



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2025 – 10:12 AM JST

PDB ID : 8ZH7 / pdb\_00008zh7  
Title : Crystal structure of N-terminal domain of N-methyl-D-aspartate receptor subunit NR1 in complex with patient-derived antibody  
Authors : Nomura, N.; Kumazaki, K.; Amano, Y.  
Deposited on : 2024-05-10  
Resolution : 3.50 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.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

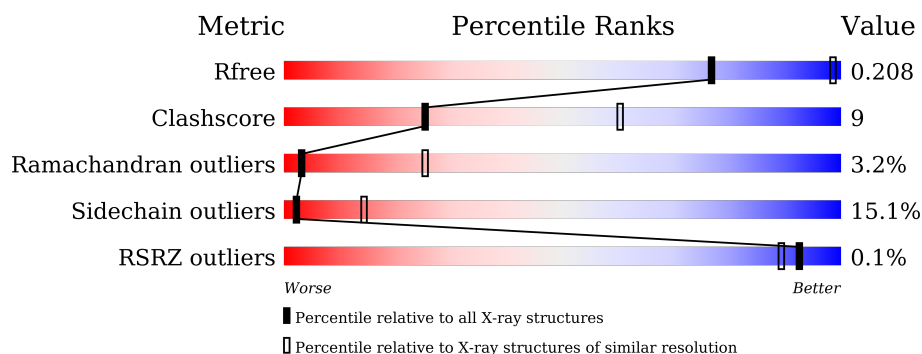
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	
1	D	384	
1	G	384	
1	J	384	
2	B	250	
2	E	250	

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Mol	Chain	Length	Quality of chain
2	H	250	<p>60% 24% • 14%</p>
2	K	250	<p>63% 21% • 14%</p>
3	C	236	<p>55% 31% • • 10%</p>
3	F	236	<p>61% 25% 5% 10%</p>
3	I	236	<p>64% 24% • 10%</p>
3	L	236	<p>69% 20% • 10%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24484 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			
1	D	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			
1	G	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			
1	J	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	394	VAL	-	expression tag	UNP Q05586
A	395	ASP	-	expression tag	UNP Q05586
A	396	GLY	-	expression tag	UNP Q05586
A	397	GLY	-	expression tag	UNP Q05586
A	398	GLY	-	expression tag	UNP Q05586
A	399	GLY	-	expression tag	UNP Q05586
A	400	GLY	-	expression tag	UNP Q05586
A	401	LEU	-	expression tag	UNP Q05586
A	402	VAL	-	expression tag	UNP Q05586
A	403	PRO	-	expression tag	UNP Q05586
A	404	ARG	-	expression tag	UNP Q05586
D	394	VAL	-	expression tag	UNP Q05586
D	395	ASP	-	expression tag	UNP Q05586
D	396	GLY	-	expression tag	UNP Q05586
D	397	GLY	-	expression tag	UNP Q05586
D	398	GLY	-	expression tag	UNP Q05586
D	399	GLY	-	expression tag	UNP Q05586
D	400	GLY	-	expression tag	UNP Q05586
D	401	LEU	-	expression tag	UNP Q05586
D	402	VAL	-	expression tag	UNP Q05586
D	403	PRO	-	expression tag	UNP Q05586

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Chain	Residue	Modelled	Actual	Comment	Reference
D	404	ARG	-	expression tag	UNP Q05586
G	394	VAL	-	expression tag	UNP Q05586
G	395	ASP	-	expression tag	UNP Q05586
G	396	GLY	-	expression tag	UNP Q05586
G	397	GLY	-	expression tag	UNP Q05586
G	398	GLY	-	expression tag	UNP Q05586
G	399	GLY	-	expression tag	UNP Q05586
G	400	GLY	-	expression tag	UNP Q05586
G	401	LEU	-	expression tag	UNP Q05586
G	402	VAL	-	expression tag	UNP Q05586
G	403	PRO	-	expression tag	UNP Q05586
G	404	ARG	-	expression tag	UNP Q05586
J	394	VAL	-	expression tag	UNP Q05586
J	395	ASP	-	expression tag	UNP Q05586
J	396	GLY	-	expression tag	UNP Q05586
J	397	GLY	-	expression tag	UNP Q05586
J	398	GLY	-	expression tag	UNP Q05586
J	399	GLY	-	expression tag	UNP Q05586
J	400	GLY	-	expression tag	UNP Q05586
J	401	LEU	-	expression tag	UNP Q05586
J	402	VAL	-	expression tag	UNP Q05586
J	403	PRO	-	expression tag	UNP Q05586
J	404	ARG	-	expression tag	UNP Q05586

- Molecule 2 is a protein called Antibody #003-102 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			
2	E	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			
2	H	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			
2	K	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			

- Molecule 3 is a protein called Antibody #003-102 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			

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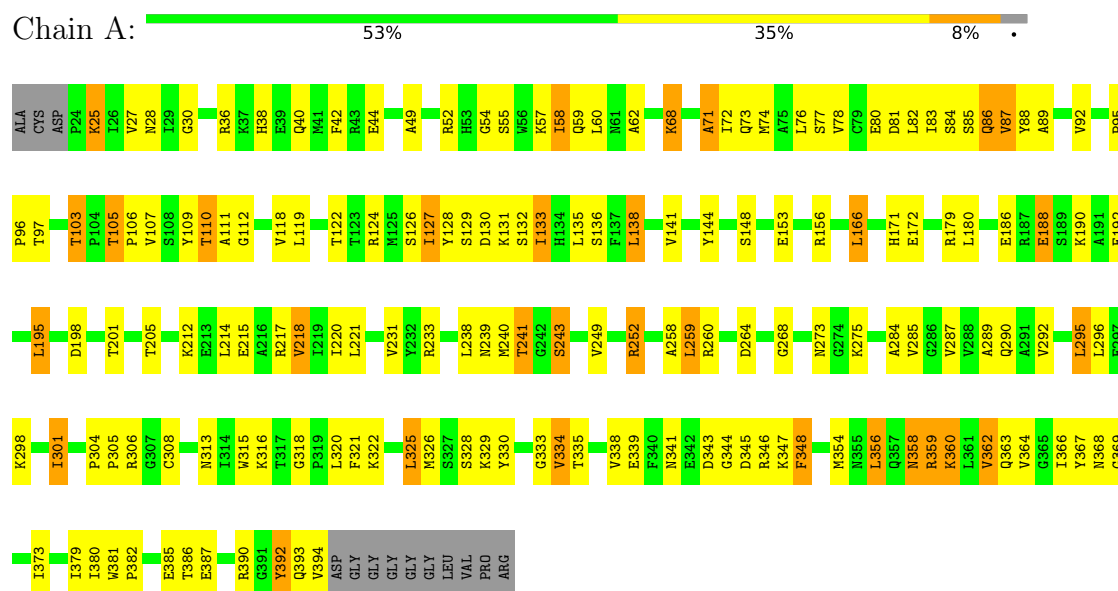
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			
3	I	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			
3	L	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			

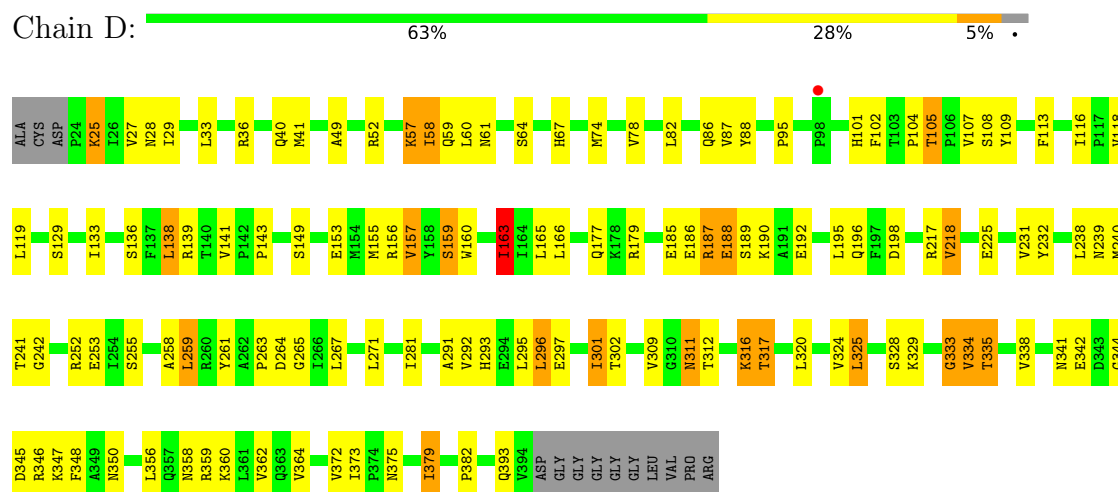
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor ionotropic, NMDA 1



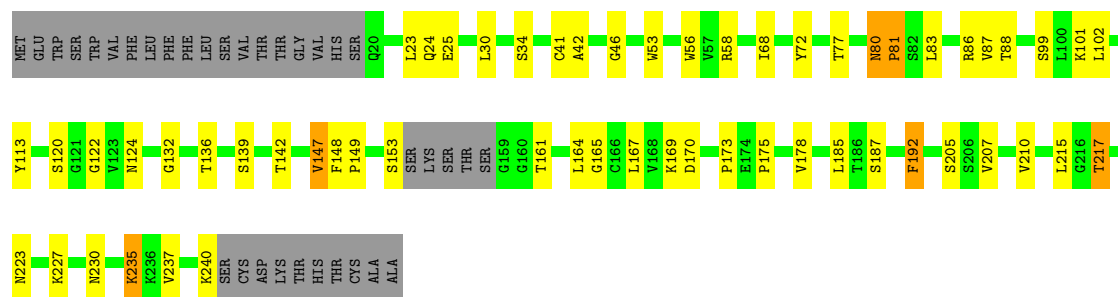
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



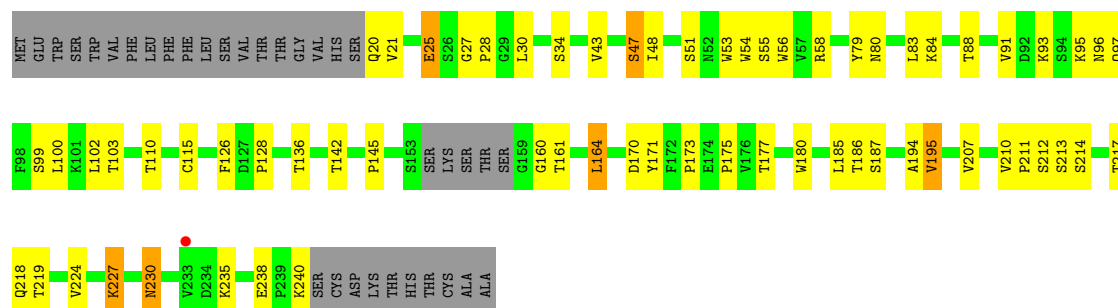
- Molecule 1: Glutamate receptor ionotropic, NMDA 1



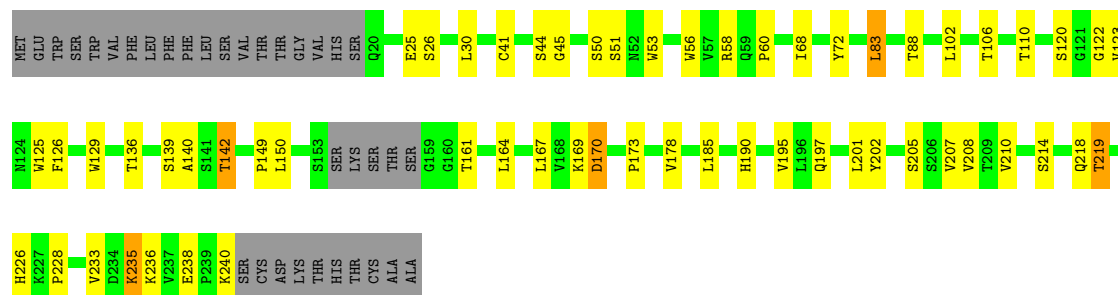




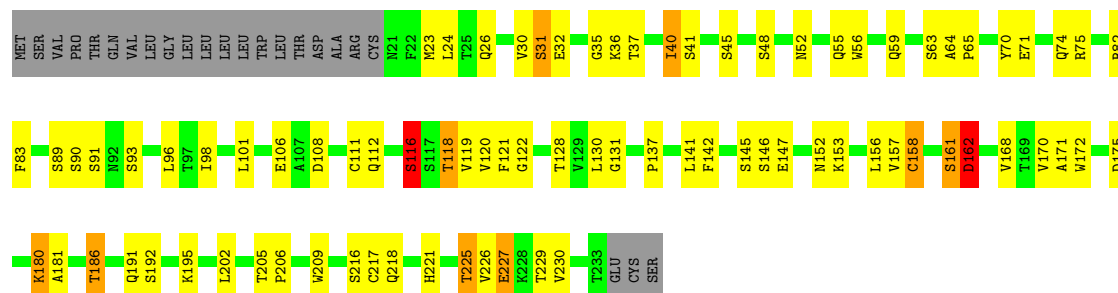
• Molecule 2: Antibody #003-102 heavy chain



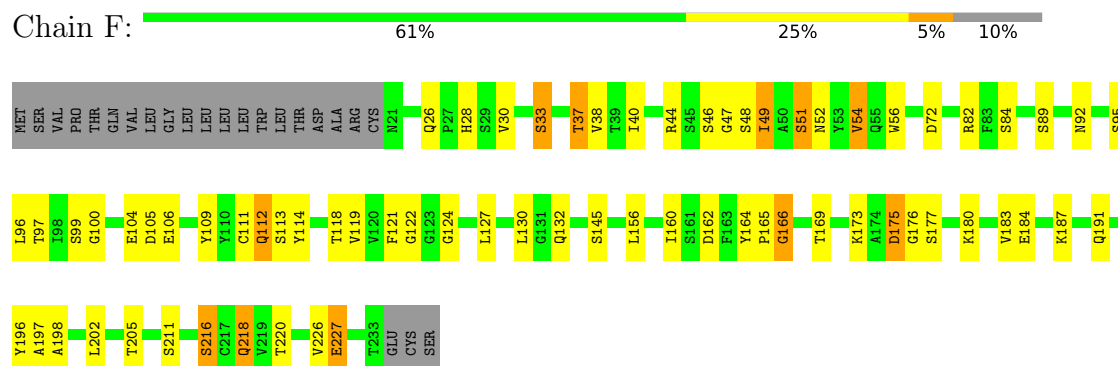
• Molecule 2: Antibody #003-102 heavy chain



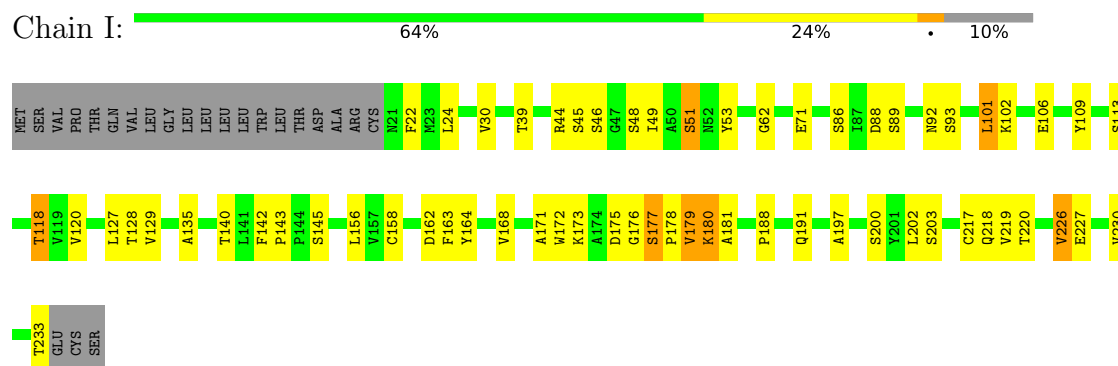
• Molecule 3: Antibody #003-102 light chain



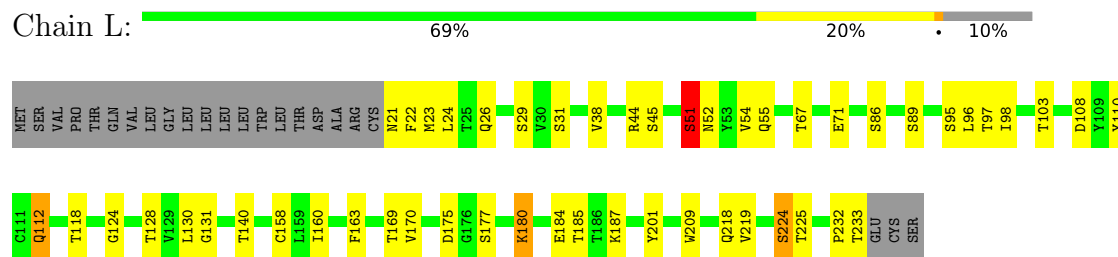
- Molecule 3: Antibody #003-102 light chain



- Molecule 3: Antibody #003-102 light chain



- Molecule 3: Antibody #003-102 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	287.01Å 287.01Å 53.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 3.50 49.71 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.71-3.50) 99.9 (49.71-3.50)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.14 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.186 , 0.227 0.170 , 0.208	Depositor DCC
$R_{free}$ test set	3158 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.024 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.83	0/2978	1.14	7/4040 (0.2%)
1	D	0.80	0/2978	1.14	13/4040 (0.3%)
1	G	0.80	0/2978	1.13	6/4040 (0.1%)
1	J	0.89	0/2978	1.18	12/4040 (0.3%)
2	B	0.82	0/1645	1.06	3/2250 (0.1%)
2	E	0.85	0/1645	1.14	9/2250 (0.4%)
2	H	0.91	0/1645	1.19	13/2250 (0.6%)
2	K	0.83	1/1645 (0.1%)	1.00	1/2250 (0.0%)
3	C	0.84	0/1641	1.13	6/2240 (0.3%)
3	F	0.89	0/1641	1.08	4/2240 (0.2%)
3	I	0.86	0/1641	1.10	5/2240 (0.2%)
3	L	0.82	0/1641	1.06	2/2240 (0.1%)
All	All	0.84	1/25056 (0.0%)	1.12	81/34120 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
3	C	0	1
3	I	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	60	PRO	CA-C	5.74	1.55	1.51

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	64	ALA	CA-C-N	8.84	130.89	119.84
3	C	64	ALA	C-N-CA	8.84	130.89	119.84
2	H	177	THR	N-CA-C	8.25	122.10	108.49
1	D	350	ASN	N-CA-C	8.04	121.28	110.35
1	A	344	GLY	N-CA-C	-7.79	101.70	112.13
1	D	379	ILE	N-CA-C	7.24	116.74	106.53
1	J	371	HIS	N-CA-C	6.99	120.06	109.23
1	J	83	ILE	N-CA-C	-6.94	105.30	113.42
1	D	88	TYR	N-CA-C	6.85	119.76	111.40
2	H	47	SER	N-CA-C	6.73	119.64	110.55
1	D	163	ILE	N-CA-C	6.67	118.08	108.48
3	I	177	SER	CA-C-N	6.61	128.10	119.84
3	I	177	SER	C-N-CA	6.61	128.10	119.84
2	H	230	ASN	N-CA-C	6.55	120.85	112.86
2	E	192	PHE	CA-C-N	6.47	126.49	119.89
2	E	192	PHE	C-N-CA	6.47	126.49	119.89
2	H	194	ALA	N-CA-C	6.47	120.23	109.95
2	E	99	SER	N-CA-C	6.41	119.14	109.41
2	B	165	GLY	N-CA-C	6.35	121.87	111.27
1	G	344	GLY	N-CA-C	-6.33	98.17	113.18
1	D	159	SER	N-CA-C	6.30	120.75	113.38
3	C	118	THR	N-CA-C	6.19	116.25	108.45
1	G	189	SER	N-CA-C	6.16	116.69	108.38
1	A	220	ILE	N-CA-C	6.12	117.84	108.71
3	I	118	THR	N-CA-C	6.12	118.08	108.96
3	C	230	VAL	N-CA-C	6.10	117.27	108.48
1	J	78	VAL	CB-CA-C	6.00	116.53	110.65
2	E	80	ASN	CA-C-N	5.99	127.32	119.84
2	E	80	ASN	C-N-CA	5.99	127.32	119.84
1	J	83	ILE	CB-CA-C	5.95	117.36	110.88
2	E	87	VAL	N-CA-C	5.93	117.98	108.85
1	A	128	TYR	N-CA-C	5.86	117.74	111.36
3	L	95	SER	N-CA-C	5.84	117.89	107.80
2	E	165	GLY	N-CA-C	5.80	119.57	111.10
1	J	137	PHE	N-CA-C	5.76	118.18	110.35
2	H	99	SER	N-CA-C	5.75	117.53	108.96
1	G	47	ASN	N-CA-C	-5.74	104.66	111.03
2	H	195	VAL	N-CA-C	5.72	115.53	106.32
1	A	362	VAL	N-CA-C	5.71	116.78	106.61
1	J	301	ILE	N-CA-C	5.67	114.53	106.53
1	D	28	ASN	N-CA-C	5.66	117.95	107.99
1	G	391	GLY	N-CA-C	-5.60	101.84	111.47
2	B	70	GLU	N-CA-C	5.59	117.58	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	210	VAL	N-CA-C	5.56	113.75	109.19
1	J	78	VAL	N-CA-C	-5.51	108.13	113.53
1	A	62	ALA	N-CA-C	5.51	117.65	107.73
3	L	163	PHE	N-CA-C	5.50	117.37	108.41
2	H	224	VAL	N-CA-C	5.44	112.03	106.21
1	J	302	THR	N-CA-C	5.40	117.06	110.41
1	D	309	VAL	N-CA-C	5.40	115.01	106.32
1	J	88	TYR	N-CA-C	5.36	119.82	113.12
2	H	126	PHE	N-CA-C	5.35	118.03	107.98
1	D	242	GLY	N-CA-C	5.33	118.49	111.03
1	G	313	ASN	N-CA-C	5.33	117.49	109.23
1	A	92	VAL	N-CA-C	5.32	115.52	107.80
2	H	27	GLY	CA-C-N	5.29	126.45	119.84
2	H	27	GLY	C-N-CA	5.29	126.45	119.84
1	J	196	GLN	N-CA-C	5.29	117.11	108.55
2	H	91	VAL	N-CA-C	5.28	120.32	109.34
1	J	116	ILE	CA-C-N	5.24	126.39	119.84
1	J	116	ILE	C-N-CA	5.24	126.39	119.84
3	I	109	TYR	N-CA-C	5.24	117.35	109.23
1	G	137	PHE	N-CA-C	5.23	117.24	107.99
2	B	105	VAL	N-CA-C	5.18	117.86	110.09
1	D	316	LYS	N-CA-C	5.17	118.69	112.38
1	D	87	VAL	N-CA-C	5.16	116.40	108.71
3	F	205	THR	CA-C-N	5.16	124.95	119.28
3	F	205	THR	C-N-CA	5.16	124.95	119.28
3	I	162	ASP	N-CA-C	5.16	118.74	111.52
3	C	229	THR	N-CA-C	5.15	117.74	108.48
2	H	58	ARG	N-CA-C	5.11	116.75	109.14
3	C	40	ILE	N-CA-C	5.09	114.82	106.72
1	A	215	GLU	N-CA-C	5.09	116.91	111.36
1	D	373	ILE	N-CA-C	5.08	113.03	107.60
3	F	184	GLU	N-CA-C	5.08	117.24	107.44
1	D	49	ALA	N-CA-C	5.06	116.80	111.28
2	H	55	SER	N-CA-C	5.06	117.40	108.75
3	F	28	HIS	N-CA-C	5.05	116.48	110.97
1	D	344	GLY	N-CA-C	-5.04	101.23	113.18
2	K	238	GLU	N-CA-C	5.03	117.23	110.29
2	E	192	PHE	N-CA-C	5.01	117.00	110.08

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	186	THR	Peptide
1	D	333	GLY	Peptide
1	G	391	GLY	Peptide
3	I	143	PRO	Peptide

## 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	2915	0	2914	75	0
1	D	2915	0	2914	57	0
1	G	2915	0	2914	73	0
1	J	2915	0	2914	77	0
2	B	1603	0	1574	23	0
2	E	1603	0	1574	23	0
2	H	1603	0	1574	18	0
2	K	1603	0	1574	19	0
3	C	1603	0	1540	41	0
3	F	1603	0	1540	32	0
3	I	1603	0	1540	27	0
3	L	1603	0	1540	19	0
All	All	24484	0	24112	460	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 9.

All (460) 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:D:138:LEU:HA	1:D:345:ASP:OD1	1.73	0.87
1:A:138:LEU:HA	1:A:345:ASP:OD1	1.75	0.85
3:I:171:ALA:HB3	3:I:218:GLN:HB3	1.58	0.85
1:D:143:PRO:HD3	1:D:346:ARG:HG2	1.60	0.83
3:F:173:LYS:HB2	3:F:216:SER:HB2	1.66	0.76
1:D:264:ASP:OD2	2:E:122:GLY:HA2	1.85	0.74
3:F:44:ARG:HH12	3:F:52:ASN:HD22	1.34	0.73
1:G:208:LEU:HB3	1:G:240:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:LEU:HD22	2:H:173:PRO:HD3	1.73	0.70
2:K:195:VAL:O	2:K:202:TYR:HA	1.92	0.69
1:A:339:GLU:O	1:A:347:LYS:HA	1.91	0.69
1:G:143:PRO:HD3	1:G:346:ARG:HG2	1.73	0.69
1:D:187:ARG:HG3	1:D:187:ARG:HH11	1.58	0.69
1:J:25:LYS:HG2	1:J:58:ILE:HG22	1.75	0.69
1:G:33:LEU:HD22	1:G:281:ILE:HD11	1.74	0.68
1:D:141:VAL:HG23	1:D:271:LEU:HD21	1.76	0.68
1:G:97:THR:HB	1:G:98:PRO:HD2	1.76	0.67
1:G:138:LEU:HD11	1:G:325:LEU:HB3	1.77	0.67
1:D:25:LYS:HG2	1:D:58:ILE:HG22	1.75	0.67
2:E:58:ARG:HB3	2:E:68:ILE:HD11	1.78	0.66
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.78	0.65
1:J:81:ASP:HB3	1:J:82:LEU:HG	1.79	0.65
3:L:170:VAL:HG22	3:L:219:VAL:HG22	1.78	0.65
1:G:267:LEU:HD21	1:G:379:ILE:HD11	1.79	0.65
3:I:168:VAL:HG12	3:I:220:THR:O	1.98	0.64
1:J:129:SER:OG	1:J:139:ARG:NH2	2.27	0.64
1:D:33:LEU:HD22	1:D:281:ILE:HD11	1.79	0.64
1:G:102:PHE:HD1	1:G:128:TYR:HH	1.45	0.63
2:H:145:PRO:HB3	2:H:171:TYR:HB3	1.79	0.63
1:A:71:ALA:HB1	1:A:106:PRO:HG3	1.80	0.63
1:D:187:ARG:O	1:D:189:SER:N	2.30	0.63
3:L:21:ASN:HB3	3:L:118:THR:CG2	2.29	0.63
1:G:124:ARG:NH1	1:G:251:GLU:OE1	2.28	0.63
1:G:264:ASP:HA	1:G:356:LEU:HD12	1.81	0.62
2:E:149:PRO:HB3	2:E:237:VAL:HG22	1.82	0.62
2:H:164:LEU:HD21	2:H:210:VAL:HG21	1.82	0.62
1:J:35:THR:OG1	1:J:38:HIS:ND1	2.33	0.61
1:J:133:ILE:HG13	1:J:134:HIS:H	1.66	0.61
1:G:356:LEU:HD23	1:G:361:LEU:CD2	2.31	0.61
1:J:138:LEU:HA	1:J:345:ASP:OD1	2.01	0.61
2:B:142:THR:HG22	2:B:229:SER:HB3	1.83	0.61
1:G:58:ILE:HG21	1:G:296:LEU:HD23	1.82	0.60
1:A:78:VAL:HA	1:A:82:LEU:HD12	1.82	0.60
3:L:51:SER:HB3	3:L:52:ASN:ND2	2.16	0.60
1:J:228:ALA:HB3	1:J:258:ALA:HB2	1.81	0.60
1:G:187:ARG:NH1	1:G:188:GLU:OE1	2.35	0.60
1:G:130:ASP:HB3	1:G:133:ILE:CG2	2.32	0.60
1:G:208:LEU:HD11	1:G:231:VAL:HG23	1.82	0.59
3:F:156:LEU:HD22	3:F:202:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:ALA:O	1:G:259:LEU:HB3	2.01	0.59
1:A:124:ARG:HD3	1:A:141:VAL:HG22	1.84	0.59
1:G:240:MET:HG2	1:G:245:TYR:CZ	2.38	0.59
1:G:289:ALA:O	1:G:292:VAL:HG12	2.03	0.59
1:J:93:SER:HB2	1:J:121:LEU:HD12	1.84	0.59
1:A:60:LEU:HD21	1:A:292:VAL:HG11	1.84	0.58
1:D:155:MET:HG2	1:D:160:TRP:HB2	1.83	0.58
1:D:301:ILE:HA	1:D:317:THR:HG21	1.85	0.58
3:F:105:ASP:O	3:F:127:LEU:HD23	2.03	0.58
1:A:241:THR:O	1:A:382:PRO:HB3	2.03	0.58
1:J:341:ASN:C	1:J:341:ASN:HD22	2.12	0.58
2:E:148:PHE:HB2	2:E:167:LEU:HB3	1.86	0.58
2:B:185:LEU:HD23	2:B:208:VAL:HG21	1.84	0.57
2:K:226:HIS:CE1	2:K:228:PRO:HB2	2.39	0.57
3:F:56:TRP:CZ3	3:F:111:CYS:HB3	2.40	0.57
1:G:356:LEU:HD11	1:G:359:ARG:HA	1.85	0.57
3:L:184:GLU:HB2	3:L:201:TYR:HB2	1.85	0.57
1:A:106:PRO:O	1:A:110:THR:OG1	2.15	0.57
3:F:160:ILE:HB	3:F:198:ALA:HB3	1.87	0.57
3:I:156:LEU:HD22	3:I:202:LEU:HD23	1.87	0.56
1:J:138:LEU:HA	1:J:345:ASP:CG	2.30	0.56
2:E:25:GLU:OE2	2:E:113:TYR:O	2.23	0.56
2:B:37:LEU:HD21	2:B:39:LEU:HD12	1.86	0.56
1:J:129:SER:OG	1:J:346:ARG:HD2	2.04	0.56
3:I:173:LYS:HA	3:I:178:PRO:HA	1.87	0.56
1:G:221:LEU:HB3	1:G:249:VAL:HG12	1.88	0.56
2:B:195:VAL:HG13	3:C:186:THR:HG22	1.88	0.56
1:J:143:PRO:HD3	1:J:346:ARG:HG2	1.88	0.56
1:D:27:VAL:HB	1:D:60:LEU:HD23	1.87	0.55
1:A:322:LYS:HE3	1:A:326:MET:HG3	1.87	0.55
1:A:111:ALA:HB3	1:A:118:VAL:CG2	2.37	0.55
1:G:27:VAL:HG11	1:G:292:VAL:HG21	1.88	0.55
3:I:88:ASP:HB3	3:I:93:SER:O	2.07	0.55
1:A:258:ALA:O	1:A:259:LEU:HB3	2.06	0.55
2:B:55:SER:OG	2:B:70:GLU:HB3	2.06	0.55
3:F:47:GLY:O	3:F:92:ASN:ND2	2.40	0.55
3:I:156:LEU:HB2	3:I:202:LEU:HB3	1.89	0.55
2:B:67:TRP:CD2	3:C:119:VAL:HB	2.42	0.55
1:D:163:ILE:HG22	1:D:218:VAL:HG13	1.89	0.55
1:A:205:THR:HG23	1:A:238:LEU:HD11	1.89	0.55
1:A:259:LEU:HD23	1:A:260:ARG:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:HA	1:D:345:ASP:CG	2.31	0.55
1:D:232:TYR:HB3	1:D:261:TYR:O	2.06	0.55
1:G:338:VAL:HG13	1:G:347:LYS:HD2	1.88	0.55
1:A:335:THR:HB	1:A:347:LYS:HZ3	1.71	0.54
3:C:26:GLN:HE21	3:C:122:GLY:HA3	1.72	0.54
1:G:92:VAL:HG11	1:G:104:PRO:HB3	1.89	0.54
1:G:130:ASP:HB3	1:G:133:ILE:HG21	1.89	0.54
2:K:110:THR:HG23	2:K:136:THR:HA	1.89	0.54
1:A:126:SER:N	1:A:172:GLU:OE1	2.35	0.54
1:G:364:VAL:HG21	1:G:379:ILE:HD12	1.90	0.54
2:B:37:LEU:HB3	2:B:102:LEU:HB3	1.90	0.54
2:H:211:PRO:C	2:H:213:SER:H	2.15	0.53
1:A:133:ILE:O	1:D:113:PHE:CZ	2.61	0.53
2:H:79:TYR:OH	2:H:88:THR:HA	2.08	0.53
3:C:141:LEU:HD22	3:C:217:CYS:HB2	1.88	0.53
1:J:33:LEU:HD13	1:J:38:HIS:HB3	1.91	0.53
3:C:118:THR:OG1	3:C:119:VAL:N	2.40	0.53
3:F:106:GLU:HG3	3:F:127:LEU:O	2.08	0.53
1:J:119:LEU:HD22	1:J:138:LEU:HB2	1.91	0.53
1:J:221:LEU:HB3	1:J:249:VAL:HG12	1.91	0.53
3:I:53:TYR:HD2	3:I:71:GLU:HA	1.74	0.53
1:J:32:VAL:HA	1:J:65:VAL:O	2.09	0.53
2:B:48:ILE:HG13	2:B:54:TRP:NE1	2.23	0.53
1:A:86:GLN:HE21	1:A:304:PRO:HD2	1.74	0.52
3:F:218:GLN:HA	3:F:227:GLU:HG2	1.90	0.52
1:J:152:PHE:HE1	1:J:187:ARG:HD2	1.74	0.52
1:A:76:LEU:O	1:A:80:GLU:N	2.41	0.52
1:D:29:ILE:HD11	1:D:60:LEU:HD22	1.92	0.52
1:J:28:ASN:O	1:J:88:TYR:HB2	2.10	0.52
1:J:78:VAL:HG21	1:J:107:VAL:HG22	1.92	0.52
2:K:30:LEU:HD23	2:K:142:THR:OG1	2.10	0.52
1:A:78:VAL:HG21	1:A:107:VAL:HG13	1.91	0.52
1:J:108:SER:HA	1:J:118:VAL:HG21	1.92	0.52
1:J:162:HIS:O	1:J:218:VAL:HG13	2.10	0.52
1:A:284:ALA:HA	1:A:287:VAL:HG22	1.92	0.52
3:C:106:GLU:HG3	3:C:128:THR:HA	1.92	0.52
1:G:33:LEU:HD13	1:G:38:HIS:HB3	1.92	0.52
1:J:320:LEU:O	1:J:324:VAL:HG23	2.10	0.52
2:E:164:LEU:HD13	2:E:237:VAL:HB	1.92	0.51
1:G:92:VAL:CG2	1:G:107:VAL:HG11	2.40	0.51
1:G:124:ARG:NH1	1:G:271:LEU:HD22	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:VAL:HG11	1:J:104:PRO:HG3	1.92	0.51
1:J:215:GLU:O	1:J:393:GLN:N	2.43	0.51
3:L:44:ARG:HH12	3:L:52:ASN:HD22	1.57	0.51
1:G:267:LEU:HD21	1:G:379:ILE:CD1	2.39	0.51
1:G:162:HIS:O	1:G:218:VAL:HG13	2.11	0.51
1:J:150:VAL:HG11	1:J:269:LEU:HD21	1.92	0.51
1:A:358:ASN:OD1	2:B:53:TRP:CE2	2.64	0.51
3:L:26:GLN:HE22	3:L:110:TYR:HA	1.75	0.51
1:D:153:GLU:HB3	1:D:372:VAL:HG23	1.91	0.51
1:J:91:LEU:HD11	1:J:284:ALA:O	2.11	0.51
1:G:231:VAL:HA	1:G:234:ALA:HB3	1.93	0.51
1:A:96:PRO:HB2	1:A:275:LYS:HE2	1.93	0.51
1:D:157:VAL:C	1:D:159:SER:H	2.19	0.51
1:J:266:ILE:C	1:J:267:LEU:HD12	2.36	0.51
3:L:21:ASN:HB3	3:L:118:THR:HG22	1.92	0.51
1:D:129:SER:OG	1:D:139:ARG:NH2	2.43	0.50
2:E:41:CYS:HB2	2:E:56:TRP:CH2	2.46	0.50
1:D:57:LYS:HE2	1:D:57:LYS:H	1.75	0.50
3:F:169:THR:HB	3:F:220:THR:HB	1.93	0.50
1:G:204:VAL:HG11	1:G:231:VAL:HB	1.93	0.50
3:F:109:TYR:O	3:F:124:GLY:HA2	2.11	0.50
1:G:60:LEU:HD21	1:G:292:VAL:HG11	1.93	0.50
1:G:260:ARG:HD2	3:I:51:SER:HB3	1.94	0.50
1:D:129:SER:OG	1:D:346:ARG:HD2	2.12	0.50
1:J:155:MET:HA	1:J:160:TRP:CD1	2.47	0.50
1:J:66:THR:O	1:J:68:LYS:HE2	2.11	0.50
1:A:260:ARG:NH1	3:C:52:ASN:HD21	2.09	0.50
3:C:75:ARG:HD3	3:C:83:PHE:O	2.12	0.50
2:E:30:LEU:HD13	2:E:173:PRO:HG3	1.93	0.50
2:K:149:PRO:HD3	2:K:235:LYS:HD3	1.93	0.50
3:C:26:GLN:NE2	3:C:122:GLY:HA3	2.27	0.50
1:A:68:LYS:HG2	1:A:73:GLN:HB3	1.94	0.50
1:J:358:ASN:OD1	2:K:53:TRP:CE2	2.65	0.50
1:J:133:ILE:HG13	1:J:134:HIS:N	2.25	0.49
1:J:266:ILE:HG22	1:J:356:LEU:HB2	1.93	0.49
3:L:55:GLN:HB2	3:L:112:GLN:HB3	1.94	0.49
1:A:368:ASN:O	1:A:369:GLY:C	2.54	0.49
3:I:163:PHE:CE2	3:I:168:VAL:HG13	2.47	0.49
1:D:108:SER:HA	1:D:118:VAL:HG21	1.92	0.49
1:J:302:THR:HG21	1:J:316:LYS:H	1.76	0.49
3:I:135:ALA:HB3	3:I:164:TYR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:VAL:HG12	1:J:222:SER:H	1.76	0.49
1:G:102:PHE:HD1	1:G:128:TYR:OH	1.95	0.49
1:J:324:VAL:O	1:J:327:SER:OG	2.24	0.49
1:J:187:ARG:NH1	1:J:189:SER:OG	2.46	0.49
1:A:338:VAL:HG13	1:A:347:LYS:HD2	1.95	0.49
1:G:315:TRP:O	1:G:318:GLY:N	2.46	0.49
3:I:191:GLN:HE21	3:I:197:ALA:HB2	1.77	0.49
1:J:25:LYS:HG2	1:J:58:ILE:CG2	2.41	0.49
3:I:22:PHE:O	3:I:120:VAL:HG21	2.13	0.48
1:J:320:LEU:HG	1:J:323:ARG:HH21	1.78	0.48
1:D:187:ARG:NH1	1:D:189:SER:OG	2.46	0.48
1:J:144:TYR:CE2	1:J:252:ARG:HD3	2.48	0.48
1:A:38:HIS:O	1:A:42:PHE:N	2.46	0.48
1:A:85:SER:O	1:A:87:VAL:N	2.47	0.48
1:A:25:LYS:HG2	1:A:58:ILE:HG22	1.96	0.48
1:G:259:LEU:O	1:G:359:ARG:NH1	2.41	0.48
3:I:219:VAL:N	3:I:226:VAL:O	2.43	0.48
2:E:124:ASN:HB2	3:F:114:TYR:CD2	2.48	0.48
2:E:147:VAL:HB	2:E:235:LYS:HD2	1.95	0.48
1:G:387:GLU:H	1:G:387:GLU:CD	2.20	0.48
3:C:55:GLN:HE21	3:C:71:GLU:H	1.62	0.48
1:D:320:LEU:O	1:D:324:VAL:HG23	2.13	0.48
3:F:183:VAL:HG22	3:F:202:LEU:HD13	1.95	0.48
1:A:315:TRP:O	1:A:318:GLY:N	2.46	0.48
3:C:55:GLN:HG3	3:C:70:TYR:HA	1.95	0.48
3:C:82:ARG:O	3:C:98:ILE:HA	2.13	0.48
1:A:305:PRO:HD3	1:A:315:TRP:CD1	2.48	0.48
1:D:253:GLU:O	1:D:258:ALA:HB1	2.14	0.48
1:G:358:ASN:HD21	2:H:53:TRP:CG	2.31	0.48
1:J:138:LEU:HA	1:J:345:ASP:OD2	2.13	0.48
1:J:153:GLU:O	1:J:156:ARG:HB2	2.13	0.48
1:A:166:LEU:HA	1:A:195:LEU:O	2.14	0.48
1:G:85:SER:O	1:G:87:VAL:N	2.47	0.48
3:I:180:LYS:HE2	3:I:181:ALA:H	1.78	0.48
1:J:77:SER:O	1:J:81:ASP:HB2	2.14	0.47
1:A:212:LYS:HB2	1:A:240:MET:SD	2.53	0.47
1:A:381:TRP:HB2	1:A:385:GLU:HB2	1.97	0.47
2:B:170:ASP:HB3	2:B:201:LEU:HD13	1.97	0.47
1:G:85:SER:O	1:G:86:GLN:C	2.57	0.47
3:F:132:GLN:HB2	3:F:164:TYR:CE2	2.49	0.47
1:J:301:ILE:HD13	1:J:301:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:PRO:HB3	2:B:171:TYR:HB3	1.95	0.47
1:D:358:ASN:OD1	2:E:53:TRP:CD1	2.68	0.47
1:A:129:SER:OG	1:A:346:ARG:HD2	2.14	0.47
2:B:67:TRP:CG	3:C:119:VAL:HB	2.50	0.47
2:H:48:ILE:HA	2:H:54:TRP:CZ2	2.50	0.47
1:J:119:LEU:HD22	1:J:138:LEU:CB	2.45	0.47
3:L:209:TRP:CE2	3:L:232:PRO:HA	2.49	0.47
3:F:37:THR:HG23	3:F:99:SER:HA	1.97	0.47
1:G:174:ARG:HD2	1:G:178:LYS:HZ1	1.80	0.47
1:G:356:LEU:HD23	1:G:361:LEU:HD21	1.96	0.47
1:D:265:GLY:O	1:D:267:LEU:HD12	2.14	0.47
2:E:192:PHE:HE1	2:E:207:VAL:HG12	1.78	0.47
1:G:340:PHE:HB3	1:G:345:ASP:HB2	1.96	0.47
1:J:33:LEU:HD22	1:J:281:ILE:HD11	1.96	0.47
1:J:121:LEU:HD22	1:J:284:ALA:CB	2.45	0.47
3:F:40:ILE:HD12	3:F:96:LEU:HD23	1.96	0.47
2:H:227:LYS:HE3	2:H:230:ASN:HA	1.97	0.47
1:J:105:THR:HG22	1:J:109:TYR:CE2	2.50	0.47
1:A:74:MET:HG2	1:A:103:THR:HG22	1.97	0.46
1:A:295:LEU:HD12	1:A:321:PHE:CD1	2.50	0.46
3:C:35:GLY:N	3:C:101:LEU:O	2.46	0.46
3:I:106:GLU:HG3	3:I:128:THR:HA	1.97	0.46
1:J:117:PRO:HG2	1:J:321:PHE:HB3	1.97	0.46
3:L:218:GLN:HE21	3:L:225:THR:HG21	1.80	0.46
3:C:180:LYS:HD2	3:C:181:ALA:H	1.80	0.46
2:H:160:GLY:HA2	2:H:212:SER:HB2	1.96	0.46
2:K:126:PHE:O	2:K:129:TRP:NE1	2.44	0.46
1:A:298:LYS:O	1:A:301:ILE:HD12	2.15	0.46
3:C:218:GLN:HE21	3:C:225:THR:CG2	2.29	0.46
1:J:150:VAL:HG13	1:J:367:TYR:CD1	2.50	0.46
1:A:112:GLY:HA2	1:A:136:SER:OG	2.15	0.46
1:A:268:GLY:O	1:A:354:MET:HB2	2.16	0.46
1:D:238:LEU:HB2	1:D:240:MET:CE	2.45	0.46
1:D:258:ALA:O	1:D:259:LEU:HB3	2.15	0.46
2:H:218:GLN:HG3	2:H:219:THR:N	2.30	0.46
3:C:156:LEU:HD13	3:C:202:LEU:HD23	1.97	0.46
3:I:30:VAL:O	3:I:127:LEU:HD12	2.16	0.46
3:I:217:CYS:O	3:I:227:GLU:HA	2.15	0.46
1:J:279:ALA:HB1	1:J:334:VAL:CG2	2.46	0.46
3:F:48:SER:OG	3:F:49:ILE:N	2.49	0.46
3:F:112:GLN:HG3	3:F:121:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:118:THR:HG23	3:I:120:VAL:HG23	1.98	0.46
3:C:31:SER:HB2	3:C:130:LEU:HG	1.97	0.46
1:D:364:VAL:HG21	1:D:379:ILE:HD12	1.96	0.46
2:E:53:TRP:CH2	2:E:72:TYR:HB2	2.50	0.46
1:G:97:THR:HB	1:G:98:PRO:CD	2.43	0.46
2:B:25:GLU:HB3	2:B:115:CYS:SG	2.56	0.45
3:C:91:SER:OG	3:C:93:SER:OG	2.30	0.45
1:G:174:ARG:HD2	1:G:178:LYS:NZ	2.31	0.45
3:C:36:LYS:HB3	3:C:37:THR:H	1.54	0.45
1:D:102:PHE:O	1:D:105:THR:OG1	2.32	0.45
3:F:51:SER:HB3	3:F:52:ASN:ND2	2.32	0.45
1:G:144:TYR:HB2	1:G:172:GLU:OE2	2.17	0.45
1:A:198:ASP:O	1:A:201:THR:HG22	2.17	0.45
2:B:26:SER:HB3	2:B:40:THR:HB	1.98	0.45
1:G:322:LYS:HA	1:G:325:LEU:HB2	1.97	0.45
2:K:58:ARG:HB3	2:K:68:ILE:HD11	1.99	0.45
1:A:392:TYR:O	1:A:394:VAL:N	2.49	0.45
2:E:83:LEU:HD11	2:E:86:ARG:NH2	2.31	0.45
3:I:172:TRP:O	3:I:179:VAL:N	2.43	0.45
1:J:150:VAL:HG11	1:J:269:LEU:CD2	2.46	0.45
1:J:272:ILE:HD12	1:J:350:ASN:HB3	1.98	0.45
2:K:219:THR:HG23	2:K:236:LYS:HE2	1.99	0.45
1:A:335:THR:HB	1:A:347:LYS:NZ	2.32	0.45
3:C:24:LEU:HD13	3:C:111:CYS:SG	2.57	0.45
2:K:214:SER:HB2	2:K:218:GLN:HB2	1.99	0.45
2:E:178:VAL:HA	2:E:223:ASN:O	2.16	0.45
2:K:41:CYS:HB2	2:K:56:TRP:CH2	2.52	0.45
3:L:22:PHE:HE2	3:L:24:LEU:HD21	1.82	0.45
1:D:241:THR:HG23	1:D:263:PRO:HB3	1.99	0.45
1:D:291:ALA:CB	1:D:325:LEU:HD13	2.47	0.45
3:I:106:GLU:HB2	3:I:129:VAL:HG23	1.99	0.45
2:K:53:TRP:CH2	2:K:72:TYR:HB2	2.52	0.45
1:A:133:ILE:HD12	1:D:311:ASN:O	2.16	0.45
3:F:156:LEU:HB2	3:F:202:LEU:HB3	1.98	0.45
1:G:212:LYS:HG3	1:G:245:TYR:OH	2.17	0.45
1:J:150:VAL:O	1:J:153:GLU:HB2	2.17	0.45
1:J:358:ASN:OD1	1:J:358:ASN:N	2.50	0.45
2:K:68:ILE:HG23	2:K:83:LEU:HD23	1.98	0.45
3:L:21:ASN:HB3	3:L:118:THR:HG21	1.99	0.45
3:L:180:LYS:CE	3:L:180:LYS:H	2.29	0.45
3:C:70:TYR:O	3:C:74:GLN:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ASP:HB3	1:G:133:ILE:HG22	1.98	0.44
1:G:187:ARG:HD2	1:G:188:GLU:HG3	1.99	0.44
1:G:221:LEU:HB3	1:G:249:VAL:CG1	2.46	0.44
1:J:350:ASN:N	1:J:350:ASN:HD22	2.15	0.44
3:C:56:TRP:CD2	3:C:96:LEU:HB2	2.52	0.44
1:D:67:HIS:CE1	1:D:95:PRO:HD2	2.52	0.44
1:G:343:ASP:OD2	1:G:346:ARG:NH2	2.50	0.44
1:D:187:ARG:HH11	1:D:187:ARG:CG	2.29	0.44
2:K:197:GLN:HG2	3:L:184:GLU:HG3	1.99	0.44
3:C:171:ALA:HB3	3:C:218:GLN:HB3	1.99	0.44
2:B:90:SER:O	2:B:98:PHE:HB2	2.18	0.44
2:B:181:ASN:HD22	2:B:185:LEU:HD13	1.82	0.44
3:F:44:ARG:HG2	3:F:46:SER:O	2.17	0.44
3:F:166:GLY:HA3	3:F:196:TYR:CD2	2.53	0.44
3:I:102:LYS:O	3:I:129:VAL:HG21	2.16	0.44
3:I:177:SER:HA	3:I:178:PRO:HD3	1.84	0.44
2:K:30:LEU:HD22	2:K:173:PRO:HD3	1.98	0.44
1:A:78:VAL:HG12	1:A:83:ILE:HG13	2.00	0.44
1:J:130:ASP:O	1:J:133:ILE:HG22	2.17	0.44
1:A:212:LYS:HE2	1:A:239:ASN:O	2.17	0.44
3:C:205:THR:O	3:C:206:PRO:C	2.61	0.44
3:I:24:LEU:HD23	3:I:44:ARG:HB2	1.99	0.44
3:I:30:VAL:O	3:I:127:LEU:HA	2.18	0.44
1:A:30:GLY:N	1:A:89:ALA:O	2.50	0.44
1:A:360:LYS:HA	3:C:116:SER:HA	2.00	0.44
1:J:39:GLU:HG2	1:J:64:SER:HB2	1.99	0.44
1:J:86:GLN:NE2	1:J:303:ASP:HB3	2.32	0.44
1:A:192:GLU:OE2	1:A:214:LEU:HD13	2.18	0.44
3:C:206:PRO:O	3:C:209:TRP:HB3	2.18	0.44
3:F:54:VAL:O	3:F:72:ASP:HA	2.17	0.44
2:H:48:ILE:HB	2:H:96:ASN:OD1	2.18	0.44
2:K:170:ASP:HB3	2:K:201:LEU:HD13	2.00	0.44
3:F:38:VAL:O	3:F:97:THR:HA	2.17	0.43
2:B:59:GLN:HB2	2:B:65:LEU:HD23	2.00	0.43
1:D:333:GLY:O	1:D:334:VAL:HG22	2.18	0.43
3:F:191:GLN:HE21	3:F:197:ALA:HB2	1.83	0.43
1:G:143:PRO:HD2	1:G:146:HIS:CD2	2.52	0.43
2:H:43:VAL:HB	2:H:96:ASN:ND2	2.34	0.43
1:J:150:VAL:HG22	1:J:367:TYR:CE2	2.54	0.43
1:D:264:ASP:OD2	2:E:122:GLY:CA	2.61	0.43
1:J:167:VAL:HG12	1:J:222:SER:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HG21	1:A:296:LEU:HD23	2.00	0.43
1:A:105:THR:CB	1:A:106:PRO:HD2	2.49	0.43
3:C:112:GLN:HG3	3:C:121:PHE:CE1	2.54	0.43
1:D:74:MET:O	1:D:78:VAL:HG23	2.18	0.43
1:A:348:PHE:CD1	1:A:348:PHE:N	2.87	0.43
1:D:104:PRO:O	1:D:105:THR:C	2.61	0.43
1:D:358:ASN:OD1	2:E:53:TRP:CE2	2.72	0.43
1:J:114:TYR:CD1	1:J:305:PRO:HG2	2.54	0.43
1:G:347:LYS:HE2	1:G:349:ALA:HB2	2.00	0.43
3:C:217:CYS:O	3:C:227:GLU:HA	2.19	0.43
1:J:165:LEU:HD21	1:J:177:GLN:HB2	2.01	0.43
1:G:129:SER:O	1:G:130:ASP:O	2.36	0.43
1:D:291:ALA:HB3	1:D:325:LEU:HD13	2.00	0.42
1:G:271:LEU:HD23	1:G:274:GLY:HA3	1.99	0.42
1:D:149:SER:OG	1:D:179:ARG:NH2	2.52	0.42
1:G:131:LYS:HG2	1:G:343:ASP:OD1	2.19	0.42
1:G:335:THR:HB	1:G:347:LYS:HZ1	1.84	0.42
2:H:56:TRP:CD1	2:H:100:LEU:HB2	2.54	0.42
1:J:114:TYR:CG	1:J:305:PRO:HG2	2.54	0.42
1:J:337:ARG:O	1:J:347:LYS:HE3	2.19	0.42
1:A:77:SER:O	1:A:81:ASP:HB2	2.19	0.42
3:C:161:SER:O	3:C:162:ASP:HB2	2.18	0.42
1:G:169:ASP:OD1	1:G:174:ARG:NH1	2.52	0.42
1:G:340:PHE:HA	1:G:346:ARG:O	2.18	0.42
3:C:191:GLN:HB2	3:C:195:LYS:O	2.19	0.42
1:D:78:VAL:HG13	1:D:82:LEU:HD12	2.00	0.42
2:E:24:GLN:O	2:E:42:ALA:N	2.53	0.42
1:G:166:LEU:O	1:G:221:LEU:HA	2.19	0.42
1:G:224:SER:HG	1:G:227:ASP:H	1.62	0.42
2:H:21:VAL:O	2:H:128:PRO:HG3	2.19	0.42
1:A:289:ALA:HA	1:A:292:VAL:HG12	2.01	0.42
3:C:142:PHE:HB2	3:C:157:VAL:HB	2.01	0.42
2:E:80:ASN:HA	2:E:81:PRO:HD2	1.86	0.42
3:F:48:SER:O	3:F:51:SER:HB2	2.18	0.42
2:H:30:LEU:HD12	2:H:136:THR:O	2.19	0.42
2:H:164:LEU:HD12	2:H:180:TRP:CH2	2.54	0.42
1:J:105:THR:HB	1:J:106:PRO:CD	2.49	0.42
2:B:195:VAL:CG1	3:C:186:THR:HG22	2.49	0.42
3:C:118:THR:HG23	3:C:120:VAL:HG23	2.00	0.42
1:D:264:ASP:O	1:D:382:PRO:HA	2.20	0.42
1:D:335:THR:HB	1:D:347:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:370:THR:HB	1:J:371:HIS:CE1	2.55	0.42
1:G:141:VAL:CG2	1:G:271:LEU:HD21	2.50	0.42
1:J:301:ILE:HG12	1:J:301:ILE:O	2.19	0.42
1:A:359:ARG:HD2	1:A:359:ARG:HA	1.85	0.42
1:G:92:VAL:HG21	1:G:107:VAL:HG11	2.01	0.42
1:G:324:VAL:O	1:G:328:SER:OG	2.38	0.42
1:J:243:SER:H	1:J:383:GLY:HA3	1.84	0.42
1:J:264:ASP:OD2	2:K:122:GLY:HA2	2.19	0.42
2:K:150:LEU:HD11	2:K:167:LEU:HB2	2.01	0.42
1:A:72:ILE:HD12	1:D:105:THR:HG23	2.02	0.42
1:A:127:ILE:HA	1:A:171:HIS:CE1	2.55	0.42
2:E:169:LYS:HB3	2:E:170:ASP:OD1	2.19	0.42
3:L:21:ASN:CB	3:L:118:THR:CG2	2.96	0.42
1:A:364:VAL:HG21	1:A:379:ILE:HD12	2.02	0.42
3:C:56:TRP:CZ3	3:C:111:CYS:HB3	2.55	0.42
3:C:137:PRO:HD3	3:C:221:HIS:CD2	2.55	0.42
3:C:158:CYS:HB2	3:C:172:TRP:CZ2	2.55	0.42
1:D:338:VAL:HA	1:D:347:LYS:HE3	2.02	0.42
1:J:279:ALA:HB1	1:J:334:VAL:HG21	2.02	0.42
3:L:38:VAL:HG12	3:L:98:ILE:HB	2.02	0.42
1:A:49:ALA:HA	1:A:52:ARG:HB2	2.02	0.41
1:A:305:PRO:HD3	1:A:315:TRP:CG	2.55	0.41
2:B:142:THR:HG23	2:B:173:PRO:HD3	2.02	0.41
1:G:71:ALA:HB1	1:G:106:PRO:HG3	2.02	0.41
3:I:188:PRO:HA	3:I:197:ALA:O	2.20	0.41
1:J:155:MET:HA	1:J:160:TRP:HD1	1.85	0.41
1:D:185:GLU:O	1:D:187:ARG:N	2.46	0.41
1:G:36:ARG:HA	1:G:39:GLU:HB2	2.02	0.41
3:I:49:ILE:N	3:I:92:ASN:OD1	2.53	0.41
1:A:273:ASN:HB2	1:A:335:THR:HG23	2.02	0.41
3:F:164:TYR:HA	3:F:165:PRO:HA	1.90	0.41
1:G:355:ASN:HB2	1:G:364:VAL:HG21	2.01	0.41
1:J:56:TRP:HB2	1:J:57:LYS:HE2	2.02	0.41
1:J:109:TYR:CE1	1:J:134:HIS:HE1	2.38	0.41
1:A:356:LEU:HD11	1:A:359:ARG:HA	2.02	0.41
2:B:226:HIS:HB3	2:B:231:THR:HB	2.03	0.41
3:C:40:ILE:HD12	3:C:96:LEU:HD23	2.01	0.41
3:F:82:ARG:HB3	3:F:99:SER:O	2.20	0.41
1:G:86:GLN:OE1	1:G:303:ASP:HB3	2.20	0.41
1:A:109:TYR:CE2	1:D:109:TYR:HB3	2.55	0.41
1:A:148:SER:HB3	1:A:180:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:183:VAL:HG22	3:F:202:LEU:CD1	2.51	0.41
2:H:25:GLU:OE2	2:H:115:CYS:SG	2.79	0.41
2:H:80:ASN:O	2:H:83:LEU:N	2.50	0.41
1:A:28:ASN:O	1:A:88:TYR:HB2	2.21	0.41
1:D:60:LEU:HD21	1:D:292:VAL:HG11	2.03	0.41
2:E:88:THR:HB	2:E:101:LYS:HB2	2.02	0.41
1:J:92:VAL:O	1:J:121:LEU:HG	2.21	0.41
1:J:155:MET:HE1	1:J:184:LEU:HD21	2.02	0.41
1:A:111:ALA:HB3	1:A:118:VAL:HG21	2.02	0.41
3:F:26:GLN:HE21	3:F:122:GLY:HA3	1.85	0.41
2:K:30:LEU:HD21	2:K:140:ALA:O	2.20	0.41
3:L:31:SER:HB2	3:L:130:LEU:HG	2.03	0.41
1:A:144:TYR:CZ	1:A:252:ARG:HD3	2.56	0.41
1:G:70:ASN:HD21	1:G:72:ILE:HG22	1.85	0.41
1:J:244:GLY:HA2	1:J:389:PRO:HB3	2.02	0.41
1:A:153:GLU:HG3	1:A:367:TYR:HE1	1.85	0.41
1:D:375:ASN:OD1	1:D:375:ASN:C	2.64	0.41
3:F:33:SER:HA	3:F:130:LEU:HB2	2.03	0.41
1:G:304:PRO:HA	1:G:315:TRP:CG	2.56	0.41
1:A:76:LEU:HG	1:D:133:ILE:HG12	2.03	0.41
2:B:148:PHE:HB3	3:C:145:SER:OG	2.21	0.41
1:D:58:ILE:HG21	1:D:296:LEU:HD23	2.02	0.41
1:G:141:VAL:HG23	1:G:271:LEU:HD21	2.03	0.41
1:D:241:THR:HG23	1:D:263:PRO:CB	2.51	0.40
3:I:101:LEU:HD22	3:I:129:VAL:HG22	2.02	0.40
3:L:31:SER:HB3	3:L:128:THR:HB	2.03	0.40
1:A:105:THR:CB	1:A:106:PRO:CD	2.99	0.40
1:A:304:PRO:HG3	1:A:315:TRP:CZ3	2.56	0.40
1:A:322:LYS:HA	1:A:325:LEU:HB2	2.03	0.40
2:B:208:VAL:O	2:B:210:VAL:HG13	2.21	0.40
3:C:32:GLU:HA	3:C:130:LEU:HD12	2.02	0.40
1:A:95:PRO:HA	1:A:96:PRO:HD3	1.99	0.40
1:A:105:THR:HB	1:A:106:PRO:CD	2.51	0.40
2:B:185:LEU:CD2	2:B:208:VAL:HG21	2.48	0.40
1:G:362:VAL:HB	1:G:377:ARG:HH12	1.86	0.40
3:L:55:GLN:HE21	3:L:71:GLU:H	1.68	0.40
3:C:71:GLU:HB2	3:C:74:GLN:HB2	2.03	0.40
1:D:293:HIS:O	1:D:297:GLU:HB2	2.21	0.40
1:D:358:ASN:OD1	2:E:53:TRP:NE1	2.55	0.40
2:E:113:TYR:O	2:E:132:GLY:HA2	2.22	0.40
3:F:118:THR:OG1	3:F:119:VAL:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:345:ASP:CG	1:J:345:ASP:O	2.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/384 (96%)	288 (78%)	64 (17%)	17 (5%)	2	18
1	D	369/384 (96%)	313 (85%)	49 (13%)	7 (2%)	6	34
1	G	369/384 (96%)	295 (80%)	54 (15%)	20 (5%)	1	14
1	J	369/384 (96%)	298 (81%)	56 (15%)	15 (4%)	2	20
2	B	212/250 (85%)	191 (90%)	20 (9%)	1 (0%)	25	59
2	E	212/250 (85%)	182 (86%)	23 (11%)	7 (3%)	3	25
2	H	212/250 (85%)	171 (81%)	34 (16%)	7 (3%)	3	25
2	K	212/250 (85%)	183 (86%)	26 (12%)	3 (1%)	9	40
3	C	211/236 (89%)	183 (87%)	21 (10%)	7 (3%)	3	25
3	F	211/236 (89%)	185 (88%)	20 (10%)	6 (3%)	4	27
3	I	211/236 (89%)	178 (84%)	28 (13%)	5 (2%)	5	30
3	L	211/236 (89%)	185 (88%)	21 (10%)	5 (2%)	5	30
All	All	3168/3480 (91%)	2652 (84%)	416 (13%)	100 (3%)	3	25

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	393	GLN
3	C	116	SER

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Mol	Chain	Res	Type
3	C	162	ASP
1	D	188	GLU
1	D	239	ASN
1	G	54	GLY
1	G	86	GLN
1	G	97	THR
1	G	130	ASP
1	G	306	ARG
1	G	343	ASP
2	H	34	SER
1	J	134	HIS
1	J	205	THR
1	J	334	VAL
1	A	131	LYS
1	A	243	SER
1	A	306	ARG
1	A	334	VAL
1	A	363	GLN
3	C	175	ASP
1	D	86	GLN
1	D	252	ARG
2	E	139	SER
2	E	187	SER
3	F	51	SER
3	F	166	GLY
1	G	131	LYS
1	G	133	ILE
1	G	259	LEU
1	G	334	VAL
2	H	84	LYS
2	H	110	THR
2	H	170	ASP
1	J	86	GLN
1	J	133	ILE
1	J	239	ASN
1	J	252	ARG
1	J	369	GLY
3	L	175	ASP
1	A	25	LYS
1	A	54	GLY
1	A	71	ALA
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	188	GLU
1	A	316	LYS
1	A	330	TYR
2	B	170	ASP
3	C	152	ASN
1	D	25	LYS
1	D	186	GLU
3	F	162	ASP
3	F	176	GLY
1	G	374	PRO
1	G	393	GLN
3	I	45	SER
3	I	51	SER
3	I	176	GLY
1	J	25	LYS
1	J	55	SER
1	J	332	ASP
2	K	170	ASP
3	L	51	SER
1	A	252	ARG
3	C	45	SER
3	C	65	PRO
1	D	334	VAL
2	E	46	GLY
2	E	217	THR
2	E	230	ASN
3	F	175	ASP
1	G	25	LYS
1	G	188	GLU
1	G	333	GLY
1	G	368	ASN
1	G	389	PRO
2	H	28	PRO
2	H	51	SER
2	H	175	PRO
1	J	117	PRO
1	J	278	SER
1	G	69	PRO
1	G	132	SER
3	I	175	ASP
1	J	159	SER
2	K	51	SER

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Mol	Chain	Res	Type
3	L	224	SER
3	I	62	GLY
1	J	56	TRP
1	G	263	PRO
3	L	124	GLY
1	A	333	GLY
3	C	131	GLY
1	A	218	VAL
2	E	81	PRO
2	K	45	GLY
3	L	131	GLY
3	F	100	GLY
2	E	175	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/325 (98%)	255 (80%)	63 (20%)	1	6
1	D	318/325 (98%)	263 (83%)	55 (17%)	1	9
1	G	318/325 (98%)	251 (79%)	67 (21%)	1	5
1	J	318/325 (98%)	264 (83%)	54 (17%)	1	10
2	B	184/215 (86%)	162 (88%)	22 (12%)	4	20
2	E	184/215 (86%)	167 (91%)	17 (9%)	7	29
2	H	184/215 (86%)	162 (88%)	22 (12%)	4	20
2	K	184/215 (86%)	157 (85%)	27 (15%)	2	15
3	C	185/206 (90%)	160 (86%)	25 (14%)	3	18
3	F	185/206 (90%)	164 (89%)	21 (11%)	4	22
3	I	185/206 (90%)	167 (90%)	18 (10%)	6	27
3	L	185/206 (90%)	162 (88%)	23 (12%)	4	20
All	All	2748/2984 (92%)	2334 (85%)	414 (15%)	2	14

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	36	ARG
1	A	40	GLN
1	A	44	GLU
1	A	55	SER
1	A	57	LYS
1	A	58	ILE
1	A	59	GLN
1	A	68	LYS
1	A	84	SER
1	A	87	VAL
1	A	97	THR
1	A	103	THR
1	A	105	THR
1	A	110	THR
1	A	119	LEU
1	A	122	THR
1	A	127	ILE
1	A	132	SER
1	A	133	ILE
1	A	135	LEU
1	A	138	LEU
1	A	156	ARG
1	A	166	LEU
1	A	179	ARG
1	A	186	GLU
1	A	188	GLU
1	A	190	LYS
1	A	195	LEU
1	A	217	ARG
1	A	218	VAL
1	A	231	VAL
1	A	233	ARG
1	A	241	THR
1	A	243	SER
1	A	259	LEU
1	A	264	ASP
1	A	285	VAL
1	A	290	GLN
1	A	295	LEU
1	A	301	ILE
1	A	308	CYS

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Mol	Chain	Res	Type
1	A	313	ASN
1	A	320	LEU
1	A	325	LEU
1	A	328	SER
1	A	329	LYS
1	A	334	VAL
1	A	341	ASN
1	A	343	ASP
1	A	348	PHE
1	A	356	LEU
1	A	358	ASN
1	A	359	ARG
1	A	360	LYS
1	A	362	VAL
1	A	366	ILE
1	A	373	ILE
1	A	380	ILE
1	A	386	THR
1	A	387	GLU
1	A	390	ARG
1	A	392	TYR
2	B	38	SER
2	B	48	ILE
2	B	77	THR
2	B	85	SER
2	B	94	SER
2	B	97	GLN
2	B	102	LEU
2	B	109	ASP
2	B	136	THR
2	B	138	SER
2	B	142	THR
2	B	161	THR
2	B	185	LEU
2	B	195	VAL
2	B	196	LEU
2	B	199	SER
2	B	207	VAL
2	B	212	SER
2	B	215	LEU
2	B	227	LYS
2	B	235	LYS

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Mol	Chain	Res	Type
2	B	240	LYS
3	C	23	MET
3	C	30	VAL
3	C	31	SER
3	C	41	SER
3	C	48	SER
3	C	59	GLN
3	C	63	SER
3	C	89	SER
3	C	90	SER
3	C	108	ASP
3	C	116	SER
3	C	146	SER
3	C	147	GLU
3	C	153	LYS
3	C	158	CYS
3	C	161	SER
3	C	162	ASP
3	C	168	VAL
3	C	170	VAL
3	C	180	LYS
3	C	192	SER
3	C	216	SER
3	C	225	THR
3	C	226	VAL
3	C	227	GLU
1	D	36	ARG
1	D	40	GLN
1	D	41	MET
1	D	52	ARG
1	D	57	LYS
1	D	58	ILE
1	D	59	GLN
1	D	61	ASN
1	D	64	SER
1	D	101	HIS
1	D	105	THR
1	D	107	VAL
1	D	116	ILE
1	D	119	LEU
1	D	136	SER
1	D	138	LEU

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Mol	Chain	Res	Type
1	D	156	ARG
1	D	157	VAL
1	D	163	ILE
1	D	165	LEU
1	D	166	LEU
1	D	177	GLN
1	D	187	ARG
1	D	188	GLU
1	D	190	LYS
1	D	192	GLU
1	D	195	LEU
1	D	196	GLN
1	D	198	ASP
1	D	217	ARG
1	D	218	VAL
1	D	225	GLU
1	D	231	VAL
1	D	255	SER
1	D	259	LEU
1	D	295	LEU
1	D	296	LEU
1	D	301	ILE
1	D	302	THR
1	D	311	ASN
1	D	312	THR
1	D	316	LYS
1	D	317	THR
1	D	325	LEU
1	D	328	SER
1	D	329	LYS
1	D	335	THR
1	D	341	ASN
1	D	342	GLU
1	D	348	PHE
1	D	356	LEU
1	D	359	ARG
1	D	360	LYS
1	D	362	VAL
1	D	393	GLN
2	E	23	LEU
2	E	34	SER
2	E	77	THR

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Mol	Chain	Res	Type
2	E	102	LEU
2	E	120	SER
2	E	136	THR
2	E	142	THR
2	E	147	VAL
2	E	153	SER
2	E	161	THR
2	E	185	LEU
2	E	205	SER
2	E	215	LEU
2	E	217	THR
2	E	227	LYS
2	E	235	LYS
2	E	240	LYS
3	F	30	VAL
3	F	33	SER
3	F	37	THR
3	F	49	ILE
3	F	54	VAL
3	F	84	SER
3	F	89	SER
3	F	95	SER
3	F	104	GLU
3	F	112	GLN
3	F	113	SER
3	F	145	SER
3	F	175	ASP
3	F	177	SER
3	F	180	LYS
3	F	187	LYS
3	F	211	SER
3	F	216	SER
3	F	218	GLN
3	F	226	VAL
3	F	227	GLU
1	G	34	SER
1	G	57	LYS
1	G	58	ILE
1	G	59	GLN
1	G	63	THR
1	G	66	THR
1	G	70	ASN

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Mol	Chain	Res	Type
1	G	72	ILE
1	G	76	LEU
1	G	81	ASP
1	G	84	SER
1	G	87	VAL
1	G	93	SER
1	G	99	ASN
1	G	103	THR
1	G	105	THR
1	G	119	LEU
1	G	122	THR
1	G	129	SER
1	G	131	LYS
1	G	138	LEU
1	G	148	SER
1	G	165	LEU
1	G	166	LEU
1	G	177	GLN
1	G	180	LEU
1	G	187	ARG
1	G	188	GLU
1	G	190	LYS
1	G	195	LEU
1	G	210	GLU
1	G	217	ARG
1	G	218	VAL
1	G	219	ILE
1	G	221	LEU
1	G	230	THR
1	G	231	VAL
1	G	241	THR
1	G	248	LEU
1	G	259	LEU
1	G	269	LEU
1	G	282	SER
1	G	294	GLU
1	G	295	LEU
1	G	296	LEU
1	G	297	GLU
1	G	301	ILE
1	G	302	THR
1	G	312	THR

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Mol	Chain	Res	Type
1	G	320	LEU
1	G	325	LEU
1	G	326	MET
1	G	329	LYS
1	G	334	VAL
1	G	335	THR
1	G	341	ASN
1	G	348	PHE
1	G	356	LEU
1	G	359	ARG
1	G	360	LYS
1	G	362	VAL
1	G	366	ILE
1	G	373	ILE
1	G	376	ASP
1	G	377	ARG
1	G	387	GLU
1	G	390	ARG
2	H	20	GLN
2	H	25	GLU
2	H	47	SER
2	H	93	LYS
2	H	95	LYS
2	H	97	GLN
2	H	102	LEU
2	H	103	THR
2	H	142	THR
2	H	161	THR
2	H	164	LEU
2	H	185	LEU
2	H	186	THR
2	H	187	SER
2	H	195	VAL
2	H	207	VAL
2	H	214	SER
2	H	217	THR
2	H	227	LYS
2	H	235	LYS
2	H	238	GLU
2	H	240	LYS
3	I	39	THR
3	I	46	SER

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Mol	Chain	Res	Type
3	I	48	SER
3	I	86	SER
3	I	89	SER
3	I	101	LEU
3	I	113	SER
3	I	140	THR
3	I	142	PHE
3	I	145	SER
3	I	158	CYS
3	I	179	VAL
3	I	180	LYS
3	I	200	SER
3	I	203	SER
3	I	226	VAL
3	I	230	VAL
3	I	233	THR
1	J	39	GLU
1	J	57	LYS
1	J	58	ILE
1	J	64	SER
1	J	68	LYS
1	J	81	ASP
1	J	85	SER
1	J	91	LEU
1	J	105	THR
1	J	108	SER
1	J	116	ILE
1	J	119	LEU
1	J	121	LEU
1	J	122	THR
1	J	149	SER
1	J	156	ARG
1	J	166	LEU
1	J	188	GLU
1	J	190	LYS
1	J	192	GLU
1	J	205	THR
1	J	207	LEU
1	J	215	GLU
1	J	217	ARG
1	J	218	VAL
1	J	231	VAL

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Mol	Chain	Res	Type
1	J	241	THR
1	J	246	VAL
1	J	259	LEU
1	J	264	ASP
1	J	275	LYS
1	J	282	SER
1	J	285	VAL
1	J	294	GLU
1	J	295	LEU
1	J	301	ILE
1	J	308	CYS
1	J	312	THR
1	J	320	LEU
1	J	328	SER
1	J	329	LYS
1	J	334	VAL
1	J	338	VAL
1	J	341	ASN
1	J	342	GLU
1	J	348	PHE
1	J	350	ASN
1	J	352	SER
1	J	358	ASN
1	J	359	ARG
1	J	366	ILE
1	J	373	ILE
1	J	380	ILE
1	J	390	ARG
2	K	25	GLU
2	K	26	SER
2	K	44	SER
2	K	50	SER
2	K	83	LEU
2	K	88	THR
2	K	102	LEU
2	K	106	THR
2	K	120	SER
2	K	123	VAL
2	K	125	TRP
2	K	139	SER
2	K	142	THR
2	K	161	THR

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Mol	Chain	Res	Type
2	K	164	LEU
2	K	169	LYS
2	K	178	VAL
2	K	185	LEU
2	K	190	HIS
2	K	205	SER
2	K	207	VAL
2	K	208	VAL
2	K	210	VAL
2	K	219	THR
2	K	233	VAL
2	K	235	LYS
2	K	240	LYS
3	L	23	MET
3	L	29	SER
3	L	45	SER
3	L	51	SER
3	L	54	VAL
3	L	67	THR
3	L	86	SER
3	L	89	SER
3	L	96	LEU
3	L	97	THR
3	L	103	THR
3	L	108	ASP
3	L	112	GLN
3	L	140	THR
3	L	158	CYS
3	L	160	ILE
3	L	169	THR
3	L	177	SER
3	L	180	LYS
3	L	185	THR
3	L	187	LYS
3	L	224	SER
3	L	233	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	59	GLN

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Mol	Chain	Res	Type
1	A	70	ASN
1	A	290	GLN
1	A	311	ASN
1	A	313	ASN
1	A	341	ASN
1	A	350	ASN
1	A	357	GLN
2	B	24	GLN
2	B	52	ASN
2	B	181	ASN
2	B	190	HIS
2	B	226	HIS
3	C	26	GLN
3	C	52	ASN
3	C	55	GLN
3	C	92	ASN
3	C	150	GLN
3	C	191	GLN
3	C	194	ASN
3	C	218	GLN
3	C	221	HIS
1	D	47	ASN
1	D	48	GLN
1	D	59	GLN
1	D	61	ASN
1	D	67	HIS
1	D	196	GLN
1	D	293	HIS
1	D	311	ASN
1	D	350	ASN
1	D	393	GLN
2	E	223	ASN
3	F	26	GLN
3	F	52	ASN
3	F	58	GLN
3	F	59	GLN
3	F	74	GLN
3	F	191	GLN
1	G	67	HIS
1	G	101	HIS
1	G	162	HIS
1	G	171	HIS

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Mol	Chain	Res	Type
1	G	270	GLN
1	G	276	ASN
1	G	300	ASN
2	H	22	GLN
2	H	190	HIS
2	H	223	ASN
3	I	21	ASN
3	I	55	GLN
3	I	152	ASN
3	I	191	GLN
3	I	194	ASN
1	J	50	ASN
1	J	61	ASN
1	J	86	GLN
1	J	134	HIS
1	J	162	HIS
1	J	270	GLN
1	J	273	ASN
1	J	300	ASN
1	J	311	ASN
1	J	350	ASN
1	J	358	ASN
2	K	52	ASN
2	K	59	GLN
2	K	76	ASN
2	K	190	HIS
2	K	225	ASN
3	L	26	GLN
3	L	52	ASN
3	L	55	GLN
3	L	74	GLN
3	L	132	GLN
3	L	193	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	371/384 (96%)	-0.97	0 <span>100</span> <span>100</span>	77, 121, 155, 209	0
1	D	371/384 (96%)	-0.89	1 (0%) <span>90</span> <span>82</span>	82, 130, 186, 225	0
1	G	371/384 (96%)	-1.00	0 <span>100</span> <span>100</span>	81, 118, 149, 192	0
1	J	371/384 (96%)	-0.77	1 (0%) <span>90</span> <span>82</span>	71, 131, 185, 291	0
2	B	216/250 (86%)	-0.99	0 <span>100</span> <span>100</span>	90, 127, 155, 183	0
2	E	216/250 (86%)	-0.98	0 <span>100</span> <span>100</span>	100, 135, 165, 212	0
2	H	216/250 (86%)	-0.88	1 (0%) <span>87</span> <span>75</span>	103, 131, 170, 198	0
2	K	216/250 (86%)	-1.03	0 <span>100</span> <span>100</span>	93, 124, 149, 163	0
3	C	213/236 (90%)	-1.00	0 <span>100</span> <span>100</span>	96, 130, 157, 175	0
3	F	213/236 (90%)	-0.89	0 <span>100</span> <span>100</span>	105, 146, 181, 200	0
3	I	213/236 (90%)	-0.99	0 <span>100</span> <span>100</span>	97, 142, 173, 190	0
3	L	213/236 (90%)	-1.02	0 <span>100</span> <span>100</span>	94, 133, 160, 173	0
All	All	3200/3480 (91%)	-0.94	3 (0%) <span>92</span> <span>89</span>	71, 129, 169, 291	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	90	ILE	4.0
2	H	233	VAL	2.9
1	D	98	PRO	2.6

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.