



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2017 – 12:56 PM EDT

PDB ID : 5BJT  
Title : Crystal structure of human FcRn with a peptide inhibitor at multiple sites  
Authors : Nienaber, V.; Badger, J.  
Deposited on : 2016-10-23  
Resolution : 3.20 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

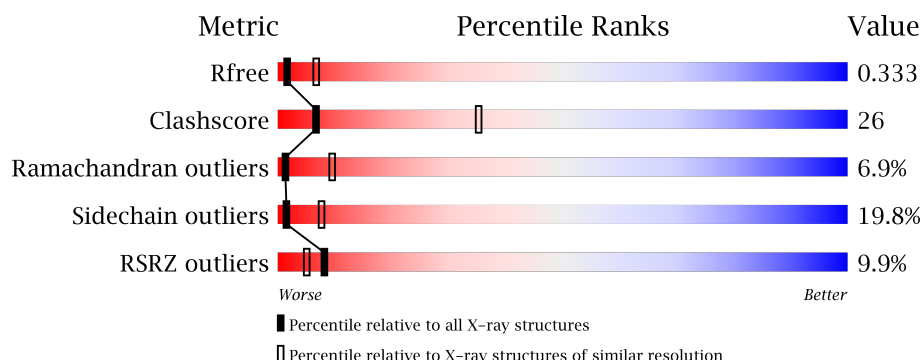
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	267	
1	C	267	
1	E	267	
1	G	267	
2	B	99	

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Mol	Chain	Length	Quality of chain
2	D	99	<div><div>2%</div><div><div></div><div>52%</div><div>41%</div><div>7%</div></div></div>
2	F	99	<div><div>2%</div><div><div></div><div>52%</div><div>41%</div><div>6%</div></div></div>
2	H	99	<div><div>67%</div><div><div></div><div>54%</div><div>41%</div><div></div></div></div>
3	P	19	<div><div>11%</div><div><div></div><div>74%</div><div>16%</div></div></div>
3	Q	19	<div><div>37%</div><div><div></div><div>32%</div><div>16%</div><div>16%</div></div></div>
3	R	19	<div><div>26%</div><div><div></div><div>37%</div><div>21%</div><div>16%</div></div></div>
3	S	19	<div><div>5%</div><div><div></div><div>32%</div><div>42%</div><div>11%</div><div>16%</div></div></div>
3	T	19	<div><div>58%</div><div><div></div><div>26%</div><div>16%</div></div></div>
3	U	19	<div><div>42%</div><div><div></div><div>37%</div><div>5%</div><div>16%</div></div></div>
3	V	19	<div><div>37%</div><div><div></div><div>37%</div><div>11%</div><div>16%</div></div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11486 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1970	1262	334	366	8			
1	C	263	Total	C	N	O	S	0	0	0
			1958	1252	330	368	8			
1	E	263	Total	C	N	O	S	0	0	0
			1964	1261	332	363	8			
1	G	263	Total	C	N	O	S	0	0	0
			1659	1055	293	306	5			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			792	504	131	154	3			
2	D	99	Total	C	N	O	S	0	0	0
			774	495	127	149	3			
2	F	99	Total	C	N	O	S	0	0	0
			775	497	131	144	3			
2	H	99	Total	C	N	O	S	0	0	0
			801	508	134	156	3			

- Molecule 3 is a protein called peptide inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	16	Total	C	N	O	S	0	0	0
			115	77	18	18	2			
3	Q	16	Total	C	N	O	S	0	0	0
			121	80	21	18	2			
3	R	16	Total	C	N	O	S	0	0	0
			121	80	21	18	2			
3	S	16	Total	C	N	O	S	0	0	0
			112	72	20	18	2			

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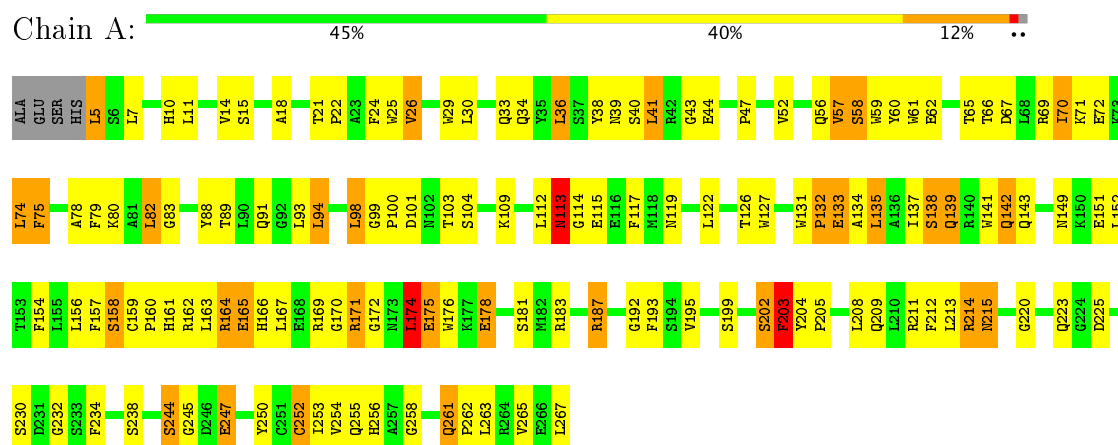
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	16	Total 106	C 69	N 17	O 18	S 2	0	0	0
3	U	16	Total 112	C 72	N 20	O 18	S 2	0	0	0
3	V	16	Total 106	C 69	N 17	O 18	S 2	0	0	0

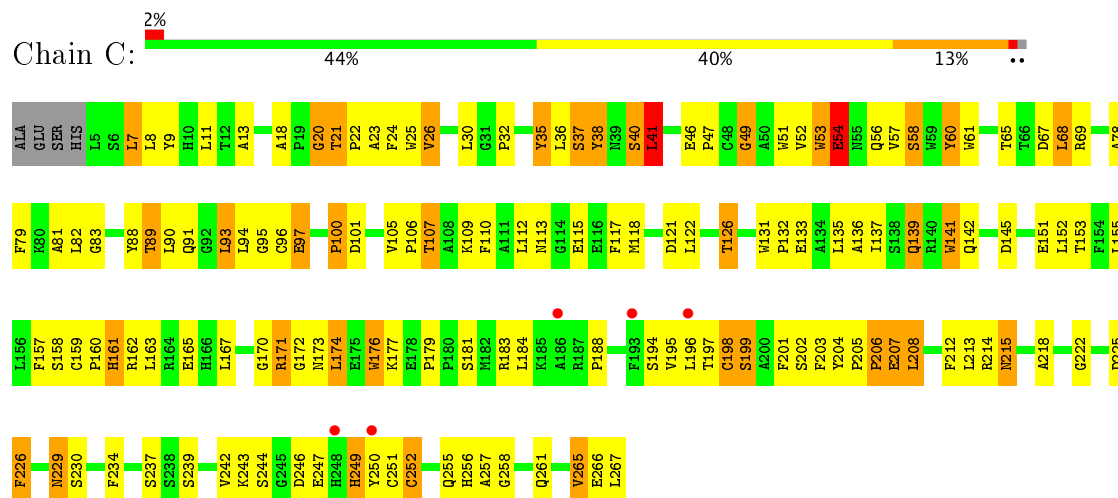
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

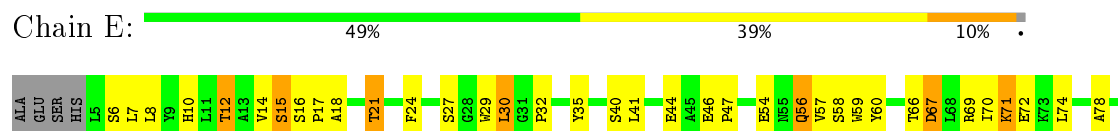
#### • Molecule 1: IgG receptor FcRn large subunit p51

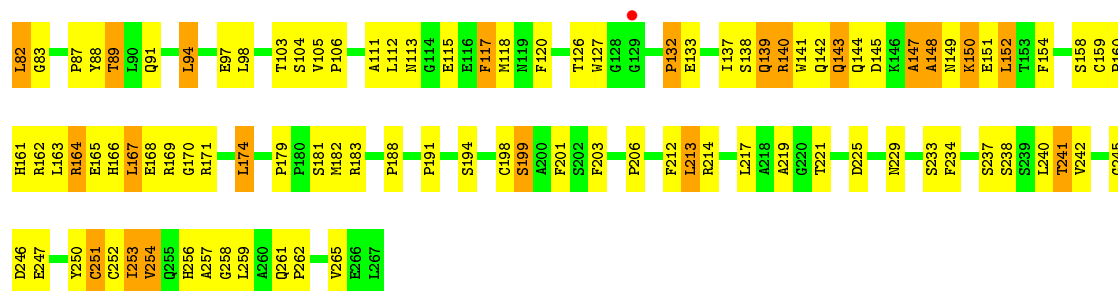


#### • Molecule 1: IgG receptor FcRn large subunit p51

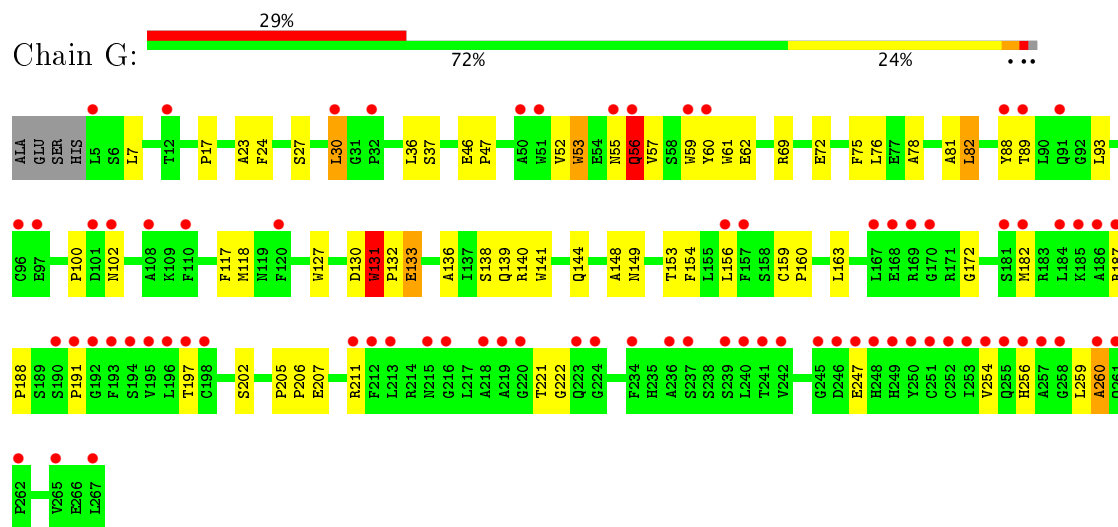


#### • Molecule 1: IgG receptor FcRn large subunit p51

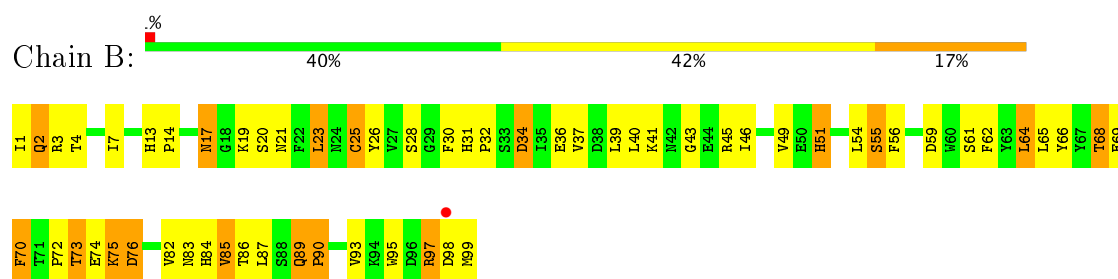




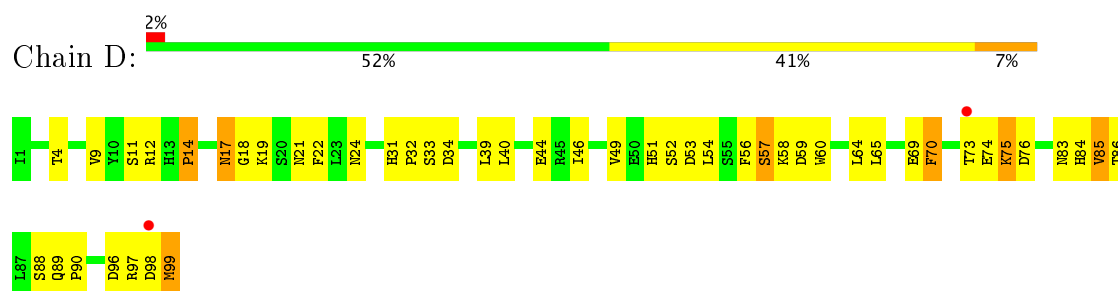
- Molecule 1: IgG receptor FcRn large subunit p51



- Molecule 2: Beta-2-microglobulin

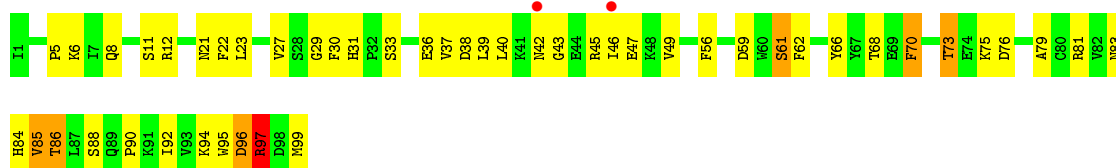


- Molecule 2: Beta-2-microglobulin

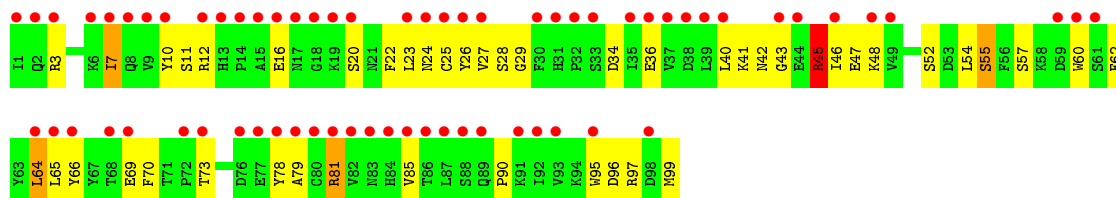


- Molecule 2: Beta-2-microglobulin

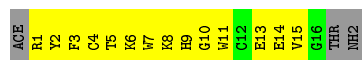




- Molecule 2: Beta-2-microglobulin



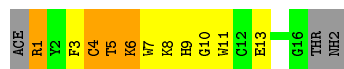
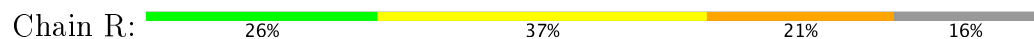
- Molecule 3: peptide inhibitor



- Molecule 3: peptide inhibitor



- Molecule 3: peptide inhibitor



- Molecule 3: peptide inhibitor



- Molecule 3: peptide inhibitor



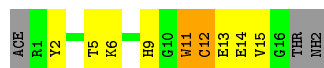
- Molecule 3: peptide inhibitor

Chain U:  42% 37% 5% 16%



- Molecule 3: peptide inhibitor

Chain V:  37% 37% 11% 16%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.92Å 176.15Å 245.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 3.20 49.25 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.9 (49.27-3.20) 99.6 (49.25-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.252 , 0.339 0.247 , 0.333	Depositor DCC
$R_{free}$ test set	1886 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.1	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 82.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

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	0.95	1/2031 (0.0%)	0.97	2/2776 (0.1%)
1	C	0.97	3/2021 (0.1%)	1.00	3/2765 (0.1%)
1	E	0.85	1/2027 (0.0%)	0.92	1/2773 (0.0%)
1	G	0.61	0/1708	0.69	0/2368
2	B	0.82	0/815	0.92	0/1112
2	D	0.83	0/797	0.94	0/1091
2	F	0.68	0/798	0.87	0/1091
2	H	0.70	0/824	0.72	0/1122
3	P	1.06	0/120	1.11	0/165
3	Q	1.06	0/126	1.25	0/172
3	R	1.00	1/126 (0.8%)	0.97	0/172
3	S	1.11	0/115	1.11	0/156
3	T	1.03	1/109 (0.9%)	0.96	0/149
3	U	0.87	0/115	1.02	0/156
3	V	1.17	0/109	1.39	2/149 (1.3%)
All	All	0.85	7/11841 (0.1%)	0.92	8/16217 (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	C	0	1
1	E	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	TRP	CB-CG	-6.92	1.37	1.50
3	T	12	CYS	CB-SG	-6.00	1.72	1.82
1	E	198	CYS	CB-SG	-5.70	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	4	CYS	CB-SG	5.69	1.92	1.82
1	C	165	GLU	CG-CD	5.51	1.60	1.51
1	A	252	CYS	CB-SG	-5.15	1.73	1.81
1	C	252	CYS	CB-SG	-5.09	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	164	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	C	93	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	E	253	ILE	CB-CA-C	-5.60	100.41	111.60
1	C	162	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	V	5	THR	CB-CA-C	-5.37	97.09	111.60
3	V	11	TRP	N-CA-C	5.21	125.06	111.00
1	A	41	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	20	GLY	Peptide
1	E	219	ALA	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	1970	0	1797	118	0
1	C	1958	0	1752	128	0
1	E	1964	0	1767	104	1
1	G	1659	0	1220	39	0
2	B	792	0	711	62	0
2	D	774	0	680	35	0
2	F	775	0	691	33	0
2	H	801	0	721	23	0
3	P	115	0	82	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	121	0	93	11	0
3	R	121	0	93	10	0
3	S	112	0	85	18	0
3	T	106	0	74	2	0
3	U	112	0	85	5	0
3	V	106	0	74	2	0
All	All	11486	0	9925	558	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 26.

All (558) 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)
2:B:89:GLN:HA	1:C:139:GLN:NE2	1.59	1.15
1:E:143:GLN:HE21	1:E:143:GLN:HA	1.11	1.15
1:A:149:ASN:HD21	3:P:14:GLU:HA	1.05	1.14
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.11	1.12
1:E:164:ARG:HH21	1:E:164:ARG:HB2	1.02	1.09
1:E:164:ARG:HH21	1:E:164:ARG:CB	1.66	1.08
1:A:171:ARG:HH21	1:A:171:ARG:CG	1.70	1.05
1:C:197:THR:HG21	2:D:99:MET:HB2	1.09	1.04
2:B:31:HIS:CD2	2:B:62:PHE:HE2	1.77	1.03
2:B:54:LEU:HG	2:B:64:LEU:HD12	1.08	1.02
1:A:171:ARG:NH2	1:A:171:ARG:HG3	1.54	1.01
1:A:158:SER:O	1:A:162:ARG:HG3	1.61	1.00
1:E:143:GLN:NE2	1:E:143:GLN:HA	1.78	0.98
1:A:171:ARG:HG3	1:A:171:ARG:HH21	0.81	0.98
2:B:31:HIS:CD2	2:B:62:PHE:CE2	2.52	0.96
1:C:157:PHE:O	1:C:160:PRO:HD2	1.66	0.94
1:C:197:THR:CG2	2:D:99:MET:HB2	1.98	0.94
2:B:54:LEU:HG	2:B:64:LEU:CD1	1.98	0.93
1:E:213:LEU:HD11	1:E:253:ILE:HD11	1.47	0.93
1:A:103:THR:HG21	3:S:1:ARG:HD3	1.51	0.93
1:E:143:GLN:HE21	1:E:143:GLN:CA	1.82	0.92
1:A:78:ALA:HB1	1:A:137:ILE:HD13	1.53	0.91
2:H:45:ARG:H	2:H:45:ARG:HD3	1.34	0.91
2:B:54:LEU:CG	2:B:64:LEU:HD12	1.98	0.91
1:E:164:ARG:NH2	1:E:164:ARG:HB2	1.85	0.91
1:A:149:ASN:ND2	3:P:14:GLU:HA	1.85	0.91
1:C:197:THR:HG21	2:D:99:MET:CB	1.98	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:NH1	1:A:187:ARG:HG3	1.78	0.90
1:C:26:VAL:HG21	1:C:68:LEU:HD22	1.54	0.90
2:B:89:GLN:HA	1:C:139:GLN:HE21	1.32	0.89
1:C:207:GLU:CD	1:C:207:GLU:H	1.77	0.88
1:E:161:HIS:HD2	3:R:11:TRP:CZ3	1.95	0.85
3:Q:1:ARG:HH21	3:Q:1:ARG:HG3	1.42	0.84
1:E:18:ALA:O	1:E:21:THR:HB	1.77	0.84
1:G:127:TRP:HB2	1:G:138:SER:HB2	1.60	0.83
1:E:12:THR:HG23	1:E:91:GLN:HG2	1.58	0.83
3:Q:1:ARG:NH2	3:Q:1:ARG:HG3	1.94	0.83
1:C:132:PRO:HA	1:C:135:LEU:HD12	1.60	0.82
1:A:159:CYS:HB3	1:A:160:PRO:HD3	1.59	0.82
1:A:18:ALA:O	1:A:21:THR:HB	1.79	0.82
2:B:54:LEU:HD21	2:B:62:PHE:HB3	1.62	0.81
1:A:114:GLY:N	2:B:31:HIS:CE1	2.48	0.81
1:E:7:LEU:HB2	1:E:163:LEU:HD13	1.62	0.81
1:C:266:GLU:HA	1:C:266:GLU:OE1	1.78	0.81
2:D:73:THR:HG22	2:D:74:GLU:H	1.46	0.80
1:A:187:ARG:HH11	1:A:187:ARG:CG	1.94	0.79
1:E:30:LEU:HD22	1:E:35:TYR:CD1	2.19	0.78
1:A:202:SER:O	1:A:234:PHE:O	2.02	0.77
2:F:40:LEU:HB2	2:F:79:ALA:HB3	1.65	0.77
1:C:171:ARG:HB3	1:C:171:ARG:CZ	2.15	0.76
1:C:199:SER:HB2	1:C:201:PHE:HE1	1.50	0.76
1:C:252:CYS:O	1:C:265:VAL:HG23	1.85	0.76
2:F:33:SER:HB3	2:F:62:PHE:CE1	2.21	0.75
3:Q:7:TRP:CE3	3:Q:11:TRP:O	2.39	0.75
3:R:3:PHE:HA	3:U:13:GLU:O	1.87	0.74
1:A:47:PRO:HG2	1:A:52:VAL:HG22	1.68	0.74
2:D:17:ASN:O	2:D:19:LYS:N	2.18	0.74
1:A:29:TRP:CZ3	1:A:34:GLN:HB2	2.22	0.73
1:C:89:THR:O	1:C:89:THR:HG22	1.89	0.72
1:A:79:PHE:O	1:A:82:LEU:HB2	1.90	0.71
1:C:7:LEU:HD12	1:C:9:TYR:CE1	2.25	0.71
1:C:30:LEU:HD22	1:C:35:TYR:CD1	2.26	0.71
2:B:64:LEU:CD2	2:B:66:TYR:CE1	2.73	0.71
1:E:206:PRO:HG3	1:E:234:PHE:CE1	2.25	0.71
1:C:157:PHE:O	1:C:159:CYS:N	2.23	0.71
2:H:10:TYR:HB3	2:H:99:MET:HG3	1.72	0.71
2:D:17:ASN:ND2	2:D:17:ASN:H	1.89	0.71
1:G:130:ASP:OD1	1:G:131:TRP:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:3:PHE:O	3:S:15:VAL:HA	1.90	0.71
1:C:188:PRO:HA	1:C:194:SER:HA	1.73	0.70
1:C:67:ASP:O	1:C:69:ARG:N	2.24	0.70
1:E:74:LEU:O	1:E:141:TRP:NE1	2.25	0.70
1:A:202:SER:OG	1:A:203:PHE:N	2.17	0.70
1:C:208:LEU:HD23	1:C:208:LEU:O	1.92	0.70
1:C:203:PHE:CZ	1:C:208:LEU:HD13	2.27	0.69
1:E:161:HIS:CD2	3:R:11:TRP:CZ3	2.80	0.69
1:C:18:ALA:O	1:C:21:THR:HB	1.93	0.69
3:P:8:LYS:O	3:P:10:GLY:N	2.25	0.69
1:C:176:TRP:CD1	1:C:177:LYS:N	2.60	0.69
2:B:64:LEU:HD22	2:B:66:TYR:CE1	2.27	0.69
1:C:82:LEU:HD11	1:C:133:GLU:HB2	1.74	0.69
1:G:36:LEU:HD23	1:G:37:SER:N	2.07	0.68
2:D:73:THR:HG22	2:D:74:GLU:N	2.09	0.68
1:A:98:LEU:HD22	1:A:103:THR:O	1.94	0.67
1:E:56:GLN:HG2	1:E:60:TYR:CD2	2.30	0.67
1:A:103:THR:HG21	3:S:1:ARG:CD	2.23	0.67
1:C:53:TRP:O	1:C:54:GLU:C	2.28	0.67
1:E:188:PRO:HA	1:E:194:SER:HA	1.76	0.67
1:A:151:GLU:O	1:A:154:PHE:HB3	1.95	0.67
2:D:97:ARG:O	2:D:99:MET:N	2.26	0.67
2:B:51:HIS:CD2	2:B:51:HIS:O	2.48	0.67
1:A:10:HIS:HB3	2:B:56:PHE:CE2	2.30	0.67
2:D:21:ASN:HB3	2:D:70:PHE:CE1	2.30	0.66
1:C:65:THR:O	1:C:69:ARG:HG3	1.96	0.66
1:A:211:ARG:HG2	1:A:253:ILE:HB	1.77	0.66
2:B:37:VAL:HB	2:B:66:TYR:CE1	2.30	0.66
2:F:6:LYS:HE2	2:F:8:GLN:HE21	1.59	0.66
2:F:49:VAL:HG22	2:F:68:THR:HB	1.77	0.66
1:E:164:ARG:CB	1:E:164:ARG:NH2	2.50	0.66
2:B:83:ASN:ND2	2:B:90:PRO:HD3	2.11	0.65
1:E:256:HIS:CD2	1:E:258:GLY:H	2.12	0.65
1:E:229:ASN:ND2	1:E:233:SER:OG	2.29	0.65
2:B:36:GLU:HB2	1:C:132:PRO:HB3	1.79	0.65
2:B:89:GLN:HA	1:C:139:GLN:HE22	1.58	0.65
2:H:41:LYS:HB2	2:H:46:ILE:HG12	1.79	0.65
1:E:57:VAL:O	1:E:59:TRP:N	2.29	0.65
1:E:126:THR:HG23	1:E:142:GLN:HE21	1.62	0.65
2:F:99:MET:HG3	2:F:99:MET:O	1.97	0.65
2:F:6:LYS:HE2	2:F:8:GLN:NE2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:O	1:A:171:ARG:HB2	1.98	0.64
2:B:31:HIS:NE2	2:B:62:PHE:HE2	1.95	0.64
2:D:84:HIS:O	2:D:86:THR:N	2.30	0.64
3:P:1:ARG:HA	3:S:15:VAL:O	1.98	0.64
1:G:127:TRP:CB	1:G:138:SER:HB2	2.27	0.63
1:E:87:PRO:HG2	1:G:53:TRP:CE3	2.33	0.63
1:E:147:ALA:O	1:E:149:ASN:N	2.32	0.63
2:B:49:VAL:O	2:B:49:VAL:HG12	1.99	0.63
1:E:54:GLU:OE1	1:E:56:GLN:NE2	2.27	0.63
2:B:76:ASP:OD1	2:B:76:ASP:N	2.20	0.63
2:B:54:LEU:CD2	2:B:62:PHE:HB3	2.27	0.62
2:H:12:ARG:HB2	2:H:22:PHE:HB2	1.81	0.62
1:E:87:PRO:HG2	1:G:53:TRP:CD2	2.35	0.62
1:A:103:THR:CG2	3:S:1:ARG:HD3	2.28	0.62
2:D:17:ASN:C	2:D:19:LYS:H	2.03	0.62
1:A:261:GLN:HB3	1:A:262:PRO:HD2	1.82	0.62
1:A:74:LEU:HD23	1:A:141:TRP:CD1	2.35	0.61
1:C:176:TRP:O	1:C:177:LYS:HG3	2.00	0.61
1:A:171:ARG:HD3	1:A:175:GLU:OE1	2.01	0.61
3:P:7:TRP:CE3	3:P:11:TRP:O	2.53	0.61
1:E:78:ALA:HB1	1:E:137:ILE:HG12	1.83	0.61
1:G:133:GLU:OE1	1:G:133:GLU:N	2.34	0.61
1:A:56:GLN:C	1:A:58:SER:H	2.03	0.61
1:C:207:GLU:OE1	1:C:207:GLU:N	2.32	0.61
1:C:157:PHE:O	1:C:158:SER:C	2.39	0.61
1:C:35:TYR:C	1:C:35:TYR:CD2	2.74	0.61
1:A:171:ARG:NH2	1:A:171:ARG:CG	2.39	0.61
1:A:213:LEU:O	1:A:250:TYR:HA	2.00	0.61
1:C:117:PHE:CZ	1:C:118:MET:HE3	2.37	0.60
1:G:141:TRP:O	1:G:144:GLN:HB2	2.00	0.60
1:E:212:PHE:CD2	1:E:240:LEU:HD22	2.36	0.60
3:R:5:THR:O	3:R:6:LYS:CB	2.49	0.60
1:A:24:PHE:HE1	1:A:75:PHE:CD2	2.19	0.60
2:D:31:HIS:ND1	2:D:32:PRO:HA	2.17	0.59
1:A:256:HIS:CD2	1:A:258:GLY:H	2.20	0.59
1:A:139:GLN:HA	1:A:142:GLN:HB2	1.85	0.59
1:E:147:ALA:O	1:E:148:ALA:C	2.41	0.59
1:C:159:CYS:HB3	1:C:160:PRO:HD3	1.84	0.59
1:C:199:SER:HB2	1:C:201:PHE:CE1	2.36	0.59
3:P:2:TYR:O	3:S:14:GLU:HA	2.03	0.58
1:A:38:TYR:OH	1:A:43:GLY:HA2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:PHE:HA	1:E:158:SER:OG	2.03	0.58
1:C:126:THR:HG22	1:C:142:GLN:NE2	2.18	0.58
2:D:59:ASP:O	2:D:60:TRP:HB2	2.03	0.58
1:C:207:GLU:CD	1:C:207:GLU:N	2.53	0.58
1:C:36:LEU:HD23	1:C:37:SER:N	2.19	0.58
3:Q:1:ARG:CG	3:Q:1:ARG:HH21	2.14	0.58
1:C:243:LYS:O	1:C:246:ASP:HB2	2.04	0.58
1:C:9:TYR:HE2	1:C:36:LEU:HD13	1.69	0.58
2:D:96:ASP:CG	2:D:99:MET:HG2	2.23	0.58
3:V:2:TYR:HD1	3:V:15:VAL:HB	1.67	0.58
1:A:30:LEU:HD23	1:A:174:LEU:HD11	1.86	0.57
2:B:51:HIS:CG	2:B:51:HIS:O	2.56	0.57
1:A:214:ARG:NH1	1:A:215:ASN:HD21	2.02	0.57
1:C:7:LEU:CD1	1:C:9:TYR:CE1	2.86	0.57
2:H:45:ARG:HD3	2:H:45:ARG:N	2.10	0.57
1:A:47:PRO:HG2	1:A:52:VAL:CG2	2.35	0.57
1:A:193:PHE:CE2	3:U:16:GLY:HA3	2.39	0.57
1:C:110:PHE:CD1	1:C:110:PHE:N	2.72	0.57
1:G:160:PRO:O	1:G:163:LEU:HB3	2.05	0.57
1:A:30:LEU:HD21	1:A:166:HIS:HB3	1.87	0.57
2:H:46:ILE:HG22	2:H:48:LYS:H	1.69	0.57
1:A:62:GLU:O	1:A:66:THR:HG23	2.05	0.56
2:F:73:THR:HB	2:F:75:LYS:H	1.70	0.56
2:D:73:THR:CG2	2:D:74:GLU:H	2.18	0.56
1:E:182:MET:HG3	1:E:265:VAL:HG21	1.86	0.56
1:A:214:ARG:NH1	1:A:215:ASN:ND2	2.54	0.56
1:A:91:GLN:NE2	2:B:56:PHE:CD2	2.74	0.56
2:B:39:LEU:HD12	2:B:68:THR:HG22	1.88	0.56
1:C:82:LEU:HD11	1:C:133:GLU:CB	2.36	0.56
1:E:213:LEU:HB3	1:E:217:LEU:O	2.06	0.56
1:A:223:GLN:O	1:A:238:SER:HA	2.06	0.56
2:D:97:ARG:C	2:D:99:MET:H	2.09	0.55
2:B:82:VAL:HG12	2:B:87:LEU:HD11	1.88	0.55
1:C:252:CYS:HB3	1:C:265:VAL:HB	1.88	0.55
3:P:4:CYS:SG	3:P:6:LYS:O	2.65	0.55
1:A:40:SER:HB2	1:A:72:GLU:OE1	2.05	0.55
2:D:83:ASN:OD1	2:D:90:PRO:HG3	2.05	0.55
2:H:11:SER:HA	2:H:23:LEU:HA	1.88	0.55
1:A:7:LEU:HD12	1:A:30:LEU:HD12	1.89	0.55
2:B:59:ASP:N	2:B:59:ASP:OD1	2.40	0.55
1:C:30:LEU:CD2	1:C:35:TYR:CD1	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LEU:HD13	1:G:30:LEU:HG	1.87	0.55
1:C:89:THR:O	1:C:89:THR:CG2	2.55	0.55
2:B:39:LEU:O	2:B:46:ILE:HG13	2.07	0.55
1:E:10:HIS:HB3	2:F:56:PHE:CE2	2.42	0.55
1:E:247:GLU:H	1:E:247:GLU:CD	2.10	0.55
1:E:213:LEU:HD11	1:E:253:ILE:CD1	2.30	0.54
1:E:159:CYS:HB3	1:E:160:PRO:HD3	1.89	0.54
3:R:5:THR:O	3:R:5:THR:HG22	2.05	0.54
1:A:122:LEU:N	1:A:122:LEU:HD12	2.23	0.54
1:A:127:TRP:O	1:A:138:SER:HB2	2.07	0.54
2:B:72:PRO:HB2	2:B:97:ARG:HH22	1.72	0.54
1:E:14:VAL:HG12	1:E:89:THR:HG23	1.89	0.54
2:F:29:GLY:HA2	2:F:61:SER:HB2	1.90	0.54
1:C:88:TYR:HA	1:C:113:ASN:HD21	1.72	0.54
1:A:58:SER:C	1:A:60:TYR:H	2.11	0.54
1:C:204:TYR:CD2	1:C:205:PRO:HA	2.43	0.54
2:F:36:GLU:HB2	2:F:83:ASN:HB3	1.89	0.54
1:A:65:THR:O	1:A:66:THR:C	2.45	0.54
1:E:229:ASN:HD22	1:E:233:SER:C	2.11	0.54
1:C:203:PHE:CE2	1:C:208:LEU:HD13	2.43	0.54
1:C:13:ALA:HA	1:C:23:ALA:O	2.08	0.53
2:F:59:ASP:OD1	2:F:61:SER:OG	2.26	0.53
2:B:64:LEU:HD22	2:B:66:TYR:HE1	1.72	0.53
2:D:34:ASP:O	2:D:84:HIS:HD2	1.91	0.53
1:A:245:GLY:N	1:A:247:GLU:OE2	2.42	0.53
1:E:82:LEU:CD2	1:E:137:ILE:HD11	2.39	0.53
2:H:10:TYR:HB3	2:H:99:MET:CG	2.38	0.53
1:C:117:PHE:CZ	1:C:118:MET:CE	2.92	0.53
1:C:78:ALA:HB1	1:C:137:ILE:HD13	1.91	0.53
1:E:27:SER:OG	1:E:29:TRP:NE1	2.37	0.53
2:D:21:ASN:HB3	2:D:70:PHE:HE1	1.74	0.52
1:C:157:PHE:O	1:C:160:PRO:CD	2.50	0.52
1:A:165:GLU:HG2	1:A:169:ARG:HH11	1.75	0.52
3:P:3:PHE:HA	3:S:13:GLU:O	2.08	0.52
2:B:26:TYR:HB2	2:B:65:LEU:HD13	1.91	0.52
1:C:214:ARG:HA	1:C:249:HIS:O	2.10	0.52
1:G:81:ALA:O	1:G:136:ALA:HB1	2.10	0.52
1:C:201:PHE:CD2	2:D:14:PRO:HD3	2.45	0.52
2:D:59:ASP:C	2:D:59:ASP:OD1	2.47	0.52
1:A:25:TRP:HA	1:A:38:TYR:O	2.10	0.52
1:C:176:TRP:HD1	1:C:177:LYS:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LYS:HE3	1:E:94:LEU:CD2	2.39	0.52
1:A:112:LEU:HB2	1:A:117:PHE:CE1	2.45	0.52
1:A:89:THR:HB	1:A:113:ASN:HA	1.91	0.52
1:C:67:ASP:C	1:C:69:ARG:H	2.13	0.52
1:A:10:HIS:CD2	1:A:29:TRP:NE1	2.78	0.52
1:C:251:CYS:HB2	1:C:265:VAL:O	2.11	0.51
2:F:21:ASN:HB3	2:F:70:PHE:CE1	2.45	0.51
1:A:22:PRO:HB3	1:A:39:ASN:HB2	1.92	0.51
2:B:17:ASN:HA	2:B:72:PRO:O	2.11	0.51
2:H:78:TYR:O	2:H:95:TRP:HB3	2.10	0.51
1:A:212:PHE:HB2	1:A:220:GLY:O	2.10	0.51
1:C:11:LEU:HD12	1:C:11:LEU:N	2.25	0.51
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.46	0.51
2:B:41:LYS:O	2:B:43:GLY:N	2.40	0.51
1:E:71:LYS:HE3	1:E:94:LEU:HD22	1.91	0.51
2:B:25:CYS:HB3	2:B:39:LEU:HD21	1.91	0.51
1:C:126:THR:HG22	1:C:142:GLN:HE21	1.76	0.51
1:A:36:LEU:C	1:A:36:LEU:HD23	2.30	0.51
2:B:19:LYS:HG2	2:B:20:SER:N	2.25	0.51
1:C:126:THR:HA	1:C:142:GLN:HE21	1.75	0.51
2:D:17:ASN:H	2:D:17:ASN:HD22	1.57	0.51
2:F:37:VAL:HB	2:F:66:TYR:CE1	2.45	0.51
1:C:153:THR:OG1	3:Q:15:VAL:HG22	2.11	0.51
1:C:126:THR:CG2	1:C:142:GLN:NE2	2.74	0.51
1:G:127:TRP:CE2	1:G:141:TRP:HE3	2.29	0.51
2:B:72:PRO:HB2	2:B:97:ARG:NH2	2.26	0.50
1:C:196:LEU:HD12	1:C:242:VAL:HG13	1.93	0.50
1:E:246:ASP:O	1:E:247:GLU:C	2.48	0.50
2:F:95:TRP:CE2	2:F:97:ARG:HA	2.46	0.50
3:S:14:GLU:O	3:S:15:VAL:HG13	2.11	0.50
1:C:97:GLU:HG3	1:C:105:VAL:HB	1.92	0.50
1:C:13:ALA:HB2	1:C:24:PHE:HD1	1.75	0.50
1:E:241:THR:O	3:S:1:ARG:NH2	2.45	0.50
3:Q:3:PHE:O	3:Q:15:VAL:HA	2.11	0.50
1:E:112:LEU:N	1:E:115:GLU:O	2.45	0.50
2:F:96:ASP:C	2:F:96:ASP:OD1	2.50	0.50
2:B:89:GLN:CA	1:C:139:GLN:HE21	2.17	0.50
1:C:184:LEU:O	1:C:184:LEU:HG	2.12	0.50
1:E:112:LEU:HB2	1:E:117:PHE:CE2	2.45	0.50
2:F:95:TRP:NE1	2:F:97:ARG:HA	2.27	0.50
1:A:113:ASN:HA	2:B:31:HIS:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:THR:HA	1:C:142:GLN:NE2	2.27	0.50
1:G:75:PHE:O	1:G:78:ALA:HB3	2.10	0.50
1:A:205:PRO:O	1:A:256:HIS:HE1	1.95	0.49
1:E:161:HIS:HD2	3:R:11:TRP:CH2	2.30	0.49
2:F:38:ASP:HB2	2:F:81:ARG:CB	2.42	0.49
2:H:78:TYR:HB2	2:H:95:TRP:CE3	2.47	0.49
1:A:149:ASN:HD21	3:P:14:GLU:CA	1.98	0.49
1:E:199:SER:HB2	1:E:201:PHE:HE1	1.77	0.49
1:A:112:LEU:HB2	1:A:117:PHE:CD1	2.47	0.49
1:C:107:THR:HG22	1:C:109:LYS:HD2	1.94	0.49
1:C:49:GLY:O	1:C:52:VAL:HG23	2.12	0.49
1:E:151:GLU:O	1:E:152:LEU:C	2.50	0.49
1:A:164:ARG:HA	1:A:167:LEU:HD12	1.94	0.49
1:A:71:LYS:HE3	1:A:94:LEU:HD21	1.93	0.49
1:C:40:SER:O	1:C:41:LEU:C	2.48	0.49
1:C:201:PHE:CG	2:D:14:PRO:HD3	2.47	0.49
1:E:214:ARG:HA	1:E:250:TYR:HA	1.94	0.49
1:A:157:PHE:HZ	3:S:13:GLU:O	1.95	0.49
1:A:159:CYS:HB3	1:A:160:PRO:CD	2.38	0.49
2:D:57:SER:OG	2:D:58:LYS:N	2.45	0.49
1:E:256:HIS:CG	1:E:257:ALA:N	2.80	0.49
1:E:69:ARG:O	1:E:72:GLU:HB3	2.13	0.49
1:C:35:TYR:CZ	1:C:36:LEU:HB2	2.47	0.49
1:E:7:LEU:CD2	1:E:162:ARG:HB3	2.42	0.49
3:R:8:LYS:O	3:R:10:GLY:N	2.46	0.49
1:C:171:ARG:HA	1:C:174:LEU:HB2	1.95	0.49
1:C:213:LEU:O	1:C:250:TYR:HA	2.13	0.49
2:F:73:THR:C	2:F:75:LYS:H	2.16	0.49
2:H:45:ARG:CD	2:H:45:ARG:H	2.17	0.49
1:E:166:HIS:O	1:E:167:LEU:C	2.50	0.49
1:E:212:PHE:CE2	1:E:240:LEU:HB2	2.48	0.49
1:C:256:HIS:CD2	1:C:258:GLY:H	2.31	0.49
1:A:151:GLU:O	1:A:154:PHE:N	2.45	0.49
1:E:120:PHE:HD1	1:E:127:TRP:CD1	2.30	0.49
2:F:6:LYS:CE	2:F:8:GLN:HE21	2.25	0.49
1:A:33:GLN:HG3	1:A:204:TYR:OH	2.12	0.48
2:B:84:HIS:O	2:B:86:THR:N	2.41	0.48
1:G:159:CYS:HB3	1:G:160:PRO:HD3	1.95	0.48
1:A:149:ASN:HA	1:A:152:LEU:HD12	1.95	0.48
1:C:24:PHE:O	1:C:25:TRP:HB3	2.12	0.48
2:B:3:ARG:O	2:B:30:PHE:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:CYS:O	1:C:237:SER:HA	2.13	0.48
1:C:60:TYR:C	1:C:60:TYR:CD1	2.87	0.48
3:Q:7:TRP:CZ3	3:Q:11:TRP:O	2.67	0.48
1:A:11:LEU:HG	1:A:26:VAL:HG13	1.95	0.48
1:C:213:LEU:HD23	1:C:218:ALA:HA	1.95	0.48
1:A:202:SER:HG	1:A:203:PHE:H	1.58	0.48
1:A:38:TYR:HE1	1:A:44:GLU:N	2.12	0.48
1:E:199:SER:HB2	1:E:201:PHE:CE1	2.48	0.48
2:F:95:TRP:CD1	2:F:95:TRP:C	2.83	0.48
2:B:73:THR:HG22	2:B:75:LYS:H	1.77	0.48
1:C:47:PRO:HB3	1:C:61:TRP:CZ2	2.48	0.48
2:B:49:VAL:HG22	2:B:68:THR:HB	1.96	0.48
1:C:95:GLY:O	1:C:106:PRO:HA	2.14	0.48
1:C:206:PRO:O	1:C:207:GLU:C	2.51	0.48
2:H:40:LEU:HD11	2:H:81:ARG:HB2	1.96	0.48
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.14	0.47
1:G:7:LEU:HB2	1:G:163:LEU:HD13	1.96	0.47
1:C:203:PHE:O	1:C:234:PHE:N	2.43	0.47
1:G:37:SER:HB3	1:G:46:GLU:O	2.14	0.47
1:A:230:SER:C	1:A:232:GLY:H	2.15	0.47
1:A:38:TYR:CE1	1:A:44:GLU:N	2.82	0.47
1:C:53:TRP:O	1:C:54:GLU:O	2.32	0.47
2:H:25:CYS:HB3	2:H:66:TYR:HB2	1.96	0.47
1:C:176:TRP:C	1:C:176:TRP:CD1	2.87	0.47
1:G:131:TRP:HA	1:G:132:PRO:HD2	1.73	0.47
3:Q:12:CYS:HB3	3:Q:13:GLU:H	1.37	0.47
1:A:80:LYS:C	1:A:82:LEU:H	2.18	0.47
1:C:226:PHE:HE1	1:C:234:PHE:CD2	2.33	0.47
1:C:9:TYR:HE2	1:C:36:LEU:CD1	2.27	0.47
1:E:56:GLN:OE1	1:E:169:ARG:HD3	2.15	0.47
2:F:73:THR:C	2:F:75:LYS:N	2.68	0.47
1:E:141:TRP:HA	1:E:144:GLN:HG2	1.97	0.47
2:F:22:PHE:HA	2:F:68:THR:O	2.14	0.47
1:G:17:PRO:HG3	1:G:23:ALA:HB2	1.95	0.47
1:G:211:ARG:HA	1:G:221:THR:HA	1.97	0.47
1:C:101:ASP:OD2	1:C:101:ASP:N	2.46	0.47
1:E:97:GLU:O	1:E:97:GLU:HG2	2.13	0.47
2:F:84:HIS:ND1	2:F:86:THR:OG1	2.40	0.47
1:G:154:PHE:CD1	1:G:154:PHE:O	2.68	0.47
1:A:171:ARG:HD2	1:A:172:GLY:N	2.30	0.47
2:B:26:TYR:HB2	2:B:65:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD11	1:A:164:ARG:HG3	1.96	0.46
1:A:171:ARG:HD2	1:A:171:ARG:C	2.35	0.46
1:A:214:ARG:HH11	1:A:215:ASN:HD21	1.63	0.46
1:A:192:GLY:C	1:A:244:SER:HB2	2.35	0.46
1:E:112:LEU:O	1:E:115:GLU:N	2.44	0.46
1:C:266:GLU:OE1	1:C:266:GLU:CA	2.50	0.46
1:E:89:THR:OG1	1:E:113:ASN:OD1	2.26	0.46
3:S:12:CYS:O	3:S:13:GLU:CB	2.62	0.46
1:A:132:PRO:HB2	1:A:133:GLU:OE2	2.16	0.46
1:G:156:LEU:O	1:G:160:PRO:HD2	2.15	0.46
2:H:54:LEU:HG	2:H:64:LEU:HG	1.98	0.46
1:C:229:ASN:HD21	1:C:234:PHE:C	2.19	0.46
1:C:20:GLY:O	1:C:41:LEU:HD11	2.15	0.46
2:D:59:ASP:O	2:D:60:TRP:CB	2.63	0.46
2:D:84:HIS:C	2:D:86:THR:H	2.19	0.46
2:H:52:SER:OG	2:H:65:LEU:HB3	2.16	0.46
3:T:3:PHE:O	3:T:15:VAL:HA	2.16	0.46
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.51	0.46
1:A:114:GLY:H	2:B:31:HIS:CE1	2.27	0.46
1:E:261:GLN:HB3	1:E:262:PRO:HD2	1.96	0.46
1:G:55:ASN:O	1:G:57:VAL:N	2.48	0.46
1:E:117:PHE:CD1	1:E:118:MET:N	2.77	0.46
1:E:143:GLN:NE2	1:E:143:GLN:CA	2.52	0.46
1:E:12:THR:O	1:E:24:PHE:HA	2.16	0.46
1:E:252:CYS:O	1:E:265:VAL:N	2.45	0.46
2:B:73:THR:O	2:B:75:LYS:N	2.49	0.46
1:C:56:GLN:O	1:C:58:SER:N	2.49	0.46
1:C:93:LEU:HD13	2:D:56:PHE:HE1	1.80	0.46
1:C:22:PRO:HB2	1:C:40:SER:OG	2.15	0.46
1:C:121:ASP:C	1:C:121:ASP:OD2	2.54	0.46
1:C:141:TRP:O	1:C:142:GLN:C	2.51	0.46
1:E:170:GLY:O	1:E:174:LEU:HD22	2.16	0.46
1:G:118:MET:SD	1:G:138:SER:HB3	2.55	0.46
2:H:40:LEU:HD12	2:H:79:ALA:HB3	1.98	0.46
1:A:171:ARG:CD	1:A:171:ARG:C	2.84	0.45
1:C:243:LYS:O	1:C:246:ASP:CB	2.64	0.45
1:C:22:PRO:HD3	1:C:41:LEU:HD21	1.97	0.45
1:E:147:ALA:O	1:E:150:LYS:N	2.49	0.45
1:E:256:HIS:CG	1:E:257:ALA:H	2.33	0.45
3:R:4:CYS:O	3:R:6:LYS:N	2.49	0.45
3:P:4:CYS:HB3	3:P:7:TRP:NE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD22	2:B:62:PHE:HD1	1.81	0.45
1:A:211:ARG:CG	1:A:253:ILE:HB	2.45	0.45
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.68	0.45
1:C:35:TYR:CE2	1:C:36:LEU:HB2	2.52	0.45
1:A:11:LEU:HD13	1:A:94:LEU:HD22	1.99	0.45
1:A:122:LEU:H	1:A:122:LEU:HD12	1.82	0.45
1:E:250:TYR:O	1:E:251:CYS:HB3	2.16	0.45
1:A:245:GLY:H	1:A:247:GLU:CD	2.20	0.45
2:B:31:HIS:NE2	2:B:62:PHE:CE2	2.80	0.45
1:C:215:ASN:N	1:C:249:HIS:O	2.36	0.45
2:F:36:GLU:HG3	1:G:172:GLY:HA2	1.99	0.45
1:G:82:LEU:HB3	1:G:88:TYR:CZ	2.52	0.45
2:H:7:ILE:HG23	2:H:27:VAL:HG22	1.97	0.45
1:A:67:ASP:OD2	1:A:162:ARG:NH2	2.50	0.45
1:A:69:ARG:O	1:A:70:ILE:C	2.53	0.45
1:C:222:GLY:HA3	1:C:239:SER:O	2.17	0.45
1:A:176:TRP:CZ2	1:A:178:GLU:HG3	2.52	0.45
1:C:171:ARG:NH2	1:C:171:ARG:HB3	2.32	0.45
1:C:171:ARG:NE	1:C:171:ARG:O	2.50	0.45
1:E:247:GLU:OE2	1:E:247:GLU:N	2.50	0.45
2:F:96:ASP:O	2:F:99:MET:HB3	2.17	0.45
3:P:14:GLU:O	3:P:15:VAL:HG13	2.17	0.45
1:C:112:LEU:N	1:C:115:GLU:O	2.49	0.45
1:E:242:VAL:HG12	1:E:250:TYR:CE1	2.51	0.45
2:F:39:LEU:HB3	2:F:46:ILE:HD12	1.99	0.45
2:F:39:LEU:O	2:F:46:ILE:HG13	2.17	0.45
1:A:10:HIS:CD2	1:A:29:TRP:HE1	2.35	0.44
1:C:38:TYR:HB2	1:C:68:LEU:HD13	1.99	0.44
1:A:115:GLU:OE2	2:B:1:ILE:HG23	2.17	0.44
1:E:78:ALA:O	1:E:82:LEU:HD22	2.17	0.44
1:E:7:LEU:O	1:E:8:LEU:HD23	2.17	0.44
1:G:24:PHE:CE2	1:G:72:GLU:HB2	2.52	0.44
1:A:137:ILE:O	1:A:138:SER:C	2.56	0.44
1:E:152:LEU:HD12	1:E:152:LEU:HA	1.79	0.44
1:G:205:PRO:HA	1:G:206:PRO:HD3	1.76	0.44
3:P:14:GLU:O	3:P:15:VAL:CG1	2.65	0.44
1:A:252:CYS:HB3	1:A:265:VAL:HB	1.99	0.44
1:C:65:THR:CG2	1:C:69:ARG:HD2	2.48	0.44
1:G:47:PRO:HB3	1:G:61:TRP:CH2	2.52	0.44
2:H:24:ASN:HA	2:H:66:TYR:O	2.17	0.44
1:C:51:TRP:CE3	1:C:54:GLU:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:LEU:HD21	1:C:155:LEU:HD12	2.00	0.44
1:E:82:LEU:HD21	1:E:137:ILE:HD11	1.98	0.44
2:F:84:HIS:O	2:F:85:VAL:C	2.55	0.44
1:G:259:LEU:O	1:G:260:ALA:HB2	2.18	0.44
3:P:3:PHE:O	3:P:15:VAL:HA	2.18	0.44
3:S:8:LYS:C	3:S:10:GLY:H	2.19	0.44
3:S:14:GLU:O	3:S:15:VAL:CG1	2.66	0.44
1:E:117:PHE:HD1	1:E:117:PHE:H	1.65	0.44
1:G:36:LEU:HG	1:G:61:TRP:HZ3	1.83	0.44
1:C:184:LEU:HD23	1:C:266:GLU:C	2.38	0.44
1:G:82:LEU:HB3	1:G:88:TYR:OH	2.18	0.44
3:R:7:TRP:CE3	3:R:11:TRP:O	2.70	0.44
2:B:73:THR:C	2:B:75:LYS:H	2.20	0.43
1:C:131:TRP:HB3	1:C:133:GLU:OE2	2.18	0.43
1:G:36:LEU:HD23	1:G:37:SER:H	1.78	0.43
1:E:164:ARG:HH21	1:E:164:ARG:CG	2.27	0.43
1:E:105:VAL:HG22	3:U:1:ARG:HG2	2.00	0.43
2:H:54:LEU:HD21	2:H:62:PHE:HB3	2.00	0.43
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.54	0.43
1:E:242:VAL:HG12	1:E:250:TYR:CZ	2.54	0.43
1:G:47:PRO:HB3	1:G:61:TRP:CZ2	2.53	0.43
1:A:157:PHE:O	1:A:160:PRO:HD2	2.18	0.43
3:Q:12:CYS:O	3:Q:13:GLU:CB	2.66	0.43
3:V:11:TRP:O	3:V:12:CYS:SG	2.76	0.43
2:B:7:ILE:HB	2:B:93:VAL:HG21	2.00	0.43
1:C:94:LEU:HA	1:C:107:THR:O	2.19	0.43
1:E:179:PRO:HB3	1:E:259:LEU:HD21	2.00	0.43
1:G:187:ARG:HA	1:G:188:PRO:HD3	1.76	0.43
1:C:157:PHE:C	1:C:159:CYS:N	2.69	0.43
1:A:131:TRP:HA	1:A:132:PRO:HD2	1.58	0.43
1:A:165:GLU:HG2	1:A:169:ARG:NH1	2.33	0.43
2:D:40:LEU:HA	2:D:44:GLU:O	2.19	0.43
1:E:17:PRO:HB3	1:E:21:THR:HG22	2.01	0.43
3:S:8:LYS:C	3:S:10:GLY:N	2.71	0.43
1:A:163:LEU:O	1:A:167:LEU:HD12	2.18	0.43
1:C:151:GLU:O	1:C:152:LEU:C	2.57	0.43
2:D:39:LEU:O	2:D:46:ILE:HG13	2.19	0.43
1:E:240:LEU:HD11	3:S:1:ARG:NH1	2.34	0.43
1:A:57:VAL:HG23	1:A:60:TYR:HB2	2.01	0.42
2:B:19:LYS:HG2	2:B:20:SER:H	1.84	0.42
1:E:97:GLU:CG	1:E:97:GLU:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:3:PHE:O	3:S:15:VAL:CA	2.65	0.42
1:C:161:HIS:O	1:C:163:LEU:N	2.52	0.42
2:D:11:SER:HA	2:D:22:PHE:O	2.19	0.42
1:A:82:LEU:HB3	1:A:88:TYR:CE1	2.54	0.42
1:E:139:GLN:O	1:E:140:ARG:C	2.58	0.42
1:E:203:PHE:N	1:E:203:PHE:CD1	2.87	0.42
2:F:94:LYS:O	2:F:96:ASP:N	2.53	0.42
3:Q:1:ARG:O	3:Q:1:ARG:HG2	2.18	0.42
1:C:35:TYR:OH	1:C:36:LEU:HD12	2.19	0.42
2:F:33:SER:HB3	2:F:62:PHE:CD1	2.54	0.42
2:D:9:VAL:HA	2:D:24:ASN:O	2.19	0.42
1:E:71:LYS:NZ	1:E:151:GLU:OE1	2.51	0.42
1:E:161:HIS:O	1:E:165:GLU:HB2	2.19	0.42
2:H:41:LYS:O	2:H:42:ASN:HB2	2.20	0.42
2:H:78:TYR:HB2	2:H:95:TRP:HE3	1.85	0.42
2:D:39:LEU:O	2:D:40:LEU:HD23	2.20	0.42
2:D:73:THR:HG22	2:D:75:LYS:H	1.85	0.42
1:E:163:LEU:O	1:E:164:ARG:C	2.58	0.42
1:E:35:TYR:O	1:E:47:PRO:HA	2.20	0.42
1:C:38:TYR:CE1	1:C:68:LEU:O	2.73	0.42
1:C:179:PRO:HA	1:C:256:HIS:CD2	2.55	0.42
1:E:245:GLY:HA2	1:E:247:GLU:OE2	2.19	0.42
1:E:98:LEU:HD23	1:E:103:THR:O	2.20	0.42
3:S:4:CYS:HA	3:S:15:VAL:HG12	2.02	0.42
2:B:23:LEU:HD23	2:B:39:LEU:HD13	2.01	0.42
2:B:32:PRO:HB2	2:B:34:ASP:OD2	2.20	0.42
1:E:15:SER:OG	1:E:88:TYR:N	2.52	0.42
1:C:181:SER:HB2	1:C:201:PHE:HB2	2.03	0.41
1:E:14:VAL:HG12	1:E:89:THR:CG2	2.49	0.41
3:R:1:ARG:HA	3:U:15:VAL:O	2.19	0.41
3:U:7:TRP:HE3	3:U:10:GLY:HA2	1.85	0.41
2:B:13:HIS:HB3	2:B:14:PRO:CD	2.49	0.41
1:C:90:LEU:HD12	1:C:91:GLN:N	2.35	0.41
1:E:118:MET:HE1	1:E:137:ILE:HG21	2.01	0.41
3:Q:3:PHE:HA	3:T:13:GLU:O	2.20	0.41
1:A:163:LEU:O	1:A:163:LEU:HD12	2.20	0.41
2:B:21:ASN:HB3	2:B:70:PHE:HE1	1.84	0.41
1:C:226:PHE:CE1	1:C:234:PHE:CD2	3.08	0.41
1:C:212:PHE:HA	1:C:251:CYS:O	2.20	0.41
1:E:30:LEU:CD2	1:E:35:TYR:CD1	2.96	0.41
2:B:95:TRP:CG	2:B:95:TRP:O	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:C	1:C:81:ALA:N	2.73	0.41
1:A:99:GLY:O	1:A:101:ASP:N	2.53	0.41
1:A:254:VAL:HG13	1:A:263:LEU:HB3	2.02	0.41
1:G:60:TYR:C	1:G:62:GLU:H	2.23	0.41
1:C:196:LEU:HD12	1:C:242:VAL:CG1	2.51	0.41
2:D:39:LEU:HD12	2:D:49:VAL:HG23	2.02	0.41
2:F:37:VAL:HG11	2:F:66:TYR:CD1	2.56	0.41
3:S:12:CYS:HB3	3:S:13:GLU:H	1.61	0.41
1:A:230:SER:C	1:A:232:GLY:N	2.74	0.41
1:A:10:HIS:O	1:A:26:VAL:HA	2.20	0.41
2:B:2:GLN:HA	2:B:31:HIS:O	2.21	0.41
1:A:65:THR:HG22	1:A:66:THR:N	2.34	0.41
2:B:26:TYR:CZ	2:B:28:SER:HB3	2.56	0.41
2:B:68:THR:OG1	2:B:69:GLU:O	2.38	0.41
2:D:51:HIS:HA	2:D:65:LEU:O	2.20	0.41
1:E:12:THR:HG23	1:E:91:GLN:CG	2.40	0.41
2:F:85:VAL:HG23	1:G:55:ASN:HD22	1.85	0.41
1:A:170:GLY:O	1:A:171:ARG:C	2.59	0.41
2:B:69:GLU:O	2:B:70:PHE:HB3	2.21	0.41
1:C:132:PRO:O	1:C:136:ALA:N	2.46	0.41
1:E:213:LEU:CB	1:E:217:LEU:O	2.69	0.41
1:E:182:MET:SD	1:E:254:VAL:HG11	2.61	0.41
1:G:24:PHE:HB2	1:G:76:LEU:HD21	2.02	0.40
2:H:26:TYR:CE2	2:H:28:SER:HB3	2.56	0.40
1:A:126:THR:HA	1:A:142:GLN:HE22	1.86	0.40
1:A:134:ALA:O	1:A:135:LEU:C	2.59	0.40
1:E:166:HIS:O	1:E:168:GLU:N	2.53	0.40
1:G:27:SER:CB	2:H:55:SER:OG	2.69	0.40
1:A:244:SER:HA	1:A:247:GLU:OE1	2.21	0.40
1:C:249:HIS:ND1	1:C:249:HIS:N	2.69	0.40
2:F:5:PRO:HB3	2:F:30:PHE:HB3	2.04	0.40
1:A:176:TRP:CE2	1:A:178:GLU:HG3	2.56	0.40
1:A:254:VAL:CG1	1:A:263:LEU:HB3	2.52	0.40
1:A:10:HIS:HD2	2:B:55:SER:HB3	1.85	0.40
1:C:78:ALA:HB1	1:C:137:ILE:CD1	2.51	0.40
1:E:111:ALA:HA	1:E:115:GLU:O	2.21	0.40
1:E:167:LEU:HD12	1:E:167:LEU:HA	1.84	0.40
1:E:17:PRO:CB	1:E:21:THR:HG22	2.52	0.40
1:G:56:GLN:HB2	1:G:56:GLN:HE21	1.79	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:E:259:LEU:O	1:E:259:LEU:O[3_555]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/267 (98%)	213 (82%)	34 (13%)	14 (5%)	2	17
1	C	261/267 (98%)	207 (79%)	36 (14%)	18 (7%)	1	9
1	E	261/267 (98%)	209 (80%)	35 (13%)	17 (6%)	1	11
1	G	261/267 (98%)	181 (69%)	65 (25%)	15 (6%)	2	16
2	B	97/99 (98%)	68 (70%)	23 (24%)	6 (6%)	2	13
2	D	97/99 (98%)	80 (82%)	11 (11%)	6 (6%)	2	13
2	F	97/99 (98%)	75 (77%)	15 (16%)	7 (7%)	1	9
2	H	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	9
3	P	14/19 (74%)	7 (50%)	5 (36%)	2 (14%)	0	1
3	Q	14/19 (74%)	8 (57%)	4 (29%)	2 (14%)	0	1
3	R	14/19 (74%)	7 (50%)	3 (21%)	4 (29%)	0	0
3	S	14/19 (74%)	10 (71%)	2 (14%)	2 (14%)	0	1
3	T	14/19 (74%)	10 (71%)	4 (29%)	0	100	100
3	U	14/19 (74%)	11 (79%)	2 (14%)	1 (7%)	1	9
3	V	14/19 (74%)	8 (57%)	1 (7%)	5 (36%)	0	0
All	All	1530/1597 (96%)	1171 (76%)	253 (16%)	106 (7%)	1	9

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	83	GLY
1	A	100	PRO

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Mol	Chain	Res	Type
1	A	132	PRO
1	A	203	PHE
1	A	215	ASN
1	A	247	GLU
2	B	17	ASN
2	B	85	VAL
2	B	98	ASP
1	C	21	THR
1	C	57	VAL
1	C	58	SER
1	C	68	LEU
1	C	100	PRO
2	D	52	SER
2	D	85	VAL
2	D	98	ASP
1	E	15	SER
1	E	58	SER
2	F	85	VAL
2	F	88	SER
2	H	97	ARG
3	P	9	HIS
3	Q	6	LYS
3	Q	13	GLU
3	R	5	THR
3	R	6	LYS
3	R	9	HIS
3	V	6	LYS
1	A	57	VAL
1	A	59	TRP
2	B	90	PRO
1	C	83	GLY
1	C	247	GLU
1	C	257	ALA
2	D	18	GLY
2	D	75	LYS
2	D	76	ASP
1	E	40	SER
1	E	132	PRO
1	E	147	ALA
1	E	148	ALA
1	E	167	LEU
1	E	221	THR

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Mol	Chain	Res	Type
2	F	97	ARG
1	G	53	TRP
1	G	56	GLN
1	G	100	PRO
1	G	131	TRP
1	G	222	GLY
1	G	260	ALA
2	H	29	GLY
3	P	13	GLU
3	R	13	GLU
3	S	13	GLU
3	U	6	LYS
3	V	9	HIS
3	V	13	GLU
1	A	142	GLN
1	A	143	GLN
1	A	174	LEU
1	A	261	GLN
1	C	141	TRP
1	C	173	ASN
1	C	202	SER
1	C	215	ASN
1	G	102	ASN
1	G	148	ALA
2	H	34	ASP
3	V	12	CYS
1	A	113	ASN
2	B	74	GLU
1	C	54	GLU
1	C	161	HIS
1	E	106	PRO
1	E	237	SER
2	F	31	HIS
2	F	43	GLY
2	F	47	GLU
1	G	202	SER
1	G	207	GLU
1	G	256	HIS
2	H	45	ARG
2	H	90	PRO
3	S	6	LYS
2	B	75	LYS

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Mol	Chain	Res	Type
1	C	49	GLY
1	E	16	SER
1	G	191	PRO
1	G	197	THR
1	G	247	GLU
1	C	172	GLY
1	C	206	PRO
1	E	67	ASP
1	E	225	ASP
1	G	254	VAL
2	H	43	GLY
2	H	60	TRP
3	V	14	GLU
1	C	170	GLY
1	E	83	GLY
2	F	90	PRO
1	E	32	PRO
1	E	191	PRO
1	E	70	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	192/220 (87%)	149 (78%)	43 (22%)	1	5
1	C	189/220 (86%)	149 (79%)	40 (21%)	1	6
1	E	187/220 (85%)	151 (81%)	36 (19%)	1	9
1	G	99/220 (45%)	83 (84%)	16 (16%)	3	13
2	B	85/94 (90%)	66 (78%)	19 (22%)	1	5
2	D	80/94 (85%)	65 (81%)	15 (19%)	2	9
2	F	79/94 (84%)	65 (82%)	14 (18%)	2	10
2	H	86/94 (92%)	70 (81%)	16 (19%)	2	9
3	P	8/15 (53%)	7 (88%)	1 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	9/15 (60%)	6 (67%)	3 (33%)	0	0
3	R	9/15 (60%)	8 (89%)	1 (11%)	7	30
3	S	8/15 (53%)	7 (88%)	1 (12%)	5	24
3	T	7/15 (47%)	6 (86%)	1 (14%)	4	18
3	U	8/15 (53%)	6 (75%)	2 (25%)	1	2
3	V	7/15 (47%)	7 (100%)	0	100	100
All	All	1053/1361 (77%)	845 (80%)	208 (20%)	1	8

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	14	VAL
1	A	15	SER
1	A	26	VAL
1	A	36	LEU
1	A	41	LEU
1	A	70	ILE
1	A	74	LEU
1	A	75	PHE
1	A	82	LEU
1	A	93	LEU
1	A	94	LEU
1	A	98	LEU
1	A	104	SER
1	A	109	LYS
1	A	113	ASN
1	A	119	ASN
1	A	133	GLU
1	A	135	LEU
1	A	138	SER
1	A	139	GLN
1	A	156	LEU
1	A	158	SER
1	A	161	HIS
1	A	165	GLU
1	A	171	ARG
1	A	174	LEU
1	A	175	GLU
1	A	178	GLU

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Mol	Chain	Res	Type
1	A	181	SER
1	A	183	ARG
1	A	187	ARG
1	A	195	VAL
1	A	199	SER
1	A	202	SER
1	A	203	PHE
1	A	208	LEU
1	A	209	GLN
1	A	214	ARG
1	A	225	ASP
1	A	244	SER
1	A	255	GLN
1	A	267	LEU
2	B	2	GLN
2	B	4	THR
2	B	23	LEU
2	B	25	CYS
2	B	34	ASP
2	B	40	LEU
2	B	45	ARG
2	B	51	HIS
2	B	55	SER
2	B	61	SER
2	B	64	LEU
2	B	68	THR
2	B	70	PHE
2	B	73	THR
2	B	76	ASP
2	B	85	VAL
2	B	89	GLN
2	B	97	ARG
2	B	99	MET
1	C	7	LEU
1	C	8	LEU
1	C	26	VAL
1	C	32	PRO
1	C	35	TYR
1	C	37	SER
1	C	38	TYR
1	C	40	SER
1	C	41	LEU

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Mol	Chain	Res	Type
1	C	46	GLU
1	C	54	GLU
1	C	60	TYR
1	C	89	THR
1	C	96	CYS
1	C	97	GLU
1	C	100	PRO
1	C	107	THR
1	C	126	THR
1	C	139	GLN
1	C	145	ASP
1	C	167	LEU
1	C	171	ARG
1	C	174	LEU
1	C	176	TRP
1	C	183	ARG
1	C	195	VAL
1	C	198	CYS
1	C	199	SER
1	C	207	GLU
1	C	208	LEU
1	C	225	ASP
1	C	226	PHE
1	C	229	ASN
1	C	230	SER
1	C	244	SER
1	C	249	HIS
1	C	255	GLN
1	C	261	GLN
1	C	265	VAL
1	C	267	LEU
2	D	4	THR
2	D	12	ARG
2	D	14	PRO
2	D	17	ASN
2	D	33	SER
2	D	53	ASP
2	D	54	LEU
2	D	57	SER
2	D	64	LEU
2	D	69	GLU
2	D	70	PHE

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Mol	Chain	Res	Type
2	D	85	VAL
2	D	88	SER
2	D	89	GLN
2	D	99	MET
1	E	6	SER
1	E	12	THR
1	E	21	THR
1	E	30	LEU
1	E	41	LEU
1	E	44	GLU
1	E	46	GLU
1	E	56	GLN
1	E	66	THR
1	E	67	ASP
1	E	71	LYS
1	E	82	LEU
1	E	89	THR
1	E	94	LEU
1	E	104	SER
1	E	117	PHE
1	E	132	PRO
1	E	133	GLU
1	E	138	SER
1	E	139	GLN
1	E	140	ARG
1	E	143	GLN
1	E	145	ASP
1	E	150	LYS
1	E	152	LEU
1	E	164	ARG
1	E	171	ARG
1	E	174	LEU
1	E	181	SER
1	E	183	ARG
1	E	199	SER
1	E	213	LEU
1	E	238	SER
1	E	241	THR
1	E	251	CYS
1	E	254	VAL
2	F	11	SER
2	F	12	ARG

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Mol	Chain	Res	Type
2	F	23	LEU
2	F	27	VAL
2	F	42	ASN
2	F	45	ARG
2	F	61	SER
2	F	70	PHE
2	F	73	THR
2	F	76	ASP
2	F	86	THR
2	F	92	ILE
2	F	96	ASP
2	F	97	ARG
1	G	30	LEU
1	G	52	VAL
1	G	56	GLN
1	G	59	TRP
1	G	69	ARG
1	G	82	LEU
1	G	89	THR
1	G	93	LEU
1	G	117	PHE
1	G	131	TRP
1	G	133	GLU
1	G	139	GLN
1	G	140	ARG
1	G	149	ASN
1	G	153	THR
1	G	182	MET
2	H	3	ARG
2	H	7	ILE
2	H	16	GLU
2	H	20	SER
2	H	36	GLU
2	H	45	ARG
2	H	47	GLU
2	H	55	SER
2	H	57	SER
2	H	64	LEU
2	H	69	GLU
2	H	70	PHE
2	H	73	THR
2	H	81	ARG

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Mol	Chain	Res	Type
2	H	85	VAL
2	H	96	ASP
3	P	5	THR
3	Q	1	ARG
3	Q	5	THR
3	Q	15	VAL
3	R	1	ARG
3	S	1	ARG
3	T	5	THR
3	U	1	ARG
3	U	5	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	34	GLN
1	A	139	GLN
1	A	149	ASN
1	A	173	ASN
1	A	209	GLN
1	A	215	ASN
1	A	223	GLN
1	A	235	HIS
1	A	256	HIS
2	B	31	HIS
2	B	51	HIS
1	C	113	ASN
1	C	142	GLN
1	C	149	ASN
1	C	173	ASN
1	C	229	ASN
1	C	235	HIS
1	C	256	HIS
2	D	2	GLN
2	D	17	ASN
1	E	10	HIS
1	E	91	GLN
1	E	142	GLN
1	E	143	GLN
1	E	161	HIS
1	E	173	ASN

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Mol	Chain	Res	Type
1	E	229	ASN
1	E	235	HIS
1	E	256	HIS
2	F	2	GLN
2	F	8	GLN
1	G	10	HIS
1	G	55	ASN
1	G	56	GLN
1	G	91	GLN
2	H	2	GLN
2	H	31	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	263/267 (98%)	-0.04	0 <span>100</span> <span>100</span>	30, 48, 67, 80	0
1	C	263/267 (98%)	0.08	5 (1%) <span>67</span> <span>52</span>	27, 47, 73, 86	0
1	E	263/267 (98%)	-0.08	1 (0%) <span>92</span> <span>89</span>	33, 51, 66, 72	0
1	G	263/267 (98%)	1.43	77 (29%) <span>1</span> <span>1</span>	69, 115, 169, 171	0
2	B	99/99 (100%)	0.16	1 (1%) <span>82</span> <span>72</span>	36, 56, 78, 83	0
2	D	99/99 (100%)	0.17	2 (2%) <span>65</span> <span>50</span>	26, 57, 74, 85	0
2	F	99/99 (100%)	0.33	2 (2%) <span>65</span> <span>50</span>	38, 64, 83, 91	0
2	H	99/99 (100%)	2.65	66 (66%) <span>0</span> <span>0</span>	105, 144, 164, 166	0
3	P	16/19 (84%)	-0.00	0 <span>100</span> <span>100</span>	43, 53, 57, 59	0
3	Q	16/19 (84%)	-0.02	0 <span>100</span> <span>100</span>	42, 48, 57, 60	0
3	R	16/19 (84%)	-0.02	0 <span>100</span> <span>100</span>	54, 61, 65, 65	0
3	S	16/19 (84%)	0.21	1 (6%) <span>21</span> <span>12</span>	46, 60, 65, 66	0
3	T	16/19 (84%)	0.04	0 <span>100</span> <span>100</span>	43, 62, 66, 67	0
3	U	16/19 (84%)	0.25	0 <span>100</span> <span>100</span>	48, 64, 79, 82	0
3	V	16/19 (84%)	0.15	0 <span>100</span> <span>100</span>	50, 60, 68, 69	0
All	All	1560/1597 (97%)	0.45	155 (9%) <span>8</span> <span>5</span>	26, 57, 161, 171	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	251	CYS	12.5
2	H	24	ASN	8.0
1	G	246	ASP	7.4
1	G	252	CYS	7.4
2	H	82	VAL	7.3
2	H	16	GLU	7.0
1	G	258	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
1	G	186	ALA	6.2
2	H	83	ASN	6.1
1	G	257	ALA	5.6
2	H	79	ALA	5.3
1	G	241	THR	5.3
2	H	68	THR	5.0
2	H	78	TYR	5.0
2	H	49	VAL	5.0
1	G	55	ASN	5.0
1	G	236	ALA	5.0
1	G	248	HIS	4.9
2	H	8	GLN	4.9
2	H	7	ILE	4.9
2	H	39	LEU	4.9
1	G	56	GLN	4.8
1	G	237	SER	4.6
1	G	256	HIS	4.6
1	G	254	VAL	4.6
1	G	185	LYS	4.5
1	G	250	TYR	4.5
2	H	66	TYR	4.4
1	G	102	ASN	4.4
1	G	190	SER	4.3
2	H	37	VAL	4.3
1	G	220	GLY	4.3
1	G	247	GLU	4.3
1	G	191	PRO	4.3
2	H	35	ILE	4.2
1	G	156	LEU	4.2
2	H	14	PRO	4.2
1	G	213	LEU	4.2
2	H	23	LEU	4.2
1	G	193	PHE	4.1
1	C	196	LEU	4.1
2	H	31	HIS	4.0
2	H	81	ARG	4.0
1	G	30	LEU	4.0
1	G	219	ALA	3.9
1	G	50	ALA	3.9
2	H	9	VAL	3.9
2	H	43	GLY	3.8
2	H	72	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	245	GLY	3.7
1	G	260	ALA	3.7
1	G	196	LEU	3.6
2	H	73	THR	3.6
1	G	184	LEU	3.6
1	G	101	ASP	3.6
1	G	242	VAL	3.5
2	H	17	ASN	3.5
1	G	218	ALA	3.5
1	G	194	SER	3.5
2	H	6	LYS	3.4
1	G	224	GLY	3.4
2	H	36	GLU	3.4
2	H	65	LEU	3.4
1	G	192	GLY	3.4
1	G	32	PRO	3.3
2	H	88	SER	3.3
2	H	13	HIS	3.3
2	H	95	TRP	3.3
2	H	48	LYS	3.3
1	G	198	CYS	3.2
1	G	215	ASN	3.2
2	H	85	VAL	3.2
2	H	2	GLN	3.2
2	H	98	ASP	3.2
2	H	92	ILE	3.1
1	G	212	PHE	3.1
1	G	240	LEU	3.1
2	H	64	LEU	3.0
2	H	38	ASP	3.0
2	H	84	HIS	3.0
2	H	20	SER	3.0
1	G	96	CYS	3.0
2	H	3	ARG	2.9
2	H	69	GLU	2.9
2	H	25	CYS	2.9
2	D	98	ASP	2.8
1	G	255	GLN	2.8
2	H	77	GLU	2.8
1	G	211	ARG	2.8
1	G	195	VAL	2.8
1	G	261	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	15	ALA	2.8
1	G	182	MET	2.7
2	H	40	LEU	2.7
2	H	30	PHE	2.7
2	H	86	THR	2.7
2	H	26	TYR	2.7
1	G	97	GLU	2.7
1	G	197	THR	2.6
1	C	250	TYR	2.6
2	H	59	ASP	2.6
1	G	253	ILE	2.6
1	G	108	ALA	2.6
1	C	193	PHE	2.6
2	H	10	TYR	2.6
1	G	12	THR	2.6
1	G	167	LEU	2.6
2	H	18	GLY	2.5
1	G	187	ARG	2.5
1	G	51	TRP	2.5
1	G	59	TRP	2.5
1	G	223	GLN	2.5
2	H	60	TRP	2.5
1	G	157	PHE	2.5
2	H	44	GLU	2.4
1	E	129	GLY	2.4
2	H	27	VAL	2.4
1	G	170	GLY	2.4
2	H	93	VAL	2.4
1	G	267	LEU	2.4
2	F	46	ILE	2.4
3	S	10	GLY	2.4
1	C	186	ALA	2.4
2	H	80	CYS	2.4
2	B	98	ASP	2.3
1	G	60	TYR	2.3
1	C	248	HIS	2.3
1	G	88	TYR	2.3
2	H	33	SER	2.3
2	D	73	THR	2.3
2	H	12	ARG	2.3
1	G	249	HIS	2.3
1	G	110	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	91	LYS	2.3
1	G	265	VAL	2.3
2	H	89	GLN	2.2
2	H	61	SER	2.2
1	G	234	PHE	2.2
1	G	262	PRO	2.2
1	G	5	LEU	2.2
2	H	19	LYS	2.2
1	G	89	THR	2.2
1	G	169	ARG	2.2
2	H	76	ASP	2.1
2	H	87	LEU	2.1
1	G	181	SER	2.1
1	G	239	SER	2.1
2	F	42	ASN	2.1
2	H	1	ILE	2.1
1	G	120	PHE	2.1
2	H	32	PRO	2.0
1	G	168	GLU	2.0
2	H	46	ILE	2.0
1	G	91	GLN	2.0
1	G	216	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.