



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2022 – 02:38 PM EDT

PDB ID : 6UJI  
Title : Low resolution crystal structure (5.5 Å) of the anthrax toxin protective antigen heptamer prepore D425A mutant  
Authors : Lovell, S.; Mehzabeen, N.; Battaile, K.P.; Bann, J.G.  
Deposited on : 2019-10-03  
Resolution : 5.50 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

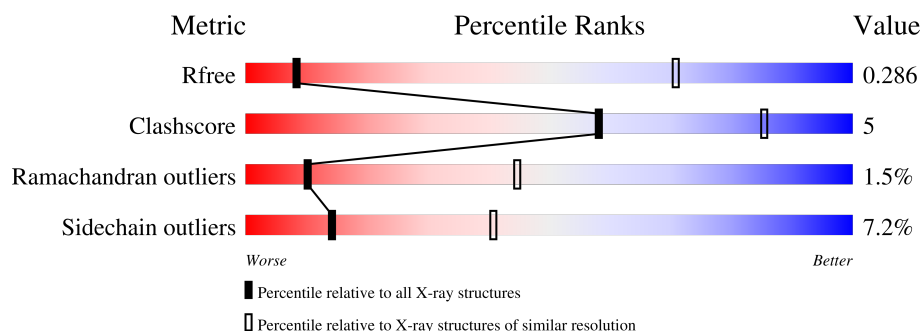
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 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	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	568	67% 15% • 17%
1	B	568	72% 18% • 9%
1	C	568	57% 11% 32%
1	D	568	77% 16% • 5%
1	E	568	71% 19% • 9%
1	F	568	68% 13% • 18%
1	G	568	73% 17% • 8%

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Mol	Chain	Length	Quality of chain
1	H	568	 69%17%13%
1	I	568	 74%18%7%
1	J	568	 67%15%17%
1	K	568	 68%16%14%
1	L	568	 57%14%29%
1	M	568	 65%18%17%
1	N	568	 65%18%15%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53490 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 Protective antigen PA-63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3712	2316	650	740	6			
1	B	519	Total	C	N	O	S	0	0	0
			4114	2578	710	820	6			
1	C	388	Total	C	N	O	S	0	0	0
			3083	1929	539	609	6			
1	D	539	Total	C	N	O	S	0	0	0
			4265	2672	735	852	6			
1	E	516	Total	C	N	O	S	0	0	0
			4089	2564	704	815	6			
1	F	467	Total	C	N	O	S	0	0	0
			3688	2316	641	725	6			
1	G	520	Total	C	N	O	S	0	0	0
			4125	2583	710	826	6			
1	H	493	Total	C	N	O	S	0	0	0
			3894	2434	678	776	6			
1	I	529	Total	C	N	O	S	0	0	0
			4189	2622	724	837	6			
1	J	470	Total	C	N	O	S	0	0	0
			3718	2322	649	741	6			
1	K	488	Total	C	N	O	S	0	0	0
			3867	2419	673	769	6			
1	L	404	Total	C	N	O	S	0	0	0
			3189	1992	555	637	5			
1	M	473	Total	C	N	O	S	0	0	0
			3749	2345	656	742	6			
1	N	480	Total	C	N	O	S	0	0	0
			3808	2375	663	764	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	ALA	ASP	engineered mutation	UNP P13423

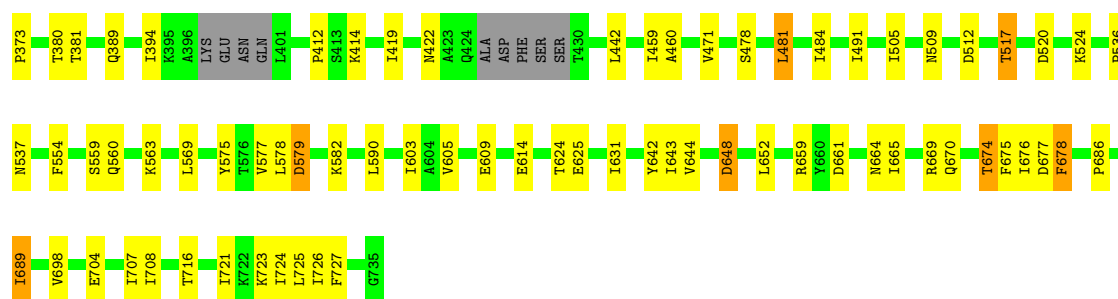
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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	ALA	ASP	engineered mutation	UNP P13423
C	425	ALA	ASP	engineered mutation	UNP P13423
D	425	ALA	ASP	engineered mutation	UNP P13423
E	425	ALA	ASP	engineered mutation	UNP P13423
F	425	ALA	ASP	engineered mutation	UNP P13423
G	425	ALA	ASP	engineered mutation	UNP P13423
H	425	ALA	ASP	engineered mutation	UNP P13423
I	425	ALA	ASP	engineered mutation	UNP P13423
J	425	ALA	ASP	engineered mutation	UNP P13423
K	425	ALA	ASP	engineered mutation	UNP P13423
L	425	ALA	ASP	engineered mutation	UNP P13423
M	425	ALA	ASP	engineered mutation	UNP P13423
N	425	ALA	ASP	engineered mutation	UNP P13423

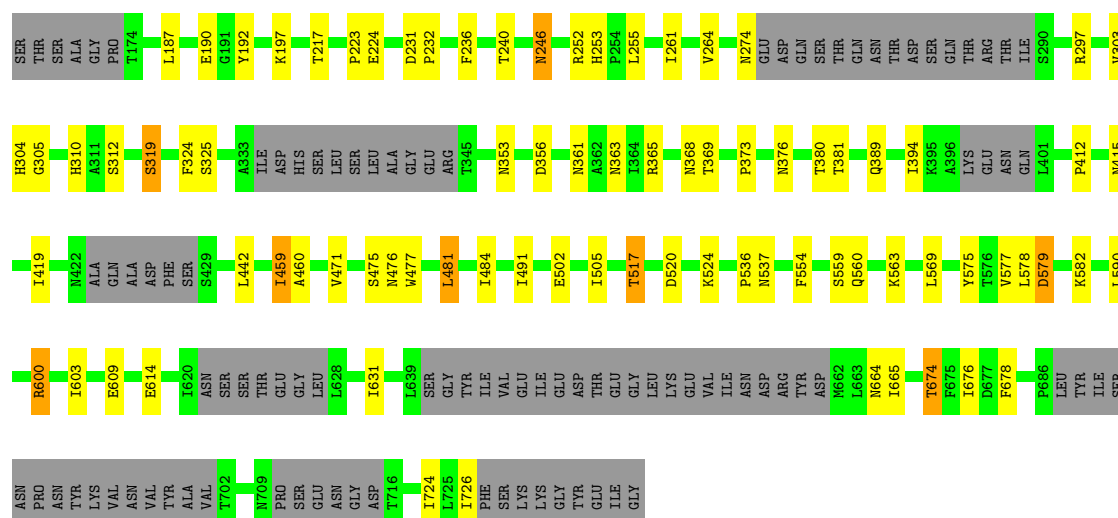






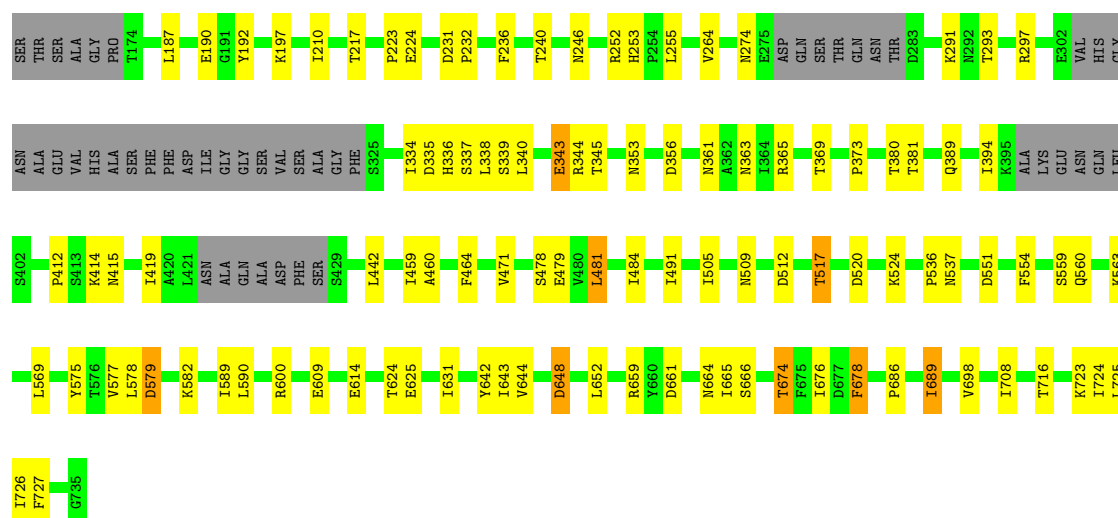
• Molecule 1: Protective antigen PA-63

Chain F: 68% 13% 18%



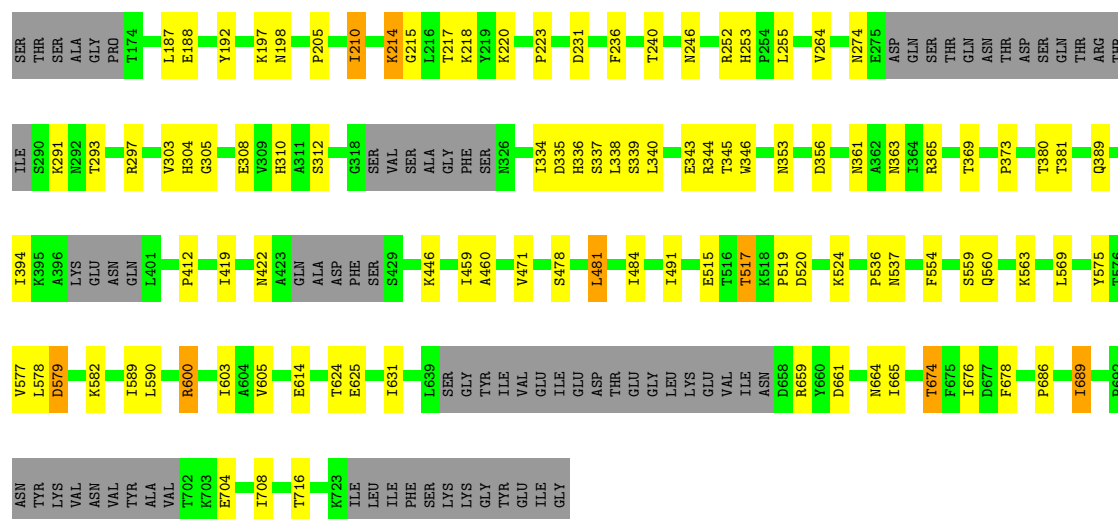
• Molecule 1: Protective antigen PA-63

Chain G: 73% 17% 8%



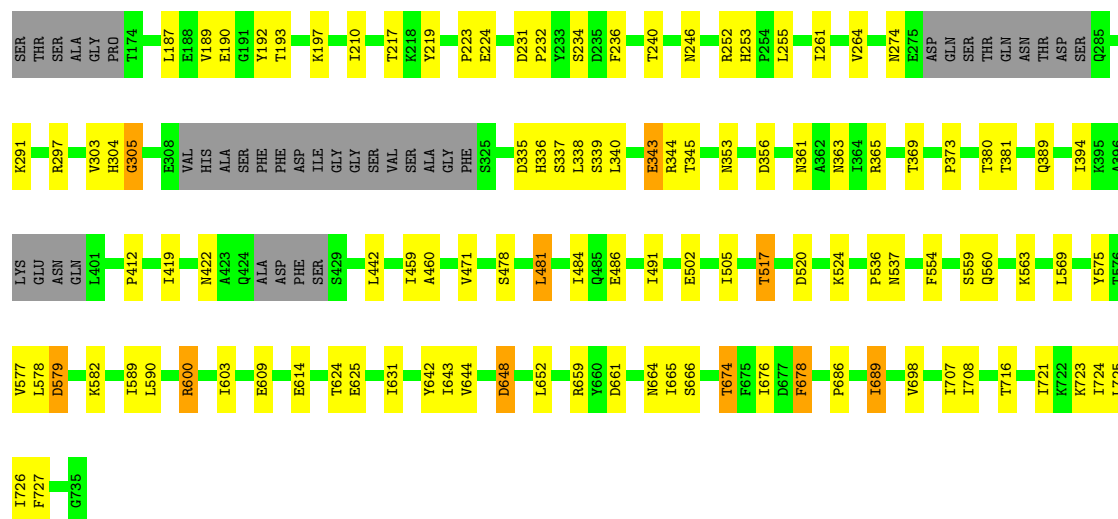
• Molecule 1: Protective antigen PA-63

Chain H:  69% 17% 13%



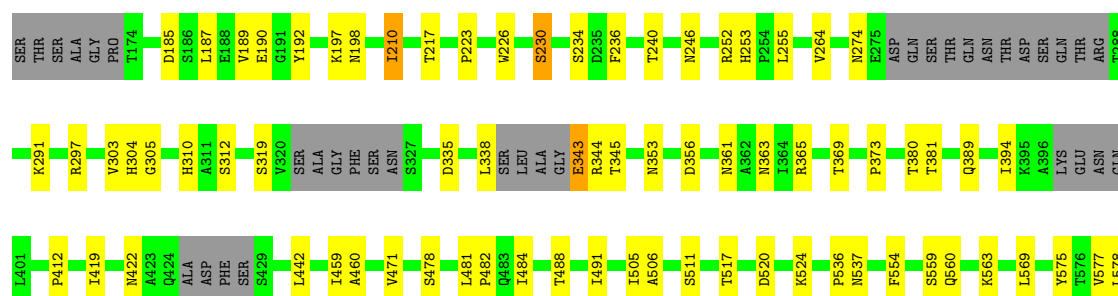
• Molecule 1: Protective antigen PA-63

Chain I:  74% 18% 7%



• Molecule 1: Protective antigen PA-63

Chain J:  67% 15% 17%





Response	Percentage
Good country	65%
Not a good country	18%
Don't know	17%



Response	Percentage
Yes	65%
No	18%
Don't know	15%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.18Å 144.25Å 304.82Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	44.83 – 5.50 49.78 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.83-5.50) 99.3 (49.78-5.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 5.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.251 , 0.278 0.268 , 0.286	Depositor DCC
$R_{free}$ test set	2250 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	183.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 204.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	53490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	257.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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](#)

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	0.37	0/3771	0.58	0/5109
1	B	0.37	0/4181	0.58	0/5667
1	C	0.36	0/3134	0.58	0/4250
1	D	0.35	0/4336	0.58	0/5877
1	E	0.36	0/4156	0.58	0/5633
1	F	0.37	0/3746	0.58	0/5072
1	G	0.35	0/4192	0.57	0/5681
1	H	0.36	0/3958	0.57	0/5364
1	I	0.35	0/4257	0.58	0/5770
1	J	0.38	0/3776	0.60	0/5112
1	K	0.38	0/3926	0.58	0/5314
1	L	0.40	0/3237	0.60	0/4388
1	M	0.39	0/3811	0.60	0/5166
1	N	0.39	0/3868	0.60	0/5243
All	All	0.37	0/54349	0.58	0/73646

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	3712	0	3666	39	0
1	B	4114	0	4098	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3083	0	3058	20	0
1	D	4265	0	4229	40	0
1	E	4089	0	4071	46	0
1	F	3688	0	3679	29	0
1	G	4125	0	4102	42	0
1	H	3894	0	3852	37	0
1	I	4189	0	4164	45	0
1	J	3718	0	3673	31	0
1	K	3867	0	3860	39	0
1	L	3189	0	3177	33	0
1	M	3749	0	3697	40	0
1	N	3808	0	3769	45	0
All	All	53490	0	53095	507	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 5.

All (507) 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:642:TYR:HB2	1:G:665:ILE:HD11	1.57	0.87
1:I:642:TYR:HB2	1:I:665:ILE:HD11	1.58	0.83
1:B:642:TYR:HB2	1:B:665:ILE:HD11	1.60	0.81
1:N:297:ARG:HD3	1:N:369:THR:HG21	1.68	0.75
1:K:481:LEU:H	1:K:482:PRO:HD2	1.56	0.71
1:E:642:TYR:HB2	1:E:665:ILE:HD11	1.74	0.68
1:D:642:TYR:HB2	1:D:665:ILE:HD11	1.78	0.65
1:L:187:LEU:HB3	1:L:192:TYR:HB3	1.79	0.65
1:I:337:SER:HA	1:I:661:ASP:HB2	1.81	0.62
1:E:648:ASP:HB2	1:E:652:LEU:H	1.65	0.62
1:B:648:ASP:HB2	1:B:652:LEU:H	1.64	0.61
1:E:325:SER:HB2	1:F:415:ASN:ND2	2.15	0.61
1:D:648:ASP:HB2	1:D:652:LEU:H	1.66	0.61
1:I:648:ASP:HB2	1:I:652:LEU:H	1.64	0.60
1:M:451:ASP:HB3	1:N:416:LEU:HD23	1.83	0.60
1:L:382:SER:HB3	1:L:393:THR:HG22	1.84	0.60
1:L:224:GLU:HB2	1:L:517:THR:HG21	1.83	0.59
1:N:575:TYR:HA	1:N:578:LEU:HD13	1.82	0.59
1:L:189:VAL:HG11	1:M:198:ASN:HB3	1.83	0.59
1:N:624:THR:HG21	1:N:689:ILE:HD11	1.85	0.59
1:G:648:ASP:HB2	1:G:652:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:VAL:HG11	1:L:198:ASN:HB3	1.85	0.58
1:C:183:ILE:HG23	1:C:203:LEU:HD21	1.86	0.58
1:G:337:SER:HA	1:G:661:ASP:HB2	1.86	0.58
1:E:337:SER:HA	1:E:661:ASP:HB2	1.86	0.57
1:L:231:ASP:HB2	1:L:232:PRO:HD2	1.86	0.57
1:A:337:SER:HA	1:A:661:ASP:HB2	1.87	0.57
1:B:337:SER:HA	1:B:661:ASP:HB2	1.86	0.57
1:I:642:TYR:HE2	1:I:666:SER:HB3	1.70	0.57
1:N:353:ASN:H	1:N:356:ASP:HB2	1.70	0.57
1:D:336:HIS:HB3	1:D:708:ILE:HG22	1.86	0.56
1:G:353:ASN:H	1:G:356:ASP:HB2	1.70	0.56
1:A:353:ASN:H	1:A:356:ASP:HB2	1.70	0.56
1:D:353:ASN:H	1:D:356:ASP:HB2	1.70	0.56
1:J:353:ASN:H	1:J:356:ASP:HB2	1.70	0.56
1:K:353:ASN:H	1:K:356:ASP:HB2	1.70	0.56
1:F:353:ASN:H	1:F:356:ASP:HB2	1.70	0.56
1:M:223:PRO:HD2	1:M:517:THR:HG22	1.88	0.56
1:H:337:SER:HA	1:H:661:ASP:HB2	1.86	0.56
1:K:337:SER:HA	1:K:661:ASP:HB2	1.86	0.56
1:L:353:ASN:H	1:L:356:ASP:HB2	1.70	0.56
1:C:353:ASN:H	1:C:356:ASP:HB2	1.71	0.56
1:B:665:ILE:HD12	1:B:676:ILE:HG23	1.88	0.55
1:B:642:TYR:HE2	1:B:666:SER:HB3	1.71	0.55
1:E:353:ASN:H	1:E:356:ASP:HB2	1.71	0.55
1:G:642:TYR:HE2	1:G:666:SER:HB3	1.70	0.55
1:H:253:HIS:CD2	1:H:255:LEU:H	2.24	0.55
1:H:353:ASN:H	1:H:356:ASP:HB2	1.70	0.55
1:M:353:ASN:H	1:M:356:ASP:HB2	1.70	0.55
1:L:490:ARG:HE	1:L:504:ARG:HH21	1.55	0.55
1:M:337:SER:HA	1:M:661:ASP:HB2	1.88	0.55
1:A:724:ILE:HG22	1:A:725:LEU:H	1.72	0.55
1:A:575:TYR:HA	1:A:578:LEU:HD13	1.89	0.55
1:N:246:ASN:HB2	1:N:373:PRO:HG3	1.89	0.55
1:D:575:TYR:HA	1:D:578:LEU:HD13	1.89	0.55
1:B:575:TYR:HA	1:B:578:LEU:HD13	1.89	0.55
1:D:291:LYS:HE2	1:D:339:SER:HB2	1.89	0.55
1:E:575:TYR:HA	1:E:578:LEU:HD13	1.89	0.55
1:L:575:TYR:HA	1:L:578:LEU:HD13	1.89	0.55
1:M:665:ILE:HD12	1:M:676:ILE:HG23	1.89	0.55
1:E:644:VAL:HG11	1:E:678:PHE:HB3	1.89	0.55
1:I:353:ASN:H	1:I:356:ASP:HB2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:665:ILE:HD12	1:I:676:ILE:HG23	1.89	0.55
1:L:509:ASN:HD22	1:L:585:ALA:HB3	1.72	0.54
1:B:223:PRO:HD2	1:B:517:THR:HG22	1.90	0.54
1:B:353:ASN:H	1:B:356:ASP:HB2	1.70	0.54
1:H:575:TYR:HA	1:H:578:LEU:HD13	1.89	0.54
1:F:575:TYR:HA	1:F:578:LEU:HD13	1.90	0.54
1:G:575:TYR:HA	1:G:578:LEU:HD13	1.89	0.54
1:C:337:SER:HA	1:C:661:ASP:HB2	1.89	0.54
1:K:575:TYR:HA	1:K:578:LEU:HD13	1.89	0.54
1:N:187:LEU:HB3	1:N:192:TYR:HB3	1.90	0.54
1:N:524:LYS:HD2	1:N:579:ASP:HB3	1.88	0.54
1:C:575:TYR:HA	1:C:578:LEU:HD13	1.89	0.53
1:M:575:TYR:HA	1:M:578:LEU:HD13	1.89	0.53
1:M:479:GLU:HG3	1:N:471:VAL:HG23	1.89	0.53
1:D:189:VAL:HG11	1:E:198:ASN:HB3	1.90	0.53
1:D:642:TYR:HE2	1:D:666:SER:HB3	1.73	0.53
1:I:246:ASN:HB2	1:I:373:PRO:HG3	1.91	0.53
1:K:291:LYS:HB3	1:K:335:ASP:HB3	1.91	0.53
1:E:246:ASN:HB2	1:E:373:PRO:HG3	1.91	0.53
1:J:575:TYR:HA	1:J:578:LEU:HD13	1.90	0.53
1:K:340:LEU:HB2	1:K:343:GLU:HB3	1.91	0.53
1:A:291:LYS:HB3	1:A:335:ASP:HB3	1.91	0.52
1:D:625:GLU:HG2	1:D:686:PRO:HB3	1.91	0.52
1:G:340:LEU:HB2	1:G:343:GLU:HB3	1.91	0.52
1:I:189:VAL:HG11	1:J:198:ASN:HB3	1.91	0.52
1:L:488:THR:HG22	1:L:506:ALA:HA	1.90	0.52
1:E:187:LEU:HB3	1:E:192:TYR:HB3	1.92	0.52
1:G:291:LYS:HB3	1:G:335:ASP:HB3	1.91	0.52
1:H:625:GLU:HG2	1:H:686:PRO:HB3	1.90	0.52
1:N:625:GLU:HG2	1:N:686:PRO:HB3	1.90	0.52
1:I:625:GLU:HG2	1:I:686:PRO:HB3	1.91	0.52
1:B:340:LEU:HB2	1:B:343:GLU:HB3	1.91	0.52
1:L:291:LYS:HB3	1:L:335:ASP:HB3	1.90	0.52
1:E:291:LYS:HB3	1:E:335:ASP:HB3	1.91	0.52
1:B:520:ASP:HB3	1:B:582:LYS:HE2	1.92	0.52
1:I:340:LEU:HB2	1:I:343:GLU:HB3	1.91	0.52
1:N:336:HIS:HE1	1:N:663:LEU:HB2	1.74	0.52
1:G:644:VAL:HG11	1:G:678:PHE:HB3	1.91	0.52
1:H:340:LEU:HB2	1:H:343:GLU:HB3	1.91	0.52
1:I:291:LYS:HB3	1:I:335:ASP:HB3	1.92	0.52
1:I:520:ASP:HB3	1:I:582:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:520:ASP:HB3	1:F:582:LYS:HE2	1.92	0.52
1:K:481:LEU:H	1:K:482:PRO:CD	2.22	0.52
1:C:291:LYS:HB3	1:C:335:ASP:HB3	1.92	0.51
1:E:631:ILE:HD12	1:E:674:THR:HB	1.92	0.51
1:F:246:ASN:HB2	1:F:373:PRO:HG3	1.92	0.51
1:B:481:LEU:HA	1:B:484:ILE:HD12	1.92	0.51
1:D:291:LYS:HB3	1:D:335:ASP:HB3	1.93	0.51
1:G:253:HIS:HE1	1:G:255:LEU:HD12	1.75	0.51
1:G:631:ILE:HD12	1:G:674:THR:HB	1.92	0.51
1:J:246:ASN:HB2	1:J:373:PRO:HG3	1.92	0.51
1:M:491:ILE:HD12	1:M:505:ILE:HD13	1.91	0.51
1:A:451:ASP:HB3	1:B:416:LEU:HD23	1.92	0.51
1:G:246:ASN:HB2	1:G:373:PRO:HG3	1.92	0.51
1:B:631:ILE:HD12	1:B:674:THR:HB	1.92	0.51
1:C:520:ASP:HB3	1:C:582:LYS:HE2	1.93	0.51
1:A:520:ASP:HB3	1:A:582:LYS:HE2	1.92	0.51
1:B:246:ASN:HB2	1:B:373:PRO:HG3	1.91	0.51
1:D:319:SER:HA	1:E:414:LYS:HG3	1.93	0.51
1:M:520:ASP:HB3	1:M:582:LYS:HE2	1.92	0.51
1:E:509:ASN:HD22	1:E:512:ASP:H	1.57	0.51
1:I:644:VAL:HG11	1:I:678:PHE:HB3	1.92	0.51
1:K:631:ILE:HD12	1:K:674:THR:HB	1.93	0.51
1:N:631:ILE:HD12	1:N:674:THR:HB	1.93	0.51
1:A:631:ILE:HD12	1:A:674:THR:HB	1.93	0.51
1:L:238:LYS:HD3	1:L:254:PRO:HA	1.92	0.51
1:L:340:LEU:HB2	1:L:343:GLU:HB3	1.92	0.51
1:A:246:ASN:HB2	1:A:373:PRO:HG3	1.92	0.51
1:H:246:ASN:HB2	1:H:373:PRO:HG3	1.92	0.51
1:K:520:ASP:HB3	1:K:582:LYS:HE2	1.93	0.50
1:B:291:LYS:HB3	1:B:335:ASP:HB3	1.92	0.50
1:C:226:TRP:CZ2	1:C:234:SER:HB3	2.47	0.50
1:H:291:LYS:HB3	1:H:335:ASP:HB3	1.91	0.50
1:I:631:ILE:HD12	1:I:674:THR:HB	1.92	0.50
1:N:520:ASP:HB3	1:N:582:LYS:HE2	1.93	0.50
1:B:625:GLU:HG2	1:B:686:PRO:HB3	1.92	0.50
1:K:488:THR:HG22	1:K:506:ALA:HA	1.94	0.50
1:B:488:THR:HG22	1:B:506:ALA:HA	1.93	0.50
1:C:246:ASN:HB2	1:C:373:PRO:HG3	1.93	0.50
1:F:319:SER:HA	1:G:414:LYS:HG3	1.92	0.50
1:G:223:PRO:HD2	1:G:517:THR:HG22	1.94	0.50
1:H:631:ILE:HD12	1:H:674:THR:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:520:ASP:HB3	1:L:582:LYS:HE2	1.93	0.50
1:N:340:LEU:HB2	1:N:343:GLU:HB3	1.91	0.50
1:G:520:ASP:HB3	1:G:582:LYS:HE2	1.92	0.50
1:K:665:ILE:HD12	1:K:676:ILE:HG23	1.93	0.50
1:D:223:PRO:HD2	1:D:517:THR:HG22	1.94	0.50
1:D:246:ASN:HB2	1:D:373:PRO:HG3	1.93	0.50
1:G:509:ASN:HD22	1:G:512:ASP:H	1.58	0.50
1:L:506:ALA:HB1	1:L:518:LYS:HE3	1.92	0.50
1:D:631:ILE:HD12	1:D:674:THR:HB	1.93	0.50
1:J:520:ASP:HB3	1:J:582:LYS:HE2	1.94	0.50
1:K:246:ASN:HB2	1:K:373:PRO:HG3	1.92	0.50
1:K:509:ASN:HD22	1:K:512:ASP:H	1.60	0.50
1:E:625:GLU:HG2	1:E:686:PRO:HB3	1.93	0.49
1:G:625:GLU:HG2	1:G:686:PRO:HB3	1.93	0.49
1:D:520:ASP:HB3	1:D:582:LYS:HE2	1.93	0.49
1:E:520:ASP:HB3	1:E:582:LYS:HE2	1.93	0.49
1:F:481:LEU:HA	1:F:484:ILE:HD12	1.95	0.49
1:H:665:ILE:HD12	1:H:676:ILE:HG23	1.94	0.49
1:J:291:LYS:HB3	1:J:335:ASP:HB3	1.94	0.49
1:E:253:HIS:HE1	1:E:255:LEU:HD12	1.76	0.49
1:I:223:PRO:HD2	1:I:517:THR:HG22	1.94	0.49
1:N:253:HIS:HE1	1:N:255:LEU:HD12	1.78	0.49
1:B:187:LEU:HB3	1:B:192:TYR:HB3	1.95	0.49
1:F:631:ILE:HD12	1:F:674:THR:HB	1.93	0.49
1:I:253:HIS:HE1	1:I:255:LEU:HD12	1.77	0.49
1:F:223:PRO:HD2	1:F:517:THR:HG22	1.95	0.49
1:H:520:ASP:HB3	1:H:582:LYS:HE2	1.94	0.49
1:K:223:PRO:HD2	1:K:517:THR:HG22	1.94	0.49
1:D:253:HIS:HE1	1:D:255:LEU:HD12	1.77	0.49
1:G:187:LEU:HB3	1:G:192:TYR:HB3	1.95	0.49
1:G:291:LYS:HE2	1:G:339:SER:HB2	1.95	0.49
1:N:403:GLN:HB2	1:N:411:TYR:HE1	1.77	0.49
1:A:235:ASP:HA	1:A:238:LYS:HE3	1.94	0.49
1:D:644:VAL:HG11	1:D:678:PHE:HB3	1.95	0.49
1:G:665:ILE:HD12	1:G:676:ILE:HG23	1.95	0.49
1:K:236:PHE:O	1:K:240:THR:HG22	2.13	0.48
1:M:460:ALA:HA	1:M:471:VAL:HA	1.95	0.48
1:N:366:TYR:HB2	1:N:411:TYR:HB3	1.94	0.48
1:B:644:VAL:HG11	1:B:678:PHE:HB3	1.94	0.48
1:J:253:HIS:HE1	1:J:255:LEU:HD12	1.78	0.48
1:M:187:LEU:HB3	1:M:192:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:HIS:HE1	1:C:255:LEU:HD12	1.78	0.48
1:E:223:PRO:HD2	1:E:517:THR:HG22	1.95	0.48
1:F:236:PHE:O	1:F:240:THR:HG22	2.13	0.48
1:I:291:LYS:HE2	1:I:339:SER:HB2	1.95	0.48
1:I:575:TYR:HA	1:I:578:LEU:HD13	1.95	0.48
1:J:631:ILE:HD12	1:J:674:THR:HB	1.95	0.48
1:J:665:ILE:HD12	1:J:676:ILE:HG23	1.95	0.48
1:A:253:HIS:HE1	1:A:255:LEU:HD12	1.78	0.48
1:B:189:VAL:HG11	1:C:198:ASN:HB3	1.96	0.48
1:M:659:ARG:HG2	1:M:716:THR:HB	1.95	0.48
1:A:236:PHE:O	1:A:240:THR:HG22	2.14	0.48
1:N:223:PRO:HD2	1:N:517:THR:HG22	1.95	0.48
1:K:291:LYS:HE2	1:K:339:SER:HB2	1.96	0.48
1:K:659:ARG:HG2	1:K:716:THR:HB	1.95	0.48
1:E:338:LEU:HD21	1:E:659:ARG:HH12	1.79	0.48
1:G:236:PHE:O	1:G:240:THR:HG22	2.14	0.48
1:L:261:ILE:HD13	1:L:502:GLU:HB3	1.96	0.48
1:E:659:ARG:HG2	1:E:716:THR:HB	1.96	0.47
1:G:659:ARG:HG2	1:G:716:THR:HB	1.96	0.47
1:D:338:LEU:HD23	1:D:343:GLU:HG3	1.95	0.47
1:E:291:LYS:HE2	1:E:339:SER:HB2	1.96	0.47
1:F:253:HIS:HE1	1:F:255:LEU:HD12	1.79	0.47
1:M:261:ILE:HB	1:M:369:THR:HG23	1.96	0.47
1:I:236:PHE:O	1:I:240:THR:HG22	2.14	0.47
1:M:297:ARG:HD3	1:M:369:THR:HG21	1.96	0.47
1:B:291:LYS:HE2	1:B:339:SER:HB2	1.96	0.47
1:E:365:ARG:HG2	1:E:412:PRO:HG2	1.97	0.47
1:J:482:PRO:HB2	1:K:246:ASN:HD21	1.80	0.47
1:K:231:ASP:HB2	1:K:232:PRO:HD2	1.96	0.47
1:L:291:LYS:HE2	1:L:339:SER:HB2	1.97	0.47
1:L:365:ARG:HG2	1:L:412:PRO:HG2	1.97	0.47
1:M:291:LYS:HB3	1:M:335:ASP:HB3	1.95	0.47
1:M:365:ARG:HG2	1:M:412:PRO:HG2	1.97	0.47
1:A:305:GLY:HA2	1:B:670:GLN:HG3	1.97	0.47
1:B:659:ARG:HG2	1:B:716:THR:HB	1.96	0.47
1:A:223:PRO:HD2	1:A:517:THR:HG22	1.96	0.47
1:C:365:ARG:HG2	1:C:412:PRO:HG2	1.97	0.47
1:M:569:LEU:HB3	1:M:577:VAL:HG11	1.97	0.47
1:N:184:PRO:HG2	1:N:187:LEU:HG	1.97	0.47
1:C:236:PHE:O	1:C:240:THR:HG22	2.15	0.47
1:D:337:SER:HA	1:D:661:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:481:LEU:HA	1:M:484:ILE:HD12	1.96	0.47
1:N:297:ARG:CD	1:N:369:THR:HG21	2.42	0.47
1:D:236:PHE:O	1:D:240:THR:HG22	2.15	0.46
1:I:659:ARG:HG2	1:I:716:THR:HB	1.97	0.46
1:J:187:LEU:HB3	1:J:192:TYR:HB3	1.98	0.46
1:D:643:ILE:HD12	1:D:723:LYS:HB3	1.98	0.46
1:E:236:PHE:O	1:E:240:THR:HG22	2.15	0.46
1:I:224:GLU:HB2	1:I:517:THR:HG21	1.97	0.46
1:N:240:THR:HG23	1:N:242:ARG:H	1.81	0.46
1:J:365:ARG:HG2	1:J:412:PRO:HG2	1.97	0.46
1:N:446:LYS:HB2	1:N:708:ILE:HD13	1.97	0.46
1:A:365:ARG:HG2	1:A:412:PRO:HG2	1.98	0.46
1:G:643:ILE:HD12	1:G:723:LYS:HB3	1.98	0.46
1:J:189:VAL:HG22	1:J:223:PRO:HG3	1.98	0.46
1:K:365:ARG:HG2	1:K:412:PRO:HG2	1.96	0.46
1:C:223:PRO:HD2	1:C:517:THR:HG22	1.98	0.46
1:G:569:LEU:HB3	1:G:577:VAL:HG11	1.97	0.46
1:A:224:GLU:HB2	1:A:517:THR:HG21	1.98	0.46
1:B:264:VAL:HG21	1:B:381:THR:HG21	1.98	0.46
1:D:569:LEU:HB3	1:D:577:VAL:HG11	1.97	0.46
1:H:303:VAL:HA	1:H:600:ARG:HH21	1.79	0.46
1:I:365:ARG:HG2	1:I:412:PRO:HG2	1.98	0.46
1:J:491:ILE:HD12	1:J:505:ILE:HD13	1.97	0.46
1:B:609:GLU:HG2	1:B:724:ILE:HG12	1.98	0.46
1:D:665:ILE:HD12	1:D:676:ILE:HG23	1.98	0.46
1:F:569:LEU:HB3	1:F:577:VAL:HG11	1.98	0.46
1:H:481:LEU:HA	1:H:484:ILE:HD12	1.98	0.46
1:I:569:LEU:HB3	1:I:577:VAL:HG11	1.98	0.46
1:M:336:HIS:HB3	1:M:708:ILE:HG22	1.98	0.46
1:N:338:LEU:HD21	1:N:659:ARG:HH12	1.80	0.46
1:B:338:LEU:HD21	1:B:659:ARG:HH12	1.81	0.46
1:H:218:LYS:HE2	1:H:220:LYS:HE3	1.97	0.46
1:H:291:LYS:HE2	1:H:339:SER:HB2	1.97	0.46
1:I:303:VAL:HA	1:I:600:ARG:HH21	1.81	0.46
1:L:336:HIS:HB3	1:L:708:ILE:HG22	1.98	0.46
1:B:365:ARG:HG2	1:B:412:PRO:HG2	1.98	0.46
1:D:365:ARG:HG2	1:D:412:PRO:HG2	1.97	0.46
1:F:264:VAL:HG21	1:F:381:THR:HG21	1.98	0.46
1:H:255:LEU:HD21	1:H:519:PRO:HD2	1.96	0.46
1:H:659:ARG:HG2	1:H:716:THR:HB	1.96	0.46
1:L:368:ASN:HD22	1:L:407:PRO:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:ARG:HG2	1:A:716:THR:HB	1.98	0.45
1:H:236:PHE:O	1:H:240:THR:HG22	2.15	0.45
1:J:569:LEU:HB3	1:J:577:VAL:HG11	1.98	0.45
1:M:207:ILE:HG22	1:M:209:ASN:H	1.82	0.45
1:B:569:LEU:HB3	1:B:577:VAL:HG11	1.98	0.45
1:D:187:LEU:HB3	1:D:192:TYR:HB3	1.97	0.45
1:G:264:VAL:HG21	1:G:381:THR:HG21	1.98	0.45
1:G:365:ARG:HG2	1:G:412:PRO:HG2	1.98	0.45
1:K:338:LEU:HD21	1:K:659:ARG:HH12	1.81	0.45
1:K:569:LEU:HB3	1:K:577:VAL:HG11	1.98	0.45
1:M:605:VAL:HB	1:M:704:GLU:HB3	1.98	0.45
1:A:187:LEU:HB3	1:A:192:TYR:HB3	1.98	0.45
1:H:192:TYR:HA	1:H:205:PRO:HA	1.97	0.45
1:I:624:THR:HG21	1:I:689:ILE:HD11	1.97	0.45
1:I:698:VAL:HB	1:I:727:PHE:HB3	1.97	0.45
1:M:189:VAL:HG11	1:N:198:ASN:HB3	1.98	0.45
1:N:218:LYS:HE2	1:N:220:LYS:HE2	1.98	0.45
1:D:698:VAL:HB	1:D:727:PHE:HB3	1.98	0.45
1:J:236:PHE:O	1:J:240:THR:HG22	2.15	0.45
1:K:187:LEU:HB3	1:K:192:TYR:HB3	1.99	0.45
1:L:189:VAL:HG21	1:M:200:ARG:HE	1.80	0.45
1:G:336:HIS:HB3	1:G:708:ILE:HG22	1.99	0.45
1:L:482:PRO:HB2	1:M:246:ASN:HD21	1.82	0.45
1:N:224:GLU:HB2	1:N:517:THR:HG21	1.99	0.45
1:E:340:LEU:HB2	1:E:343:GLU:HB3	1.97	0.45
1:F:365:ARG:HG2	1:F:412:PRO:HG2	1.97	0.45
1:I:486:GLU:HG3	1:J:246:ASN:HD22	1.81	0.45
1:K:609:GLU:HG2	1:K:724:ILE:HG12	1.98	0.45
1:L:525:GLU:O	1:L:529:ILE:HG12	2.16	0.45
1:E:224:GLU:HB2	1:E:517:THR:HG21	1.99	0.45
1:F:224:GLU:HB2	1:F:517:THR:HG21	1.99	0.45
1:G:338:LEU:HD21	1:G:659:ARG:HH12	1.81	0.45
1:G:609:GLU:HG2	1:G:724:ILE:HG12	1.98	0.45
1:K:189:VAL:HG13	1:L:199:LYS:HG2	1.98	0.45
1:L:569:LEU:HB3	1:L:577:VAL:HG11	1.99	0.45
1:E:643:ILE:HD12	1:E:723:LYS:HB3	1.98	0.45
1:E:698:VAL:HB	1:E:727:PHE:HB3	1.98	0.45
1:H:569:LEU:HB3	1:H:577:VAL:HG11	1.98	0.45
1:K:336:HIS:HB3	1:K:708:ILE:HG22	1.99	0.45
1:C:569:LEU:HB3	1:C:577:VAL:HG11	1.98	0.45
1:F:609:GLU:HG2	1:F:724:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:338:LEU:HD21	1:I:659:ARG:HH12	1.81	0.45
1:M:405:LEU:HD13	1:M:411:TYR:HB2	1.98	0.45
1:N:524:LYS:HG3	1:N:540:LEU:HD13	1.99	0.45
1:B:643:ILE:HD12	1:B:723:LYS:HB3	1.99	0.45
1:E:336:HIS:HB3	1:E:708:ILE:HG22	1.99	0.45
1:G:224:GLU:HB2	1:G:517:THR:HG21	1.99	0.45
1:G:481:LEU:HA	1:G:484:ILE:HD12	1.98	0.45
1:A:264:VAL:HG21	1:A:381:THR:HG21	1.99	0.44
1:A:459:ILE:HG12	1:A:477:TRP:CD1	2.52	0.44
1:H:264:VAL:HG21	1:H:381:THR:HG21	1.99	0.44
1:H:310:HIS:CD2	1:H:312:SER:HB2	2.53	0.44
1:I:336:HIS:HB3	1:I:708:ILE:HG22	1.99	0.44
1:B:336:HIS:HB3	1:B:708:ILE:HG22	1.98	0.44
1:M:224:GLU:HB2	1:M:517:THR:HG21	1.99	0.44
1:B:524:LYS:HB2	1:B:579:ASP:HA	1.99	0.44
1:C:187:LEU:HB3	1:C:192:TYR:HB3	1.99	0.44
1:D:264:VAL:HG21	1:D:381:THR:HG21	2.00	0.44
1:F:187:LEU:HB3	1:F:192:TYR:HB3	1.99	0.44
1:H:338:LEU:HD21	1:H:659:ARG:HH12	1.83	0.44
1:A:336:HIS:HB3	1:A:708:ILE:HG22	2.00	0.44
1:E:554:PHE:HB2	1:E:559:SER:HB2	2.00	0.44
1:I:643:ILE:HD12	1:I:723:LYS:HB3	1.99	0.44
1:N:236:PHE:O	1:N:240:THR:HG22	2.17	0.44
1:N:569:LEU:HB3	1:N:577:VAL:HG11	1.98	0.44
1:E:184:PRO:HG2	1:E:187:LEU:HG	1.99	0.44
1:E:569:LEU:HB3	1:E:577:VAL:HG11	1.99	0.44
1:I:231:ASP:HB2	1:I:232:PRO:HD2	2.00	0.44
1:I:460:ALA:HA	1:I:471:VAL:HA	2.00	0.44
1:J:264:VAL:HG21	1:J:381:THR:HG21	1.99	0.44
1:K:253:HIS:HE1	1:K:255:LEU:HD12	1.83	0.44
1:A:554:PHE:HB2	1:A:559:SER:HB2	2.00	0.44
1:D:481:LEU:HA	1:D:484:ILE:HD12	2.00	0.44
1:G:698:VAL:HB	1:G:727:PHE:HB3	1.99	0.44
1:L:248:SER:HB2	1:L:371:THR:HG22	2.00	0.44
1:A:481:LEU:HA	1:A:484:ILE:HD12	1.99	0.44
1:C:264:VAL:HG21	1:C:381:THR:HG21	1.98	0.44
1:I:609:GLU:HG2	1:I:724:ILE:HG12	1.98	0.44
1:D:609:GLU:HG2	1:D:724:ILE:HG12	2.00	0.44
1:E:609:GLU:HG2	1:E:724:ILE:HG12	1.99	0.44
1:H:198:ASN:HB3	1:N:189:VAL:HG11	1.99	0.44
1:L:524:LYS:HB2	1:L:579:ASP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:490:ARG:HH21	1:M:588:ASN:HD21	1.66	0.44
1:N:666:SER:HB2	1:N:674:THR:HG22	2.00	0.44
1:K:224:GLU:HB2	1:K:517:THR:HG21	1.99	0.44
1:L:189:VAL:HG13	1:M:199:LYS:HG2	2.00	0.44
1:N:460:ALA:HA	1:N:471:VAL:HA	2.00	0.44
1:A:569:LEU:HB3	1:A:577:VAL:HG11	1.98	0.43
1:I:187:LEU:HB3	1:I:192:TYR:HB3	2.00	0.43
1:I:193:THR:HA	1:I:219:TYR:HD2	1.82	0.43
1:I:481:LEU:HA	1:I:484:ILE:HD12	1.99	0.43
1:K:554:PHE:HB2	1:K:559:SER:HB2	2.00	0.43
1:A:613:LYS:HG2	1:A:725:LEU:HB3	2.00	0.43
1:E:264:VAL:HG21	1:E:381:THR:HG21	1.99	0.43
1:K:297:ARG:HD3	1:K:369:THR:HG21	2.01	0.43
1:H:297:ARG:HD3	1:H:369:THR:HG21	2.01	0.43
1:I:264:VAL:HG21	1:I:381:THR:HG21	1.99	0.43
1:J:460:ALA:HA	1:J:471:VAL:HA	2.00	0.43
1:M:338:LEU:HD21	1:M:659:ARG:HH12	1.83	0.43
1:N:401:LEU:HD13	1:N:411:TYR:CE1	2.53	0.43
1:N:605:VAL:HB	1:N:704:GLU:HB3	2.00	0.43
1:A:189:VAL:HG11	1:B:198:ASN:HB3	2.00	0.43
1:B:460:ALA:HA	1:B:471:VAL:HA	2.01	0.43
1:B:554:PHE:HB2	1:B:559:SER:HB2	2.01	0.43
1:B:698:VAL:HB	1:B:727:PHE:HB3	1.99	0.43
1:F:554:PHE:HB2	1:F:559:SER:HB2	2.00	0.43
1:K:264:VAL:HG21	1:K:381:THR:HG21	1.99	0.43
1:E:481:LEU:HA	1:E:484:ILE:HD12	1.99	0.43
1:E:605:VAL:HB	1:E:704:GLU:HB3	2.01	0.43
1:E:665:ILE:HD12	1:E:676:ILE:HG23	2.00	0.43
1:N:481:LEU:HA	1:N:484:ILE:HD12	1.99	0.43
1:A:613:LYS:HE2	1:A:725:LEU:HB2	2.00	0.43
1:G:297:ARG:HD3	1:G:369:THR:HG21	2.01	0.43
1:H:336:HIS:HB3	1:H:708:ILE:HG22	2.00	0.43
1:H:524:LYS:HB2	1:H:579:ASP:HA	2.00	0.43
1:J:223:PRO:HD2	1:J:517:THR:HG22	2.00	0.43
1:J:303:VAL:HA	1:J:600:ARG:HH21	1.83	0.43
1:M:264:VAL:HG21	1:M:381:THR:HG21	1.99	0.43
1:M:609:GLU:HG2	1:M:724:ILE:HG12	1.99	0.43
1:D:554:PHE:HB2	1:D:559:SER:HB2	2.00	0.43
1:L:223:PRO:HD2	1:L:517:THR:HG22	2.00	0.43
1:M:460:ALA:HB2	1:M:471:VAL:HG22	2.01	0.43
1:M:488:THR:HG22	1:M:506:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:HD3	1:B:369:THR:HG21	2.01	0.43
1:C:460:ALA:HA	1:C:471:VAL:HA	2.00	0.43
1:C:524:LYS:HB2	1:C:579:ASP:HA	2.01	0.43
1:J:297:ARG:HD3	1:J:369:THR:HG21	2.00	0.43
1:J:310:HIS:CD2	1:J:312:SER:HB2	2.54	0.43
1:B:224:GLU:HB2	1:B:517:THR:HG21	2.00	0.43
1:D:217:THR:HB	1:D:219:TYR:CZ	2.54	0.43
1:H:554:PHE:HB2	1:H:559:SER:HB2	2.00	0.43
1:B:231:ASP:HB2	1:B:232:PRO:HD2	1.99	0.43
1:J:605:VAL:HB	1:J:704:GLU:HB3	2.01	0.43
1:L:554:PHE:HB2	1:L:559:SER:HB2	2.01	0.43
1:D:460:ALA:HA	1:D:471:VAL:HA	2.00	0.42
1:E:624:THR:HG21	1:E:689:ILE:HD11	2.01	0.42
1:H:605:VAL:HB	1:H:704:GLU:HB3	2.01	0.42
1:H:624:THR:HG21	1:H:689:ILE:HD11	2.01	0.42
1:J:524:LYS:HB2	1:J:579:ASP:HA	2.01	0.42
1:M:707:ILE:HG12	1:M:721:ILE:HG12	2.01	0.42
1:C:491:ILE:HD12	1:C:505:ILE:HD13	2.01	0.42
1:E:187:LEU:HD22	1:E:205:PRO:HB3	2.00	0.42
1:G:524:LYS:HB2	1:G:579:ASP:HA	2.00	0.42
1:I:491:ILE:HG12	1:I:589:ILE:HB	2.01	0.42
1:K:524:LYS:HB2	1:K:579:ASP:HA	2.01	0.42
1:E:524:LYS:HB2	1:E:579:ASP:HA	2.00	0.42
1:G:554:PHE:HB2	1:G:559:SER:HB2	2.00	0.42
1:J:554:PHE:HB2	1:J:559:SER:HB2	2.00	0.42
1:A:231:ASP:HB2	1:A:232:PRO:HD2	2.02	0.42
1:D:524:LYS:HB2	1:D:579:ASP:HA	2.00	0.42
1:F:325:SER:HB2	1:G:415:ASN:HD22	1.84	0.42
1:H:491:ILE:HG12	1:H:589:ILE:HB	2.02	0.42
1:I:554:PHE:HB2	1:I:559:SER:HB2	2.00	0.42
1:N:207:ILE:HB	1:N:210:ILE:HG12	2.01	0.42
1:F:297:ARG:HD3	1:F:369:THR:HG21	2.00	0.42
1:F:665:ILE:HD12	1:F:676:ILE:HG23	2.02	0.42
1:H:460:ALA:HA	1:H:471:VAL:HA	2.01	0.42
1:A:524:LYS:HB2	1:A:579:ASP:HA	2.00	0.42
1:C:297:ARG:HD3	1:C:369:THR:HG21	2.01	0.42
1:D:224:GLU:HB2	1:D:517:THR:HG21	2.00	0.42
1:F:303:VAL:HA	1:F:600:ARG:HH21	1.84	0.42
1:I:524:LYS:HB2	1:I:579:ASP:HA	2.01	0.42
1:J:488:THR:HG22	1:J:506:ALA:HA	2.02	0.42
1:N:193:THR:HA	1:N:219:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:HA	1:A:600:ARG:HH21	1.85	0.42
1:I:297:ARG:HD3	1:I:369:THR:HG21	2.02	0.42
1:K:491:ILE:HG12	1:K:589:ILE:HB	2.02	0.42
1:D:303:VAL:HA	1:D:600:ARG:HH21	1.85	0.42
1:D:310:HIS:CD2	1:D:312:SER:HB2	2.55	0.42
1:E:491:ILE:HD12	1:E:505:ILE:HD13	2.02	0.42
1:F:460:ALA:HA	1:F:471:VAL:HA	2.00	0.42
1:G:460:ALA:HA	1:G:471:VAL:HA	2.00	0.42
1:H:293:THR:HG22	1:H:334:ILE:HA	2.02	0.42
1:L:264:VAL:HG21	1:L:381:THR:HG21	2.00	0.42
1:D:605:VAL:HB	1:D:704:GLU:HB3	2.02	0.42
1:J:338:LEU:HD23	1:J:343:GLU:HG3	2.02	0.42
1:J:481:LEU:HA	1:J:484:ILE:HD12	2.01	0.42
1:K:605:VAL:HB	1:K:704:GLU:HB3	2.01	0.42
1:N:491:ILE:HG12	1:N:589:ILE:HB	2.02	0.42
1:A:477:TRP:HB3	1:A:481:LEU:HD12	2.02	0.41
1:F:310:HIS:CD2	1:F:312:SER:HB2	2.55	0.41
1:M:524:LYS:HB2	1:M:579:ASP:HA	2.00	0.41
1:N:554:PHE:HB2	1:N:559:SER:HB2	2.01	0.41
1:A:319:SER:HA	1:B:414:LYS:HG3	2.01	0.41
1:E:675:PHE:CZ	1:E:677:ASP:HB2	2.55	0.41
1:E:707:ILE:HG12	1:E:721:ILE:HG12	2.02	0.41
1:G:231:ASP:HB2	1:G:232:PRO:HD2	2.02	0.41
1:M:238:LYS:HB2	1:M:252:ARG:O	2.20	0.41
1:N:374:ILE:HD12	1:N:405:LEU:HD23	2.01	0.41
1:A:460:ALA:HA	1:A:471:VAL:HA	2.00	0.41
1:E:460:ALA:HA	1:E:471:VAL:HA	2.01	0.41
1:G:491:ILE:HG12	1:G:589:ILE:HB	2.02	0.41
1:A:305:GLY:HA2	1:B:670:GLN:HE21	1.86	0.41
1:B:491:ILE:HD12	1:B:505:ILE:HD13	2.02	0.41
1:F:524:LYS:HB2	1:F:579:ASP:HA	2.01	0.41
1:A:297:ARG:HD3	1:A:369:THR:HG21	2.02	0.41
1:G:293:THR:HG22	1:G:334:ILE:HA	2.03	0.41
1:H:365:ARG:HG2	1:H:412:PRO:HG2	2.02	0.41
1:A:491:ILE:HD12	1:A:505:ILE:HD13	2.03	0.41
1:B:605:VAL:HB	1:B:704:GLU:HB3	2.03	0.41
1:D:491:ILE:HD12	1:D:505:ILE:HD13	2.03	0.41
1:M:554:PHE:HB2	1:M:559:SER:HB2	2.01	0.41
1:N:365:ARG:HG2	1:N:412:PRO:HG2	2.02	0.41
1:N:400:GLN:HG3	1:N:401:LEU:N	2.35	0.41
1:F:491:ILE:HD12	1:F:505:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:491:ILE:HD12	1:I:505:ILE:HD13	2.02	0.41
1:N:494:ASN:HB2	1:N:498:LEU:HA	2.01	0.41
1:K:707:ILE:HG12	1:K:721:ILE:HG12	2.02	0.41
1:L:515:GLU:HA	1:L:518:LYS:HD3	2.03	0.41
1:B:228:THR:HG23	1:B:518:LYS:HG2	2.02	0.41
1:D:297:ARG:HD3	1:D:369:THR:HG21	2.02	0.41
1:F:459:ILE:HG12	1:F:477:TRP:CD1	2.55	0.41
1:G:624:THR:HG21	1:G:689:ILE:HD11	2.02	0.41
1:M:243:ILE:HG21	1:M:252:ARG:HD2	2.03	0.41
1:A:491:ILE:HG12	1:A:589:ILE:HB	2.03	0.41
1:B:293:THR:HG22	1:B:334:ILE:HA	2.03	0.41
1:H:210:ILE:O	1:H:214:LYS:HB2	2.21	0.41
1:H:223:PRO:HD2	1:H:517:THR:HG22	2.03	0.41
1:I:261:ILE:HD13	1:I:502:GLU:HB3	2.03	0.41
1:A:513:PRO:HG2	1:B:239:VAL:O	2.22	0.40
1:E:297:ARG:HD3	1:E:369:THR:HG21	2.02	0.40
1:M:303:VAL:HG23	1:N:670:GLN:HG2	2.03	0.40
1:B:411:TYR:HB3	1:B:412:PRO:HD3	2.04	0.40
1:D:293:THR:HG22	1:D:334:ILE:HA	2.03	0.40
1:E:231:ASP:HB2	1:E:232:PRO:HD2	2.03	0.40
1:F:231:ASP:HB2	1:F:232:PRO:HD2	2.03	0.40
1:F:261:ILE:HD13	1:F:502:GLU:HB3	2.04	0.40
1:G:491:ILE:HD12	1:G:505:ILE:HD13	2.03	0.40
1:I:305:GLY:HA2	1:J:670:GLN:HG3	2.02	0.40
1:J:226:TRP:CZ2	1:J:234:SER:HB2	2.56	0.40
1:E:293:THR:HG22	1:E:334:ILE:HA	2.03	0.40
1:H:346:TRP:CZ2	1:H:446:LYS:HE3	2.57	0.40
1:K:460:ALA:HA	1:K:471:VAL:HA	2.02	0.40
1:N:710:PRO:HG3	1:N:716:THR:HG22	2.02	0.40
1:A:310:HIS:CD2	1:A:312:SER:HB2	2.56	0.40
1:B:346:TRP:CZ2	1:B:446:LYS:HE3	2.57	0.40
1:B:380:THR:HG23	1:B:395:LYS:HB2	2.04	0.40
1:I:707:ILE:HG12	1:I:721:ILE:HG12	2.04	0.40
1:K:293:THR:HG22	1:K:334:ILE:HA	2.04	0.40
1:K:620:ILE:HD11	1:K:630:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/568 (80%)	407 (90%)	39 (9%)	9 (2%)	7	37
1	B	509/568 (90%)	454 (89%)	49 (10%)	6 (1%)	13	49
1	C	374/568 (66%)	335 (90%)	35 (9%)	4 (1%)	14	51
1	D	529/568 (93%)	473 (89%)	49 (9%)	7 (1%)	12	47
1	E	506/568 (89%)	457 (90%)	43 (8%)	6 (1%)	13	49
1	F	449/568 (79%)	402 (90%)	41 (9%)	6 (1%)	12	47
1	G	510/568 (90%)	460 (90%)	45 (9%)	5 (1%)	15	53
1	H	479/568 (84%)	424 (88%)	46 (10%)	9 (2%)	8	38
1	I	519/568 (91%)	460 (89%)	52 (10%)	7 (1%)	12	47
1	J	452/568 (80%)	401 (89%)	39 (9%)	12 (3%)	5	31
1	K	474/568 (84%)	424 (90%)	44 (9%)	6 (1%)	12	47
1	L	388/568 (68%)	347 (89%)	36 (9%)	5 (1%)	12	47
1	M	459/568 (81%)	403 (88%)	48 (10%)	8 (2%)	9	41
1	N	466/568 (82%)	415 (89%)	40 (9%)	11 (2%)	6	33
All	All	6569/7952 (83%)	5862 (89%)	606 (9%)	101 (2%)	10	45

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	587	MET
1	N	413	SER
1	B	422	ASN
1	I	304	HIS
1	J	715	ASP
1	K	481	LEU
1	L	506	ALA
1	A	197	LYS
1	A	304	HIS

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Mol	Chain	Res	Type
1	A	389	GLN
1	A	422	ASN
1	B	197	LYS
1	B	389	GLN
1	C	197	LYS
1	C	389	GLN
1	D	197	LYS
1	D	389	GLN
1	E	389	GLN
1	F	197	LYS
1	F	304	HIS
1	F	389	GLN
1	G	197	LYS
1	G	389	GLN
1	H	197	LYS
1	H	214	LYS
1	H	215	GLY
1	H	304	HIS
1	H	389	GLN
1	H	422	ASN
1	I	197	LYS
1	I	389	GLN
1	I	422	ASN
1	J	197	LYS
1	J	230	SER
1	J	304	HIS
1	J	389	GLN
1	J	422	ASN
1	J	711	SER
1	K	197	LYS
1	K	389	GLN
1	K	506	ALA
1	L	197	LYS
1	L	389	GLN
1	M	197	LYS
1	M	389	GLN
1	N	197	LYS
1	N	208	SER
1	N	389	GLN
1	N	422	ASN
1	N	544	GLY
1	A	345	THR

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Mol	Chain	Res	Type
1	B	345	THR
1	C	345	THR
1	D	304	HIS
1	D	319	SER
1	D	345	THR
1	E	345	THR
1	E	422	ASN
1	G	345	THR
1	H	345	THR
1	I	345	THR
1	J	345	THR
1	K	345	THR
1	L	345	THR
1	M	304	HIS
1	M	345	THR
1	N	345	THR
1	N	498	LEU
1	N	536	PRO
1	N	538	GLY
1	A	319	SER
1	A	536	PRO
1	B	238	LYS
1	B	536	PRO
1	C	536	PRO
1	D	536	PRO
1	E	326	ASN
1	E	536	PRO
1	F	319	SER
1	F	536	PRO
1	G	464	PHE
1	G	536	PRO
1	H	536	PRO
1	I	536	PRO
1	J	210	ILE
1	J	319	SER
1	J	536	PRO
1	K	536	PRO
1	L	536	PRO
1	M	536	PRO
1	A	305	GLY
1	A	306	ASN
1	E	197	LYS

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Mol	Chain	Res	Type
1	F	305	GLY
1	H	305	GLY
1	I	305	GLY
1	D	305	GLY
1	J	305	GLY
1	M	305	GLY
1	M	467	GLY
1	N	532	GLY

### 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	418/504 (83%)	389 (93%)	29 (7%)	15	42
1	B	465/504 (92%)	434 (93%)	31 (7%)	16	42
1	C	349/504 (69%)	327 (94%)	22 (6%)	18	44
1	D	482/504 (96%)	448 (93%)	34 (7%)	14	41
1	E	462/504 (92%)	429 (93%)	33 (7%)	14	41
1	F	416/504 (82%)	385 (92%)	31 (8%)	13	39
1	G	468/504 (93%)	435 (93%)	33 (7%)	14	41
1	H	439/504 (87%)	408 (93%)	31 (7%)	14	41
1	I	473/504 (94%)	440 (93%)	33 (7%)	15	41
1	J	419/504 (83%)	389 (93%)	30 (7%)	14	41
1	K	438/504 (87%)	406 (93%)	32 (7%)	14	40
1	L	362/504 (72%)	335 (92%)	27 (8%)	13	39
1	M	419/504 (83%)	383 (91%)	36 (9%)	10	34
1	N	432/504 (86%)	396 (92%)	36 (8%)	11	36
All	All	6042/7056 (86%)	5604 (93%)	438 (7%)	14	41

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	GLU
1	A	210	ILE
1	A	246	ASN
1	A	252	ARG
1	A	274	ASN
1	A	308	GLU
1	A	324	PHE
1	A	344	ARG
1	A	361	ASN
1	A	363	ASN
1	A	380	THR
1	A	394	ILE
1	A	419	ILE
1	A	442	LEU
1	A	459	ILE
1	A	478	SER
1	A	481	LEU
1	A	517	THR
1	A	537	ASN
1	A	560	GLN
1	A	563	LYS
1	A	579	ASP
1	A	590	LEU
1	A	600	ARG
1	A	603	ILE
1	A	614	GLU
1	A	630	ASN
1	A	664	ASN
1	A	674	THR
1	B	190	GLU
1	B	210	ILE
1	B	274	ASN
1	B	285	GLN
1	B	344	ARG
1	B	361	ASN
1	B	363	ASN
1	B	380	THR
1	B	394	ILE
1	B	419	ILE
1	B	442	LEU
1	B	459	ILE
1	B	466	ASN
1	B	478	SER

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Mol	Chain	Res	Type
1	B	490	ARG
1	B	517	THR
1	B	537	ASN
1	B	560	GLN
1	B	563	LYS
1	B	579	ASP
1	B	590	LEU
1	B	603	ILE
1	B	614	GLU
1	B	648	ASP
1	B	664	ASN
1	B	670	GLN
1	B	674	THR
1	B	678	PHE
1	B	689	ILE
1	B	725	LEU
1	B	726	ILE
1	C	210	ILE
1	C	252	ARG
1	C	274	ASN
1	C	344	ARG
1	C	361	ASN
1	C	363	ASN
1	C	368	ASN
1	C	380	THR
1	C	394	ILE
1	C	419	ILE
1	C	442	LEU
1	C	459	ILE
1	C	478	SER
1	C	481	LEU
1	C	517	THR
1	C	537	ASN
1	C	560	GLN
1	C	563	LYS
1	C	579	ASP
1	C	590	LEU
1	C	593	ASP
1	C	664	ASN
1	D	190	GLU
1	D	210	ILE
1	D	246	ASN

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Mol	Chain	Res	Type
1	D	252	ARG
1	D	274	ASN
1	D	343	GLU
1	D	344	ARG
1	D	361	ASN
1	D	363	ASN
1	D	380	THR
1	D	394	ILE
1	D	419	ILE
1	D	442	LEU
1	D	459	ILE
1	D	478	SER
1	D	481	LEU
1	D	517	THR
1	D	537	ASN
1	D	560	GLN
1	D	563	LYS
1	D	579	ASP
1	D	590	LEU
1	D	600	ARG
1	D	603	ILE
1	D	614	GLU
1	D	648	ASP
1	D	659	ARG
1	D	661	ASP
1	D	664	ASN
1	D	674	THR
1	D	678	PHE
1	D	689	ILE
1	D	725	LEU
1	D	726	ILE
1	E	190	GLU
1	E	195	ASP
1	E	203	LEU
1	E	234	SER
1	E	252	ARG
1	E	274	ASN
1	E	344	ARG
1	E	361	ASN
1	E	363	ASN
1	E	380	THR
1	E	394	ILE

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Mol	Chain	Res	Type
1	E	419	ILE
1	E	442	LEU
1	E	459	ILE
1	E	478	SER
1	E	481	LEU
1	E	517	THR
1	E	537	ASN
1	E	560	GLN
1	E	563	LYS
1	E	579	ASP
1	E	590	LEU
1	E	603	ILE
1	E	614	GLU
1	E	648	ASP
1	E	664	ASN
1	E	669	ARG
1	E	670	GLN
1	E	674	THR
1	E	678	PHE
1	E	689	ILE
1	E	725	LEU
1	E	726	ILE
1	F	190	GLU
1	F	217	THR
1	F	246	ASN
1	F	252	ARG
1	F	274	ASN
1	F	324	PHE
1	F	361	ASN
1	F	363	ASN
1	F	368	ASN
1	F	376	ASN
1	F	380	THR
1	F	394	ILE
1	F	419	ILE
1	F	442	LEU
1	F	459	ILE
1	F	475	SER
1	F	476	ASN
1	F	481	LEU
1	F	517	THR
1	F	537	ASN

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Mol	Chain	Res	Type
1	F	560	GLN
1	F	563	LYS
1	F	579	ASP
1	F	590	LEU
1	F	600	ARG
1	F	603	ILE
1	F	614	GLU
1	F	664	ASN
1	F	674	THR
1	F	678	PHE
1	F	726	ILE
1	G	190	GLU
1	G	210	ILE
1	G	217	THR
1	G	252	ARG
1	G	274	ASN
1	G	343	GLU
1	G	344	ARG
1	G	361	ASN
1	G	363	ASN
1	G	380	THR
1	G	394	ILE
1	G	419	ILE
1	G	442	LEU
1	G	459	ILE
1	G	478	SER
1	G	479	GLU
1	G	481	LEU
1	G	517	THR
1	G	537	ASN
1	G	551	ASP
1	G	560	GLN
1	G	563	LYS
1	G	579	ASP
1	G	590	LEU
1	G	600	ARG
1	G	614	GLU
1	G	648	ASP
1	G	664	ASN
1	G	674	THR
1	G	678	PHE
1	G	689	ILE

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Mol	Chain	Res	Type
1	G	725	LEU
1	G	726	ILE
1	H	187	LEU
1	H	188	GLU
1	H	210	ILE
1	H	217	THR
1	H	231	ASP
1	H	252	ARG
1	H	274	ASN
1	H	308	GLU
1	H	344	ARG
1	H	361	ASN
1	H	363	ASN
1	H	380	THR
1	H	394	ILE
1	H	419	ILE
1	H	459	ILE
1	H	478	SER
1	H	481	LEU
1	H	515	GLU
1	H	517	THR
1	H	537	ASN
1	H	560	GLN
1	H	563	LYS
1	H	579	ASP
1	H	590	LEU
1	H	600	ARG
1	H	603	ILE
1	H	614	GLU
1	H	664	ASN
1	H	674	THR
1	H	678	PHE
1	H	689	ILE
1	I	190	GLU
1	I	210	ILE
1	I	217	THR
1	I	234	SER
1	I	252	ARG
1	I	274	ASN
1	I	343	GLU
1	I	344	ARG
1	I	361	ASN

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Mol	Chain	Res	Type
1	I	363	ASN
1	I	380	THR
1	I	394	ILE
1	I	419	ILE
1	I	442	LEU
1	I	459	ILE
1	I	478	SER
1	I	481	LEU
1	I	517	THR
1	I	537	ASN
1	I	560	GLN
1	I	563	LYS
1	I	579	ASP
1	I	590	LEU
1	I	600	ARG
1	I	603	ILE
1	I	614	GLU
1	I	648	ASP
1	I	664	ASN
1	I	674	THR
1	I	678	PHE
1	I	689	ILE
1	I	725	LEU
1	I	726	ILE
1	J	185	ASP
1	J	190	GLU
1	J	210	ILE
1	J	217	THR
1	J	230	SER
1	J	252	ARG
1	J	274	ASN
1	J	343	GLU
1	J	344	ARG
1	J	361	ASN
1	J	363	ASN
1	J	380	THR
1	J	394	ILE
1	J	419	ILE
1	J	442	LEU
1	J	459	ILE
1	J	478	SER
1	J	511	SER

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Mol	Chain	Res	Type
1	J	537	ASN
1	J	560	GLN
1	J	563	LYS
1	J	579	ASP
1	J	590	LEU
1	J	600	ARG
1	J	603	ILE
1	J	614	GLU
1	J	664	ASN
1	J	670	GLN
1	J	674	THR
1	J	678	PHE
1	K	190	GLU
1	K	210	ILE
1	K	217	THR
1	K	230	SER
1	K	252	ARG
1	K	274	ASN
1	K	343	GLU
1	K	344	ARG
1	K	361	ASN
1	K	363	ASN
1	K	380	THR
1	K	394	ILE
1	K	419	ILE
1	K	442	LEU
1	K	459	ILE
1	K	480	VAL
1	K	481	LEU
1	K	515	GLU
1	K	517	THR
1	K	537	ASN
1	K	560	GLN
1	K	563	LYS
1	K	579	ASP
1	K	590	LEU
1	K	600	ARG
1	K	603	ILE
1	K	614	GLU
1	K	664	ASN
1	K	674	THR
1	K	678	PHE

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Mol	Chain	Res	Type
1	K	725	LEU
1	K	726	ILE
1	L	190	GLU
1	L	194	VAL
1	L	210	ILE
1	L	228	THR
1	L	244	ASP
1	L	274	ASN
1	L	296	SER
1	L	343	GLU
1	L	344	ARG
1	L	361	ASN
1	L	376	ASN
1	L	380	THR
1	L	382	SER
1	L	394	ILE
1	L	419	ILE
1	L	442	LEU
1	L	459	ILE
1	L	464	PHE
1	L	481	LEU
1	L	512	ASP
1	L	537	ASN
1	L	560	GLN
1	L	563	LYS
1	L	579	ASP
1	L	590	LEU
1	L	614	GLU
1	L	705	ASN
1	M	190	GLU
1	M	210	ILE
1	M	217	THR
1	M	230	SER
1	M	250	GLU
1	M	252	ARG
1	M	274	ASN
1	M	344	ARG
1	M	361	ASN
1	M	363	ASN
1	M	376	ASN
1	M	380	THR
1	M	394	ILE

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Mol	Chain	Res	Type
1	M	400	GLN
1	M	402	SER
1	M	419	ILE
1	M	442	LEU
1	M	459	ILE
1	M	481	LEU
1	M	517	THR
1	M	537	ASN
1	M	560	GLN
1	M	563	LYS
1	M	579	ASP
1	M	584	ASN
1	M	587	MET
1	M	590	LEU
1	M	600	ARG
1	M	603	ILE
1	M	614	GLU
1	M	664	ASN
1	M	674	THR
1	M	678	PHE
1	M	689	ILE
1	M	725	LEU
1	M	726	ILE
1	N	190	GLU
1	N	203	LEU
1	N	209	ASN
1	N	210	ILE
1	N	214	LYS
1	N	252	ARG
1	N	274	ASN
1	N	343	GLU
1	N	344	ARG
1	N	361	ASN
1	N	363	ASN
1	N	380	THR
1	N	394	ILE
1	N	399	ASN
1	N	419	ILE
1	N	442	LEU
1	N	459	ILE
1	N	478	SER
1	N	481	LEU

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Mol	Chain	Res	Type
1	N	517	THR
1	N	534	ASN
1	N	560	GLN
1	N	563	LYS
1	N	579	ASP
1	N	590	LEU
1	N	593	ASP
1	N	603	ILE
1	N	614	GLU
1	N	653	LYS
1	N	657	ASN
1	N	664	ASN
1	N	674	THR
1	N	678	PHE
1	N	689	ILE
1	N	702	THR
1	N	706	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	C	246	ASN
1	C	485	GLN
1	D	246	ASN
1	D	483	GLN
1	D	485	GLN
1	E	485	GLN
1	E	509	ASN
1	E	657	ASN
1	F	246	ASN
1	F	485	GLN
1	G	485	GLN
1	G	509	ASN
1	G	553	ASN
1	H	485	GLN
1	I	483	GLN
1	I	543	GLN
1	J	476	ASN
1	J	509	ASN
1	K	438	GLN
1	K	509	ASN

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Mol	Chain	Res	Type
1	L	368	ASN
1	L	509	ASN
1	M	246	ASN
1	M	483	GLN
1	N	246	ASN
1	N	376	ASN
1	N	454	GLN
1	N	483	GLN
1	N	485	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.