL:HG13	2:D:401:Z80:H4	1.85	0.58
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.84	0.58
1:A:227:SER:OG	1:A:228:PHE:N	2.37	0.58
1:B:299:ARG:HA	1:B:301:ARG:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:SER:O	1:D:231:ARG:HD3	2.02	0.58
1:B:284:HIS:HE1	1:B:291:VAL:HG13	1.68	0.58
1:C:284:HIS:CE1	1:C:291:VAL:HG13	2.39	0.58
1:D:227:SER:OG	1:D:228:PHE:N	2.37	0.58
1:G:284:HIS:CE1	1:G:291:VAL:HG13	2.38	0.58
1:H:79:ILE:HD11	1:H:131:GLU:HB3	1.85	0.58
1:J:227:SER:OG	1:J:228:PHE:N	2.36	0.58
1:B:224:TRP:NE1	1:B:301:ARG:HB3	2.18	0.58
1:B:227:SER:O	1:B:231:ARG:HD3	2.03	0.58
1:A:38:TYR:CZ	1:A:105:ARG:HD2	2.39	0.58
1:J:155:GLU:HG3	1:J:161:TRP:NE1	2.19	0.57
1:D:224:TRP:NE1	1:D:301:ARG:HB3	2.19	0.57
1:D:287:GLN:OE1	1:D:287:GLN:N	2.37	0.57
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.87	0.57
1:E:147:VAL:HG13	2:E:401:Z80:H4	1.85	0.57
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.86	0.57
1:E:126:PHE:CZ	2:E:401:Z80:H2	2.39	0.57
1:B:227:SER:OG	1:B:228:PHE:N	2.38	0.57
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.85	0.57
1:C:227:SER:O	1:C:231:ARG:HD3	2.04	0.57
1:F:14:VAL:O	1:F:141:ARG:N	2.34	0.57
1:F:28:THR:HB	1:F:256:LEU:HD21	1.87	0.57
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.69	0.57
1:J:79:ILE:HD11	1:J:131:GLU:HB3	1.87	0.57
1:A:79:ILE:HD11	1:A:131:GLU:HB3	1.87	0.57
1:E:14:VAL:O	1:E:141:ARG:N	2.32	0.57
1:G:38:TYR:CZ	1:G:105:ARG:HD2	2.40	0.57
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.86	0.57
1:G:287:GLN:CD	1:G:289:ASN:O	2.43	0.57
1:B:161:TRP:O	1:B:198:VAL:N	2.36	0.56
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.86	0.56
1:F:227:SER:OG	1:F:228:PHE:N	2.38	0.56
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.40	0.56
1:H:227:SER:OG	1:H:228:PHE:N	2.38	0.56
1:J:227:SER:O	1:J:231:ARG:HD3	2.04	0.56
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.86	0.56
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.87	0.56
1:J:66:TRP:CE3	1:J:71:LEU:HD12	2.40	0.56
1:D:14:VAL:O	1:D:141:ARG:N	2.34	0.56
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.86	0.56
1:H:14:VAL:O	1:H:141:ARG:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:H	1:A:155:GLU:CD	2.08	0.56
1:A:126:PHE:CZ	2:A:401:Z80:H2	2.41	0.56
1:C:28:THR:HB	1:C:256:LEU:HD21	1.88	0.56
1:D:79:ILE:HD11	1:D:131:GLU:HB3	1.86	0.56
1:I:79:ILE:HD11	1:I:131:GLU:HB3	1.87	0.56
1:G:227:SER:OG	1:G:228:PHE:N	2.38	0.56
1:J:155:GLU:HA	1:J:158:ASP:HB2	1.88	0.56
1:B:238:LEU:HB3	1:B:273:ILE:HD13	1.86	0.55
1:C:51:PRO:HD2	1:C:56:LEU:HD23	1.89	0.55
1:F:227:SER:O	1:F:231:ARG:HD3	2.05	0.55
1:J:155:GLU:OE1	2:J:401:Z80:H15	2.07	0.55
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.89	0.55
1:B:249:THR:HG23	1:B:253:LEU:HD22	1.88	0.55
1:J:299:ARG:HA	1:J:301:ARG:HG3	1.89	0.55
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.88	0.55
1:F:151:ASN:ND2	1:F:155:GLU:OE1	2.40	0.55
1:D:216:ILE:O	1:D:219:SER:HB3	2.07	0.55
1:F:81:VAL:O	1:J:105:ARG:NH2	2.40	0.55
1:B:14:VAL:O	1:B:141:ARG:N	2.31	0.55
1:D:238:LEU:HB3	1:D:273:ILE:HD13	1.87	0.55
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.89	0.55
1:I:28:THR:HB	1:I:256:LEU:HD21	1.89	0.55
1:A:155:GLU:HG3	1:A:161:TRP:HD1	1.67	0.55
1:B:105:ARG:NH2	1:C:81:VAL:O	2.40	0.55
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.22	0.54
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.26	0.54
1:J:126:PHE:CZ	2:J:401:Z80:H2	2.42	0.54
1:G:227:SER:O	1:G:231:ARG:HD3	2.07	0.54
1:D:155:GLU:HG3	1:D:161:TRP:NE1	2.20	0.54
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.37	0.54
1:A:152:ILE:HA	1:A:155:GLU:OE2	2.07	0.54
1:I:227:SER:O	1:I:231:ARG:HD3	2.07	0.54
1:A:147:VAL:HG11	2:A:401:Z80:H4	1.90	0.54
1:H:227:SER:O	1:H:231:ARG:HD3	2.08	0.54
1:B:167:SER:HB2	1:B:194:ARG:HG3	1.89	0.54
1:C:224:TRP:NE1	1:C:301:ARG:HB3	2.23	0.54
1:E:174:ARG:HH11	1:E:187:GLU:HG3	1.73	0.54
1:H:155:GLU:HG3	1:H:161:TRP:NE1	2.21	0.54
1:A:287:GLN:OE1	1:A:287:GLN:N	2.41	0.53
1:A:284:HIS:CE1	1:A:291:VAL:HG13	2.43	0.53
1:G:79:ILE:HD11	1:G:131:GLU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:GLN:HG2	1:J:289:ASN:O	2.08	0.53
1:H:28:THR:HB	1:H:256:LEU:HD21	1.89	0.53
1:H:151:ASN:ND2	2:H:401:Z80:H15	2.23	0.53
1:H:64:GLU:HA	1:H:67:ILE:HD12	1.91	0.53
1:A:28:THR:HB	1:A:256:LEU:HD21	1.90	0.53
1:A:81:VAL:O	1:E:105:ARG:NH2	2.42	0.53
1:A:240:LEU:HD23	1:E:241:THR:HA	1.91	0.53
1:G:14:VAL:O	1:G:141:ARG:N	2.35	0.53
1:J:151:ASN:ND2	1:J:162:ILE:HG12	2.22	0.53
1:J:119:PHE:CB	1:J:260:THR:HB	2.38	0.53
1:B:152:ILE:HA	1:B:155:GLU:OE2	2.07	0.53
1:I:119:PHE:CB	1:I:260:THR:HB	2.39	0.53
1:J:284:HIS:HE1	1:J:291:VAL:HG13	1.74	0.53
1:B:153:ASP:H	1:B:155:GLU:CD	2.13	0.53
1:E:28:THR:HB	1:E:256:LEU:HD21	1.91	0.53
1:E:158:ASP:OD2	2:E:401:Z80:H13	2.09	0.53
1:G:122:ASP:HB3	1:G:124:GLN:OE1	2.09	0.52
1:A:238:LEU:HB3	1:A:273:ILE:HD13	1.91	0.52
1:G:119:PHE:HB3	1:G:260:THR:HB	1.91	0.52
1:J:28:THR:HB	1:J:256:LEU:HD21	1.91	0.52
1:F:294:ASP:HB3	1:F:297:ILE:CG2	2.40	0.52
1:I:88:GLY:HA2	1:J:84:SER:HB3	1.92	0.52
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.90	0.52
1:E:161:TRP:O	1:E:198:VAL:N	2.38	0.52
1:G:119:PHE:CB	1:G:260:THR:HB	2.39	0.52
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.45	0.52
1:A:147:VAL:CG1	2:A:401:Z80:H4	2.40	0.52
1:D:151:ASN:CG	1:D:155:GLU:OE2	2.48	0.52
1:G:238:LEU:HB3	1:G:273:ILE:HD13	1.92	0.52
1:H:294:ASP:HB3	1:H:297:ILE:CG2	2.40	0.52
1:A:151:ASN:HA	1:A:155:GLU:OE2	2.11	0.51
1:A:155:GLU:HG3	1:A:161:TRP:NE1	2.24	0.51
1:B:122:ASP:HB2	1:B:199:ARG:HB2	1.92	0.51
1:D:279:LEU:HD22	1:D:297:ILE:HD11	1.91	0.51
1:J:126:PHE:HE1	1:J:197:ALA:HB3	1.75	0.51
1:A:126:PHE:HE1	1:A:197:ALA:HB3	1.75	0.51
1:C:66:TRP:CE3	1:C:71:LEU:HD12	2.45	0.51
1:E:155:GLU:HB3	2:E:401:Z80:C16	2.39	0.51
1:F:95:PHE:HE1	1:F:101:ILE:HD12	1.75	0.51
1:C:79:ILE:HD11	1:C:131:GLU:HB3	1.93	0.51
1:D:119:PHE:HB3	1:D:260:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:TRP:O	1:D:198:VAL:N	2.41	0.51
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.93	0.51
1:H:147:VAL:HG13	2:H:401:Z80:H4	1.92	0.51
1:D:263:ASP:O	1:D:267:ILE:HG12	2.11	0.51
1:F:155:GLU:HB3	2:F:401:Z80:C15	2.39	0.51
1:F:161:TRP:HB2	1:F:198:VAL:HB	1.92	0.51
1:C:205:LEU:HD23	1:C:209:ILE:HG13	1.92	0.51
1:C:253:LEU:HD21	1:C:262:ILE:HD12	1.93	0.51
1:F:208:PHE:O	1:F:245:TYR:OH	2.28	0.51
1:F:238:LEU:HB3	1:F:273:ILE:HD13	1.92	0.51
1:I:161:TRP:O	1:I:198:VAL:N	2.40	0.51
1:J:155:GLU:HB3	2:J:401:Z80:H15	1.91	0.51
1:D:127:VAL:HG22	1:D:194:ARG:HB3	1.93	0.51
1:E:151:ASN:CG	1:E:155:GLU:OE2	2.49	0.51
1:G:208:PHE:O	1:G:245:TYR:OH	2.28	0.51
1:H:66:TRP:HE3	1:H:71:LEU:HD12	1.76	0.51
1:J:56:LEU:HD13	1:J:57:ILE:N	2.26	0.51
1:A:161:TRP:O	1:A:198:VAL:N	2.37	0.51
1:B:287:GLN:N	1:B:287:GLN:OE1	2.43	0.50
1:C:66:TRP:HE3	1:C:71:LEU:HD12	1.75	0.50
1:A:93:MET:HB2	1:A:101:ILE:HB	1.93	0.50
1:C:14:VAL:O	1:C:141:ARG:N	2.38	0.50
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.28	0.50
1:G:167:SER:HB2	1:G:194:ARG:O	2.12	0.50
1:D:161:TRP:HB2	1:D:198:VAL:HB	1.92	0.50
1:H:151:ASN:CG	1:H:155:GLU:OE2	2.50	0.50
1:I:127:VAL:HG22	1:I:194:ARG:HB3	1.92	0.50
1:I:119:PHE:HB3	1:I:260:THR:HB	1.93	0.50
1:I:51:PRO:HD2	1:I:56:LEU:HD23	1.94	0.50
1:A:14:VAL:O	1:A:141:ARG:N	2.39	0.50
1:A:158:ASP:OD2	2:A:401:Z80:H14	2.12	0.50
1:D:28:THR:HB	1:D:256:LEU:HD21	1.94	0.50
1:G:91:ARG:HD3	1:H:134:SER:HB3	1.93	0.50
1:A:122:ASP:HB3	1:A:124:GLN:OE1	2.12	0.50
1:B:119:PHE:HB3	1:B:260:THR:HB	1.94	0.50
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.76	0.50
1:H:66:TRP:CE3	1:H:71:LEU:HD12	2.46	0.50
1:I:287:GLN:N	1:I:287:GLN:OE1	2.45	0.50
1:E:155:GLU:HG3	1:E:161:TRP:NE1	2.26	0.50
1:F:205:LEU:HD23	1:F:209:ILE:HG13	1.93	0.50
1:G:71:LEU:HD11	1:G:94:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:TRP:N	1:F:198:VAL:O	2.30	0.49
1:H:119:PHE:HB3	1:H:260:THR:HB	1.94	0.49
1:A:151:ASN:HD22	2:A:401:Z80:H15	1.77	0.49
1:B:216:ILE:O	1:B:219:SER:HB3	2.12	0.49
1:E:126:PHE:HE1	1:E:197:ALA:HB3	1.78	0.49
1:I:112:ASN:ND2	1:I:125:GLN:O	2.46	0.49
1:I:91:ARG:HD3	1:J:134:SER:HB3	1.93	0.49
1:A:88:GLY:HA2	1:B:84:SER:HB3	1.93	0.49
1:C:284:HIS:HE1	1:C:291:VAL:HG13	1.77	0.49
1:G:159:GLU:HB3	1:G:160:TRP:CD1	2.47	0.49
1:J:294:ASP:HB3	1:J:297:ILE:CG2	2.42	0.49
1:E:161:TRP:HB2	1:E:198:VAL:HB	1.95	0.49
1:F:159:GLU:HB3	1:F:160:TRP:CD1	2.47	0.49
1:F:301:ARG:HH12	1:G:285:HIS:HE2	1.60	0.49
1:G:284:HIS:HE1	1:G:291:VAL:HG13	1.75	0.49
1:A:91:ARG:HD3	1:B:134:SER:HB3	1.95	0.49
1:B:38:TYR:CZ	1:B:105:ARG:HD2	2.48	0.49
1:G:162:ILE:HA	1:G:197:ALA:HA	1.95	0.49
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.94	0.49
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.28	0.49
1:H:56:LEU:HD13	1:H:57:ILE:N	2.28	0.49
1:D:159:GLU:HB3	1:D:160:TRP:CD1	2.47	0.49
1:B:155:GLU:HB3	2:B:401:Z80:H13	1.94	0.49
1:E:216:ILE:O	1:E:219:SER:HB3	2.13	0.49
1:H:162:ILE:HA	1:H:197:ALA:HA	1.95	0.49
1:F:153:ASP:H	1:F:155:GLU:CD	2.16	0.48
1:E:249:THR:HG23	1:E:253:LEU:HD22	1.94	0.48
1:F:294:ASP:HB3	1:F:297:ILE:HG22	1.95	0.48
1:C:294:ASP:HB3	1:C:297:ILE:CG2	2.43	0.48
1:D:157:ILE:HD11	1:E:117:ARG:NE	2.29	0.48
1:F:162:ILE:HA	1:F:197:ALA:HA	1.95	0.48
1:G:216:ILE:O	1:G:219:SER:HB3	2.13	0.48
1:H:119:PHE:CB	1:H:260:THR:HB	2.43	0.48
1:A:78:PHE:O	1:A:81:VAL:HG12	2.14	0.48
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.31	0.48
1:I:66:TRP:CE3	1:I:71:LEU:HD12	2.49	0.48
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.32	0.48
1:G:294:ASP:HB3	1:G:297:ILE:CG2	2.44	0.48
1:A:216:ILE:O	1:A:219:SER:HB3	2.14	0.48
1:B:28:THR:HB	1:B:256:LEU:HD21	1.96	0.48
1:G:151:ASN:HA	1:G:155:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:SER:HB2	1:G:186:ASN:ND2	2.29	0.48
1:G:263:ASP:O	1:G:267:ILE:HG12	2.13	0.48
1:H:151:ASN:ND2	1:H:155:GLU:OE2	2.46	0.48
1:I:14:VAL:O	1:I:141:ARG:N	2.38	0.48
1:C:155:GLU:HG3	1:C:161:TRP:HD1	1.75	0.48
1:I:95:PHE:HE1	1:I:101:ILE:HD12	1.78	0.48
1:I:159:GLU:HB3	1:I:160:TRP:CD1	2.48	0.48
1:I:238:LEU:HB3	1:I:273:ILE:HD13	1.96	0.48
1:A:122:ASP:HB2	1:A:199:ARG:HB2	1.96	0.48
1:B:119:PHE:CB	1:B:260:THR:HB	2.44	0.48
1:B:175:TYR:O	1:B:186:ASN:ND2	2.46	0.48
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.31	0.48
1:J:161:TRP:O	1:J:198:VAL:N	2.47	0.48
1:B:205:LEU:HA	1:B:209:ILE:HB	1.96	0.47
1:C:151:ASN:HD22	2:C:401:Z80:H15	1.79	0.47
1:C:97:ASP:OD2	1:C:99:ARG:NH1	2.47	0.47
1:E:162:ILE:HA	1:E:197:ALA:HA	1.95	0.47
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.31	0.47
1:D:212:LEU:HB2	1:D:245:TYR:CE2	2.48	0.47
1:G:160:TRP:CD1	2:G:401:Z80:H1	2.50	0.47
1:B:235:SER:HB3	1:B:277:ILE:HD11	1.96	0.47
1:D:294:ASP:HB3	1:D:297:ILE:HG22	1.94	0.47
1:A:56:LEU:HD13	1:A:57:ILE:N	2.29	0.47
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.44	0.47
1:B:56:LEU:HD13	1:B:57:ILE:N	2.29	0.47
1:D:71:LEU:HD11	1:D:94:LEU:HD21	1.97	0.47
1:G:56:LEU:HD13	1:G:57:ILE:N	2.29	0.47
1:H:78:PHE:O	1:H:81:VAL:HG12	2.14	0.47
1:A:134:SER:OG	1:E:59:GLU:OE2	2.33	0.47
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.61	0.47
1:F:126:PHE:CZ	2:F:401:Z80:H2	2.50	0.47
1:G:209:ILE:HG23	1:G:265:MET:HE1	1.96	0.47
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.33	0.47
1:D:14:VAL:HG21	1:D:138:GLN:NE2	2.30	0.47
1:D:76:LEU:HB3	1:D:130:LEU:HD11	1.96	0.47
1:E:238:LEU:HB3	1:E:273:ILE:HD13	1.96	0.47
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.62	0.47
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.79	0.47
1:J:161:TRP:HB2	1:J:198:VAL:HB	1.96	0.47
1:C:161:TRP:O	1:C:198:VAL:N	2.43	0.47
1:F:289:ASN:OD1	1:F:292:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:ASN:O	1:F:290:GLY:C	2.53	0.47
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.33	0.47
1:J:27:ASN:HB3	1:J:32:THR:HB	1.96	0.47
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.50	0.47
1:D:155:GLU:HB3	2:D:401:Z80:H13	1.95	0.47
1:I:141:ARG:HD2	1:I:142:PHE:CE2	2.50	0.47
1:A:159:GLU:HB3	1:A:160:TRP:CD1	2.49	0.47
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.50	0.47
1:I:38:TYR:CZ	1:I:105:ARG:HD2	2.50	0.47
1:J:119:PHE:HB2	1:J:260:THR:HB	1.97	0.47
1:C:294:ASP:O	1:C:297:ILE:HG22	2.16	0.46
1:D:78:PHE:O	1:D:81:VAL:HG12	2.14	0.46
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.97	0.46
1:F:126:PHE:CE1	2:F:401:Z80:H18	2.50	0.46
1:H:178:LEU:HD13	1:H:178:LEU:HA	1.75	0.46
1:I:208:PHE:O	1:I:245:TYR:OH	2.30	0.46
1:I:56:LEU:HD13	1:I:57:ILE:N	2.29	0.46
1:A:224:TRP:HE1	1:A:301:ARG:HB3	1.79	0.46
1:A:263:ASP:O	1:A:267:ILE:HG12	2.15	0.46
1:A:66:TRP:CE3	1:A:71:LEU:HD12	2.50	0.46
1:D:56:LEU:HD13	1:D:57:ILE:N	2.31	0.46
1:E:155:GLU:OE1	2:E:401:Z80:H12	2.15	0.46
1:F:174:ARG:HH11	1:F:187:GLU:HG3	1.80	0.46
1:F:216:ILE:O	1:F:219:SER:HB3	2.15	0.46
1:J:119:PHE:HB3	1:J:260:THR:HB	1.97	0.46
1:C:56:LEU:HD13	1:C:57:ILE:N	2.30	0.46
1:F:220:TRP:CE3	1:F:305:PRO:HG3	2.50	0.46
1:F:93:MET:HB2	1:F:101:ILE:HB	1.96	0.46
1:G:153:ASP:H	1:G:155:GLU:CD	2.18	0.46
1:D:284:HIS:CE1	1:D:291:VAL:HG13	2.50	0.46
1:I:301:ARG:HH12	1:J:285:HIS:HE2	1.63	0.46
1:A:95:PHE:HE1	1:A:101:ILE:HD12	1.79	0.46
1:E:287:GLN:N	1:E:287:GLN:OE1	2.48	0.46
1:H:294:ASP:HB3	1:H:297:ILE:HG22	1.97	0.46
1:I:147:VAL:HG13	2:I:401:Z80:H4	1.98	0.46
1:E:151:ASN:HA	1:E:155:GLU:OE2	2.16	0.46
1:F:284:HIS:CE1	1:F:291:VAL:HG13	2.51	0.46
1:I:216:ILE:O	1:I:219:SER:HB3	2.15	0.46
1:J:147:VAL:HG13	2:J:401:Z80:H4	1.98	0.46
1:H:173:ILE:O	1:H:187:GLU:HA	2.14	0.46
1:A:66:TRP:HE3	1:A:71:LEU:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:ND2	1:B:162:ILE:H	2.14	0.46
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.98	0.46
1:C:88:GLY:HA2	1:D:84:SER:HB3	1.98	0.46
1:E:153:ASP:H	1:E:155:GLU:CD	2.18	0.46
1:G:260:THR:O	1:G:264:GLN:HG3	2.16	0.46
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.49	0.46
1:H:248:TYR:HE1	1:I:250:SER:OG	1.99	0.46
1:J:72:TRP:CZ3	1:J:74:PRO:HB3	2.51	0.46
1:C:147:VAL:CG1	2:C:401:Z80:H4	2.42	0.46
1:A:294:ASP:HB3	1:A:297:ILE:HG22	1.97	0.45
1:C:301:ARG:HH12	1:D:285:HIS:HE2	1.64	0.45
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.81	0.45
1:F:155:GLU:OE2	1:F:161:TRP:CD1	2.69	0.45
1:G:28:THR:HB	1:G:256:LEU:HD21	1.97	0.45
1:J:263:ASP:O	1:J:267:ILE:HG12	2.16	0.45
1:C:28:THR:HA	1:C:116:PHE:CE1	2.51	0.45
1:D:208:PHE:O	1:D:245:TYR:OH	2.32	0.45
1:G:294:ASP:HB3	1:G:297:ILE:HG22	1.97	0.45
1:J:141:ARG:HD2	1:J:142:PHE:CE2	2.51	0.45
1:C:263:ASP:O	1:C:267:ILE:HG12	2.17	0.45
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.34	0.45
1:G:66:TRP:CE3	1:G:71:LEU:HD12	2.52	0.45
1:I:78:PHE:O	1:I:81:VAL:HG12	2.16	0.45
1:D:294:ASP:HB3	1:D:297:ILE:CG2	2.46	0.45
1:G:153:ASP:N	1:G:155:GLU:OE2	2.49	0.45
1:H:141:ARG:HD2	1:H:142:PHE:CE2	2.52	0.45
1:J:158:ASP:OD2	2:J:401:Z80:H13	2.16	0.45
1:A:167:SER:CB	1:A:194:ARG:HG3	2.46	0.45
1:B:263:ASP:O	1:B:267:ILE:HG12	2.16	0.45
2:J:401:Z80:H9	2:J:401:Z80:H16	1.63	0.45
1:B:132:PRO:HD2	1:B:189:SER:O	2.16	0.45
1:B:167:SER:CB	1:B:194:ARG:HG3	2.46	0.45
1:D:119:PHE:CB	1:D:260:THR:HB	2.47	0.45
1:E:141:ARG:HD2	1:E:142:PHE:CE2	2.52	0.45
1:G:152:ILE:HA	1:G:155:GLU:OE2	2.16	0.45
1:H:126:PHE:CZ	2:H:401:Z80:H2	2.52	0.45
1:J:151:ASN:ND2	1:J:162:ILE:H	2.14	0.45
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.35	0.45
1:D:38:TYR:CZ	1:D:105:ARG:HD2	2.52	0.45
1:E:235:SER:HB3	1:E:277:ILE:HD11	1.99	0.45
1:I:66:TRP:HE3	1:I:71:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PRO:HB3	1:C:270:TYR:CE1	2.52	0.45
1:G:132:PRO:HD2	1:G:189:SER:O	2.15	0.45
1:G:149:THR:HB	2:G:401:Z80:H16	1.98	0.45
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.79	0.45
1:A:279:LEU:HD22	1:A:297:ILE:HD11	1.97	0.45
1:C:119:PHE:HB3	1:C:260:THR:HB	1.98	0.45
1:D:155:GLU:CD	1:D:155:GLU:H	2.08	0.45
1:H:126:PHE:HE1	1:H:197:ALA:HB3	1.82	0.45
1:J:216:ILE:O	1:J:219:SER:HB3	2.16	0.45
1:B:208:PHE:O	1:B:245:TYR:OH	2.33	0.44
1:C:155:GLU:HG3	1:C:161:TRP:HE1	1.81	0.44
1:J:294:ASP:HB3	1:J:297:ILE:HG22	1.98	0.44
1:C:123:ARG:HG3	1:C:198:VAL:HG22	1.99	0.44
1:G:141:ARG:HD2	1:G:142:PHE:CE2	2.52	0.44
1:H:157:ILE:HD11	1:I:117:ARG:NE	2.32	0.44
1:B:116:PHE:HB2	1:B:258:TYR:HE1	1.82	0.44
1:C:208:PHE:O	1:C:245:TYR:OH	2.31	0.44
1:F:155:GLU:HG2	1:F:155:GLU:H	1.27	0.44
1:F:91:ARG:HD3	1:G:134:SER:HB3	1.98	0.44
1:G:248:TYR:HD1	1:H:247:PHE:HA	1.82	0.44
1:J:167:SER:HB2	1:J:194:ARG:HG3	1.99	0.44
1:J:66:TRP:CZ3	1:J:94:LEU:HD13	2.52	0.44
1:C:161:TRP:HB2	1:C:198:VAL:HB	1.99	0.44
1:F:263:ASP:O	1:F:267:ILE:HG12	2.17	0.44
1:J:294:ASP:O	1:J:297:ILE:HG22	2.17	0.44
1:B:294:ASP:HB3	1:B:297:ILE:HG22	1.99	0.44
1:C:78:PHE:O	1:C:81:VAL:HG12	2.18	0.44
1:D:260:THR:O	1:D:264:GLN:HG3	2.18	0.44
1:E:14:VAL:HG21	1:E:138:GLN:NE2	2.32	0.44
1:G:78:PHE:O	1:G:81:VAL:HG12	2.17	0.44
1:H:161:TRP:HB2	1:H:198:VAL:HB	1.99	0.44
1:A:27:ASN:HB3	1:A:32:THR:HB	2.00	0.44
1:B:76:LEU:HB3	1:B:130:LEU:HD11	2.00	0.44
1:B:199:ARG:O	1:B:201:PRO:HD3	2.18	0.44
1:B:301:ARG:HH12	1:C:285:HIS:HE2	1.65	0.44
1:C:141:ARG:HD2	1:C:142:PHE:CE2	2.52	0.44
1:D:284:HIS:HB3	1:D:285:HIS:ND1	2.32	0.44
1:F:151:ASN:ND2	2:F:401:Z80:H15	2.28	0.44
1:J:17:SER:HA	1:J:144:ASP:O	2.17	0.44
1:A:161:TRP:HB2	1:A:198:VAL:HB	2.00	0.44
1:G:167:SER:CB	1:G:194:ARG:HG3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:LEU:HB3	1:J:130:LEU:HD11	2.00	0.44
1:C:248:TYR:HD1	1:D:247:PHE:HA	1.83	0.44
1:D:44:THR:HG23	1:D:99:ARG:HB3	2.00	0.44
1:E:112:ASN:OD1	1:E:113:ASP:N	2.51	0.44
2:G:401:Z80:H17	2:G:401:Z80:H9	1.64	0.44
1:E:159:GLU:HB3	1:E:160:TRP:CD1	2.53	0.44
1:E:44:THR:HG23	1:E:99:ARG:HB3	2.00	0.44
1:G:27:ASN:HB3	1:G:32:THR:HB	2.00	0.44
1:J:44:THR:HG23	1:J:99:ARG:HB3	2.00	0.44
1:A:14:VAL:HG21	1:A:138:GLN:NE2	2.32	0.43
1:A:260:THR:O	1:A:264:GLN:HG3	2.18	0.43
1:E:173:ILE:O	1:E:187:GLU:HA	2.18	0.43
1:H:95:PHE:HE1	1:H:101:ILE:HD12	1.83	0.43
1:B:260:THR:O	1:B:264:GLN:HG3	2.17	0.43
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.53	0.43
1:F:126:PHE:HE1	1:F:197:ALA:HB3	1.83	0.43
1:I:294:ASP:HB3	1:I:297:ILE:CG2	2.48	0.43
1:B:157:ILE:HD11	1:C:117:ARG:NE	2.32	0.43
1:I:126:PHE:HE1	1:I:197:ALA:HB3	1.84	0.43
1:B:91:ARG:HD3	1:C:134:SER:HB3	2.00	0.43
1:D:17:SER:HA	1:D:144:ASP:O	2.18	0.43
1:G:58:VAL:HB	1:G:92:LEU:HB2	1.99	0.43
1:I:123:ARG:C	1:I:124:GLN:NE2	2.72	0.43
1:A:157:ILE:HD11	1:B:117:ARG:NE	2.33	0.43
1:H:216:ILE:O	1:H:219:SER:HB3	2.18	0.43
1:B:178:LEU:HD13	1:B:178:LEU:HA	1.82	0.43
1:E:178:LEU:HD13	1:E:178:LEU:HA	1.79	0.43
1:F:127:VAL:HG22	1:F:194:ARG:CB	2.48	0.43
1:A:151:ASN:ND2	1:A:155:GLU:OE2	2.52	0.43
1:B:179:SER:HB2	1:B:186:ASN:ND2	2.33	0.43
1:B:162:ILE:HA	1:B:197:ALA:HA	2.01	0.43
1:C:212:LEU:HB2	1:C:245:TYR:CE2	2.54	0.43
1:D:88:GLY:HA2	1:E:84:SER:HB3	2.00	0.43
1:G:76:LEU:HB3	1:G:130:LEU:HD11	2.00	0.43
1:B:118:LEU:HA	1:B:261:VAL:HG23	2.00	0.43
1:D:178:LEU:HD13	1:D:178:LEU:HA	1.82	0.43
1:I:256:LEU:HD12	1:I:260:THR:HG22	2.00	0.43
1:J:14:VAL:HG21	1:J:138:GLN:NE2	2.34	0.43
1:J:268:ALA:HB1	1:J:308:PHE:CE1	2.53	0.43
1:A:14:VAL:HG13	1:A:43:TRP:HD1	1.83	0.43
1:B:159:GLU:HG3	1:C:257:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:ASP:H	1:H:155:GLU:CD	2.22	0.43
1:A:97:ASP:OD2	1:A:99:ARG:NH1	2.52	0.43
1:C:14:VAL:HG21	1:C:138:GLN:NE2	2.34	0.43
1:F:141:ARG:HD2	1:F:142:PHE:CE2	2.54	0.43
1:H:260:THR:O	1:H:264:GLN:HG3	2.19	0.43
1:I:157:ILE:HD11	1:J:117:ARG:NE	2.34	0.43
1:A:141:ARG:HD2	1:A:142:PHE:CE2	2.53	0.42
1:A:167:SER:HB2	1:A:194:ARG:HG3	2.00	0.42
1:D:253:LEU:HD21	1:D:262:ILE:HD12	2.00	0.42
1:E:119:PHE:CB	1:E:260:THR:HB	2.49	0.42
1:E:224:TRP:HE1	1:E:301:ARG:HB3	1.84	0.42
1:E:78:PHE:O	1:E:81:VAL:HG12	2.19	0.42
1:F:78:PHE:O	1:F:81:VAL:HG12	2.19	0.42
1:H:72:TRP:CZ3	1:H:74:PRO:HB3	2.54	0.42
1:I:260:THR:N	1:I:263:ASP:HB2	2.34	0.42
1:J:175:TYR:O	1:J:186:ASN:ND2	2.46	0.42
1:A:133:PHE:CE2	1:E:91:ARG:HG2	2.54	0.42
1:B:126:PHE:CE1	2:B:401:Z80:H2	2.54	0.42
1:D:95:PHE:HE1	1:D:101:ILE:HD12	1.84	0.42
1:D:66:TRP:CE3	1:D:71:LEU:HD12	2.55	0.42
1:E:27:ASN:HB3	1:E:32:THR:HB	2.01	0.42
1:F:122:ASP:HB2	1:F:199:ARG:HB2	2.01	0.42
1:G:95:PHE:HE1	1:G:101:ILE:HD12	1.85	0.42
1:G:253:LEU:HD21	1:G:262:ILE:HD12	2.01	0.42
1:I:92:LEU:HA	1:I:92:LEU:HD23	1.88	0.42
1:J:273:ILE:O	1:J:277:ILE:HG13	2.19	0.42
1:B:14:VAL:HG21	1:B:138:GLN:NE2	2.34	0.42
1:C:294:ASP:HB3	1:C:297:ILE:HG22	2.01	0.42
1:D:141:ARG:HD2	1:D:142:PHE:CE2	2.54	0.42
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.82	0.42
1:E:160:TRP:CD1	2:E:401:Z80:C5	3.03	0.42
1:F:284:HIS:HB3	1:F:285:HIS:ND1	2.34	0.42
1:A:285:HIS:HE2	1:E:301:ARG:HH12	1.66	0.42
1:G:14:VAL:HG21	1:G:138:GLN:NE2	2.35	0.42
1:G:93:MET:HB2	1:G:101:ILE:HB	2.01	0.42
1:H:225:LEU:HB2	1:H:231:ARG:HG3	2.01	0.42
1:J:154:ASN:C	1:J:156:GLU:H	2.21	0.42
1:B:212:LEU:HB2	1:B:245:TYR:CE2	2.54	0.42
1:F:151:ASN:HD21	1:F:161:TRP:HA	1.84	0.42
1:J:16:VAL:HA	1:J:40:VAL:O	2.20	0.42
1:J:78:PHE:O	1:J:81:VAL:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLU:OE2	1:D:284:HIS:NE2	2.50	0.42
1:F:119:PHE:CB	1:F:260:THR:HB	2.50	0.42
1:H:27:ASN:HB3	1:H:32:THR:HB	2.00	0.42
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.55	0.42
1:I:119:PHE:HB2	1:I:260:THR:HB	2.02	0.42
1:A:151:ASN:HD21	1:A:161:TRP:HA	1.85	0.42
1:C:157:ILE:HD11	1:D:117:ARG:NE	2.35	0.42
1:G:167:SER:HB3	1:G:194:ARG:HG3	2.02	0.42
1:F:241:THR:HA	1:G:240:LEU:HD23	2.01	0.42
1:H:155:GLU:OE1	2:H:401:Z80:H12	2.19	0.42
1:I:13:ASP:HB3	1:I:141:ARG:HE	1.85	0.42
1:J:155:GLU:HA	1:J:158:ASP:N	2.31	0.42
1:J:179:SER:HB2	1:J:186:ASN:ND2	2.35	0.42
1:J:260:THR:O	1:J:264:GLN:HG3	2.18	0.42
1:B:225:LEU:HB2	1:B:231:ARG:HG3	2.00	0.42
1:A:248:TYR:HE1	1:B:250:SER:OG	2.03	0.42
1:C:179:SER:HB2	1:C:186:ASN:ND2	2.34	0.42
1:F:147:VAL:HG13	2:F:401:Z80:CL1	2.57	0.42
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.88	0.42
1:H:238:LEU:HB3	1:H:273:ILE:CD1	2.49	0.42
1:I:72:TRP:CZ3	1:I:74:PRO:HB3	2.55	0.42
1:J:284:HIS:HB3	1:J:285:HIS:ND1	2.34	0.42
1:B:13:ASP:HB3	1:B:141:ARG:HE	1.85	0.42
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.83	0.42
1:C:287:GLN:HG2	1:C:289:ASN:O	2.20	0.42
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.55	0.42
1:D:27:ASN:HB3	1:D:32:THR:HB	2.01	0.42
1:D:160:TRP:CD1	2:D:401:Z80:C5	3.02	0.42
1:D:72:TRP:CZ3	1:D:74:PRO:HB3	2.55	0.42
1:E:263:ASP:O	1:E:267:ILE:HG12	2.20	0.42
1:F:117:ARG:NE	1:J:157:ILE:HD11	2.34	0.42
1:F:253:LEU:HD21	1:F:262:ILE:HD12	2.02	0.42
1:I:14:VAL:HG21	1:I:138:GLN:NE2	2.35	0.42
1:H:88:GLY:HA2	1:I:84:SER:HB3	2.01	0.42
1:J:238:LEU:HB3	1:J:273:ILE:CD1	2.48	0.42
1:F:250:SER:OG	1:J:248:TYR:HE1	2.03	0.42
1:A:294:ASP:HB3	1:A:297:ILE:CG2	2.49	0.42
1:A:268:ALA:HB1	1:A:308:PHE:CE1	2.55	0.42
1:A:71:LEU:HD11	1:A:94:LEU:HD21	2.01	0.42
1:B:141:ARG:HD2	1:B:142:PHE:CE2	2.55	0.42
1:B:155:GLU:HB2	1:B:161:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:VAL:HA	1:D:102:TYR:O	2.20	0.42
1:A:284:HIS:NE2	1:E:226:GLU:OE2	2.53	0.42
1:E:284:HIS:HB3	1:E:285:HIS:ND1	2.34	0.42
1:F:14:VAL:HG21	1:F:138:GLN:NE2	2.35	0.42
1:G:157:ILE:HD11	1:H:117:ARG:NE	2.35	0.42
1:A:133:PHE:HE2	1:E:91:ARG:HG2	1.84	0.41
1:B:78:PHE:O	1:B:81:VAL:HG12	2.19	0.41
1:B:95:PHE:HE1	1:B:101:ILE:HD12	1.84	0.41
1:C:160:TRP:CD1	2:C:401:Z80:C5	3.03	0.41
1:C:95:PHE:HE1	1:C:101:ILE:HD12	1.84	0.41
1:E:225:LEU:HB2	1:E:231:ARG:HG3	2.01	0.41
1:F:134:SER:HB3	1:J:91:ARG:CD	2.47	0.41
1:F:221:SER:HB2	1:G:281:ILE:CD1	2.50	0.41
1:I:160:TRP:CD1	2:I:401:Z80:C5	3.03	0.41
1:I:232:LEU:O	1:I:235:SER:HB2	2.20	0.41
1:A:178:LEU:HD13	1:A:178:LEU:HA	1.80	0.41
1:C:29:LEU:HA	1:C:29:LEU:HD23	1.85	0.41
1:C:64:GLU:HA	1:C:67:ILE:HD12	2.02	0.41
1:C:58:VAL:O	1:C:91:ARG:HA	2.20	0.41
1:E:119:PHE:HB3	1:E:120:PRO:HD3	2.03	0.41
1:B:155:GLU:HB2	1:B:161:TRP:HD1	1.85	0.41
1:G:126:PHE:CE1	2:G:401:Z80:H2	2.55	0.41
1:I:59:GLU:OE2	1:J:134:SER:OG	2.38	0.41
1:B:143:SER:HB2	1:B:170:ILE:HD11	2.02	0.41
1:D:151:ASN:ND2	1:D:162:ILE:H	2.19	0.41
1:D:58:VAL:HB	1:D:92:LEU:HB2	2.03	0.41
1:G:155:GLU:HB3	2:G:401:Z80:C15	2.48	0.41
1:G:178:LEU:HA	1:G:178:LEU:HD13	1.77	0.41
1:H:226:GLU:OE2	1:I:284:HIS:NE2	2.54	0.41
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.82	0.41
1:A:58:VAL:O	1:A:91:ARG:HA	2.21	0.41
2:B:401:Z80:H16	2:B:401:Z80:H9	1.58	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.90	0.41
1:E:132:PRO:HD2	1:E:189:SER:O	2.20	0.41
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
1:I:169:HIS:O	1:I:170:ILE:HB	2.20	0.41
1:I:287:GLN:HG2	1:I:289:ASN:O	2.21	0.41
1:I:294:ASP:HB3	1:I:297:ILE:HG22	2.02	0.41
1:C:122:ASP:HB2	1:C:199:ARG:HB2	2.02	0.41
1:C:13:ASP:HB3	1:C:141:ARG:HE	1.86	0.41
1:C:256:LEU:HD12	1:C:260:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:SER:HB2	1:D:194:ARG:HG3	2.02	0.41
1:D:17:SER:HB2	1:D:40:VAL:CG2	2.50	0.41
1:A:240:LEU:CD2	1:E:241:THR:HA	2.51	0.41
1:G:151:ASN:ND2	1:G:162:ILE:H	2.19	0.41
1:B:151:ASN:ND2	1:B:155:GLU:OE1	2.54	0.41
1:C:155:GLU:CG	1:C:161:TRP:CD1	2.96	0.41
1:C:205:LEU:HA	1:C:209:ILE:HB	2.02	0.41
1:C:72:TRP:CZ3	1:C:74:PRO:HB3	2.55	0.41
1:E:56:LEU:HD13	1:E:57:ILE:N	2.35	0.41
1:G:160:TRP:CD1	2:G:401:Z80:C5	3.04	0.41
1:I:173:ILE:O	1:I:187:GLU:HA	2.20	0.41
1:B:153:ASP:O	1:B:155:GLU:HG2	2.20	0.41
1:F:97:ASP:OD2	1:F:99:ARG:NH1	2.54	0.41
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.21	0.41
1:I:263:ASP:O	1:I:267:ILE:HG12	2.21	0.41
1:A:153:ASP:N	1:A:155:GLU:OE2	2.54	0.41
1:D:268:ALA:HB1	1:D:308:PHE:CE1	2.56	0.41
1:D:91:ARG:HD3	1:E:134:SER:HB3	2.02	0.41
1:J:155:GLU:CG	1:J:161:TRP:HD1	2.29	0.41
1:A:13:ASP:HB3	1:A:141:ARG:HE	1.85	0.41
1:A:284:HIS:HB3	1:A:285:HIS:ND1	2.35	0.41
1:D:169:HIS:O	1:D:170:ILE:HB	2.20	0.41
1:D:132:PRO:HD2	1:D:189:SER:O	2.21	0.41
1:F:153:ASP:HB3	1:F:154:ASN:H	1.65	0.41
1:F:167:SER:HB2	1:F:194:ARG:HG3	2.03	0.41
1:G:159:GLU:OE2	1:H:29:LEU:HD21	2.19	0.41
1:H:268:ALA:HB1	1:H:308:PHE:CE1	2.55	0.41
1:J:238:LEU:HA	1:J:238:LEU:HD13	1.94	0.41
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.55	0.41
1:F:160:TRP:CD1	2:F:401:Z80:C5	3.04	0.41
1:G:176:ASP:OD1	1:G:176:ASP:N	2.54	0.41
1:H:114:MET:HE2	1:H:124:GLN:HG2	2.03	0.41
1:H:160:TRP:CD1	2:H:401:Z80:C5	3.04	0.41
1:I:44:THR:HG23	1:I:99:ARG:HB3	2.03	0.41
1:J:178:LEU:HD13	1:J:178:LEU:HA	1.81	0.41
1:D:174:ARG:HD3	1:D:174:ARG:HH21	1.71	0.40
1:D:120:PRO:O	1:D:201:PRO:HB3	2.21	0.40
1:F:56:LEU:HD13	1:F:57:ILE:N	2.36	0.40
1:F:66:TRP:HE3	1:F:71:LEU:HD12	1.85	0.40
1:F:248:TYR:HE1	1:G:250:SER:OG	2.03	0.40
1:H:263:ASP:O	1:H:267:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:ASP:OD2	1:H:99:ARG:NH1	2.54	0.40
1:E:161:TRP:N	1:E:198:VAL:O	2.34	0.40
1:G:155:GLU:HG3	1:G:161:TRP:NE1	2.36	0.40
1:H:14:VAL:HG21	1:H:138:GLN:NE2	2.35	0.40
1:I:105:ARG:NH2	1:J:81:VAL:O	2.54	0.40
1:I:224:TRP:HE1	1:I:301:ARG:HB3	1.85	0.40
1:A:126:PHE:CE1	2:A:401:Z80:H18	2.57	0.40
1:E:175:TYR:O	1:E:186:ASN:ND2	2.50	0.40
1:H:205:LEU:HA	1:H:209:ILE:HB	2.03	0.40
1:H:209:ILE:HG23	1:H:265:MET:HE1	2.02	0.40
1:H:240:LEU:HD23	1:H:240:LEU:HA	1.88	0.40
1:H:92:LEU:HA	1:H:92:LEU:HD23	1.92	0.40
1:I:28:THR:HB	1:I:256:LEU:CD2	2.51	0.40
1:I:28:THR:HA	1:I:116:PHE:CE1	2.57	0.40
1:A:119:PHE:HB3	1:A:120:PRO:HD3	2.03	0.40
1:J:147:VAL:CG1	2:J:401:Z80:H4	2.51	0.40
1:A:162:ILE:HA	1:A:197:ALA:HA	2.03	0.40
1:A:284:HIS:HE1	1:A:291:VAL:HG13	1.83	0.40
1:C:224:TRP:CD1	1:C:224:TRP:N	2.89	0.40
1:D:126:PHE:HE1	1:D:197:ALA:HB3	1.87	0.40
1:E:151:ASN:ND2	1:E:155:GLU:OE2	2.55	0.40
1:F:157:ILE:HD11	1:G:117:ARG:NE	2.37	0.40
1:J:14:VAL:HB	1:J:140:LEU:HD23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:ASN:ND2	1:H:288:ALA:O[1_455]	2.19	0.01

## 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%)	264 (87%)	39 (13%)	2 (1%)	26	72
1	B	305/307 (99%)	263 (86%)	40 (13%)	2 (1%)	26	72
1	C	305/307 (99%)	265 (87%)	38 (12%)	2 (1%)	26	72
1	D	305/307 (99%)	265 (87%)	38 (12%)	2 (1%)	26	72
1	E	305/307 (99%)	263 (86%)	40 (13%)	2 (1%)	26	72
1	F	305/307 (99%)	265 (87%)	38 (12%)	2 (1%)	26	72
1	G	305/307 (99%)	266 (87%)	37 (12%)	2 (1%)	26	72
1	H	305/307 (99%)	263 (86%)	40 (13%)	2 (1%)	26	72
1	I	305/307 (99%)	266 (87%)	36 (12%)	3 (1%)	19	66
1	J	305/307 (99%)	265 (87%)	37 (12%)	3 (1%)	19	66
All	All	3050/3070 (99%)	2645 (87%)	383 (13%)	22 (1%)	26	72

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	167	SER
1	J	152	ILE
1	J	155	GLU
1	D	153	ASP
1	E	153	ASP
1	G	170	ILE
1	H	153	ASP
1	I	153	ASP
1	A	153	ASP
1	B	153	ASP
1	C	153	ASP
1	F	153	ASP
1	G	153	ASP
1	D	170	ILE
1	E	170	ILE
1	H	170	ILE
1	I	170	ILE
1	A	170	ILE
1	C	170	ILE
1	F	170	ILE
1	J	170	ILE
1	B	170	ILE

### 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%)	267 (97%)	7 (3%)	54	83
1	B	275/275 (100%)	268 (98%)	7 (2%)	55	84
1	C	275/275 (100%)	266 (97%)	9 (3%)	45	80
1	D	275/275 (100%)	265 (96%)	10 (4%)	42	79
1	E	275/275 (100%)	265 (96%)	10 (4%)	42	79
1	F	275/275 (100%)	267 (97%)	8 (3%)	50	82
1	G	275/275 (100%)	267 (97%)	8 (3%)	50	82
1	H	275/275 (100%)	269 (98%)	6 (2%)	60	86
1	I	274/275 (100%)	266 (97%)	8 (3%)	50	82
1	J	275/275 (100%)	267 (97%)	8 (3%)	50	82
All	All	2748/2750 (100%)	2667 (97%)	81 (3%)	50	82

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	138	GLN
1	A	206	TRP
1	A	228	PHE
1	A	255	ARG
1	A	258	TYR
1	A	304	PHE
1	B	29	LEU
1	B	53	ASP
1	B	138	GLN
1	B	206	TRP
1	B	228	PHE
1	B	255	ARG
1	B	258	TYR
1	C	29	LEU
1	C	53	ASP

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Mol	Chain	Res	Type
1	C	138	GLN
1	C	150	GLU
1	C	206	TRP
1	C	228	PHE
1	C	255	ARG
1	C	258	TYR
1	C	287	GLN
1	D	29	LEU
1	D	53	ASP
1	D	138	GLN
1	D	150	GLU
1	D	163	ARG
1	D	206	TRP
1	D	228	PHE
1	D	255	ARG
1	D	299	ARG
1	D	304	PHE
1	E	29	LEU
1	E	53	ASP
1	E	91	ARG
1	E	138	GLN
1	E	150	GLU
1	E	206	TRP
1	E	207	SER
1	E	228	PHE
1	E	255	ARG
1	E	304	PHE
1	F	29	LEU
1	F	53	ASP
1	F	91	ARG
1	F	138	GLN
1	F	150	GLU
1	F	206	TRP
1	F	255	ARG
1	F	304	PHE
1	G	29	LEU
1	G	91	ARG
1	G	138	GLN
1	G	150	GLU
1	G	206	TRP
1	G	228	PHE
1	G	255	ARG

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Mol	Chain	Res	Type
1	G	304	PHE
1	H	65	ARG
1	H	138	GLN
1	H	206	TRP
1	H	228	PHE
1	H	255	ARG
1	H	287	GLN
1	I	53	ASP
1	I	91	ARG
1	I	119	PHE
1	I	124	GLN
1	I	138	GLN
1	I	150	GLU
1	I	206	TRP
1	I	255	ARG
1	J	91	ARG
1	J	138	GLN
1	J	150	GLU
1	J	206	TRP
1	J	228	PHE
1	J	255	ARG
1	J	258	TYR
1	J	299	ARG

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

Mol	Chain	Res	Type
1	A	21	ASN
1	A	151	ASN
1	B	151	ASN
1	C	151	ASN
1	D	151	ASN
1	E	151	ASN
1	F	151	ASN
1	G	151	ASN
1	H	151	ASN
1	H	287	GLN
1	I	124	GLN
1	I	151	ASN
1	J	151	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 ⓘ

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	Z80	A	401	-	23,23,23	4.09	5 (21%)	32,32,32	1.79	4 (12%)
2	Z80	B	401	-	23,23,23	4.14	5 (21%)	32,32,32	1.77	4 (12%)
2	Z80	C	401	-	23,23,23	4.08	5 (21%)	32,32,32	1.69	4 (12%)
2	Z80	D	401	-	23,23,23	4.01	5 (21%)	32,32,32	1.44	1 (3%)
2	Z80	E	401	-	23,23,23	4.05	5 (21%)	32,32,32	1.68	3 (9%)
2	Z80	F	401	-	23,23,23	4.18	5 (21%)	32,32,32	1.64	4 (12%)
2	Z80	G	401	-	23,23,23	4.14	5 (21%)	32,32,32	1.71	3 (9%)
2	Z80	H	401	-	23,23,23	4.12	5 (21%)	32,32,32	1.46	2 (6%)
2	Z80	I	401	-	23,23,23	4.08	5 (21%)	32,32,32	1.62	4 (12%)
2	Z80	J	401	-	23,23,23	4.10	5 (21%)	32,32,32	1.74	3 (9%)

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	Z80	A	401	-	-	0/6/18/18	0/2/3/3
2	Z80	B	401	-	-	0/6/18/18	0/2/3/3
2	Z80	C	401	-	-	0/6/18/18	0/2/3/3
2	Z80	D	401	-	-	0/6/18/18	0/3/3/3
2	Z80	E	401	-	-	0/6/18/18	0/2/3/3
2	Z80	F	401	-	-	0/6/18/18	0/2/3/3
2	Z80	G	401	-	-	0/6/18/18	0/2/3/3
2	Z80	H	401	-	-	0/6/18/18	0/3/3/3
2	Z80	I	401	-	-	0/6/18/18	0/2/3/3
2	Z80	J	401	-	-	0/6/18/18	0/2/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	Z80	C3-S1	-7.90	1.61	1.76
2	G	401	Z80	C2-S1	-7.75	1.62	1.76
2	I	401	Z80	C3-S1	-7.75	1.62	1.76
2	D	401	Z80	C3-S1	-7.71	1.62	1.76
2	C	401	Z80	C3-S1	-7.71	1.62	1.76
2	E	401	Z80	C2-S1	-7.69	1.62	1.76
2	H	401	Z80	C3-S1	-7.69	1.62	1.76
2	H	401	Z80	C2-S1	-7.68	1.62	1.76
2	E	401	Z80	C3-S1	-7.67	1.62	1.76
2	B	401	Z80	C3-S1	-7.66	1.62	1.76
2	F	401	Z80	C2-S1	-7.66	1.62	1.76
2	F	401	Z80	C3-S1	-7.66	1.62	1.76
2	A	401	Z80	C2-S1	-7.66	1.62	1.76
2	A	401	Z80	C3-S1	-7.62	1.62	1.76
2	I	401	Z80	C2-S1	-7.62	1.62	1.76
2	C	401	Z80	C2-S1	-7.55	1.62	1.76
2	D	401	Z80	C2-S1	-7.54	1.62	1.76
2	J	401	Z80	C3-S1	-7.50	1.62	1.76
2	B	401	Z80	C2-S1	-7.49	1.62	1.76
2	J	401	Z80	C2-S1	-7.38	1.62	1.76
2	H	401	Z80	C17-C1	2.23	1.43	1.39
2	D	401	Z80	C17-C1	2.27	1.43	1.39
2	G	401	Z80	C17-C1	2.34	1.43	1.39
2	E	401	Z80	C17-C1	2.37	1.43	1.39
2	F	401	Z80	C17-C1	2.39	1.43	1.39
2	C	401	Z80	C17-C1	2.40	1.43	1.39
2	I	401	Z80	C17-C1	2.42	1.43	1.39
2	B	401	Z80	C17-C1	2.44	1.43	1.39
2	A	401	Z80	C17-C1	2.45	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	Z80	C17-C1	2.57	1.44	1.39
2	D	401	Z80	C1-N1	10.43	1.57	1.40
2	I	401	Z80	C1-N1	10.63	1.58	1.40
2	E	401	Z80	C1-N1	10.74	1.58	1.40
2	C	401	Z80	C1-N1	10.76	1.58	1.40
2	H	401	Z80	C1-N1	10.77	1.58	1.40
2	A	401	Z80	C1-N1	10.82	1.58	1.40
2	G	401	Z80	C1-N1	10.88	1.58	1.40
2	B	401	Z80	C1-N1	10.92	1.58	1.40
2	J	401	Z80	C1-N1	10.99	1.58	1.40
2	E	401	Z80	C4-N1	11.02	1.58	1.40
2	D	401	Z80	C4-N1	11.11	1.58	1.40
2	F	401	Z80	C1-N1	11.11	1.59	1.40
2	A	401	Z80	C4-N1	11.28	1.59	1.40
2	C	401	Z80	C4-N1	11.33	1.59	1.40
2	I	401	Z80	C4-N1	11.34	1.59	1.40
2	J	401	Z80	C4-N1	11.41	1.59	1.40
2	G	401	Z80	C4-N1	11.48	1.59	1.40
2	H	401	Z80	C4-N1	11.61	1.59	1.40
2	F	401	Z80	C4-N1	11.68	1.59	1.40
2	B	401	Z80	C4-N1	11.71	1.59	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	Z80	C12-N1-C4	-5.59	111.10	118.99
2	G	401	Z80	C12-N1-C4	-5.31	111.49	118.99
2	E	401	Z80	C12-N1-C4	-5.30	111.50	118.99
2	C	401	Z80	C12-N1-C4	-5.24	111.58	118.99
2	J	401	Z80	C12-N1-C4	-5.14	111.73	118.99
2	B	401	Z80	C12-N1-C4	-5.00	111.93	118.99
2	I	401	Z80	C12-N1-C4	-4.22	113.02	118.99
2	F	401	Z80	C12-N1-C4	-3.71	113.75	118.99
2	B	401	Z80	C12-N1-C1	-3.14	114.56	118.99
2	I	401	Z80	C12-N1-C1	-2.47	115.50	118.99
2	G	401	Z80	C12-N1-C1	-2.41	115.59	118.99
2	A	401	Z80	C12-N1-C1	-2.24	115.83	118.99
2	C	401	Z80	C12-N1-C1	-2.01	116.14	118.99
2	F	401	Z80	C8-C9-C10	2.10	121.50	119.22
2	C	401	Z80	C8-C9-C10	2.10	121.51	119.22
2	H	401	Z80	C8-C9-C10	2.15	121.56	119.22
2	J	401	Z80	C8-C9-C10	2.26	121.68	119.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	Z80	C14-C13-C12	2.27	120.50	112.85
2	A	401	Z80	C8-C9-C10	2.29	121.71	119.22
2	E	401	Z80	C8-C9-C10	2.31	121.73	119.22
2	I	401	Z80	C13-C14-N2	2.39	119.79	113.83
2	F	401	Z80	C14-C13-C12	2.57	121.51	112.85
2	F	401	Z80	C3-S1-C2	5.22	113.65	100.68
2	E	401	Z80	C3-S1-C2	5.53	114.41	100.68
2	I	401	Z80	C3-S1-C2	5.58	114.53	100.68
2	H	401	Z80	C3-S1-C2	5.63	114.65	100.68
2	D	401	Z80	C3-S1-C2	5.68	114.79	100.68
2	J	401	Z80	C3-S1-C2	5.82	115.13	100.68
2	C	401	Z80	C3-S1-C2	5.87	115.26	100.68
2	B	401	Z80	C3-S1-C2	5.95	115.44	100.68
2	G	401	Z80	C3-S1-C2	6.06	115.73	100.68
2	A	401	Z80	C3-S1-C2	6.25	116.20	100.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	Z80	7	0
2	B	401	Z80	6	0
2	C	401	Z80	5	0
2	D	401	Z80	4	0
2	E	401	Z80	7	0
2	F	401	Z80	8	0
2	G	401	Z80	9	0
2	H	401	Z80	6	0
2	I	401	Z80	3	0
2	J	401	Z80	7	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%)	-0.11	13 (4%)	40	32	49, 88, 191, 243	0
1	B	307/307 (100%)	-0.19	11 (3%)	46	37	48, 87, 193, 241	0
1	C	307/307 (100%)	-0.10	13 (4%)	40	32	46, 86, 192, 243	0
1	D	307/307 (100%)	-0.21	10 (3%)	50	40	44, 86, 192, 241	0
1	E	307/307 (100%)	-0.37	5 (1%)	74	66	48, 86, 192, 242	0
1	F	307/307 (100%)	-0.18	14 (4%)	36	29	53, 89, 191, 242	0
1	G	307/307 (100%)	-0.19	12 (3%)	43	35	49, 87, 192, 241	0
1	H	307/307 (100%)	-0.21	13 (4%)	40	32	49, 88, 194, 257	0
1	I	307/307 (100%)	-0.29	7 (2%)	64	54	45, 88, 191, 242	0
1	J	307/307 (100%)	-0.17	14 (4%)	36	29	48, 89, 196, 242	0
All	All	3070/3070 (100%)	-0.20	112 (3%)	46	37	44, 87, 194, 257	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	GLY	6.6
1	H	291	VAL	5.8
1	H	289	ASN	5.8
1	C	317	ILE	5.6
1	G	152	ILE	5.6
1	B	289	ASN	5.6
1	I	180	SER	5.4
1	H	151	ASN	5.3
1	H	152	ILE	5.2
1	H	290	GLY	4.9
1	F	287	GLN	4.9
1	B	290	GLY	4.6
1	G	290	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	305	PRO	4.5
1	E	291	VAL	4.4
1	D	179	SER	4.3
1	A	178	LEU	4.3
1	J	306	LEU	4.1
1	F	288	ALA	4.1
1	C	314	VAL	4.0
1	D	182	GLN	3.9
1	H	288	ALA	3.9
1	J	307	GLY	3.9
1	C	312	GLY	3.8
1	C	306	LEU	3.8
1	F	179	SER	3.8
1	I	182	GLN	3.8
1	F	290	GLY	3.6
1	C	313	CYS	3.6
1	D	180	SER	3.6
1	I	181	VAL	3.6
1	D	176	ASP	3.5
1	A	177	HIS	3.5
1	E	288	ALA	3.4
1	C	315	LEU	3.4
1	F	289	ASN	3.4
1	F	180	SER	3.3
1	C	316	VAL	3.3
1	E	289	ASN	3.3
1	I	179	SER	3.2
1	B	291	VAL	3.2
1	J	310	ALA	3.2
1	D	178	LEU	3.2
1	C	152	ILE	3.1
1	J	309	LEU	3.1
1	I	183	PRO	3.1
1	J	291	VAL	3.0
1	H	164	GLY	3.0
1	J	290	GLY	3.0
1	D	291	VAL	2.9
1	B	153	ASP	2.9
1	D	163	ARG	2.9
1	H	315	LEU	2.8
1	B	149	THR	2.8
1	C	288	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	303	ALA	2.8
1	G	153	ASP	2.7
1	A	297	ILE	2.7
1	D	157	ILE	2.7
1	H	312	GLY	2.7
1	J	304	PHE	2.7
1	F	316	VAL	2.7
1	G	149	THR	2.7
1	C	151	ASN	2.7
1	B	296	LEU	2.7
1	A	176	ASP	2.7
1	G	313	CYS	2.7
1	H	293	ASP	2.6
1	F	317	ILE	2.6
1	A	179	SER	2.6
1	C	302	LEU	2.6
1	J	312	GLY	2.6
1	G	315	LEU	2.6
1	F	182	GLN	2.5
1	J	164	GLY	2.5
1	A	165	LYS	2.5
1	H	165	LYS	2.5
1	J	308	PHE	2.5
1	G	314	VAL	2.5
1	F	286	ARG	2.5
1	J	154	ASN	2.4
1	H	309	LEU	2.4
1	A	49	LYS	2.4
1	B	151	ASN	2.4
1	B	288	ALA	2.4
1	A	175	TYR	2.4
1	G	297	ILE	2.4
1	A	314	VAL	2.4
1	A	315	LEU	2.3
1	I	288	ALA	2.3
1	F	166	ALA	2.3
1	J	157	ILE	2.3
1	D	177	HIS	2.3
1	G	155	GLU	2.2
1	D	151	ASN	2.2
1	G	151	ASN	2.2
1	C	139	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	292	GLU	2.2
1	A	286	ARG	2.2
1	F	165	LYS	2.2
1	B	313	CYS	2.2
1	F	291	VAL	2.2
1	H	292	GLU	2.2
1	B	294	ASP	2.1
1	C	289	ASN	2.1
1	B	152	ILE	2.1
1	I	177	HIS	2.0
1	A	186	ASN	2.0
1	E	49	LYS	2.0
1	A	53	ASP	2.0
1	G	157	ILE	2.0
1	F	178	LEU	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	Z80	B	401	21/21	0.71	0.86	4.48	53,125,138,159	21
2	Z80	G	401	21/21	0.84	0.83	3.56	15,111,180,217	21
2	Z80	D	401	21/21	0.91	0.45	1.96	50,84,133,254	21
2	Z80	A	401	21/21	0.93	0.42	1.60	56,101,149,209	0
2	Z80	E	401	21/21	0.91	0.32	1.45	53,83,143,202	0
2	Z80	C	401	21/21	0.91	0.40	1.35	64,107,145,306	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	Z80	F	401	21/21	0.91	0.38	1.14	23,94,128,261	0
2	Z80	H	401	21/21	0.90	0.47	1.05	61,95,146,229	0
2	Z80	I	401	21/21	0.91	0.28	0.56	50,103,145,284	21
2	Z80	J	401	21/21	0.94	0.29	-0.03	29,73,109,228	21

## 6.5 Other polymers [i](#)

There are no such residues in this entry.