



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:06 AM BST

PDB ID : 6RUT
Title : Mycoplasma Genitalium Heterodimer Nap Complex (P140-P110 globular)
Authors : Fita, I.; Aparicio, D.
Deposited on : 2019-05-29
Resolution : 2.65 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

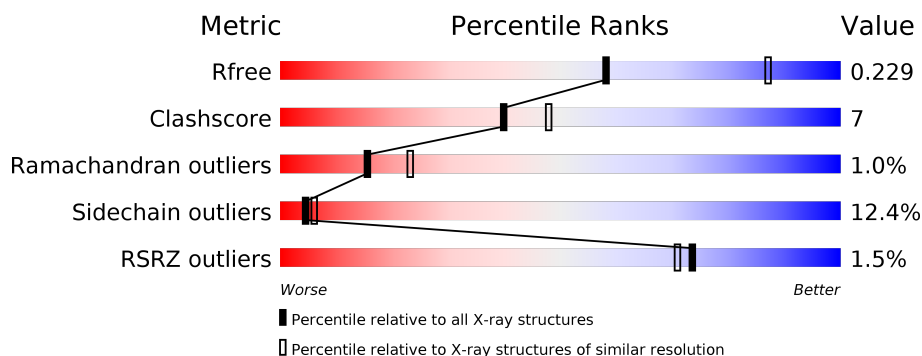
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 ≥ 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	A	802	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 79% 16% • • </div> </div>
1	C	802	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 77% 17% • • </div> </div>
1	E	802	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 79% 16% • • </div> </div>
1	G	802	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 78% 17% • • </div> </div>
2	B	1334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 69% 22% • 5% </div> </div>
2	D	1334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 69% 22% • 5% </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	1334	<div><div><div>3%</div><div>67%</div><div>22%</div><div>6%</div></div></div>
2	H	1334	<div><div><div>3%</div><div>67%</div><div>23%</div><div>7%</div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 64181 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6013	3758	1009	1240	6			
1	C	779	Total	C	N	O	S	0	0	0
			5999	3751	1006	1236	6			
1	E	783	Total	C	N	O	S	0	0	0
			6017	3760	1010	1241	6			
1	G	784	Total	C	N	O	S	0	0	0
			6023	3763	1011	1243	6			

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1268	Total	C	N	O	S	0	0	0
			9938	6303	1679	1942	14			
2	D	1265	Total	C	N	O	S	0	0	0
			9918	6293	1676	1935	14			
2	F	1250	Total	C	N	O	S	0	0	0
			9822	6242	1658	1909	13			
2	H	1247	Total	C	N	O	S	0	0	0
			9798	6228	1654	1903	13			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	121	Total	O	0	0
			121	121		
3	C	87	Total	O	0	0
			87	87		
3	D	137	Total	O	0	0
			137	137		

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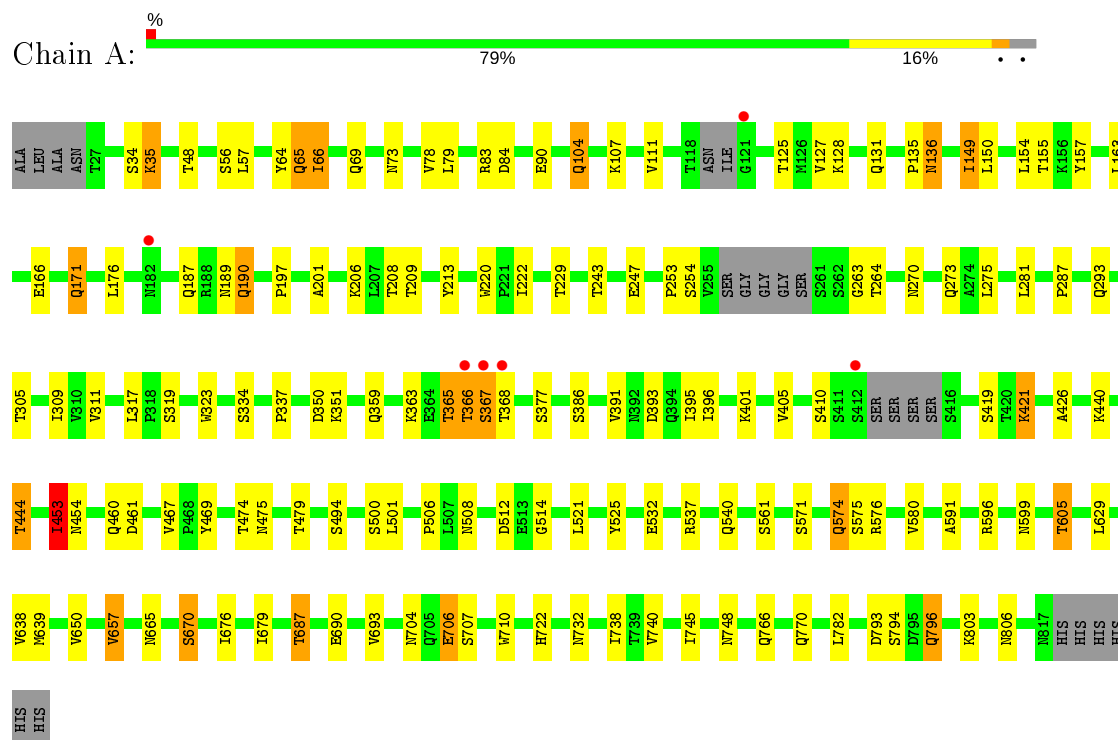
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	69	Total 69	O 69	0	0
3	F	70	Total 70	O 70	0	0
3	G	49	Total 49	O 49	0	0
3	H	58	Total 58	O 58	0	0

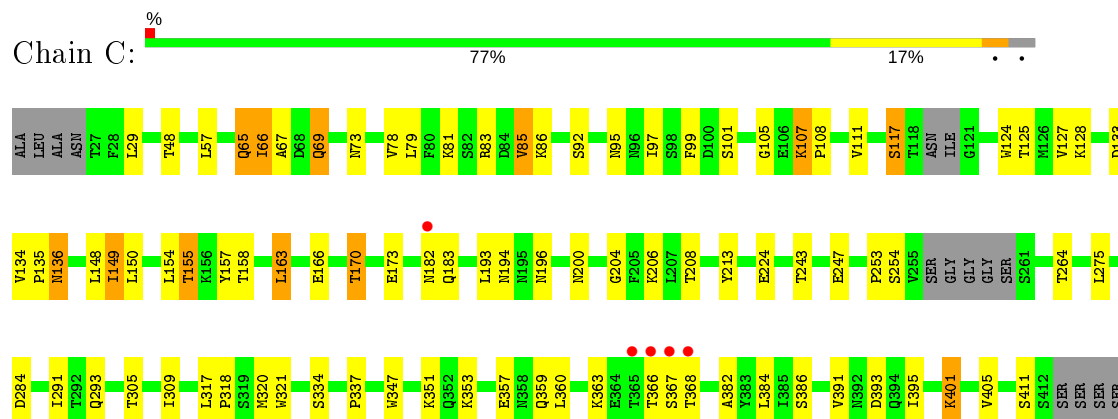
3 Residue-property plots [i](#)

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: Mgp-operon protein 3



• Molecule 1: Mgp-operon protein 3

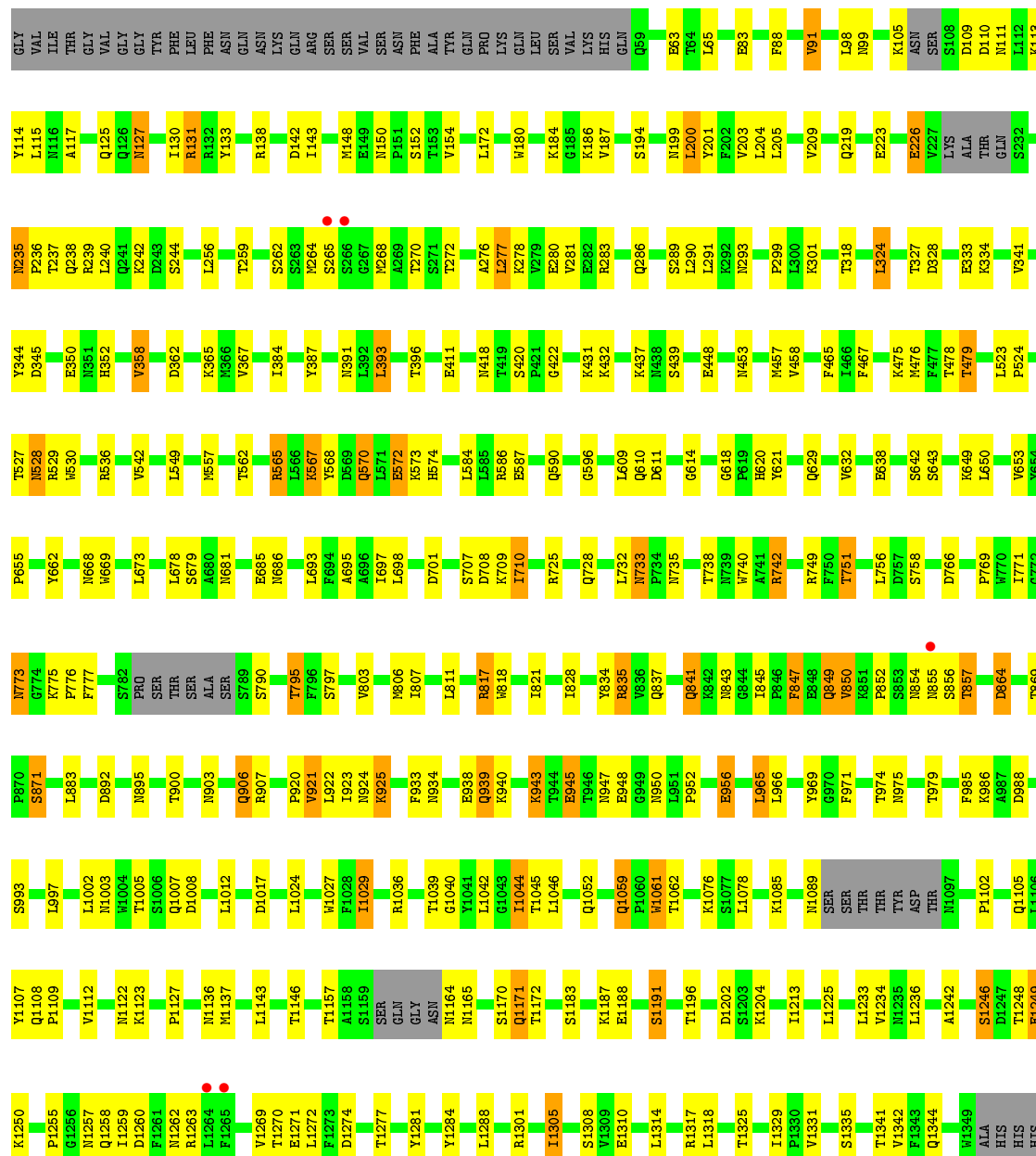




HIS
HIS
HIS

• Molecule 2: Adhesin P1

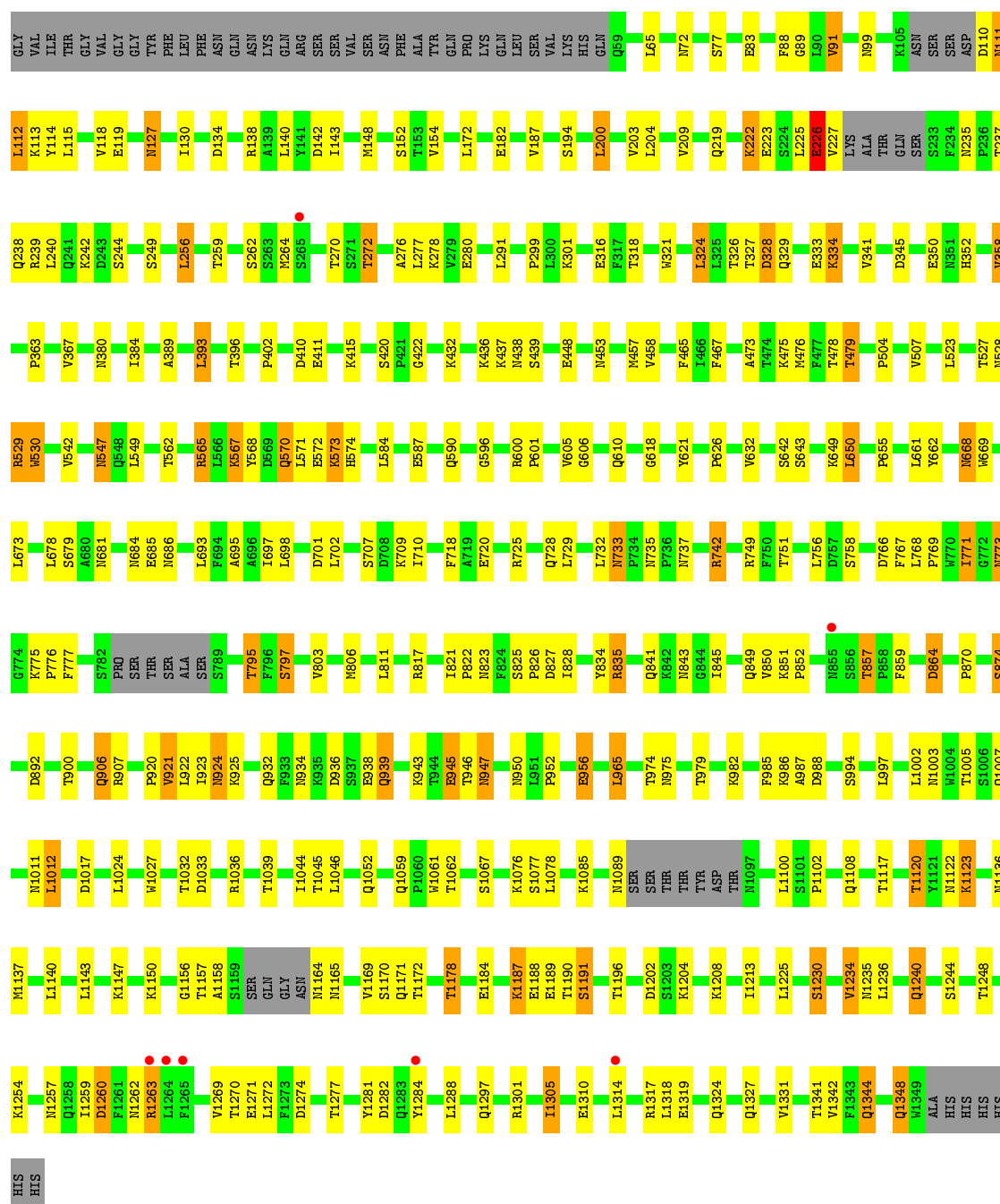
Chain B:  69% 22% 5%



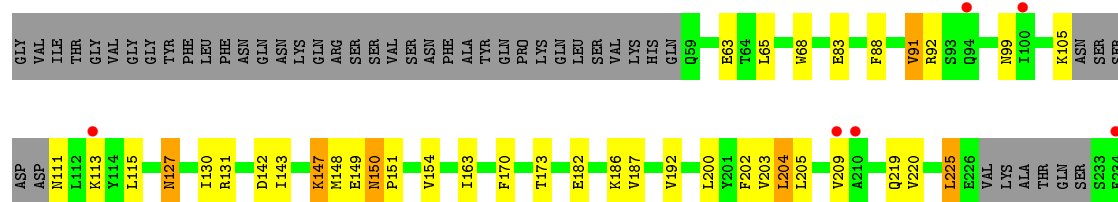
HIS
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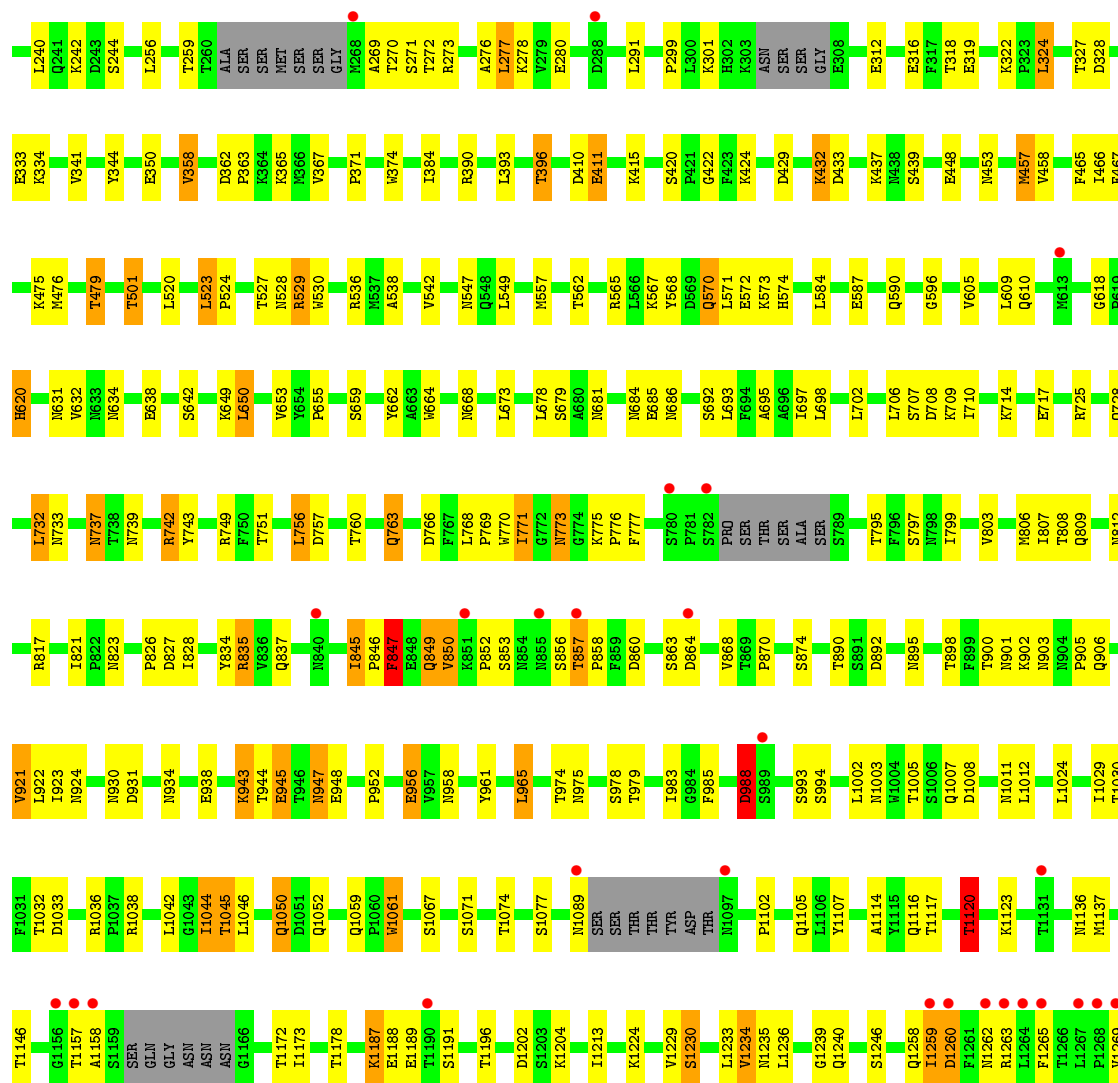
• Molecule 2: Adhesin P1

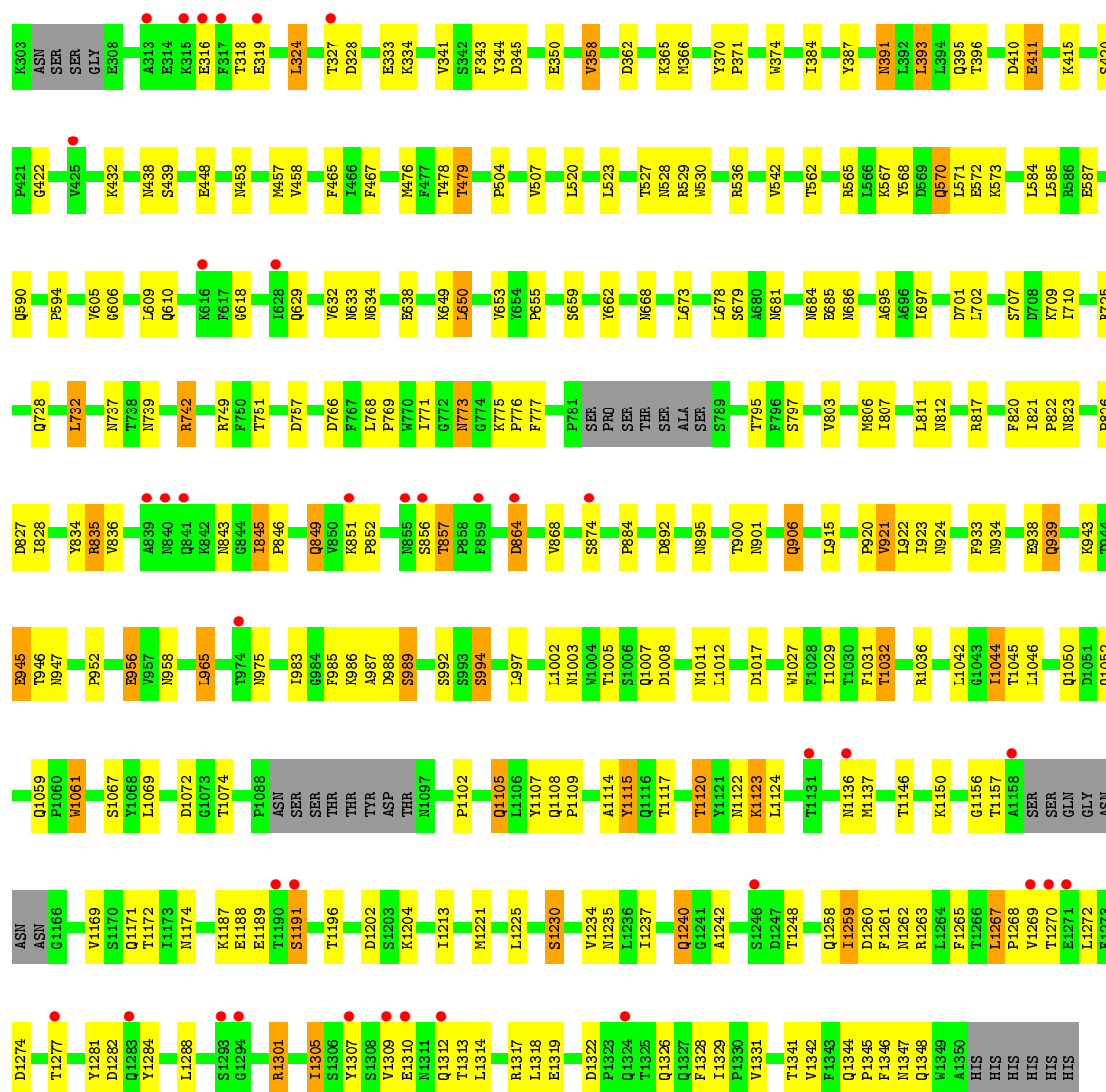
Chain D:  69% 22% 5%



• Molecule 2: Adhesin P1







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.00Å 157.28Å 192.37Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	121.66 – 2.65 150.67 – 2.65	Depositor EDS
% Data completeness (in resolution range)	73.2 (121.66-2.65) 73.3 (150.67-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.187 , 0.224 0.199 , 0.229	Depositor DCC
R_{free} test set	9457 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	64181	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.48	0/6136	0.74	0/8340
1	C	0.48	0/6122	0.74	0/8321
1	E	0.47	0/6141	0.74	0/8347
1	G	0.48	0/6147	0.74	1/8355 (0.0%)
2	B	0.50	0/10187	0.76	1/13863 (0.0%)
2	D	0.49	0/10167	0.76	4/13836 (0.0%)
2	F	0.46	0/10069	0.73	2/13701 (0.0%)
2	H	0.48	1/10044 (0.0%)	0.72	2/13668 (0.0%)
All	All	0.48	1/65013 (0.0%)	0.74	10/88431 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1115	TYR	CA-C	7.32	1.72	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1165	ASN	C-N-CA	7.25	137.53	122.30
2	H	989	SER	CA-CB-OG	-5.95	95.13	111.20
2	D	530	TRP	N-CA-C	-5.77	95.43	111.00
1	G	367	SER	C-N-CA	5.75	136.09	121.70
2	B	856	SER	C-N-CA	5.64	135.79	121.70
2	H	856	SER	C-N-CA	5.36	135.10	121.70
2	F	538	ALA	N-CA-C	-5.31	96.66	111.00
2	D	225	LEU	C-N-CA	5.18	134.65	121.70
2	F	1120	THR	CB-CA-C	-5.12	97.79	111.60
2	D	226	GLU	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

There are no planarity outliers.

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	6013	0	5805	61	0
1	C	5999	0	5794	71	0
1	E	6017	0	5809	62	0
1	G	6023	0	5814	90	0
2	B	9938	0	9645	145	0
2	D	9918	0	9631	163	0
2	F	9822	0	9548	155	0
2	H	9798	0	9529	199	0
3	A	62	0	0	0	0
3	B	121	0	0	2	0
3	C	87	0	0	0	0
3	D	137	0	0	5	0
3	E	69	0	0	0	0
3	F	70	0	0	1	0
3	G	49	0	0	0	0
3	H	58	0	0	2	0
All	All	64181	0	61575	915	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (915) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:812:ASP:OD2	1:G:815:LEU:CD1	1.72	1.35
1:G:255:VAL:HG23	1:G:726:GLN:HB3	1.19	1.11
1:G:812:ASP:OD2	1:G:815:LEU:HD13	1.36	1.09
1:G:812:ASP:OD2	1:G:815:LEU:HD12	1.54	1.06
1:G:460:GLN:CA	2:H:812:ASN:HD21	1.68	1.05
1:E:73:ASN:HD21	1:E:327:ARG:HH22	1.05	1.01
1:G:460:GLN:N	2:H:812:ASN:HD21	1.57	1.01
2:H:989:SER:OG	2:H:1115:TYR:CA	2.08	1.01
1:C:66:ILE:HD11	1:C:69:GLN:HG3	1.43	0.99
2:B:527:THR:HG23	2:B:678:LEU:HD23	1.46	0.97
2:H:989:SER:CB	2:H:1115:TYR:O	2.13	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:ASP:OD1	2:B:614:GLY:HA2	1.66	0.96
1:G:255:VAL:HG22	1:G:261:SER:HB2	1.49	0.95
1:C:440:LYS:O	1:C:444:THR:HG23	1.72	0.90
1:E:66:ILE:HD11	1:E:69:GLN:HG3	1.53	0.90
2:B:280:GLU:HG3	2:B:650:LEU:HD12	1.55	0.89
2:D:685:GLU:HG3	2:D:686:ASN:H	1.37	0.88
1:G:460:GLN:HA	2:H:812:ASN:HD21	1.38	0.87
1:G:460:GLN:CA	2:H:812:ASN:ND2	2.37	0.87
2:H:1265:PHE:HA	2:H:1312:GLN:NE2	1.89	0.86
2:F:1344:GLN:HG3	2:F:1348:GLN:HB3	1.57	0.86
2:D:852:PRO:HB2	2:D:857:THR:HG22	1.57	0.84
2:H:527:THR:HG23	2:H:678:LEU:HD23	1.59	0.84
2:H:1301:ARG:HG3	2:H:1301:ARG:HH21	1.39	0.84
1:E:540:GLN:HG2	1:E:579:PRO:HA	1.58	0.84
1:G:460:GLN:HA	2:H:812:ASN:ND2	1.93	0.83
2:H:1265:PHE:HB3	2:H:1312:GLN:HE21	1.44	0.83
2:H:318:THR:HG23	2:H:319:GLU:H	1.42	0.82
1:A:440:LYS:O	1:A:444:THR:HG23	1.80	0.82
1:G:66:ILE:HD11	1:G:69:GLN:HG3	1.62	0.82
2:H:1267:LEU:H	2:H:1267:LEU:HD12	1.44	0.82
1:G:749:GLN:HA	1:G:749:GLN:HE21	1.46	0.81
2:H:989:SER:OG	2:H:1115:TYR:C	2.18	0.81
1:G:540:GLN:HG2	1:G:579:PRO:HA	1.63	0.81
2:D:1344:GLN:HG3	2:D:1348:GLN:HB3	1.63	0.80
1:G:652:THR:HG21	1:G:657:VAL:CG1	2.11	0.80
2:D:1301:ARG:HG3	2:D:1301:ARG:HH21	1.45	0.79
2:H:1265:PHE:CA	2:H:1312:GLN:NE2	2.45	0.78
2:F:1005:THR:HG22	2:F:1007:GLN:H	1.49	0.78
2:B:524:PRO:HD2	2:B:557:MET:CE	2.14	0.78
1:G:255:VAL:CG2	1:G:261:SER:HB2	2.12	0.78
2:B:766:ASP:OD2	2:B:797:SER:HB3	1.84	0.78
2:H:989:SER:HB3	2:H:1115:TYR:O	1.84	0.77
2:D:527:THR:HG23	2:D:678:LEU:HD23	1.66	0.77
2:F:988:ASP:OD2	2:F:993:SER:HB2	1.85	0.77
2:F:527:THR:HG23	2:F:678:LEU:HD23	1.67	0.76
1:G:255:VAL:CG2	1:G:726:GLN:HB3	2.10	0.76
2:B:1305:ILE:HD11	2:B:1317:ARG:HB3	1.68	0.76
2:F:1301:ARG:HG3	2:F:1301:ARG:HH21	1.49	0.76
2:D:766:ASP:OD2	2:D:797:SER:HB3	1.86	0.76
1:A:66:ILE:HD12	1:A:78:VAL:HG13	1.67	0.75
2:F:845:ILE:HG23	2:F:849:GLN:OE1	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:HB2	1:A:599:ASN:ND2	2.01	0.75
2:H:852:PRO:HB2	2:H:857:THR:HG22	1.67	0.75
1:A:366:THR:HG22	1:A:494:SER:HA	1.65	0.75
1:G:460:GLN:N	2:H:812:ASN:ND2	2.35	0.75
2:H:845:ILE:HG21	2:H:849:GLN:OE1	1.85	0.75
2:B:924:ASN:HB2	2:B:985:PHE:HA	1.69	0.75
2:D:1254:LYS:HB3	2:D:1259:ILE:CD1	2.16	0.74
2:D:695:ALA:HB3	2:D:751:THR:HG22	1.68	0.74
2:H:989:SER:OG	2:H:1115:TYR:CB	2.36	0.74
1:A:596:ARG:HB2	1:A:599:ASN:HD22	1.53	0.74
2:B:988:ASP:OD1	2:B:993:SER:HB2	1.88	0.74
2:D:1005:THR:HG22	2:D:1007:GLN:H	1.51	0.74
1:E:65:GLN:HE22	1:E:83:ARG:HG3	1.51	0.74
2:B:524:PRO:HD2	2:B:557:MET:HE2	1.70	0.74
2:B:65:LEU:HB3	2:B:91:VAL:HG13	1.70	0.73
2:H:989:SER:OG	2:H:1115:TYR:O	2.04	0.73
1:G:66:ILE:HD11	1:G:69:GLN:CG	2.18	0.73
1:C:66:ILE:HD11	1:C:69:GLN:CG	2.16	0.73
1:G:652:THR:HG21	1:G:657:VAL:HG12	1.71	0.73
2:F:773:ASN:HD22	2:F:775:LYS:HB2	1.52	0.72
1:G:652:THR:CG2	1:G:657:VAL:CG1	2.66	0.72
1:A:136:ASN:H	1:A:136:ASN:HD22	1.36	0.72
2:H:989:SER:OG	2:H:1115:TYR:HB2	1.90	0.72
2:H:1265:PHE:CB	2:H:1312:GLN:HE21	2.03	0.72
1:G:73:ASN:HD21	1:G:327:ARG:HH22	1.37	0.72
1:G:66:ILE:HD12	1:G:78:VAL:HG13	1.72	0.71
2:H:989:SER:OG	2:H:1115:TYR:N	2.22	0.71
1:A:65:GLN:HE22	1:A:83:ARG:HG3	1.55	0.71
2:F:763:GLN:HE22	2:F:799:ILE:HD13	1.56	0.71
2:B:1269:VAL:HA	2:B:1272:LEU:HD12	1.73	0.71
2:H:100:ILE:O	2:H:103:VAL:HG22	1.91	0.71
2:F:1305:ILE:HD11	2:F:1317:ARG:HB3	1.73	0.71
2:F:857:THR:HG23	2:F:858:PRO:HD2	1.72	0.71
2:H:65:LEU:HB3	2:H:91:VAL:HG13	1.71	0.71
2:F:150:ASN:H	2:F:151:PRO:HD3	1.54	0.70
2:H:138:ARG:HG2	2:H:1242:ALA:HB1	1.73	0.70
2:D:850:VAL:CG2	2:D:859:PHE:HB3	2.20	0.70
2:D:773:ASN:HD21	2:D:975:ASN:HB3	1.55	0.70
2:D:773:ASN:HD22	2:D:775:LYS:HB2	1.55	0.70
2:D:685:GLU:HG3	2:D:686:ASN:N	2.07	0.70
2:F:278:LYS:HB2	2:F:650:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:773:ASN:HD21	2:F:975:ASN:HB3	1.57	0.69
2:D:1254:LYS:HB3	2:D:1259:ILE:HD11	1.75	0.69
2:B:773:ASN:HD22	2:B:775:LYS:HB2	1.56	0.69
1:C:454:ASN:ND2	1:C:467:VAL:H	1.91	0.69
1:C:65:GLN:HE22	1:C:83:ARG:HG3	1.58	0.69
2:H:1005:THR:HG22	2:H:1007:GLN:H	1.57	0.68
2:H:845:ILE:HG23	2:H:849:GLN:NE2	2.09	0.68
1:E:410:SER:HB2	1:E:421:LYS:HG3	1.75	0.68
2:F:362:ASP:HB3	2:F:365:LYS:HG2	1.76	0.68
2:H:845:ILE:CG2	2:H:849:GLN:HE22	2.06	0.68
2:H:1265:PHE:CA	2:H:1312:GLN:HE21	2.04	0.68
1:C:808:LEU:HD11	2:D:702:LEU:HD12	1.76	0.67
2:D:835:ARG:HD3	2:D:845:ILE:HG21	1.75	0.67
2:D:946:THR:HA	2:D:1120:THR:CG2	2.24	0.67
1:G:410:SER:HB2	1:G:421:LYS:HG3	1.75	0.67
2:F:1230:SER:HB3	2:F:1235:ASN:ND2	2.09	0.67
2:H:103:VAL:HG21	2:H:118:VAL:HG22	1.75	0.67
1:A:155:THR:HG22	1:A:157:TYR:H	1.58	0.67
2:B:262:SER:HB2	2:B:643:SER:HB3	1.77	0.67
2:B:1246:SER:O	2:B:1249:GLU:OE2	2.12	0.67
1:E:73:ASN:ND2	1:E:327:ARG:HH22	1.85	0.67
2:F:127:ASN:HD21	2:F:147:LYS:HE3	1.60	0.67
1:G:704:ASN:HB3	1:G:707:SER:HB2	1.76	0.67
1:C:596:ARG:HB2	1:C:599:ASN:ND2	2.10	0.66
2:D:226:GLU:HG2	2:D:239:ARG:HH21	1.59	0.66
2:H:1265:PHE:HA	2:H:1312:GLN:HE22	1.58	0.66
1:C:454:ASN:HD22	1:C:467:VAL:H	1.42	0.66
2:D:65:LEU:HB3	2:D:91:VAL:HG13	1.78	0.66
1:G:766:GLN:O	2:H:742:ARG:HD2	1.95	0.65
2:F:1003:ASN:HB3	2:F:1102:PRO:HG2	1.77	0.65
2:F:424:LYS:HG2	2:F:433:ASP:HA	1.76	0.65
2:D:226:GLU:HG2	2:D:239:ARG:NH2	2.11	0.65
2:H:422:GLY:HA2	2:H:439:SER:OG	1.97	0.65
2:F:857:THR:HG23	2:F:858:PRO:CD	2.27	0.65
2:H:1305:ILE:HD11	2:H:1317:ARG:HB3	1.78	0.64
2:B:1109:PRO:HB3	2:B:1137:MET:HE1	1.78	0.64
2:B:527:THR:HG23	2:B:678:LEU:CD2	2.24	0.64
2:B:835:ARG:HD3	2:B:845:ILE:HG21	1.80	0.64
2:H:131:ARG:HB2	2:H:142:ASP:OD1	1.96	0.64
2:F:924:ASN:HB2	2:F:985:PHE:HA	1.78	0.64
1:G:347:TRP:HH2	1:G:401:LYS:HG3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1265:PHE:HB3	2:H:1312:GLN:NE2	2.10	0.64
2:D:822:PRO:HB2	2:D:1189:GLU:HB2	1.80	0.64
2:F:341:VAL:HG22	2:F:358:VAL:HB	1.80	0.64
2:H:366:MET:HG3	2:H:370:TYR:HE1	1.61	0.63
2:H:845:ILE:CG2	2:H:849:GLN:NE2	2.61	0.63
1:G:652:THR:CG2	1:G:657:VAL:HG12	2.28	0.63
1:A:687:THR:HG23	1:A:690:GLU:OE1	1.98	0.63
2:D:223:GLU:HG3	2:D:478:THR:OG1	1.98	0.63
2:H:280:GLU:HG3	2:H:650:LEU:HD12	1.79	0.63
2:H:114:TYR:CE2	2:H:217:ASN:ND2	2.67	0.62
1:E:574:GLN:HE21	1:E:575:SER:H	1.46	0.62
1:C:411:SER:H	1:C:421:LYS:HE3	1.63	0.62
2:B:341:VAL:HG22	2:B:358:VAL:HB	1.82	0.62
2:F:766:ASP:OD2	2:F:797:SER:HB3	1.99	0.62
2:B:921:VAL:HG13	2:B:965:LEU:HD13	1.81	0.62
1:A:104:GLN:OE1	1:A:104:GLN:HA	2.00	0.62
2:D:326:THR:OG1	2:D:329:GLN:HG3	1.99	0.62
1:G:661:PHE:CE1	1:G:668:LEU:HD23	2.35	0.62
2:D:65:LEU:HD21	2:D:127:ASN:HB3	1.82	0.62
2:F:244:SER:HB2	2:F:568:TYR:O	2.00	0.62
1:A:794:SER:H	1:A:796:GLN:HE22	1.48	0.61
2:H:1268:PRO:HB3	2:H:1309:VAL:HG13	1.80	0.61
2:H:366:MET:HG3	2:H:370:TYR:CE1	2.35	0.61
2:D:280:GLU:HG3	2:D:650:LEU:HD12	1.82	0.61
1:E:155:THR:HG23	1:E:157:TYR:H	1.64	0.61
2:F:1011:ASN:HD22	2:F:1067:SER:H	1.46	0.61
1:C:596:ARG:HB2	1:C:599:ASN:HD22	1.65	0.61
2:D:1269:VAL:HA	2:D:1272:LEU:HD12	1.83	0.61
2:F:280:GLU:HG3	2:F:650:LEU:HD12	1.81	0.61
2:F:901:ASN:HB3	2:F:958:ASN:HD21	1.66	0.61
2:H:773:ASN:HD22	2:H:775:LYS:HB2	1.64	0.61
2:B:1005:THR:HG22	2:B:1007:GLN:H	1.65	0.61
2:B:1248:THR:HB	2:B:1331:VAL:HG13	1.82	0.61
2:B:934:ASN:O	2:B:938:GLU:HB2	2.00	0.61
2:D:823:ASN:HD22	2:D:825:SER:H	1.48	0.61
2:H:822:PRO:HB2	2:H:1189:GLU:HB2	1.82	0.61
2:B:278:LYS:HB2	2:B:650:LEU:HD11	1.83	0.61
2:F:1269:VAL:HA	2:F:1272:LEU:HD12	1.82	0.61
2:F:837:GLN:HG3	2:F:846:PRO:HD2	1.83	0.61
2:H:1301:ARG:CG	2:H:1301:ARG:HH21	2.10	0.61
1:A:365:THR:O	1:A:367:SER:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ILE:HD12	1:C:78:VAL:HG13	1.83	0.60
2:D:226:GLU:HG3	2:D:239:ARG:NE	2.15	0.60
2:F:318:THR:HG23	2:F:319:GLU:H	1.65	0.60
2:H:114:TYR:HE2	2:H:217:ASN:ND2	1.98	0.60
2:H:924:ASN:HB2	2:H:985:PHE:HA	1.82	0.60
1:A:460:GLN:HG3	2:B:895:ASN:HB2	1.83	0.60
1:G:460:GLN:H	2:H:812:ASN:HD21	1.48	0.60
1:E:460:GLN:HA	2:F:812:ASN:OD1	2.01	0.60
1:C:405:VAL:HG11	1:C:426:ALA:HB2	1.84	0.60
1:C:766:GLN:O	2:D:742:ARG:HD2	2.02	0.60
1:A:187:GLN:O	1:A:190:GLN:HG2	2.02	0.59
1:E:346:ASP:HB3	1:E:573:THR:O	2.02	0.59
2:H:110:ASP:HA	2:H:220:VAL:HG13	1.83	0.59
2:D:262:SER:HB2	2:D:643:SER:HB3	1.84	0.59
1:C:318:PRO:HB3	1:C:382:ALA:HB1	1.84	0.59
2:F:276:ALA:HB2	2:F:655:PRO:HD3	1.85	0.59
2:H:845:ILE:HG23	2:H:849:GLN:HE22	1.65	0.59
2:H:989:SER:HA	2:H:1114:ALA:HB1	1.84	0.59
2:D:570:GLN:HG3	2:D:573:LYS:HE3	1.83	0.59
1:A:135:PRO:HB3	1:A:337:PRO:HG2	1.85	0.59
1:E:66:ILE:HD12	1:E:78:VAL:HG13	1.83	0.59
1:A:670:SER:HA	1:A:679:ILE:HG22	1.85	0.59
1:C:531:GLN:HE22	1:C:593:GLY:H	1.50	0.59
2:D:590:GLN:CD	2:D:906:GLN:HG2	2.23	0.59
2:B:807:ILE:HG21	2:B:828:ILE:HD12	1.85	0.59
1:G:460:GLN:HG3	2:H:895:ASN:HB2	1.84	0.59
1:A:166:GLU:HG3	1:A:206:LYS:HB2	1.85	0.59
2:B:237:THR:HG22	2:B:1108:GLN:HG3	1.85	0.59
2:F:115:LEU:HD11	2:F:324:LEU:HD22	1.83	0.59
2:D:341:VAL:HG22	2:D:358:VAL:HB	1.85	0.58
1:C:704:ASN:HB3	1:C:707:SER:HB2	1.84	0.58
1:G:386:SER:HB3	1:G:626:SER:OG	2.03	0.58
2:F:777:PHE:HB3	2:F:795:THR:CG2	2.33	0.58
1:C:525:TYR:CE1	1:C:591:ALA:HB1	2.39	0.58
2:D:1011:ASN:HD22	2:D:1067:SER:H	1.52	0.58
2:H:773:ASN:HD21	2:H:975:ASN:HB3	1.68	0.58
1:C:574:GLN:HE21	1:C:575:SER:H	1.51	0.58
2:D:1301:ARG:HG3	2:D:1301:ARG:NH2	2.18	0.58
2:F:1259:ILE:HG12	2:F:1260:ASP:H	1.69	0.58
2:F:65:LEU:HB3	2:F:91:VAL:HG13	1.86	0.58
2:H:115:LEU:HD11	2:H:324:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1255:PRO:HB2	2:B:1257:ASN:OD1	2.04	0.57
2:F:620:HIS:CD2	2:F:620:HIS:H	2.20	0.57
2:B:1260:ASP:OD2	2:B:1263:ARG:HB2	2.04	0.57
1:C:521:LEU:HD23	1:C:580:VAL:HG23	1.87	0.57
2:D:1305:ILE:HD11	2:D:1317:ARG:HB3	1.86	0.57
2:F:988:ASP:OD1	2:F:1114:ALA:HA	2.04	0.57
1:E:525:TYR:HE1	1:E:591:ALA:HB1	1.69	0.57
2:D:924:ASN:HB2	2:D:985:PHE:HA	1.85	0.57
2:H:742:ARG:HH11	2:H:742:ARG:HG2	1.70	0.57
2:D:244:SER:HB2	2:D:568:TYR:O	2.04	0.57
2:B:524:PRO:HD2	2:B:557:MET:HE1	1.85	0.57
2:B:268:MET:HB2	2:B:871:SER:OG	2.04	0.57
1:G:308:HIS:CD2	1:G:326:GLU:OE2	2.58	0.57
1:A:561:SER:HB3	2:D:1178:THR:HG21	1.87	0.56
2:D:1248:THR:HB	2:D:1331:VAL:HG13	1.85	0.56
2:B:226:GLU:HB2	2:B:239:ARG:CZ	2.35	0.56
2:F:1305:ILE:HD11	2:F:1317:ARG:CB	2.35	0.56
2:F:186:LYS:HB3	2:F:205:LEU:HB3	1.87	0.56
2:D:1027:TRP:CE3	2:D:1046:LEU:HB3	2.40	0.56
2:F:1029:ILE:HD11	2:F:1044:ILE:HG12	1.86	0.56
2:H:151:PRO:HG3	2:H:180:TRP:CE2	2.40	0.56
2:B:235:ASN:HD22	2:B:236:PRO:HD2	1.70	0.56
2:H:299:PRO:HD2	2:H:605:VAL:HG12	1.87	0.56
1:C:514:GLY:HA2	1:C:605:THR:O	2.05	0.56
2:D:240:LEU:HB2	2:D:584:LEU:HD22	1.87	0.56
2:F:742:ARG:HG2	2:F:742:ARG:HH11	1.71	0.56
1:C:347:TRP:HH2	1:C:401:LYS:HG3	1.71	0.56
2:D:1254:LYS:HB3	2:D:1259:ILE:HD13	1.85	0.56
2:D:892:ASP:HA	2:D:900:THR:HG23	1.88	0.56
2:D:934:ASN:O	2:D:938:GLU:HB2	2.05	0.56
2:F:68:TRP:CD1	2:F:92:ARG:HB2	2.41	0.56
2:B:115:LEU:HD11	2:B:324:LEU:HD22	1.87	0.56
2:H:1268:PRO:HB3	2:H:1309:VAL:CG1	2.35	0.56
2:D:334:LYS:HE3	3:D:1414:HOH:O	2.05	0.55
1:E:66:ILE:HD11	1:E:69:GLN:CG	2.32	0.55
2:F:845:ILE:CG2	2:F:849:GLN:OE1	2.53	0.55
1:G:369:ASN:HA	1:G:371:HIS:CD2	2.41	0.55
2:H:892:ASP:HA	2:H:900:THR:HG23	1.87	0.55
2:B:773:ASN:HB3	2:B:775:LYS:H	1.71	0.55
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.88	0.55
2:B:528:ASN:ND2	2:B:530:TRP:HE3	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1003:ASN:HB3	2:H:1102:PRO:HG2	1.88	0.55
2:B:611:ASP:OD1	2:B:614:GLY:CA	2.47	0.55
2:D:693:LEU:HD21	2:D:1024:LEU:HD22	1.89	0.55
2:F:476:MET:H	2:F:479:THR:HG22	1.72	0.55
2:H:528:ASN:OD1	2:H:530:TRP:O	2.24	0.55
2:B:1046:LEU:HD12	2:B:1213:ILE:HD12	1.87	0.55
2:H:114:TYR:HE2	2:H:217:ASN:HD21	1.54	0.55
2:H:527:THR:HG23	2:H:678:LEU:CD2	2.35	0.55
2:D:278:LYS:HB2	2:D:650:LEU:HD11	1.88	0.55
1:E:525:TYR:CE1	1:E:591:ALA:HB1	2.42	0.55
2:F:739:ASN:O	2:F:742:ARG:HB2	2.06	0.55
2:H:1237:ILE:O	2:H:1240:GLN:HB2	2.06	0.55
2:H:393:LEU:HD12	2:H:571:LEU:HD11	1.88	0.55
2:H:695:ALA:HB3	2:H:751:THR:HG22	1.88	0.55
2:H:807:ILE:HG21	2:H:828:ILE:HD12	1.88	0.55
2:H:835:ARG:NE	2:H:849:GLN:OE1	2.40	0.55
2:B:777:PHE:O	2:B:795:THR:HG22	2.06	0.55
2:B:849:GLN:HE22	2:B:883:LEU:HD12	1.72	0.55
2:D:476:MET:H	2:D:479:THR:HG22	1.71	0.55
2:D:806:MET:HG3	2:D:827:ASP:OD1	2.05	0.55
2:H:849:GLN:HG2	2:H:1122:ASN:O	2.07	0.55
2:B:590:GLN:OE1	2:B:906:GLN:HG2	2.06	0.55
2:H:989:SER:HG	2:H:1115:TYR:N	2.03	0.55
1:C:135:PRO:HB3	1:C:337:PRO:HG2	1.88	0.55
2:F:150:ASN:H	2:F:151:PRO:CD	2.20	0.54
1:C:29:LEU:HD21	1:C:124:TRP:HZ2	1.72	0.54
1:C:149:ILE:HG23	1:C:213:TYR:HB3	1.90	0.54
1:C:697:THR:HG21	1:C:719:LYS:HD2	1.88	0.54
2:D:946:THR:HA	2:D:1120:THR:HG21	1.88	0.54
1:G:155:THR:HG23	1:G:157:TYR:H	1.73	0.54
2:B:240:LEU:HB2	2:B:584:LEU:HD22	1.88	0.54
2:H:946:THR:HA	2:H:1120:THR:CG2	2.38	0.54
2:D:777:PHE:O	2:D:795:THR:HG22	2.06	0.54
2:H:1230:SER:HB3	2:H:1235:ASN:ND2	2.21	0.54
2:B:391:ASN:HD22	2:B:418:ASN:HD22	1.56	0.54
2:D:773:ASN:HB3	2:D:775:LYS:H	1.72	0.54
2:H:1029:ILE:HD11	2:H:1044:ILE:HG12	1.90	0.54
2:H:835:ARG:NH2	2:H:884:PRO:O	2.40	0.54
1:E:460:GLN:HG3	2:F:895:ASN:HB2	1.89	0.54
2:B:773:ASN:HD21	2:B:975:ASN:HB3	1.71	0.54
2:H:1046:LEU:HD12	2:H:1213:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD12	1:A:78:VAL:CG1	2.37	0.54
2:B:695:ALA:HB3	2:B:751:THR:HG22	1.90	0.54
1:E:149:ILE:HG23	1:E:213:TYR:HB3	1.90	0.54
2:F:769:PRO:HA	2:F:776:PRO:HA	1.88	0.54
1:C:652:THR:HG21	1:C:657:VAL:HG12	1.90	0.54
1:G:369:ASN:HB3	1:G:497:LYS:HE2	1.90	0.54
1:A:66:ILE:HD11	1:A:69:GLN:HB3	1.90	0.53
2:F:714:LYS:HA	2:F:717:GLU:HG3	1.90	0.53
2:F:777:PHE:O	2:F:795:THR:HG22	2.08	0.53
2:H:777:PHE:O	2:H:795:THR:HG22	2.08	0.53
2:H:422:GLY:CA	2:H:439:SER:OG	2.57	0.53
1:G:804:ASN:HD21	1:G:807:GLY:H	1.55	0.53
2:F:773:ASN:HB3	2:F:775:LYS:H	1.73	0.53
1:G:582:TYR:HB2	1:G:588:ILE:HG21	1.91	0.53
2:H:1259:ILE:HG12	2:H:1260:ASP:H	1.73	0.53
2:F:570:GLN:HG3	2:F:573:LYS:HE3	1.90	0.53
2:F:271:SER:HB2	2:F:868:VAL:HG22	1.90	0.53
2:D:272:THR:HG21	2:D:864:ASP:HB3	1.89	0.53
2:H:994:SER:OG	2:H:1137:MET:CE	2.57	0.53
1:E:151:GLU:HB2	1:E:213:TYR:CE1	2.43	0.53
1:E:574:GLN:NE2	1:E:575:SER:H	2.07	0.53
2:H:476:MET:HB2	2:H:479:THR:HB	1.91	0.53
2:B:1003:ASN:HB3	2:B:1102:PRO:HG2	1.91	0.53
2:B:194:SER:HB2	2:B:200:LEU:HB3	1.91	0.53
1:C:794:SER:H	1:C:796:GLN:HE22	1.57	0.53
2:F:150:ASN:N	2:F:151:PRO:HD3	2.24	0.53
2:H:1011:ASN:HD22	2:H:1067:SER:H	1.56	0.53
2:H:1313:THR:HG22	2:H:1344:GLN:HB3	1.91	0.53
2:B:1008:ASP:HB3	2:B:1061:TRP:CD1	2.44	0.53
2:F:1046:LEU:HD12	2:F:1213:ILE:HD12	1.90	0.53
2:F:952:PRO:HG2	2:F:956:GLU:HG2	1.91	0.53
2:H:1263:ARG:O	2:H:1267:LEU:HD11	2.10	0.53
2:B:1301:ARG:HG3	2:B:1301:ARG:HH21	1.73	0.52
1:C:117:SER:OG	1:C:125:THR:HG22	2.10	0.52
2:F:1301:ARG:NH2	2:F:1301:ARG:HG3	2.23	0.52
1:G:460:GLN:O	2:H:812:ASN:ND2	2.42	0.52
2:D:1062:THR:HG21	2:D:1085:LYS:HB2	1.91	0.52
2:D:870:PRO:HD2	2:D:874:SER:O	2.09	0.52
2:D:920:PRO:HB2	2:D:997:LEU:HG	1.92	0.52
2:B:1234:VAL:HG13	2:B:1236:LEU:HG	1.91	0.52
2:B:476:MET:H	2:B:479:THR:HG22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ASN:O	2:D:817:ARG:HD2	2.10	0.52
2:D:1305:ILE:HD11	2:D:1317:ARG:CB	2.40	0.52
2:D:822:PRO:HB2	2:D:1189:GLU:CB	2.40	0.52
2:D:222:LYS:HE2	2:D:321:TRP:HA	1.92	0.52
1:G:66:ILE:HD12	1:G:78:VAL:CG1	2.38	0.52
2:H:766:ASP:OD2	2:H:797:SER:HB3	2.10	0.52
2:B:590:GLN:CD	2:B:906:GLN:HG2	2.29	0.52
2:H:989:SER:HG	2:H:1115:TYR:HB2	1.73	0.52
2:H:994:SER:OG	2:H:1137:MET:HE2	2.10	0.52
2:H:131:ARG:HD2	2:H:139:ALA:HB1	1.92	0.52
2:H:244:SER:HB2	2:H:568:TYR:O	2.10	0.52
1:A:281:LEU:H	1:A:293:GLN:HE22	1.57	0.52
1:G:272:LYS:HE3	1:G:285:GLN:NE2	2.25	0.52
1:C:155:THR:HG23	1:C:157:TYR:H	1.74	0.52
2:D:226:GLU:HG3	2:D:239:ARG:HE	1.74	0.52
2:D:845:ILE:HG23	2:D:849:GLN:HE22	1.75	0.52
2:D:821:ILE:HD11	2:D:828:ILE:HD11	1.91	0.52
1:E:767:SER:HB2	1:E:809:PHE:CD1	2.45	0.52
2:F:903:ASN:HB2	2:F:905:PRO:HD2	1.91	0.52
2:B:769:PRO:HA	2:B:776:PRO:HA	1.92	0.51
1:G:514:GLY:HA2	1:G:605:THR:O	2.10	0.51
2:H:1105:GLN:HB3	2:H:1107:TYR:CE2	2.45	0.51
2:H:277:LEU:HB2	2:H:653:VAL:HB	1.92	0.51
2:B:903:ASN:O	2:B:907:ARG:HG3	2.10	0.51
1:C:85:VAL:HG23	1:C:107:LYS:O	2.11	0.51
2:D:1046:LEU:HD12	2:D:1213:ILE:HD12	1.92	0.51
2:H:457:MET:HA	2:H:465:PHE:O	2.09	0.51
1:C:166:GLU:HG3	1:C:206:LYS:HB2	1.92	0.51
2:D:237:THR:HG22	2:D:1108:GLN:HG3	1.90	0.51
1:E:521:LEU:HD23	1:E:580:VAL:HG23	1.92	0.51
1:G:347:TRP:CH2	1:G:401:LYS:HG3	2.43	0.51
2:D:112:LEU:HB3	3:D:1515:HOH:O	2.11	0.51
1:A:197:PRO:HD2	1:A:453:ILE:HD11	1.92	0.51
2:B:920:PRO:HB2	2:B:997:LEU:HG	1.93	0.51
1:E:767:SER:HB2	1:E:809:PHE:HD1	1.76	0.51
2:F:549:LEU:HD23	2:F:698:LEU:HB2	1.91	0.51
2:H:820:PHE:CE2	2:H:895:ASN:HA	2.46	0.51
1:E:293:GLN:HA	1:E:293:GLN:NE2	2.25	0.51
2:F:127:ASN:HD21	2:F:147:LYS:CE	2.24	0.51
2:H:278:LYS:HB2	2:H:650:LEU:HD11	1.92	0.51
2:H:341:VAL:HG22	2:H:358:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1005:THR:HG23	3:B:1422:HOH:O	2.10	0.51
1:C:357:GLU:HA	1:C:360:LEU:HD12	1.93	0.51
1:E:545:GLY:HA3	1:E:573:THR:HG22	1.93	0.51
2:F:299:PRO:HD2	2:F:605:VAL:HG12	1.93	0.51
1:G:454:ASN:ND2	1:G:467:VAL:H	2.09	0.51
1:G:101:SER:HB3	1:G:106:GLU:OE1	2.11	0.51
1:G:194:ASN:HB2	1:G:483:LYS:HD2	1.92	0.51
1:A:514:GLY:HA2	1:A:605:THR:HG23	1.93	0.50
1:A:766:GLN:O	2:B:742:ARG:HD2	2.11	0.50
2:D:758:SER:HA	2:D:907:ARG:NH1	2.26	0.50
1:E:196:ASN:HA	1:E:482:ILE:HG23	1.93	0.50
2:F:807:ILE:HG21	2:F:828:ILE:HD12	1.93	0.50
1:G:175:HIS:HB3	1:G:191:HIS:CD2	2.45	0.50
2:F:574:HIS:CE1	2:F:596:GLY:HA3	2.46	0.50
1:G:782:LEU:HD22	1:G:788:ALA:HB2	1.93	0.50
2:H:296:ALA:HA	2:H:384:ILE:HG21	1.92	0.50
2:H:934:ASN:O	2:H:938:GLU:HB2	2.11	0.50
2:B:283:ARG:HD2	2:B:290:LEU:HD23	1.92	0.50
1:C:148:LEU:HD11	1:C:502:ILE:HG13	1.93	0.50
1:E:734:GLY:HA2	1:E:774:GLN:O	2.11	0.50
2:F:1050:GLN:HG3	3:F:1444:HOH:O	2.10	0.50
2:F:664:TRP:CD1	2:F:898:THR:HG22	2.46	0.50
2:B:244:SER:HB2	2:B:568:TYR:O	2.12	0.50
2:D:134:ASP:HB3	2:D:140:LEU:HD21	1.92	0.50
2:B:362:ASP:HB3	2:B:365:LYS:HG2	1.92	0.50
1:C:767:SER:HB2	1:C:809:PHE:HD1	1.76	0.50
2:H:296:ALA:HA	2:H:384:ILE:CG2	2.42	0.50
2:H:476:MET:H	2:H:479:THR:HG22	1.76	0.50
2:B:268:MET:HG3	2:B:638:GLU:OE1	2.11	0.50
2:D:1076:LYS:HB3	2:D:1169:VAL:CG1	2.42	0.50
2:D:921:VAL:HG13	2:D:965:LEU:HD13	1.94	0.50
2:H:585:LEU:HD12	2:H:1105:GLN:HG3	1.94	0.50
2:B:286:GLN:OE1	2:B:289:SER:HB3	2.10	0.50
1:G:808:LEU:HD11	2:H:702:LEU:HD12	1.93	0.50
1:C:693:VAL:HG21	1:C:738:ILE:HD11	1.93	0.50
2:D:110:ASP:HB3	3:D:1515:HOH:O	2.11	0.50
2:F:590:GLN:CD	2:F:906:GLN:HG2	2.32	0.50
2:H:952:PRO:HG2	2:H:956:GLU:HG2	1.93	0.50
2:D:1230:SER:HB3	2:D:1235:ASN:ND2	2.27	0.50
2:F:1008:ASP:HB3	2:F:1061:TRP:CD1	2.46	0.50
2:H:387:TYR:O	2:H:391:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ASN:O	2:B:817:ARG:HD2	2.12	0.49
1:A:693:VAL:HG21	1:A:738:ILE:HD11	1.94	0.49
2:B:111:ASN:O	2:B:115:LEU:HG	2.12	0.49
2:B:138:ARG:HG2	2:B:1242:ALA:HB1	1.94	0.49
2:D:528:ASN:OD1	2:D:530:TRP:O	2.29	0.49
2:D:1003:ASN:HB3	2:D:1102:PRO:HG2	1.93	0.49
2:D:851:LYS:HD3	2:D:1123:LYS:HZ2	1.77	0.49
2:F:994:SER:HB2	2:F:1137:MET:CE	2.43	0.49
1:G:65:GLN:HE22	1:G:83:ARG:HG2	1.76	0.49
2:H:362:ASP:HB3	2:H:365:LYS:HG2	1.93	0.49
2:H:852:PRO:HB2	2:H:857:THR:CG2	2.40	0.49
1:G:149:ILE:HG23	1:G:213:TYR:HB3	1.94	0.49
2:H:769:PRO:HA	2:H:776:PRO:HA	1.94	0.49
1:C:525:TYR:HE1	1:C:591:ALA:HB1	1.76	0.49
2:D:823:ASN:ND2	2:D:825:SER:H	2.11	0.49
2:H:1109:PRO:HB3	2:H:1137:MET:HE3	1.93	0.49
1:E:454:ASN:ND2	1:E:467:VAL:H	2.10	0.49
2:H:1150:LYS:HE2	2:H:1156:GLY:HA2	1.95	0.49
2:H:821:ILE:HG22	2:H:823:ASN:H	1.77	0.49
2:D:402:PRO:HG2	2:D:415:LYS:O	2.12	0.49
1:E:127:VAL:HG12	1:E:128:LYS:HG3	1.94	0.49
2:H:1008:ASP:HB3	2:H:1061:TRP:CD1	2.48	0.49
2:H:240:LEU:HB2	2:H:584:LEU:HD22	1.95	0.49
2:B:1233:LEU:HD21	2:B:1329:ILE:HG21	1.94	0.49
2:B:277:LEU:HB2	2:B:653:VAL:HB	1.94	0.49
2:B:952:PRO:HG2	2:B:956:GLU:HG2	1.94	0.49
1:C:767:SER:HB2	1:C:809:PHE:CD1	2.47	0.49
2:D:806:MET:HG2	2:D:826:PRO:HG2	1.95	0.49
2:H:115:LEU:HD22	2:H:209:VAL:HG11	1.94	0.49
1:A:474:THR:HG21	1:A:479:THR:CG2	2.42	0.49
2:F:994:SER:HB2	2:F:1137:MET:HE2	1.95	0.49
2:F:65:LEU:HD21	2:F:127:ASN:HB3	1.95	0.49
2:B:693:LEU:HD21	2:B:1024:LEU:HD22	1.95	0.49
2:B:1305:ILE:HD11	2:B:1317:ARG:CB	2.40	0.49
2:D:850:VAL:HG23	2:D:859:PHE:HB3	1.92	0.49
2:D:936:ASP:HB2	3:D:1520:HOH:O	2.12	0.49
2:H:295:PHE:HB3	3:H:1407:HOH:O	2.11	0.49
2:H:920:PRO:HB2	2:H:997:LEU:HG	1.95	0.49
1:C:117:SER:OG	1:C:125:THR:CG2	2.60	0.48
2:H:114:TYR:C	2:H:114:TYR:CD1	2.86	0.48
2:B:1029:ILE:HD11	2:B:1044:ILE:HG12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:697:ILE:HD12	2:D:749:ARG:HB2	1.94	0.48
2:F:821:ILE:HG22	2:F:823:ASN:H	1.77	0.48
2:F:806:MET:HG3	2:F:827:ASP:OD1	2.13	0.48
2:H:68:TRP:CD1	2:H:92:ARG:HB2	2.48	0.48
1:A:127:VAL:HG12	1:A:128:LYS:HG3	1.94	0.48
2:B:969:TYR:HB3	2:B:971:PHE:CD1	2.48	0.48
1:C:133:ASP:O	1:C:337:PRO:HD3	2.13	0.48
2:D:852:PRO:HB2	2:D:857:THR:CG2	2.35	0.48
2:F:742:ARG:NH1	2:F:742:ARG:HG2	2.29	0.48
2:B:98:LEU:HD12	2:B:125:GLN:HG2	1.94	0.48
1:C:359:GLN:HG2	1:C:405:VAL:HG12	1.96	0.48
2:D:475:LYS:HD2	2:D:479:THR:O	2.13	0.48
1:E:86:LYS:HB2	1:E:105:GLY:HA3	1.95	0.48
2:F:240:LEU:HB2	2:F:584:LEU:HD22	1.95	0.48
2:B:742:ARG:HH11	2:B:742:ARG:HG2	1.79	0.48
1:C:111:VAL:HG11	1:C:309:ILE:HG21	1.96	0.48
2:D:1240:GLN:HA	2:D:1240:GLN:OE1	2.13	0.48
2:D:946:THR:HA	2:D:1120:THR:HG23	1.94	0.48
2:F:327:THR:HG22	2:F:410:ASP:OD2	2.13	0.48
1:G:767:SER:HB2	1:G:809:PHE:CD1	2.48	0.48
1:E:693:VAL:HG21	1:E:738:ILE:HD11	1.96	0.48
2:H:821:ILE:HD13	2:H:826:PRO:HA	1.96	0.48
1:A:521:LEU:HD23	1:A:580:VAL:HG23	1.96	0.48
2:H:191:VAL:HG22	2:H:203:VAL:HG12	1.96	0.48
2:B:259:THR:HG22	2:B:278:LYS:HD3	1.94	0.48
1:G:767:SER:HB2	1:G:809:PHE:HD1	1.77	0.48
2:H:1281:TYR:HB2	2:H:1284:TYR:HD2	1.79	0.48
2:H:235:ASN:HD22	2:H:236:PRO:HD2	1.79	0.48
2:B:180:TRP:O	2:B:184:LYS:HB2	2.14	0.48
2:D:328:ASP:HB2	3:D:1424:HOH:O	2.13	0.48
1:E:293:GLN:HA	1:E:293:GLN:HE21	1.79	0.48
1:E:581:PRO:HG3	1:E:654:GLY:HA3	1.96	0.48
2:D:1254:LYS:CB	2:D:1259:ILE:HD11	2.43	0.47
1:E:136:ASN:H	1:E:136:ASN:HD22	1.61	0.47
2:H:1003:ASN:ND2	2:H:1146:THR:HG21	2.29	0.47
2:H:1305:ILE:HD11	2:H:1317:ARG:CB	2.43	0.47
2:H:504:PRO:HG2	2:H:507:VAL:HG23	1.96	0.47
2:D:393:LEU:HD23	2:D:565:ARG:HD2	1.95	0.47
2:D:299:PRO:HD2	2:D:605:VAL:HG12	1.96	0.47
2:D:947:ASN:HD22	2:D:947:ASN:H	1.63	0.47
2:F:1067:SER:HB3	2:F:1077:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1187:LYS:O	2:F:1196:THR:HG21	2.14	0.47
2:F:467:PHE:CG	2:F:542:VAL:HG21	2.49	0.47
2:F:277:LEU:HB2	2:F:653:VAL:HB	1.96	0.47
1:G:792:LYS:HE3	1:G:797:ASN:HD21	1.79	0.47
2:H:773:ASN:HB3	2:H:775:LYS:H	1.79	0.47
1:A:474:THR:HG21	1:A:479:THR:HG21	1.97	0.47
2:D:1076:LYS:HB3	2:D:1169:VAL:HG12	1.96	0.47
2:D:327:THR:HG22	2:D:410:ASP:OD2	2.13	0.47
2:F:847:PHE:CD2	2:F:850:VAL:HB	2.50	0.47
2:B:393:LEU:HD23	2:B:565:ARG:HD2	1.96	0.47
2:D:457:MET:HA	2:D:465:PHE:O	2.14	0.47
1:E:460:GLN:CA	2:F:812:ASN:OD1	2.63	0.47
2:F:422:GLY:HA2	2:F:439:SER:HB2	1.97	0.47
2:F:693:LEU:HD21	2:F:1024:LEU:HD22	1.97	0.47
2:H:78:LEU:O	2:H:87:SER:HA	2.14	0.47
1:A:710:TRP:HB2	1:A:740:VAL:HB	1.96	0.47
1:E:294:LEU:O	1:E:298:SER:HB2	2.15	0.47
2:F:947:ASN:H	2:F:947:ASN:HD22	1.61	0.47
1:G:281:LEU:H	1:G:293:GLN:HE22	1.62	0.47
2:H:1265:PHE:O	2:H:1312:GLN:NE2	2.47	0.47
2:H:851:LYS:HD3	2:H:1123:LYS:HZ2	1.79	0.47
2:D:1032:THR:HG22	2:D:1033:ASP:OD1	2.14	0.47
2:D:111:ASN:O	2:D:115:LEU:HG	2.14	0.47
2:D:411:GLU:HB3	2:D:415:LYS:HD3	1.97	0.47
1:E:281:LEU:H	1:E:293:GLN:HE22	1.62	0.47
1:E:514:GLY:HA2	1:E:605:THR:O	2.15	0.47
2:H:114:TYR:HE1	2:H:118:VAL:HG21	1.79	0.47
2:B:65:LEU:HD21	2:B:127:ASN:HB3	1.96	0.47
2:D:835:ARG:HB2	2:D:845:ILE:HD13	1.97	0.47
2:F:1229:VAL:HG22	2:F:1239:GLY:HA2	1.96	0.47
1:C:293:GLN:HA	1:C:293:GLN:OE1	2.14	0.47
2:F:457:MET:HA	2:F:465:PHE:O	2.14	0.47
2:F:524:PRO:HD2	2:F:557:MET:CE	2.45	0.47
2:H:237:THR:HG22	2:H:1108:GLN:HG3	1.97	0.47
1:A:410:SER:HB2	1:A:421:LYS:HG3	1.96	0.47
1:A:650:VAL:HG13	1:A:657:VAL:HG13	1.96	0.47
2:B:570:GLN:HG3	2:B:573:LYS:HE3	1.97	0.47
2:B:735:ASN:HB2	2:B:738:THR:HG23	1.97	0.47
2:F:834:TYR:CZ	2:F:945:GLU:HG3	2.49	0.47
2:F:934:ASN:O	2:F:938:GLU:HB2	2.15	0.47
1:A:273:GLN:HG2	1:A:722:HIS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1191:SER:HB3	2:B:1196:THR:HG23	1.97	0.47
2:D:1067:SER:HB3	2:D:1077:SER:OG	2.15	0.47
1:G:151:GLU:HB2	1:G:213:TYR:CE1	2.50	0.47
2:H:520:LEU:HD23	2:H:757:ASP:HA	1.95	0.47
2:H:697:ILE:HD12	2:H:749:ARG:HB2	1.96	0.47
2:H:901:ASN:HB3	2:H:958:ASN:HD21	1.80	0.47
1:A:706:GLU:H	1:A:706:GLU:HG2	1.48	0.46
1:C:723:ASP:OD2	1:C:727:THR:HB	2.15	0.46
1:C:66:ILE:HD12	1:C:78:VAL:CG1	2.46	0.46
2:F:429:ASP:HB3	2:F:432:LYS:HD3	1.96	0.46
2:H:590:GLN:CD	2:H:906:GLN:HG2	2.36	0.46
1:A:171:GLN:NE2	1:A:201:ALA:HB3	2.29	0.46
2:F:835:ARG:HD3	2:F:845:ILE:HG21	1.96	0.46
2:F:943:LYS:HB3	2:F:948:GLU:HB2	1.97	0.46
1:A:405:VAL:HG11	1:A:426:ALA:HB2	1.98	0.46
1:C:471:GLY:O	1:C:481:PRO:HA	2.15	0.46
1:E:216:LEU:HA	1:E:290:VAL:HB	1.96	0.46
1:G:652:THR:CG2	1:G:657:VAL:HG13	2.44	0.46
2:H:946:THR:HA	2:H:1120:THR:HG21	1.98	0.46
1:A:135:PRO:HA	1:A:337:PRO:HD2	1.97	0.46
1:A:363:LYS:O	1:A:363:LYS:HG2	2.15	0.46
2:B:387:TYR:O	2:B:391:ASN:HB2	2.15	0.46
2:D:1191:SER:HB3	2:D:1196:THR:HG23	1.97	0.46
2:D:226:GLU:CG	2:D:239:ARG:NE	2.78	0.46
2:F:1188:GLU:HG2	2:F:1189:GLU:HG2	1.96	0.46
1:G:735:PHE:CD1	1:G:776:LEU:HB2	2.51	0.46
2:B:1027:TRP:CE3	2:B:1046:LEU:HB3	2.50	0.46
2:B:1260:ASP:CG	2:B:1263:ARG:HB2	2.35	0.46
2:B:939:GLN:HE21	2:B:950:ASN:HB2	1.80	0.46
1:C:204:GLY:HA3	1:C:424:ALA:O	2.16	0.46
2:D:574:HIS:CE1	2:D:596:GLY:HA3	2.50	0.46
2:D:685:GLU:CG	2:D:686:ASN:H	2.18	0.46
1:C:808:LEU:HD23	2:D:742:ARG:HG2	1.96	0.46
1:E:704:ASN:HB3	1:E:707:SER:HB2	1.97	0.46
2:B:777:PHE:HB3	2:B:795:THR:CG2	2.46	0.46
2:D:567:LYS:HD3	2:D:621:TYR:CE2	2.51	0.46
1:E:472:ASN:HD22	1:E:478:THR:HB	1.79	0.46
1:E:574:GLN:HE21	1:E:575:SER:N	2.12	0.46
2:H:1274:ASP:HB3	2:H:1277:THR:HG22	1.98	0.46
2:H:271:SER:HB2	2:H:868:VAL:HG22	1.97	0.46
1:A:704:ASN:HB3	1:A:707:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:VAL:HG13	2:H:131:ARG:NH1	2.31	0.46
2:H:634:ASN:O	2:H:638:GLU:HB2	2.15	0.46
1:A:506:PRO:HB2	1:A:540:GLN:HA	1.97	0.46
1:A:525:TYR:CE1	1:A:591:ALA:HB1	2.50	0.46
2:F:634:ASN:O	2:F:638:GLU:HB2	2.16	0.46
2:H:203:VAL:HG13	2:H:343:PHE:CE1	2.50	0.46
2:D:345:ASP:HA	2:D:352:HIS:O	2.16	0.46
2:D:733:ASN:HD22	2:D:733:ASN:H	1.64	0.46
2:D:821:ILE:HG22	2:D:823:ASN:H	1.80	0.46
1:G:363:LYS:HG3	1:G:374:HIS:CE1	2.50	0.46
1:C:170:THR:HG22	1:C:173:GLU:H	1.81	0.46
2:D:547:ASN:H	2:D:547:ASN:HD22	1.62	0.46
2:D:626:PRO:HG3	2:D:661:LEU:HG	1.98	0.46
1:G:671:THR:HG21	1:G:676:ILE:HG12	1.97	0.46
1:G:801:ILE:HD13	1:G:815:LEU:O	2.15	0.46
2:H:1261:PHE:CD2	2:H:1265:PHE:HE2	2.34	0.46
2:H:318:THR:CG2	2:H:319:GLU:H	2.18	0.46
2:H:777:PHE:HB3	2:H:795:THR:CG2	2.46	0.46
2:D:111:ASN:HA	2:D:114:TYR:HB3	1.97	0.45
2:D:422:GLY:HA2	2:D:439:SER:HB2	1.98	0.45
1:E:766:GLN:O	2:F:742:ARG:HD2	2.16	0.45
2:F:390:ARG:HD3	2:F:396:THR:O	2.16	0.45
1:G:135:PRO:HB3	1:G:337:PRO:HG2	1.96	0.45
2:B:1059:GLN:HG2	3:B:1521:HOH:O	2.16	0.45
2:B:892:ASP:HA	2:B:900:THR:HG23	1.97	0.45
1:G:368:THR:O	1:G:369:ASN:HB2	2.16	0.45
2:H:806:MET:HG2	2:H:826:PRO:HG2	1.98	0.45
1:A:366:THR:HG22	1:A:494:SER:CA	2.42	0.45
2:B:697:ILE:HD12	2:B:749:ARG:HB2	1.98	0.45
1:C:196:ASN:HA	1:C:482:ILE:HG23	1.98	0.45
2:D:259:THR:HG22	2:D:278:LYS:HD3	1.99	0.45
2:F:1234:VAL:HG13	2:F:1236:LEU:HG	1.98	0.45
2:F:1274:ASP:HB3	2:F:1277:THR:HG22	1.97	0.45
2:B:1112:VAL:HA	2:B:1127:PRO:HA	1.97	0.45
2:B:852:PRO:HB2	2:B:857:THR:HG22	1.99	0.45
2:B:272:THR:HG21	2:B:864:ASP:HB3	1.99	0.45
2:D:1147:LYS:HA	2:D:1150:LYS:HD3	1.97	0.45
2:F:806:MET:HG2	2:F:826:PRO:HG2	1.98	0.45
2:F:892:ASP:HA	2:F:900:THR:HG23	1.99	0.45
2:H:276:ALA:HB2	2:H:655:PRO:HD3	1.99	0.45
2:H:570:GLN:HG3	2:H:573:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:SER:HB3	1:C:626:SER:OG	2.16	0.45
2:D:1078:LEU:HD22	2:D:1225:LEU:HD23	1.99	0.45
2:H:203:VAL:HG13	2:H:343:PHE:HE1	1.81	0.45
2:H:91:VAL:HG12	2:H:129:ALA:HB3	1.99	0.45
1:A:396:ILE:HG22	1:A:629:LEU:HD21	1.99	0.45
2:B:1274:ASP:HB3	2:B:1277:THR:HG22	1.99	0.45
1:C:506:PRO:HB2	1:C:540:GLN:HA	1.99	0.45
2:D:1234:VAL:HG13	2:D:1236:LEU:HG	1.99	0.45
2:D:939:GLN:NE2	2:D:950:ASN:HB2	2.32	0.45
1:E:405:VAL:HG11	1:E:426:ALA:HB2	1.99	0.45
2:B:668:ASN:HB2	2:B:669:TRP:CE3	2.51	0.45
2:D:1301:ARG:HH22	2:D:1319:GLU:CD	2.20	0.45
2:D:223:GLU:HG2	2:D:1100:LEU:HD23	1.98	0.45
2:D:72:ASN:HB2	2:D:473:ALA:HB2	1.98	0.45
2:F:1003:ASN:ND2	2:F:1146:THR:HG21	2.31	0.45
2:H:1269:VAL:HG11	2:H:1307:TYR:HB2	1.99	0.45
2:H:244:SER:HB3	2:H:571:LEU:HB2	1.97	0.45
2:D:600:ARG:HG2	2:D:669:TRP:CH2	2.52	0.45
2:D:529:ARG:NH2	2:D:729:LEU:O	2.50	0.45
2:D:952:PRO:HG2	2:D:956:GLU:HG2	1.98	0.45
2:F:272:THR:HG21	2:F:864:ASP:HB3	1.99	0.45
1:G:184:TRP:CD2	1:G:199:PRO:HB3	2.51	0.45
2:H:114:TYR:CE1	2:H:118:VAL:HG21	2.52	0.45
2:H:1269:VAL:HA	2:H:1272:LEU:HD12	1.98	0.45
1:A:574:GLN:HE21	1:A:575:SER:H	1.64	0.45
2:B:834:TYR:OH	2:B:945:GLU:HG2	2.17	0.45
1:C:193:LEU:HD21	1:C:485:ALA:HB3	1.98	0.45
2:F:1265:PHE:CZ	2:F:1288:LEU:HD21	2.52	0.45
2:F:225:LEU:O	2:F:225:LEU:HG	2.17	0.45
1:G:521:LEU:HD23	1:G:580:VAL:HG23	1.98	0.45
1:C:194:ASN:HB2	1:C:483:LYS:HD3	1.99	0.44
2:D:767:PHE:CZ	2:D:1208:LYS:HG2	2.52	0.44
2:H:1265:PHE:CB	2:H:1312:GLN:NE2	2.70	0.44
1:C:136:ASN:HD22	1:C:136:ASN:H	1.66	0.44
2:F:557:MET:SD	2:F:692:SER:HB2	2.58	0.44
2:B:152:SER:HB2	2:B:172:LEU:HD22	1.99	0.44
2:D:363:PRO:O	2:D:367:VAL:HG23	2.17	0.44
2:F:244:SER:HB3	2:F:571:LEU:HB2	1.98	0.44
1:G:749:GLN:HA	1:G:749:GLN:NE2	2.24	0.44
1:A:469:TYR:CE1	2:B:818:TRP:HD1	2.34	0.44
1:C:170:THR:OG1	1:C:200:ASN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:467:PHE:CD1	2:D:542:VAL:HG21	2.52	0.44
2:D:504:PRO:HG2	2:D:507:VAL:HG23	1.99	0.44
2:D:565:ARG:HG3	2:D:601:PRO:HB3	1.99	0.44
2:F:834:TYR:HE1	2:F:944:THR:HG23	1.83	0.44
2:B:299:PRO:HB2	2:B:609:LEU:HD12	2.00	0.44
2:D:994:SER:HB2	2:D:1137:MET:HE2	1.98	0.44
2:D:226:GLU:CG	2:D:239:ARG:HE	2.30	0.44
2:D:256:LEU:HD13	2:D:606:GLY:HA3	1.99	0.44
2:H:739:ASN:O	2:H:742:ARG:HB2	2.16	0.44
2:H:915:LEU:O	2:H:1027:TRP:CD1	2.71	0.44
1:C:67:ALA:HB2	1:C:81:LYS:HG2	2.00	0.44
2:F:1029:ILE:HD12	2:F:1046:LEU:HD21	2.00	0.44
2:F:1178:THR:HG22	1:G:566:THR:HG21	1.99	0.44
1:A:34:SER:HB2	1:A:65:GLN:HB2	1.99	0.44
2:F:529:ARG:CZ	2:F:732:LEU:HD23	2.48	0.44
1:G:434:ASP:OD1	1:G:469:TYR:HA	2.18	0.44
2:B:1040:GLY:HA3	2:B:1183:SER:HB3	2.00	0.44
2:B:186:LYS:HB3	2:B:205:LEU:HB3	1.99	0.44
2:B:933:PHE:HZ	2:B:939:GLN:HG2	1.81	0.44
2:D:467:PHE:CG	2:D:542:VAL:HG21	2.53	0.44
2:F:363:PRO:O	2:F:367:VAL:HG23	2.16	0.44
2:F:476:MET:HB2	2:F:479:THR:HB	1.99	0.44
1:G:73:ASN:HD21	1:G:327:ARG:NH2	2.08	0.44
2:H:806:MET:HG3	2:H:827:ASP:OD1	2.18	0.44
2:B:223:GLU:HG3	2:B:478:THR:OG1	2.18	0.44
2:D:1274:ASP:HB3	2:D:1277:THR:HG22	2.00	0.44
2:F:706:LEU:HD13	2:F:743:TYR:CD2	2.53	0.44
2:H:822:PRO:HB2	2:H:1189:GLU:CB	2.47	0.44
2:B:536:ARG:NH1	2:B:686:ASN:HB3	2.33	0.43
2:B:758:SER:HA	2:B:907:ARG:NH1	2.33	0.43
2:B:956:GLU:H	2:B:956:GLU:HG3	1.56	0.43
2:D:194:SER:HB2	2:D:200:LEU:HB3	1.99	0.43
2:F:1233:LEU:HD21	2:F:1329:ILE:HG21	2.00	0.43
1:G:261:SER:CB	1:G:726:GLN:HB2	2.47	0.43
1:G:406:GLY:HA2	1:G:499:ASN:O	2.18	0.43
2:H:585:LEU:CD1	2:H:1105:GLN:HG3	2.48	0.43
2:H:152:SER:HB2	2:H:172:LEU:HD22	2.00	0.43
2:B:834:TYR:CZ	2:B:945:GLU:HG2	2.53	0.43
2:D:380:ASN:HA	2:D:718:PHE:CZ	2.53	0.43
1:G:171:GLN:HG2	1:G:184:TRP:HH2	1.83	0.43
2:B:939:GLN:HE21	2:B:950:ASN:HD22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:549:LEU:HD23	2:D:698:LEU:HB2	1.99	0.43
2:H:1191:SER:HB3	2:H:1196:THR:HG23	2.01	0.43
2:B:1078:LEU:HD22	2:B:1225:LEU:HD23	1.99	0.43
2:B:115:LEU:HD22	2:B:209:VAL:HG11	2.01	0.43
2:H:732:LEU:HD13	2:H:732:LEU:HA	1.92	0.43
1:A:222:ILE:HD12	1:A:270:ASN:HD21	1.82	0.43
1:A:35:LYS:HE2	1:A:64:TYR:O	2.19	0.43
1:A:461:ASP:HB3	2:B:811:LEU:HD13	2.01	0.43
1:C:461:ASP:HB3	2:D:811:LEU:HD13	2.01	0.43
2:F:695:ALA:HB3	2:F:751:THR:HG22	1.99	0.43
2:F:770:TRP:HE3	2:F:773:ASN:HB2	1.83	0.43
2:H:223:GLU:HG3	2:H:478:THR:OG1	2.19	0.43
2:H:327:THR:HG22	2:H:410:ASP:OD2	2.18	0.43
2:B:1281:TYR:HB2	2:B:1284:TYR:CD2	2.53	0.43
2:B:574:HIS:CE1	2:B:596:GLY:HA3	2.54	0.43
2:B:567:LYS:HD3	2:B:621:TYR:CE2	2.53	0.43
2:F:299:PRO:HB2	2:F:609:LEU:HD12	2.01	0.43
1:G:489:LYS:HE2	1:G:491:ASP:HB2	1.99	0.43
2:H:1281:TYR:HD2	2:H:1284:TYR:HE2	1.67	0.43
2:D:932:GLN:HB2	2:D:982:LYS:HB3	1.99	0.43
2:F:527:THR:HG23	2:F:678:LEU:CD2	2.44	0.43
2:H:1032:THR:HG21	3:H:1401:HOH:O	2.17	0.43
2:H:921:VAL:HG13	2:H:965:LEU:HD13	2.00	0.43
1:C:127:VAL:HG12	1:C:128:LYS:HG3	2.01	0.43
2:D:769:PRO:HA	2:D:776:PRO:HA	2.01	0.43
2:F:1105:GLN:HB2	2:F:1107:TYR:CE2	2.54	0.43
2:F:923:ILE:HD12	2:F:983:ILE:HG22	2.00	0.43
2:H:371:PRO:HD2	2:H:374:TRP:CD2	2.54	0.43
2:B:114:TYR:O	2:B:117:ALA:HB3	2.19	0.43
2:B:467:PHE:CG	2:B:542:VAL:HG21	2.54	0.43
1:C:320:MET:HB2	1:C:321:TRP:CE3	2.54	0.43
2:D:119:GLU:HG2	2:D:209:VAL:HG23	2.00	0.43
2:D:389:ALA:O	2:D:393:LEU:HB2	2.18	0.43
2:F:411:GLU:HB3	2:F:415:LYS:HD3	2.00	0.43
1:G:351:LYS:HG2	1:G:355:PHE:HE2	1.84	0.43
1:G:475:ASN:O	2:H:817:ARG:HD2	2.18	0.43
2:H:1322:ASP:HB2	2:H:1329:ILE:HG12	2.00	0.43
2:H:272:THR:HG21	2:H:864:ASP:HB3	2.01	0.43
1:C:99:PHE:CZ	1:C:108:PRO:HB3	2.54	0.43
2:F:192:VAL:HG12	2:F:202:PHE:HB2	2.00	0.43
2:F:921:VAL:HG13	2:F:965:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:LEU:HD22	2:D:209:VAL:HG11	2.01	0.42
1:E:88:LYS:HE3	1:E:100:ASP:HA	2.01	0.42
1:E:166:GLU:HG3	1:E:206:LYS:HB2	2.01	0.42
2:F:520:LEU:HD23	2:F:757:ASP:HA	2.01	0.42
2:F:860:ASP:O	2:F:863:SER:HB3	2.19	0.42
2:H:467:PHE:CG	2:H:542:VAL:HG21	2.54	0.42
2:B:549:LEU:HD23	2:B:698:LEU:HB2	1.99	0.42
2:F:523:LEU:HG	2:F:557:MET:CE	2.49	0.42
2:F:697:ILE:HD12	2:F:749:ARG:HB2	2.00	0.42
1:G:545:GLY:HA3	1:G:573:THR:HG22	2.01	0.42
2:D:835:ARG:HB3	2:D:1122:ASN:HA	2.02	0.42
1:E:636:ASN:HA	1:E:637:PRO:HD3	1.96	0.42
1:G:66:ILE:HD11	1:G:69:GLN:HG2	1.98	0.42
2:B:281:VAL:HG22	2:B:293:ASN:HA	2.00	0.42
2:D:945:GLU:HG3	2:D:945:GLU:H	1.40	0.42
1:G:167:LYS:HE2	1:G:202:SER:HB2	2.01	0.42
1:G:785:GLU:HB3	1:G:803:LYS:HZ2	1.85	0.42
2:H:1261:PHE:O	2:H:1263:ARG:N	2.53	0.42
2:H:536:ARG:NH1	2:H:686:ASN:HB3	2.35	0.42
1:A:149:ILE:HG23	1:A:213:TYR:HB3	2.02	0.42
1:A:155:THR:CG2	1:A:157:TYR:H	2.28	0.42
1:A:454:ASN:ND2	1:A:467:VAL:H	2.17	0.42
2:B:1062:THR:HG21	2:B:1085:LYS:HB2	2.02	0.42
2:B:131:ARG:HD2	2:B:133:TYR:CE1	2.54	0.42
2:D:821:ILE:HD11	2:D:828:ILE:CD1	2.49	0.42
2:D:77:SER:HA	2:D:89:GLY:HA2	2.02	0.42
2:D:939:GLN:HE21	2:D:950:ASN:HB2	1.84	0.42
2:F:269:ALA:HA	2:F:870:PRO:HA	2.00	0.42
2:H:256:LEU:HD13	2:H:606:GLY:HA3	2.01	0.42
2:D:244:SER:HB3	2:D:571:LEU:HB2	2.01	0.42
2:D:834:TYR:CZ	2:D:945:GLU:HG2	2.54	0.42
1:E:792:LYS:HE3	1:E:797:ASN:HD21	1.84	0.42
2:B:837:GLN:HB3	2:B:841:GLN:HB3	2.02	0.42
1:C:651:LEU:HA	1:C:651:LEU:HD23	1.90	0.42
1:C:812:ASP:OD2	1:C:815:LEU:HG	2.20	0.42
2:D:114:TYR:O	2:D:118:VAL:HG23	2.19	0.42
2:D:1281:TYR:HB2	2:D:1284:TYR:HD2	1.83	0.42
1:E:216:LEU:HB3	1:E:291:ILE:HB	2.01	0.42
2:F:475:LYS:HD2	2:F:479:THR:O	2.20	0.42
2:F:890:THR:HA	2:F:902:LYS:HE3	2.01	0.42
1:A:311:VAL:HB	1:A:323:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:LYS:HD2	2:B:479:THR:O	2.20	0.42
2:B:821:ILE:HD11	2:B:828:ILE:HD11	2.01	0.42
1:C:347:TRP:CH2	1:C:401:LYS:HG3	2.53	0.42
2:D:1012:LEU:HD23	2:D:1012:LEU:HA	1.93	0.42
2:D:1150:LYS:HE2	2:D:1156:GLY:HA2	2.02	0.42
2:D:115:LEU:HD11	2:D:324:LEU:HD22	2.02	0.42
2:D:152:SER:HB2	2:D:172:LEU:HD22	2.02	0.42
2:D:668:ASN:HB2	2:D:669:TRP:CE3	2.54	0.42
1:E:697:THR:HB	1:E:715:ASP:O	2.19	0.42
2:F:115:LEU:HD22	2:F:209:VAL:HG11	2.02	0.42
2:B:528:ASN:HD22	2:B:530:TRP:HE3	1.65	0.42
2:B:943:LYS:HB3	2:B:948:GLU:HB2	2.01	0.42
1:E:170:THR:HG22	1:E:173:GLU:H	1.85	0.42
1:E:436:LYS:HB2	1:E:441:ASP:HB3	2.01	0.42
2:F:170:PHE:CZ	2:F:344:TYR:HB3	2.55	0.42
2:F:756:LEU:HD12	2:F:760:THR:HG22	2.01	0.42
2:F:845:ILE:HA	2:F:846:PRO:HD3	1.93	0.42
2:H:299:PRO:HB2	2:H:609:LEU:HD12	2.02	0.42
1:A:136:ASN:H	1:A:136:ASN:ND2	2.11	0.41
1:A:253:PRO:HD2	1:A:263:GLY:HA3	2.02	0.41
1:A:359:GLN:HG2	1:A:405:VAL:HG12	2.01	0.41
1:C:347:TRP:CD1	1:C:353:LYS:HG3	2.55	0.41
2:F:771:ILE:HG13	2:F:771:ILE:H	1.69	0.41
1:G:67:ALA:HB2	1:G:81:LYS:HG2	2.01	0.41
2:H:923:ILE:HD12	2:H:983:ILE:HG22	2.00	0.41
2:D:222:LYS:CE	2:D:321:TRP:HA	2.51	0.41
1:G:165:LYS:HD2	1:G:510:TYR:HB3	2.01	0.41
2:B:733:ASN:H	2:B:733:ASN:ND2	2.18	0.41
1:C:86:LYS:HB2	1:C:105:GLY:HA3	2.02	0.41
2:D:226:GLU:HB3	2:D:227:VAL:H	1.43	0.41
2:F:1281:TYR:HB2	2:F:1284:TYR:HD2	1.86	0.41
2:F:808:THR:HG21	2:F:817:ARG:NH2	2.35	0.41
2:H:201:TYR:CE1	2:H:345:ASP:HB3	2.56	0.41
2:H:933:PHE:HZ	2:H:939:GLN:HG2	1.85	0.41
1:A:639:MET:HB2	1:A:748:ASN:O	2.20	0.41
2:B:327:THR:HG21	2:B:367:VAL:HG21	2.02	0.41
2:F:475:LYS:HE3	2:F:1005:THR:HG21	2.03	0.41
1:G:261:SER:O	1:G:263:GLY:N	2.53	0.41
2:H:1031:PHE:CE2	2:H:1044:ILE:HD11	2.56	0.41
2:B:710:ILE:HD12	2:B:740:TRP:HA	2.02	0.41
1:C:581:PRO:HG3	1:C:654:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASN:O	1:E:146:LYS:HB2	2.21	0.41
1:E:347:TRP:HH2	1:E:401:LYS:HG3	1.86	0.41
1:E:650:VAL:HG13	1:E:657:VAL:HG13	2.03	0.41
2:F:524:PRO:HD2	2:F:557:MET:HE2	2.03	0.41
2:H:1281:TYR:HD2	2:H:1284:TYR:CE2	2.39	0.41
2:B:924:ASN:HB3	2:B:925:LYS:HG2	2.02	0.41
2:D:834:TYR:OH	2:D:945:GLU:HG2	2.21	0.41
1:E:706:GLU:N	1:E:706:GLU:OE1	2.54	0.41
2:F:528:ASN:OD1	2:F:530:TRP:O	2.39	0.41
1:G:411:SER:H	1:G:421:LYS:HE3	1.85	0.41
2:H:162:PRO:HG3	2:H:344:TYR:CE2	2.55	0.41
2:H:834:TYR:OH	2:H:945:GLU:HG2	2.20	0.41
2:B:391:ASN:ND2	2:B:418:ASN:HD22	2.18	0.41
2:B:422:GLY:HA2	2:B:439:SER:HB2	2.02	0.41
2:B:835:ARG:HB3	2:B:1122:ASN:HA	2.03	0.41
2:F:111:ASN:OD1	2:F:220:VAL:HG13	2.21	0.41
2:F:424:LYS:HD2	2:F:432:LYS:O	2.21	0.41
2:F:457:MET:HG3	2:F:466:ILE:HG13	2.02	0.41
2:H:1027:TRP:CE3	2:H:1046:LEU:HB3	2.56	0.41
2:H:151:PRO:HG3	2:H:180:TRP:CZ2	2.55	0.41
2:H:395:GLN:HE22	2:H:565:ARG:HD3	1.86	0.41
2:H:835:ARG:CZ	2:H:849:GLN:OE1	2.68	0.41
1:E:204:GLY:HA3	1:E:424:ALA:O	2.20	0.41
2:F:371:PRO:HD2	2:F:374:TRP:CD2	2.55	0.41
1:G:661:PHE:HE1	1:G:668:LEU:HD23	1.80	0.41
2:H:845:ILE:HG21	2:H:849:GLN:CD	2.39	0.41
2:B:1076:LYS:HE3	2:B:1171:GLN:HG3	2.02	0.41
2:B:945:GLU:H	2:B:945:GLU:HG3	1.38	0.41
1:G:135:PRO:HA	1:G:337:PRO:HD2	2.02	0.41
1:G:28:PHE:HE2	1:G:42:PRO:HA	1.86	0.41
1:A:220:TRP:O	1:A:287:PRO:HG2	2.20	0.41
2:B:276:ALA:HB2	2:B:655:PRO:HD3	2.01	0.41
2:D:851:LYS:HA	2:D:1123:LYS:NZ	2.36	0.41
2:D:923:ILE:HG22	2:D:1140:LEU:HG	2.03	0.41
1:E:808:LEU:HD11	2:F:702:LEU:HD12	2.03	0.41
2:F:536:ARG:NH1	2:F:686:ASN:HB3	2.36	0.41
2:F:664:TRP:HB2	2:F:898:THR:HA	2.03	0.41
1:G:433:LEU:HD23	1:G:534:LEU:HD11	2.03	0.41
1:G:461:ASP:HB3	2:H:811:LEU:HD13	2.03	0.41
2:H:987:ALA:HB1	2:H:1115:TYR:CG	2.55	0.41
2:B:457:MET:HA	2:B:465:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:PHE:CE1	2:B:850:VAL:HB	2.56	0.41
1:G:131:GLN:HG2	1:G:132:LEU:N	2.36	0.41
2:H:1221:MET:HB2	2:H:1225:LEU:HD11	2.03	0.41
2:H:131:ARG:HG2	2:H:133:TYR:CZ	2.56	0.41
2:H:411:GLU:HB3	2:H:415:LYS:HD3	2.03	0.41
2:B:345:ASP:HA	2:B:352:HIS:O	2.21	0.40
2:B:742:ARG:HG2	2:B:742:ARG:NH1	2.35	0.40
1:C:253:PRO:HG3	2:F:737:ASN:HD22	1.85	0.40
2:D:1260:ASP:OD1	2:D:1263:ARG:HB2	2.21	0.40
2:F:204:LEU:HD23	2:F:204:LEU:HA	1.98	0.40
2:H:180:TRP:O	2:H:184:LYS:HB2	2.21	0.40
2:H:834:TYR:CZ	2:H:945:GLU:HG2	2.55	0.40
2:H:945:GLU:HG3	2:H:945:GLU:H	1.36	0.40
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.03	0.40
2:B:199:ASN:O	2:B:344:TYR:HA	2.21	0.40
1:E:165:LYS:HB3	1:E:205:PHE:HB2	2.03	0.40
1:E:605:THR:HG22	1:E:606:THR:HG23	2.03	0.40
1:G:293:GLN:NE2	1:G:293:GLN:HA	2.35	0.40
2:H:1248:THR:HB	2:H:1331:VAL:HG13	2.03	0.40
2:H:594:PRO:HG2	2:H:1124:LEU:HD22	2.03	0.40
2:B:1105:GLN:HB2	2:B:1107:TYR:CE2	2.56	0.40
1:C:158:THR:CG2	1:C:163:LEU:HD13	2.52	0.40
1:C:97:ILE:HG22	1:C:134:VAL:HB	2.03	0.40
1:E:135:PRO:HB3	1:E:337:PRO:HG2	2.03	0.40
1:E:98:SER:HA	1:E:134:VAL:HG21	2.03	0.40
2:F:1038:ARG:HE	2:F:1038:ARG:HB2	1.63	0.40
2:F:1116:GLN:HB2	2:F:1120:THR:HA	2.03	0.40
2:F:501:THR:HG21	2:F:708:ASP:C	2.41	0.40
2:B:1234:VAL:CG1	2:B:1236:LEU:HG	2.51	0.40
2:B:923:ILE:HD11	2:B:966:LEU:HD21	2.04	0.40
1:C:782:LEU:HD22	1:C:788:ALA:HB2	2.03	0.40
1:E:143:GLN:HA	1:E:146:LYS:HE3	2.02	0.40
2:F:1030:THR:HB	2:F:1045:THR:OG1	2.22	0.40
2:F:467:PHE:CD1	2:F:542:VAL:HG21	2.56	0.40
2:F:756:LEU:HD12	2:F:760:THR:CG2	2.51	0.40
1:G:216:LEU:HD22	1:G:291:ILE:HD12	2.04	0.40
2:B:1003:ASN:ND2	2:B:1146:THR:HG21	2.37	0.40
2:B:201:TYR:CE1	2:B:345:ASP:HB3	2.57	0.40
2:B:572:GLU:HG2	2:B:572:GLU:H	1.57	0.40
2:B:940:LYS:HB2	2:B:948:GLU:HB3	2.04	0.40
2:D:276:ALA:HB2	2:D:655:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:VAL:HG11	1:E:309:ILE:HG21	2.03	0.40
2:H:742:ARG:NH1	2:H:742:ARG:HG2	2.34	0.40

There are no symmetry-related clashes.

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	773/802 (96%)	717 (93%)	50 (6%)	6 (1%)	19	29
1	C	771/802 (96%)	715 (93%)	48 (6%)	8 (1%)	15	23
1	E	777/802 (97%)	710 (91%)	60 (8%)	7 (1%)	17	26
1	G	778/802 (97%)	719 (92%)	50 (6%)	9 (1%)	13	19
2	B	1256/1334 (94%)	1162 (92%)	87 (7%)	7 (1%)	25	37
2	D	1253/1334 (94%)	1157 (92%)	84 (7%)	12 (1%)	15	23
2	F	1234/1334 (92%)	1139 (92%)	80 (6%)	15 (1%)	13	19
2	H	1231/1334 (92%)	1125 (91%)	91 (7%)	15 (1%)	13	19
All	All	8073/8544 (94%)	7444 (92%)	550 (7%)	79 (1%)	15	23

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	THR
1	A	367	SER
1	C	368	THR
2	D	618	GLY
2	D	1157	THR
2	D	1158	ALA
2	F	150	ASN
2	F	847	PHE

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Mol	Chain	Res	Type
2	F	857	THR
2	F	1157	THR
2	F	1158	ALA
1	G	262	SER
1	G	368	THR
1	G	783	SER
1	G	784	GLU
2	H	618	GLY
2	H	1157	THR
2	H	1262	ASN
1	A	368	THR
1	A	512	ASP
2	B	618	GLY
2	B	854	ASN
1	C	795	ASP
2	D	987	ALA
1	E	795	ASP
2	F	618	GLY
2	F	988	ASP
2	F	1259	ILE
1	G	782	LEU
1	G	795	ASP
2	H	1188	GLU
2	H	1259	ILE
2	H	1347	ASN
2	B	847	PHE
2	B	1188	GLU
1	C	182	ASN
1	C	284	ASP
2	D	1188	GLU
1	E	284	ASP
1	E	367	SER
2	F	684	ASN
2	F	1258	GLN
2	F	1263	ARG
2	F	1326	GLN
1	G	232	GLY
2	H	1326	GLN
1	A	365	THR
2	D	226	GLU
2	D	1263	ARG
1	E	232	GLY

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Mol	Chain	Res	Type
1	E	453	ILE
2	H	684	ASN
2	H	1258	GLN
2	B	586	ARG
1	C	367	SER
1	C	446	ASP
1	C	453	ILE
2	D	1187	LYS
1	E	368	THR
1	G	453	ILE
1	G	563	GLY
2	H	874	SER
2	B	855	ASN
1	C	563	GLY
2	D	264	MET
2	D	684	ASN
1	E	167	LYS
2	F	852	PRO
2	F	874	SER
2	H	97	ASN
2	H	1187	LYS
1	A	453	ILE
2	B	143	ILE
2	D	771	ILE
2	H	846	PRO
2	F	143	ILE
2	H	836	VAL
2	H	1345	PRO
2	D	143	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	685/701 (98%)	615 (90%)	70 (10%)	7	10
1	C	683/701 (97%)	616 (90%)	67 (10%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	684/701 (98%)	612 (90%)	72 (10%)	7	10
1	G	685/701 (98%)	624 (91%)	61 (9%)	9	14
2	B	1112/1171 (95%)	955 (86%)	157 (14%)	3	4
2	D	1109/1171 (95%)	949 (86%)	160 (14%)	3	3
2	F	1097/1171 (94%)	938 (86%)	159 (14%)	3	3
2	H	1093/1171 (93%)	951 (87%)	142 (13%)	4	5
All	All	7148/7488 (96%)	6260 (88%)	888 (12%)	4	6

All (888) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	48	THR
1	A	56	SER
1	A	57	LEU
1	A	65	GLN
1	A	66	ILE
1	A	73	ASN
1	A	79	LEU
1	A	84	ASP
1	A	90	GLU
1	A	104	GLN
1	A	107	LYS
1	A	125	THR
1	A	131	GLN
1	A	136	ASN
1	A	149	ILE
1	A	150	LEU
1	A	154	LEU
1	A	163	LEU
1	A	171	GLN
1	A	176	LEU
1	A	189	ASN
1	A	190	GLN
1	A	208	THR
1	A	209	THR
1	A	229	THR
1	A	243	THR
1	A	247	GLU
1	A	254	SER

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Mol	Chain	Res	Type
1	A	264	THR
1	A	275	LEU
1	A	305	THR
1	A	317	LEU
1	A	319	SER
1	A	334	SER
1	A	350	ASP
1	A	351	LYS
1	A	377	SER
1	A	386	SER
1	A	391	VAL
1	A	393	ASP
1	A	395	ILE
1	A	401	LYS
1	A	419	SER
1	A	421	LYS
1	A	444	THR
1	A	453	ILE
1	A	500	SER
1	A	508	ASN
1	A	532	GLU
1	A	537	ARG
1	A	571	SER
1	A	574	GLN
1	A	576	ARG
1	A	605	THR
1	A	638	VAL
1	A	657	VAL
1	A	665	ASN
1	A	670	SER
1	A	676	ILE
1	A	687	THR
1	A	706	GLU
1	A	732	ASN
1	A	745	ILE
1	A	770	GLN
1	A	782	LEU
1	A	793	ASP
1	A	796	GLN
1	A	803	LYS
1	A	806	ASN
2	B	63	GLU

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Mol	Chain	Res	Type
2	B	83	GLU
2	B	88	PHE
2	B	91	VAL
2	B	99	ASN
2	B	105	LYS
2	B	109	ASP
2	B	110	ASP
2	B	113	LYS
2	B	127	ASN
2	B	130	ILE
2	B	131	ARG
2	B	142	ASP
2	B	148	MET
2	B	150	ASN
2	B	154	VAL
2	B	187	VAL
2	B	200	LEU
2	B	203	VAL
2	B	204	LEU
2	B	219	GLN
2	B	226	GLU
2	B	235	ASN
2	B	238	GLN
2	B	242	LYS
2	B	256	LEU
2	B	264	MET
2	B	265	SER
2	B	270	THR
2	B	277	LEU
2	B	291	LEU
2	B	301	LYS
2	B	318	THR
2	B	324	LEU
2	B	328	ASP
2	B	333	GLU
2	B	334	LYS
2	B	350	GLU
2	B	358	VAL
2	B	384	ILE
2	B	393	LEU
2	B	396	THR
2	B	411	GLU

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Mol	Chain	Res	Type
2	B	420	SER
2	B	431	LYS
2	B	432	LYS
2	B	437	LYS
2	B	448	GLU
2	B	453	ASN
2	B	458	VAL
2	B	479	THR
2	B	523	LEU
2	B	528	ASN
2	B	529	ARG
2	B	562	THR
2	B	565	ARG
2	B	567	LYS
2	B	570	GLN
2	B	572	GLU
2	B	587	GLU
2	B	610	GLN
2	B	620	HIS
2	B	629	GLN
2	B	632	VAL
2	B	642	SER
2	B	649	LYS
2	B	662	TYR
2	B	673	LEU
2	B	679	SER
2	B	681	ASN
2	B	685	GLU
2	B	701	ASP
2	B	707	SER
2	B	708	ASP
2	B	709	LYS
2	B	710	ILE
2	B	725	ARG
2	B	728	GLN
2	B	732	LEU
2	B	733	ASN
2	B	742	ARG
2	B	751	THR
2	B	756	LEU
2	B	771	ILE
2	B	773	ASN

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Mol	Chain	Res	Type
2	B	790	SER
2	B	795	THR
2	B	803	VAL
2	B	806	MET
2	B	817	ARG
2	B	835	ARG
2	B	841	GLN
2	B	843	ASN
2	B	849	GLN
2	B	850	VAL
2	B	857	THR
2	B	864	ASP
2	B	869	THR
2	B	871	SER
2	B	906	GLN
2	B	921	VAL
2	B	922	LEU
2	B	925	LYS
2	B	939	GLN
2	B	943	LYS
2	B	945	GLU
2	B	947	ASN
2	B	956	GLU
2	B	965	LEU
2	B	974	THR
2	B	979	THR
2	B	986	LYS
2	B	1002	LEU
2	B	1012	LEU
2	B	1017	ASP
2	B	1029	ILE
2	B	1036	ARG
2	B	1039	THR
2	B	1042	LEU
2	B	1044	ILE
2	B	1045	THR
2	B	1052	GLN
2	B	1059	GLN
2	B	1061	TRP
2	B	1089	ASN
2	B	1123	LYS
2	B	1136	ASN

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Mol	Chain	Res	Type
2	B	1143	LEU
2	B	1157	THR
2	B	1164	ASN
2	B	1165	ASN
2	B	1170	SER
2	B	1171	GLN
2	B	1172	THR
2	B	1187	LYS
2	B	1191	SER
2	B	1202	ASP
2	B	1204	LYS
2	B	1246	SER
2	B	1249	GLU
2	B	1250	LYS
2	B	1258	GLN
2	B	1259	ILE
2	B	1262	ASN
2	B	1270	THR
2	B	1271	GLU
2	B	1288	LEU
2	B	1305	ILE
2	B	1308	SER
2	B	1310	GLU
2	B	1314	LEU
2	B	1318	LEU
2	B	1325	THR
2	B	1335	SER
2	B	1341	THR
2	B	1342	VAL
2	B	1344	GLN
1	C	48	THR
1	C	57	LEU
1	C	65	GLN
1	C	66	ILE
1	C	69	GLN
1	C	73	ASN
1	C	79	LEU
1	C	85	VAL
1	C	92	SER
1	C	95	ASN
1	C	101	SER
1	C	107	LYS

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Mol	Chain	Res	Type
1	C	117	SER
1	C	136	ASN
1	C	149	ILE
1	C	150	LEU
1	C	154	LEU
1	C	155	THR
1	C	163	LEU
1	C	170	THR
1	C	183	GLN
1	C	208	THR
1	C	224	GLU
1	C	243	THR
1	C	247	GLU
1	C	254	SER
1	C	264	THR
1	C	275	LEU
1	C	291	ILE
1	C	305	THR
1	C	317	LEU
1	C	334	SER
1	C	351	LYS
1	C	363	LYS
1	C	366	THR
1	C	384	LEU
1	C	391	VAL
1	C	393	ASP
1	C	395	ILE
1	C	401	LYS
1	C	421	LYS
1	C	444	THR
1	C	446	ASP
1	C	483	LYS
1	C	496	VAL
1	C	537	ARG
1	C	540	GLN
1	C	571	SER
1	C	574	GLN
1	C	576	ARG
1	C	580	VAL
1	C	638	VAL
1	C	639	MET
1	C	657	VAL

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Mol	Chain	Res	Type
1	C	670	SER
1	C	674	ASN
1	C	676	ILE
1	C	716	SER
1	C	719	LYS
1	C	732	ASN
1	C	745	ILE
1	C	782	LEU
1	C	785	GLU
1	C	793	ASP
1	C	796	GLN
1	C	806	ASN
1	C	813	THR
2	D	83	GLU
2	D	88	PHE
2	D	91	VAL
2	D	99	ASN
2	D	111	ASN
2	D	112	LEU
2	D	113	LYS
2	D	127	ASN
2	D	130	ILE
2	D	138	ARG
2	D	142	ASP
2	D	148	MET
2	D	154	VAL
2	D	182	GLU
2	D	187	VAL
2	D	200	LEU
2	D	203	VAL
2	D	204	LEU
2	D	219	GLN
2	D	222	LYS
2	D	226	GLU
2	D	235	ASN
2	D	238	GLN
2	D	242	LYS
2	D	249	SER
2	D	256	LEU
2	D	270	THR
2	D	272	THR
2	D	277	LEU

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Mol	Chain	Res	Type
2	D	291	LEU
2	D	301	LYS
2	D	316	GLU
2	D	318	THR
2	D	324	LEU
2	D	328	ASP
2	D	333	GLU
2	D	334	LYS
2	D	350	GLU
2	D	358	VAL
2	D	384	ILE
2	D	393	LEU
2	D	396	THR
2	D	420	SER
2	D	432	LYS
2	D	436	LYS
2	D	437	LYS
2	D	438	ASN
2	D	448	GLU
2	D	453	ASN
2	D	458	VAL
2	D	479	THR
2	D	523	LEU
2	D	529	ARG
2	D	547	ASN
2	D	562	THR
2	D	565	ARG
2	D	567	LYS
2	D	570	GLN
2	D	572	GLU
2	D	573	LYS
2	D	587	GLU
2	D	610	GLN
2	D	632	VAL
2	D	642	SER
2	D	649	LYS
2	D	650	LEU
2	D	662	TYR
2	D	668	ASN
2	D	673	LEU
2	D	679	SER
2	D	681	ASN

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Mol	Chain	Res	Type
2	D	701	ASP
2	D	707	SER
2	D	709	LYS
2	D	710	ILE
2	D	720	GLU
2	D	725	ARG
2	D	728	GLN
2	D	732	LEU
2	D	733	ASN
2	D	735	ASN
2	D	737	ASN
2	D	742	ARG
2	D	756	LEU
2	D	768	LEU
2	D	771	ILE
2	D	773	ASN
2	D	795	THR
2	D	797	SER
2	D	803	VAL
2	D	835	ARG
2	D	841	GLN
2	D	843	ASN
2	D	857	THR
2	D	864	ASP
2	D	874	SER
2	D	906	GLN
2	D	921	VAL
2	D	922	LEU
2	D	924	ASN
2	D	925	LYS
2	D	939	GLN
2	D	943	LYS
2	D	945	GLU
2	D	947	ASN
2	D	956	GLU
2	D	965	LEU
2	D	974	THR
2	D	979	THR
2	D	986	LYS
2	D	988	ASP
2	D	1002	LEU
2	D	1012	LEU

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Mol	Chain	Res	Type
2	D	1017	ASP
2	D	1036	ARG
2	D	1039	THR
2	D	1044	ILE
2	D	1045	THR
2	D	1052	GLN
2	D	1059	GLN
2	D	1061	TRP
2	D	1089	ASN
2	D	1117	THR
2	D	1120	THR
2	D	1123	LYS
2	D	1136	ASN
2	D	1143	LEU
2	D	1164	ASN
2	D	1170	SER
2	D	1171	GLN
2	D	1172	THR
2	D	1178	THR
2	D	1184	GLU
2	D	1187	LYS
2	D	1190	THR
2	D	1191	SER
2	D	1202	ASP
2	D	1204	LYS
2	D	1230	SER
2	D	1234	VAL
2	D	1240	GLN
2	D	1244	SER
2	D	1257	ASN
2	D	1260	ASP
2	D	1262	ASN
2	D	1270	THR
2	D	1271	GLU
2	D	1282	ASP
2	D	1288	LEU
2	D	1297	GLN
2	D	1305	ILE
2	D	1310	GLU
2	D	1314	LEU
2	D	1318	LEU
2	D	1324	GLN

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Mol	Chain	Res	Type
2	D	1327	GLN
2	D	1341	THR
2	D	1342	VAL
2	D	1344	GLN
2	D	1348	GLN
1	E	27	THR
1	E	31	LYS
1	E	48	THR
1	E	57	LEU
1	E	65	GLN
1	E	66	ILE
1	E	69	GLN
1	E	79	LEU
1	E	102	THR
1	E	103	SER
1	E	136	ASN
1	E	149	ILE
1	E	150	LEU
1	E	154	LEU
1	E	155	THR
1	E	163	LEU
1	E	165	LYS
1	E	170	THR
1	E	186	SER
1	E	187	GLN
1	E	211	ASN
1	E	217	SER
1	E	226	ILE
1	E	243	THR
1	E	247	GLU
1	E	254	SER
1	E	264	THR
1	E	275	LEU
1	E	284	ASP
1	E	305	THR
1	E	317	LEU
1	E	330	GLN
1	E	331	GLU
1	E	346	ASP
1	E	349	GLU
1	E	351	LYS
1	E	363	LYS

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Mol	Chain	Res	Type
1	E	366	THR
1	E	391	VAL
1	E	393	ASP
1	E	395	ILE
1	E	401	LYS
1	E	409	SER
1	E	419	SER
1	E	421	LYS
1	E	472	ASN
1	E	490	LYS
1	E	496	VAL
1	E	537	ARG
1	E	540	GLN
1	E	574	GLN
1	E	575	SER
1	E	576	ARG
1	E	580	VAL
1	E	595	LYS
1	E	604	VAL
1	E	605	THR
1	E	638	VAL
1	E	640	SER
1	E	657	VAL
1	E	680	SER
1	E	705	GLN
1	E	706	GLU
1	E	732	ASN
1	E	733	MET
1	E	745	ILE
1	E	770	GLN
1	E	772	THR
1	E	782	LEU
1	E	796	GLN
1	E	806	ASN
1	E	813	THR
2	F	63	GLU
2	F	83	GLU
2	F	88	PHE
2	F	91	VAL
2	F	99	ASN
2	F	105	LYS
2	F	113	LYS

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Mol	Chain	Res	Type
2	F	127	ASN
2	F	130	ILE
2	F	131	ARG
2	F	142	ASP
2	F	147	LYS
2	F	148	MET
2	F	149	GLU
2	F	154	VAL
2	F	163	ILE
2	F	173	THR
2	F	182	GLU
2	F	187	VAL
2	F	200	LEU
2	F	203	VAL
2	F	204	LEU
2	F	219	GLN
2	F	225	LEU
2	F	242	LYS
2	F	256	LEU
2	F	259	THR
2	F	270	THR
2	F	273	ARG
2	F	277	LEU
2	F	291	LEU
2	F	301	LYS
2	F	312	GLU
2	F	316	GLU
2	F	322	LYS
2	F	324	LEU
2	F	328	ASP
2	F	333	GLU
2	F	334	LYS
2	F	350	GLU
2	F	358	VAL
2	F	384	ILE
2	F	393	LEU
2	F	396	THR
2	F	411	GLU
2	F	420	SER
2	F	432	LYS
2	F	437	LYS
2	F	448	GLU

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Mol	Chain	Res	Type
2	F	453	ASN
2	F	457	MET
2	F	458	VAL
2	F	479	THR
2	F	501	THR
2	F	523	LEU
2	F	529	ARG
2	F	547	ASN
2	F	562	THR
2	F	565	ARG
2	F	567	LYS
2	F	570	GLN
2	F	572	GLU
2	F	587	GLU
2	F	610	GLN
2	F	620	HIS
2	F	631	ASN
2	F	632	VAL
2	F	642	SER
2	F	649	LYS
2	F	650	LEU
2	F	659	SER
2	F	662	TYR
2	F	668	ASN
2	F	673	LEU
2	F	679	SER
2	F	681	ASN
2	F	685	GLU
2	F	707	SER
2	F	709	LYS
2	F	710	ILE
2	F	725	ARG
2	F	728	GLN
2	F	732	LEU
2	F	733	ASN
2	F	737	ASN
2	F	742	ARG
2	F	756	LEU
2	F	763	GLN
2	F	768	LEU
2	F	771	ILE
2	F	773	ASN

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Mol	Chain	Res	Type
2	F	803	VAL
2	F	809	GLN
2	F	835	ARG
2	F	845	ILE
2	F	847	PHE
2	F	849	GLN
2	F	850	VAL
2	F	853	SER
2	F	856	SER
2	F	921	VAL
2	F	922	LEU
2	F	930	ASN
2	F	931	ASP
2	F	943	LYS
2	F	945	GLU
2	F	947	ASN
2	F	956	GLU
2	F	961	TYR
2	F	965	LEU
2	F	974	THR
2	F	978	SER
2	F	979	THR
2	F	988	ASP
2	F	1002	LEU
2	F	1012	LEU
2	F	1032	THR
2	F	1033	ASP
2	F	1036	ARG
2	F	1042	LEU
2	F	1044	ILE
2	F	1045	THR
2	F	1050	GLN
2	F	1052	GLN
2	F	1059	GLN
2	F	1061	TRP
2	F	1071	SER
2	F	1074	THR
2	F	1089	ASN
2	F	1117	THR
2	F	1120	THR
2	F	1123	LYS
2	F	1136	ASN

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Mol	Chain	Res	Type
2	F	1172	THR
2	F	1173	ILE
2	F	1187	LYS
2	F	1191	SER
2	F	1202	ASP
2	F	1204	LYS
2	F	1224	LYS
2	F	1230	SER
2	F	1234	VAL
2	F	1240	GLN
2	F	1246	SER
2	F	1260	ASP
2	F	1262	ASN
2	F	1270	THR
2	F	1271	GLU
2	F	1282	ASP
2	F	1288	LEU
2	F	1305	ILE
2	F	1310	GLU
2	F	1314	LEU
2	F	1318	LEU
2	F	1328	PHE
2	F	1337	THR
2	F	1341	THR
2	F	1342	VAL
2	F	1348	GLN
1	G	56	SER
1	G	57	LEU
1	G	65	GLN
1	G	66	ILE
1	G	69	GLN
1	G	79	LEU
1	G	90	GLU
1	G	101	SER
1	G	102	THR
1	G	107	LYS
1	G	118	THR
1	G	149	ILE
1	G	150	LEU
1	G	155	THR
1	G	159	LEU
1	G	163	LEU

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Mol	Chain	Res	Type
1	G	165	LYS
1	G	170	THR
1	G	186	SER
1	G	224	GLU
1	G	243	THR
1	G	247	GLU
1	G	254	SER
1	G	275	LEU
1	G	284	ASP
1	G	291	ILE
1	G	305	THR
1	G	317	LEU
1	G	326	GLU
1	G	331	GLU
1	G	332	ASN
1	G	351	LYS
1	G	363	LYS
1	G	366	THR
1	G	391	VAL
1	G	395	ILE
1	G	396	ILE
1	G	401	LYS
1	G	419	SER
1	G	421	LYS
1	G	496	VAL
1	G	500	SER
1	G	531	GLN
1	G	537	ARG
1	G	540	GLN
1	G	567	LYS
1	G	574	GLN
1	G	576	ARG
1	G	580	VAL
1	G	605	THR
1	G	638	VAL
1	G	652	THR
1	G	657	VAL
1	G	665	ASN
1	G	671	THR
1	G	676	ILE
1	G	732	ASN
1	G	745	ILE

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Mol	Chain	Res	Type
1	G	749	GLN
1	G	796	GLN
1	G	806	ASN
2	H	63	GLU
2	H	83	GLU
2	H	88	PHE
2	H	91	VAL
2	H	95	ASN
2	H	96	ASP
2	H	105	LYS
2	H	113	LYS
2	H	114	TYR
2	H	127	ASN
2	H	130	ILE
2	H	131	ARG
2	H	148	MET
2	H	149	GLU
2	H	154	VAL
2	H	163	ILE
2	H	187	VAL
2	H	200	LEU
2	H	204	LEU
2	H	219	GLN
2	H	242	LYS
2	H	256	LEU
2	H	259	THR
2	H	270	THR
2	H	277	LEU
2	H	291	LEU
2	H	301	LYS
2	H	316	GLU
2	H	324	LEU
2	H	328	ASP
2	H	333	GLU
2	H	334	LYS
2	H	350	GLU
2	H	358	VAL
2	H	391	ASN
2	H	393	LEU
2	H	396	THR
2	H	411	GLU
2	H	420	SER

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Mol	Chain	Res	Type
2	H	432	LYS
2	H	438	ASN
2	H	448	GLU
2	H	453	ASN
2	H	458	VAL
2	H	479	THR
2	H	523	LEU
2	H	529	ARG
2	H	562	THR
2	H	567	LYS
2	H	570	GLN
2	H	572	GLU
2	H	587	GLU
2	H	610	GLN
2	H	629	GLN
2	H	632	VAL
2	H	633	ASN
2	H	649	LYS
2	H	650	LEU
2	H	659	SER
2	H	662	TYR
2	H	668	ASN
2	H	673	LEU
2	H	679	SER
2	H	681	ASN
2	H	685	GLU
2	H	701	ASP
2	H	707	SER
2	H	709	LYS
2	H	710	ILE
2	H	725	ARG
2	H	728	GLN
2	H	732	LEU
2	H	737	ASN
2	H	742	ARG
2	H	768	LEU
2	H	771	ILE
2	H	773	ASN
2	H	803	VAL
2	H	835	ARG
2	H	843	ASN
2	H	845	ILE

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Mol	Chain	Res	Type
2	H	849	GLN
2	H	857	THR
2	H	864	ASP
2	H	906	GLN
2	H	921	VAL
2	H	922	LEU
2	H	939	GLN
2	H	943	LYS
2	H	945	GLU
2	H	947	ASN
2	H	956	GLU
2	H	965	LEU
2	H	986	LYS
2	H	988	ASP
2	H	992	SER
2	H	994	SER
2	H	1002	LEU
2	H	1012	LEU
2	H	1017	ASP
2	H	1032	THR
2	H	1036	ARG
2	H	1042	LEU
2	H	1044	ILE
2	H	1045	THR
2	H	1050	GLN
2	H	1052	GLN
2	H	1059	GLN
2	H	1061	TRP
2	H	1069	LEU
2	H	1072	ASP
2	H	1074	THR
2	H	1105	GLN
2	H	1117	THR
2	H	1120	THR
2	H	1123	LYS
2	H	1136	ASN
2	H	1169	VAL
2	H	1171	GLN
2	H	1172	THR
2	H	1174	ASN
2	H	1191	SER
2	H	1202	ASP

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Mol	Chain	Res	Type
2	H	1204	LYS
2	H	1230	SER
2	H	1234	VAL
2	H	1240	GLN
2	H	1267	LEU
2	H	1270	THR
2	H	1282	ASP
2	H	1288	LEU
2	H	1301	ARG
2	H	1305	ILE
2	H	1310	GLU
2	H	1314	LEU
2	H	1318	LEU
2	H	1319	GLU
2	H	1328	PHE
2	H	1341	THR
2	H	1342	VAL
2	H	1346	PHE
2	H	1348	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	136	ASN
1	A	171	GLN
1	A	194	ASN
1	A	211	ASN
1	A	270	ASN
1	A	293	GLN
1	A	392	ASN
1	A	394	GLN
1	A	454	ASN
1	A	460	GLN
1	A	530	ASN
1	A	531	GLN
1	A	574	GLN
1	A	599	ASN
1	A	662	ASN
1	A	665	ASN
1	A	722	HIS
1	A	748	ASN

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Mol	Chain	Res	Type
1	A	796	GLN
1	A	797	ASN
1	A	806	ASN
2	B	99	ASN
2	B	127	ASN
2	B	144	ASN
2	B	218	ASN
2	B	235	ASN
2	B	302	HIS
2	B	360	HIS
2	B	391	ASN
2	B	395	GLN
2	B	462	ASN
2	B	528	ASN
2	B	548	GLN
2	B	570	GLN
2	B	582	GLN
2	B	610	GLN
2	B	620	HIS
2	B	684	ASN
2	B	728	GLN
2	B	733	ASN
2	B	735	ASN
2	B	745	ASN
2	B	748	GLN
2	B	773	ASN
2	B	841	GLN
2	B	849	GLN
2	B	895	ASN
2	B	908	ASN
2	B	924	ASN
2	B	932	GLN
2	B	939	GLN
2	B	1011	ASN
2	B	1119	ASN
2	B	1165	ASN
2	B	1258	GLN
2	B	1327	GLN
2	B	1333	ASN
1	C	104	GLN
1	C	136	ASN
1	C	182	ASN

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Mol	Chain	Res	Type
1	C	183	GLN
1	C	211	ASN
1	C	394	GLN
1	C	454	ASN
1	C	530	ASN
1	C	531	GLN
1	C	574	GLN
1	C	599	ASN
1	C	662	ASN
1	C	665	ASN
1	C	796	GLN
1	C	797	ASN
1	C	804	ASN
2	D	59	GLN
2	D	84	ASN
2	D	127	ASN
2	D	235	ASN
2	D	241	GLN
2	D	360	HIS
2	D	395	GLN
2	D	547	ASN
2	D	548	GLN
2	D	570	GLN
2	D	620	HIS
2	D	631	ASN
2	D	684	ASN
2	D	728	GLN
2	D	733	ASN
2	D	773	ASN
2	D	823	ASN
2	D	939	GLN
2	D	947	ASN
2	D	975	ASN
2	D	1011	ASN
2	D	1119	ASN
2	D	1311	ASN
2	D	1324	GLN
2	D	1333	ASN
1	E	65	GLN
1	E	73	ASN
1	E	136	ASN
1	E	143	GLN

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Mol	Chain	Res	Type
1	E	293	GLN
1	E	330	GLN
1	E	454	ASN
1	E	472	ASN
1	E	530	ASN
1	E	574	GLN
1	E	599	ASN
1	E	662	ASN
1	E	665	ASN
1	E	732	ASN
1	E	748	ASN
1	E	797	ASN
1	E	804	ASN
2	F	127	ASN
2	F	144	ASN
2	F	235	ASN
2	F	352	HIS
2	F	360	HIS
2	F	391	ASN
2	F	395	GLN
2	F	418	ASN
2	F	547	ASN
2	F	570	GLN
2	F	580	GLN
2	F	620	HIS
2	F	631	ASN
2	F	634	ASN
2	F	684	ASN
2	F	728	GLN
2	F	748	GLN
2	F	763	GLN
2	F	773	ASN
2	F	823	ASN
2	F	939	GLN
2	F	947	ASN
2	F	958	ASN
2	F	1011	ASN
2	F	1108	GLN
2	F	1171	GLN
2	F	1235	ASN
2	F	1311	ASN
2	F	1347	ASN

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Mol	Chain	Res	Type
2	F	1348	GLN
1	G	65	GLN
1	G	72	HIS
1	G	73	ASN
1	G	180	GLN
1	G	183	GLN
1	G	285	GLN
1	G	293	GLN
1	G	308	HIS
1	G	392	ASN
1	G	454	ASN
1	G	574	GLN
1	G	662	ASN
1	G	665	ASN
1	G	749	GLN
1	G	766	GLN
1	G	797	ASN
1	G	804	ASN
1	G	814	GLN
2	H	95	ASN
2	H	97	ASN
2	H	235	ASN
2	H	360	HIS
2	H	391	ASN
2	H	395	GLN
2	H	418	ASN
2	H	570	GLN
2	H	631	ASN
2	H	634	ASN
2	H	728	GLN
2	H	735	ASN
2	H	773	ASN
2	H	812	ASN
2	H	823	ASN
2	H	932	GLN
2	H	939	GLN
2	H	947	ASN
2	H	958	ASN
2	H	1011	ASN
2	H	1311	ASN
2	H	1312	GLN
2	H	1333	ASN

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Mol	Chain	Res	Type
2	H	1348	GLN

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 monosaccharides 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, 95th 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 ²)	Q<0.9
1	A	781/802 (97%)	-0.55	6 (0%) 86 85	8, 29, 71, 112	0
1	C	779/802 (97%)	-0.55	6 (0%) 86 85	9, 28, 73, 99	0
1	E	783/802 (97%)	-0.58	6 (0%) 86 85	7, 29, 68, 109	0
1	G	784/802 (97%)	-0.53	7 (0%) 84 83	8, 32, 69, 105	0
2	B	1268/1334 (95%)	-0.51	5 (0%) 92 93	7, 29, 76, 130	0
2	D	1265/1334 (94%)	-0.57	7 (0%) 89 89	6, 27, 73, 118	0
2	F	1250/1334 (93%)	-0.19	42 (3%) 45 41	9, 44, 103, 136	0
2	H	1247/1334 (93%)	-0.03	46 (3%) 41 38	14, 55, 115, 149	0
All	All	8157/8544 (95%)	-0.41	125 (1%) 73 71	6, 34, 91, 149	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	856	SER	7.1
1	A	367	SER	6.8
2	F	1265	PHE	6.1
2	H	855	ASN	6.0
2	H	1294	GLY	6.0
1	E	366	THR	5.3
2	F	268	MET	5.3
1	A	366	THR	4.7
1	C	365	THR	4.6
2	D	265	SER	4.6
2	B	1264	LEU	4.6
2	H	839	ALA	4.5
2	F	1294	GLY	4.2
2	H	110	ASP	4.2
2	F	288	ASP	4.1
1	G	793	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	412	SER	3.9
1	G	795	ASP	3.9
2	B	266	SER	3.9
2	H	1190	THR	3.9
1	C	366	THR	3.8
2	H	243	ASP	3.8
2	F	1269	VAL	3.7
2	B	265	SER	3.6
2	H	840	ASN	3.5
2	F	1283	GLN	3.5
2	F	1324	GLN	3.5
2	H	227	VAL	3.3
2	B	1265	PHE	3.3
2	D	1264	LEU	3.3
2	H	1312	GLN	3.3
2	H	1271	GLU	3.3
1	C	493	LYS	3.3
1	E	181	ALA	3.3
2	H	1277	THR	3.2
2	H	425	VAL	3.2
2	F	1097	ASN	3.2
2	H	1158	ALA	3.2
2	H	288	ASP	3.1
2	H	616	LYS	3.1
2	F	782	SER	3.0
2	F	1264	LEU	3.0
2	H	859	PHE	3.0
1	E	367	SER	3.0
2	H	874	SER	3.0
2	H	974	THR	3.0
2	F	1262	ASN	3.0
2	H	1191	SER	3.0
2	H	1270	THR	3.0
2	F	1268	PRO	3.0
2	D	855	ASN	3.0
2	D	1284	TYR	3.0
2	H	841	GLN	2.9
2	F	855	ASN	2.9
2	F	1158	ALA	2.9
2	H	1283	GLN	2.9
1	E	368	THR	2.9
1	G	366	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	319	GLU	2.8
2	B	855	ASN	2.8
2	F	613	MET	2.8
2	F	1310	GLU	2.8
2	H	316	GLU	2.8
2	H	1310	GLU	2.8
1	C	368	THR	2.8
1	A	121	GLY	2.8
2	H	256	LEU	2.7
2	F	94	GLN	2.7
2	F	1263	ARG	2.7
2	F	210	ALA	2.7
2	F	989	SER	2.7
2	D	1263	ARG	2.7
2	F	1323	PRO	2.6
2	F	1285	VAL	2.6
1	C	367	SER	2.6
2	H	1324	GLN	2.6
2	D	1265	PHE	2.6
2	F	864	ASP	2.6
2	F	1267	LEU	2.6
2	F	113	LYS	2.6
2	H	317	PHE	2.6
2	F	1312	GLN	2.5
1	C	182	ASN	2.5
1	A	182	ASN	2.5
2	F	840	ASN	2.5
1	E	365	THR	2.5
2	H	276	ALA	2.4
2	F	1190	THR	2.4
2	F	1270	THR	2.4
2	F	1156	GLY	2.4
2	F	1305	ILE	2.4
2	H	149	GLU	2.4
2	F	1259	ILE	2.3
2	H	1246	SER	2.3
2	H	1136	ASN	2.3
2	D	1314	LEU	2.3
1	A	368	THR	2.3
2	F	1157	THR	2.3
2	H	864	ASP	2.3
2	F	209	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	1293	SER	2.3
2	F	851	LYS	2.3
2	H	145	LEU	2.2
2	H	59	GLN	2.2
2	F	780	SER	2.2
2	F	1260	ASP	2.2
2	F	1089	ASN	2.2
2	F	1131	THR	2.2
1	G	179	GLY	2.1
2	F	857	THR	2.1
2	H	1307	TYR	2.1
2	H	851	LYS	2.1
1	G	794	SER	2.1
1	G	494	SER	2.1
2	H	1269	VAL	2.1
2	H	327	THR	2.1
2	F	234	PHE	2.1
2	F	100	ILE	2.1
2	H	628	ILE	2.1
1	G	495	THR	2.1
2	H	315	LYS	2.0
2	H	313	ALA	2.0
2	H	1131	THR	2.0
1	E	182	ASN	2.0
2	H	1309	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.