



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 06:31 PM EDT

PDB ID : 4N90  
Title : Crystal structure of ternary complex of TRAIL, DR5, and Fab fragment from a DR5 agonist antibody  
Authors : Huang, X.  
Deposited on : 2013-10-18  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

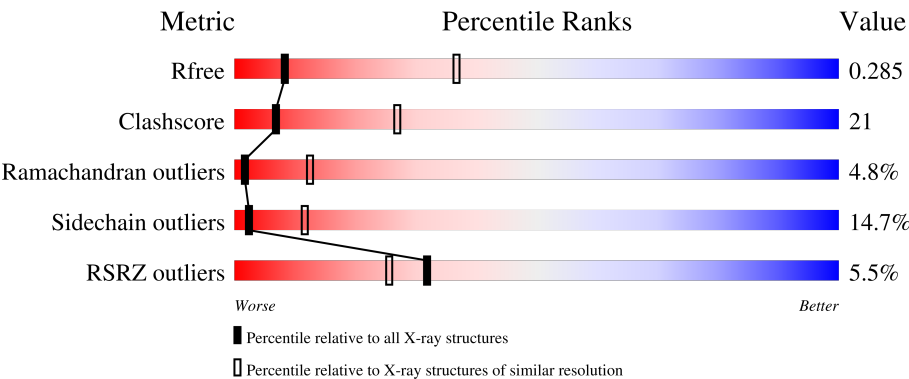
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 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 3.30 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))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	R	126	<div><div>3%</div><div><div></div><div>55%</div><div>26%</div><div>5%</div><div>14%</div></div></div>
1	S	126	<div><div>3%</div><div><div></div><div>51%</div><div>25%</div><div>8%</div><div>16%</div></div></div>
1	T	126	<div><div>6%</div><div><div></div><div>43%</div><div>37%</div><div>6%</div><div>15%</div></div></div>
2	A	168	<div><div>6%</div><div><div></div><div>52%</div><div>33%</div><div>6%</div><div>8%</div></div></div>
2	B	168	<div><div>2%</div><div><div></div><div>53%</div><div>32%</div><div>7%</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	C	168	<div><div></div><div>5%</div><div>49%</div><div>35%</div><div>8%</div><div>8%</div></div>
3	E	215	<div><div></div><div>2%</div><div>60%</div><div>35%</div><div></div><div></div></div>
3	G	215	<div><div></div><div>11%</div><div>59%</div><div>32%</div><div>8%</div><div></div></div>
3	I	215	<div><div></div><div>8%</div><div>56%</div><div>34%</div><div>7%</div><div></div></div>
4	D	224	<div><div></div><div>2%</div><div>46%</div><div>38%</div><div>11%</div><div></div></div>
4	F	224	<div><div></div><div>8%</div><div>49%</div><div>36%</div><div>10%</div><div></div></div>
4	H	224	<div><div></div><div>4%</div><div>45%</div><div>38%</div><div>12%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15934 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 Tumor necrosis factor receptor superfamily member 10B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	108	Total	C	N	O	S	0	0	0
			833	498	150	169	16			
1	S	106	Total	C	N	O	S	0	0	0
			814	486	145	167	16			
1	T	107	Total	C	N	O	S	0	0	0
			824	492	148	168	16			

- Molecule 2 is a protein called Tumor necrosis factor ligand superfamily member 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	155	Total	C	N	O	S	0	0	0
			1278	813	221	240	4			
2	B	155	Total	C	N	O	S	0	0	0
			1274	811	221	238	4			
2	C	154	Total	C	N	O	S	0	1	0
			1276	812	223	237	4			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1623	1015	275	329	4			
3	G	214	Total	C	N	O	S	0	0	0
			1615	1012	271	328	4			
3	I	214	Total	C	N	O	S	0	0	0
			1615	1012	271	328	4			

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1616	1021	269	321	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1575	998	258	314	5			
4	H	215	Total	C	N	O	S	0	0	0
			1590	1007	262	316	5			

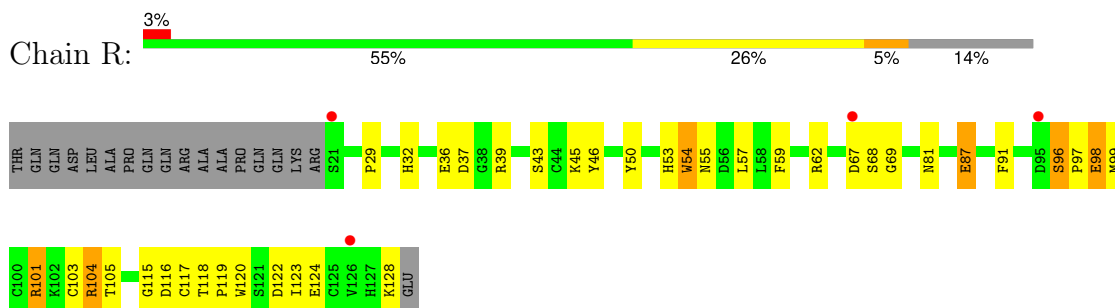
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

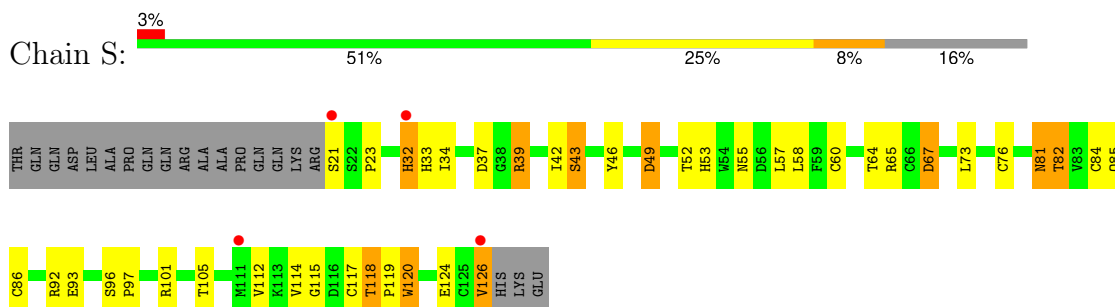
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

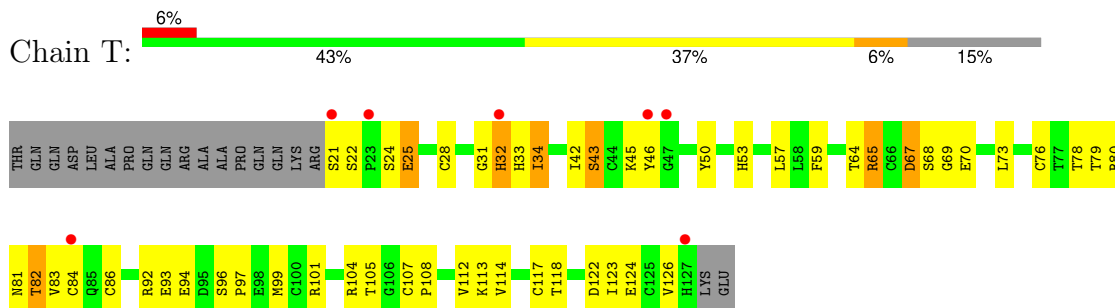
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

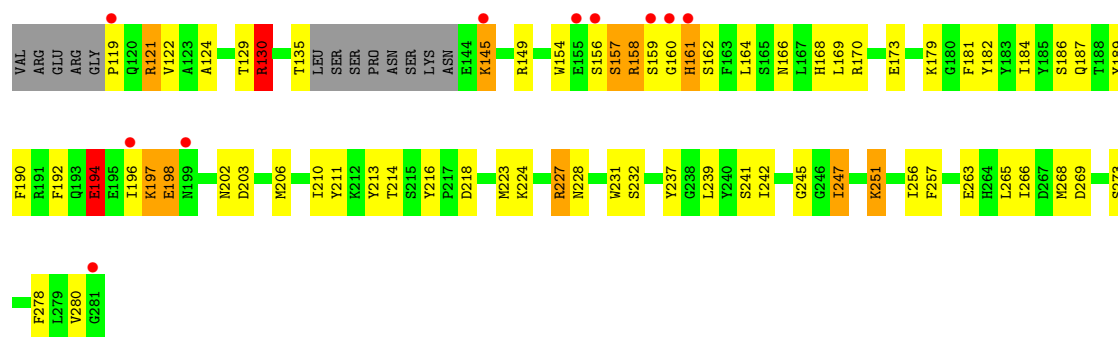


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

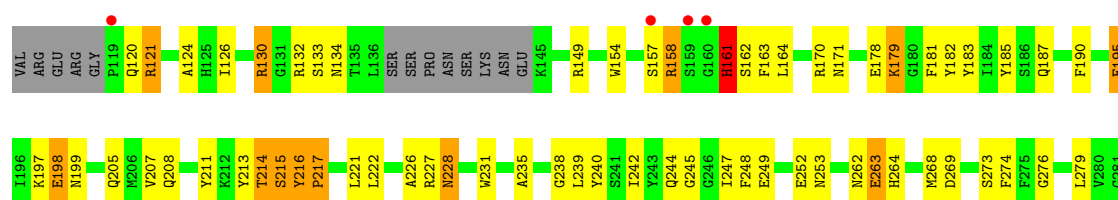


- Molecule 2: Tumor necrosis factor ligand superfamily member 10

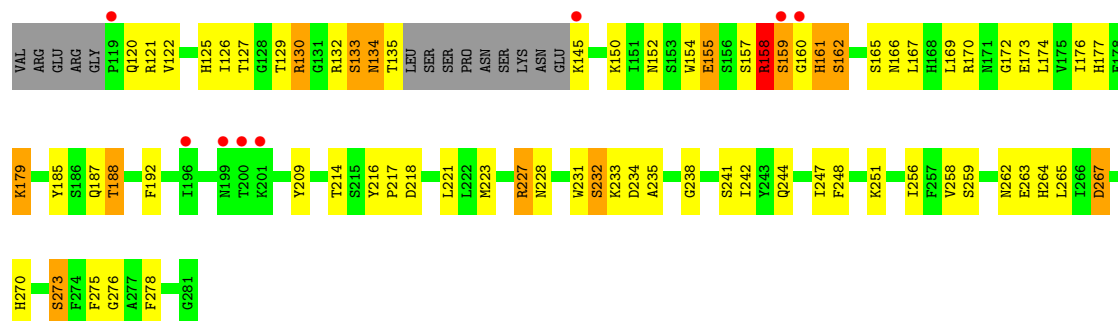




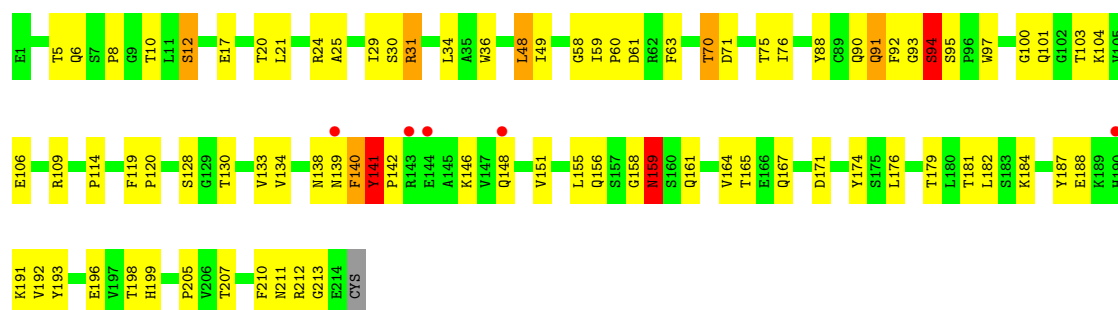
- Molecule 2: Tumor necrosis factor ligand superfamily member 10



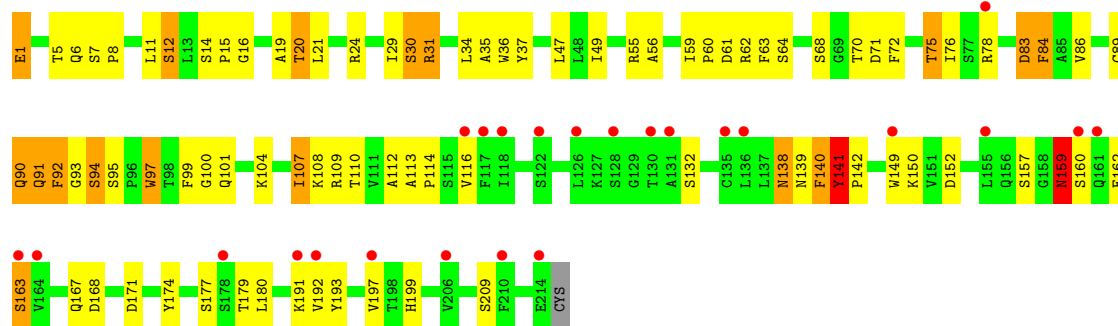
- Molecule 2: Tumor necrosis factor ligand superfamily member 10



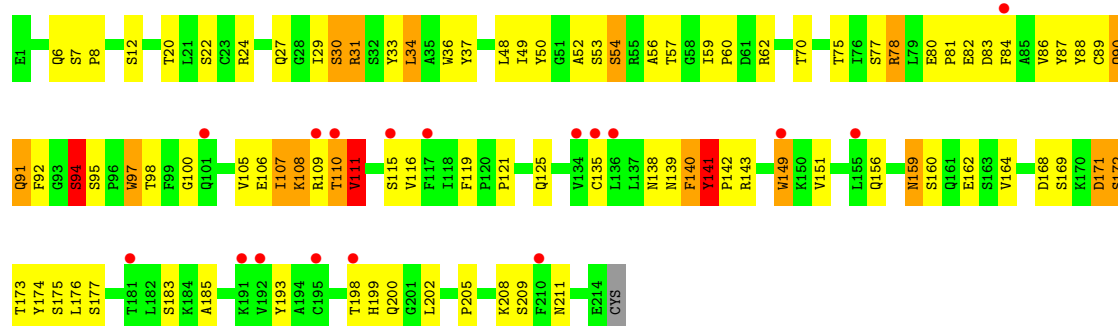
- Molecule 3: Fab light chain



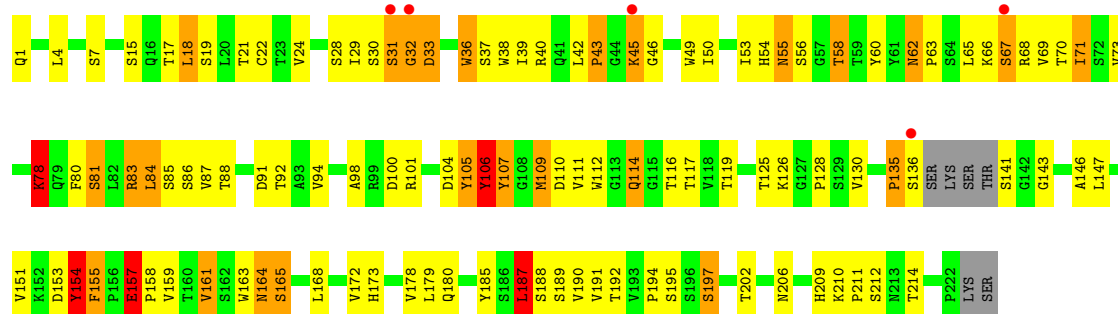
- Molecule 3: Fab light chain



• Molecule 3: Fab light chain



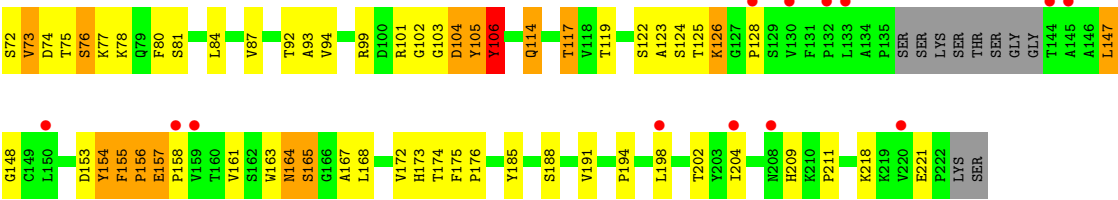
• Molecule 4: Fab heavy chain



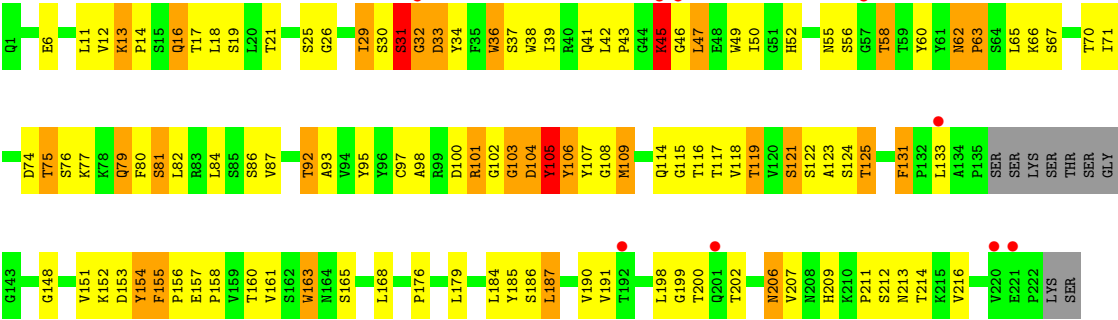
• Molecule 4: Fab heavy chain







● Molecule 4: Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.01Å 152.01Å 613.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 99.0 (50.00-3.30)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.229 , 0.286 0.229 , 0.285	Depositor DCC
$R_{free}$ test set	3233 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.2	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	15934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% 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: ZN

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	R	0.66	3/851 (0.4%)	0.69	0/1150
1	S	0.69	3/831 (0.4%)	0.74	0/1124
1	T	0.65	1/842 (0.1%)	0.75	1/1139 (0.1%)
2	A	0.61	1/1309 (0.1%)	0.74	0/1758
2	B	0.63	0/1305	0.76	0/1753
2	C	0.66	1/1311 (0.1%)	0.81	1/1760 (0.1%)
3	E	0.60	1/1660 (0.1%)	0.80	2/2258 (0.1%)
3	G	0.52	1/1652 (0.1%)	0.72	2/2249 (0.1%)
3	I	0.55	2/1652 (0.1%)	0.78	2/2249 (0.1%)
4	D	0.62	1/1657 (0.1%)	0.87	4/2267 (0.2%)
4	F	0.63	3/1616 (0.2%)	0.77	1/2216 (0.0%)
4	H	0.64	3/1631 (0.2%)	0.80	0/2233
All	All	0.62	20/16317 (0.1%)	0.78	13/22156 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	E	0	2
3	G	0	2
3	I	0	2
4	D	0	4
4	F	0	4
4	H	0	4
All	All	0	19

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	36	TRP	CD2-CE2	6.55	1.49	1.41
4	H	49	TRP	CD2-CE2	6.01	1.48	1.41
1	S	32	HIS	CB-CG	5.84	1.60	1.50
3	G	97	TRP	CD2-CE2	5.64	1.48	1.41
1	R	120	TRP	CD2-CE2	5.61	1.48	1.41
3	E	97	TRP	CD2-CE2	5.60	1.48	1.41
4	F	36	TRP	CD2-CE2	5.57	1.48	1.41
1	S	67	ASP	CB-CG	5.54	1.63	1.51
4	F	163	TRP	CD2-CE2	5.39	1.47	1.41
3	I	97	TRP	CD2-CE2	5.37	1.47	1.41
4	D	36	TRP	CD2-CE2	5.32	1.47	1.41
1	R	67	ASP	CB-CG	5.31	1.62	1.51
2	C	154	TRP	CD2-CE2	5.28	1.47	1.41
1	S	120	TRP	CD2-CE2	5.22	1.47	1.41
4	H	163	TRP	CD2-CE2	5.15	1.47	1.41
1	T	32	HIS	CB-CG	5.13	1.59	1.50
1	R	54	TRP	CD2-CE2	5.09	1.47	1.41
2	A	154	TRP	CD2-CE2	5.07	1.47	1.41
4	F	49	TRP	CD2-CE2	5.07	1.47	1.41
3	I	149	TRP	CD2-CE2	5.01	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	95	SER	N-CA-C	-8.99	86.72	111.00
3	E	141	TYR	N-CA-C	7.51	131.29	111.00
4	F	155	PHE	N-CA-C	6.98	129.83	111.00
3	I	95	SER	N-CA-C	-6.81	92.61	111.00
3	G	95	SER	N-CA-C	-6.54	93.33	111.00
4	D	155	PHE	N-CA-CB	-6.26	99.33	110.60
4	D	18	LEU	CA-CB-CG	5.93	128.95	115.30
3	I	141	TYR	N-CA-C	5.55	125.97	111.00
4	D	187	LEU	CA-CB-CG	5.54	128.05	115.30
4	D	157	GLU	N-CA-C	5.40	125.58	111.00
1	T	67	ASP	CB-CG-OD1	5.30	123.07	118.30
2	C	158	ARG	N-CA-C	5.29	125.28	111.00
3	G	141	TYR	N-CA-C	5.28	125.26	111.00

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	155	GLU	Peptide

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Mol	Chain	Res	Type	Group
4	D	106	TYR	Peptide
4	D	154	TYR	Peptide
4	D	164	ASN	Peptide
4	D	67	SER	Peptide
3	E	140	PHE	Peptide
3	E	94	SER	Peptide
4	F	104	ASP	Peptide
4	F	106	TYR	Peptide
4	F	154	TYR	Peptide
4	F	42	LEU	Peptide
3	G	140	PHE	Peptide
3	G	94	SER	Peptide
4	H	104	ASP	Peptide
4	H	106	TYR	Peptide
4	H	154	TYR	Peptide
4	H	202	THR	Peptide
3	I	140	PHE	Peptide
3	I	94	SER	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	R	833	0	755	28	0
1	S	814	0	735	30	0
1	T	824	0	742	35	0
2	A	1278	0	1226	63	0
2	B	1274	0	1222	74	0
2	C	1276	0	1229	50	0
3	E	1623	0	1548	59	1
3	G	1615	0	1538	59	0
3	I	1615	0	1538	71	0
4	D	1616	0	1556	89	0
4	F	1575	0	1498	63	0
4	H	1590	0	1527	91	0
5	A	1	0	0	0	0
All	All	15934	0	15114	650	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 21.

All (650) 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:157:SER:HA	2:B:158:ARG:NH2	1.47	1.28
2:B:158:ARG:HG2	2:B:158:ARG:HH11	1.09	1.14
1:T:64:THR:O	1:T:82:THR:HG21	1.61	1.01
4:D:42:LEU:HB3	4:D:43:PRO:HD2	1.40	1.00
3:I:156:GLN:HB3	3:I:159:ASN:HD21	1.33	0.94
3:E:10:THR:HG22	3:E:104:LYS:HB3	1.50	0.93
3:E:148:GLN:NE2	3:E:155:LEU:CD1	2.33	0.92
2:A:158:ARG:HD2	2:A:158:ARG:O	1.71	0.90
1:T:65:ARG:HH22	3:I:97:TRP:HE1	1.14	0.90
4:F:45:LYS:HG2	4:F:46:GLY:H	1.37	0.90
1:R:53:HIS:NE2	2:C:218:ASP:OD2	2.05	0.89
4:D:54:HIS:HD2	4:D:56:SER:H	1.19	0.87
4:H:30:SER:O	4:H:31:SER:HB2	1.75	0.86
4:F:45:LYS:CG	4:F:46:GLY:H	1.88	0.85
1:S:76:CYS:HB2	1:S:82:THR:HG22	1.59	0.85
4:D:54:HIS:CD2	4:D:56:SER:H	1.96	0.84
3:E:21:LEU:HD23	3:E:103:THR:HB	1.57	0.84
2:B:157:SER:HA	2:B:158:ARG:CZ	2.07	0.84
2:A:228:ASN:HD22	2:B:239:LEU:H	1.24	0.83
3:G:168:ASP:HB3	3:G:171:ASP:HB3	1.60	0.83
4:D:65:LEU:HB3	4:D:69:VAL:CG2	2.08	0.83
4:H:32:GLY:HA2	4:H:55:ASN:HD21	1.42	0.83
3:E:148:GLN:NE2	3:E:155:LEU:HD11	1.93	0.83
3:G:92:PHE:HD2	3:G:92:PHE:N	1.77	0.82
3:E:114:PRO:HD3	3:E:199:HIS:CD2	2.15	0.82
3:E:146:LYS:HE3	3:E:148:GLN:OE1	1.78	0.82
1:R:46:TYR:H	4:D:58:THR:HG21	1.42	0.81
2:B:158:ARG:HG2	2:B:158:ARG:NH1	1.87	0.81
4:D:4:LEU:HD12	4:D:111:VAL:HG12	1.60	0.81
3:G:6:GLN:HE21	3:G:100:GLY:HA3	1.44	0.81
1:S:46:TYR:H	4:F:58:THR:HG21	1.46	0.80
3:E:148:GLN:HE21	3:E:155:LEU:CD1	1.95	0.80
4:H:18:LEU:HD11	4:H:118:VAL:HG11	1.64	0.80
2:B:158:ARG:HB3	2:B:162:SER:O	1.82	0.79
2:B:249:GLU:OE1	2:C:158:ARG:HD3	1.81	0.79
4:H:92:THR:HG23	4:H:119:THR:HA	1.65	0.79
2:A:192:PHE:HE1	2:A:194:GLU:HG2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:64:THR:H	1:S:81:ASN:HD21	1.30	0.78
3:G:92:PHE:N	3:G:92:PHE:CD2	2.50	0.78
3:I:30:SER:O	3:I:31:ARG:HB2	1.84	0.77
3:E:140:PHE:O	3:E:174:TYR:N	2.17	0.77
1:T:46:TYR:H	4:H:58:THR:HG21	1.48	0.77
3:I:56:ALA:HB3	3:I:59:ILE:HD13	1.67	0.77
2:A:192:PHE:CE1	2:A:194:GLU:HG2	2.20	0.76
4:F:92:THR:HG23	4:F:119:THR:HA	1.68	0.76
2:B:158:ARG:O	2:B:161:HIS:ND1	2.19	0.76
2:B:247:ILE:HD11	2:C:278:PHE:HD2	1.51	0.76
3:G:177:SER:HB3	4:F:175:PHE:CE1	2.19	0.75
3:E:164:VAL:HG22	3:E:176:LEU:HD12	1.69	0.75
4:H:154:TYR:O	4:H:155:PHE:HB2	1.85	0.75
3:E:184:LYS:O	3:E:188:GLU:HG2	1.87	0.74
3:G:62:ARG:HD2	3:G:78:ARG:O	1.87	0.74
3:G:91:GLN:NE2	3:G:93:GLY:H	1.86	0.74
3:E:91:GLN:NE2	3:E:93:GLY:H	1.85	0.74
4:D:45:LYS:NZ	4:D:46:GLY:H	1.86	0.74
4:D:168:LEU:HD21	4:D:191:VAL:HG11	1.68	0.74
2:A:161:HIS:HE1	2:C:221:LEU:O	1.70	0.73
3:I:140:PHE:O	3:I:174:TYR:N	2.21	0.73
3:E:29:ILE:HD11	3:E:34:LEU:HD12	1.70	0.73
4:F:154:TYR:CE2	4:F:185:TYR:HB2	2.24	0.73
3:I:107:ILE:HD12	3:I:172:SER:HA	1.70	0.73
4:D:50:ILE:HG23	4:D:65:LEU:HD13	1.71	0.73
1:R:96:SER:N	1:R:97:PRO:HD3	2.04	0.73
3:G:20:THR:HG23	3:G:75:THR:HG23	1.69	0.73
4:H:156:PRO:HD2	4:H:211:PRO:HB2	1.71	0.73
2:A:158:ARG:HD3	2:A:162:SER:H	1.54	0.72
4:D:65:LEU:HB3	4:D:69:VAL:HG21	1.71	0.72
4:H:30:SER:HB3	4:H:75:THR:HG21	1.70	0.72
3:I:140:PHE:O	3:I:173:THR:HB	1.91	0.71
1:T:92:ARG:HG3	1:T:92:ARG:HH11	1.56	0.71
3:E:30:SER:O	3:E:31:ARG:HB2	1.89	0.71
3:E:30:SER:O	3:E:31:ARG:CB	2.37	0.71
1:T:65:ARG:NH2	3:I:97:TRP:HE1	1.88	0.70
3:G:1:GLU:HG3	3:G:1:GLU:O	1.91	0.70
4:H:29:ILE:HG13	4:H:75:THR:HG23	1.72	0.70
4:D:98:ALA:HB3	4:D:109:MET:HE2	1.73	0.70
4:F:101:ARG:HB2	4:F:106:TYR:HB2	1.73	0.70
3:I:50:TYR:O	3:I:54:SER:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:145:LYS:NZ	2:A:218:ASP:OD2	2.22	0.70
2:A:129:THR:O	2:A:130:ARG:HB3	1.91	0.70
1:R:32:HIS:HA	1:R:43:SER:HA	1.75	0.69
4:F:34:TYR:HE1	4:F:104:ASP:OD2	1.76	0.69
4:D:92:THR:HG23	4:D:119:THR:HA	1.74	0.69
3:I:168:ASP:HB3	3:I:171:ASP:HB3	1.72	0.69
1:S:67:ASP:OD2	2:B:269:ASP:OD2	2.09	0.69
1:S:114:VAL:HB	1:S:124:GLU:HB3	1.75	0.69
4:F:45:LYS:HG2	4:F:46:GLY:N	2.08	0.69
4:D:62:ASN:HD22	4:D:63:PRO:HD2	1.58	0.68
4:H:6:GLU:HB3	4:H:116:THR:HG23	1.75	0.68
4:F:34:TYR:CE1	4:F:104:ASP:OD2	2.46	0.68
3:I:37:TYR:HE1	3:I:90:GLN:HE21	1.41	0.68
2:A:158:ARG:HD3	2:A:162:SER:N	2.09	0.68
1:S:115:GLY:H	1:S:124:GLU:HB3	1.59	0.68
2:A:129:THR:HG22	2:A:130:ARG:H	1.59	0.68
3:G:191:LYS:HG3	3:G:192:VAL:HG23	1.76	0.68
4:H:77:LYS:O	4:H:79:GLN:HG3	1.93	0.68
4:D:187:LEU:HD23	4:D:188:SER:N	2.09	0.68
3:G:140:PHE:O	3:G:174:TYR:N	2.24	0.67
4:F:168:LEU:HD21	4:F:191:VAL:HG11	1.75	0.67
2:A:192:PHE:HB3	2:A:265:LEU:HD22	1.77	0.67
4:D:146:ALA:HB2	4:D:192:THR:HG22	1.77	0.67
2:A:179:LYS:HG3	2:A:251:LYS:HA	1.77	0.67
4:F:45:LYS:CD	4:F:46:GLY:H	2.08	0.67
3:G:160:SER:HA	3:G:179:THR:O	1.94	0.66
4:H:14:PRO:HD3	4:H:121:SER:C	2.15	0.66
3:G:37:TYR:HE1	3:G:90:GLN:HG2	1.59	0.66
3:E:93:GLY:O	3:E:94:SER:HB3	1.94	0.66
3:E:8:PRO:O	3:E:103:THR:HG23	1.96	0.66
4:H:38:TRP:HB3	4:H:50:ILE:HD12	1.77	0.66
2:B:214:THR:HG22	2:B:216:TYR:HB3	1.77	0.65
3:E:6:GLN:HE22	3:E:88:TYR:HA	1.61	0.65
4:H:101:ARG:HH11	4:H:101:ARG:CG	2.09	0.65
1:S:52:THR:OG1	1:S:53:HIS:HD2	1.79	0.65
2:A:129:THR:O	2:A:130:ARG:CB	2.45	0.65
4:H:36:TRP:HB3	4:H:80:PHE:CE1	2.32	0.65
2:A:158:ARG:NH2	2:A:161:HIS:HD2	1.94	0.65
2:A:181:PHE:CE2	2:B:121:ARG:HD2	2.32	0.65
2:A:157:SER:OG	2:A:158:ARG:N	2.26	0.64
4:F:45:LYS:CG	4:F:46:GLY:N	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:53:ILE:HD13	4:F:72:SER:HA	1.78	0.64
3:G:90:GLN:HG3	3:G:92:PHE:HE2	1.61	0.64
4:H:133:LEU:HB2	4:H:148:GLY:O	1.98	0.64
3:E:191:LYS:HG3	3:E:192:VAL:HG23	1.79	0.64
4:H:168:LEU:HD21	4:H:191:VAL:HG11	1.80	0.64
1:S:81:ASN:HD22	1:S:82:THR:H	1.47	0.63
2:A:119:PRO:N	2:A:121:ARG:HD2	2.13	0.63
4:F:103:GLY:C	4:F:105:TYR:N	2.51	0.63
3:I:84:PHE:CG	3:I:107:ILE:HG12	2.34	0.63
1:R:96:SER:CB	1:R:101:ARG:NH1	2.61	0.63
4:F:154:TYR:CE2	4:F:185:TYR:CB	2.82	0.63
2:A:158:ARG:HD2	2:A:158:ARG:C	2.16	0.62
3:G:29:ILE:HD11	3:G:34:LEU:HD12	1.80	0.62
4:F:65:LEU:O	4:F:67:SER:N	2.32	0.62
3:I:168:ASP:CB	3:I:171:ASP:HB3	2.29	0.62
3:G:91:GLN:C	3:G:92:PHE:HD2	2.03	0.62
1:R:96:SER:N	1:R:97:PRO:CD	2.63	0.62
2:A:158:ARG:NE	2:A:161:HIS:HA	2.15	0.62
4:H:156:PRO:HD2	4:H:211:PRO:CB	2.28	0.62
3:G:12:SER:HB3	3:G:108:LYS:HE3	1.82	0.62
4:D:56:SER:OG	4:D:58:THR:HG22	2.01	0.61
3:G:19:ALA:HB3	3:G:76:ILE:HB	1.83	0.61
1:R:96:SER:HB2	1:R:101:ARG:NH1	2.15	0.61
2:B:207:VAL:HG13	2:B:226:ALA:HB2	1.81	0.61
1:T:107:CYS:SG	1:T:113:LYS:HB2	2.40	0.61
4:F:74:ASP:OD1	4:F:76:SER:OG	2.16	0.61
1:R:96:SER:H	1:R:97:PRO:HD3	1.64	0.61
1:S:118:THR:O	1:S:120:TRP:N	2.34	0.61
4:D:194:PRO:HB2	4:D:197:SER:HB2	1.82	0.61
1:R:91:PHE:CZ	1:R:122:ASP:HB2	2.35	0.60
4:H:121:SER:HB3	4:H:123:ALA:HB2	1.84	0.60
1:T:57:LEU:HD11	2:B:216:TYR:CE1	2.36	0.60
3:E:138:ASN:HD21	4:D:173:HIS:HD2	1.47	0.60
4:D:42:LEU:CB	4:D:43:PRO:HD2	2.22	0.60
3:I:81:PRO:HA	3:I:84:PHE:CE1	2.35	0.60
3:G:90:GLN:NE2	3:G:99:PHE:CZ	2.69	0.60
1:T:78:THR:HG23	1:T:79:THR:HG23	1.84	0.60
2:A:227:ARG:CZ	2:B:240:TYR:HE2	2.14	0.60
2:B:158:ARG:HH11	2:B:158:ARG:CG	2.00	0.60
1:T:108:PRO:HG3	2:B:199:ASN:HB3	1.83	0.60
4:F:73:VAL:HG12	4:F:80:PHE:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:209:HIS:HD2	4:F:211:PRO:HD2	1.67	0.60
4:H:62:ASN:C	4:H:62:ASN:HD22	2.05	0.60
4:F:74:ASP:HB3	4:F:77:LYS:HB2	1.84	0.60
3:E:156:GLN:HB3	3:E:159:ASN:HD21	1.67	0.60
4:H:106:TYR:O	4:H:107:TYR:HB2	2.02	0.59
2:C:167:LEU:HD23	2:C:176:ILE:HD13	1.85	0.59
3:G:6:GLN:NE2	3:G:89:CYS:H	2.01	0.59
2:A:187:GLN:O	2:A:273:SER:HA	2.02	0.59
3:G:107:ILE:HG13	3:G:167:GLN:NE2	2.18	0.59
2:C:126:ILE:HA	2:C:162:SER:HB3	1.84	0.59
3:G:142:PRO:HD2	3:G:199:HIS:CE1	2.37	0.59
4:F:164:ASN:HB2	4:F:167:ALA:HB3	1.83	0.59
3:I:48:LEU:HD23	3:I:59:ILE:HG12	1.84	0.59
1:R:37:ASP:OD1	1:R:39:ARG:HG2	2.02	0.59
2:B:205:GLN:O	2:B:262:ASN:ND2	2.36	0.59
3:E:188:GLU:OE2	3:E:188:GLU:HA	2.03	0.59
4:F:5:GLN:HG3	4:F:114:GLN:OE1	2.03	0.58
3:I:109:ARG:C	3:I:110:THR:CG2	2.71	0.58
2:A:160:GLY:O	2:A:161:HIS:HB2	2.02	0.58
2:A:228:ASN:ND2	2:B:239:LEU:H	1.98	0.58
4:D:98:ALA:HB3	4:D:109:MET:CE	2.32	0.58
4:H:93:ALA:O	4:H:95:TYR:HD1	1.86	0.58
1:S:114:VAL:HG21	1:S:126:VAL:HG13	1.85	0.58
2:C:262:ASN:HB3	2:C:265:LEU:HD12	1.84	0.58
2:C:157:SER:O	2:C:159:SER:N	2.30	0.58
3:I:30:SER:O	3:I:31:ARG:CB	2.52	0.58
2:C:132:ARG:HB3	2:C:270:HIS:CE1	2.38	0.58
1:R:59:PHE:CE2	2:A:158:ARG:HB3	2.38	0.58
4:D:62:ASN:HD22	4:D:63:PRO:CD	2.17	0.58
4:F:161:VAL:HG11	4:F:174:THR:HG21	1.86	0.58
4:H:74:ASP:HB3	4:H:77:LYS:HB2	1.85	0.58
1:T:28:CYS:SG	1:T:34:ILE:HG22	2.44	0.58
4:F:154:TYR:CD2	4:F:185:TYR:HB2	2.39	0.58
4:H:18:LEU:CD1	4:H:118:VAL:HG11	2.32	0.57
4:H:45:LYS:CG	4:H:46:GLY:H	2.17	0.57
4:H:93:ALA:O	4:H:95:TYR:CD1	2.57	0.57
4:D:130:VAL:HG12	4:D:130:VAL:O	2.02	0.57
3:G:90:GLN:HG3	3:G:92:PHE:CE2	2.39	0.57
3:G:168:ASP:CB	3:G:171:ASP:HB3	2.33	0.57
1:S:76:CYS:CB	1:S:82:THR:HG22	2.32	0.57
3:E:60:PRO:HG2	3:E:63:PHE:HD2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:HIS:HD2	4:D:56:SER:N	1.97	0.57
2:B:238:GLY:O	2:B:239:LEU:HD23	2.04	0.57
2:C:232:SER:C	2:C:234:ASP:H	2.08	0.57
4:H:151:VAL:CG1	4:H:207:VAL:HG11	2.34	0.57
2:A:122:VAL:HG22	2:A:166:ASN:HB2	1.87	0.57
4:F:32:GLY:HA2	4:F:55:ASN:OD1	2.05	0.57
4:D:45:LYS:HZ2	4:D:45:LYS:HB3	1.69	0.56
3:G:90:GLN:NE2	3:G:99:PHE:CE2	2.72	0.56
4:H:13:LYS:O	4:H:16:GLN:HB2	2.05	0.56
4:H:62:ASN:C	4:H:62:ASN:ND2	2.58	0.56
1:T:50:TYR:CZ	1:T:81:ASN:HB2	2.40	0.56
2:B:157:SER:CA	2:B:158:ARG:CZ	2.81	0.56
3:E:148:GLN:HE21	3:E:155:LEU:HD12	1.69	0.56
4:F:53:ILE:CD1	4:F:72:SER:HA	2.35	0.56
1:S:37:ASP:OD2	1:S:39:ARG:HB3	2.05	0.56
1:T:76:CYS:HB2	1:T:82:THR:HG22	1.88	0.56
4:D:141:SER:O	4:D:143:GLY:HA2	2.05	0.56
2:A:184:ILE:O	2:A:245:GLY:HA2	2.06	0.56
4:F:54:HIS:HD2	4:F:56:SER:OG	1.89	0.56
4:D:4:LEU:CD2	4:D:22:CYS:SG	2.94	0.56
3:G:150:LYS:O	3:G:193:TYR:HA	2.06	0.56
3:I:107:ILE:CD1	3:I:172:SER:HA	2.35	0.56
1:R:46:TYR:N	4:D:58:THR:HG21	2.18	0.56
4:H:45:LYS:HG3	4:H:46:GLY:N	2.21	0.56
4:F:94:VAL:HG22	4:F:117:THR:HB	1.88	0.56
1:T:86:CYS:SG	1:T:92:ARG:HB2	2.45	0.56
1:T:104:ARG:HB2	1:T:123:ILE:HD11	1.87	0.56
2:C:223:MET:HB3	2:C:244:GLN:OE1	2.06	0.56
4:D:65:LEU:CB	4:D:69:VAL:HG21	2.36	0.55
4:D:187:LEU:HD23	4:D:187:LEU:C	2.26	0.55
3:E:167:GLN:HG3	3:E:174:TYR:CE2	2.42	0.55
3:E:196:GLU:HG3	3:E:207:THR:OG1	2.07	0.55
3:I:159:ASN:HD22	3:I:159:ASN:H	1.54	0.55
4:H:11:LEU:HD22	4:H:125:THR:HG22	1.89	0.55
3:I:12:SER:HB3	3:I:108:LYS:HD2	1.89	0.55
2:A:214:THR:HG23	2:A:216:TYR:H	1.72	0.55
4:D:42:LEU:HB3	4:D:43:PRO:CD	2.26	0.55
4:D:128:PRO:HD2	4:D:214:THR:HG21	1.89	0.55
3:I:109:ARG:C	3:I:110:THR:HG22	2.27	0.55
3:E:48:LEU:HD23	3:E:59:ILE:HG12	1.88	0.55
3:I:84:PHE:CZ	3:I:107:ILE:HG23	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:29:ILE:HG22	4:H:36:TRP:CE2	2.41	0.55
3:G:97:TRP:CD1	3:G:97:TRP:N	2.73	0.55
2:B:222:LEU:HD22	2:B:248:PHE:CD2	2.42	0.55
3:G:116:VAL:HG21	3:G:197:VAL:HG21	1.89	0.55
3:I:82:GLU:O	3:I:84:PHE:N	2.40	0.55
2:A:278:PHE:HE1	2:A:280:VAL:HG12	1.72	0.54
3:G:91:GLN:HE21	3:G:93:GLY:H	1.55	0.54
4:F:175:PHE:HD1	4:F:188:SER:HB2	1.72	0.54
2:B:158:ARG:NH1	2:B:158:ARG:N	2.54	0.54
4:D:24:VAL:HB	4:D:78:LYS:HG3	1.88	0.54
4:H:101:ARG:CG	4:H:101:ARG:NH1	2.67	0.54
4:H:45:LYS:HG3	4:H:46:GLY:H	1.72	0.54
3:G:138:ASN:HD21	4:F:173:HIS:CD2	2.25	0.54
3:E:63:PHE:CE1	3:E:76:ILE:HG12	2.43	0.54
4:D:98:ALA:CB	4:D:109:MET:HE2	2.37	0.54
1:T:99:MET:HB2	2:B:205:GLN:NE2	2.22	0.54
2:C:125:HIS:O	2:C:162:SER:HA	2.08	0.54
2:B:190:PHE:HB2	2:B:240:TYR:HB2	1.89	0.54
2:C:129:THR:O	2:C:130:ARG:CB	2.56	0.54
1:S:84:CYS:HB2	2:B:134:ASN:HD21	1.73	0.54
1:T:57:LEU:HD11	2:B:216:TYR:CD1	2.42	0.54
4:H:209:HIS:HB3	4:H:214:THR:HB	1.90	0.54
1:S:23:PRO:HG3	1:S:39:ARG:O	2.08	0.53
4:H:101:ARG:NH1	4:H:101:ARG:HG2	2.24	0.53
4:H:148:GLY:HA2	4:H:163:TRP:CZ2	2.43	0.53
4:D:161:VAL:HG21	4:D:189:SER:HB2	1.90	0.53
4:F:54:HIS:CD2	4:F:56:SER:H	2.25	0.53
3:I:6:GLN:HE22	3:I:88:TYR:HA	1.73	0.53
2:B:197:LYS:NZ	3:G:24:ARG:HH22	2.06	0.53
3:E:159:ASN:HD22	3:E:159:ASN:H	1.56	0.53
4:F:31:SER:O	4:F:33:ASP:N	2.42	0.53
3:E:91:GLN:HE22	3:E:93:GLY:H	1.57	0.53
4:H:33:ASP:HB3	4:H:104:ASP:OD2	2.09	0.53
1:R:53:HIS:CB	2:C:217:PRO:HG2	2.39	0.53
4:D:106:TYR:O	4:D:107:TYR:HB2	2.09	0.53
4:H:209:HIS:HD2	4:H:211:PRO:HD2	1.74	0.53
1:R:98:GLU:OE2	1:R:98:GLU:HA	2.08	0.53
1:S:52:THR:OG1	1:S:53:HIS:CD2	2.62	0.53
3:I:135:CYS:HB2	3:I:149:TRP:CH2	2.44	0.52
3:G:149:TRP:CD2	3:G:180:LEU:HD22	2.44	0.52
2:A:227:ARG:CZ	2:B:240:TYR:CE2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:PRO:O	4:D:136:SER:CB	2.57	0.52
3:I:156:GLN:HB3	3:I:159:ASN:ND2	2.15	0.52
2:B:181:PHE:HE1	2:B:249:GLU:HB2	1.75	0.52
3:I:81:PRO:O	3:I:84:PHE:HD1	1.92	0.52
4:H:103:GLY:C	4:H:105:TYR:N	2.63	0.52
1:T:67:ASP:O	1:T:70:GLU:HG3	2.09	0.52
4:H:209:HIS:CD2	4:H:211:PRO:HD2	2.45	0.52
2:C:166:ASN:C	2:C:177:HIS:HD1	2.12	0.52
3:E:29:ILE:HD11	3:E:34:LEU:CD1	2.39	0.52
2:C:150:LYS:NZ	2:C:173:GLU:OE2	2.43	0.51
4:D:163:TRP:O	4:D:165:SER:N	2.43	0.51
1:S:55:ASN:HB2	1:S:57:LEU:HG	1.93	0.51
1:T:64:THR:O	1:T:82:THR:CG2	2.46	0.51
2:C:126:ILE:HD13	2:C:174:LEU:HD21	1.91	0.51
4:D:43:PRO:O	4:D:45:LYS:HB2	2.10	0.51
1:T:92:ARG:HG3	1:T:92:ARG:NH1	2.25	0.51
2:B:157:SER:C	2:B:158:ARG:CZ	2.79	0.51
2:B:158:ARG:O	2:B:161:HIS:CE1	2.63	0.51
3:I:97:TRP:N	3:I:97:TRP:CD1	2.75	0.51
4:D:4:LEU:HD23	4:D:22:CYS:SG	2.51	0.51
4:D:32:GLY:HA2	4:D:55:ASN:OD1	2.11	0.51
2:C:152:ASN:HA	2:C:172:GLY:HA3	1.92	0.51
4:D:4:LEU:HD22	4:D:22:CYS:SG	2.50	0.51
3:I:91:GLN:HE22	3:I:94:SER:H	1.57	0.51
4:H:151:VAL:HG13	4:H:207:VAL:HG11	1.92	0.51
1:T:96:SER:OG	1:T:101:ARG:NH1	2.43	0.51
2:A:181:PHE:CD2	2:B:121:ARG:HD2	2.46	0.51
2:B:268:MET:O	2:B:269:ASP:C	2.49	0.51
3:E:193:TYR:HB2	3:E:210:PHE:CE1	2.46	0.51
1:T:64:THR:OG1	2:C:133:SER:O	2.28	0.51
4:F:61:TYR:CE2	4:F:69:VAL:HG12	2.46	0.51
4:H:52:HIS:C	4:H:71:ILE:HD11	2.31	0.51
1:S:81:ASN:HD22	1:S:82:THR:N	2.09	0.51
4:D:172:VAL:HG22	4:D:191:VAL:HG22	1.93	0.51
3:G:34:LEU:HD23	3:G:35:ALA:N	2.26	0.51
3:I:84:PHE:CE1	3:I:107:ILE:HG23	2.45	0.51
4:D:210:LYS:O	4:D:212:SER:N	2.44	0.50
4:F:157:GLU:H	4:F:158:PRO:CD	2.24	0.50
3:I:49:ILE:HA	3:I:54:SER:O	2.11	0.50
3:I:110:THR:O	3:I:110:THR:OG1	2.29	0.50
1:T:53:HIS:CB	2:B:217:PRO:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:PRO:HD2	3:E:199:HIS:CE1	2.46	0.50
4:H:13:LYS:HA	4:H:121:SER:O	2.12	0.50
4:D:45:LYS:HZ3	4:D:46:GLY:H	1.59	0.50
4:F:126:LYS:HD2	4:F:155:PHE:HB2	1.93	0.50
4:F:204:ILE:HA	4:F:218:LYS:O	2.11	0.50
1:S:96:SER:CB	1:S:101:ARG:HH11	2.25	0.50
2:A:247:ILE:HG13	2:B:185:TYR:OH	2.12	0.50
2:B:130:ARG:O	2:B:130:ARG:HG3	2.11	0.50
3:E:21:LEU:HD23	3:E:103:THR:CB	2.35	0.50
4:D:151:VAL:HG11	4:D:159:VAL:HG11	1.93	0.50
4:F:62:ASN:HB3	4:F:65:LEU:HD12	1.93	0.49
4:H:165:SER:H	4:H:206:ASN:HD21	1.61	0.49
4:D:65:LEU:HB3	4:D:69:VAL:HG23	1.88	0.49
3:G:36:TRP:HB2	3:G:49:ILE:HB	1.94	0.49
3:I:116:VAL:HG12	3:I:208:LYS:HG3	1.95	0.49
2:C:232:SER:C	2:C:234:ASP:N	2.66	0.49
3:E:6:GLN:HE21	3:E:100:GLY:HA3	1.77	0.49
4:D:151:VAL:HG12	4:D:154:TYR:CE1	2.48	0.49
4:D:179:LEU:HB2	4:D:185:TYR:CE2	2.47	0.49
4:F:18:LEU:HB2	4:F:87:VAL:HG11	1.94	0.49
2:B:211:TYR:CD1	2:B:221:LEU:HA	2.48	0.49
3:I:6:GLN:HE21	3:I:100:GLY:HA3	1.77	0.49
3:I:29:ILE:HD11	3:I:34:LEU:HD12	1.94	0.49
4:H:148:GLY:HA2	4:H:163:TRP:CH2	2.46	0.49
4:D:39:ILE:HD13	4:D:109:MET:HE1	1.95	0.49
4:D:157:GLU:HG3	4:D:185:TYR:CE1	2.47	0.49
2:B:252:GLU:HG2	2:B:253:ASN:ND2	2.28	0.49
4:D:126:LYS:O	4:D:154:TYR:HA	2.12	0.49
3:G:37:TYR:CE1	3:G:90:GLN:HG2	2.45	0.49
1:R:103:CYS:HA	1:R:122:ASP:OD1	2.11	0.49
4:D:28:SER:OG	4:D:78:LYS:HE2	2.12	0.49
4:F:101:ARG:O	4:F:103:GLY:N	2.41	0.49
3:I:37:TYR:CE1	3:I:90:GLN:NE2	2.81	0.49
3:G:24:ARG:HA	3:G:70:THR:O	2.11	0.49
3:I:80:GLU:O	3:I:84:PHE:CE1	2.66	0.49
2:B:179:LYS:O	2:B:179:LYS:HG3	2.12	0.48
4:D:29:ILE:H	4:D:78:LYS:HD2	1.78	0.48
2:B:158:ARG:HA	2:B:162:SER:H	1.78	0.48
4:D:100:ASP:OD1	4:D:101:ARG:O	2.31	0.48
3:G:56:ALA:HB3	3:G:59:ILE:HD13	1.95	0.48
1:R:53:HIS:HB3	2:C:217:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:156:SER:O	2:A:157:SER:HB3	2.12	0.48
2:B:158:ARG:NH1	2:B:158:ARG:H	2.11	0.48
4:D:45:LYS:NZ	4:D:46:GLY:N	2.60	0.48
4:D:55:ASN:C	4:D:55:ASN:ND2	2.66	0.48
4:H:31:SER:HB3	4:H:33:ASP:OD2	2.14	0.48
4:H:100:ASP:HB2	4:H:109:MET:HE3	1.94	0.48
3:E:191:LYS:HG3	3:E:192:VAL:CG2	2.42	0.48
4:H:101:ARG:O	4:H:103:GLY:N	2.47	0.48
1:T:21:SER:HB3	1:T:22:SER:H	1.52	0.48
1:T:59:PHE:CE2	2:C:158:ARG:HB2	2.48	0.48
2:A:182:TYR:O	2:A:247:ILE:HA	2.14	0.48
3:E:114:PRO:HA	3:E:140:PHE:HB3	1.96	0.48
3:E:138:ASN:HD21	4:D:173:HIS:CD2	2.30	0.48
3:E:161:GLN:HE22	4:D:180:GLN:HA	1.78	0.47
4:D:109:MET:HG3	4:D:112:TRP:CZ2	2.49	0.47
4:H:39:ILE:HD11	4:H:109:MET:SD	2.54	0.47
2:C:209:TYR:HB2	2:C:259:SER:HB3	1.95	0.47
4:F:14:PRO:O	4:F:16:GLN:N	2.46	0.47
3:G:30:SER:O	3:G:31:ARG:CB	2.62	0.47
4:F:62:ASN:HD22	4:F:63:PRO:HD2	1.79	0.47
4:H:74:ASP:OD1	4:H:76:SER:OG	2.32	0.47
1:T:53:HIS:HB3	2:B:217:PRO:HG2	1.97	0.47
1:T:68:SER:OG	1:T:69:GLY:N	2.47	0.47
2:B:187:GLN:O	2:B:273:SER:HA	2.14	0.47
4:H:179:LEU:HB2	4:H:185:TYR:CE2	2.49	0.47
1:R:50:TYR:CZ	1:R:81:ASN:HB2	2.50	0.47
2:B:247:ILE:HD11	2:C:278:PHE:CD2	2.41	0.47
4:D:65:LEU:O	4:D:67:SER:N	2.47	0.47
3:I:81:PRO:HA	3:I:84:PHE:HE1	1.79	0.47
2:B:228:ASN:HD22	2:B:228:ASN:H	1.61	0.47
3:E:60:PRO:HG2	3:E:63:PHE:CD2	2.47	0.47
3:I:82:GLU:C	3:I:84:PHE:H	2.18	0.47
2:B:231:TRP:CG	2:C:235:ALA:HA	2.50	0.47
4:D:45:LYS:HZ2	4:D:46:GLY:H	1.59	0.47
3:G:59:ILE:HG23	3:G:63:PHE:CD2	2.50	0.47
4:F:165:SER:O	4:F:165:SER:OG	2.32	0.47
3:I:36:TRP:HB2	3:I:49:ILE:HB	1.97	0.47
3:I:176:LEU:HD23	3:I:177:SER:N	2.30	0.47
2:B:183:TYR:OH	2:B:245:GLY:HA3	2.14	0.47
4:F:34:TYR:CD2	4:F:99:ARG:HD2	2.50	0.47
4:F:41:GLN:HB2	4:F:47:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:118:THR:HB	1:R:119:PRO:HD2	1.97	0.47
2:B:183:TYR:CZ	2:B:245:GLY:HA3	2.50	0.47
2:C:223:MET:HG3	2:C:248:PHE:CZ	2.50	0.47
3:E:119:PHE:HA	3:E:120:PRO:HD3	1.76	0.47
4:F:14:PRO:C	4:F:16:GLN:H	2.18	0.47
4:H:152:LYS:HG2	4:H:153:ASP:OD1	2.14	0.47
1:S:49:ASP:HB2	1:S:60:CYS:HB2	1.96	0.47
2:C:160:GLY:O	2:C:270:HIS:CD2	2.68	0.47
2:C:267:ASP:OD1	2:C:267:ASP:C	2.53	0.47
4:D:110:ASP:OD1	4:D:111:VAL:HG23	2.15	0.47
4:H:6:GLU:CD	4:H:115:GLY:HA2	2.35	0.47
2:B:231:TRP:CD2	2:C:235:ALA:HA	2.50	0.46
2:C:187:GLN:HA	2:C:242:ILE:O	2.15	0.46
3:I:24:ARG:HA	3:I:70:THR:O	2.15	0.46
4:H:56:SER:OG	4:H:58:THR:HG22	2.15	0.46
1:S:81:ASN:ND2	1:S:82:THR:H	2.11	0.46
2:A:239:LEU:H	2:C:228:ASN:ND2	2.12	0.46
2:B:182:TYR:CZ	2:B:279:LEU:HD13	2.49	0.46
3:E:21:LEU:HD12	3:E:21:LEU:N	2.30	0.46
3:G:141:TYR:HA	3:G:142:PRO:HA	1.50	0.46
3:E:159:ASN:HD22	3:E:159:ASN:N	2.13	0.46
4:H:148:GLY:HA3	4:H:190:VAL:HA	1.96	0.46
4:H:157:GLU:N	4:H:158:PRO:HD2	2.31	0.46
2:A:187:GLN:HA	2:A:242:ILE:O	2.15	0.46
2:A:211:TYR:HB2	2:A:257:PHE:CE1	2.51	0.46
3:I:143:ARG:NH2	3:I:164:VAL:HG21	2.29	0.46
1:S:81:ASN:ND2	1:S:82:THR:N	2.64	0.46
1:T:73:LEU:HB3	1:T:83:VAL:HG12	1.98	0.46
2:B:187:GLN:HA	2:B:242:ILE:O	2.15	0.46
4:F:40:ARG:HD3	4:F:50:ILE:HD11	1.97	0.46
1:S:85:GLN:HG2	1:S:86:CYS:N	2.30	0.46
2:A:161:HIS:CE1	2:C:221:LEU:O	2.60	0.46
4:D:114:GLN:H	4:D:114:GLN:NE2	2.12	0.46
3:I:81:PRO:HA	3:I:84:PHE:CD1	2.51	0.46
1:S:65:ARG:NH2	3:G:92:PHE:O	2.49	0.46
2:B:228:ASN:H	2:B:228:ASN:ND2	2.14	0.46
3:G:163:SER:OG	4:F:176:PRO:HG2	2.15	0.46
4:H:151:VAL:HG22	4:H:207:VAL:HG21	1.97	0.46
2:B:158:ARG:CZ	2:B:158:ARG:N	2.79	0.46
4:D:84:LEU:HD13	4:D:87:VAL:HG12	1.96	0.46
3:I:6:GLN:NE2	3:I:89:CYS:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:33:TYR:O	3:I:91:GLN:HA	2.16	0.46
3:I:140:PHE:CE1	3:I:175:SER:HA	2.50	0.46
2:B:214:THR:HG23	2:B:215:SER:N	2.29	0.46
3:E:120:PRO:HB3	3:E:210:PHE:CE2	2.51	0.46
3:E:114:PRO:HD3	3:E:199:HIS:HD2	1.76	0.45
3:E:164:VAL:HG12	3:E:165:THR:O	2.15	0.45
4:D:31:SER:O	4:D:33:ASP:N	2.49	0.45
4:H:45:LYS:CG	4:H:46:GLY:N	2.79	0.45
4:H:212:SER:O	4:H:213:ASN:HB2	2.16	0.45
4:D:55:ASN:C	4:D:55:ASN:HD22	2.19	0.45
4:D:62:ASN:C	4:D:62:ASN:ND2	2.69	0.45
3:G:142:PRO:HD2	3:G:199:HIS:HE1	1.80	0.45
1:T:24:SER:O	1:T:25:GLU:HB2	2.15	0.45
3:I:111:VAL:HG13	3:I:142:PRO:HD3	1.98	0.45
2:B:208:GLN:HE21	2:B:244:GLN:HE21	1.65	0.45
2:C:169:LEU:HD13	2:C:174:LEU:HD23	1.99	0.45
3:E:90:GLN:NE2	3:E:92:PHE:HE2	2.15	0.45
4:H:155:PHE:HA	4:H:156:PRO:HA	1.76	0.45
2:C:256:ILE:HG13	2:C:275:PHE:HZ	1.82	0.45
3:G:6:GLN:HE22	3:G:89:CYS:H	1.64	0.45
4:H:92:THR:CG2	4:H:119:THR:HA	2.42	0.45
2:A:210:ILE:HD12	2:A:223:MET:CE	2.46	0.45
2:C:160:GLY:O	2:C:161:HIS:HB2	2.16	0.45
2:A:190:PHE:CE1	2:A:206:MET:HB3	2.53	0.44
2:B:149:ARG:HD3	2:B:263:GLU:HG2	1.98	0.44
2:B:183:TYR:CE2	2:B:185:TYR:HB3	2.52	0.44
3:I:84:PHE:CE2	3:I:107:ILE:HA	2.52	0.44
4:H:62:ASN:O	4:H:63:PRO:C	2.56	0.44
2:C:214:THR:HG23	2:C:216:TYR:H	1.83	0.44
2:C:264:HIS:HB2	3:I:27:GLN:HG2	1.99	0.44
4:F:123:ALA:HB1	4:F:126:LYS:NZ	2.33	0.44
4:H:151:VAL:HG11	4:H:207:VAL:HG11	2.00	0.44
3:E:211:ASN:O	3:E:213:GLY:N	2.50	0.44
3:G:86:VAL:HG22	3:G:104:LYS:HG3	1.99	0.44
4:H:18:LEU:HD23	4:H:19:SER:N	2.32	0.44
4:H:30:SER:CB	4:H:75:THR:HG21	2.43	0.44
1:R:123:ILE:O	1:R:123:ILE:HG13	2.17	0.44
3:I:119:PHE:CD2	4:H:133:LEU:HB3	2.53	0.44
1:R:115:GLY:HA3	1:R:124:GLU:HB2	2.00	0.44
2:B:181:PHE:CE1	2:B:249:GLU:HB2	2.51	0.44
3:E:12:SER:HA	3:E:106:GLU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:ARG:HH22	4:D:91:ASP:CG	2.21	0.44
3:G:159:ASN:HD22	3:G:159:ASN:H	1.65	0.44
3:G:162:GLU:O	3:G:163:SER:HB2	2.17	0.44
4:F:128:PRO:HG3	4:F:209:HIS:HD1	1.83	0.44
3:I:37:TYR:OH	4:H:109:MET:HG3	2.18	0.44
3:I:151:VAL:HG22	3:I:193:TYR:CD2	2.53	0.44
4:H:98:ALA:HB3	4:H:109:MET:HE2	1.99	0.44
1:R:62:ARG:HH21	2:A:159:SER:HB3	1.82	0.44
1:S:96:SER:N	1:S:97:PRO:HD3	2.32	0.44
2:A:122:VAL:HG22	2:A:166:ASN:CB	2.46	0.44
2:A:158:ARG:CZ	2:A:161:HIS:HA	2.48	0.44
2:A:268:MET:O	2:A:269:ASP:C	2.56	0.44
3:E:187:TYR:HA	3:E:193:TYR:OH	2.17	0.44
4:F:13:LYS:HB2	4:F:16:GLN:CG	2.48	0.44
4:F:45:LYS:CD	4:F:46:GLY:N	2.79	0.44
1:R:36:GLU:HG2	1:R:37:ASP:H	1.83	0.44
1:S:33:HIS:N	1:S:42:ILE:O	2.51	0.44
2:C:188:THR:HA	2:C:273:SER:HB3	1.99	0.44
2:A:129:THR:HG22	2:A:130:ARG:N	2.31	0.44
3:G:90:GLN:HB3	3:G:99:PHE:CD2	2.53	0.44
3:I:84:PHE:CD2	3:I:105:VAL:HG12	2.53	0.44
3:I:92:PHE:CD1	4:H:107:TYR:HB3	2.53	0.44
4:H:125:THR:HB	4:H:156:PRO:HD3	1.99	0.44
2:B:185:TYR:CZ	2:B:276:GLY:HA3	2.53	0.43
4:F:155:PHE:CD2	4:F:156:PRO:HA	2.53	0.43
3:I:92:PHE:CZ	4:H:108:GLY:HA2	2.53	0.43
4:H:131:PHE:HE2	4:H:152:LYS:HD3	1.82	0.43
4:D:62:ASN:HD22	4:D:62:ASN:C	2.21	0.43
3:G:112:ALA:HB3	3:G:140:PHE:HA	2.00	0.43
4:H:154:TYR:HB2	4:H:209:HIS:CE1	2.53	0.43
3:G:11:LEU:HD23	3:G:11:LEU:HA	1.81	0.43
4:H:47:LEU:N	4:H:47:LEU:HD23	2.33	0.43
3:I:91:GLN:CD	3:I:91:GLN:O	2.56	0.43
4:D:104:ASP:O	4:D:105:TYR:HB3	2.19	0.43
4:D:126:LYS:HD3	4:D:153:ASP:O	2.19	0.43
4:H:50:ILE:HG23	4:H:65:LEU:CD1	2.48	0.43
4:H:186:SER:O	4:H:187:LEU:HB2	2.19	0.43
2:C:185:TYR:CE1	2:C:276:GLY:HA3	2.54	0.43
2:C:192:PHE:CE1	2:C:238:GLY:HA3	2.53	0.43
3:E:93:GLY:O	3:E:94:SER:CB	2.64	0.43
4:D:53:ILE:HB	4:D:71:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:29:ILE:HG22	4:F:36:TRP:CE2	2.54	0.43
4:F:39:ILE:HG23	4:F:48:GLU:O	2.19	0.43
4:H:12:VAL:HG21	4:H:18:LEU:HA	2.00	0.43
2:A:124:ALA:HB1	2:A:164:LEU:HD23	2.01	0.43
2:B:195:GLU:OE1	2:B:197:LYS:HE3	2.19	0.43
4:D:38:TRP:HB3	4:D:50:ILE:HD12	2.00	0.43
4:F:154:TYR:CE2	4:F:185:TYR:HB3	2.54	0.43
3:I:59:ILE:HA	3:I:60:PRO:HD2	1.66	0.43
1:T:33:HIS:N	1:T:42:ILE:O	2.51	0.43
2:B:197:LYS:HZ1	3:G:24:ARG:HH22	1.67	0.43
3:I:141:TYR:HB2	3:I:173:THR:HG22	2.00	0.43
2:A:224:LYS:NZ	2:B:133:SER:OG	2.52	0.43
3:E:48:LEU:HD23	3:E:48:LEU:HA	1.87	0.43
4:H:31:SER:O	4:H:55:ASN:ND2	2.52	0.43
1:R:29:PRO:HB3	1:R:54:TRP:CH2	2.54	0.42
2:A:227:ARG:NH2	2:C:227[A]:ARG:HH12	2.17	0.42
4:D:17:THR:HG22	4:D:85:SER:HA	2.00	0.42
4:D:104:ASP:O	4:D:105:TYR:CB	2.67	0.42
3:I:171:ASP:O	3:I:172:SER:HB2	2.19	0.42
2:C:179:LYS:HB2	2:C:251:LYS:HA	2.01	0.42
4:F:42:LEU:HD23	4:F:93:ALA:HB2	2.01	0.42
3:I:7:SER:HA	3:I:8:PRO:HA	1.84	0.42
2:A:197:LYS:NZ	3:E:24:ARG:HH12	2.16	0.42
4:D:101:ARG:HG3	4:D:106:TYR:CD1	2.54	0.42
3:E:134:VAL:HG22	3:E:179:THR:HG23	2.01	0.42
3:E:151:VAL:HG22	3:E:193:TYR:HD2	1.85	0.42
3:G:114:PRO:HD3	3:G:199:HIS:HD2	1.83	0.42
3:I:37:TYR:HE1	3:I:90:GLN:NE2	2.09	0.42
4:H:157:GLU:HG3	4:H:185:TYR:CZ	2.54	0.42
1:R:99:MET:HG2	2:A:237:TYR:CG	2.54	0.42
3:E:36:TRP:HB2	3:E:49:ILE:HB	2.01	0.42
3:G:113:ALA:HA	3:G:114:PRO:HD3	1.92	0.42
1:S:96:SER:HB3	1:S:101:ARG:HH11	1.84	0.42
2:A:196:ILE:H	2:A:196:ILE:HG13	1.62	0.42
2:B:124:ALA:HB1	2:B:164:LEU:HD23	2.02	0.42
3:I:183:SER:C	3:I:185:ALA:H	2.23	0.42
1:S:46:TYR:N	4:F:58:THR:HG21	2.24	0.42
2:A:173:GLU:HG2	2:A:257:PHE:HB3	2.02	0.42
2:B:126:ILE:HA	2:B:162:SER:HB3	2.01	0.42
3:E:25:ALA:O	3:E:70:THR:HG22	2.20	0.42
4:D:62:ASN:HD22	4:D:63:PRO:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:172:VAL:HA	4:D:190:VAL:O	2.20	0.42
3:I:159:ASN:H	3:I:159:ASN:ND2	2.17	0.42
1:T:31:GLY:HA2	1:T:78:THR:O	2.20	0.42
1:T:64:THR:HB	1:T:82:THR:HG23	2.02	0.42
4:D:49:TRP:CE3	4:D:62:ASN:HB2	2.55	0.42
4:D:209:HIS:HB3	4:D:214:THR:HB	2.02	0.42
4:F:155:PHE:CG	4:F:156:PRO:HA	2.55	0.42
3:I:90:GLN:CD	3:I:92:PHE:CE2	2.93	0.42
2:C:258:VAL:CG1	2:C:259:SER:N	2.83	0.42
4:D:54:HIS:CD2	4:D:56:SER:N	2.77	0.42
4:H:123:ALA:O	4:H:124:SER:HB2	2.19	0.42
1:T:32:HIS:HA	1:T:43:SER:HA	2.02	0.41
2:A:190:PHE:CE2	2:A:266:ILE:HD11	2.55	0.41
4:D:33:ASP:HB3	4:D:104:ASP:CG	2.40	0.41
4:D:39:ILE:CD1	4:D:109:MET:HE1	2.50	0.41
3:G:15:PRO:HD3	3:G:108:LYS:O	2.20	0.41
4:F:62:ASN:HD22	4:F:63:PRO:CD	2.33	0.41
4:F:172:VAL:HG22	4:F:191:VAL:HG22	2.01	0.41
1:S:32:HIS:HA	1:S:43:SER:HA	2.02	0.41
2:B:263:GLU:HG3	2:B:264:HIS:N	2.34	0.41
3:E:24:ARG:NH1	3:E:71:ASP:OD1	2.53	0.41
4:D:36:TRP:HB3	4:D:80:PHE:CE1	2.54	0.41
2:A:278:PHE:HD2	2:C:247:ILE:HD11	1.85	0.41
4:H:41:GLN:O	4:H:93:ALA:HB1	2.20	0.41
1:R:118:THR:HB	1:R:119:PRO:CD	2.50	0.41
2:B:182:TYR:CE2	2:B:279:LEU:HD13	2.55	0.41
3:E:146:LYS:HB3	3:E:198:THR:HB	2.02	0.41
4:D:81:SER:HB3	4:D:83:ARG:HH11	1.85	0.41
4:H:32:GLY:CA	4:H:55:ASN:HD21	2.24	0.41
4:H:34:TYR:HE1	4:H:104:ASP:HB3	1.86	0.41
2:A:227:ARG:NH2	2:C:227[A]:ARG:NH1	2.68	0.41
2:A:265:LEU:HA	2:A:265:LEU:HD23	1.86	0.41
2:C:227[A]:ARG:NH2	2:C:228:ASN:O	2.53	0.41
2:C:231:TRP:O	2:C:232:SER:C	2.57	0.41
1:R:69:GLY:O	1:R:87:GLU:HB3	2.21	0.41
1:S:92:ARG:HD2	1:S:97:PRO:HA	2.03	0.41
2:A:227:ARG:HD3	2:B:239:LEU:O	2.19	0.41
4:D:19:SER:OG	4:D:83:ARG:NH2	2.53	0.41
3:I:48:LEU:HD11	3:I:87:TYR:HE1	1.85	0.41
4:H:38:TRP:CZ3	4:H:97:CYS:HB3	2.55	0.41
1:T:112:VAL:N	1:T:126:VAL:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:GLY:C	3:E:59:ILE:HD12	2.41	0.41
2:A:197:LYS:HB3	2:A:198:GLU:H	1.50	0.41
2:B:157:SER:HA	2:B:158:ARG:HH21	1.66	0.41
3:G:7:SER:HA	3:G:8:PRO:HA	1.81	0.41
4:F:54:HIS:CG	4:F:55:ASN:N	2.89	0.41
4:H:84:LEU:HD23	4:H:84:LEU:HA	1.82	0.41
1:S:118:THR:C	1:S:120:TRP:H	2.24	0.41
1:T:93:GLU:HG2	1:T:94:GLU:N	2.35	0.41
2:A:227:ARG:NH1	2:B:240:TYR:CE2	2.89	0.41
2:B:126:ILE:HA	2:B:162:SER:CB	2.51	0.41
4:D:40:ARG:HA	4:D:94:VAL:O	2.21	0.41
4:D:210:LYS:C	4:D:212:SER:H	2.23	0.41
3:G:34:LEU:HD13	3:G:72:PHE:CG	2.56	0.41
3:I:62:ARG:HD2	3:I:78:ARG:O	2.21	0.41
2:A:189:TYR:OH	2:A:239:LEU:HD22	2.20	0.41
2:A:231:TRP:CD2	2:B:235:ALA:HA	2.56	0.41
3:G:83:ASP:O	3:G:84:PHE:C	2.60	0.41
2:B:126:ILE:HD12	2:B:154:TRP:CB	2.51	0.40
3:I:125:GLN:HG3	4:H:131:PHE:CE2	2.56	0.40
4:H:14:PRO:HD3	4:H:122:SER:N	2.35	0.40
2:A:149:ARG:HD3	2:A:263:GLU:HG2	2.04	0.40
2:A:169:LEU:HD12	2:A:169:LEU:HA	1.83	0.40
2:C:192:PHE:HB3	2:C:265:LEU:HD22	2.03	0.40
3:G:60:PRO:C	3:G:62:ARG:N	2.74	0.40
4:H:154:TYR:O	4:H:184:LEU:HB3	2.21	0.40
1:R:104:ARG:HD2	1:R:122:ASP:OD2	2.21	0.40
1:T:84:CYS:HB2	2:C:134:ASN:HD21	1.86	0.40
4:F:147:LEU:HB2	4:F:148:GLY:H	1.63	0.40
3:I:110:THR:O	3:I:111:VAL:C	2.58	0.40
3:I:199:HIS:HB3	3:I:202:LEU:HD12	2.04	0.40
4:D:56:SER:OG	4:D:58:THR:CG2	2.69	0.40
4:H:13:LYS:O	4:H:16:GLN:N	2.54	0.40
4:H:71:ILE:HA	4:H:81:SER:O	2.21	0.40
1:R:55:ASN:OD1	1:R:57:LEU:HB2	2.20	0.40
2:A:164:LEU:HD13	2:A:168:HIS:HA	2.02	0.40
2:B:154:TRP:CZ3	2:B:274:PHE:HA	2.57	0.40
2:C:122:VAL:HA	2:C:165:SER:O	2.21	0.40
3:G:132:SER:HA	3:G:180:LEU:O	2.21	0.40
3:I:12:SER:HA	3:I:106:GLU:O	2.22	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)
3:E:17:GLU:OE1	3:E:17:GLU:OE1[12_545]	2.18	0.02

## 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	R	106/126 (84%)	98 (92%)	6 (6%)	2 (2%)	6	29
1	S	104/126 (82%)	90 (86%)	13 (12%)	1 (1%)	13	42
1	T	105/126 (83%)	89 (85%)	13 (12%)	3 (3%)	3	22
2	A	151/168 (90%)	129 (85%)	16 (11%)	6 (4%)	2	16
2	B	151/168 (90%)	133 (88%)	14 (9%)	4 (3%)	4	23
2	C	151/168 (90%)	132 (87%)	14 (9%)	5 (3%)	3	19
3	E	212/215 (99%)	181 (85%)	23 (11%)	8 (4%)	2	17
3	G	212/215 (99%)	177 (84%)	25 (12%)	10 (5%)	2	13
3	I	212/215 (99%)	178 (84%)	20 (9%)	14 (7%)	1	7
4	D	214/224 (96%)	175 (82%)	26 (12%)	13 (6%)	1	9
4	F	210/224 (94%)	167 (80%)	28 (13%)	15 (7%)	1	7
4	H	211/224 (94%)	162 (77%)	32 (15%)	17 (8%)	1	5
All	All	2039/2199 (93%)	1711 (84%)	230 (11%)	98 (5%)	2	12

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	119	PRO
2	A	130	ARG
2	A	161	HIS
2	B	198	GLU
2	C	158	ARG
3	E	94	SER
3	E	139	ASN

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Mol	Chain	Res	Type
3	E	141	TYR
3	E	212	ARG
4	D	66	LYS
4	D	105	TYR
4	D	165	SER
3	G	84	PHE
3	G	141	TYR
4	F	32	GLY
4	F	66	LYS
4	F	156	PRO
4	F	157	GLU
3	I	30	SER
3	I	83	ASP
3	I	139	ASN
3	I	141	TYR
3	I	172	SER
4	H	31	SER
4	H	43	PRO
4	H	66	LYS
4	H	67	SER
4	H	87	VAL
4	H	105	TYR
4	H	155	PHE
4	H	187	LEU
1	R	68	SER
1	T	97	PRO
2	A	157	SER
2	A	194	GLU
2	A	197	LYS
2	B	161	HIS
2	C	130	ARG
2	C	133	SER
2	C	161	HIS
2	C	233	LYS
3	E	31	ARG
4	D	32	GLY
4	D	135	PRO
3	G	31	ARG
3	G	61	ASP
3	G	83	ASP
3	G	139	ASN
4	F	15	SER

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Mol	Chain	Res	Type
4	F	105	TYR
4	F	153	ASP
4	F	164	ASN
3	I	31	ARG
4	H	102	GLY
1	T	122	ASP
2	A	198	GLU
2	B	217	PRO
3	E	159	ASN
4	D	78	LYS
4	D	107	TYR
4	D	158	PRO
3	G	16	GLY
3	G	94	SER
3	G	163	SER
4	F	106	TYR
3	I	53	SER
3	I	159	ASN
1	T	25	GLU
4	D	43	PRO
4	D	164	ASN
3	G	159	ASN
4	F	31	SER
4	F	76	SER
4	F	194	PRO
4	F	198	LEU
3	I	52	ALA
3	I	171	ASP
2	B	215	SER
4	D	106	TYR
4	F	122	SER
3	I	77	SER
4	H	45	LYS
4	H	63	PRO
4	H	103	GLY
4	D	211	PRO
4	F	102	GLY
4	H	198	LEU
3	E	158	GLY
3	I	111	VAL
4	H	32	GLY
4	D	157	GLU

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Mol	Chain	Res	Type
4	H	26	GLY
4	H	176	PRO
1	R	96	SER
3	I	205	PRO
3	I	121	PRO
4	H	199	GLY
3	E	205	PRO

### 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	R	99/114 (87%)	90 (91%)	9 (9%)	7	27
1	S	97/114 (85%)	82 (84%)	15 (16%)	2	10
1	T	98/114 (86%)	87 (89%)	11 (11%)	5	19
2	A	137/149 (92%)	120 (88%)	17 (12%)	4	16
2	B	136/149 (91%)	117 (86%)	19 (14%)	3	13
2	C	137/149 (92%)	118 (86%)	19 (14%)	3	13
3	E	179/185 (97%)	161 (90%)	18 (10%)	6	23
3	G	178/185 (96%)	152 (85%)	26 (15%)	2	12
3	I	178/185 (96%)	152 (85%)	26 (15%)	2	12
4	D	181/192 (94%)	143 (79%)	38 (21%)	1	4
4	F	175/192 (91%)	147 (84%)	28 (16%)	2	9
4	H	178/192 (93%)	142 (80%)	36 (20%)	1	4
All	All	1773/1920 (92%)	1511 (85%)	262 (15%)	2	11

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	45	LYS
1	R	87	GLU
1	R	98	GLU

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Mol	Chain	Res	Type
1	R	101	ARG
1	R	104	ARG
1	R	105	THR
1	R	116	ASP
1	R	117	CYS
1	R	128	LYS
1	S	21	SER
1	S	34	ILE
1	S	39	ARG
1	S	43	SER
1	S	49	ASP
1	S	58	LEU
1	S	73	LEU
1	S	81	ASN
1	S	82	THR
1	S	93	GLU
1	S	105	THR
1	S	112	VAL
1	S	117	CYS
1	S	118	THR
1	S	126	VAL
1	T	34	ILE
1	T	43	SER
1	T	45	LYS
1	T	65	ARG
1	T	80	ARG
1	T	82	THR
1	T	105	THR
1	T	114	VAL
1	T	117	CYS
1	T	118	THR
1	T	124	GLU
2	A	121	ARG
2	A	130	ARG
2	A	135	THR
2	A	145	LYS
2	A	158	ARG
2	A	170	ARG
2	A	186	SER
2	A	194	GLU
2	A	202	ASN
2	A	203	ASP

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Mol	Chain	Res	Type
2	A	213	TYR
2	A	227	ARG
2	A	232	SER
2	A	241	SER
2	A	247	ILE
2	A	251	LYS
2	A	256	ILE
2	B	120	GLN
2	B	121	ARG
2	B	130	ARG
2	B	132	ARG
2	B	158	ARG
2	B	161	HIS
2	B	163	PHE
2	B	170	ARG
2	B	171	ASN
2	B	178	GLU
2	B	179	LYS
2	B	195	GLU
2	B	198	GLU
2	B	213	TYR
2	B	214	THR
2	B	216	TYR
2	B	227	ARG
2	B	228	ASN
2	B	263	GLU
2	C	120	GLN
2	C	121	ARG
2	C	127	THR
2	C	134	ASN
2	C	135	THR
2	C	145	LYS
2	C	155	GLU
2	C	159	SER
2	C	162	SER
2	C	170	ARG
2	C	179	LYS
2	C	188	THR
2	C	227[A]	ARG
2	C	227[B]	ARG
2	C	232	SER
2	C	241	SER

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Mol	Chain	Res	Type
2	C	263	GLU
2	C	267	ASP
2	C	273	SER
3	E	5	THR
3	E	12	SER
3	E	20	THR
3	E	48	LEU
3	E	61	ASP
3	E	70	THR
3	E	75	THR
3	E	91	GLN
3	E	101	GLN
3	E	109	ARG
3	E	128	SER
3	E	130	THR
3	E	133	VAL
3	E	141	TYR
3	E	159	ASN
3	E	171	ASP
3	E	181	THR
3	E	182	LEU
4	D	1	GLN
4	D	7	SER
4	D	15	SER
4	D	18	LEU
4	D	21	THR
4	D	30	SER
4	D	31	SER
4	D	33	ASP
4	D	37	SER
4	D	45	LYS
4	D	55	ASN
4	D	58	THR
4	D	60	TYR
4	D	62	ASN
4	D	70	THR
4	D	71	ILE
4	D	73	VAL
4	D	78	LYS
4	D	81	SER
4	D	83	ARG
4	D	84	LEU

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Mol	Chain	Res	Type
4	D	86	SER
4	D	88	THR
4	D	109	MET
4	D	114	GLN
4	D	116	THR
4	D	117	THR
4	D	125	THR
4	D	147	LEU
4	D	154	TYR
4	D	155	PHE
4	D	161	VAL
4	D	178	VAL
4	D	187	LEU
4	D	195	SER
4	D	197	SER
4	D	202	THR
4	D	206	ASN
3	G	1	GLU
3	G	5	THR
3	G	12	SER
3	G	14	SER
3	G	20	THR
3	G	21	LEU
3	G	30	SER
3	G	47	LEU
3	G	55	ARG
3	G	64	SER
3	G	68	SER
3	G	71	ASP
3	G	75	THR
3	G	90	GLN
3	G	91	GLN
3	G	92	PHE
3	G	101	GLN
3	G	107	ILE
3	G	109	ARG
3	G	110	THR
3	G	138	ASN
3	G	141	TYR
3	G	152	ASP
3	G	157	SER
3	G	159	ASN

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Mol	Chain	Res	Type
3	G	209	SER
4	F	1	GLN
4	F	7	SER
4	F	17	THR
4	F	21	THR
4	F	23	THR
4	F	28	SER
4	F	29	ILE
4	F	30	SER
4	F	34	TYR
4	F	37	SER
4	F	45	LYS
4	F	52	HIS
4	F	62	ASN
4	F	70	THR
4	F	73	VAL
4	F	75	THR
4	F	78	LYS
4	F	81	SER
4	F	84	LEU
4	F	114	GLN
4	F	117	THR
4	F	124	SER
4	F	125	THR
4	F	126	LYS
4	F	147	LEU
4	F	165	SER
4	F	202	THR
4	F	221	GLU
3	I	20	THR
3	I	22	SER
3	I	34	LEU
3	I	54	SER
3	I	57	THR
3	I	75	THR
3	I	78	ARG
3	I	86	VAL
3	I	90	GLN
3	I	91	GLN
3	I	94	SER
3	I	98	THR
3	I	107	ILE

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Mol	Chain	Res	Type
3	I	108	LYS
3	I	110	THR
3	I	111	VAL
3	I	115	SER
3	I	138	ASN
3	I	141	TYR
3	I	160	SER
3	I	162	GLU
3	I	169	SER
3	I	198	THR
3	I	200	GLN
3	I	209	SER
3	I	211	ASN
4	H	13	LYS
4	H	16	GLN
4	H	17	THR
4	H	21	THR
4	H	25	SER
4	H	29	ILE
4	H	31	SER
4	H	33	ASP
4	H	37	SER
4	H	42	LEU
4	H	45	LYS
4	H	47	LEU
4	H	58	THR
4	H	60	TYR
4	H	62	ASN
4	H	70	THR
4	H	75	THR
4	H	79	GLN
4	H	81	SER
4	H	82	LEU
4	H	86	SER
4	H	92	THR
4	H	101	ARG
4	H	105	TYR
4	H	109	MET
4	H	114	GLN
4	H	117	THR
4	H	119	THR
4	H	121	SER

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Mol	Chain	Res	Type
4	H	125	THR
4	H	131	PHE
4	H	160	THR
4	H	161	VAL
4	H	200	THR
4	H	206	ASN
4	H	216	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	33	HIS
1	S	53	HIS
1	S	81	ASN
1	T	33	HIS
1	T	48	GLN
2	A	161	HIS
2	A	228	ASN
2	A	253	ASN
2	A	262	ASN
2	A	264	HIS
2	A	270	HIS
2	B	134	ASN
2	B	193	GLN
2	B	208	GLN
2	B	228	ASN
2	B	253	ASN
2	B	262	ASN
2	B	270	HIS
2	C	134	ASN
2	C	193	GLN
2	C	208	GLN
2	C	228	ASN
2	C	253	ASN
3	E	6	GLN
3	E	43	GLN
3	E	91	GLN
3	E	138	ASN
3	E	148	GLN
3	E	159	ASN
3	E	161	GLN
3	E	199	HIS

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Mol	Chain	Res	Type
4	D	41	GLN
4	D	54	HIS
4	D	62	ASN
4	D	114	GLN
3	G	6	GLN
3	G	43	GLN
3	G	90	GLN
3	G	91	GLN
3	G	138	ASN
3	G	139	ASN
3	G	156	GLN
3	G	159	ASN
4	F	5	GLN
4	F	54	HIS
4	F	62	ASN
3	I	6	GLN
3	I	27	GLN
3	I	39	GLN
3	I	43	GLN
3	I	90	GLN
3	I	91	GLN
3	I	138	ASN
3	I	159	ASN
3	I	200	GLN
4	H	54	HIS
4	H	55	ASN
4	H	62	ASN
4	H	79	GLN
4	H	114	GLN
4	H	206	ASN
4	H	209	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	R	108/126 (85%)	0.10	4 (3%) 45 33	39, 71, 149, 167	0
1	S	106/126 (84%)	0.34	4 (3%) 44 33	49, 71, 152, 169	0
1	T	107/126 (84%)	0.43	7 (6%) 26 21	44, 72, 139, 168	0
2	A	155/168 (92%)	-0.09	10 (6%) 26 21	32, 55, 121, 202	0
2	B	155/168 (92%)	-0.10	4 (2%) 57 42	34, 51, 109, 164	0
2	C	154/168 (91%)	-0.10	8 (5%) 34 27	26, 54, 107, 181	1 (0%)
3	E	214/215 (99%)	-0.20	5 (2%) 61 46	28, 55, 103, 117	0
3	G	214/215 (99%)	0.57	24 (11%) 11 11	43, 94, 158, 175	0
3	I	214/215 (99%)	0.44	17 (7%) 20 18	28, 85, 140, 154	0
4	D	218/224 (97%)	-0.17	5 (2%) 61 46	36, 55, 94, 113	0
4	F	214/224 (95%)	0.52	18 (8%) 18 17	51, 92, 141, 166	0
4	H	215/224 (95%)	0.30	9 (4%) 41 31	29, 74, 113, 136	0
All	All	2074/2199 (94%)	0.17	115 (5%) 32 25	26, 68, 139, 202	1 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	135	CYS	5.8
3	G	136	LEU	4.7
2	B	159	SER	4.5
4	F	44	GLY	4.4
1	S	126	VAL	4.2
4	H	45	LYS	4.1
2	A	196	ILE	4.1
3	E	148	GLN	4.0
2	A	159	SER	4.0
4	F	132	PRO	3.7
2	C	196	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	43	PRO	3.7
2	B	157	SER	3.7
3	G	192	VAL	3.7
3	G	178	SER	3.6
3	I	115	SER	3.5
2	A	155	GLU	3.5
4	D	32	GLY	3.5
3	G	128	SER	3.4
2	A	160	GLY	3.4
3	G	117	PHE	3.4
1	S	32	HIS	3.4
2	A	156	SER	3.4
3	I	135	CYS	3.3
4	F	130	VAL	3.3
4	F	208	ASN	3.3
4	F	133	LEU	3.3
2	C	145	LYS	3.2
3	G	164	VAL	3.2
4	H	32	GLY	3.2
3	G	163	SER	3.2
1	T	21	SER	3.1
1	S	21	SER	3.1
3	I	117	PHE	3.1
2	A	119	PRO	3.1
4	D	136	SER	3.1
4	F	150	LEU	3.1
2	A	281	GLY	3.0
3	E	143	ARG	3.0
4	F	159	VAL	3.0
2	C	201	LYS	3.0
4	D	31	SER	3.0
3	I	191	LYS	3.0
3	I	155	LEU	3.0
2	C	159	SER	3.0
3	I	101	GLN	2.9
4	F	45	LYS	2.9
3	G	214	GLU	2.9
1	R	67	ASP	2.9
3	I	192	VAL	2.9
4	F	32	GLY	2.8
3	G	149	TRP	2.8
3	G	210	PHE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	119	PRO	2.8
3	E	144	GLU	2.8
3	I	181	THR	2.8
1	T	47	GLY	2.7
4	H	221	GLU	2.7
1	S	111	MET	2.7
1	T	84	CYS	2.7
3	I	84	PHE	2.6
3	G	160	SER	2.6
2	C	200	THR	2.6
1	R	126	VAL	2.6
4	H	201	GLN	2.6
3	G	161	GLN	2.6
3	E	190	HIS	2.5
4	F	198	LEU	2.5
4	H	46	GLY	2.5
4	D	45	LYS	2.5
3	G	118	ILE	2.5
2	A	199	ASN	2.5
4	H	57	GLY	2.5
2	B	119	PRO	2.5
3	I	136	LEU	2.5
4	H	192	THR	2.5
1	R	21	SER	2.5
4	F	220	VAL	2.5
2	A	145	LYS	2.4
4	F	158	PRO	2.4
2	A	161	HIS	2.3
3	G	197	VAL	2.3
4	H	220	VAL	2.3
3	G	191	LYS	2.3
3	G	130	THR	2.3
4	F	144	THR	2.3
4	F	204	ILE	2.3
2	C	199	ASN	2.3
1	T	32	HIS	2.3
3	G	116	VAL	2.3
4	F	31	SER	2.3
1	R	95	ASP	2.2
1	T	127	HIS	2.2
3	I	109	ARG	2.2
4	H	133	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	78	ARG	2.2
1	T	23	PRO	2.2
3	G	126	LEU	2.2
1	T	46	TYR	2.2
3	I	195	CYS	2.2
4	F	145	ALA	2.2
4	F	128	PRO	2.2
3	I	198	THR	2.2
2	B	160	GLY	2.1
4	D	67	SER	2.1
3	G	131	ALA	2.1
3	G	206	VAL	2.1
3	I	110	THR	2.1
3	E	139	ASN	2.1
2	C	160	GLY	2.1
3	I	134	VAL	2.1
3	G	122	SER	2.0
3	I	210	PHE	2.0
3	I	149	TRP	2.0
3	G	155	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	ZN	A	301	1/1	0.99	0.02	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.