



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:29 PM GMT

PDB ID : 3KL9
Title : Crystal structure of PepA from Streptococcus pneumoniae
Authors : Kim, K.K.; Lee, S.; Kim, D.
Deposited on : 2009-11-07
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

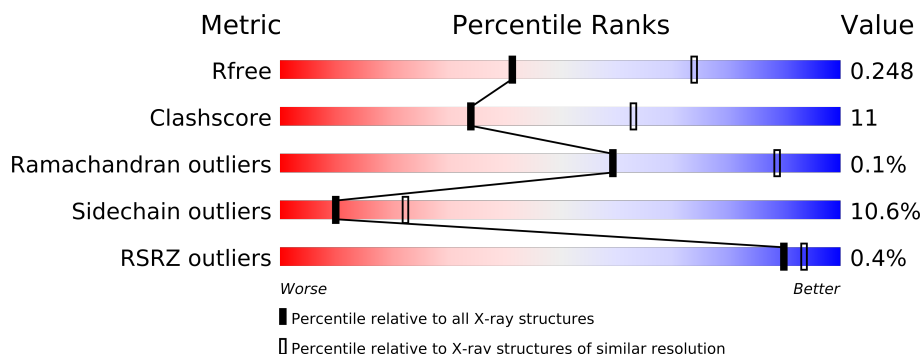
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	355	
1	B	355	
1	C	355	
1	D	355	
1	E	355	
1	F	355	
1	G	355	
1	H	355	
1	I	355	
1	J	355	
1	K	355	
1	L	355	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31329 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutamyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2577	1635	434	498	10			
1	B	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	C	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	D	340	Total	C	N	O	S	0	0	0
			2577	1635	434	498	10			
1	E	340	Total	C	N	O	S	0	0	0
			2577	1635	434	498	10			
1	F	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	G	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	H	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	I	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	J	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			
1	K	340	Total	C	N	O	S	0	0	0
			2577	1635	434	498	10			
1	L	337	Total	C	N	O	S	0	0	0
			2556	1623	431	493	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
B	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
C	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
D	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
E	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
G	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
H	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
I	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
J	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
K	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7
L	0	SER	-	EXPRESSION TAG	UNP Q8DNJ7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total 46	O 46	0	0
3	B	45	Total 45	O 45	0	0

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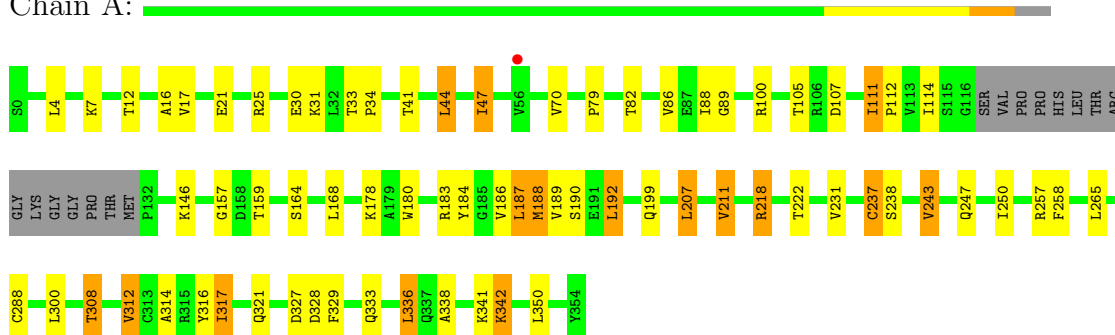
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	50	Total 50	O 50	0	0
3	D	44	Total 44	O 44	0	0
3	E	44	Total 44	O 44	0	0
3	F	45	Total 45	O 45	0	0
3	G	47	Total 47	O 47	0	0
3	H	36	Total 36	O 36	0	0
3	I	50	Total 50	O 50	0	0
3	J	45	Total 45	O 45	0	0
3	K	54	Total 54	O 54	0	0
3	L	43	Total 43	O 43	0	0

3 Residue-property plots

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

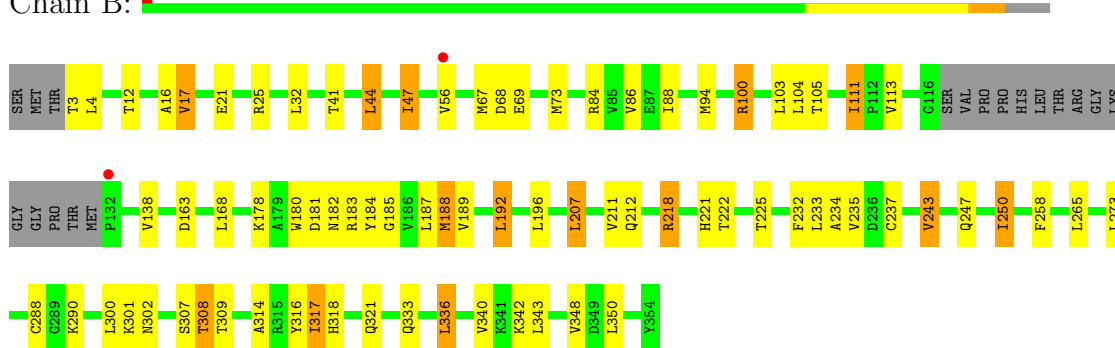
- Molecule 1: Glutamyl aminopeptidase

Chain A:



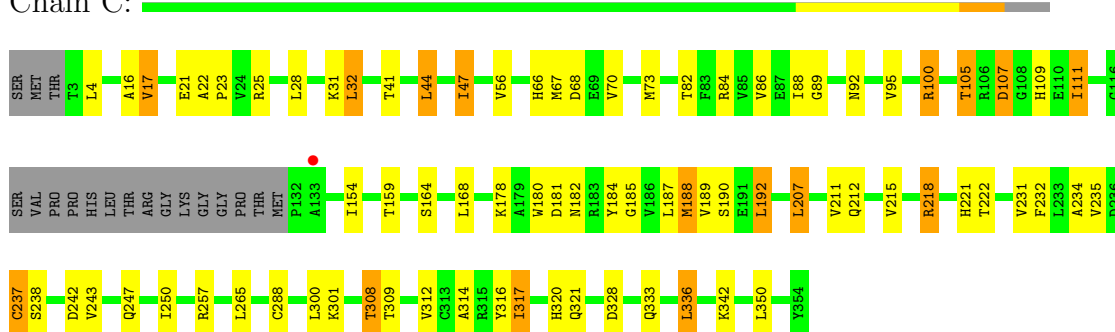
- Molecule 1: Glutamyl aminopeptidase

Chain B:



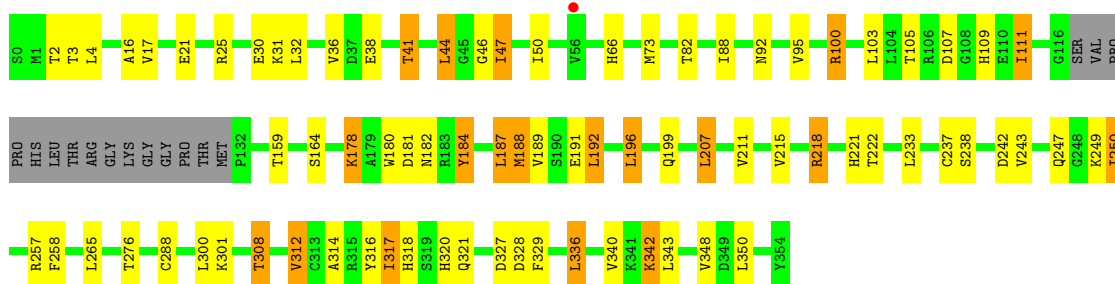
- Molecule 1: Glutamyl aminopeptidase

Chain C:



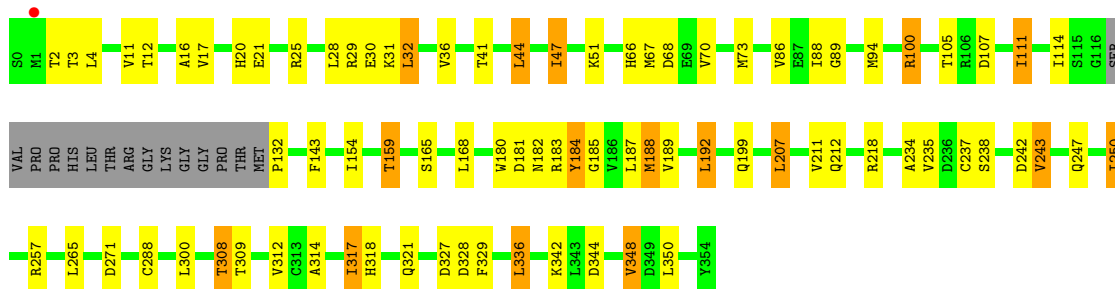
- Molecule 1: Glutamyl aminopeptidase

Chain D:



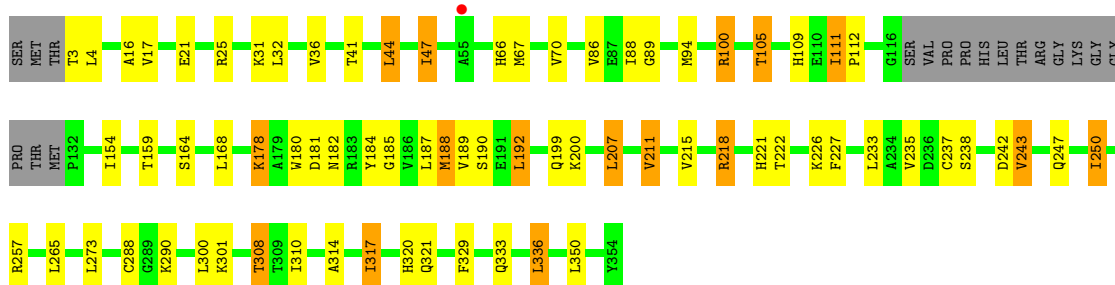
- Molecule 1: Glutamyl aminopeptidase

Chain E:



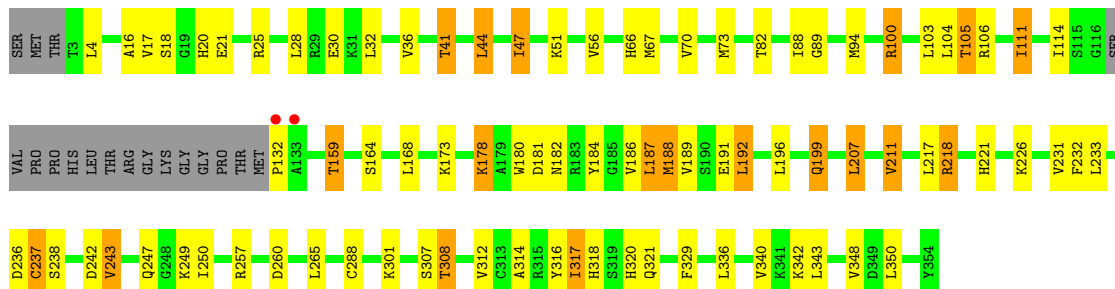
- Molecule 1: Glutamyl aminopeptidase

Chain F:



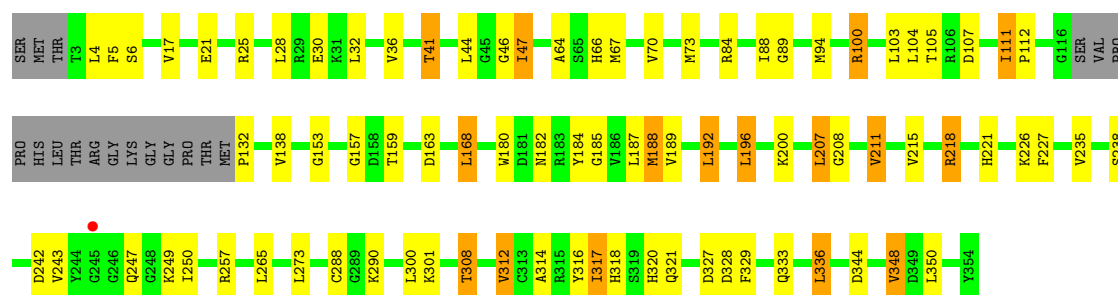
- Molecule 1: Glutamyl aminopeptidase

Chain G:



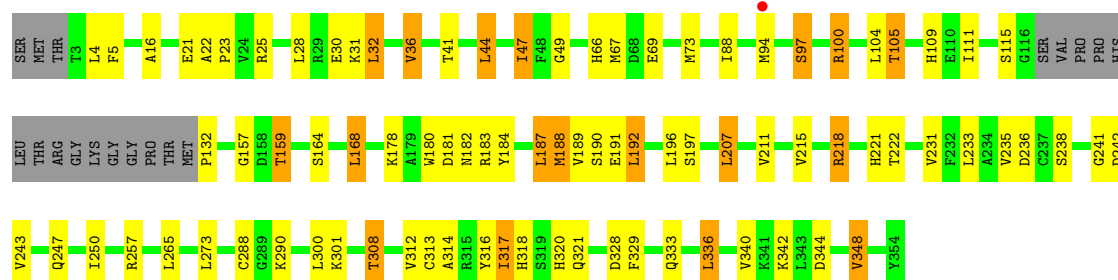
- Molecule 1: Glutamyl aminopeptidase

Chain H:



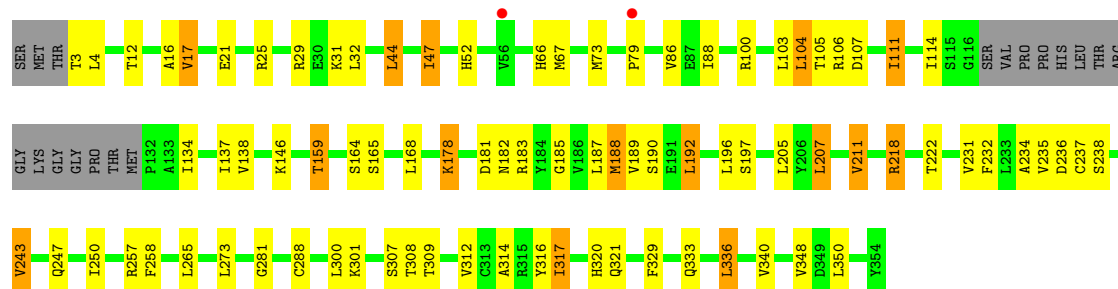
• Molecule 1: Glutamyl aminopeptidase

Chain I:



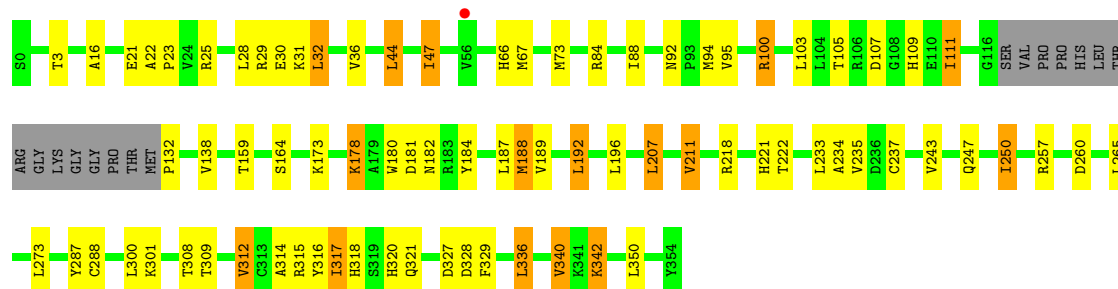
• Molecule 1: Glutamyl aminopeptidase

Chain J:



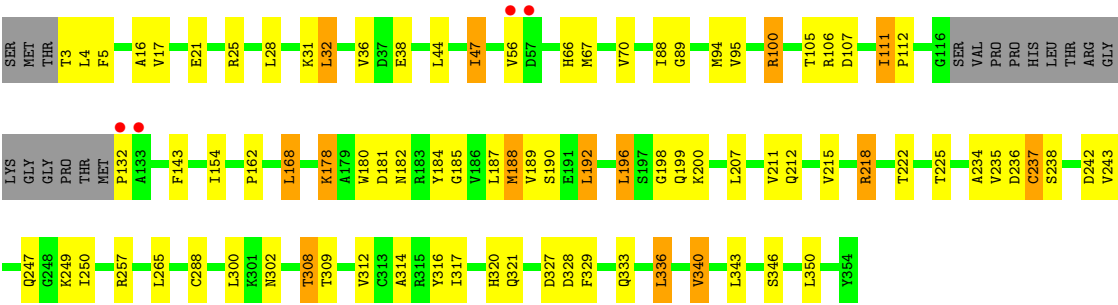
• Molecule 1: Glutamyl aminopeptidase

Chain K:



• Molecule 1: Glutamyl aminopeptidase

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	138.30Å 118.34Å 160.30Å 90.00° 106.35° 90.00°	Depositor
Resolution (Å)	44.43 – 2.70 44.43 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.43-2.70) 99.1 (44.43-2.69)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.200 , 0.247 0.203 , 0.248	Depositor DCC
R_{free} test set	6890 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 0.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 137116 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31329	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/2629	0.62	0/3558
1	B	0.42	0/2608	0.62	0/3530
1	C	0.41	0/2608	0.62	0/3530
1	D	0.42	0/2629	0.61	0/3558
1	E	0.41	0/2629	0.60	0/3558
1	F	0.43	0/2608	0.62	0/3530
1	G	0.42	0/2608	0.61	0/3530
1	H	0.42	0/2608	0.60	0/3530
1	I	0.41	0/2608	0.61	0/3530
1	J	0.43	0/2608	0.62	0/3530
1	K	0.42	0/2629	0.60	0/3558
1	L	0.42	0/2608	0.62	0/3530
All	All	0.42	0/31380	0.61	0/42472

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2577	0	2550	51	0
1	B	2556	0	2526	59	0
1	C	2556	0	2526	68	0
1	D	2577	0	2550	58	0
1	E	2577	0	2550	63	0
1	F	2556	0	2526	49	0
1	G	2556	0	2526	65	0
1	H	2556	0	2526	68	0
1	I	2556	0	2526	74	0
1	J	2556	0	2526	65	0
1	K	2577	0	2550	63	0
1	L	2556	0	2526	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	46	0	0	0	0
3	B	45	0	0	0	0
3	C	50	0	0	1	0
3	D	44	0	0	0	0
3	E	44	0	0	1	0
3	F	45	0	0	1	0
3	G	47	0	0	1	0
3	H	36	0	0	1	0
3	I	50	0	0	0	0
3	J	45	0	0	3	0
3	K	54	0	0	3	0
3	L	43	0	0	2	0
All	All	31329	0	30408	664	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (664) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:100:ARG:NH1	1:L:321:GLN:HE22	1.42	1.17
1:E:321:GLN:HE22	1:H:100:ARG:NH1	1.47	1.11
1:C:100:ARG:HH11	1:C:100:ARG:HG3	1.00	1.11
1:K:73:MET:HB2	1:K:88:ILE:HD11	1.35	1.08
1:J:25:ARG:HG3	1:J:47:ILE:HG12	1.31	1.08
1:E:73:MET:HB2	1:E:88:ILE:HD11	1.37	1.05
1:C:100:ARG:NH1	1:J:321:GLN:HE22	1.58	1.02
1:A:188:MET:HE2	1:A:333:GLN:HB2	1.36	1.01
1:C:188:MET:HE2	1:C:333:GLN:HB2	1.45	0.99
1:F:100:ARG:NH1	1:K:321:GLN:HE22	1.64	0.96
1:A:321:GLN:HE22	1:D:100:ARG:NH1	1.65	0.94
1:B:100:ARG:NH1	1:G:321:GLN:HE22	1.65	0.94
1:B:73:MET:HB2	1:B:88:ILE:HD11	1.50	0.94
1:K:25:ARG:HG3	1:K:47:ILE:HG12	1.48	0.93
1:H:73:MET:HB2	1:H:88:ILE:HD11	1.50	0.93
1:A:100:ARG:HH11	1:D:321:GLN:HE22	1.17	0.92
1:B:321:GLN:HE22	1:G:100:ARG:HH11	1.17	0.92
1:I:321:GLN:HE22	1:L:100:ARG:NH1	1.67	0.92
1:F:321:GLN:HE22	1:K:100:ARG:NH1	1.67	0.91
1:K:100:ARG:HG3	1:K:100:ARG:HH11	1.35	0.91
1:C:100:ARG:HG3	1:C:100:ARG:NH1	1.80	0.90
1:I:321:GLN:HE22	1:L:100:ARG:HH11	1.16	0.89
1:I:100:ARG:HG3	1:I:100:ARG:HH11	1.35	0.89
1:E:100:ARG:HH11	1:H:321:GLN:HE22	1.20	0.89
1:K:265:LEU:HD13	1:K:308:THR:HG23	1.56	0.88
1:B:321:GLN:HE22	1:G:100:ARG:NH1	1.70	0.88
1:A:321:GLN:HE22	1:D:100:ARG:HH11	1.22	0.88
1:H:250:ILE:HD11	1:H:314:ALA:HA	1.56	0.87
1:I:188:MET:HE2	1:I:333:GLN:HB2	1.57	0.87
1:F:100:ARG:HH11	1:K:321:GLN:HE22	1.16	0.86
1:I:100:ARG:NH1	1:L:321:GLN:NE2	2.24	0.86
1:K:250:ILE:HD11	1:K:314:ALA:HA	1.56	0.84
1:D:100:ARG:HH11	1:D:100:ARG:HG3	1.41	0.84
1:L:25:ARG:HG3	1:L:47:ILE:HG12	1.60	0.84
1:J:265:LEU:HD13	1:J:308:THR:CG2	2.07	0.84
1:C:25:ARG:HG3	1:C:47:ILE:HG12	1.58	0.84
1:G:265:LEU:HD13	1:G:308:THR:HG23	1.60	0.83
1:D:73:MET:HB2	1:D:88:ILE:HD11	1.60	0.83
1:K:265:LEU:HD13	1:K:308:THR:CG2	2.09	0.83
1:G:250:ILE:HD11	1:G:314:ALA:HA	1.61	0.82
1:I:250:ILE:HD11	1:I:314:ALA:HA	1.62	0.81
1:I:100:ARG:HH11	1:L:321:GLN:HE22	1.23	0.80
1:B:100:ARG:HH11	1:G:321:GLN:HE22	1.27	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:265:LEU:HD13	1:B:308:THR:CG2	2.11	0.80
1:K:342:LYS:HE3	3:K:383:HOH:O	1.82	0.80
1:E:189:VAL:HG13	1:E:207:LEU:HD22	1.62	0.79
1:L:265:LEU:HD13	1:L:308:THR:HG23	1.61	0.79
1:G:189:VAL:HG13	1:G:207:LEU:HD22	1.62	0.79
1:C:73:MET:HB2	1:C:88:ILE:HD11	1.63	0.78
1:D:73:MET:HB2	1:D:88:ILE:CD1	2.12	0.78
1:A:188:MET:HE2	1:A:333:GLN:CB	2.14	0.78
1:E:321:GLN:NE2	1:H:100:ARG:NH1	2.29	0.78
1:F:265:LEU:HD13	1:F:308:THR:HG23	1.65	0.78
1:F:265:LEU:HD13	1:F:308:THR:CG2	2.14	0.78
1:I:73:MET:HB2	1:I:88:ILE:HD11	1.66	0.78
1:F:273:LEU:HD11	1:F:308:THR:HG21	1.65	0.76
1:A:189:VAL:HG13	1:A:207:LEU:HD22	1.65	0.76
1:L:105:THR:HG22	1:L:107:ASP:H	1.51	0.76
1:K:73:MET:HB2	1:K:88:ILE:CD1	2.16	0.75
1:C:265:LEU:HD13	1:C:308:THR:HG23	1.68	0.75
1:B:265:LEU:HD13	1:B:308:THR:HG23	1.66	0.75
1:C:100:ARG:HH12	1:J:321:GLN:HE22	1.34	0.74
1:C:265:LEU:HD13	1:C:308:THR:CG2	2.17	0.74
1:L:16:ALA:HB1	1:L:21:GLU:HA	1.68	0.74
1:A:250:ILE:HD11	1:A:314:ALA:HA	1.69	0.74
1:A:105:THR:HG22	1:A:107:ASP:H	1.53	0.74
1:B:25:ARG:HG3	1:B:47:ILE:HG12	1.69	0.73
1:E:21:GLU:CD	1:E:211:VAL:HG23	2.08	0.73
1:C:250:ILE:HD11	1:C:314:ALA:HA	1.69	0.73
1:A:188:MET:CE	1:A:333:GLN:HB2	2.18	0.73
1:C:100:ARG:NH1	1:J:321:GLN:NE2	2.36	0.72
1:D:21:GLU:CD	1:D:211:VAL:HG23	2.09	0.72
1:B:73:MET:HB2	1:B:88:ILE:CD1	2.19	0.72
1:J:25:ARG:HG3	1:J:47:ILE:CG1	2.15	0.72
1:A:100:ARG:NH1	1:D:321:GLN:HE22	1.88	0.72
1:I:25:ARG:HG3	1:I:47:ILE:HG12	1.71	0.71
1:E:100:ARG:NH1	1:H:321:GLN:HE22	1.88	0.71
1:F:189:VAL:HG13	1:F:207:LEU:HD22	1.71	0.71
1:I:100:ARG:HH11	1:L:321:GLN:NE2	1.88	0.71
1:H:73:MET:HB2	1:H:88:ILE:CD1	2.20	0.71
1:K:100:ARG:CG	1:K:100:ARG:HH11	2.04	0.71
1:H:47:ILE:HD11	1:H:67:MET:SD	2.31	0.70
1:K:189:VAL:HG13	1:K:207:LEU:HD22	1.73	0.70
1:K:100:ARG:HG3	1:K:100:ARG:NH1	2.01	0.70
1:J:73:MET:HB2	1:J:88:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:247:GLN:NE2	1:G:288:CYS:H	1.90	0.70
1:A:44:LEU:HB3	1:A:211:VAL:HG11	1.73	0.70
1:H:105:THR:HG22	1:H:107:ASP:H	1.56	0.70
1:H:25:ARG:HG3	1:H:47:ILE:HG12	1.74	0.69
1:A:25:ARG:HG3	1:A:47:ILE:HG12	1.75	0.69
1:H:265:LEU:HD13	1:H:308:THR:HG23	1.74	0.69
1:C:321:GLN:HE22	1:J:100:ARG:NH1	1.91	0.69
1:J:250:ILE:HD11	1:J:314:ALA:HA	1.76	0.68
1:E:165:SER:O	1:H:100:ARG:NH2	2.27	0.68
1:J:273:LEU:HD11	1:J:308:THR:HG21	1.75	0.68
1:G:221:HIS:HA	1:G:301:LYS:HD2	1.76	0.68
1:G:100:ARG:HH11	1:G:100:ARG:HG3	1.58	0.67
1:E:218:ARG:HB3	1:F:300:LEU:HD21	1.75	0.67
1:I:132:PRO:HG3	1:L:94:MET:CE	2.24	0.67
1:B:247:GLN:NE2	1:B:288:CYS:H	1.92	0.67
1:E:250:ILE:HD11	1:E:314:ALA:HA	1.76	0.67
1:E:73:MET:HB2	1:E:88:ILE:CD1	2.22	0.66
1:I:189:VAL:HG13	1:I:207:LEU:HD22	1.76	0.66
1:I:312:VAL:HG22	1:I:328:ASP:HB3	1.77	0.66
1:L:189:VAL:HG13	1:L:207:LEU:CD2	2.24	0.66
1:E:265:LEU:HD13	1:E:308:THR:HG23	1.76	0.66
1:D:100:ARG:HG3	1:D:100:ARG:NH1	2.09	0.66
1:F:321:GLN:HE22	1:K:100:ARG:HH11	1.44	0.66
1:H:182:ASN:ND2	1:H:185:GLY:H	1.94	0.66
1:I:192:LEU:HG	1:I:336:LEU:HD13	1.77	0.66
1:C:192:LEU:HG	1:C:336:LEU:HD13	1.79	0.66
1:C:21:GLU:CD	1:C:211:VAL:HG23	2.16	0.66
1:K:247:GLN:NE2	1:K:288:CYS:H	1.94	0.66
1:J:105:THR:HG22	1:J:107:ASP:H	1.62	0.65
1:K:100:ARG:O	1:K:320:HIS:HE1	1.79	0.65
1:G:265:LEU:HD13	1:G:308:THR:CG2	2.26	0.65
1:G:66:HIS:CE1	1:G:182:ASN:HB2	2.32	0.65
1:I:100:ARG:HG3	1:I:100:ARG:NH1	2.10	0.65
1:C:321:GLN:HE22	1:J:100:ARG:HH11	1.44	0.65
1:I:188:MET:HE3	1:I:188:MET:HA	1.79	0.64
1:B:25:ARG:HG3	1:B:47:ILE:CG1	2.28	0.64
1:G:44:LEU:HB3	1:G:211:VAL:HG11	1.79	0.64
1:B:21:GLU:CD	1:B:211:VAL:HG23	2.17	0.64
1:L:21:GLU:CD	1:L:211:VAL:HG23	2.16	0.64
1:I:321:GLN:NE2	1:L:100:ARG:HH11	1.93	0.64
1:I:273:LEU:HD11	1:I:308:THR:HG21	1.79	0.64
1:H:192:LEU:HD22	1:H:196:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:94:MET:CE	1:H:132:PRO:HG3	2.28	0.64
1:L:36:VAL:HG12	1:L:38:GLU:H	1.63	0.63
1:D:265:LEU:HD13	1:D:308:THR:HG23	1.79	0.63
1:D:44:LEU:HD22	1:D:222:THR:HG21	1.79	0.63
1:D:36:VAL:HG13	1:D:50:ILE:O	1.98	0.63
1:D:16:ALA:HB1	1:D:21:GLU:HA	1.80	0.63
1:B:218:ARG:HB3	1:C:300:LEU:HD21	1.81	0.63
1:E:321:GLN:HE22	1:H:100:ARG:HH11	1.39	0.63
1:B:188:MET:HE1	1:B:333:GLN:HB2	1.80	0.63
1:J:16:ALA:HB1	1:J:21:GLU:HA	1.79	0.63
1:F:105:THR:HG22	1:F:109:HIS:H	1.63	0.62
1:K:44:LEU:HB3	1:K:211:VAL:HG11	1.80	0.62
1:J:247:GLN:NE2	1:J:288:CYS:H	1.97	0.62
1:C:16:ALA:HB1	1:C:21:GLU:HA	1.81	0.62
1:E:192:LEU:HG	1:E:336:LEU:HD13	1.82	0.62
1:C:66:HIS:CE1	1:C:182:ASN:HB2	2.34	0.62
1:D:189:VAL:HG13	1:D:207:LEU:HD22	1.80	0.62
1:D:100:ARG:HH11	1:D:100:ARG:CG	2.10	0.62
1:F:188:MET:HG2	1:F:235:VAL:HG11	1.80	0.62
1:L:314:ALA:HB3	1:L:317:ILE:CD1	2.29	0.62
1:D:312:VAL:HG22	1:D:328:ASP:HB3	1.81	0.61
1:A:237:CYS:SG	1:A:317:ILE:HD11	2.40	0.61
1:B:94:MET:SD	1:G:94:MET:CE	2.88	0.61
1:H:188:MET:HE1	1:H:333:GLN:HB2	1.82	0.61
1:F:247:GLN:NE2	1:F:288:CYS:H	1.97	0.61
1:L:336:LEU:O	1:L:340:VAL:HG13	2.00	0.61
1:G:100:ARG:NH1	1:G:100:ARG:HG3	2.14	0.61
1:E:211:VAL:HG22	1:E:212:GLN:HG3	1.80	0.61
1:G:100:ARG:HH11	1:G:100:ARG:CG	2.13	0.61
1:D:180:TRP:CE2	1:D:184:TYR:HB2	2.36	0.61
1:C:188:MET:HE2	1:C:333:GLN:CB	2.26	0.61
1:E:25:ARG:HG3	1:E:47:ILE:HG12	1.82	0.61
1:J:21:GLU:CD	1:J:211:VAL:HG22	2.21	0.61
1:A:188:MET:CE	1:A:333:GLN:HE21	2.14	0.60
1:I:73:MET:HB2	1:I:88:ILE:CD1	2.31	0.60
1:H:192:LEU:HG	1:H:336:LEU:HD13	1.82	0.60
1:E:47:ILE:HD11	1:E:67:MET:SD	2.40	0.60
1:B:317:ILE:HG23	1:B:318:HIS:CD2	2.36	0.60
1:K:164:SER:HB3	1:K:178:LYS:HB3	1.83	0.60
1:C:100:ARG:HH11	1:C:100:ARG:CG	1.91	0.60
1:I:221:HIS:HA	1:I:301:LYS:HD2	1.81	0.60
1:H:226:LYS:HD3	1:H:227:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:317:ILE:HG23	1:G:318:HIS:CD2	2.36	0.60
1:I:188:MET:HG2	1:I:235:VAL:HG11	1.84	0.60
1:A:16:ALA:HB1	1:A:21:GLU:HA	1.85	0.59
1:I:314:ALA:HB3	1:I:317:ILE:CD1	2.33	0.59
1:I:265:LEU:HD13	1:I:308:THR:HG23	1.85	0.59
1:B:314:ALA:HB3	1:B:317:ILE:CD1	2.33	0.59
1:E:312:VAL:HG22	1:E:328:ASP:HB3	1.84	0.59
1:B:100:ARG:HH11	1:G:321:GLN:NE2	2.00	0.59
1:L:66:HIS:CE1	1:L:182:ASN:HB2	2.38	0.59
1:J:314:ALA:HB3	1:J:317:ILE:CD1	2.33	0.59
1:A:218:ARG:HB3	1:B:300:LEU:HD21	1.84	0.59
1:I:100:ARG:HH12	1:L:321:GLN:HE22	1.46	0.58
1:B:250:ILE:HD11	1:B:314:ALA:HA	1.84	0.58
1:F:321:GLN:HE22	1:K:100:ARG:HH12	1.47	0.58
1:K:107:ASP:OD1	1:K:109:HIS:HD2	1.87	0.58
1:F:238:SER:OG	1:F:257:ARG:NH2	2.37	0.58
1:J:52:HIS:HE1	3:J:383:HOH:O	1.85	0.58
1:L:225:THR:HA	1:L:302:ASN:HD21	1.68	0.58
1:C:189:VAL:HG13	1:C:207:LEU:HD22	1.84	0.58
1:I:132:PRO:HG3	1:L:94:MET:HE1	1.85	0.58
1:I:44:LEU:HB3	1:I:211:VAL:HG11	1.84	0.58
1:B:192:LEU:HG	1:B:336:LEU:HD13	1.85	0.58
1:B:189:VAL:HG13	1:B:207:LEU:HD22	1.85	0.58
1:E:94:MET:HE2	1:H:132:PRO:HG3	1.85	0.58
1:E:105:THR:HG22	1:E:107:ASP:H	1.67	0.58
1:G:25:ARG:HG3	1:G:47:ILE:HG12	1.84	0.58
1:F:188:MET:HE1	1:F:333:GLN:HB2	1.84	0.57
1:H:265:LEU:HD13	1:H:308:THR:CG2	2.33	0.57
1:L:211:VAL:HG22	1:L:212:GLN:HG3	1.86	0.57
1:J:188:MET:HE1	1:J:333:GLN:HB2	1.86	0.57
1:L:238:SER:OG	1:L:257:ARG:NH2	2.37	0.57
1:D:238:SER:OG	1:D:257:ARG:NH2	2.38	0.57
1:D:218:ARG:HB3	1:L:300:LEU:HD21	1.87	0.57
1:A:188:MET:HE2	1:A:333:GLN:HE21	1.69	0.56
1:E:132:PRO:HG3	1:H:94:MET:CE	2.35	0.56
1:D:250:ILE:HD11	1:D:314:ALA:HA	1.87	0.56
1:D:66:HIS:CE1	1:D:182:ASN:HB2	2.39	0.56
1:D:105:THR:HB	1:D:109:HIS:HB2	1.87	0.56
1:L:44:LEU:HD22	1:L:222:THR:HG21	1.87	0.56
1:J:17:VAL:HG13	1:J:88:ILE:HG21	1.87	0.56
1:I:238:SER:OG	1:I:257:ARG:NH2	2.38	0.56
1:D:36:VAL:HG12	1:D:38:GLU:H	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:164:SER:HB3	1:J:178:LYS:HB3	1.86	0.56
1:L:192:LEU:HD22	1:L:196:LEU:HD22	1.88	0.56
1:F:25:ARG:HG3	1:F:47:ILE:HG12	1.86	0.56
1:L:196:LEU:HD21	1:L:340:VAL:HG21	1.88	0.56
1:D:196:LEU:HD21	1:D:340:VAL:HG21	1.87	0.56
1:I:215:VAL:HG23	1:I:218:ARG:HG3	1.87	0.56
1:D:44:LEU:HB3	1:D:211:VAL:HG11	1.88	0.56
1:K:44:LEU:HD22	1:K:222:THR:HG21	1.88	0.56
1:E:321:GLN:HE22	1:H:100:ARG:HH12	1.47	0.55
1:A:12:THR:O	1:A:178:LYS:NZ	2.37	0.55
1:E:314:ALA:HB3	1:E:317:ILE:CD1	2.35	0.55
1:D:192:LEU:HD22	1:D:196:LEU:HD22	1.87	0.55
1:E:44:LEU:HB3	1:E:211:VAL:HG11	1.89	0.55
1:A:21:GLU:CD	1:A:211:VAL:HG22	2.26	0.55
1:L:314:ALA:HB3	1:L:317:ILE:HD11	1.89	0.55
1:D:192:LEU:HG	1:D:336:LEU:HD13	1.88	0.55
1:L:25:ARG:HG3	1:L:47:ILE:CG1	2.36	0.55
1:J:44:LEU:HD22	1:J:222:THR:HG21	1.89	0.55
1:C:247:GLN:NE2	1:C:288:CYS:H	2.04	0.55
1:B:196:LEU:HD21	1:B:340:VAL:HG21	1.88	0.55
1:A:321:GLN:NE2	1:D:100:ARG:HH11	1.98	0.55
1:F:192:LEU:HG	1:F:336:LEU:HD13	1.88	0.55
1:H:314:ALA:HB3	1:H:317:ILE:HD11	1.89	0.55
1:G:188:MET:CE	1:G:329:PHE:CE1	2.90	0.55
1:B:188:MET:HG2	1:B:235:VAL:HG11	1.89	0.55
1:D:73:MET:CB	1:D:88:ILE:HD11	2.34	0.55
1:E:180:TRP:CE2	1:E:184:TYR:HB2	2.42	0.55
1:A:192:LEU:HG	1:A:336:LEU:HD13	1.89	0.55
1:J:238:SER:OG	1:J:257:ARG:NH2	2.40	0.55
1:E:247:GLN:NE2	1:E:288:CYS:H	2.04	0.54
1:C:221:HIS:HA	1:C:301:LYS:HD2	1.89	0.54
1:H:100:ARG:HG3	1:H:100:ARG:HH11	1.72	0.54
1:K:66:HIS:CE1	1:K:182:ASN:HB2	2.43	0.54
1:F:100:ARG:HH11	1:K:321:GLN:NE2	1.95	0.54
1:I:132:PRO:HG3	1:L:94:MET:HE2	1.88	0.54
1:J:73:MET:HB2	1:J:88:ILE:CD1	2.36	0.54
1:F:215:VAL:O	1:F:218:ARG:NH1	2.40	0.54
1:A:238:SER:OG	1:A:257:ARG:NH2	2.40	0.54
1:F:47:ILE:HD11	1:F:67:MET:SD	2.48	0.54
1:B:69:GLU:OE1	1:B:178:LYS:HE2	2.08	0.54
1:B:225:THR:HA	1:B:302:ASN:HD21	1.72	0.54
1:I:100:ARG:O	1:I:320:HIS:HE1	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:25:ARG:HG3	1:K:47:ILE:CG1	2.31	0.53
1:H:17:VAL:HG13	1:H:88:ILE:HG21	1.90	0.53
1:K:180:TRP:CE2	1:K:184:TYR:HB2	2.43	0.53
1:G:28:LEU:HD11	1:G:186:VAL:HG13	1.91	0.53
1:A:180:TRP:CE2	1:A:184:TYR:HB2	2.43	0.53
1:H:215:VAL:HG23	1:H:218:ARG:HG3	1.90	0.53
1:H:100:ARG:HB3	1:H:163:ASP:HB3	1.89	0.53
1:H:314:ALA:HB3	1:H:317:ILE:CD1	2.37	0.53
1:I:97:SER:O	1:I:115:SER:OG	2.18	0.53
1:L:250:ILE:HD11	1:L:314:ALA:HA	1.90	0.53
1:L:180:TRP:CE2	1:L:184:TYR:HB2	2.43	0.53
1:A:31:LYS:HD3	1:A:190:SER:OG	2.08	0.53
1:K:192:LEU:HD22	1:K:196:LEU:HD22	1.91	0.53
1:F:221:HIS:HA	1:F:301:LYS:HD2	1.91	0.53
1:F:44:LEU:HD22	1:F:222:THR:HG21	1.89	0.53
1:I:188:MET:HE1	1:I:329:PHE:CE1	2.43	0.53
1:D:103:LEU:HB3	1:D:111:ILE:HG13	1.90	0.53
1:G:73:MET:HB2	1:G:88:ILE:HD11	1.91	0.53
1:L:47:ILE:HD11	1:L:67:MET:SD	2.49	0.53
1:D:215:VAL:HG23	1:D:218:ARG:HG3	1.90	0.53
1:H:312:VAL:HG22	1:H:328:ASP:HB3	1.90	0.53
1:G:237:CYS:SG	1:G:317:ILE:HD11	2.49	0.52
1:A:44:LEU:HD22	1:A:222:THR:HG21	1.91	0.52
1:F:180:TRP:CE2	1:F:184:TYR:HB2	2.44	0.52
1:H:103:LEU:HB3	1:H:111:ILE:HG13	1.91	0.52
1:B:321:GLN:NE2	1:G:100:ARG:HH11	1.97	0.52
1:I:188:MET:HE2	1:I:333:GLN:HE21	1.74	0.52
1:D:164:SER:HB3	1:D:178:LYS:HB3	1.90	0.52
1:J:29:ARG:HD2	3:J:382:HOH:O	2.09	0.52
1:J:265:LEU:HD13	1:J:308:THR:HG21	1.90	0.52
1:H:105:THR:HG22	1:H:107:ASP:N	2.25	0.52
1:B:16:ALA:HB1	1:B:21:GLU:HA	1.92	0.52
1:C:312:VAL:HG22	1:C:328:ASP:HB3	1.91	0.52
1:H:21:GLU:CD	1:H:211:VAL:HG22	2.29	0.52
1:L:100:ARG:O	1:L:320:HIS:HE1	1.92	0.52
1:B:211:VAL:HG22	1:B:212:GLN:HG3	1.92	0.52
1:B:84:ARG:NH2	1:B:138:VAL:HG22	2.25	0.52
1:I:47:ILE:HD11	1:I:67:MET:SD	2.50	0.52
1:J:218:ARG:HB3	1:K:300:LEU:HD21	1.91	0.52
1:G:180:TRP:CE2	1:G:184:TYR:HB2	2.45	0.51
1:A:79:PRO:HA	1:A:146:LYS:HB2	1.91	0.51
1:H:317:ILE:HG23	1:H:318:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:47:ILE:HD11	1:K:67:MET:SD	2.51	0.51
1:H:250:ILE:HD11	1:H:314:ALA:CA	2.34	0.51
1:K:317:ILE:HG23	1:K:318:HIS:CD2	2.46	0.51
1:J:103:LEU:HB3	1:J:111:ILE:HG13	1.92	0.51
1:G:317:ILE:HG23	1:G:318:HIS:HD2	1.75	0.51
1:A:199:GLN:OE1	1:A:341:LYS:HE3	2.09	0.51
1:C:31:LYS:HD3	1:C:190:SER:OG	2.10	0.51
1:H:188:MET:HG2	1:H:235:VAL:HG11	1.92	0.51
1:D:314:ALA:HB3	1:D:317:ILE:CD1	2.41	0.51
1:D:196:LEU:HD21	1:D:340:VAL:CG2	2.41	0.51
1:L:31:LYS:HD3	1:L:190:SER:OG	2.11	0.51
1:J:336:LEU:O	1:J:340:VAL:HG13	2.11	0.51
1:F:250:ILE:HD11	1:F:314:ALA:HA	1.93	0.51
1:D:107:ASP:OD1	1:D:109:HIS:HD2	1.94	0.51
1:F:188:MET:HE3	1:F:329:PHE:CE1	2.46	0.51
1:L:182:ASN:HD21	1:L:236:ASP:HA	1.76	0.51
1:H:44:LEU:HB3	1:H:211:VAL:HG11	1.92	0.51
1:L:182:ASN:ND2	1:L:236:ASP:HA	2.26	0.51
1:K:188:MET:HE2	1:K:329:PHE:CZ	2.46	0.51
1:I:188:MET:CE	1:I:333:GLN:HE21	2.23	0.50
1:B:44:LEU:HB3	1:B:211:VAL:HG11	1.93	0.50
1:J:100:ARG:O	1:J:320:HIS:HE1	1.94	0.50
1:G:47:ILE:HD11	1:G:67:MET:SD	2.51	0.50
1:F:31:LYS:HD3	1:F:190:SER:OG	2.11	0.50
1:L:100:ARG:HH11	1:L:100:ARG:HG3	1.75	0.50
1:E:189:VAL:HG13	1:E:207:LEU:CD2	2.40	0.50
1:G:73:MET:HB2	1:G:88:ILE:CD1	2.41	0.50
1:C:237:CYS:SG	1:C:317:ILE:HD11	2.51	0.50
1:D:247:GLN:NE2	1:D:288:CYS:H	2.08	0.50
1:G:238:SER:OG	1:G:257:ARG:NH2	2.44	0.50
1:H:84:ARG:NH2	1:H:138:VAL:HG22	2.27	0.50
1:L:247:GLN:NE2	1:L:288:CYS:H	2.10	0.50
1:H:344:ASP:O	1:H:348:VAL:HG13	2.12	0.50
1:H:238:SER:OG	1:H:257:ARG:NH2	2.45	0.50
1:L:17:VAL:HG13	1:L:88:ILE:HG21	1.93	0.50
1:I:44:LEU:HD22	1:I:222:THR:HG21	1.93	0.50
1:G:242:ASP:OD1	1:G:243:VAL:N	2.45	0.50
1:I:66:HIS:CE1	1:I:182:ASN:HB2	2.46	0.50
1:G:100:ARG:O	1:G:320:HIS:HE1	1.95	0.50
1:E:16:ALA:HB1	1:E:21:GLU:HA	1.94	0.50
1:G:16:ALA:HB1	1:G:21:GLU:HA	1.94	0.50
1:L:188:MET:HE3	1:L:329:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:189:VAL:HG13	1:L:207:LEU:HD22	1.91	0.50
1:I:182:ASN:ND2	1:I:236:ASP:HA	2.27	0.50
1:I:16:ALA:O	1:I:69:GLU:HG2	2.11	0.49
1:C:250:ILE:HD11	1:C:314:ALA:CA	2.41	0.49
1:A:82:THR:HG21	1:D:243:VAL:CG2	2.42	0.49
1:K:92:ASN:O	1:K:95:VAL:HG22	2.11	0.49
1:K:234:ALA:O	1:K:309:THR:HA	2.12	0.49
1:J:47:ILE:HD11	1:J:67:MET:SD	2.53	0.49
1:L:44:LEU:HB3	1:L:211:VAL:HG11	1.95	0.49
1:H:273:LEU:HD11	1:H:308:THR:HG21	1.94	0.49
1:I:301:LYS:HE2	1:I:301:LYS:HA	1.93	0.49
1:F:314:ALA:HB3	1:F:317:ILE:CD1	2.42	0.49
1:E:12:THR:HA	1:E:183:ARG:HG3	1.93	0.49
1:E:17:VAL:HG13	1:E:88:ILE:HG21	1.95	0.49
1:F:100:ARG:O	1:F:320:HIS:HE1	1.96	0.49
1:I:164:SER:HB3	1:I:178:LYS:HB3	1.93	0.49
1:B:100:ARG:HB3	1:B:163:ASP:HB3	1.95	0.49
1:D:340:VAL:HA	1:D:343:LEU:HD12	1.95	0.49
1:C:180:TRP:CE2	1:C:184:TYR:HB2	2.47	0.49
1:J:281:GLY:HA2	3:J:363:HOH:O	2.13	0.49
1:K:250:ILE:HD13	1:K:315:ARG:HG3	1.95	0.49
1:F:16:ALA:HB1	1:F:21:GLU:HA	1.94	0.49
1:C:164:SER:HB3	1:C:178:LYS:HB3	1.94	0.49
1:I:100:ARG:HG3	1:L:321:GLN:NE2	2.28	0.49
1:B:273:LEU:HD11	1:B:308:THR:HG21	1.94	0.49
1:A:265:LEU:HD13	1:A:308:THR:CG2	2.42	0.49
1:G:192:LEU:HD22	1:G:196:LEU:HD22	1.95	0.49
1:I:105:THR:HG22	1:I:109:HIS:N	2.28	0.49
1:E:265:LEU:HD13	1:E:308:THR:CG2	2.43	0.48
1:L:242:ASP:HB3	1:L:249:LYS:HA	1.93	0.48
1:C:100:ARG:NH2	1:J:165:SER:O	2.46	0.48
1:C:188:MET:HA	1:C:188:MET:HE3	1.94	0.48
1:E:94:MET:HE1	1:H:132:PRO:HG3	1.95	0.48
1:J:188:MET:HE3	1:J:329:PHE:CD1	2.47	0.48
1:F:21:GLU:CD	1:F:211:VAL:HG22	2.33	0.48
1:F:314:ALA:HB3	1:F:317:ILE:HD11	1.94	0.48
1:C:28:LEU:O	1:C:32:LEU:HB2	2.14	0.48
1:A:105:THR:HG22	1:A:107:ASP:N	2.25	0.48
1:A:265:LEU:HD13	1:A:308:THR:HG23	1.95	0.48
1:A:247:GLN:NE2	1:A:288:CYS:H	2.11	0.48
1:J:66:HIS:CE1	1:J:182:ASN:HB2	2.49	0.48
1:J:188:MET:HE3	1:J:329:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:66:HIS:CE1	1:F:182:ASN:HB2	2.48	0.48
1:C:320:HIS:HD2	3:C:361:HOH:O	1.97	0.48
1:A:243:VAL:CG2	1:D:82:THR:HG21	2.43	0.48
1:E:344:ASP:O	1:E:348:VAL:HG13	2.12	0.48
1:A:100:ARG:CG	1:D:321:GLN:NE2	2.77	0.48
1:D:17:VAL:HG13	1:D:88:ILE:HG21	1.95	0.48
1:C:44:LEU:HD22	1:C:222:THR:HG21	1.95	0.48
1:I:16:ALA:HB1	1:I:21:GLU:HA	1.95	0.48
1:I:94:MET:HE1	1:L:132:PRO:HG3	1.95	0.48
1:F:164:SER:HB3	1:F:178:LYS:HB3	1.95	0.48
1:F:321:GLN:NE2	1:K:100:ARG:HH11	2.09	0.48
1:C:17:VAL:HG13	1:C:88:ILE:HG21	1.96	0.48
1:E:105:THR:HG22	1:E:107:ASP:N	2.29	0.48
1:D:300:LEU:HD21	1:H:218:ARG:HB3	1.96	0.48
1:D:276:THR:HG23	1:D:342:LYS:HE3	1.96	0.48
1:L:265:LEU:HD13	1:L:308:THR:CG2	2.40	0.48
1:B:47:ILE:HD11	1:B:67:MET:SD	2.54	0.48
1:E:105:THR:HG21	1:E:107:ASP:OD1	2.14	0.48
1:L:100:ARG:CG	1:L:100:ARG:HH11	2.26	0.47
1:C:44:LEU:HB3	1:C:211:VAL:HG11	1.96	0.47
1:K:312:VAL:HG22	1:K:328:ASP:HB3	1.94	0.47
1:I:180:TRP:CE2	1:I:184:TYR:HB2	2.50	0.47
1:G:18:SER:O	1:G:20:HIS:HD2	1.97	0.47
1:K:273:LEU:HD11	1:K:308:THR:HG21	1.96	0.47
1:B:232:PHE:O	1:B:307:SER:HA	2.14	0.47
1:J:237:CYS:HB2	1:J:312:VAL:O	2.15	0.47
1:L:70:VAL:HG12	1:L:89:GLY:HA3	1.96	0.47
1:H:189:VAL:HG13	1:H:207:LEU:HD22	1.96	0.47
1:C:100:ARG:HH11	1:J:321:GLN:NE2	2.08	0.47
1:C:82:THR:HG21	1:J:243:VAL:CG2	2.43	0.47
1:I:317:ILE:HG23	1:I:318:HIS:CD2	2.49	0.47
1:F:182:ASN:ND2	1:F:185:GLY:H	2.13	0.47
1:I:5:PHE:CD2	1:I:168:LEU:HD13	2.49	0.47
1:E:94:MET:CE	1:H:94:MET:SD	3.02	0.47
1:L:185:GLY:HA2	1:L:235:VAL:HG12	1.96	0.47
1:A:17:VAL:HG13	1:A:88:ILE:HG21	1.96	0.47
1:A:183:ARG:HD3	1:A:186:VAL:HG21	1.97	0.47
1:K:84:ARG:NH2	1:K:138:VAL:HG22	2.29	0.47
1:F:226:LYS:HD3	1:F:227:PHE:CE2	2.49	0.47
1:L:181:ASP:HA	1:L:182:ASN:HA	1.57	0.47
1:L:234:ALA:O	1:L:309:THR:HA	2.14	0.47
1:A:300:LEU:HD21	1:C:218:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:33:THR:HB	1:A:34:PRO:HD3	1.95	0.47
1:C:188:MET:HE2	1:C:333:GLN:HE21	1.80	0.47
1:I:187:LEU:HD22	1:I:191:GLU:HG2	1.97	0.47
1:C:66:HIS:CE1	1:C:182:ASN:CB	2.97	0.47
1:A:164:SER:HB3	1:A:178:LYS:HB3	1.97	0.47
1:B:221:HIS:HA	1:B:301:LYS:HD2	1.97	0.47
1:C:70:VAL:HG12	1:C:89:GLY:HA3	1.97	0.46
1:B:180:TRP:CE2	1:B:184:TYR:HB2	2.50	0.46
1:L:100:ARG:HG3	1:L:100:ARG:NH1	2.31	0.46
1:E:114:ILE:HG21	1:H:321:GLN:HE21	1.80	0.46
1:L:181:ASP:HB2	1:L:237:CYS:SG	2.55	0.46
1:E:188:MET:CE	1:E:329:PHE:CE1	2.99	0.46
1:D:242:ASP:HB3	1:D:249:LYS:HA	1.97	0.46
1:C:22:ALA:HB3	1:C:23:PRO:HD3	1.97	0.46
1:I:218:ARG:HB3	1:J:300:LEU:HD21	1.97	0.46
1:H:242:ASP:HB3	1:H:249:LYS:HA	1.96	0.46
1:A:100:ARG:HG2	1:D:321:GLN:NE2	2.30	0.46
1:K:247:GLN:HE21	1:K:287:TYR:HA	1.81	0.46
1:B:218:ARG:HB3	1:C:300:LEU:CD2	2.46	0.46
1:J:181:ASP:HA	1:J:182:ASN:HA	1.74	0.46
1:E:29:ARG:NH2	3:E:379:HOH:O	2.49	0.46
1:L:192:LEU:HG	1:L:336:LEU:HD13	1.98	0.46
1:B:12:THR:HA	1:B:183:ARG:HG3	1.98	0.46
1:G:105:THR:HG23	3:G:357:HOH:O	2.15	0.46
1:C:105:THR:HB	1:C:109:HIS:HB2	1.98	0.46
1:K:257:ARG:NH1	1:K:260:ASP:HB3	2.30	0.46
1:E:132:PRO:HG3	1:H:94:MET:HE1	1.97	0.46
1:B:314:ALA:HB3	1:B:317:ILE:HD11	1.98	0.46
1:I:104:LEU:HB2	1:I:159:THR:HG23	1.96	0.46
1:E:11:VAL:HB	1:E:183:ARG:HB3	1.98	0.46
1:J:79:PRO:HA	1:J:146:LYS:HB2	1.97	0.46
1:G:314:ALA:HB3	1:G:317:ILE:CD1	2.45	0.45
1:C:234:ALA:O	1:C:309:THR:HA	2.16	0.45
1:C:66:HIS:HD2	1:C:68:ASP:OD1	1.98	0.45
1:F:44:LEU:HB3	1:F:211:VAL:HG11	1.97	0.45
1:G:164:SER:HB3	1:G:178:LYS:HB3	1.97	0.45
1:F:17:VAL:HG13	1:F:88:ILE:HG21	1.97	0.45
1:B:17:VAL:HG13	1:B:88:ILE:HG21	1.98	0.45
1:E:28:LEU:O	1:E:32:LEU:HB2	2.17	0.45
1:I:31:LYS:HD3	1:I:190:SER:OG	2.16	0.45
1:E:271:ASP:OD1	1:G:106:ARG:NH1	2.46	0.45
1:J:265:LEU:HD13	1:J:308:THR:HG23	1.96	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:265:LEU:HD13	1:C:308:THR:HG21	1.94	0.45
1:F:94:MET:CE	1:K:132:PRO:HG3	2.47	0.45
1:L:5:PHE:CD2	1:L:168:LEU:HD13	2.51	0.45
1:I:21:GLU:CD	1:I:211:VAL:HG23	2.37	0.45
1:B:243:VAL:HG22	1:G:82:THR:HG21	1.99	0.45
1:G:182:ASN:HD21	1:G:236:ASP:HA	1.81	0.45
1:D:265:LEU:HD13	1:D:308:THR:CG2	2.44	0.45
1:C:237:CYS:HB2	1:C:312:VAL:O	2.17	0.45
1:F:70:VAL:HG12	1:F:89:GLY:HA3	1.98	0.45
1:B:234:ALA:O	1:B:309:THR:HA	2.16	0.45
1:E:321:GLN:NE2	1:H:100:ARG:HH11	2.05	0.45
1:J:314:ALA:HB3	1:J:317:ILE:HD13	1.97	0.45
1:H:247:GLN:NE2	1:H:288:CYS:H	2.15	0.45
1:H:5:PHE:CD2	1:H:168:LEU:HD13	2.51	0.45
1:C:107:ASP:C	1:C:107:ASP:OD1	2.55	0.45
1:H:66:HIS:CE1	1:H:182:ASN:HB2	2.51	0.45
1:J:192:LEU:HG	1:J:336:LEU:HD13	1.98	0.45
1:D:221:HIS:HA	1:D:301:LYS:HD2	1.99	0.45
1:E:70:VAL:HG12	1:E:89:GLY:HA3	1.99	0.45
1:J:12:THR:HA	1:J:183:ARG:HG3	1.99	0.45
1:B:111:ILE:HD11	1:B:113:VAL:HG23	1.98	0.45
1:C:73:MET:HB2	1:C:88:ILE:CD1	2.40	0.44
1:K:336:LEU:O	1:K:340:VAL:HG13	2.16	0.44
1:C:82:THR:OG1	1:C:84:ARG:NH2	2.50	0.44
1:I:22:ALA:HB3	1:I:23:PRO:HD3	1.99	0.44
1:J:105:THR:HG22	1:J:107:ASP:N	2.29	0.44
1:I:238:SER:O	1:I:313:CYS:HA	2.17	0.44
1:C:215:VAL:HG23	1:C:218:ARG:HG3	1.99	0.44
1:G:51:LYS:NZ	1:G:199:GLN:O	2.50	0.44
1:J:104:LEU:HB2	1:J:159:THR:HG23	1.98	0.44
1:G:257:ARG:HD3	1:G:260:ASP:OD2	2.17	0.44
1:H:320:HIS:HD2	3:H:381:HOH:O	2.00	0.44
1:C:21:GLU:CG	1:C:211:VAL:HG23	2.47	0.44
1:B:94:MET:SD	1:G:94:MET:HE3	2.57	0.44
1:F:247:GLN:HE21	1:F:288:CYS:H	1.65	0.44
1:K:188:MET:CE	1:K:329:PHE:CE1	3.01	0.44
1:K:103:LEU:HB3	1:K:111:ILE:HG13	1.98	0.44
1:B:68:ASP:N	1:B:68:ASP:OD1	2.50	0.44
1:L:105:THR:HG22	1:L:106:ARG:N	2.32	0.44
1:G:182:ASN:ND2	1:G:236:ASP:HA	2.32	0.44
1:G:17:VAL:CG1	1:G:18:SER:N	2.80	0.44
1:C:92:ASN:O	1:C:95:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:241:GLY:O	1:I:242:ASP:C	2.56	0.44
1:A:114:ILE:HG21	1:D:321:GLN:HE21	1.83	0.44
1:K:308:THR:HB	1:K:309:THR:H	1.65	0.44
1:C:321:GLN:NE2	1:J:100:ARG:HH11	2.12	0.44
1:A:338:ALA:O	1:A:342:LYS:HB2	2.17	0.44
1:H:301:LYS:HA	1:H:301:LYS:HE2	1.99	0.44
1:K:221:HIS:HA	1:K:301:LYS:HD2	2.00	0.44
1:I:344:ASP:O	1:I:348:VAL:HG13	2.17	0.44
1:F:242:ASP:OD1	1:F:243:VAL:N	2.51	0.44
1:E:188:MET:HG2	1:E:235:VAL:HG11	2.00	0.44
1:H:100:ARG:HG3	1:H:100:ARG:NH1	2.33	0.43
1:J:100:ARG:HG2	1:J:114:ILE:HG22	2.00	0.43
1:K:16:ALA:HB1	1:K:21:GLU:HA	2.00	0.43
1:D:317:ILE:HG23	1:D:318:HIS:CD2	2.53	0.43
1:G:340:VAL:HA	1:G:343:LEU:HD12	2.00	0.43
1:B:181:ASP:HA	1:B:182:ASN:HA	1.76	0.43
1:H:300:LEU:HD21	1:L:218:ARG:HB3	1.99	0.43
1:H:41:THR:HA	1:H:46:GLY:O	2.18	0.43
1:B:321:GLN:HE22	1:G:100:ARG:HG3	1.83	0.43
1:I:182:ASN:HD21	1:I:236:ASP:HA	1.82	0.43
1:A:188:MET:HE3	1:A:329:PHE:CZ	2.53	0.43
1:I:196:LEU:HD21	1:I:340:VAL:HG21	2.00	0.43
1:E:111:ILE:HD13	1:E:143:PHE:CZ	2.53	0.43
1:I:247:GLN:NE2	1:I:288:CYS:H	2.16	0.43
1:G:41:THR:O	1:G:226:LYS:HE2	2.19	0.43
1:D:181:ASP:HA	1:D:182:ASN:HA	1.73	0.43
1:H:111:ILE:HA	1:H:112:PRO:HD3	1.89	0.43
1:G:181:ASP:HA	1:G:182:ASN:HA	1.69	0.43
1:I:28:LEU:O	1:I:32:LEU:HB2	2.17	0.43
1:H:70:VAL:HG12	1:H:89:GLY:HA3	2.00	0.43
1:K:314:ALA:HB3	1:K:317:ILE:CD1	2.49	0.43
1:C:308:THR:HB	1:C:309:THR:H	1.69	0.43
1:H:188:MET:HE3	1:H:329:PHE:CE1	2.54	0.43
1:J:188:MET:HG2	1:J:235:VAL:HG11	2.01	0.43
1:K:181:ASP:HA	1:K:182:ASN:HA	1.75	0.43
1:F:310:ILE:HA	3:F:360:HOH:O	2.17	0.43
1:D:25:ARG:HG3	1:D:47:ILE:HG12	2.01	0.43
1:I:188:MET:HE1	1:I:329:PHE:CD1	2.54	0.43
1:I:69:GLU:OE1	1:I:178:LYS:HE2	2.19	0.43
1:C:238:SER:OG	1:C:257:ARG:NH2	2.51	0.43
1:K:22:ALA:HB3	1:K:23:PRO:HD3	2.01	0.43
1:E:317:ILE:HG23	1:E:318:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:200:LYS:HE2	1:F:200:LYS:HB3	1.81	0.43
1:C:211:VAL:HG22	1:C:212:GLN:HG3	2.00	0.43
1:E:111:ILE:HG12	1:E:154:ILE:HD11	2.01	0.43
1:L:312:VAL:HG22	1:L:328:ASP:HB3	2.00	0.43
1:H:180:TRP:CE2	1:H:184:TYR:HB2	2.54	0.43
1:E:242:ASP:OD1	1:E:243:VAL:N	2.52	0.43
1:J:189:VAL:HG13	1:J:207:LEU:HD22	2.00	0.43
1:L:111:ILE:HA	1:L:112:PRO:HD3	1.86	0.42
1:G:70:VAL:HG12	1:G:89:GLY:HA3	2.01	0.42
1:A:157:GLY:HA2	1:B:258:PHE:CD1	2.54	0.42
1:A:237:CYS:HB2	1:A:312:VAL:O	2.19	0.42
1:D:92:ASN:O	1:D:95:VAL:HG22	2.19	0.42
1:J:234:ALA:O	1:J:309:THR:HA	2.18	0.42
1:A:70:VAL:HG12	1:A:89:GLY:HA3	2.01	0.42
1:J:105:THR:HG22	1:J:106:ARG:N	2.35	0.42
1:I:181:ASP:HA	1:I:182:ASN:HA	1.72	0.42
1:K:342:LYS:HE2	1:K:342:LYS:HB2	1.61	0.42
1:K:196:LEU:HD21	1:K:340:VAL:HG21	2.00	0.42
1:F:94:MET:SD	1:K:94:MET:SD	3.17	0.42
1:H:28:LEU:HD23	1:H:28:LEU:HA	1.85	0.42
1:E:66:HIS:CE1	1:E:182:ASN:HB2	2.54	0.42
1:B:94:MET:CE	1:G:132:PRO:HG3	2.49	0.42
1:G:242:ASP:HB3	1:G:249:LYS:HA	2.01	0.42
1:J:182:ASN:ND2	1:J:185:GLY:H	2.17	0.42
1:J:134:ILE:HA	1:J:137:ILE:HD12	2.01	0.42
1:I:36:VAL:HG11	1:I:49:GLY:CA	2.49	0.42
1:B:182:ASN:ND2	1:B:185:GLY:H	2.18	0.42
1:E:182:ASN:ND2	1:E:185:GLY:H	2.17	0.42
1:C:111:ILE:HG12	1:C:154:ILE:HD11	2.00	0.42
1:G:100:ARG:HA	1:G:114:ILE:HG22	2.02	0.42
1:L:340:VAL:HA	1:L:343:LEU:HD12	2.02	0.42
1:L:28:LEU:O	1:L:32:LEU:HB2	2.20	0.42
1:E:314:ALA:HB3	1:E:317:ILE:HD11	2.01	0.42
1:B:44:LEU:HD22	1:B:222:THR:HG21	2.01	0.42
1:J:182:ASN:ND2	1:J:236:ASP:HA	2.34	0.42
1:B:103:LEU:HB3	1:B:111:ILE:HG13	2.00	0.42
1:E:20:HIS:CG	1:E:159:THR:HG21	2.55	0.42
1:A:188:MET:HE2	1:A:333:GLN:CA	2.50	0.42
1:I:187:LEU:HD13	1:I:329:PHE:CZ	2.55	0.42
1:C:232:PHE:CE1	1:C:234:ALA:HB2	2.54	0.42
1:G:301:LYS:HA	1:G:301:LYS:HE2	2.02	0.42
1:K:21:GLU:CD	1:K:211:VAL:HG22	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:218:ARG:HD2	1:J:300:LEU:HD21	2.02	0.42
1:K:196:LEU:HD21	1:K:340:VAL:CG2	2.50	0.42
1:C:243:VAL:HG21	1:J:138:VAL:HG11	2.02	0.42
1:C:242:ASP:OD1	1:C:243:VAL:N	2.53	0.42
1:H:64:ALA:HA	1:H:208:GLY:O	2.20	0.42
1:C:47:ILE:HD11	1:C:67:MET:SD	2.60	0.41
1:H:105:THR:HG23	1:H:153:GLY:O	2.20	0.41
1:K:188:MET:HG2	1:K:235:VAL:HG11	2.01	0.41
1:L:111:ILE:HD13	1:L:143:PHE:CZ	2.55	0.41
1:E:300:LEU:HD21	1:G:218:ARG:HD2	2.03	0.41
1:G:103:LEU:HB3	1:G:111:ILE:HG13	2.01	0.41
1:D:258:PHE:CD1	1:H:157:GLY:HA2	2.55	0.41
1:G:232:PHE:O	1:G:307:SER:HA	2.20	0.41
1:E:66:HIS:HD2	1:E:68:ASP:OD1	2.03	0.41
1:B:188:MET:HE2	1:B:333:GLN:HE21	1.86	0.41
1:L:215:VAL:HG23	1:L:218:ARG:HG3	2.02	0.41
1:E:300:LEU:HD21	1:G:218:ARG:HB3	2.02	0.41
1:D:188:MET:HE3	1:D:329:PHE:CE1	2.56	0.41
1:L:200:LYS:HE2	1:L:200:LYS:HB3	1.81	0.41
1:D:187:LEU:HD22	1:D:191:GLU:HG2	2.03	0.41
1:K:29:ARG:NH2	3:K:392:HOH:O	2.52	0.41
1:G:66:HIS:CE1	1:G:182:ASN:CB	3.02	0.41
1:L:247:GLN:NE2	3:L:523:HOH:O	2.44	0.41
1:I:180:TRP:HA	1:I:180:TRP:CE3	2.55	0.41
1:K:257:ARG:HH11	1:K:260:ASP:HB3	1.85	0.41
1:L:111:ILE:HG12	1:L:154:ILE:HD11	2.02	0.41
1:E:234:ALA:O	1:E:309:THR:HA	2.20	0.41
1:K:28:LEU:O	1:K:32:LEU:HB2	2.20	0.41
1:L:162:PRO:O	1:L:178:LYS:HE3	2.20	0.41
1:B:94:MET:HE1	1:G:94:MET:SD	2.61	0.41
1:G:187:LEU:HD22	1:G:191:GLU:HG2	2.02	0.41
1:I:300:LEU:HD21	1:K:218:ARG:HB3	2.02	0.41
1:I:97:SER:HB3	1:L:95:VAL:HG12	2.01	0.41
1:H:100:ARG:O	1:H:320:HIS:HE1	2.04	0.41
1:L:188:MET:HE2	1:L:333:GLN:HE21	1.85	0.41
1:B:343:LEU:HD22	1:B:348:VAL:HG12	2.03	0.41
1:E:238:SER:OG	1:E:257:ARG:NH2	2.53	0.41
1:D:100:ARG:O	1:D:320:HIS:HE1	2.03	0.41
1:F:321:GLN:NE2	1:K:100:ARG:NH1	2.49	0.41
1:K:100:ARG:CG	1:K:100:ARG:NH1	2.71	0.41
1:J:44:LEU:HB3	1:J:211:VAL:HG11	2.03	0.41
1:C:181:ASP:HA	1:C:182:ASN:HA	1.72	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:333:GLN:HA	1:H:333:GLN:NE2	2.36	0.41
1:E:105:THR:CG2	1:E:107:ASP:OD1	2.69	0.41
1:B:196:LEU:HD21	1:B:340:VAL:CG2	2.50	0.41
1:H:221:HIS:HA	1:H:301:LYS:HD2	2.02	0.41
1:F:111:ILE:HG12	1:F:154:ILE:HD11	2.02	0.41
1:F:111:ILE:HA	1:F:112:PRO:HD3	2.01	0.41
1:A:111:ILE:HA	1:A:112:PRO:HD3	1.93	0.41
1:J:31:LYS:HD3	1:J:190:SER:OG	2.20	0.41
1:C:188:MET:HG2	1:C:235:VAL:HG11	2.02	0.41
1:I:157:GLY:HA2	1:J:258:PHE:CD1	2.55	0.41
1:G:104:LEU:HB2	1:G:159:THR:HG23	2.02	0.41
1:D:41:THR:HA	1:D:46:GLY:O	2.20	0.41
1:D:73:MET:HB2	1:D:88:ILE:HD12	1.97	0.40
1:A:258:PHE:CZ	1:A:288:CYS:HB2	2.56	0.40
1:E:181:ASP:HA	1:E:182:ASN:HA	1.76	0.40
1:J:232:PHE:O	1:J:307:SER:HA	2.21	0.40
1:B:321:GLN:NE2	1:G:100:ARG:HG3	2.37	0.40
1:B:258:PHE:CZ	1:B:288:CYS:HB2	2.57	0.40
1:A:312:VAL:HG22	1:A:328:ASP:HB3	2.03	0.40
1:K:109:HIS:CD2	3:K:391:HOH:O	2.74	0.40
1:G:188:MET:HE2	1:G:329:PHE:CZ	2.56	0.40
1:G:257:ARG:HH11	1:G:260:ASP:HB3	1.86	0.40
1:F:181:ASP:HA	1:F:182:ASN:HA	1.71	0.40
1:J:205:LEU:HD21	1:J:207:LEU:HG	2.03	0.40
1:E:51:LYS:NZ	1:E:199:GLN:O	2.54	0.40
1:C:188:MET:CE	1:C:333:GLN:HE21	2.33	0.40
1:J:192:LEU:HD22	1:J:196:LEU:HD22	2.03	0.40
1:A:7:LYS:HB3	1:A:187:LEU:HD21	2.03	0.40
1:C:182:ASN:ND2	1:C:185:GLY:H	2.19	0.40
1:J:301:LYS:HA	1:J:301:LYS:HE2	2.03	0.40
1:I:183:ARG:HD3	1:I:183:ARG:HA	1.86	0.40
1:I:188:MET:HG2	1:I:235:VAL:CG1	2.51	0.40
1:L:211:VAL:HG12	3:L:384:HOH:O	2.20	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	336/355 (95%)	324 (96%)	12 (4%)	0	100	100
1	B	333/355 (94%)	323 (97%)	9 (3%)	1 (0%)	50	82
1	C	333/355 (94%)	321 (96%)	12 (4%)	0	100	100
1	D	336/355 (95%)	328 (98%)	8 (2%)	0	100	100
1	E	336/355 (95%)	321 (96%)	15 (4%)	0	100	100
1	F	333/355 (94%)	322 (97%)	11 (3%)	0	100	100
1	G	333/355 (94%)	324 (97%)	9 (3%)	0	100	100
1	H	333/355 (94%)	324 (97%)	9 (3%)	0	100	100
1	I	333/355 (94%)	320 (96%)	11 (3%)	2 (1%)	33	66
1	J	333/355 (94%)	322 (97%)	11 (3%)	0	100	100
1	K	336/355 (95%)	328 (98%)	8 (2%)	0	100	100
1	L	333/355 (94%)	320 (96%)	10 (3%)	3 (1%)	25	55
All	All	4008/4260 (94%)	3877 (97%)	125 (3%)	6 (0%)	59	89

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	97	SER
1	L	199	GLN
1	B	56	VAL
1	I	197	SER
1	L	198	GLY
1	L	56	VAL

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	273/285 (96%)	247 (90%)	26 (10%)	12	28
1	B	270/285 (95%)	241 (89%)	29 (11%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	270/285 (95%)	243 (90%)	27 (10%)	11	25
1	D	273/285 (96%)	240 (88%)	33 (12%)	7	17
1	E	273/285 (96%)	243 (89%)	30 (11%)	9	21
1	F	270/285 (95%)	240 (89%)	30 (11%)	9	20
1	G	270/285 (95%)	235 (87%)	35 (13%)	6	15
1	H	270/285 (95%)	240 (89%)	30 (11%)	9	20
1	I	270/285 (95%)	243 (90%)	27 (10%)	11	25
1	J	270/285 (95%)	244 (90%)	26 (10%)	12	27
1	K	273/285 (96%)	243 (89%)	30 (11%)	9	21
1	L	270/285 (95%)	248 (92%)	22 (8%)	17	36
All	All	3252/3420 (95%)	2907 (89%)	345 (11%)	10	22

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	30	GLU
1	A	41	THR
1	A	44	LEU
1	A	47	ILE
1	A	86	VAL
1	A	111	ILE
1	A	159	THR
1	A	168	LEU
1	A	187	LEU
1	A	188	MET
1	A	192	LEU
1	A	207	LEU
1	A	211	VAL
1	A	218	ARG
1	A	231	VAL
1	A	237	CYS
1	A	243	VAL
1	A	308	THR
1	A	312	VAL
1	A	316	TYR
1	A	317	ILE
1	A	327	ASP

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Mol	Chain	Res	Type
1	A	336	LEU
1	A	342	LYS
1	A	350	LEU
1	B	3	THR
1	B	4	LEU
1	B	17	VAL
1	B	32	LEU
1	B	41	THR
1	B	44	LEU
1	B	47	ILE
1	B	86	VAL
1	B	100	ARG
1	B	104	LEU
1	B	105	THR
1	B	111	ILE
1	B	168	LEU
1	B	187	LEU
1	B	188	MET
1	B	192	LEU
1	B	207	LEU
1	B	218	ARG
1	B	233	LEU
1	B	237	CYS
1	B	243	VAL
1	B	250	ILE
1	B	290	LYS
1	B	308	THR
1	B	316	TYR
1	B	317	ILE
1	B	336	LEU
1	B	342	LYS
1	B	350	LEU
1	C	4	LEU
1	C	17	VAL
1	C	32	LEU
1	C	41	THR
1	C	44	LEU
1	C	47	ILE
1	C	56	VAL
1	C	86	VAL
1	C	100	ARG
1	C	105	THR

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Mol	Chain	Res	Type
1	C	107	ASP
1	C	111	ILE
1	C	159	THR
1	C	168	LEU
1	C	187	LEU
1	C	188	MET
1	C	192	LEU
1	C	207	LEU
1	C	218	ARG
1	C	231	VAL
1	C	237	CYS
1	C	308	THR
1	C	316	TYR
1	C	317	ILE
1	C	336	LEU
1	C	342	LYS
1	C	350	LEU
1	D	2	THR
1	D	3	THR
1	D	4	LEU
1	D	30	GLU
1	D	31	LYS
1	D	32	LEU
1	D	41	THR
1	D	44	LEU
1	D	47	ILE
1	D	100	ARG
1	D	111	ILE
1	D	159	THR
1	D	178	LYS
1	D	184	TYR
1	D	187	LEU
1	D	188	MET
1	D	192	LEU
1	D	196	LEU
1	D	199	GLN
1	D	207	LEU
1	D	218	ARG
1	D	233	LEU
1	D	237	CYS
1	D	250	ILE
1	D	308	THR

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Mol	Chain	Res	Type
1	D	312	VAL
1	D	316	TYR
1	D	317	ILE
1	D	327	ASP
1	D	336	LEU
1	D	342	LYS
1	D	348	VAL
1	D	350	LEU
1	E	2	THR
1	E	3	THR
1	E	4	LEU
1	E	30	GLU
1	E	31	LYS
1	E	32	LEU
1	E	36	VAL
1	E	41	THR
1	E	44	LEU
1	E	47	ILE
1	E	86	VAL
1	E	100	ARG
1	E	111	ILE
1	E	159	THR
1	E	168	LEU
1	E	184	TYR
1	E	187	LEU
1	E	188	MET
1	E	192	LEU
1	E	207	LEU
1	E	237	CYS
1	E	243	VAL
1	E	250	ILE
1	E	308	THR
1	E	317	ILE
1	E	327	ASP
1	E	336	LEU
1	E	342	LYS
1	E	348	VAL
1	E	350	LEU
1	F	3	THR
1	F	4	LEU
1	F	32	LEU
1	F	36	VAL

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Mol	Chain	Res	Type
1	F	41	THR
1	F	44	LEU
1	F	47	ILE
1	F	86	VAL
1	F	100	ARG
1	F	105	THR
1	F	111	ILE
1	F	159	THR
1	F	168	LEU
1	F	178	LYS
1	F	187	LEU
1	F	188	MET
1	F	192	LEU
1	F	199	GLN
1	F	207	LEU
1	F	211	VAL
1	F	218	ARG
1	F	233	LEU
1	F	237	CYS
1	F	243	VAL
1	F	250	ILE
1	F	290	LYS
1	F	308	THR
1	F	317	ILE
1	F	336	LEU
1	F	350	LEU
1	G	4	LEU
1	G	30	GLU
1	G	32	LEU
1	G	36	VAL
1	G	41	THR
1	G	44	LEU
1	G	47	ILE
1	G	56	VAL
1	G	100	ARG
1	G	105	THR
1	G	111	ILE
1	G	159	THR
1	G	168	LEU
1	G	173	LYS
1	G	178	LYS
1	G	187	LEU

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Mol	Chain	Res	Type
1	G	188	MET
1	G	192	LEU
1	G	199	GLN
1	G	207	LEU
1	G	211	VAL
1	G	217	LEU
1	G	218	ARG
1	G	231	VAL
1	G	233	LEU
1	G	237	CYS
1	G	243	VAL
1	G	308	THR
1	G	312	VAL
1	G	316	TYR
1	G	317	ILE
1	G	336	LEU
1	G	342	LYS
1	G	348	VAL
1	G	350	LEU
1	H	4	LEU
1	H	6	SER
1	H	30	GLU
1	H	32	LEU
1	H	36	VAL
1	H	41	THR
1	H	47	ILE
1	H	100	ARG
1	H	104	LEU
1	H	111	ILE
1	H	159	THR
1	H	168	LEU
1	H	187	LEU
1	H	188	MET
1	H	192	LEU
1	H	196	LEU
1	H	200	LYS
1	H	207	LEU
1	H	211	VAL
1	H	218	ARG
1	H	243	VAL
1	H	290	LYS
1	H	308	THR

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Mol	Chain	Res	Type
1	H	312	VAL
1	H	316	TYR
1	H	317	ILE
1	H	327	ASP
1	H	336	LEU
1	H	348	VAL
1	H	350	LEU
1	I	4	LEU
1	I	30	GLU
1	I	32	LEU
1	I	36	VAL
1	I	41	THR
1	I	44	LEU
1	I	47	ILE
1	I	100	ARG
1	I	105	THR
1	I	111	ILE
1	I	159	THR
1	I	168	LEU
1	I	187	LEU
1	I	188	MET
1	I	192	LEU
1	I	207	LEU
1	I	218	ARG
1	I	231	VAL
1	I	233	LEU
1	I	243	VAL
1	I	290	LYS
1	I	308	THR
1	I	316	TYR
1	I	317	ILE
1	I	336	LEU
1	I	342	LYS
1	I	348	VAL
1	J	3	THR
1	J	4	LEU
1	J	17	VAL
1	J	32	LEU
1	J	44	LEU
1	J	47	ILE
1	J	86	VAL
1	J	104	LEU

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Mol	Chain	Res	Type
1	J	111	ILE
1	J	159	THR
1	J	168	LEU
1	J	178	LYS
1	J	187	LEU
1	J	188	MET
1	J	192	LEU
1	J	197	SER
1	J	207	LEU
1	J	211	VAL
1	J	218	ARG
1	J	231	VAL
1	J	243	VAL
1	J	316	TYR
1	J	317	ILE
1	J	336	LEU
1	J	348	VAL
1	J	350	LEU
1	K	3	THR
1	K	30	GLU
1	K	31	LYS
1	K	32	LEU
1	K	36	VAL
1	K	44	LEU
1	K	47	ILE
1	K	100	ARG
1	K	105	THR
1	K	111	ILE
1	K	159	THR
1	K	173	LYS
1	K	178	LYS
1	K	187	LEU
1	K	188	MET
1	K	192	LEU
1	K	207	LEU
1	K	211	VAL
1	K	233	LEU
1	K	237	CYS
1	K	243	VAL
1	K	250	ILE
1	K	312	VAL
1	K	316	TYR

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Mol	Chain	Res	Type
1	K	317	ILE
1	K	327	ASP
1	K	336	LEU
1	K	340	VAL
1	K	342	LYS
1	K	350	LEU
1	L	3	THR
1	L	4	LEU
1	L	32	LEU
1	L	47	ILE
1	L	100	ARG
1	L	111	ILE
1	L	168	LEU
1	L	178	LYS
1	L	187	LEU
1	L	188	MET
1	L	192	LEU
1	L	196	LEU
1	L	218	ARG
1	L	237	CYS
1	L	243	VAL
1	L	308	THR
1	L	316	TYR
1	L	327	ASP
1	L	336	LEU
1	L	340	VAL
1	L	346	SER
1	L	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	66	HIS
1	A	182	ASN
1	A	247	GLN
1	A	320	HIS
1	A	321	GLN
1	A	333	GLN
1	A	337	GLN
1	B	20	HIS
1	B	66	HIS

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Mol	Chain	Res	Type
1	B	182	ASN
1	B	199	GLN
1	B	247	GLN
1	B	302	ASN
1	B	320	HIS
1	B	321	GLN
1	B	333	GLN
1	B	337	GLN
1	C	66	HIS
1	C	109	HIS
1	C	182	ASN
1	C	247	GLN
1	C	320	HIS
1	C	321	GLN
1	C	333	GLN
1	C	337	GLN
1	D	20	HIS
1	D	66	HIS
1	D	109	HIS
1	D	182	ASN
1	D	199	GLN
1	D	247	GLN
1	D	302	ASN
1	D	320	HIS
1	D	321	GLN
1	D	333	GLN
1	D	337	GLN
1	E	20	HIS
1	E	66	HIS
1	E	109	HIS
1	E	182	ASN
1	E	247	GLN
1	E	320	HIS
1	E	321	GLN
1	F	66	HIS
1	F	182	ASN
1	F	199	GLN
1	F	247	GLN
1	F	263	HIS
1	F	320	HIS
1	F	321	GLN
1	F	333	GLN

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Mol	Chain	Res	Type
1	F	337	GLN
1	G	20	HIS
1	G	66	HIS
1	G	182	ASN
1	G	199	GLN
1	G	247	GLN
1	G	302	ASN
1	G	320	HIS
1	G	321	GLN
1	G	333	GLN
1	G	337	GLN
1	H	20	HIS
1	H	66	HIS
1	H	182	ASN
1	H	247	GLN
1	H	320	HIS
1	H	321	GLN
1	H	333	GLN
1	H	337	GLN
1	I	20	HIS
1	I	66	HIS
1	I	182	ASN
1	I	199	GLN
1	I	247	GLN
1	I	302	ASN
1	I	320	HIS
1	I	321	GLN
1	I	333	GLN
1	I	337	GLN
1	J	20	HIS
1	J	66	HIS
1	J	182	ASN
1	J	199	GLN
1	J	247	GLN
1	J	320	HIS
1	J	321	GLN
1	J	333	GLN
1	J	337	GLN
1	K	20	HIS
1	K	109	HIS
1	K	182	ASN
1	K	247	GLN

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Mol	Chain	Res	Type
1	K	320	HIS
1	K	321	GLN
1	K	333	GLN
1	K	337	GLN
1	L	66	HIS
1	L	182	ASN
1	L	247	GLN
1	L	302	ASN
1	L	320	HIS
1	L	321	GLN
1	L	333	GLN
1	L	337	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/355 (95%)	-0.36	1 (0%) 91 95	20, 27, 37, 44	0
1	B	337/355 (94%)	-0.35	2 (0%) 86 90	20, 26, 35, 39	0
1	C	337/355 (94%)	-0.36	1 (0%) 91 95	20, 27, 37, 42	0
1	D	340/355 (95%)	-0.28	1 (0%) 91 95	21, 27, 36, 44	0
1	E	340/355 (95%)	-0.33	1 (0%) 91 95	19, 27, 36, 47	0
1	F	337/355 (94%)	-0.34	1 (0%) 91 95	21, 27, 36, 42	0
1	G	337/355 (94%)	-0.39	2 (0%) 86 90	21, 26, 34, 39	0
1	H	337/355 (94%)	-0.28	1 (0%) 91 95	22, 29, 38, 45	0
1	I	337/355 (94%)	-0.34	1 (0%) 91 95	22, 28, 36, 42	0
1	J	337/355 (94%)	-0.31	2 (0%) 86 90	20, 27, 36, 44	0
1	K	340/355 (95%)	-0.40	1 (0%) 91 95	20, 26, 35, 41	0
1	L	337/355 (94%)	-0.16	4 (1%) 75 81	23, 30, 39, 46	0
All	All	4056/4260 (95%)	-0.32	18 (0%) 90 93	19, 27, 37, 47	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	56	VAL	3.6
1	E	1	MET	3.2
1	D	56	VAL	3.2
1	L	57	ASP	3.1
1	I	94	MET	3.1
1	J	56	VAL	3.1
1	K	56	VAL	2.6
1	J	79	PRO	2.3
1	G	132	PRO	2.3
1	H	245	GLY	2.3
1	L	132	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	133	ALA	2.2
1	C	133	ALA	2.1
1	F	55	ALA	2.0
1	B	56	VAL	2.0
1	B	132	PRO	2.0
1	G	133	ALA	2.0
1	A	56	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	D	356	1/1	0.10	-1.66	73,73,73,73	0
2	ZN	G	355	1/1	0.09	-2.03	81,81,81,81	0
2	ZN	K	355	1/1	0.09	-2.45	69,69,69,69	0
2	ZN	F	355	1/1	0.07	-2.96	73,73,73,73	0
2	ZN	L	356	1/1	0.06	-3.10	74,74,74,74	0
2	ZN	A	355	1/1	0.06	-3.30	63,63,63,63	0
2	ZN	K	356	1/1	0.08	-3.37	65,65,65,65	0
2	ZN	B	355	1/1	0.07	-3.44	77,77,77,77	0
2	ZN	H	355	1/1	0.07	-3.49	78,78,78,78	0
2	ZN	I	356	1/1	0.06	-3.69	69,69,69,69	0
2	ZN	I	355	1/1	0.05	-3.83	63,63,63,63	0
2	ZN	D	355	1/1	0.06	-3.87	61,61,61,61	0
2	ZN	J	356	1/1	0.07	-3.98	68,68,68,68	0
2	ZN	C	356	1/1	0.06	-4.05	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	J	355	1/1	0.05	-4.24	67,67,67,67	0
2	ZN	E	355	1/1	0.06	-4.38	63,63,63,63	0
2	ZN	H	356	1/1	0.04	-5.04	70,70,70,70	0
2	ZN	G	356	1/1	0.05	-5.15	65,65,65,65	0
2	ZN	F	356	1/1	0.04	-5.31	63,63,63,63	0
2	ZN	C	355	1/1	0.05	-5.50	65,65,65,65	0
2	ZN	L	355	1/1	0.04	-5.77	73,73,73,73	0
2	ZN	B	356	1/1	0.04	-6.20	57,57,57,57	0
2	ZN	E	356	1/1	0.07	-7.01	75,75,75,75	0
2	ZN	A	356	1/1	0.03	-10.90	64,64,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.