



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:42 PM UTC

PDB ID : 9EA9 / pdb\_00009ea9  
Title : Crystal structure of BoNT/A-NTNH-HA70 -VHH\_F12-VHH\_H7-Fab\_NTN  
H complex  
Authors : Lam, K.H.; Gao, L.; Jin, R.  
Deposited on : 2024-11-10  
Resolution : 2.93 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

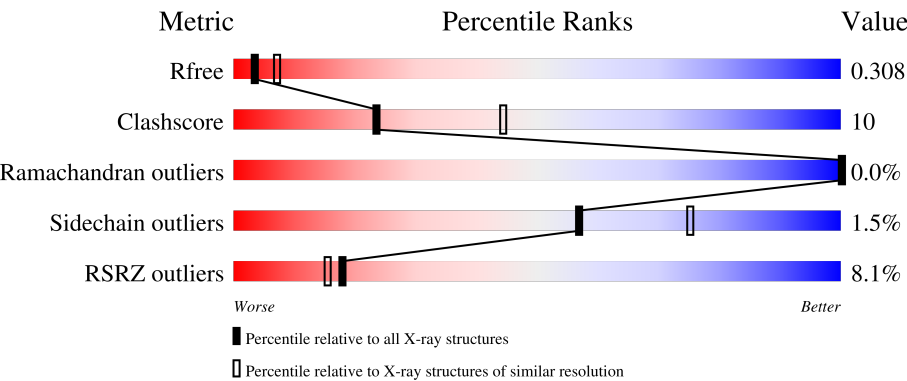
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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))
$R_{free}$	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	A	1296	<div><div>5%</div><div><div></div><div>75%</div><div>23%</div><div>.</div></div></div>
2	B	1194	<div><div>4%</div><div><div></div><div>75%</div><div>23%</div><div>..</div></div></div>
3	C	128	<div><div>11%</div><div><div></div><div>64%</div><div>27%</div><div>9%</div></div></div>
4	F	121	<div><div>3%</div><div><div></div><div>74%</div><div>19%</div><div>6%</div></div></div>
5	D	626	<div><div>%</div><div><div></div><div>20%</div><div>8%</div><div>72%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	G	626	
5	H	626	
5	I	626	
5	J	626	
6	E	626	
7	K	105	
8	M	117	
9	N	94	
10	L	103	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	SO4	A	1301	-	-	X	-
11	SO4	E	701	-	-	X	-
13	MG	E	705	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 39218 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0	0
			10371	6651	1716	1971	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	VAL	variant	UNP P0DPI0
A	224	GLN	GLU	conflict	UNP P0DPI0
A	363	ALA	ARG	conflict	UNP P0DPI0
A	366	PHE	TYR	conflict	UNP P0DPI0

- Molecule 2 is a protein called Non-toxic nonhemagglutinin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1187	Total	C	N	O	S	0	0	0
			9671	6194	1553	1892	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	426	SER	THR	conflict	UNP Q45914
B	1194	PRO	-	expression tag	UNP Q45914

- Molecule 3 is a protein called Nanobody ciA-F12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	117	Total	C	N	O	S	0	0	0
			873	540	153	176	4			

- Molecule 4 is a protein called Nanobody ciA-H7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	114	Total	C	N	O	S	0	0	0
			853	529	151	168	5			

- Molecule 5 is a protein called HA-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	169	Total	C	N	O	S	0	0	0
			1376	891	223	260	2			
5	J	421	Total	C	N	O	S	0	0	0
			3366	2121	564	676	5			
5	D	174	Total	C	N	O	S	0	0	0
			1409	914	228	265	2			
5	G	169	Total	C	N	O	S	0	0	0
			1382	894	223	263	2			
5	H	421	Total	C	N	O	S	0	0	0
			3363	2120	562	676	5			

- Molecule 6 is a protein called HA70/A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	421	Total	C	N	O	S	0	0	0
			3358	2115	561	677	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	575	ASP	ILE	conflict	UNP Q8KHU9
E	576	ALA	ASP	conflict	UNP Q8KHU9

- Molecule 7 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	105	Total	C	N	O	S	0	0	0
			803	505	134	162	2			

- Molecule 8 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	117	Total	C	N	O	S	0	0	0
			881	557	144	176	4			

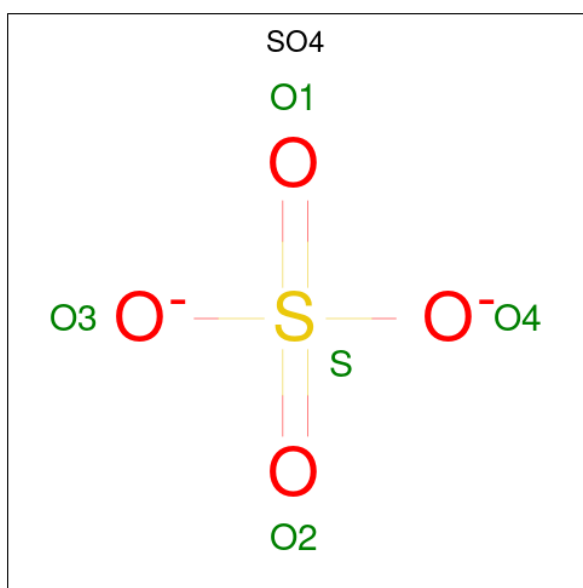
- Molecule 9 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	94	Total	C	N	O	S	8	0	0
			634	399	104	129	2			

- Molecule 10 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	103	Total	C	N	O	S	0	0	0
			752	460	129	160	3			

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Mg	0	0
			1	1		
13	B	1	Total	Mg	0	0
			1	1		
13	J	1	Total	Mg	0	0
			1	1		
13	E	6	Total	Mg	0	0
			6	6		
13	H	1	Total	Mg	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	25	Total	O	0	0
			25	25		
14	B	15	Total	O	0	0
			15	15		
14	F	4	Total	O	0	0
			4	4		
14	I	3	Total	O	0	0
			3	3		
14	J	2	Total	O	0	0
			2	2		
14	D	3	Total	O	0	0
			3	3		
14	E	8	Total	O	0	0
			8	8		

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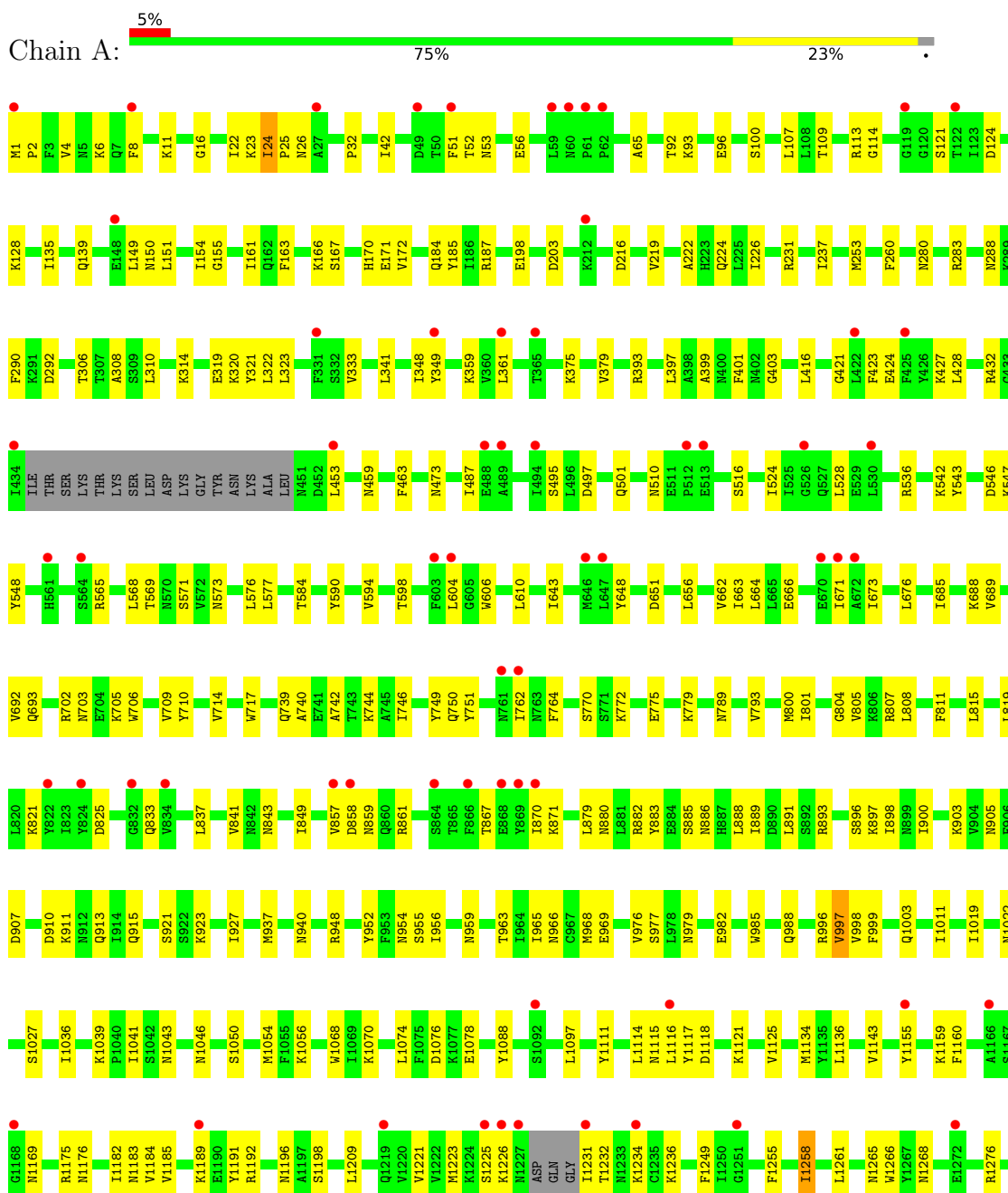
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	G	2	Total	O	0	0
			2	2		
14	H	2	Total	O	0	0
			2	2		
14	M	1	Total	O	0	0
			1	1		

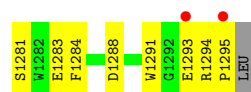


### 3 Residue-property plots

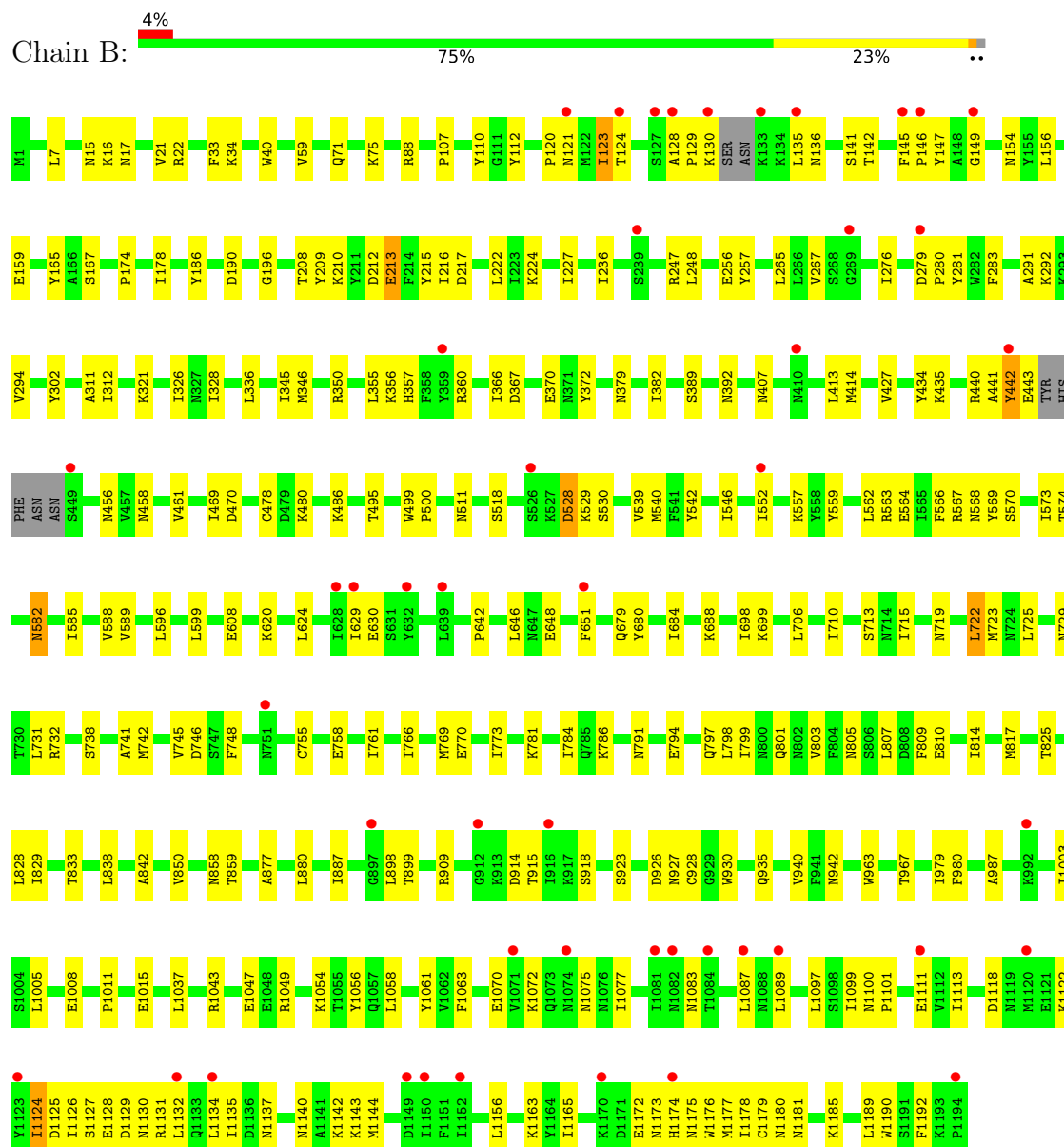
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Botulinum neurotoxin type A

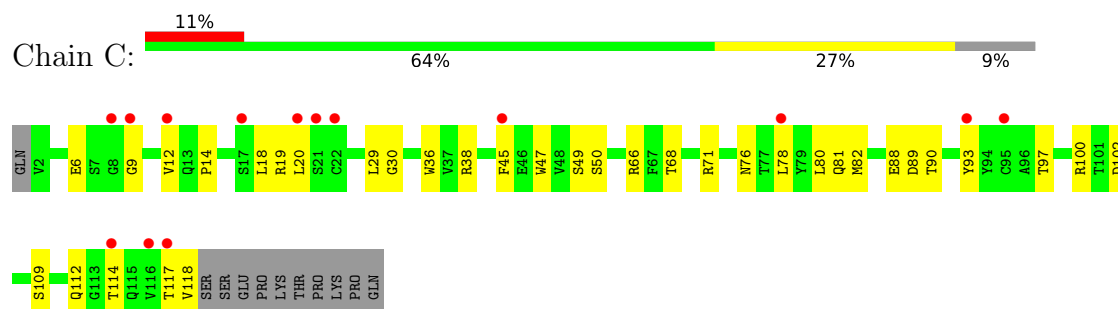




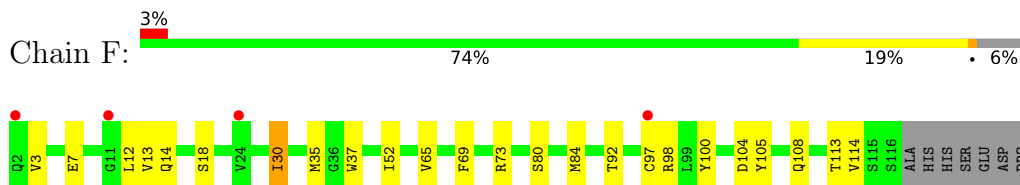
- Molecule 2: Non-toxic nonhemagglutinin type A



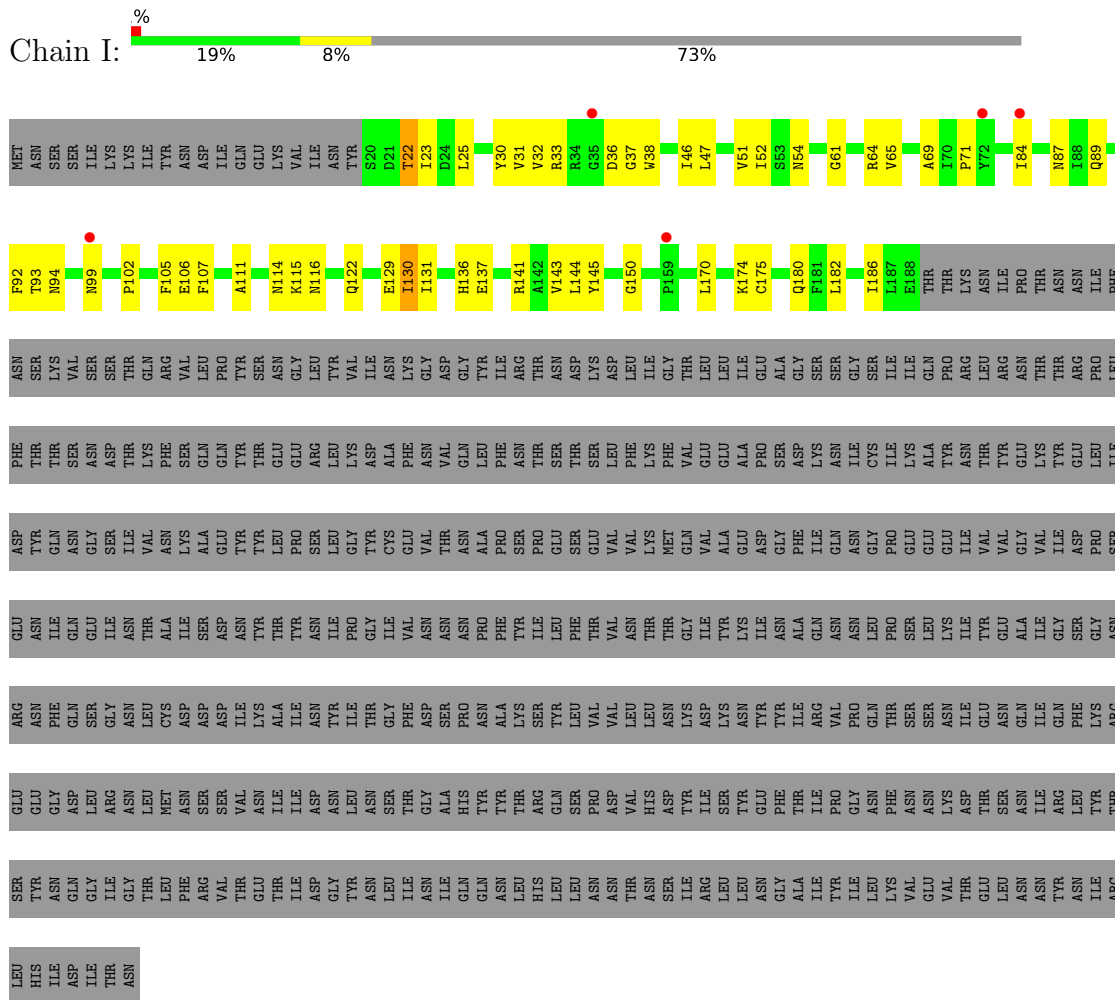
- Molecule 3: Nanobody ciA-F12



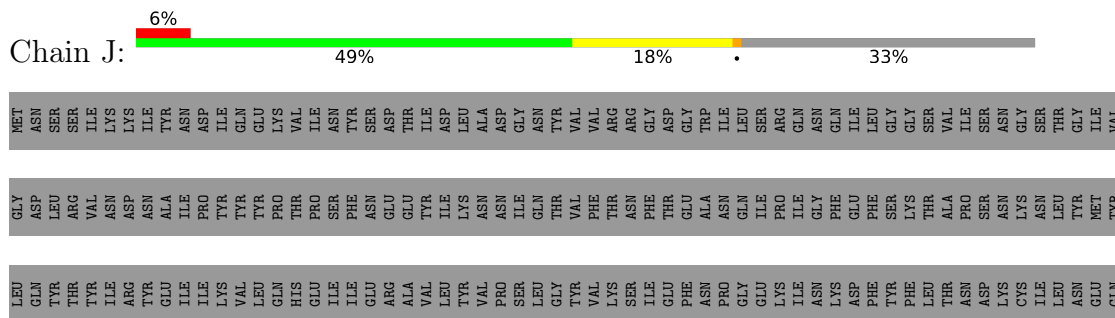
- Molecule 4: Nanobody ciA-H7

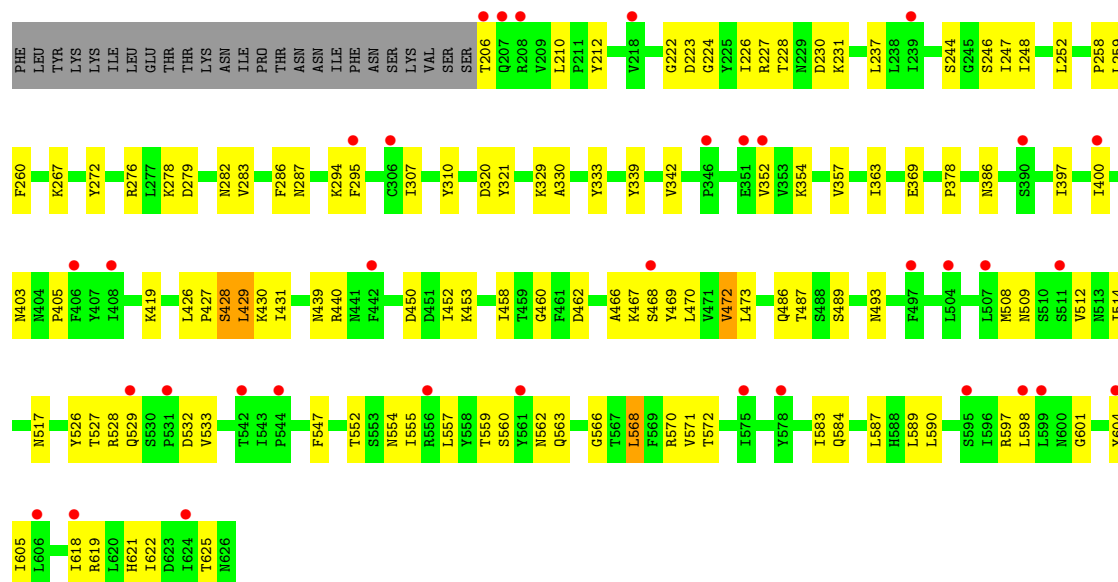


- Molecule 5: HA-70

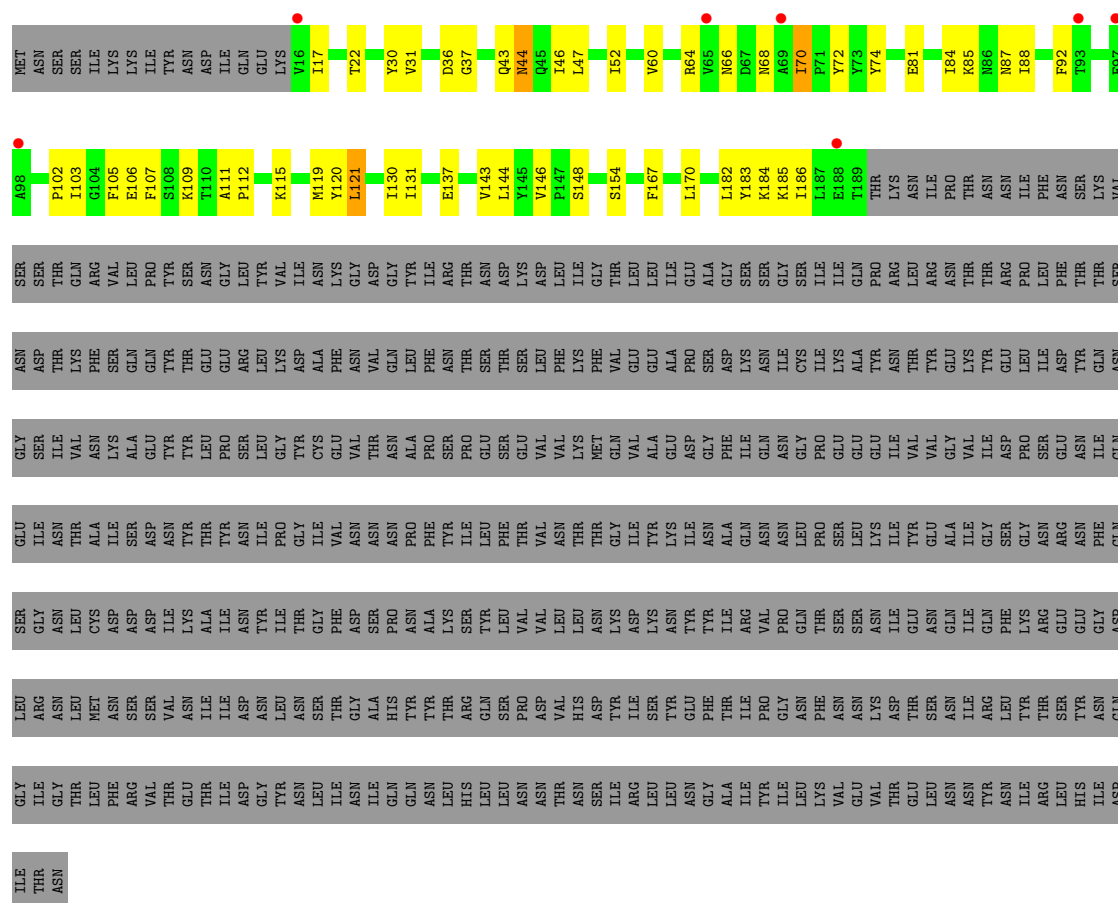


- Molecule 5: HA-70

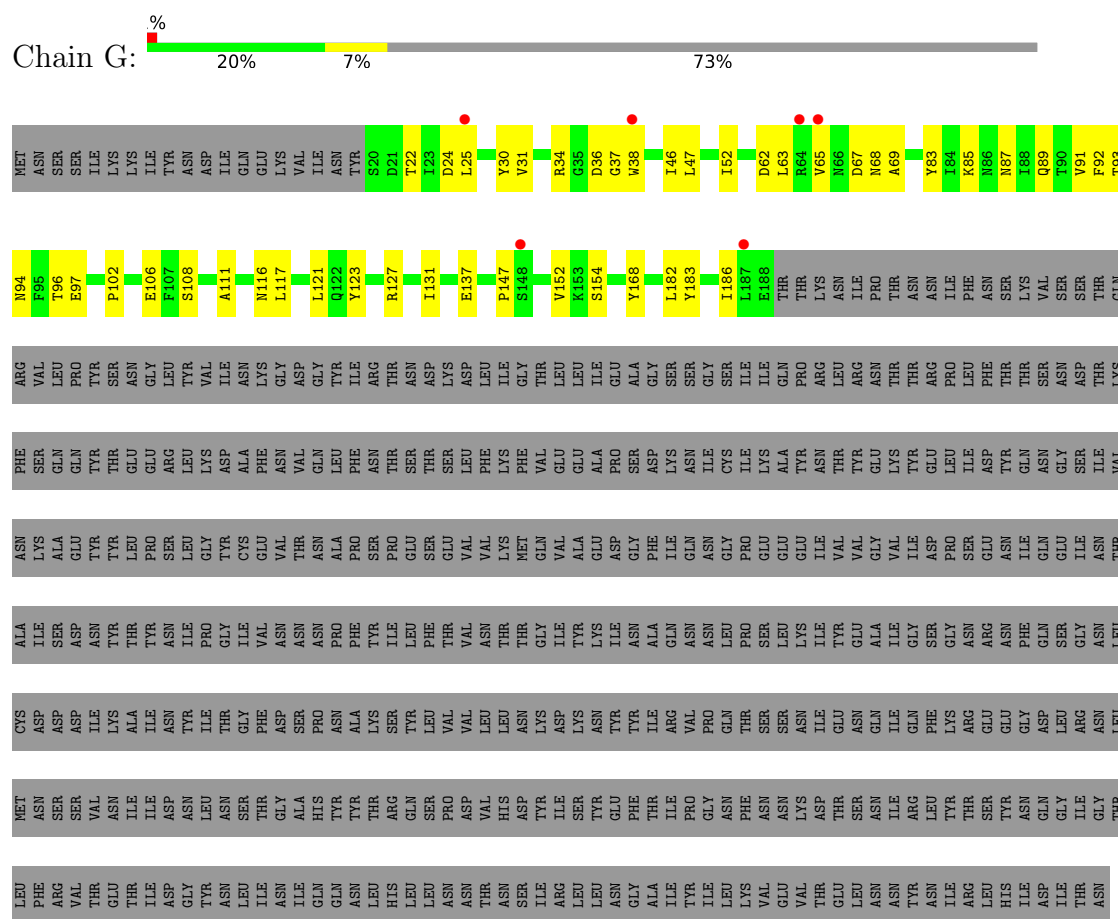




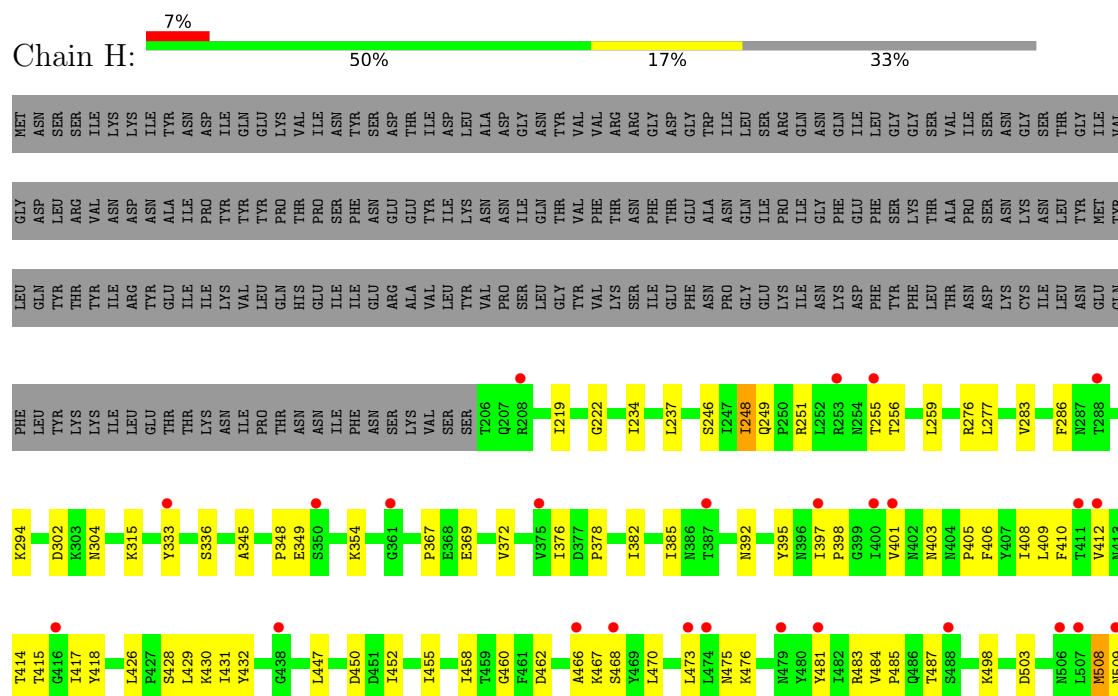
• Molecule 5: HA-70

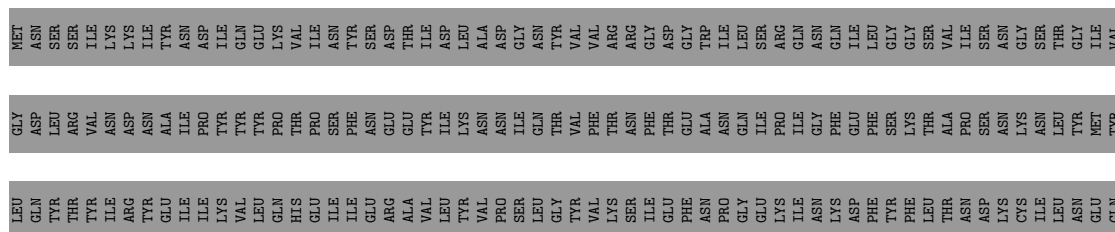
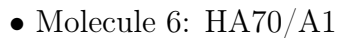


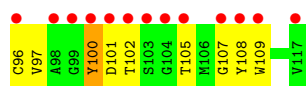
• Molecule 5: HA-70



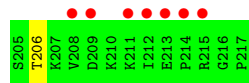
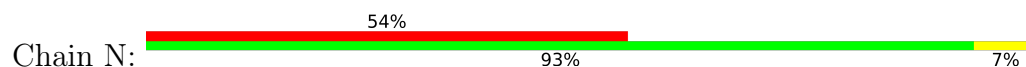
- Molecule 5: HA-70



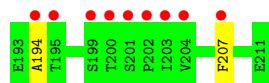
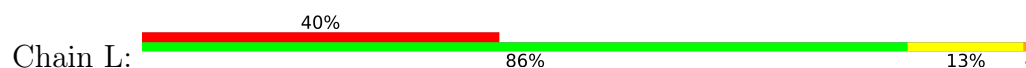




● Molecule 9: anti-NTNH Fab



● Molecule 10: anti-NTNH Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.65Å 203.65Å 479.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.61 – 2.93 99.61 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.61-2.93) 99.9 (99.61-2.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5107	Depositor
R, $R_{free}$	0.286 , 0.308 0.287 , 0.308	Depositor DCC
$R_{free}$ test set	2000 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	39218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, MG

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	0.14	0/10590	0.32	0/14338
2	B	0.15	0/9876	0.34	0/13390
3	C	0.16	0/893	0.34	0/1213
4	F	0.15	0/867	0.35	0/1167
5	D	0.16	0/1442	0.37	0/1959
5	G	0.11	0/1414	0.32	0/1919
5	H	0.14	0/3426	0.36	0/4662
5	I	0.13	0/1408	0.36	0/1911
5	J	0.13	0/3429	0.36	0/4667
6	E	0.13	0/3421	0.35	0/4657
7	K	0.29	0/821	0.50	0/1116
8	M	0.15	0/902	0.34	0/1226
9	N	0.11	0/650	0.33	0/900
10	L	0.13	0/768	0.31	0/1047
All	All	0.14	0/39907	0.34	0/54172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10371	0	10228	199	0
2	B	9671	0	9434	189	0
3	C	873	0	812	20	0
4	F	853	0	830	17	0
5	D	1409	0	1375	41	0
5	G	1382	0	1357	38	0
5	H	3363	0	3265	73	0
5	I	1376	0	1348	35	0
5	J	3366	0	3267	84	0
6	E	3358	0	3253	69	0
7	K	803	0	766	30	0
8	M	881	0	834	23	0
9	N	634	0	579	4	0
10	L	752	0	650	10	0
11	A	20	0	0	3	0
11	B	20	0	0	1	0
11	D	5	0	0	0	0
11	E	5	0	0	4	0
12	A	1	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	E	6	0	0	0	0
13	H	1	0	0	0	0
13	J	1	0	0	0	0
14	A	25	0	0	4	0
14	B	15	0	0	3	0
14	D	3	0	0	1	0
14	E	8	0	0	3	0
14	F	4	0	0	0	0
14	G	2	0	0	0	0
14	H	2	0	0	1	0
14	I	3	0	0	0	0
14	J	2	0	0	0	0
14	M	1	0	0	0	0
All	All	39218	0	37998	785	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 10.

All (785) 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)
10:L:143:ASN:HB3	10:L:145:LYS:HE2	1.47	0.96
5:J:584:GLN:HG3	5:J:587:LEU:HD11	1.48	0.92
5:I:54:ASN:HD22	5:I:114:ASN:H	1.22	0.87
1:A:903:LYS:HG3	1:A:921:SER:HB2	1.55	0.87
2:B:120:PRO:HB3	2:B:146:PRO:HD2	1.57	0.87
7:K:55:ILE:HG13	8:M:100:TYR:OH	1.77	0.84
1:A:709:VAL:HG21	1:A:808:LEU:HD21	1.61	0.82
1:A:717:TRP:HB2	1:A:800:MET:HE1	1.61	0.82
5:G:89:GLN:HG2	5:G:94:ASN:HA	1.63	0.81
1:A:952:TYR:H	1:A:1003:GLN:HE22	1.29	0.81
2:B:528:ASP:HB2	2:B:530:SER:H	1.51	0.76
5:J:562:ASN:HB2	5:J:618:ILE:HD13	1.66	0.74
1:A:24:ILE:HD11	1:A:51:PHE:CE2	2.23	0.74
5:G:92:PHE:HE1	5:G:182:LEU:HD23	1.52	0.74
5:D:84:ILE:O	5:D:88:ILE:HG12	1.89	0.73
5:H:415:THR:HG22	5:H:475:ASN:HA	1.70	0.73
1:A:880:ASN:OD1	1:A:882:ARG:NH1	2.22	0.73
5:G:117:LEU:HD21	5:G:154:SER:HB2	1.70	0.73
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.71	0.72
2:B:59:VAL:HG12	2:B:486:LYS:HD2	1.71	0.72
6:E:568:LEU:HB3	6:E:584:GLN:HB3	1.71	0.72
1:A:648:TYR:N	1:A:651:ASP:OD2	2.23	0.71
1:A:1088:TYR:HH	1:A:1231:ILE:N	1.87	0.71
5:G:94:ASN:HD21	5:G:97:GLU:HB2	1.55	0.71
5:H:529:GLN:HB3	14:H:802:HOH:O	1.91	0.70
2:B:360:ARG:HE	2:B:360:ARG:HA	1.55	0.70
7:K:47:LEU:HD22	7:K:58:ILE:CG2	2.22	0.69
1:A:473:ASN:HB2	14:A:1403:HOH:O	1.91	0.69
7:K:44:PRO:HG2	8:M:45:LEU:HD11	1.74	0.69
5:H:542:THR:HG22	5:H:603:ILE:HG12	1.74	0.69
1:A:709:VAL:CG2	1:A:808:LEU:HD21	2.23	0.69
2:B:379:ASN:HD21	2:B:858:ASN:HD21	1.40	0.68
2:B:145:PHE:HB3	2:B:146:PRO:HD3	1.76	0.68
2:B:511:ASN:HD22	2:B:530:SER:HA	1.59	0.68
5:H:259:LEU:HB2	5:H:333:TYR:HB2	1.74	0.68
6:E:249:GLN:HE21	6:E:251:ARG:H	1.42	0.68
2:B:442:TYR:HD1	2:B:443:GLU:HG3	1.59	0.68
2:B:22:ARG:NH1	2:B:159:GLU:O	2.26	0.68
5:I:52:ILE:HG13	5:I:111:ALA:HB2	1.77	0.67
7:K:34:HIS:HD2	7:K:88:GLN:HE21	1.41	0.67
5:D:44:ASN:HD21	5:D:170:LEU:HB2	1.58	0.67
5:G:89:GLN:NE2	5:G:94:ASN:OD1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:17:SER:HB3	8:M:84:ILE:HG13	1.76	0.67
1:A:24:ILE:HD11	1:A:51:PHE:HE2	1.57	0.67
2:B:486:LYS:NZ	11:B:1202:SO4:O4	2.28	0.66
5:D:183:TYR:HE2	5:H:354:LYS:HB3	1.60	0.66
5:H:543:ILE:HD12	5:H:543:ILE:H	1.60	0.66
7:K:55:ILE:HG22	7:K:58:ILE:HG12	1.77	0.66
5:G:46:ILE:HG22	5:H:283:VAL:HG12	1.76	0.66
5:D:81:GLU:CD	5:D:81:GLU:H	2.01	0.65
2:B:212:ASP:OD2	2:B:688:LYS:NZ	2.27	0.65
5:H:349:GLU:OE1	5:H:349:GLU:N	2.26	0.65
2:B:1173:ASN:O	2:B:1174:HIS:ND1	2.29	0.65
2:B:1135:ILE:HD12	2:B:1137:ASN:H	1.61	0.65
1:A:598:THR:O	1:A:750:GLN:NE2	2.29	0.65
5:G:31:VAL:HG21	5:G:91:VAL:HG21	1.79	0.65
2:B:719:ASN:O	2:B:723:MET:HG3	1.96	0.65
10:L:134:LEU:HD22	10:L:173:MET:HE1	1.79	0.65
5:D:52:ILE:HG13	5:D:111:ALA:HB2	1.79	0.64
3:C:82:MET:HE1	3:C:93:TYR:CE2	2.32	0.64
1:A:888:LEU:HB3	1:A:900:ILE:HD11	1.77	0.64
5:H:395:TYR:HE1	5:H:398:PRO:HD3	1.63	0.64
2:B:706:LEU:O	2:B:710:ILE:HG13	1.98	0.64
1:A:705:LYS:O	1:A:709:VAL:HG22	1.98	0.64
5:J:259:LEU:HB2	5:J:333:TYR:HB2	1.80	0.64
2:B:1132:LEU:HD11	2:B:1165:ILE:HD13	1.78	0.64
2:B:435:LYS:NZ	14:B:1301:HOH:O	2.31	0.64
5:I:84:ILE:HG12	5:I:130:ILE:HG13	1.79	0.64
7:K:49:LYS:H	7:K:55:ILE:HD13	1.63	0.64
2:B:784:ILE:HD13	2:B:798:LEU:HB3	1.78	0.63
2:B:979:ILE:HB	2:B:987:ALA:HB3	1.79	0.63
5:I:115:LYS:HD3	5:I:116:ASN:H	1.62	0.63
5:D:22:THR:HA	5:D:137:GLU:HA	1.79	0.63
6:E:625:THR:OG1	6:E:626:ASN:ND2	2.32	0.63
7:K:47:LEU:HD22	7:K:58:ILE:HG23	1.80	0.63
5:H:555:ILE:HD12	5:H:624:ILE:HG12	1.81	0.63
2:B:770:GLU:HA	2:B:773:ILE:HG12	1.80	0.63
1:A:673:ILE:HG22	1:A:807:ARG:HG3	1.81	0.63
6:E:405:PRO:HD3	6:E:486:GLN:HB2	1.80	0.63
4:F:98:ARG:NH2	4:F:104:ASP:OD1	2.23	0.62
1:A:1114:LEU:HB3	1:A:1283:GLU:HB2	1.81	0.62
5:J:467:LYS:HB3	5:J:514:ILE:HB	1.81	0.62
7:K:51:ALA:HB1	7:K:65:GLY:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:473:LEU:H	5:H:509:ASN:ND2	1.98	0.61
2:B:1172:GLU:H	2:B:1173:ASN:HA	1.65	0.61
5:I:170:LEU:HD21	5:I:174:LYS:HG2	1.81	0.61
6:E:385:ILE:HD11	6:E:395:TYR:HD2	1.66	0.61
2:B:914:ASP:OD1	2:B:915:THR:N	2.32	0.61
4:F:108:GLN:N	4:F:108:GLN:OE1	2.34	0.61
1:A:1115:ASN:HD21	1:A:1117:TYR:HB3	1.66	0.61
2:B:528:ASP:HB2	2:B:530:SER:N	2.15	0.61
1:A:985:TRP:HB3	1:A:997:VAL:HG22	1.82	0.61
5:J:466:ALA:HB2	5:J:528:ARG:HH21	1.66	0.61
8:M:102:THR:HB	8:M:105:THR:HG23	1.83	0.60
1:A:198:GLU:HG2	1:A:361:LEU:HD11	1.83	0.60
2:B:518:SER:HB3	2:B:540:MET:HE1	1.83	0.60
2:B:1178:ILE:HD12	2:B:1180:ASN:HB3	1.83	0.60
5:J:517:ASN:HD21	5:J:526:TYR:HE1	1.50	0.60
5:D:36:ASP:OD1	5:D:37:GLY:N	2.35	0.60
6:E:397:ILE:HD12	6:E:493:ASN:HB3	1.83	0.60
5:J:231:LYS:NZ	5:G:91:VAL:O	2.34	0.60
8:M:97:VAL:HG11	8:M:109:TRP:CE3	2.36	0.60
5:G:94:ASN:ND2	5:G:97:GLU:HB2	2.17	0.60
5:H:557:LEU:HD13	5:H:606:LEU:HD22	1.82	0.60
5:D:92:PHE:HE1	5:D:182:LEU:HD23	1.65	0.60
7:K:61:LYS:HB2	7:K:75:ASN:H	1.66	0.60
2:B:7:LEU:HD13	2:B:33:PHE:HB3	1.84	0.59
1:A:573:ASN:O	1:A:577:LEU:HD12	2.01	0.59
1:A:937:MET:HE3	1:A:1046:ASN:HB2	1.83	0.59
6:E:260:PHE:HE1	6:E:330:ALA:HB1	1.67	0.59
2:B:1072:LYS:HE2	2:B:1075:ASN:HA	1.83	0.59
5:J:428:SER:HB2	5:J:466:ALA:HB3	1.85	0.59
5:J:230:ASP:O	5:G:93:THR:OG1	2.21	0.59
8:M:6:GLN:HE22	8:M:95:TYR:HA	1.65	0.59
2:B:1070:GLU:HB2	2:B:1077:ILE:HD11	1.84	0.59
2:B:1140:ASN:O	2:B:1142:LYS:NZ	2.36	0.59
2:B:880:LEU:O	2:B:1011:PRO:HA	2.03	0.58
1:A:959:ASN:ND2	2:B:801:GLN:O	2.32	0.58
2:B:208:THR:HB	2:B:366:ILE:HD11	1.85	0.58
5:J:267:LYS:NZ	5:J:320:ASP:OD2	2.33	0.58
1:A:954:ASN:OD1	1:A:956:ILE:N	2.29	0.58
1:A:996:ARG:HD3	2:B:807:LEU:HD21	1.83	0.58
1:A:1294:ARG:HD3	1:A:1295:PRO:HD2	1.83	0.58
2:B:624:LEU:HD11	2:B:761:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1097:LEU:HB2	2:B:1113:ILE:HG12	1.85	0.58
1:A:710:TYR:O	1:A:714:VAL:HG23	2.03	0.58
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.85	0.58
1:A:1265:ASN:OD1	1:A:1268:ASN:ND2	2.37	0.58
5:J:462:ASP:OD2	5:J:529:GLN:NE2	2.36	0.58
1:A:1115:ASN:HD22	1:A:1118:ASP:H	1.52	0.58
5:H:543:ILE:HD11	5:H:604:TYR:CD2	2.39	0.58
6:E:207:GLN:NE2	14:E:802:HOH:O	2.33	0.58
2:B:838:LEU:HD13	2:B:859:THR:HG21	1.85	0.58
5:D:30:TYR:HB2	5:D:131:ILE:HG13	1.86	0.57
5:J:559:THR:HB	5:J:618:ILE:HD11	1.86	0.57
3:C:68:THR:HG22	3:C:81:GLN:HB3	1.86	0.57
5:D:70:ILE:HD13	5:D:72:TYR:HE1	1.70	0.57
1:A:1097:LEU:HD21	1:A:1223:MET:HB3	1.86	0.57
5:H:554:ASN:HB3	5:H:625:THR:HG23	1.86	0.57
3:C:97:THR:HG21	3:C:109:SER:H	1.70	0.57
10:L:113:VAL:HG22	10:L:134:LEU:HG	1.87	0.57
5:I:47:LEU:HD23	5:I:122:GLN:HA	1.87	0.56
5:J:469:TYR:CE1	5:J:512:VAL:HB	2.40	0.56
5:I:61:GLY:HA3	5:I:106:GLU:HG3	1.86	0.56
1:A:393:ARG:NH1	14:A:1401:HOH:O	2.38	0.56
5:J:222:GLY:HA2	5:J:369:GLU:HB3	1.87	0.56
5:J:431:ILE:HG21	5:J:472:VAL:HG11	1.87	0.56
5:H:560:SER:OG	5:H:621:HIS:NE2	2.39	0.56
5:J:431:ILE:HG23	5:J:458:ILE:HB	1.86	0.56
6:E:557:LEU:HD13	6:E:606:LEU:HD22	1.86	0.56
1:A:676:LEU:HB3	1:A:705:LYS:HE2	1.87	0.56
1:A:742:ALA:O	1:A:746:ILE:HG13	2.06	0.56
5:J:557:LEU:HD23	5:J:622:ILE:HG12	1.86	0.56
5:D:144:LEU:HD11	5:D:146:VAL:HG23	1.86	0.56
5:I:31:VAL:HG13	5:I:186:ILE:HD11	1.86	0.56
4:F:92:THR:HG23	4:F:113:THR:HA	1.88	0.56
5:I:71:PRO:HB2	5:I:144:LEU:HD11	1.88	0.56
1:A:779:LYS:NZ	11:A:1301:SO4:S	2.71	0.55
5:D:31:VAL:HG13	5:D:186:ILE:HD11	1.87	0.55
8:M:51:ILE:HD13	8:M:58:THR:HG22	1.88	0.55
6:E:559:THR:HG23	6:E:589:LEU:HB3	1.88	0.55
8:M:71:THR:HG23	8:M:80:TYR:HB2	1.88	0.55
1:A:24:ILE:HG22	1:A:135:ILE:HG22	1.88	0.55
6:E:249:GLN:NE2	6:E:251:ARG:H	2.05	0.55
5:J:227:ARG:HD2	5:J:259:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:55:ASP:OD1	8:M:55:ASP:N	2.38	0.55
1:A:114:GLY:HA2	1:A:320:LYS:HG3	1.89	0.55
2:B:589:VAL:HG21	2:B:745:VAL:HG12	1.87	0.55
1:A:858:ASP:O	1:A:861:ARG:NH1	2.40	0.55
5:J:252:LEU:HB2	5:G:102:PRO:HG2	1.89	0.55
5:J:570:ARG:HH21	5:J:572:THR:HG22	1.72	0.55
5:D:105:PHE:HE2	5:D:121:LEU:HD11	1.71	0.55
6:E:615:ASN:OD1	11:E:701:SO4:S	2.64	0.55
2:B:350:ARG:NH2	2:B:746:ASP:OD1	2.40	0.54
2:B:469:ILE:HG13	6:E:253:ARG:HH11	1.72	0.54
5:J:426:LEU:HD21	5:J:467:LYS:HG2	1.89	0.54
5:G:89:GLN:HE22	5:G:96:THR:HB	1.72	0.54
5:H:527:THR:HG22	5:H:619:ARG:HG2	1.89	0.54
1:A:954:ASN:OD1	1:A:955:SER:N	2.41	0.54
2:B:470:ASP:HB2	6:E:253:ARG:HD3	1.89	0.54
5:H:430:LYS:HD3	5:H:483:ARG:HD3	1.89	0.54
2:B:147:TYR:CD2	6:E:252:LEU:HB3	2.43	0.54
2:B:773:ILE:HD13	2:B:809:PHE:HE2	1.71	0.54
1:A:1:MET:N	1:A:2:PRO:HD3	2.22	0.54
1:A:23:LYS:HD2	1:A:32:PRO:HG3	1.89	0.54
2:B:1099:ILE:HD11	2:B:1111:GLU:HB3	1.88	0.54
7:K:49:LYS:HB3	7:K:55:ILE:HD11	1.90	0.54
1:A:149:LEU:C	1:A:150:ASN:HD22	2.15	0.54
7:K:19:VAL:HG22	7:K:74:ILE:HB	1.90	0.54
5:J:223:ASP:OD1	5:J:224:GLY:N	2.40	0.54
1:A:453:LEU:HD23	1:A:453:LEU:H	1.73	0.54
3:C:90:THR:HG23	3:C:117:THR:HA	1.89	0.54
5:G:52:ILE:HG13	5:G:111:ALA:HB2	1.89	0.54
5:I:33:ARG:HH11	5:I:180:GLN:HE22	1.54	0.54
5:J:260:PHE:HE1	5:J:330:ALA:HB1	1.72	0.53
6:E:411:THR:HB	6:E:447:LEU:HD13	1.90	0.53
1:A:280:ASN:OD1	1:A:283:ARG:NH1	2.31	0.53
8:M:97:VAL:HG12	8:M:109:TRP:HA	1.89	0.53
1:A:167:SER:HB3	1:A:184:GLN:HE22	1.74	0.53
7:K:47:LEU:HD22	7:K:58:ILE:HG21	1.88	0.53
2:B:511:ASN:ND2	2:B:530:SER:HA	2.21	0.53
5:H:409:LEU:HG	5:H:447:LEU:HD21	1.90	0.53
5:D:88:ILE:HD11	5:D:130:ILE:HD11	1.90	0.53
1:A:1155:TYR:CD2	1:A:1293:GLU:HG2	2.43	0.53
2:B:326:ILE:HD13	2:B:456:ASN:HB2	1.91	0.53
2:B:442:TYR:CD1	2:B:443:GLU:HG3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:382:ILE:HG23	6:E:407:TYR:HB2	1.91	0.53
1:A:124:ASP:OD1	1:A:124:ASP:N	2.34	0.53
5:I:102:PRO:HB2	6:E:252:LEU:HD12	1.90	0.53
5:J:354:LYS:H	5:J:354:LYS:HD2	1.74	0.53
1:A:548:TYR:HE2	1:A:576:LEU:HD12	1.73	0.53
1:A:1226:LYS:O	1:A:1234:LYS:HB2	2.08	0.52
6:E:389:ILE:HB	6:E:412:VAL:HA	1.90	0.52
6:E:468:SER:HA	6:E:512:VAL:O	2.09	0.52
1:A:656:LEU:HD13	1:A:663:ILE:HD11	1.90	0.52
1:A:998:VAL:HB	2:B:807:LEU:HD12	1.91	0.52
6:E:402:ASN:OD1	6:E:403:ASN:ND2	2.42	0.52
1:A:319:GLU:OE2	1:A:510:ASN:ND2	2.41	0.52
2:B:283:PHE:HA	2:B:434:TYR:OH	2.09	0.52
2:B:1131:ARG:HD3	2:B:1176:TRP:HB3	1.92	0.52
4:F:7:GLU:H	4:F:108:GLN:HE22	1.56	0.52
2:B:495:THR:HG21	2:B:499:TRP:CD1	2.45	0.52
5:J:571:VAL:HG21	5:J:605:ILE:HG13	1.91	0.52
2:B:755:CYS:SG	14:B:1309:HOH:O	2.59	0.52
1:A:1176:ASN:HD22	1:A:1225:SER:H	1.56	0.52
5:H:276:ARG:NH1	5:H:378:PRO:HG3	2.25	0.52
7:K:49:LYS:HD3	7:K:55:ILE:HD11	1.90	0.52
2:B:210:LYS:HE3	2:B:213:GLU:HA	1.90	0.52
5:H:468:SER:HA	5:H:512:VAL:O	2.09	0.52
1:A:751:TYR:CE2	1:A:764:PHE:HB3	2.44	0.52
2:B:1172:GLU:N	2:B:1173:ASN:HA	2.24	0.52
2:B:1083:ASN:ND2	2:B:1175:ASN:OD1	2.36	0.51
5:D:102:PRO:O	5:H:249:GLN:NE2	2.43	0.51
5:H:429:LEU:HB2	5:H:470:LEU:HD11	1.92	0.51
7:K:55:ILE:HG13	8:M:100:TYR:HH	1.74	0.51
8:M:107:GLY:C	8:M:108:TYR:HD1	2.19	0.51
1:A:1125:VAL:HG22	1:A:1134:MET:HG2	1.93	0.51
4:F:65:VAL:HB	4:F:69:PHE:CD2	2.44	0.51
7:K:49:LYS:HE3	8:M:101:ASP:OD2	2.10	0.51
2:B:1130:ASN:O	2:B:1179:CYS:N	2.37	0.51
10:L:134:LEU:HD21	10:L:194:ALA:HB2	1.92	0.51
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.92	0.51
2:B:311:ALA:O	2:B:312:ILE:HD13	2.10	0.51
5:D:183:TYR:CE2	5:H:354:LYS:HB3	2.43	0.51
1:A:940:ASN:HB2	11:A:1301:SO4:O2	2.10	0.51
2:B:21:VAL:HG21	2:B:156:LEU:HD13	1.93	0.51
3:C:45:PHE:HB2	3:C:102:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:36:ASP:OD1	5:I:37:GLY:N	2.44	0.51
6:E:210:LEU:HB2	6:E:321:TYR:OH	2.10	0.51
2:B:781:LYS:HG3	2:B:799:ILE:HD13	1.92	0.51
4:F:14:GLN:OE1	4:F:14:GLN:N	2.44	0.51
5:H:503:ASP:HB3	5:H:580:LEU:HB2	1.93	0.51
1:A:590:TYR:O	1:A:594:VAL:HG12	2.11	0.51
4:F:12:LEU:H	4:F:12:LEU:HD23	1.75	0.51
5:H:219:ILE:HG12	5:H:372:VAL:HG13	1.93	0.51
5:H:432:TYR:HB3	5:H:455:ILE:HB	1.92	0.51
1:A:184:GLN:NE2	1:A:231:ARG:HD3	2.25	0.51
3:C:9:GLY:H	3:C:18:LEU:HD21	1.75	0.51
1:A:897:LYS:HB3	1:A:927:ILE:HB	1.92	0.50
7:K:31:ASN:HB2	7:K:51:ALA:HB2	1.93	0.50
10:L:120:SER:O	10:L:124:THR:HG23	2.12	0.50
1:A:121:SER:HB2	1:A:128:LYS:HB2	1.93	0.50
1:A:1266:TRP:HH2	1:A:1276:ARG:HB3	1.77	0.50
5:D:112:PRO:HB2	5:D:115:LYS:HD2	1.93	0.50
5:H:462:ASP:OD2	5:H:529:GLN:NE2	2.43	0.50
3:C:36:TRP:CD2	3:C:80:LEU:HD12	2.47	0.50
5:D:84:ILE:HG12	5:D:130:ILE:HG13	1.93	0.50
5:G:67:ASP:HB2	5:H:286:PHE:CZ	2.46	0.50
1:A:1196:ASN:OD1	1:A:1198:SER:OG	2.24	0.50
6:E:410:PHE:HE1	6:E:482:ILE:HG13	1.76	0.50
5:H:405:PRO:HB3	5:H:485:PRO:HA	1.94	0.50
1:A:1097:LEU:HD12	1:A:1225:SER:HB3	1.93	0.50
2:B:1124:ILE:HG23	2:B:1132:LEU:HD22	1.94	0.50
5:J:427:PRO:HG3	5:J:487:THR:HG22	1.93	0.50
6:E:574:THR:HG23	6:E:576:ALA:H	1.76	0.50
7:K:49:LYS:CD	7:K:55:ILE:HD11	2.41	0.50
8:M:30:THR:O	8:M:30:THR:OG1	2.29	0.50
1:A:709:VAL:HG21	1:A:808:LEU:HD11	1.93	0.50
1:A:568:LEU:HD22	1:A:594:VAL:HG11	1.93	0.50
1:A:569:THR:HG22	1:A:571:SER:H	1.77	0.50
2:B:389:SER:O	2:B:392:ASN:ND2	2.45	0.50
6:E:615:ASN:OD1	11:E:701:SO4:O2	2.29	0.50
2:B:346:MET:HB3	2:B:825:THR:HG23	1.92	0.50
3:C:29:LEU:HD21	3:C:78:LEU:HB2	1.93	0.50
5:J:466:ALA:CB	5:J:528:ARG:HH21	2.25	0.50
9:N:201:HIS:CE1	9:N:203:ALA:HB3	2.47	0.50
2:B:458:ASN:HB3	2:B:461:VAL:HG22	1.94	0.49
2:B:1125:ASP:OD1	2:B:1126:ILE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:81:GLU:OE1	5:D:81:GLU:N	2.34	0.49
5:H:392:ASN:OD1	5:H:498:LYS:HD3	2.12	0.49
5:H:450:ASP:HB2	5:H:452:ILE:HG13	1.93	0.49
1:A:643:ILE:HG21	1:A:664:LEU:HD23	1.94	0.49
2:B:599:LEU:HB3	2:B:608:GLU:HG2	1.94	0.49
2:B:1061:TYR:HB2	2:B:1189:LEU:HB2	1.93	0.49
3:C:29:LEU:H	3:C:76:ASN:ND2	2.10	0.49
5:I:54:ASN:ND2	5:I:114:ASN:H	2.02	0.49
1:A:96:GLU:O	1:A:100:SER:OG	2.30	0.49
1:A:821:LYS:NZ	1:A:825:ASP:OD2	2.46	0.49
1:A:969:GLU:HG3	1:A:1050:SER:HA	1.95	0.49
2:B:112:TYR:CD1	2:B:149:GLY:HA3	2.47	0.49
2:B:1172:GLU:H	2:B:1174:HIS:H	1.60	0.49
14:A:1420:HOH:O	2:B:585:ILE:HD11	2.13	0.49
2:B:256:GLU:HG3	2:B:427:VAL:HG12	1.94	0.49
5:J:554:ASN:HB3	5:J:625:THR:OG1	2.13	0.49
2:B:877:ALA:HB2	2:B:1015:GLU:HB2	1.94	0.49
3:C:14:PRO:HG3	3:C:118:VAL:HG12	1.94	0.49
5:J:429:LEU:HB2	5:J:470:LEU:HD11	1.94	0.49
5:J:560:SER:HG	5:J:621:HIS:HE2	1.60	0.49
5:H:414:THR:O	5:H:418:TYR:OH	2.25	0.49
1:A:815:LEU:HD23	1:A:819:LEU:HD13	1.94	0.49
5:I:22:THR:HA	5:I:137:GLU:HA	1.95	0.49
5:H:417:ILE:HD13	5:H:508:MET:HG2	1.94	0.49
2:B:539:VAL:HG11	2:B:698:ILE:HD11	1.95	0.49
5:J:587:LEU:HB3	5:J:589:LEU:HD21	1.95	0.49
6:E:512:VAL:HG22	6:E:538:SER:HB2	1.93	0.49
5:G:62:ASP:OD1	5:G:63:LEU:N	2.42	0.49
1:A:288:ASN:HB2	4:F:100:TYR:HD2	1.78	0.49
1:A:292:ASP:CG	4:F:98:ARG:HH12	2.21	0.49
5:J:559:THR:HG23	5:J:589:LEU:HB3	1.95	0.49
5:D:60:VAL:HG13	5:D:119:MET:HE2	1.95	0.49
5:H:401:VAL:HG21	5:H:406:PHE:CD2	2.48	0.49
2:B:582:ASN:OD1	2:B:582:ASN:N	2.46	0.48
2:B:786:LYS:HG3	8:M:52:TYR:CD2	2.48	0.48
3:C:112:GLN:OE1	3:C:112:GLN:N	2.39	0.48
5:J:210:LEU:HD23	5:J:212:TYR:CE2	2.48	0.48
2:B:291:ALA:HA	2:B:294:VAL:HG22	1.94	0.48
2:B:552:ILE:HD12	2:B:557:LYS:HB3	1.96	0.48
2:B:528:ASP:OD1	2:B:528:ASP:N	2.45	0.48
2:B:224:LYS:HB2	2:B:336:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:ASN:OD1	2:B:807:LEU:HB2	2.13	0.48
5:D:109:LYS:HE3	5:D:154:SER:HB3	1.96	0.48
2:B:15:ASN:OD1	2:B:165:TYR:OH	2.27	0.48
2:B:699:LYS:HG2	2:B:731:LEU:HD22	1.95	0.48
5:I:31:VAL:HG12	5:I:130:ILE:HD13	1.95	0.48
7:K:86:PHE:CD1	7:K:99:GLY:HA2	2.48	0.48
1:A:52:THR:HG23	1:A:528:LEU:HD21	1.95	0.48
1:A:306:THR:OG1	1:A:516:SER:O	2.26	0.48
2:B:142:THR:HG21	5:J:248:ILE:HG21	1.96	0.48
2:B:480:LYS:H	2:B:480:LYS:HD2	1.77	0.48
2:B:738:SER:O	2:B:742:MET:HG3	2.13	0.48
5:J:570:ARG:HB2	5:J:583:ILE:HD13	1.96	0.48
1:A:965:ILE:HB	1:A:976:VAL:HB	1.95	0.48
5:D:70:ILE:HD12	5:D:70:ILE:O	2.14	0.48
5:D:92:PHE:CE1	5:D:182:LEU:HD23	2.46	0.48
1:A:24:ILE:HD12	1:A:185:TYR:CE2	2.49	0.48
1:A:1266:TRP:CH2	1:A:1276:ARG:HB3	2.49	0.48
2:B:217:ASP:OD1	2:B:372:TYR:OH	2.28	0.48
9:N:182:SER:HB3	10:L:133:PHE:CD2	2.48	0.48
1:A:167:SER:HB3	1:A:184:GLN:NE2	2.29	0.48
2:B:435:LYS:HE2	2:B:630:GLU:HB2	1.94	0.48
5:J:419:LYS:HE3	5:J:469:TYR:CD2	2.48	0.48
5:J:473:LEU:H	5:J:509:ASN:ND2	2.12	0.48
5:H:543:ILE:HD13	5:H:599:LEU:O	2.14	0.48
1:A:885:SER:OG	1:A:886:ASN:N	2.47	0.47
1:A:1169:ASN:HD21	1:A:1175:ARG:HH22	1.60	0.47
5:H:415:THR:HG23	5:H:476:LYS:HG2	1.94	0.47
1:A:915:GLN:HB2	1:A:1068:TRP:CH2	2.48	0.47
2:B:356:LYS:H	2:B:356:LYS:HD2	1.79	0.47
2:B:367:ASP:HB3	2:B:370:GLU:OE1	2.14	0.47
2:B:799:ILE:O	2:B:803:VAL:HG13	2.15	0.47
2:B:1118:ASP:HB2	2:B:1122:LYS:HG2	1.95	0.47
5:H:625:THR:OG1	5:H:626:ASN:N	2.47	0.47
10:L:111:PRO:HB3	10:L:137:PHE:HB3	1.96	0.47
2:B:1135:ILE:HD12	2:B:1137:ASN:N	2.28	0.47
1:A:397:LEU:HD12	1:A:403:GLY:HA2	1.95	0.47
2:B:1127:SER:OG	2:B:1128:GLU:N	2.47	0.47
6:E:321:TYR:CE2	6:E:324:GLY:HA2	2.49	0.47
7:K:30:SER:OG	7:K:31:ASN:N	2.45	0.47
1:A:968:MET:HE1	1:A:988:GLN:HB3	1.96	0.47
1:A:979:ASN:HB3	1:A:982:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ILE:HG12	2:B:124:THR:N	2.30	0.47
1:A:42:ILE:HD13	1:A:151:LEU:HB3	1.96	0.47
1:A:804:GLY:O	1:A:808:LEU:HD12	2.15	0.47
2:B:209:TYR:CZ	2:B:216:ILE:HG13	2.49	0.47
5:H:543:ILE:HD11	5:H:604:TYR:HD2	1.77	0.47
7:K:59:PRO:HB2	7:K:62:PHE:HE2	1.79	0.47
1:A:107:LEU:HA	1:A:349:TYR:CZ	2.50	0.47
1:A:375:LYS:HB2	1:A:416:LEU:HD11	1.97	0.47
1:A:428:LEU:HD23	1:A:542:LYS:HD2	1.96	0.47
2:B:1087:LEU:HB3	2:B:1089:LEU:HD12	1.96	0.47
5:J:563:GLN:HB2	5:J:590:LEU:HD22	1.96	0.47
6:E:377:ASP:OD1	6:E:379:SER:OG	2.27	0.47
6:E:478:LYS:HD2	14:E:803:HOH:O	2.14	0.47
6:E:563:GLN:HA	6:E:590:LEU:HB2	1.96	0.47
5:G:168:TYR:OH	5:H:367:PRO:HB2	2.15	0.47
7:K:47:LEU:HA	7:K:47:LEU:HD23	1.58	0.47
2:B:128:ALA:HB3	2:B:136:ASN:HB2	1.97	0.47
5:H:304:ASN:HB2	5:H:345:ALA:HB2	1.97	0.47
5:H:403:ASN:HB3	5:H:487:THR:O	2.15	0.47
1:A:702:ARG:HH21	1:A:703:ASN:HD21	1.63	0.47
2:B:360:ARG:HA	2:B:360:ARG:NE	2.28	0.47
5:H:376:ILE:HG21	5:H:382:ILE:HD11	1.96	0.47
1:A:306:THR:HG23	1:A:308:ALA:H	1.80	0.47
1:A:915:GLN:HB2	1:A:1068:TRP:CZ3	2.50	0.47
2:B:1054:LYS:HB3	2:B:1056:TYR:CE1	2.49	0.47
5:J:279:ASP:HB3	5:J:453:LYS:HB2	1.97	0.47
1:A:867:THR:HG22	1:A:871:LYS:HD2	1.96	0.46
2:B:588:VAL:HG22	2:B:748:PHE:CE1	2.50	0.46
2:B:829:ILE:O	2:B:833:THR:OG1	2.26	0.46
5:D:44:ASN:OD1	5:D:44:ASN:N	2.48	0.46
6:E:264:ASN:OD1	6:E:266:THR:HG22	2.15	0.46
6:E:348:PRO:HA	6:E:349:GLU:HA	1.45	0.46
5:H:348:PRO:HA	5:H:349:GLU:HA	1.54	0.46
5:H:426:LEU:HD21	5:H:467:LYS:HG2	1.96	0.46
1:A:1160:PHE:CE1	1:A:1184:VAL:HG22	2.50	0.46
2:B:16:LYS:HE2	2:B:17:ASN:OD1	2.15	0.46
2:B:570:SER:O	2:B:574:THR:OG1	2.25	0.46
5:I:23:ILE:HG23	5:I:25:LEU:HB2	1.97	0.46
5:J:212:TYR:HB2	5:J:321:TYR:CD2	2.50	0.46
5:J:247:ILE:HG13	5:J:307:ILE:HD11	1.98	0.46
5:D:112:PRO:HG2	5:D:115:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:527:THR:HG22	6:E:619:ARG:HG2	1.96	0.46
8:M:35:GLN:HB3	8:M:50:THR:HG23	1.98	0.46
1:A:4:VAL:HG21	1:A:92:THR:HG23	1.96	0.46
2:B:34:LYS:HB2	2:B:40:TRP:CZ3	2.50	0.46
5:I:105:PHE:CZ	5:I:150:GLY:HA3	2.49	0.46
5:H:251:ARG:NH2	5:H:336:SER:O	2.49	0.46
1:A:6:LYS:HB3	1:A:8:PHE:CE2	2.50	0.46
5:J:552:THR:HG23	5:J:597:ARG:HH21	1.80	0.46
5:D:143:VAL:HG21	6:E:440:ARG:HA	1.98	0.46
5:H:401:VAL:HG11	5:H:406:PHE:CE2	2.51	0.46
1:A:171:GLU:HG2	1:A:172:VAL:HG13	1.98	0.46
1:A:772:LYS:HA	1:A:775:GLU:OE1	2.16	0.46
3:C:6:GLU:HB2	3:C:114:THR:OG1	2.15	0.46
5:J:405:PRO:HD3	5:J:486:GLN:HB2	1.96	0.46
1:A:361:LEU:HB2	1:A:401:PHE:CD2	2.51	0.46
1:A:879:LEU:HB3	1:A:1074:LEU:HB3	1.97	0.46
4:F:7:GLU:N	4:F:108:GLN:HE22	2.13	0.46
4:F:37:TRP:CH2	4:F:97:CYS:HB2	2.51	0.46
6:E:389:ILE:O	6:E:413:ASN:HB2	2.16	0.46
5:G:47:LEU:HD11	5:G:123:TYR:CZ	2.51	0.46
1:A:689:VAL:O	1:A:693:GLN:HG3	2.15	0.46
2:B:248:LEU:HD12	2:B:257:TYR:CZ	2.51	0.46
2:B:620:LYS:HB2	2:B:679:GLN:HE22	1.81	0.46
5:D:144:LEU:CD1	5:D:146:VAL:HG23	2.45	0.46
6:E:563:GLN:HB2	6:E:590:LEU:HD22	1.98	0.46
5:G:31:VAL:HG11	5:G:87:ASN:HB3	1.98	0.46
5:H:598:LEU:HD22	5:H:604:TYR:CZ	2.51	0.46
2:B:1043:ARG:HB3	2:B:1047:GLU:HA	1.98	0.46
5:I:64:ARG:NH1	5:I:99:ASN:OD1	2.48	0.46
6:E:222:GLY:HA2	6:E:369:GLU:HB3	1.98	0.46
6:E:432:TYR:HB3	6:E:455:ILE:HB	1.96	0.46
5:H:431:ILE:HG23	5:H:458:ILE:HB	1.96	0.46
1:A:93:LYS:NZ	1:A:379:VAL:O	2.50	0.46
2:B:713:SER:OG	2:B:715:ILE:HG13	2.15	0.46
5:I:141:ARG:NH2	5:J:439:ASN:O	2.49	0.46
5:J:248:ILE:HG12	5:J:294:LYS:HG3	1.96	0.46
5:J:272:TYR:O	5:J:276:ARG:HG2	2.16	0.46
5:G:89:GLN:NE2	5:G:96:THR:H	2.14	0.46
10:L:118:PRO:HG2	10:L:128:ALA:HB1	1.97	0.46
1:A:948:ARG:NH2	1:A:1288:ASP:OD2	2.44	0.45
2:B:935:GLN:OE1	2:B:940:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:313:TYR:HB3	6:E:333:TYR:HB3	1.97	0.45
6:E:431:ILE:HG23	6:E:458:ILE:HB	1.97	0.45
6:E:563:GLN:HB3	6:E:612:GLU:HB3	1.98	0.45
5:G:65:VAL:N	5:G:68:ASN:OD1	2.47	0.45
1:A:688:LYS:O	1:A:692:VAL:HG13	2.17	0.45
1:A:801:ILE:O	1:A:805:VAL:HG23	2.16	0.45
1:A:1121:LYS:HB3	1:A:1136:LEU:HB3	1.97	0.45
2:B:559:TYR:OH	2:B:722:LEU:HD23	2.17	0.45
4:F:30:ILE:O	4:F:30:ILE:HG13	2.16	0.45
5:G:85:LYS:HB3	5:G:85:LYS:HE3	1.70	0.45
1:A:789:ASN:O	1:A:793:VAL:HG23	2.15	0.45
1:A:1134:MET:HE3	1:A:1261:LEU:HD12	1.99	0.45
4:F:35:MET:SD	4:F:80:SER:HB2	2.56	0.45
5:H:558:TYR:CE1	5:H:621:HIS:HB2	2.51	0.45
4:F:52:ILE:HG23	4:F:73:ARG:HD2	1.99	0.45
5:D:184:LYS:NZ	14:D:801:HOH:O	2.40	0.45
1:A:11:LYS:HA	1:A:11:LYS:HD2	1.68	0.45
2:B:265:LEU:HD21	2:B:276:ILE:HG13	1.98	0.45
2:B:918:SER:HB3	2:B:1008:GLU:HB2	1.97	0.45
2:B:1132:LEU:HD12	2:B:1177:MET:HB3	1.97	0.45
5:G:30:TYR:HB2	5:G:131:ILE:HG13	1.99	0.45
5:H:508:MET:HA	5:H:509:ASN:HA	1.60	0.45
1:A:25:PRO:HA	1:A:524:ILE:HB	1.99	0.45
2:B:129:PRO:O	2:B:130:LYS:HG2	2.16	0.45
2:B:236:ILE:HG21	2:B:328:ILE:HD11	1.98	0.45
2:B:1165:ILE:HG22	2:B:1190:TRP:CZ2	2.51	0.45
5:J:227:ARG:HH21	5:J:231:LYS:HD2	1.82	0.45
1:A:751:TYR:OH	1:A:762:ILE:O	2.33	0.45
1:A:779:LYS:NZ	11:A:1301:SO4:O3	2.49	0.45
1:A:1182:ILE:HD12	1:A:1221:VAL:HG21	1.98	0.45
1:A:1189:LYS:HG2	5:J:400:ILE:HA	1.99	0.45
1:A:1236:LYS:HB3	1:A:1249:PHE:HE2	1.81	0.45
2:B:124:THR:OG1	5:G:106:GLU:OE2	2.27	0.45
5:J:563:GLN:HA	5:J:590:LEU:HB2	1.98	0.45
2:B:794:GLU:HA	2:B:797:GLN:HG2	1.98	0.45
3:C:30:GLY:HA2	3:C:71:ARG:NH1	2.32	0.45
5:J:428:SER:CB	5:J:466:ALA:HB3	2.47	0.45
6:E:223:ASP:CG	6:E:314:GLU:HG3	2.42	0.45
2:B:1144:MET:HE2	2:B:1144:MET:HB2	1.88	0.45
5:G:121:LEU:HB2	5:G:152:VAL:HG12	1.98	0.45
1:A:22:ILE:HD12	1:A:24:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HG21	1:A:260:PHE:HB2	1.99	0.45
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.52	0.45
2:B:186:TYR:CE2	2:B:478:CYS:HB3	2.52	0.45
2:B:440:ARG:N	2:B:442:TYR:CE2	2.76	0.45
3:C:38:ARG:NH2	3:C:88:GLU:O	2.50	0.45
4:F:18:SER:HA	4:F:84:MET:O	2.16	0.45
5:I:69:ALA:O	5:I:99:ASN:ND2	2.50	0.45
5:J:226:ILE:HG21	5:J:310:TYR:HB3	1.99	0.45
5:J:587:LEU:HB3	5:J:589:LEU:CD2	2.46	0.45
5:D:103:ILE:HD11	5:H:234:ILE:HG23	1.99	0.45
6:E:568:LEU:HD11	6:E:604:TYR:HB3	1.97	0.45
1:A:26:ASN:ND2	1:A:51:PHE:O	2.50	0.44
2:B:414:MET:HE2	2:B:414:MET:HB3	1.62	0.44
2:B:722:LEU:HA	2:B:725:LEU:HD12	1.99	0.44
6:E:420:ILE:HD13	6:E:482:ILE:HD11	1.98	0.44
1:A:749:TYR:CD1	1:A:749:TYR:C	2.95	0.44
2:B:528:ASP:H	2:B:529:LYS:HA	1.82	0.44
5:I:129:GLU:HG2	5:I:143:VAL:HG22	1.99	0.44
5:J:386:ASN:OD1	5:J:386:ASN:N	2.47	0.44
6:E:383:GLN:HG2	6:E:395:TYR:OH	2.17	0.44
6:E:518:LEU:HD21	6:E:622:ILE:HG21	1.98	0.44
5:G:87:ASN:O	5:G:91:VAL:HG23	2.17	0.44
5:H:517:ASN:HD21	5:H:526:TYR:HE2	1.64	0.44
10:L:134:LEU:HD13	10:L:173:MET:SD	2.57	0.44
1:A:16:GLY:HA3	1:A:139:GLN:OE1	2.17	0.44
1:A:547:LYS:HD2	1:A:547:LYS:HA	1.82	0.44
1:A:565:ARG:HB2	1:A:749:TYR:CE2	2.52	0.44
5:J:508:MET:HA	5:J:509:ASN:HA	1.65	0.44
5:J:468:SER:HA	5:J:512:VAL:O	2.18	0.44
5:J:568:LEU:HD21	5:J:604:TYR:HB3	2.00	0.44
1:A:671:ILE:HG13	1:A:673:ILE:HD13	1.99	0.44
1:A:883:TYR:CE1	1:A:911:LYS:HE3	2.52	0.44
2:B:909:ARG:HD3	2:B:963:TRP:CD1	2.52	0.44
5:J:527:THR:HG23	5:J:619:ARG:HG3	1.99	0.44
5:J:570:ARG:NH2	5:J:572:THR:HG22	2.33	0.44
6:E:536:TYR:CE1	6:E:609:GLU:HB2	2.53	0.44
5:H:467:LYS:HB2	5:H:514:ILE:HB	2.00	0.44
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	2.00	0.44
2:B:741:ALA:O	2:B:745:VAL:HG13	2.17	0.44
3:C:49:SER:OG	3:C:50:SER:N	2.50	0.44
5:I:38:TRP:CE2	5:I:175:CYS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:258:PRO:HG3	5:J:286:PHE:O	2.18	0.44
5:J:532:ASP:OD1	5:J:533:VAL:N	2.48	0.44
5:D:46:ILE:HG13	5:D:47:LEU:HD22	2.00	0.44
6:E:508:MET:HA	6:E:509:ASN:HA	1.64	0.44
2:B:141:SER:OG	6:E:294:LYS:NZ	2.49	0.44
2:B:742:MET:O	2:B:745:VAL:HG22	2.18	0.44
5:G:69:ALA:C	5:G:147:PRO:HG2	2.42	0.44
2:B:758:GLU:OE2	2:B:814:ILE:HG12	2.18	0.44
2:B:798:LEU:HD23	2:B:798:LEU:HA	1.88	0.44
5:J:397:ILE:HD12	5:J:493:ASN:HB3	2.00	0.44
6:E:227:ARG:HE	6:E:231:LYS:HD3	1.83	0.44
5:H:234:ILE:HD11	5:H:249:GLN:HG3	2.00	0.44
5:H:385:ILE:HD13	5:H:385:ILE:HA	1.87	0.44
1:A:427:LYS:HD3	1:A:543:TYR:HE2	1.82	0.43
5:J:246:SER:HA	5:J:295:PHE:O	2.18	0.43
6:E:401:VAL:HG21	6:E:406:PHE:CD1	2.52	0.43
6:E:430:LYS:HA	6:E:460:GLY:HA3	2.00	0.43
5:H:248:ILE:HG22	5:H:294:LYS:HB2	2.00	0.43
1:A:706:TRP:CE3	1:A:849:ILE:HB	2.54	0.43
1:A:896:SER:HB3	1:A:927:ILE:O	2.18	0.43
2:B:247:ARG:CZ	2:B:357:HIS:HD2	2.31	0.43
5:I:22:THR:HB	5:I:137:GLU:OE2	2.18	0.43
5:I:33:ARG:HB2	5:I:92:PHE:CZ	2.54	0.43
5:I:145:TYR:HE2	5:J:440:ARG:HG2	1.82	0.43
5:D:112:PRO:HB2	5:D:115:LYS:NZ	2.32	0.43
1:A:53:ASN:OD1	1:A:56:GLU:N	2.51	0.43
1:A:216:ASP:HB3	1:A:219:VAL:HG23	1.99	0.43
1:A:501:GLN:HG3	2:B:1063:PHE:CE1	2.53	0.43
1:A:843:ASN:HB3	2:B:935:GLN:NE2	2.33	0.43
5:D:120:TYR:OH	5:D:167:PHE:O	2.34	0.43
1:A:432:ARG:NH1	1:A:546:ASP:OD2	2.52	0.43
1:A:717:TRP:HZ3	1:A:857:VAL:HG21	1.82	0.43
2:B:121:ASN:O	2:B:121:ASN:ND2	2.52	0.43
2:B:469:ILE:HG13	2:B:470:ASP:H	1.83	0.43
2:B:569:TYR:CD1	2:B:698:ILE:HG13	2.54	0.43
2:B:923:SER:HB2	2:B:1003:ILE:HG12	2.00	0.43
7:K:96:THR:OG1	7:K:97:PHE:N	2.51	0.43
1:A:1043:ASN:OD1	1:A:1043:ASN:N	2.48	0.43
3:C:18:LEU:HD23	3:C:19:ARG:H	1.83	0.43
3:C:20:LEU:N	3:C:20:LEU:HD12	2.34	0.43
5:J:555:ILE:HG13	5:J:598:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:74:TYR:O	6:E:441:ASN:HB3	2.18	0.43
6:E:207:GLN:CD	14:E:802:HOH:O	2.61	0.43
6:E:588:HIS:O	6:E:592:ASN:HB2	2.19	0.43
5:H:599:LEU:HD12	5:H:604:TYR:OH	2.18	0.43
1:A:253:MET:HG2	1:A:459:ASN:O	2.18	0.43
1:A:322:LEU:HD23	1:A:341:LEU:HD13	2.01	0.43
1:A:463:PHE:CE1	1:A:666:GLU:HG3	2.54	0.43
2:B:1129:ASP:OD2	2:B:1131:ARG:NH2	2.51	0.43
5:J:403:ASN:O	5:J:486:GLN:NE2	2.51	0.43
5:D:107:PHE:CZ	5:H:237:LEU:HD22	2.53	0.43
6:E:615:ASN:ND2	11:E:701:SO4:O4	2.52	0.43
1:A:222:ALA:O	1:A:226:ILE:HG13	2.19	0.43
1:A:997:VAL:HG12	1:A:1039:LYS:HB2	2.00	0.43
1:A:1291:TRP:NE1	1:A:1293:GLU:OE1	2.48	0.43
2:B:107:PRO:HB3	2:B:196:GLY:C	2.44	0.43
2:B:842:ALA:HA	2:B:850:VAL:O	2.19	0.43
8:M:32:TYR:OH	8:M:100:TYR:O	2.36	0.43
1:A:1176:ASN:ND2	1:A:1225:SER:H	2.16	0.43
2:B:926:ASP:O	2:B:927:ASN:C	2.61	0.43
2:B:967:THR:HB	2:B:980:PHE:HB2	2.01	0.43
1:A:907:ASP:HB3	1:A:910:ASP:O	2.19	0.43
1:A:999:PHE:HD1	1:A:1036:ILE:HG21	1.82	0.43
2:B:210:LYS:HB2	2:B:215:TYR:CE1	2.54	0.43
4:F:13:VAL:O	4:F:114:VAL:HA	2.19	0.43
6:E:384:GLU:HG2	6:E:447:LEU:HD23	2.01	0.43
5:H:401:VAL:HG21	5:H:406:PHE:HD2	1.83	0.43
7:K:93:TRP:N	7:K:94:PRO:HD2	2.34	0.43
1:A:24:ILE:HG22	1:A:135:ILE:CG2	2.49	0.43
1:A:226:ILE:HD13	1:A:349:TYR:C	2.44	0.43
2:B:769:MET:O	2:B:773:ILE:HG23	2.18	0.43
2:B:926:ASP:O	2:B:928:CYS:HB2	2.18	0.43
2:B:1049:ARG:H	2:B:1049:ARG:HG3	1.69	0.43
5:J:287:ASN:OD1	5:J:287:ASN:N	2.49	0.43
5:J:528:ARG:HA	5:J:528:ARG:HD3	1.64	0.43
5:J:570:ARG:HG3	5:J:604:TYR:CE2	2.54	0.43
5:J:450:ASP:HB3	5:J:452:ILE:HG13	2.00	0.42
6:E:619:ARG:NH2	11:E:701:SO4:O4	2.52	0.42
2:B:123:ILE:HG12	2:B:124:THR:H	1.84	0.42
2:B:573:ILE:HD12	2:B:573:ILE:HA	1.94	0.42
2:B:786:LYS:HG3	8:M:52:TYR:HD2	1.84	0.42
5:I:22:THR:HA	5:I:136:HIS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:428:SER:OG	5:H:466:ALA:O	2.35	0.42
9:N:121:LYS:HB3	9:N:121:LYS:HE2	1.78	0.42
3:C:47:TRP:CD1	3:C:100:ARG:HA	2.54	0.42
5:J:244:SER:HB2	5:G:108:SER:HB3	2.00	0.42
6:E:385:ILE:HD11	6:E:395:TYR:CD2	2.49	0.42
5:G:24:ASP:O	5:G:25:LEU:HD23	2.18	0.42
1:A:740:ALA:O	1:A:744:LYS:HG3	2.19	0.42
1:A:837:LEU:O	1:A:841:VAL:HG23	2.19	0.42
2:B:1100:ASN:OD1	2:B:1101:PRO:HD2	2.20	0.42
7:K:55:ILE:HG22	7:K:55:ILE:O	2.19	0.42
2:B:110:TYR:OH	2:B:190:ASP:OD1	2.30	0.42
2:B:642:PRO:O	2:B:646:LEU:HB2	2.20	0.42
5:I:51:VAL:HB	5:J:339:TYR:HD1	1.84	0.42
5:G:36:ASP:OD1	5:G:37:GLY:N	2.51	0.42
5:H:410:PHE:HA	5:H:447:LEU:HD22	2.01	0.42
1:A:224:GLN:OE1	1:A:224:GLN:HA	2.20	0.42
1:A:584:THR:HA	1:A:739:GLN:HE22	1.83	0.42
2:B:71:GLN:O	2:B:75:LYS:HG3	2.19	0.42
2:B:112:TYR:HD1	2:B:149:GLY:HA3	1.85	0.42
2:B:500:PRO:HB3	2:B:596:LEU:HB3	2.01	0.42
5:I:22:THR:H	5:I:137:GLU:HG3	1.83	0.42
1:A:421:GLY:N	1:A:424:GLU:HG3	2.34	0.42
1:A:1182:ILE:O	1:A:1192:ARG:HD3	2.20	0.42
5:I:46:ILE:HB	5:J:283:VAL:HG12	2.02	0.42
5:I:107:PHE:CZ	6:E:237:LEU:HG	2.55	0.42
5:H:408:ILE:O	5:H:481:TYR:HA	2.20	0.42
1:A:1116:LEU:HD12	1:A:1281:SER:HB3	2.01	0.42
2:B:292:LYS:HE3	2:B:292:LYS:HB2	1.82	0.42
2:B:321:LYS:HE2	14:B:1305:HOH:O	2.20	0.42
2:B:648:GLU:HA	2:B:651:PHE:CD2	2.55	0.42
2:B:729:ASN:ND2	2:B:732:ARG:HH12	2.17	0.42
5:J:547:PHE:HB2	5:J:601:GLY:HA3	2.00	0.42
5:J:566:GLY:O	5:J:587:LEU:HB2	2.20	0.42
5:D:31:VAL:HG11	5:D:87:ASN:HB3	2.00	0.42
5:H:255:THR:O	5:H:256:THR:OG1	2.35	0.42
7:K:68:THR:OG1	7:K:69:ASP:OD1	2.35	0.42
7:K:69:ASP:N	7:K:69:ASP:OD1	2.53	0.42
8:M:28:THR:O	8:M:31:THR:HG22	2.19	0.42
1:A:473:ASN:CB	14:A:1403:HOH:O	2.60	0.42
1:A:689:VAL:O	1:A:692:VAL:HG22	2.20	0.42
2:B:407:ASN:HB3	2:B:413:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:LEU:HD11	2:B:1192:PHE:HE2	1.85	0.42
1:A:166:LYS:HE3	1:A:187:ARG:NH2	2.34	0.42
2:B:88:ARG:HH21	2:B:345:ILE:HD11	1.85	0.42
2:B:279:ASP:HB3	2:B:280:PRO:HD3	2.02	0.42
2:B:1058:LEU:HD21	2:B:1190:TRP:HB3	2.01	0.42
6:E:426:LEU:HG	6:E:467:LYS:HG2	2.02	0.42
7:K:33:LEU:HD22	7:K:70:PHE:CG	2.55	0.42
7:K:34:HIS:CD2	7:K:88:GLN:HE21	2.28	0.42
1:A:150:ASN:HD22	1:A:150:ASN:N	2.16	0.41
1:A:423:PHE:N	1:A:423:PHE:CD1	2.87	0.41
1:A:706:TRP:HA	1:A:808:LEU:CD2	2.50	0.41
1:A:923:LYS:HB3	1:A:1056:LYS:HG3	2.00	0.41
2:B:302:TYR:CD1	2:B:302:TYR:C	2.97	0.41
2:B:564:GLU:O	2:B:568:ASN:ND2	2.37	0.41
2:B:1163:LYS:HA	2:B:1181:ASN:OD1	2.20	0.41
5:G:83:TYR:O	5:G:87:ASN:ND2	2.35	0.41
1:A:870:ILE:HD13	1:A:870:ILE:HA	1.85	0.41
1:A:889:ILE:HA	1:A:898:ILE:HD13	2.02	0.41
1:A:1255:PHE:O	1:A:1258:ILE:HG12	2.20	0.41
2:B:154:ASN:OD1	2:B:154:ASN:N	2.53	0.41
2:B:281:TYR:HB2	2:B:441:ALA:HB1	2.02	0.41
2:B:1113:ILE:HG22	2:B:1143:LYS:HG3	2.02	0.41
5:D:30:TYR:CZ	5:D:185:LYS:HD2	2.55	0.41
5:D:85:LYS:HB3	5:D:85:LYS:HE3	1.76	0.41
5:D:106:GLU:HG2	5:H:246:SER:HB2	2.02	0.41
1:A:290:PHE:HB3	1:A:333:VAL:HG21	2.01	0.41
2:B:1163:LYS:HB2	2:B:1179:CYS:SG	2.60	0.41
1:A:606:TRP:O	1:A:610:LEU:HD23	2.20	0.41
1:A:709:VAL:HG21	1:A:808:LEU:CD2	2.40	0.41
1:A:744:LYS:HD3	1:A:770:SER:HA	2.02	0.41
1:A:857:VAL:HG12	1:A:859:ASN:H	1.84	0.41
1:A:963:THR:HA	1:A:977:SER:HA	2.02	0.41
2:B:1135:ILE:HD11	2:B:1137:ASN:O	2.20	0.41
6:E:236:THR:HG23	6:E:308:LYS:HG2	2.02	0.41
5:H:519:ASN:HA	5:H:544:PRO:HB3	2.02	0.41
1:A:833:GLN:N	1:A:833:GLN:OE1	2.53	0.41
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.55	0.41
2:B:154:ASN:HB2	2:B:167:SER:O	2.21	0.41
2:B:1129:ASP:OD1	2:B:1129:ASP:N	2.49	0.41
5:I:89:GLN:HG2	5:I:94:ASN:HA	2.01	0.41
5:J:237:LEU:HD23	5:J:237:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:237:LEU:HB2	5:J:307:ILE:HG12	2.02	0.41
5:J:276:ARG:NH1	5:J:378:PRO:HG3	2.35	0.41
6:E:518:LEU:HD12	6:E:518:LEU:HA	1.93	0.41
5:G:34:ARG:HB2	5:G:127:ARG:HB3	2.03	0.41
1:A:321:TYR:HB2	1:A:323:LEU:CD1	2.51	0.41
1:A:811:PHE:CZ	1:A:815:LEU:HD12	2.55	0.41
1:A:882:ARG:HB2	1:A:891:LEU:HD13	2.02	0.41
1:A:1027:SER:HB2	1:A:1041:ILE:HD13	2.02	0.41
2:B:766:ILE:O	2:B:770:GLU:HG2	2.20	0.41
5:J:278:LYS:O	5:J:282:ASN:HA	2.21	0.41
1:A:905:ASN:HB3	1:A:915:GLN:HB3	2.02	0.41
2:B:147:TYR:O	2:B:147:TYR:CG	2.73	0.41
2:B:817:MET:HB3	2:B:817:MET:HE3	1.82	0.41
6:E:259:LEU:HB2	6:E:333:TYR:HB2	2.02	0.41
5:G:116:ASN:OD1	5:G:116:ASN:N	2.54	0.41
5:H:397:ILE:HA	5:H:398:PRO:HD3	1.95	0.41
1:A:203:ASP:N	1:A:203:ASP:OD1	2.53	0.41
1:A:310:LEU:O	1:A:314:LYS:HG3	2.21	0.41
1:A:819:LEU:HD23	1:A:841:VAL:HG22	2.01	0.41
6:E:552:THR:HG23	6:E:597:ARG:HH21	1.85	0.41
5:G:31:VAL:O	5:G:183:TYR:HA	2.21	0.41
1:A:163:PHE:O	1:A:224:GLN:NE2	2.54	0.41
1:A:676:LEU:HB2	1:A:811:PHE:HB2	2.02	0.41
1:A:966:ASN:HB3	1:A:1054:MET:HB3	2.02	0.41
1:A:1022:ASN:HB2	1:A:1078:GLU:CD	2.46	0.41
2:B:542:TYR:O	2:B:546:ILE:HG12	2.21	0.41
2:B:563:ARG:O	2:B:567:ARG:HG3	2.21	0.41
2:B:680:TYR:O	2:B:684:ILE:HG13	2.21	0.41
2:B:1122:LYS:HB3	2:B:1134:LEU:HB3	2.02	0.41
2:B:1185:LYS:H	2:B:1185:LYS:HG2	1.67	0.41
3:C:12:VAL:O	3:C:118:VAL:HA	2.21	0.41
5:J:228:THR:HG22	5:J:363:ILE:HD11	2.03	0.41
5:J:357:VAL:HG12	5:G:182:LEU:HG	2.02	0.41
5:J:430:LYS:HA	5:J:460:GLY:HA3	2.03	0.41
5:D:43:GLN:OE1	6:E:282:ASN:ND2	2.51	0.41
6:E:271:GLN:O	6:E:275:GLU:HG2	2.21	0.41
7:K:65:GLY:HA3	7:K:70:PHE:HA	2.02	0.41
8:M:51:ILE:HD12	8:M:51:ILE:HA	1.87	0.41
1:A:109:THR:O	1:A:113:ARG:HG2	2.20	0.41
1:A:154:ILE:HG13	1:A:155:GLY:O	2.21	0.41
1:A:1134:MET:HE3	1:A:1134:MET:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:PRO:CB	2:B:178:ILE:HA	2.51	0.41
2:B:791:ASN:HA	8:M:101:ASP:O	2.21	0.41
4:F:3:VAL:HB	4:F:105:TYR:CE1	2.56	0.41
5:H:315:LYS:HG3	5:H:333:TYR:CE2	2.56	0.41
5:H:430:LYS:HA	5:H:460:GLY:HA3	2.03	0.41
1:A:1183:ASN:HA	1:A:1191:TYR:O	2.20	0.40
2:B:566:PHE:CD2	2:B:899:THR:HB	2.57	0.40
2:B:930:TRP:HA	2:B:942:ASN:O	2.22	0.40
5:J:462:ASP:CG	5:J:529:GLN:HE22	2.28	0.40
6:E:416:GLY:HA3	6:E:499:ARG:NH1	2.36	0.40
6:E:536:TYR:CD1	6:E:607:LYS:HE2	2.56	0.40
5:G:67:ASP:HB2	5:H:286:PHE:CE2	2.56	0.40
5:G:83:TYR:OH	5:G:186:ILE:HG21	2.21	0.40
5:H:533:VAL:HG12	5:H:534:HIS:ND1	2.36	0.40
1:A:1191:TYR:HB3	1:A:1209:LEU:O	2.22	0.40
3:C:66:ARG:HH22	3:C:89:ASP:CG	2.29	0.40
5:G:38:TRP:CZ2	5:G:127:ARG:HD3	2.57	0.40
5:H:222:GLY:HA2	5:H:369:GLU:HB3	2.03	0.40
7:K:38:GLN:OE1	7:K:44:PRO:HG3	2.21	0.40
1:A:399:ALA:HB2	1:A:893:ARG:HB2	2.02	0.40
1:A:685:ILE:HD12	1:A:685:ILE:H	1.86	0.40
2:B:562:LEU:HD23	2:B:898:LEU:HD23	2.03	0.40
5:I:30:TYR:HB2	5:I:131:ILE:HG12	2.03	0.40
5:I:32:VAL:HA	5:I:182:LEU:O	2.21	0.40
5:J:329:LYS:HB3	5:J:329:LYS:HE2	1.87	0.40
5:G:22:THR:HG22	5:G:137:GLU:HG3	2.04	0.40
5:H:277:LEU:HB3	5:H:283:VAL:CG2	2.50	0.40
1:A:1236:LYS:HB3	1:A:1249:PHE:CE2	2.56	0.40
2:B:227:ILE:HG22	2:B:267:VAL:HG22	2.03	0.40
2:B:1037:LEU:HA	2:B:1037:LEU:HD23	1.84	0.40
5:I:31:VAL:HG11	5:I:87:ASN:HB3	2.03	0.40
5:I:64:ARG:O	5:I:64:ARG:HD2	2.21	0.40
5:D:64:ARG:HG2	5:D:66:ASN:HB2	2.03	0.40
1:A:65:ALA:O	1:A:536:ARG:NH1	2.45	0.40
1:A:170:HIS:CG	1:A:171:GLU:N	2.89	0.40
1:A:306:THR:HG23	1:A:308:ALA:N	2.36	0.40
1:A:495:SER:OG	1:A:497:ASP:OD1	2.38	0.40
1:A:1189:LYS:HG2	5:J:400:ILE:HG23	2.03	0.40
2:B:213:GLU:HG3	2:B:382:ILE:CD1	2.52	0.40
2:B:887:ILE:HG23	2:B:1005:LEU:HB3	2.03	0.40
5:D:70:ILE:H	5:D:70:ILE:HG13	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:570:ARG:O	5:H:581:ILE:HD12	2.22	0.40
8:M:40:ARG:HH21	8:M:89:GLU:C	2.30	0.40
8:M:76:SER:OG	8:M:78:THR:OG1	2.29	0.40
9:N:201:HIS:HB3	9:N:206:THR:HB	2.03	0.40
10:L:133:PHE:C	10:L:134:LEU:HD12	2.47	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	1270/1296 (98%)	1236 (97%)	34 (3%)	0	100	100
2	B	1181/1194 (99%)	1133 (96%)	48 (4%)	0	100	100
3	C	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
4	F	112/121 (93%)	110 (98%)	1 (1%)	1 (1%)	14	34
5	D	172/626 (28%)	164 (95%)	8 (5%)	0	100	100
5	G	167/626 (27%)	161 (96%)	6 (4%)	0	100	100
5	H	419/626 (67%)	399 (95%)	20 (5%)	0	100	100
5	I	167/626 (27%)	156 (93%)	11 (7%)	0	100	100
5	J	419/626 (67%)	401 (96%)	18 (4%)	0	100	100
6	E	419/626 (67%)	403 (96%)	16 (4%)	0	100	100
7	K	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
8	M	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
9	N	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
10	L	101/103 (98%)	101 (100%)	0	0	100	100
All	All	4850/6914 (70%)	4664 (96%)	185 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	30	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	1152/1177 (98%)	1140 (99%)	12 (1%)	68	81
2	B	1101/1113 (99%)	1088 (99%)	13 (1%)	63	78
3	C	90/103 (87%)	90 (100%)	0	100	100
4	F	90/97 (93%)	90 (100%)	0	100	100
5	D	153/572 (27%)	147 (96%)	6 (4%)	28	53
5	G	153/572 (27%)	153 (100%)	0	100	100
5	H	381/572 (67%)	375 (98%)	6 (2%)	55	74
5	I	151/572 (26%)	147 (97%)	4 (3%)	40	65
5	J	381/572 (67%)	373 (98%)	8 (2%)	47	70
6	E	380/571 (66%)	374 (98%)	6 (2%)	55	74
7	K	91/94 (97%)	89 (98%)	2 (2%)	45	69
8	M	90/94 (96%)	87 (97%)	3 (3%)	33	58
9	N	68/83 (82%)	66 (97%)	2 (3%)	37	62
10	L	79/95 (83%)	77 (98%)	2 (2%)	42	66
All	All	4360/6287 (69%)	4296 (98%)	64 (2%)	57	75

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	161	ILE
1	A	348	ILE
1	A	359	LYS
1	A	487	ILE

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Mol	Chain	Res	Type
1	A	604	LEU
1	A	662	VAL
1	A	997	VAL
1	A	1076	ASP
1	A	1143	VAL
1	A	1232	THR
1	A	1258	ILE
2	B	123	ILE
2	B	135	LEU
2	B	213	GLU
2	B	222	LEU
2	B	355	LEU
2	B	442	TYR
2	B	528	ASP
2	B	582	ASN
2	B	629	ILE
2	B	722	LEU
2	B	810	GLU
2	B	828	LEU
2	B	1124	ILE
5	I	22	THR
5	I	65	VAL
5	I	93	THR
5	I	130	ILE
5	J	206	THR
5	J	342	VAL
5	J	352	VAL
5	J	428	SER
5	J	429	LEU
5	J	472	VAL
5	J	489	SER
5	J	568	LEU
5	D	17	ILE
5	D	44	ASN
5	D	68	ASN
5	D	70	ILE
5	D	121	LEU
5	D	148	SER
6	E	322	GLN
6	E	342	VAL
6	E	412	VAL
6	E	448	CYS

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Mol	Chain	Res	Type
6	E	579	ASN
6	E	625	THR
5	H	248	ILE
5	H	302	ASP
5	H	412	VAL
5	H	484	VAL
5	H	508	MET
5	H	575	ILE
7	K	55	ILE
7	K	71	THR
8	M	30	THR
8	M	96	CYS
8	M	100	TYR
9	N	138	VAL
9	N	185	VAL
10	L	145	LYS
10	L	207	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	174	ASN
1	A	184	GLN
1	A	278	GLN
1	A	315	ASN
1	A	514	ASN
1	A	573	ASN
1	A	609	GLN
1	A	703	ASN
1	A	739	GLN
1	A	753	GLN
1	A	852	GLN
1	A	859	ASN
1	A	1003	GLN
1	A	1115	ASN
1	A	1238	ASN
1	A	1257	ASN
1	A	1265	ASN
1	A	1268	ASN
2	B	93	ASN
2	B	254	ASN

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Mol	Chain	Res	Type
2	B	450	ASN
2	B	485	GLN
2	B	507	GLN
2	B	694	GLN
2	B	729	ASN
2	B	739	GLN
2	B	760	ASN
2	B	858	ASN
2	B	1010	ASN
2	B	1140	ASN
3	C	86	GLN
4	F	40	GLN
4	F	75	ASN
5	I	54	ASN
5	I	180	GLN
5	J	322	GLN
5	J	396	ASN
5	J	486	GLN
5	J	563	GLN
5	J	579	ASN
5	J	617	ASN
5	D	116	ASN
6	E	249	GLN
6	E	284	GLN
6	E	365	ASN
6	E	403	ASN
6	E	423	GLN
6	E	439	ASN
6	E	475	ASN
6	E	479	ASN
6	E	513	ASN
6	E	549	ASN
5	G	89	GLN
5	G	172	ASN
5	G	180	GLN
5	H	282	ASN
5	H	365	ASN
5	H	439	ASN
5	H	446	ASN
5	H	479	ASN
5	H	486	GLN
5	H	614	ASN

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Mol	Chain	Res	Type
7	K	88	GLN
8	M	1	GLN
8	M	35	GLN
8	M	62	GLN
10	L	135	ASN
10	L	159	ASN
10	L	188	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	SO4	A	1301	-	4,4,4	0.64	0	6,6,6	0.09	0
11	SO4	A	1304	-	4,4,4	0.72	0	6,6,6	0.39	0
11	SO4	A	1302	-	4,4,4	0.67	0	6,6,6	0.18	0
11	SO4	B	1203	-	4,4,4	0.67	0	6,6,6	0.08	0
11	SO4	D	701	-	4,4,4	0.68	0	6,6,6	0.38	0
11	SO4	A	1303	-	4,4,4	0.67	0	6,6,6	0.05	0
11	SO4	B	1201	-	4,4,4	0.67	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	SO4	E	701	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
11	SO4	B	1204	-	4,4,4	0.73	0	6,6,6	0.42	0
11	SO4	B	1202	-	4,4,4	0.66	0	6,6,6	0.22	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	701	SO4	O4-S-O3	3.06	125.39	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1301	SO4	3	0
11	E	701	SO4	4	0
11	B	1202	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	132:PRO	C	137:SER	N	10.71

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	1276/1296 (98%)	0.59	66 (5%)	33 27	35, 63, 101, 165	0
2	B	1187/1194 (99%)	0.46	47 (3%)	42 34	27, 53, 95, 176	0
3	C	117/128 (91%)	0.95	14 (11%)	9 8	56, 94, 129, 158	0
4	F	114/121 (94%)	0.49	4 (3%)	47 39	55, 68, 90, 95	0
5	D	174/626 (27%)	0.52	7 (4%)	42 34	28, 48, 87, 133	0
5	G	169/626 (26%)	0.69	6 (3%)	46 38	40, 61, 92, 113	0
5	H	421/626 (67%)	0.87	44 (10%)	11 11	32, 82, 127, 170	0
5	I	169/626 (26%)	0.50	5 (2%)	52 44	28, 49, 79, 107	0
5	J	421/626 (67%)	0.83	35 (8%)	17 15	36, 71, 124, 159	0
6	E	421/626 (67%)	0.48	9 (2%)	63 54	24, 42, 86, 169	0
7	K	105/105 (100%)	1.69	34 (32%)	1 1	96, 141, 175, 214	0
8	M	117/117 (100%)	1.39	32 (27%)	1 1	84, 116, 146, 155	0
9	N	93/94 (98%)	2.27	51 (54%)	0 0	131, 179, 209, 218	0
10	L	103/103 (100%)	1.86	41 (39%)	1 0	168, 206, 234, 274	0
All	All	4887/6914 (70%)	0.70	395 (8%)	18 15	24, 62, 150, 274	0

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	201	SER	6.4
9	N	188	SER	5.9
10	L	111	PRO	5.5
7	K	102	LEU	5.1
1	A	1225	SER	5.0
9	N	132	PRO	4.9
9	N	153	THR	4.7
9	N	199	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
9	N	208	VAL	4.7
9	N	150	GLU	4.7
9	N	152	VAL	4.5
1	A	1227	ASN	4.4
10	L	138	TYR	4.4
9	N	147	TYR	4.3
9	N	200	ALA	4.2
2	B	629	ILE	4.2
10	L	117	PRO	4.2
9	N	213	GLU	4.2
1	A	51	PHE	4.1
10	L	109	ALA	4.1
10	L	155	ASN	4.1
7	K	105	ILE	4.1
5	D	16	VAL	4.0
9	N	189	THR	4.0
5	H	575	ILE	3.9
2	B	1084	THR	3.8
1	A	832	GLY	3.8
1	A	1295	PRO	3.8
7	K	48	ILE	3.8
1	A	672	ALA	3.7
8	M	107	GLY	3.7
5	J	468	SER	3.7
1	A	647	LEU	3.7
7	K	11	LEU	3.7
1	A	119	GLY	3.7
8	M	100	TYR	3.7
10	L	112	THR	3.7
2	B	1087	LEU	3.6
7	K	85	TYR	3.6
8	M	117	VAL	3.6
9	N	179	LEU	3.6
7	K	2	ILE	3.6
9	N	185	VAL	3.6
10	L	200	THR	3.6
10	L	154	GLN	3.5
7	K	86	PHE	3.5
7	K	62	PHE	3.5
5	J	529	GLN	3.5
5	H	438	GLY	3.5
9	N	191	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
6	E	348	PRO	3.4
7	K	59	PRO	3.4
5	G	187	LEU	3.3
2	B	121	ASN	3.3
3	C	12	VAL	3.3
5	G	64	ARG	3.3
5	J	400	ILE	3.3
9	N	183	VAL	3.3
1	A	1226	LYS	3.3
5	J	406	PHE	3.3
7	K	77	VAL	3.3
8	M	87	ALA	3.3
8	M	93	VAL	3.3
8	M	99	GLY	3.3
6	E	491	ILE	3.2
1	A	512	PRO	3.2
10	L	148	ILE	3.2
10	L	146	TRP	3.2
1	A	869	TYR	3.2
10	L	203	ILE	3.2
10	L	153	ARG	3.2
1	A	434	ILE	3.2
1	A	1092	SER	3.2
9	N	144	VAL	3.2
3	C	114	THR	3.2
5	J	206	THR	3.2
9	N	142	CYS	3.1
8	M	108	TYR	3.1
2	B	127	SER	3.1
2	B	526	SER	3.1
9	N	131	ALA	3.1
5	H	541	PHE	3.1
10	L	202	PRO	3.1
9	N	190	TRP	3.1
3	C	9	GLY	3.1
5	J	239	ILE	3.1
9	N	177	TYR	3.1
6	E	529	GLN	3.1
1	A	27	ALA	3.0
10	L	177	LEU	3.0
7	K	15	PRO	3.0
8	M	14	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
8	M	41	PRO	3.0
1	A	824	TYR	3.0
9	N	143	LEU	3.0
1	A	857	VAL	3.0
9	N	154	LEU	3.0
5	J	497	PHE	3.0
5	H	253	ARG	2.9
10	L	190	TYR	2.9
10	L	158	LEU	2.9
5	I	99	ASN	2.9
9	N	192	SER	2.9
2	B	651	PHE	2.9
8	M	105	THR	2.9
10	L	191	THR	2.9
5	J	544	PRO	2.9
9	N	214	PRO	2.9
7	K	81	ASP	2.9
7	K	9	ALA	2.9
9	N	120	ALA	2.9
9	N	186	THR	2.9
3	C	22	CYS	2.9
1	A	61	PRO	2.9
2	B	1071	VAL	2.9
5	D	98	ALA	2.9
10	L	110	ALA	2.9
7	K	73	ILE	2.9
2	B	1082	ASN	2.8
8	M	64	PHE	2.8
5	H	542	THR	2.8
10	L	140	LYS	2.8
3	C	93	TYR	2.8
1	A	1166	ALA	2.8
7	K	104	ILE	2.8
1	A	1168	GLY	2.8
2	B	145	PHE	2.8
2	B	916	ILE	2.8
1	A	834	VAL	2.8
9	N	138	VAL	2.8
2	B	1150	ILE	2.8
2	B	1081	ILE	2.7
5	H	555	ILE	2.7
9	N	182	SER	2.7

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Mol	Chain	Res	Type	RSRZ
9	N	187	SER	2.7
8	M	10	GLU	2.7
2	B	1152	ILE	2.7
10	L	115	ILE	2.7
10	L	192	CYS	2.7
2	B	751	ASN	2.7
5	D	97	GLU	2.7
5	H	514	ILE	2.7
5	H	509	ASN	2.7
2	B	133	LYS	2.7
2	B	1174	HIS	2.7
2	B	359	TYR	2.7
6	E	306	CYS	2.7
2	B	410	ASN	2.7
5	H	288	THR	2.7
5	H	361	GLY	2.7
5	H	564	GLY	2.7
2	B	1111	GLU	2.7
1	A	604	LEU	2.7
5	H	400	ILE	2.6
7	K	60	SER	2.7
8	M	36	TRP	2.6
5	H	411	THR	2.6
10	L	131	VAL	2.6
10	L	169	SER	2.6
7	K	35	TRP	2.6
2	B	269	GLY	2.6
1	A	530	LEU	2.6
1	A	1272	GLU	2.6
5	J	618	ILE	2.6
9	N	209	ASP	2.6
9	N	156	TRP	2.6
2	B	149	GLY	2.6
1	A	361	LEU	2.6
9	N	171	VAL	2.6
10	L	204	VAL	2.6
2	B	912	GLY	2.6
3	C	8	GLY	2.6
5	H	474	LEU	2.6
7	K	84	VAL	2.6
9	N	139	THR	2.6
3	C	21	SER	2.5

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Mol	Chain	Res	Type	RSRZ
7	K	20	SER	2.5
2	B	130	LYS	2.5
2	B	1134	LEU	2.5
9	N	141	GLY	2.5
1	A	870	ILE	2.5
9	N	212	ILE	2.5
1	A	866	PHE	2.5
1	A	60	ASN	2.5
9	N	181	SER	2.5
7	K	47	LEU	2.5
9	N	161	LEU	2.5
5	J	604	TYR	2.5
5	H	527	THR	2.5
9	N	170	ALA	2.5
3	C	95	CYS	2.5
2	B	279	ASP	2.5
2	B	1149	ASP	2.5
1	A	864	SER	2.5
5	H	350	SER	2.5
5	H	473	LEU	2.5
1	A	49	ASP	2.5
1	A	646	MET	2.5
5	J	511	SER	2.5
1	A	331	PHE	2.5
1	A	513	GLU	2.5
1	A	603	PHE	2.5
5	J	578	TYR	2.5
7	K	71	THR	2.5
10	L	178	THR	2.5
4	F	97	CYS	2.5
5	H	583	ILE	2.4
7	K	58	ILE	2.4
3	C	17	SER	2.4
8	M	88	SER	2.4
9	N	204	SER	2.4
1	A	868	GLU	2.4
8	M	109	TRP	2.4
5	J	561	TYR	2.4
6	E	345	ALA	2.4
6	E	576	ALA	2.4
2	B	124	THR	2.4
1	A	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	639	LEU	2.4
8	M	101	ASP	2.4
8	M	104	GLY	2.4
5	G	148	SER	2.4
8	M	32	TYR	2.4
8	M	71	THR	2.4
3	C	20	LEU	2.4
2	B	552	ILE	2.4
5	J	575	ILE	2.4
8	M	96	CYS	2.4
4	F	24	VAL	2.4
7	K	65	GLY	2.4
1	A	148	GLU	2.4
2	B	128	ALA	2.4
8	M	98	ALA	2.4
5	H	333	TYR	2.4
7	K	100	THR	2.4
5	J	598	LEU	2.4
5	J	624	ILE	2.4
10	L	145	LYS	2.4
1	A	670	GLU	2.4
1	A	1293	GLU	2.4
9	N	137	SER	2.4
1	A	122	THR	2.4
1	A	453	LEU	2.4
3	C	116	VAL	2.3
9	N	211	LYS	2.3
1	A	1219	GLN	2.3
2	B	239	SER	2.3
5	H	557	LEU	2.3
10	L	187	HIS	2.3
1	A	494	ILE	2.3
5	G	65	VAL	2.3
5	H	512	VAL	2.3
8	M	37	VAL	2.3
1	A	526	GLY	2.3
1	A	1251	GLY	2.3
5	H	416	GLY	2.3
5	H	479	ASN	2.3
5	J	295	PHE	2.3
8	M	35	GLN	2.3
1	A	59	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	449	SER	2.3
5	H	606	LEU	2.3
1	A	671	ILE	2.3
9	N	178	THR	2.3
7	K	99	GLY	2.3
5	D	188	GLU	2.3
1	A	422	LEU	2.3
5	H	568	LEU	2.3
1	A	1234	LYS	2.3
2	B	632	TYR	2.3
5	H	604	TYR	2.3
10	L	184	TYR	2.3
5	I	35	GLY	2.3
5	H	466	ALA	2.3
4	F	2	GLN	2.3
8	M	63	LYS	2.3
9	N	145	LYS	2.3
8	M	47	TRP	2.3
8	M	103	SER	2.3
10	L	113	VAL	2.3
10	L	130	VAL	2.3
5	D	69	ALA	2.2
9	N	203	ALA	2.2
7	K	21	LEU	2.2
8	M	84	ILE	2.2
5	I	72	TYR	2.2
10	L	199	SER	2.2
3	C	45	PHE	2.2
7	K	97	PHE	2.2
5	G	25	LEU	2.2
5	I	159	PRO	2.2
5	J	352	VAL	2.2
5	D	93	THR	2.2
5	H	387	THR	2.2
7	K	14	THR	2.2
2	B	1123	TYR	2.2
7	K	63	GLY	2.2
1	A	8	PHE	2.2
10	L	207	PHE	2.2
2	B	1132	LEU	2.2
10	L	194	ALA	2.2
2	B	628	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
9	N	215	ARG	2.2
6	E	206	THR	2.2
1	A	349	TYR	2.2
5	J	390	SER	2.2
5	J	595	SER	2.2
1	A	1116	LEU	2.2
10	L	123	LEU	2.2
1	A	1231	ILE	2.2
5	J	207	GLN	2.2
5	J	531	PRO	2.2
7	K	3	VAL	2.2
3	C	117	THR	2.2
4	F	11	GLY	2.2
2	B	1089	LEU	2.2
5	J	504	LEU	2.2
5	H	488	SER	2.2
7	K	33	LEU	2.2
1	A	488	GLU	2.2
6	E	492	GLU	2.2
1	A	762	ILE	2.1
5	H	208	ARG	2.1
5	H	375	VAL	2.1
2	B	897	GLY	2.1
6	E	567	THR	2.1
8	M	102	THR	2.1
9	N	167	THR	2.1
10	L	133	PHE	2.1
5	J	306	CYS	2.1
5	H	468	SER	2.1
8	M	68	ALA	2.1
10	L	152	GLU	2.1
5	H	397	ILE	2.1
2	B	1074	ASN	2.1
2	B	146	PRO	2.1
1	A	858	ASP	2.1
5	H	507	LEU	2.1
5	I	84	ILE	2.1
5	J	408	ILE	2.1
9	N	197	CYS	2.1
2	B	1170	LYS	2.1
5	J	218	VAL	2.1
3	C	78	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	J	599	LEU	2.1
5	J	606	LEU	2.1
7	K	72	LEU	2.1
8	M	44	GLY	2.1
9	N	146	GLY	2.1
1	A	365	THR	2.1
5	J	442	PHE	2.1
5	J	556	ARG	2.1
7	K	76	ARG	2.1
1	A	489	ALA	2.1
5	H	523	ALA	2.1
5	H	540	GLU	2.1
5	H	578	TYR	2.1
5	D	65	VAL	2.1
2	B	1194	PRO	2.1
5	J	346	PRO	2.1
9	N	151	PRO	2.1
2	B	135	LEU	2.1
5	J	507	LEU	2.1
10	L	156	GLY	2.1
5	H	605	ILE	2.1
5	H	481	TYR	2.1
1	A	564	SER	2.0
8	M	81	MET	2.0
1	A	561	HIS	2.0
5	H	401	VAL	2.0
5	H	412	VAL	2.0
9	N	127	VAL	2.0
1	A	761	ASN	2.0
5	H	598	LEU	2.0
9	N	176	LEU	2.0
5	J	208	ARG	2.0
7	K	57	GLY	2.0
5	H	255	THR	2.0
5	J	351	GLU	2.0
1	A	822	TYR	2.0
1	A	1155	TYR	2.0
10	L	120	SER	2.0
1	A	62	PRO	2.0
8	M	11	LEU	2.0
5	H	506	ASN	2.0
1	A	425	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
5	J	542	THR	2.0
10	L	180	THR	2.0
10	L	195	THR	2.0
1	A	212	LYS	2.0
1	A	1189	LYS	2.0
2	B	992	LYS	2.0
2	B	1120	MET	2.0
5	G	38	TRP	2.0
2	B	442	TYR	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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
13	MG	E	705	1/1	0.60	0.88	89,89,89,89	1
11	SO4	B	1204	5/5	0.68	0.14	75,77,108,134	0
11	SO4	A	1304	5/5	0.74	0.11	96,100,111,132	0
13	MG	A	1306	1/1	0.81	0.29	36,36,36,36	0
11	SO4	B	1203	5/5	0.82	0.14	55,70,82,87	0
11	SO4	E	701	5/5	0.83	0.23	66,67,86,90	0
11	SO4	D	701	5/5	0.86	0.10	64,66,79,88	0
13	MG	E	707	1/1	0.86	0.29	20,20,20,20	0
11	SO4	A	1303	5/5	0.87	0.12	67,69,84,106	0
13	MG	B	1205	1/1	0.87	0.22	40,40,40,40	0
11	SO4	B	1201	5/5	0.88	0.08	59,70,88,91	0
11	SO4	B	1202	5/5	0.88	0.10	45,57,60,69	0
11	SO4	A	1301	5/5	0.89	0.12	63,64,82,90	0
11	SO4	A	1302	5/5	0.89	0.13	63,66,73,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	MG	E	703	1/1	0.90	0.14	20,20,20,20	0
13	MG	E	704	1/1	0.93	0.25	30,30,30,30	0
13	MG	H	701	1/1	0.93	0.21	14,14,14,14	0
13	MG	E	702	1/1	0.94	0.17	24,24,24,24	0
13	MG	J	701	1/1	0.94	0.23	34,34,34,34	0
12	ZN	A	1305	1/1	0.96	0.04	129,129,129,129	0
13	MG	E	706	1/1	0.97	0.41	49,49,49,49	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.