



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:20 AM UTC

PDB ID : 4GPK / pdb_00004gpk
Title : Crystal structure of NprR in complex with its cognate peptide NprX
Authors : Zouhir, S.; Guimaraes, B.; Perchat, S.; Nicaise, M.; Lereclus, D.; Nessler, S.
Deposited on : 2012-08-21
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

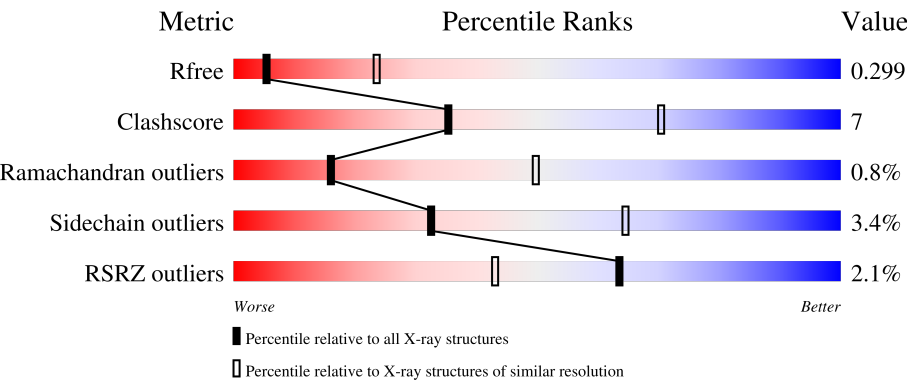
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 ≥ 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	372	% 76%16%8%
1	B	372	6% 66%23%8%
1	C	372	2% 66%23%9%
1	D	372	% 67%24%8%
1	E	372	3% 73%17%9%

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Mol	Chain	Length	Quality of chain
1	F	372	
1	G	372	
1	H	372	
1	I	372	
1	J	372	
1	K	372	
1	L	372	
2	M	8	
2	N	8	
2	O	8	
2	P	8	
2	Q	8	
2	R	8	
2	S	8	
2	T	8	
2	U	8	
2	V	8	
2	W	8	
2	X	8	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35360 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 NprR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2896	1882	465	535	14			
1	B	342	Total	C	N	O	S	0	0	0
			2882	1873	462	533	14			
1	C	340	Total	C	N	O	S	0	0	0
			2869	1869	460	526	14			
1	D	342	Total	C	N	O	S	0	0	0
			2883	1876	462	531	14			
1	E	339	Total	C	N	O	S	0	0	0
			2861	1863	459	525	14			
1	F	341	Total	C	N	O	S	0	0	0
			2875	1865	462	534	14			
1	G	345	Total	C	N	O	S	0	0	0
			2911	1893	465	539	14			
1	H	343	Total	C	N	O	S	0	0	0
			2895	1883	463	535	14			
1	I	344	Total	C	N	O	S	0	0	0
			2903	1889	464	536	14			
1	J	347	Total	C	N	O	S	0	0	0
			2929	1902	471	542	14			
1	K	340	Total	C	N	O	S	0	0	0
			2866	1863	460	529	14			
1	L	346	Total	C	N	O	S	0	0	0
			2918	1896	467	541	14			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP G5DDY8
A	424	ARG	-	expression tag	UNP G5DDY8
A	425	SER	-	expression tag	UNP G5DDY8
A	426	HIS	-	expression tag	UNP G5DDY8
A	427	HIS	-	expression tag	UNP G5DDY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	HIS	-	expression tag	UNP G5DDY8
A	429	HIS	-	expression tag	UNP G5DDY8
A	430	HIS	-	expression tag	UNP G5DDY8
A	431	HIS	-	expression tag	UNP G5DDY8
B	60	MET	-	initiating methionine	UNP G5DDY8
B	424	ARG	-	expression tag	UNP G5DDY8
B	425	SER	-	expression tag	UNP G5DDY8
B	426	HIS	-	expression tag	UNP G5DDY8
B	427	HIS	-	expression tag	UNP G5DDY8
B	428	HIS	-	expression tag	UNP G5DDY8
B	429	HIS	-	expression tag	UNP G5DDY8
B	430	HIS	-	expression tag	UNP G5DDY8
B	431	HIS	-	expression tag	UNP G5DDY8
C	60	MET	-	initiating methionine	UNP G5DDY8
C	424	ARG	-	expression tag	UNP G5DDY8
C	425	SER	-	expression tag	UNP G5DDY8
C	426	HIS	-	expression tag	UNP G5DDY8
C	427	HIS	-	expression tag	UNP G5DDY8
C	428	HIS	-	expression tag	UNP G5DDY8
C	429	HIS	-	expression tag	UNP G5DDY8
C	430	HIS	-	expression tag	UNP G5DDY8
C	431	HIS	-	expression tag	UNP G5DDY8
D	60	MET	-	initiating methionine	UNP G5DDY8
D	424	ARG	-	expression tag	UNP G5DDY8
D	425	SER	-	expression tag	UNP G5DDY8
D	426	HIS	-	expression tag	UNP G5DDY8
D	427	HIS	-	expression tag	UNP G5DDY8
D	428	HIS	-	expression tag	UNP G5DDY8
D	429	HIS	-	expression tag	UNP G5DDY8
D	430	HIS	-	expression tag	UNP G5DDY8
D	431	HIS	-	expression tag	UNP G5DDY8
E	60	MET	-	initiating methionine	UNP G5DDY8
E	424	ARG	-	expression tag	UNP G5DDY8
E	425	SER	-	expression tag	UNP G5DDY8
E	426	HIS	-	expression tag	UNP G5DDY8
E	427	HIS	-	expression tag	UNP G5DDY8
E	428	HIS	-	expression tag	UNP G5DDY8
E	429	HIS	-	expression tag	UNP G5DDY8
E	430	HIS	-	expression tag	UNP G5DDY8
E	431	HIS	-	expression tag	UNP G5DDY8
F	60	MET	-	initiating methionine	UNP G5DDY8
F	424	ARG	-	expression tag	UNP G5DDY8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	425	SER	-	expression tag	UNP G5DDY8
F	426	HIS	-	expression tag	UNP G5DDY8
F	427	HIS	-	expression tag	UNP G5DDY8
F	428	HIS	-	expression tag	UNP G5DDY8
F	429	HIS	-	expression tag	UNP G5DDY8
F	430	HIS	-	expression tag	UNP G5DDY8
F	431	HIS	-	expression tag	UNP G5DDY8
G	60	MET	-	initiating methionine	UNP G5DDY8
G	424	ARG	-	expression tag	UNP G5DDY8
G	425	SER	-	expression tag	UNP G5DDY8
G	426	HIS	-	expression tag	UNP G5DDY8
G	427	HIS	-	expression tag	UNP G5DDY8
G	428	HIS	-	expression tag	UNP G5DDY8
G	429	HIS	-	expression tag	UNP G5DDY8
G	430	HIS	-	expression tag	UNP G5DDY8
G	431	HIS	-	expression tag	UNP G5DDY8
H	60	MET	-	initiating methionine	UNP G5DDY8
H	424	ARG	-	expression tag	UNP G5DDY8
H	425	SER	-	expression tag	UNP G5DDY8
H	426	HIS	-	expression tag	UNP G5DDY8
H	427	HIS	-	expression tag	UNP G5DDY8
H	428	HIS	-	expression tag	UNP G5DDY8
H	429	HIS	-	expression tag	UNP G5DDY8
H	430	HIS	-	expression tag	UNP G5DDY8
H	431	HIS	-	expression tag	UNP G5DDY8
I	60	MET	-	initiating methionine	UNP G5DDY8
I	424	ARG	-	expression tag	UNP G5DDY8
I	425	SER	-	expression tag	UNP G5DDY8
I	426	HIS	-	expression tag	UNP G5DDY8
I	427	HIS	-	expression tag	UNP G5DDY8
I	428	HIS	-	expression tag	UNP G5DDY8
I	429	HIS	-	expression tag	UNP G5DDY8
I	430	HIS	-	expression tag	UNP G5DDY8
I	431	HIS	-	expression tag	UNP G5DDY8
J	60	MET	-	initiating methionine	UNP G5DDY8
J	424	ARG	-	expression tag	UNP G5DDY8
J	425	SER	-	expression tag	UNP G5DDY8
J	426	HIS	-	expression tag	UNP G5DDY8
J	427	HIS	-	expression tag	UNP G5DDY8
J	428	HIS	-	expression tag	UNP G5DDY8
J	429	HIS	-	expression tag	UNP G5DDY8
J	430	HIS	-	expression tag	UNP G5DDY8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	431	HIS	-	expression tag	UNP G5DDY8
K	60	MET	-	initiating methionine	UNP G5DDY8
K	424	ARG	-	expression tag	UNP G5DDY8
K	425	SER	-	expression tag	UNP G5DDY8
K	426	HIS	-	expression tag	UNP G5DDY8
K	427	HIS	-	expression tag	UNP G5DDY8
K	428	HIS	-	expression tag	UNP G5DDY8
K	429	HIS	-	expression tag	UNP G5DDY8
K	430	HIS	-	expression tag	UNP G5DDY8
K	431	HIS	-	expression tag	UNP G5DDY8
L	60	MET	-	initiating methionine	UNP G5DDY8
L	424	ARG	-	expression tag	UNP G5DDY8
L	425	SER	-	expression tag	UNP G5DDY8
L	426	HIS	-	expression tag	UNP G5DDY8
L	427	HIS	-	expression tag	UNP G5DDY8
L	428	HIS	-	expression tag	UNP G5DDY8
L	429	HIS	-	expression tag	UNP G5DDY8
L	430	HIS	-	expression tag	UNP G5DDY8
L	431	HIS	-	expression tag	UNP G5DDY8

- Molecule 2 is a protein called NprX peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	N	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	O	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	P	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	Q	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	R	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	S	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	T	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	U	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	V	8	Total	C	N	O	0	0	0
			56	34	9	13			

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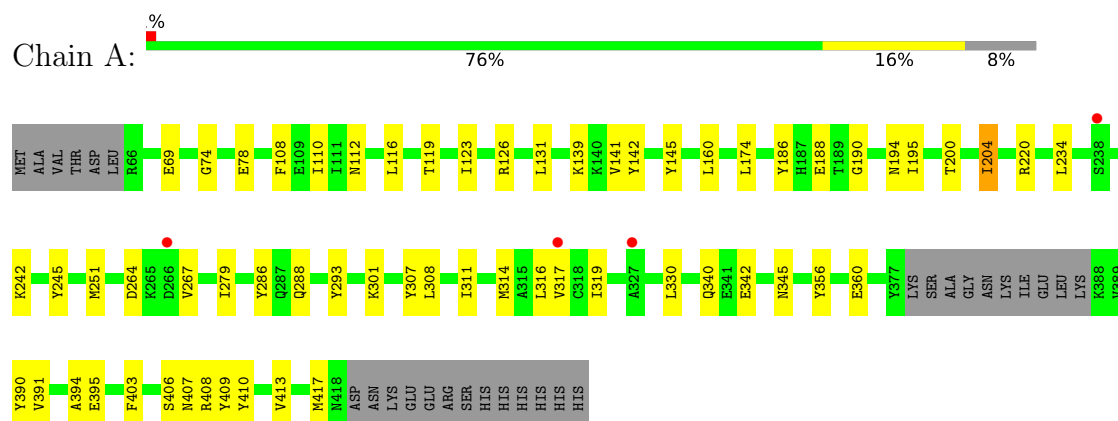
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	8	Total	C	N	O	0	0	0
			56	34	9	13			
2	X	8	Total	C	N	O	0	0	0
			56	34	9	13			

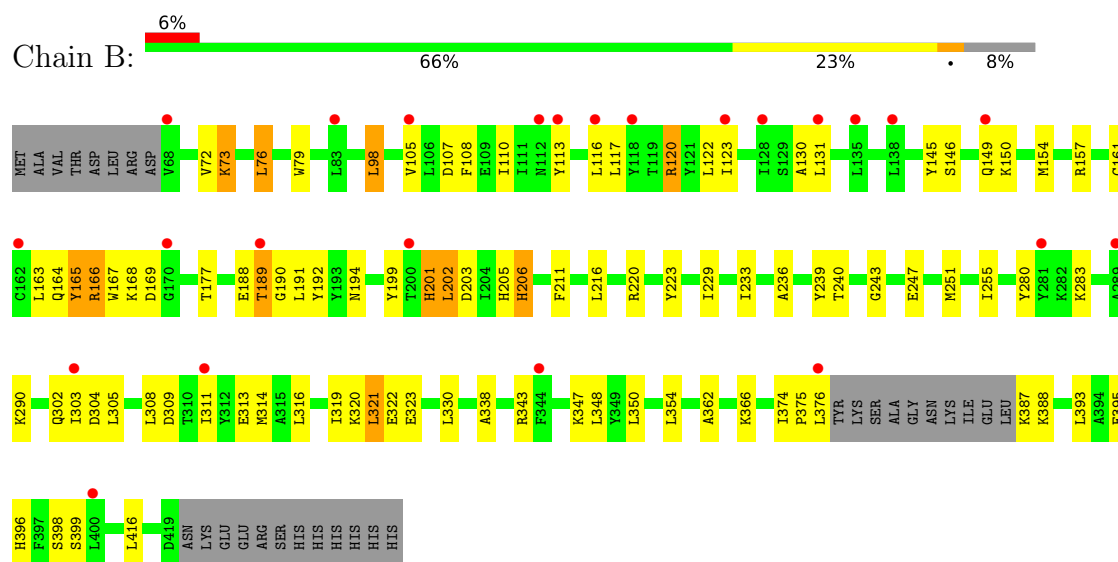
3 Residue-property plots [i](#)

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

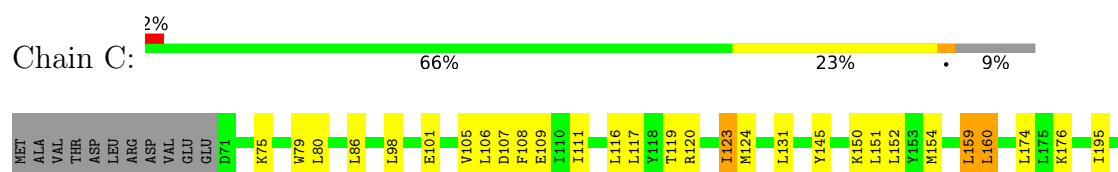
• Molecule 1: NprR

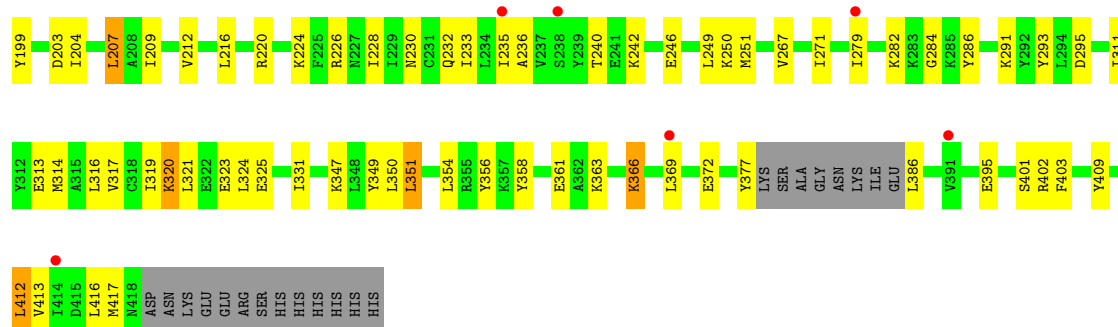


• Molecule 1: NprR

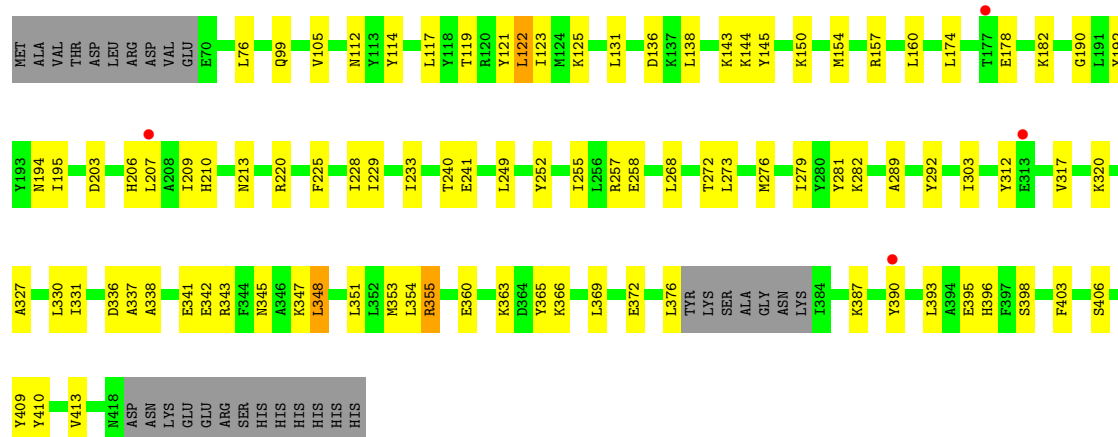


• Molecule 1: NprR

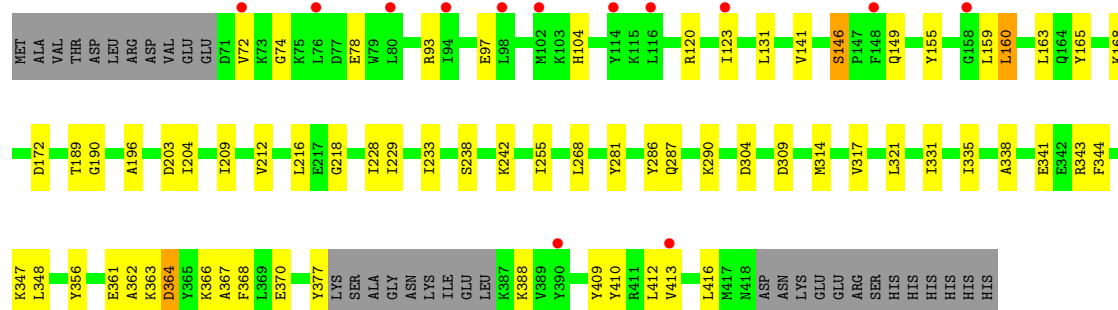




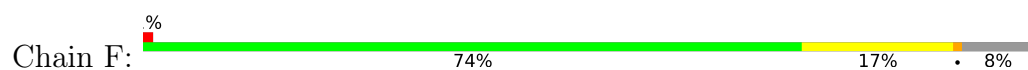
• Molecule 1: NprR

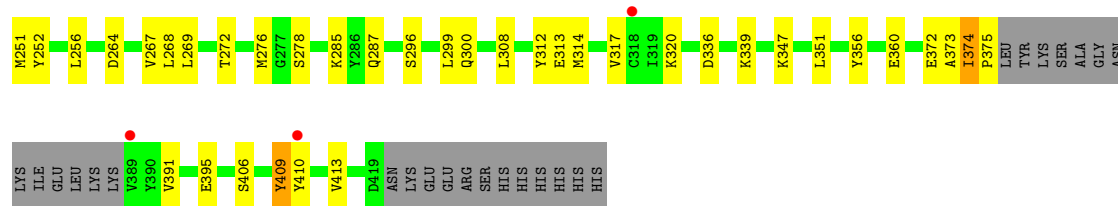


• Molecule 1: NprR

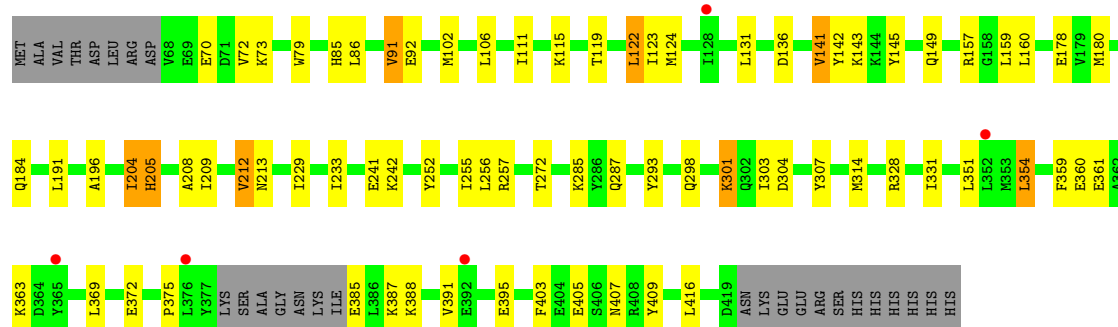
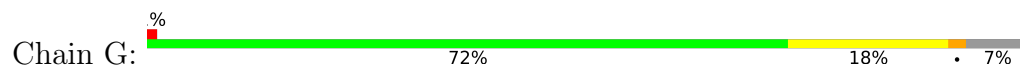


• Molecule 1: NprR

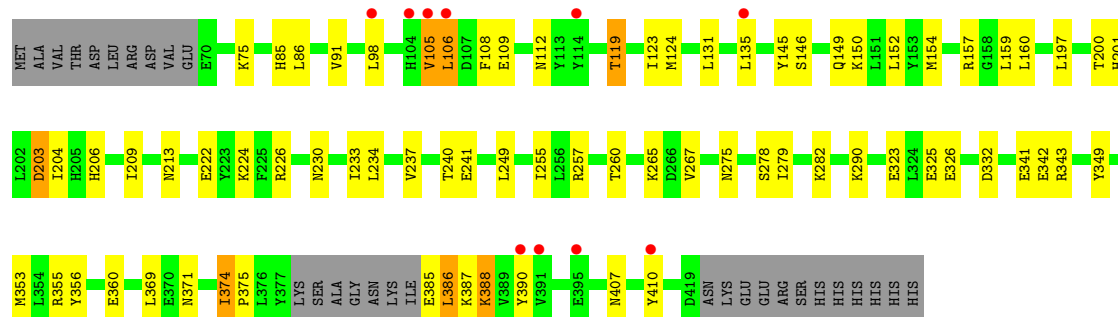




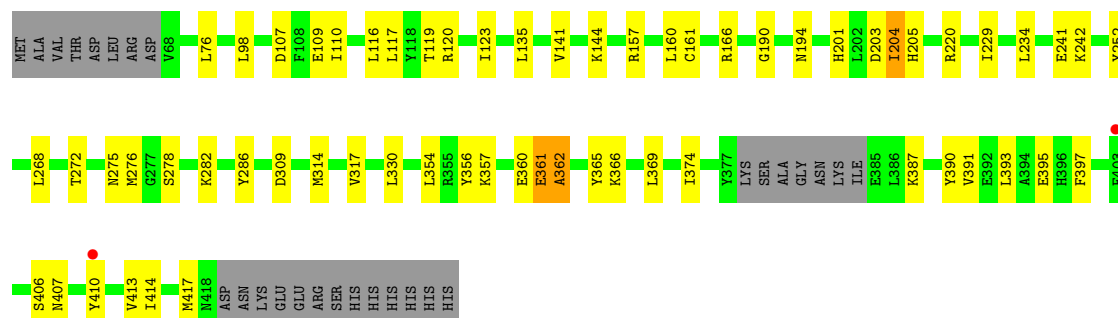
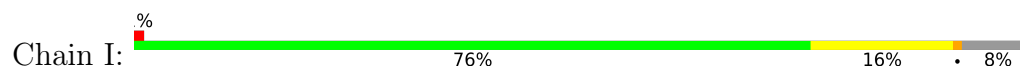
• Molecule 1: NprR



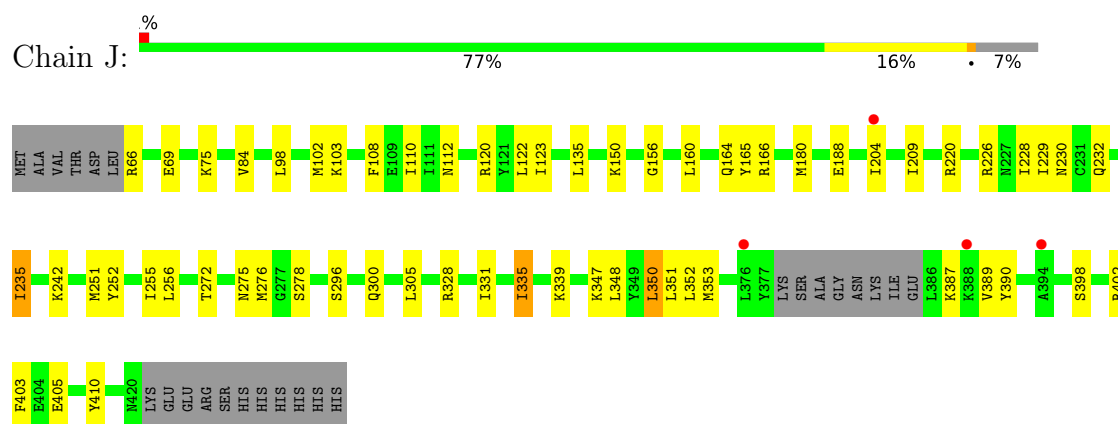
• Molecule 1: NprR



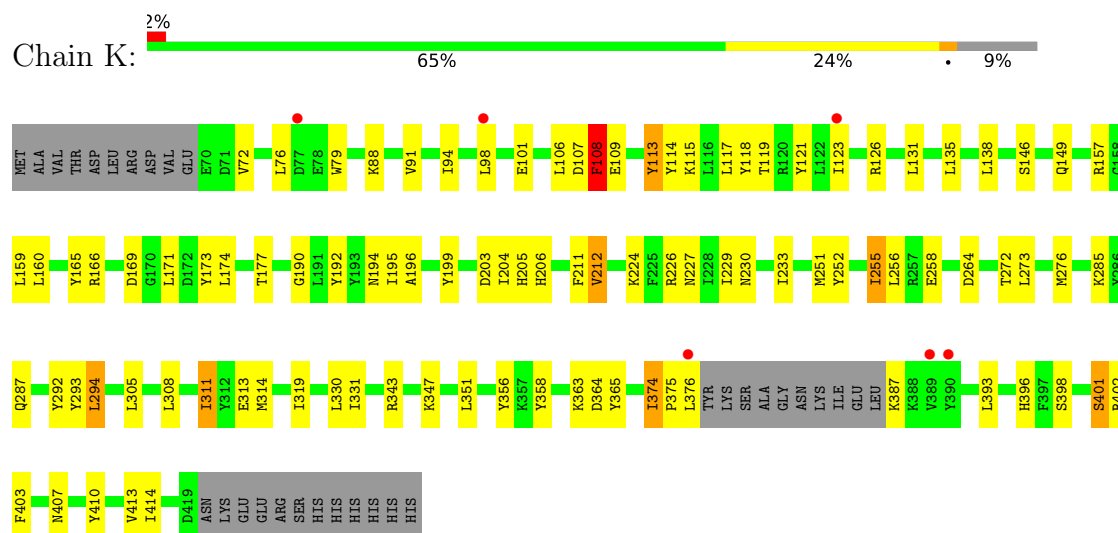
• Molecule 1: NprR



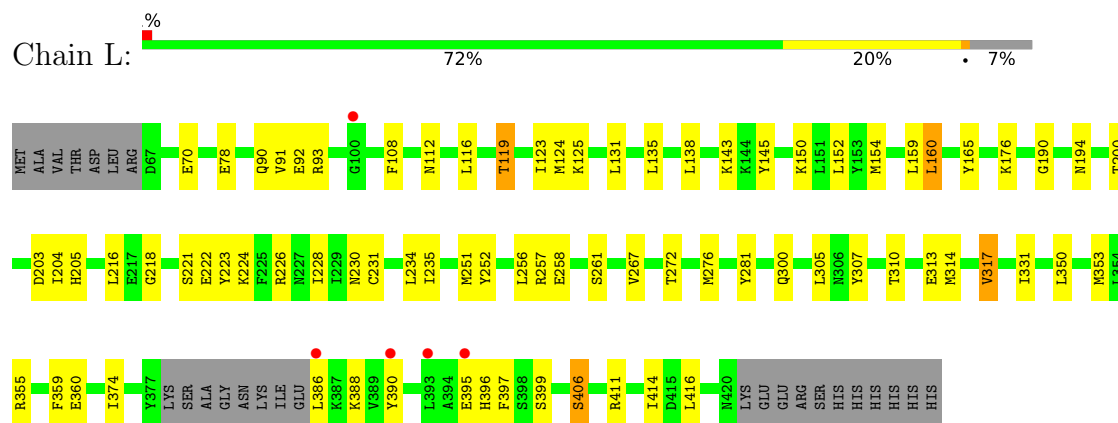
• Molecule 1: NprR



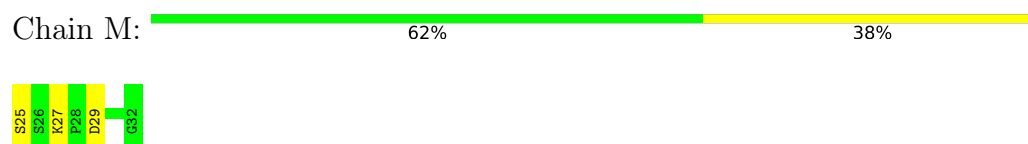
• Molecule 1: NprR



• Molecule 1: NprR



• Molecule 2: NprX peptide



● Molecule 2: NprX peptide

Chain N:  62% 25% 12%



● Molecule 2: NprX peptide

Chain O:  75% 25%



● Molecule 2: NprX peptide

Chain P:  100%

There are no outlier residues recorded for this chain.

● Molecule 2: NprX peptide

Chain Q:  75% 12% 12%



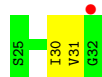
● Molecule 2: NprX peptide

Chain R:  62% 38%



● Molecule 2: NprX peptide

Chain S:  12% 75% 25%



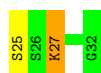
● Molecule 2: NprX peptide

Chain T:  50% 50%



● Molecule 2: NprX peptide

Chain U:  75% 12% 12%



• Molecule 2: NprX peptide

Chain V:  75% 25%



• Molecule 2: NprX peptide

Chain W:  75% 25%



• Molecule 2: NprX peptide

Chain X:  88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.24Å 133.35Å 137.50Å 108.25° 104.83° 103.83°	Depositor
Resolution (Å)	29.74 – 3.20 29.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.74-3.20) 98.6 (29.74-3.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.8_1069, BUSTER-TNT	Depositor
R, R_{free}	0.270 , 0.299 0.269 , 0.299	Depositor DCC
R_{free} test set	24330 reflections (20.00%)	wwPDB-VP
Wilson B-factor (Å ²)	116.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35360	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/2953	0.68	0/3969
1	B	0.26	0/2938	0.74	2/3948 (0.1%)
1	C	0.25	0/2926	0.66	0/3932
1	D	0.25	0/2939	0.68	0/3949
1	E	0.25	0/2918	0.70	2/3921 (0.1%)
1	F	0.26	0/2931	0.65	0/3940
1	G	0.26	0/2968	0.66	0/3989
1	H	0.25	0/2952	0.67	1/3967 (0.0%)
1	I	0.26	0/2960	0.67	2/3978 (0.1%)
1	J	0.25	0/2986	0.66	0/4013
1	K	0.27	0/2922	0.69	1/3926 (0.0%)
1	L	0.25	0/2975	0.66	2/3999 (0.1%)
2	M	0.25	0/56	0.72	0/73
2	N	0.33	0/56	0.61	0/73
2	O	0.47	0/56	0.89	0/73
2	P	0.30	0/56	0.77	0/73
2	Q	0.62	0/56	0.81	0/73
2	R	0.29	0/56	0.68	0/73
2	S	0.29	0/56	0.55	0/73
2	T	0.32	0/56	0.77	0/73
2	U	0.30	0/56	0.67	0/73
2	V	0.32	0/56	0.64	0/73
2	W	0.30	0/56	0.64	0/73
2	X	0.25	0/56	0.70	0/73
All	All	0.26	0/36040	0.68	10/48407 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	388	LYS	N-CA-C	-5.59	106.35	112.72
1	B	72	VAL	N-CA-C	-5.42	107.51	111.90
1	E	146	SER	CA-C-N	5.37	126.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	146	SER	C-N-CA	5.37	126.55	119.84
1	L	360	GLU	N-CA-C	-5.34	105.38	111.14
1	I	374	ILE	CA-C-N	-5.33	114.25	119.64
1	I	374	ILE	C-N-CA	-5.33	114.25	119.64
1	B	73	LYS	N-CA-C	-5.29	106.87	113.38
1	K	401	SER	N-CA-C	5.11	112.97	108.78
1	L	203	ASP	CB-CA-C	-5.07	110.75	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2896	0	2906	33	0
1	B	2882	0	2897	60	0
1	C	2869	0	2892	53	0
1	D	2883	0	2906	51	0
1	E	2861	0	2881	42	0
1	F	2875	0	2877	36	0
1	G	2911	0	2923	38	0
1	H	2895	0	2908	42	0
1	I	2903	0	2919	42	0
1	J	2929	0	2940	35	0
1	K	2866	0	2882	64	0
1	L	2918	0	2927	47	0
2	M	56	0	56	1	0
2	N	56	0	56	2	0
2	O	56	0	56	1	0
2	P	56	0	56	0	0
2	Q	56	0	56	2	0
2	R	56	0	56	2	0
2	S	56	0	56	0	0
2	T	56	0	56	4	0
2	U	56	0	56	2	0
2	V	56	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	56	0	56	2	0
2	X	56	0	56	0	0
All	All	35360	0	35530	527	0

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

All (527) 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:B:113:TYR:HB3	1:B:149:GLN:HG2	1.63	0.81
1:B:395:GLU:HA	1:B:398:SER:HB2	1.68	0.76
1:B:313:GLU:OE2	2:N:25:SER:N	2.20	0.75
1:K:308:LEU:HD11	1:K:347:LYS:HD3	1.70	0.74
1:D:112:ASN:HD22	1:D:145:TYR:HE1	1.33	0.73
1:C:154:MET:HE2	1:C:176:LYS:HD2	1.72	0.72
1:D:395:GLU:HG3	1:D:410:TYR:HB2	1.72	0.71
1:L:300:GLN:HE22	1:L:310:THR:HG21	1.56	0.70
1:I:356:TYR:HA	1:I:360:GLU:HB3	1.71	0.70
1:H:341:GLU:O	1:H:343:ARG:N	2.23	0.70
1:K:190:GLY:O	1:K:194:ASN:ND2	2.25	0.70
1:E:120:ARG:HA	1:E:123:ILE:HD12	1.75	0.69
1:J:331:ILE:HG13	1:J:351:LEU:HD12	1.74	0.69
1:L:119:THR:HG23	1:L:131:LEU:HD11	1.75	0.69
1:G:85:HIS:HB3	1:H:257:ARG:HD3	1.74	0.68
1:E:364:ASP:HB3	1:E:367:ALA:HB3	1.75	0.68
1:I:190:GLY:O	1:I:194:ASN:ND2	2.27	0.68
1:I:220:ARG:HH11	1:J:220:ARG:HH11	1.42	0.67
1:L:226:ARG:O	1:L:230:ASN:ND2	2.28	0.67
1:D:190:GLY:O	1:D:194:ASN:ND2	2.28	0.66
1:K:123:ILE:HG12	1:K:159:LEU:HD13	1.77	0.66
1:C:220:ARG:HH11	1:D:220:ARG:HH11	1.44	0.66
1:C:123:ILE:HD13	1:C:159:LEU:HD23	1.77	0.65
1:D:398:SER:HB2	1:D:406:SER:HB3	1.78	0.65
1:K:374:ILE:HG23	1:K:375:PRO:HD3	1.77	0.65
1:H:204:ILE:HG12	1:H:241:GLU:HB3	1.79	0.65
1:B:161:CYS:SG	1:B:166:ARG:NH1	2.70	0.64
1:B:290:LYS:HG3	1:B:314:MET:HE1	1.80	0.64
1:H:75:LYS:HB3	1:H:98:LEU:HD11	1.78	0.64
1:H:108:PHE:O	1:H:112:ASN:ND2	2.31	0.64
1:C:369:LEU:HD12	1:C:372:GLU:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:275:ASN:OD1	2:V:25:SER:N	2.31	0.64
1:I:135:LEU:HD13	1:I:157:ARG:HD2	1.80	0.64
1:L:190:GLY:O	1:L:194:ASN:ND2	2.30	0.63
1:B:190:GLY:O	1:B:194:ASN:ND2	2.31	0.63
1:J:164:GLN:OE1	1:J:166:ARG:NH2	2.32	0.62
1:C:402:ARG:HB3	1:C:403:PHE:HB3	1.81	0.62
1:G:331:ILE:HG13	1:G:351:LEU:HD12	1.80	0.62
1:C:366:LYS:HA	1:C:369:LEU:HB3	1.81	0.62
1:G:403:PHE:O	1:G:407:ASN:ND2	2.33	0.62
1:K:123:ILE:O	1:K:126:ARG:NH1	2.33	0.62
1:B:189:THR:HA	1:B:192:TYR:HD2	1.65	0.61
1:K:398:SER:HA	1:K:401:SER:HB2	1.81	0.61
1:D:252:TYR:HB3	1:D:276:MET:HE3	1.80	0.61
1:I:252:TYR:HB3	1:I:276:MET:HE2	1.81	0.61
1:C:331:ILE:HG13	1:C:351:LEU:HD12	1.83	0.61
1:L:252:TYR:HB3	1:L:276:MET:HE2	1.80	0.61
1:F:126:ARG:NH2	2:R:29:ASP:OD2	2.34	0.61
1:A:251:MET:SD	1:B:223:TYR:OH	2.58	0.61
1:E:341:GLU:HG3	1:E:343:ARG:H	1.65	0.61
1:A:116:LEU:O	1:A:119:THR:OG1	2.19	0.60
1:B:146:SER:O	1:B:150:LYS:N	2.28	0.60
1:B:229:ILE:HD11	1:B:255:ILE:HG23	1.84	0.60
1:B:113:TYR:HA	1:B:116:LEU:HB2	1.84	0.60
1:D:341:GLU:O	1:D:343:ARG:N	2.32	0.60
1:A:190:GLY:O	1:A:194:ASN:ND2	2.34	0.60
1:C:145:TYR:O	1:C:150:LYS:NZ	2.35	0.60
1:F:356:TYR:HA	1:F:360:GLU:HB2	1.82	0.60
1:K:224:LYS:HE2	1:L:257:ARG:HH22	1.67	0.59
1:G:79:TRP:HE1	1:G:91:VAL:HB	1.67	0.59
1:I:314:MET:HE3	1:I:330:LEU:HD13	1.84	0.59
1:A:245:TYR:HB3	1:A:279:ILE:HG23	1.84	0.59
1:F:372:GLU:O	1:F:374:ILE:N	2.35	0.59
1:G:141:VAL:O	1:G:143:LYS:N	2.35	0.59
1:K:98:LEU:HA	1:K:101:GLU:HB2	1.84	0.59
1:E:123:ILE:HD13	1:E:159:LEU:HD11	1.84	0.59
1:F:102:MET:HE1	1:F:110:ILE:HG22	1.85	0.59
1:K:226:ARG:O	1:K:230:ASN:ND2	2.35	0.59
1:J:252:TYR:HB3	1:J:276:MET:HE2	1.84	0.59
1:C:347:LYS:HD2	1:C:350:LEU:HD21	1.85	0.59
1:K:294:LEU:HD22	1:K:314:MET:HE1	1.85	0.59
1:L:350:LEU:HD11	1:L:386:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ARG:NH1	2:R:32:GLY:O	2.36	0.58
1:H:290:LYS:NZ	1:H:323:GLU:OE1	2.36	0.58
1:D:363:LYS:HB3	1:D:366:LYS:HE2	1.84	0.58
1:G:257:ARG:HD2	1:H:85:HIS:HB3	1.85	0.58
1:B:216:LEU:HD21	1:B:220:ARG:HE	1.68	0.58
1:H:123:ILE:HG21	1:H:159:LEU:HD23	1.84	0.58
1:K:229:ILE:HD11	1:K:255:ILE:HB	1.85	0.58
1:H:209:ILE:O	1:H:213:ASN:ND2	2.35	0.58
1:H:374:ILE:HG13	1:H:375:PRO:HD3	1.85	0.58
1:A:108:PHE:O	1:A:112:ASN:ND2	2.37	0.58
1:E:131:LEU:HD23	1:E:160:LEU:HD23	1.86	0.58
1:A:69:GLU:HG3	1:A:110:ILE:HD11	1.85	0.57
1:B:123:ILE:HG13	1:B:163:LEU:HD11	1.86	0.57
1:J:75:LYS:HG2	1:J:98:LEU:HD21	1.85	0.57
1:F:336:ASP:HA	1:F:339:LYS:HE3	1.87	0.57
1:A:395:GLU:HG2	1:A:410:TYR:CZ	2.39	0.57
1:D:338:ALA:HB1	1:D:348:LEU:HB2	1.85	0.57
1:K:72:VAL:O	1:K:76:LEU:HG	2.05	0.57
1:D:336:ASP:OD1	1:D:337:ALA:N	2.38	0.57
1:K:119:THR:HG23	1:K:131:LEU:HD11	1.85	0.57
1:J:339:LYS:HD2	1:J:348:LEU:HD11	1.87	0.57
1:K:166:ARG:NH1	1:K:169:ASP:OD2	2.38	0.57
1:B:393:LEU:O	1:B:396:HIS:ND1	2.32	0.56
1:D:182:LYS:NZ	1:D:192:TYR:OH	2.35	0.56
1:K:376:LEU:O	1:K:387:LYS:NZ	2.38	0.56
1:F:212:VAL:HG11	1:F:235:ILE:HG23	1.86	0.56
1:J:305:LEU:HB2	1:J:347:LYS:HZ2	1.71	0.56
1:B:105:VAL:HG11	1:B:110:ILE:HG21	1.87	0.56
1:D:331:ILE:HD12	1:D:355:ARG:HB2	1.88	0.56
1:K:308:LEU:HA	1:K:311:ILE:HB	1.88	0.56
1:K:375:PRO:HB2	1:K:376:LEU:HD23	1.89	0.55
1:F:164:GLN:OE1	1:F:166:ARG:NH1	2.39	0.55
1:I:357:LYS:HE2	1:I:393:LEU:HD21	1.88	0.55
1:H:145:TYR:O	1:H:150:LYS:NZ	2.32	0.55
1:L:135:LEU:HD12	1:L:160:LEU:HD12	1.87	0.55
1:F:395:GLU:HG2	1:F:406:SER:HB2	1.89	0.54
1:J:235:ILE:HG13	1:J:251:MET:HE1	1.90	0.54
1:L:204:ILE:O	1:L:205:HIS:ND1	2.40	0.54
1:F:216:LEU:HD11	1:F:228:ILE:HG23	1.90	0.54
1:H:278:SER:OG	1:H:282:LYS:NZ	2.40	0.54
1:J:350:LEU:HD23	1:J:351:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD12	1:A:319:ILE:HD11	1.90	0.54
1:F:196:ALA:HB1	1:F:212:VAL:HG23	1.90	0.54
1:D:327:ALA:HA	1:D:330:LEU:HD12	1.90	0.54
1:L:256:LEU:HD22	1:L:276:MET:HE1	1.89	0.54
1:K:393:LEU:HA	1:K:396:HIS:HB3	1.89	0.54
1:J:387:LYS:HA	1:J:390:TYR:CE2	2.43	0.54
1:B:199:TYR:HB3	1:B:205:HIS:HB2	1.90	0.53
1:I:361:GLU:HG3	1:I:362:ALA:N	2.24	0.53
1:D:99:GLN:OE1	1:D:114:TYR:OH	2.27	0.53
1:G:70:GLU:HB2	1:G:73:LYS:HG3	1.90	0.53
1:G:252:TYR:HD1	1:G:255:ILE:HD11	1.74	0.53
1:F:246:GLU:HG2	1:F:250:LYS:HE3	1.91	0.53
1:C:116:LEU:HD23	1:C:152:LEU:HB2	1.90	0.53
1:L:154:MET:HE2	1:L:176:LYS:HG2	1.90	0.53
1:E:165:TYR:OH	1:E:304:ASP:OD1	2.25	0.53
1:E:229:ILE:HD13	1:E:268:LEU:HD13	1.91	0.53
1:E:410:TYR:HA	1:E:413:VAL:HG22	1.91	0.53
1:D:207:LEU:HA	1:D:210:HIS:HB3	1.90	0.52
1:D:257:ARG:HH11	1:D:258:GLU:HG2	1.74	0.52
1:D:365:TYR:O	1:D:369:LEU:N	2.41	0.52
1:H:260:THR:HA	1:H:265:LYS:HE2	1.90	0.52
1:K:113:TYR:HD1	1:K:114:TYR:N	2.08	0.52
1:L:116:LEU:HD12	1:L:138:LEU:HD13	1.91	0.52
1:C:395:GLU:HG2	1:C:409:TYR:HD2	1.74	0.52
1:B:311:ILE:HG13	1:B:330:LEU:HD12	1.91	0.52
1:L:235:ILE:HG13	1:L:251:MET:HE1	1.91	0.52
1:K:398:SER:OG	1:K:402:ARG:O	2.24	0.52
1:G:136:ASP:OD1	1:G:157:ARG:NH2	2.42	0.52
1:G:196:ALA:HB1	1:G:212:VAL:HG23	1.91	0.52
1:K:356:TYR:O	1:K:365:TYR:OH	2.27	0.52
1:F:91:VAL:HG21	1:F:124:MET:HE1	1.91	0.52
1:B:387:LYS:HD3	1:B:416:LEU:HD23	1.91	0.52
1:J:108:PHE:O	1:J:112:ASN:ND2	2.37	0.52
1:J:226:ARG:O	1:J:230:ASN:ND2	2.42	0.52
1:K:113:TYR:HD1	1:K:113:TYR:C	2.17	0.52
1:B:321:LEU:HD23	1:B:322:GLU:H	1.75	0.52
1:J:402:ARG:HB3	1:J:403:PHE:HA	1.91	0.52
1:E:229:ILE:HD11	1:E:255:ILE:HG23	1.92	0.51
1:H:385:GLU:HA	1:H:388:LYS:HE2	1.91	0.51
1:K:196:ALA:HB1	1:K:212:VAL:HG23	1.92	0.51
1:A:174:LEU:HB3	1:A:195:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:HG21	1:A:234:LEU:HD22	1.91	0.51
1:B:192:TYR:HD1	1:B:211:PHE:HD1	1.56	0.51
1:K:194:ASN:HD21	2:W:31:VAL:HG22	1.74	0.51
1:L:218:GLY:O	1:L:221:SER:OG	2.24	0.51
1:I:366:LYS:HD3	1:I:369:LEU:HD12	1.91	0.51
1:C:235:ILE:HG23	1:C:251:MET:HE1	1.92	0.51
1:H:233:ILE:HG12	1:H:255:ILE:HD13	1.93	0.51
1:J:410:TYR:HE2	1:K:407:ASN:HD22	1.57	0.51
1:K:113:TYR:C	1:K:113:TYR:CD1	2.89	0.51
1:G:351:LEU:HD13	1:G:354:LEU:HD21	1.92	0.51
1:D:229:ILE:HD13	1:D:268:LEU:HD13	1.93	0.51
1:D:393:LEU:HA	1:D:396:HIS:HD2	1.75	0.51
1:C:233:ILE:HD13	1:C:271:ILE:HD11	1.93	0.50
1:E:209:ILE:HA	1:E:212:VAL:HG22	1.93	0.50
1:B:145:TYR:HB3	1:B:146:SER:HB2	1.94	0.50
1:C:216:LEU:HG	1:C:220:ARG:HE	1.77	0.50
1:D:209:ILE:O	1:D:213:ASN:ND2	2.36	0.50
1:A:131:LEU:HD23	1:A:160:LEU:HD23	1.93	0.50
1:J:150:LYS:HB2	1:J:180:MET:HE1	1.93	0.50
1:D:376:LEU:HD13	1:D:387:LYS:HB2	1.92	0.50
1:G:145:TYR:HB3	1:G:149:GLN:HB2	1.93	0.50
1:H:203:ASP:HB3	1:H:204:ILE:HG13	1.93	0.50
1:B:247:GLU:N	1:B:247:GLU:OE1	2.43	0.50
1:E:309:ASP:HB2	1:E:347:LYS:HE2	1.94	0.50
1:B:120:ARG:HA	1:B:123:ILE:HG22	1.93	0.49
1:B:202:LEU:HB3	1:B:205:HIS:HE1	1.77	0.49
1:C:230:ASN:HA	1:C:233:ILE:HD12	1.93	0.49
1:J:229:ILE:HD11	1:J:255:ILE:HG23	1.93	0.49
1:B:122:LEU:HD21	1:B:130:ALA:HB3	1.94	0.49
1:C:86:LEU:HG	1:C:124:MET:HE2	1.94	0.49
1:F:252:TYR:HB3	1:F:276:MET:HE3	1.94	0.49
1:H:353:MET:HE1	1:H:387:LYS:HE3	1.93	0.49
1:G:298:GLN:O	1:G:301:LYS:NZ	2.42	0.49
1:A:403:PHE:HB3	1:D:403:PHE:CE2	2.48	0.49
1:C:230:ASN:HD22	2:O:28:PRO:HB3	1.77	0.49
1:K:363:LYS:HG2	1:K:364:ASP:H	1.78	0.49
1:C:174:LEU:HB3	1:C:195:ILE:HG12	1.93	0.49
1:A:293:TYR:HB3	1:A:314:MET:HE3	1.94	0.49
1:F:285:LYS:O	1:F:287:GLN:N	2.44	0.49
1:G:180:MET:HG2	1:G:184:GLN:HE21	1.77	0.49
1:K:118:TYR:HA	1:K:121:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:HD23	1:F:160:LEU:HD23	1.94	0.49
1:G:285:LYS:O	1:G:287:GLN:N	2.44	0.49
1:B:375:PRO:HG2	1:B:376:LEU:HD12	1.94	0.49
1:F:395:GLU:HG3	1:F:410:TYR:HB2	1.95	0.49
1:J:165:TYR:CZ	1:J:305:LEU:HD23	2.48	0.49
1:B:146:SER:H	1:B:149:GLN:HB2	1.77	0.48
1:B:280:TYR:HA	1:B:283:LYS:HB3	1.95	0.48
1:D:131:LEU:HD23	1:D:160:LEU:HD23	1.95	0.48
1:G:372:GLU:HA	1:G:375:PRO:HD2	1.95	0.48
1:E:281:TYR:HD1	1:E:317:VAL:HG23	1.78	0.48
1:I:369:LEU:O	1:I:390:TYR:OH	2.30	0.48
1:B:309:ASP:HA	1:B:347:LYS:HE2	1.95	0.48
1:E:286:TYR:HB3	1:E:317:VAL:HG22	1.95	0.48
1:K:410:TYR:HA	1:K:413:VAL:HG22	1.95	0.48
1:G:293:TYR:HB3	1:G:314:MET:HE3	1.95	0.48
1:I:407:ASN:OD1	1:L:406:SER:OG	2.28	0.48
1:C:279:ILE:HA	1:C:282:LYS:HB2	1.95	0.48
1:C:246:GLU:O	1:C:250:LYS:HG2	2.14	0.48
1:H:200:THR:HG21	1:H:234:LEU:HD22	1.94	0.48
1:J:328:ARG:HA	1:J:331:ILE:HG22	1.96	0.48
1:L:395:GLU:O	1:L:399:SER:OG	2.28	0.48
1:G:369:LEU:HA	1:G:372:GLU:HB2	1.96	0.48
1:D:289:ALA:HB3	1:D:317:VAL:HG21	1.95	0.48
1:G:387:LYS:HG3	1:G:416:LEU:HG	1.96	0.48
1:I:366:LYS:HE3	1:I:397:PHE:HB2	1.96	0.48
1:L:388:LYS:HE3	1:L:416:LEU:HD11	1.95	0.48
1:B:107:ASP:OD1	1:B:108:PHE:N	2.47	0.48
1:H:197:LEU:HD23	2:T:30:ILE:HG22	1.96	0.48
1:I:252:TYR:OH	1:I:275:ASN:ND2	2.46	0.48
1:K:135:LEU:HD21	1:K:157:ARG:HD2	1.96	0.48
1:C:226:ARG:NH1	1:C:230:ASN:OD1	2.47	0.47
1:D:143:LYS:HG3	1:D:144:LYS:HG3	1.95	0.47
1:F:116:LEU:O	1:F:119:THR:OG1	2.25	0.47
1:F:150:LYS:HB2	1:F:180:MET:HE1	1.96	0.47
1:K:258:GLU:HG2	1:L:223:TYR:O	2.14	0.47
1:E:146:SER:OG	1:E:149:GLN:NE2	2.47	0.47
1:E:309:ASP:OD1	2:Q:25:SER:N	2.47	0.47
1:K:229:ILE:O	1:K:233:ILE:HG12	2.14	0.47
1:D:369:LEU:O	1:D:372:GLU:HG3	2.14	0.47
1:J:275:ASN:O	1:J:278:SER:OG	2.24	0.47
1:A:220:ARG:HH11	1:B:220:ARG:HD3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:TYR:CZ	1:C:207:LEU:HD23	2.49	0.47
1:E:356:TYR:HD2	1:E:368:PHE:HZ	1.61	0.47
1:E:189:THR:HG21	1:E:218:GLY:HA3	1.96	0.47
1:K:252:TYR:HB3	1:K:276:MET:HE3	1.95	0.47
1:E:93:ARG:O	1:E:97:GLU:HG2	2.13	0.47
1:G:204:ILE:HD12	1:G:241:GLU:HB3	1.96	0.47
1:A:307:TYR:HD2	1:A:308:LEU:HD12	1.80	0.47
1:C:107:ASP:O	1:C:109:GLU:N	2.46	0.47
1:D:229:ILE:HD11	1:D:255:ILE:HG23	1.96	0.47
1:B:73:LYS:HA	1:B:76:LEU:HB2	1.97	0.47
1:A:264:ASP:OD1	1:A:264:ASP:N	2.48	0.47
1:I:278:SER:OG	1:I:282:LYS:NZ	2.41	0.47
1:J:331:ILE:O	1:J:335:ILE:HG12	2.15	0.47
1:B:304:ASP:OD1	1:B:305:LEU:N	2.45	0.47
1:D:174:LEU:HB3	1:D:195:ILE:HG12	1.96	0.47
1:G:111:ILE:HG22	1:G:115:LYS:HZ2	1.80	0.47
1:C:75:LYS:HZ1	1:C:98:LEU:HD21	1.79	0.46
1:H:386:LEU:HD22	1:H:387:LYS:HG2	1.97	0.46
1:I:354:LEU:HA	1:I:357:LYS:HB3	1.97	0.46
1:C:286:TYR:CG	1:C:320:LYS:HD2	2.50	0.46
1:D:119:THR:O	1:D:123:ILE:HG13	2.15	0.46
1:K:331:ILE:HG13	1:K:351:LEU:HD22	1.96	0.46
1:E:338:ALA:HB3	1:E:348:LEU:HD13	1.96	0.46
1:G:385:GLU:HB3	1:G:388:LYS:HE2	1.97	0.46
1:F:409:TYR:O	1:F:413:VAL:HG13	2.15	0.46
1:G:256:LEU:HB2	1:G:272:THR:HG21	1.97	0.46
1:H:275:ASN:OD1	2:T:25:SER:N	2.49	0.46
1:C:98:LEU:HA	1:C:101:GLU:HB2	1.96	0.46
1:I:410:TYR:HE1	1:L:414:ILE:HB	1.80	0.46
1:A:356:TYR:HA	1:A:360:GLU:HB2	1.98	0.46
1:F:235:ILE:HG13	1:F:251:MET:HE1	1.97	0.46
1:D:345:ASN:HA	1:D:348:LEU:HB3	1.98	0.46
1:G:391:VAL:HG13	1:G:409:TYR:HB3	1.97	0.46
1:H:91:VAL:HG21	1:H:124:MET:HE1	1.98	0.46
1:H:332:ASP:OD1	1:H:355:ARG:NH1	2.49	0.46
1:H:356:TYR:HA	1:H:360:GLU:HB2	1.96	0.46
1:G:209:ILE:O	1:G:213:ASN:ND2	2.47	0.46
1:H:201:HIS:HA	2:T:27:LYS:HE2	1.97	0.46
1:K:285:LYS:O	1:K:287:GLN:N	2.48	0.46
1:D:240:THR:HG23	1:D:279:ILE:HG12	1.98	0.46
1:J:123:ILE:HD11	1:J:156:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:ILE:HD13	1:J:235:ILE:HG22	1.97	0.46
1:A:126:ARG:NH1	2:M:29:ASP:OD2	2.43	0.45
1:D:136:ASP:OD1	1:D:157:ARG:NH2	2.47	0.45
1:A:406:SER:HB2	1:D:403:PHE:HZ	1.82	0.45
1:B:201:HIS:CE1	2:N:27:LYS:HD3	2.50	0.45
1:K:108:PHE:N	1:K:108:PHE:CD2	2.84	0.45
1:B:188:GLU:HG2	1:B:191:LEU:H	1.81	0.45
1:C:79:TRP:CZ3	1:C:117:LEU:HB3	2.51	0.45
1:B:117:LEU:O	1:B:120:ARG:HG3	2.17	0.45
1:G:204:ILE:HG21	1:G:242:LYS:HD3	1.99	0.45
1:C:224:LYS:O	1:C:228:ILE:HG13	2.16	0.45
1:I:242:LYS:HD2	1:I:242:LYS:HA	1.73	0.45
1:J:120:ARG:HH22	1:J:188:GLU:CD	2.25	0.45
1:G:359:PHE:N	1:G:360:GLU:HA	2.31	0.45
1:H:203:ASP:HA	1:H:204:ILE:HA	1.60	0.45
1:K:131:LEU:HD23	1:K:160:LEU:HD23	1.97	0.45
1:K:165:TYR:CD2	1:K:343:ARG:HB3	2.52	0.45
1:E:196:ALA:HB1	1:E:212:VAL:HG13	1.99	0.45
1:K:293:TYR:CZ	1:K:313:GLU:HB3	2.52	0.45
1:D:366:LYS:O	1:D:369:LEU:HB2	2.17	0.45
1:E:287:GLN:HA	1:E:290:LYS:HE2	1.98	0.45
1:I:410:TYR:CE1	1:L:414:ILE:HB	2.52	0.45
1:F:119:THR:O	1:F:123:ILE:HG13	2.17	0.45
1:F:314:MET:HA	1:F:317:VAL:HG12	1.99	0.45
1:H:109:GLU:HA	1:H:112:ASN:HD22	1.82	0.45
1:B:168:LYS:HG2	1:B:202:LEU:HD21	1.98	0.44
1:E:361:GLU:HA	1:E:362:ALA:HA	1.70	0.44
1:L:108:PHE:O	1:L:112:ASN:ND2	2.50	0.44
1:A:204:ILE:HG13	1:A:242:LYS:HE3	1.99	0.44
1:B:79:TRP:CH2	1:B:98:LEU:HD13	2.52	0.44
1:B:154:MET:HA	1:B:157:ARG:HG2	1.98	0.44
1:B:347:LYS:HD2	1:B:347:LYS:HA	1.86	0.44
1:C:203:ASP:OD2	1:C:386:LEU:N	2.50	0.44
1:L:313:GLU:O	1:L:317:VAL:HG13	2.17	0.44
1:B:165:TYR:O	1:B:167:TRP:N	2.51	0.44
1:D:273:LEU:HD22	1:D:292:TYR:HD1	1.82	0.44
1:E:331:ILE:O	1:E:335:ILE:HG12	2.18	0.44
1:F:296:SER:O	1:F:300:GLN:HG3	2.17	0.44
1:K:94:ILE:O	1:K:98:LEU:HG	2.17	0.44
1:L:281:TYR:CD1	1:L:317:VAL:HG12	2.52	0.44
1:C:116:LEU:O	1:C:119:THR:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ILE:HD12	1:C:354:LEU:HD22	2.00	0.44
1:F:256:LEU:HB2	1:F:272:THR:HG21	1.99	0.44
1:L:91:VAL:HG21	1:L:124:MET:HE1	1.99	0.44
1:L:258:GLU:O	1:L:261:SER:OG	2.30	0.44
1:A:409:TYR:O	1:A:413:VAL:HG23	2.18	0.44
1:D:76:LEU:HD22	1:D:117:LEU:HD12	1.99	0.44
1:I:76:LEU:HD12	1:I:117:LEU:HD12	2.00	0.44
1:L:143:LYS:HE3	1:L:143:LYS:HB2	1.90	0.44
1:D:252:TYR:CD1	1:D:272:THR:HG23	2.53	0.44
1:E:168:LYS:NZ	1:E:172:ASP:OD2	2.50	0.44
1:E:216:LEU:HD11	1:E:228:ILE:HG23	1.99	0.44
1:I:119:THR:O	1:I:123:ILE:HG13	2.18	0.44
1:I:201:HIS:CE1	2:U:27:LYS:HG3	2.52	0.44
1:I:410:TYR:O	1:I:413:VAL:HG12	2.18	0.44
1:J:256:LEU:HD22	1:J:276:MET:HE1	2.00	0.44
1:C:356:TYR:HE2	1:C:363:LYS:HB3	1.82	0.44
1:E:388:LYS:HG3	1:E:416:LEU:HD22	1.99	0.44
1:F:67:ASP:OD1	1:F:67:ASP:N	2.51	0.44
1:H:369:LEU:HD21	1:H:390:TYR:HB2	2.00	0.44
1:J:135:LEU:HD12	1:J:160:LEU:HD22	1.99	0.44
1:K:227:ASN:HA	1:K:230:ASN:HD22	1.83	0.44
1:L:145:TYR:O	1:L:150:LYS:NZ	2.51	0.44
1:A:308:LEU:O	1:A:311:ILE:HG13	2.18	0.44
1:B:150:LYS:O	1:B:154:MET:HG2	2.18	0.44
1:C:313:GLU:HA	1:C:316:LEU:HD12	2.00	0.44
1:D:241:GLU:OE1	1:D:282:LYS:NZ	2.51	0.44
1:H:325:GLU:HG2	1:H:326:GLU:H	1.83	0.44
1:I:161:CYS:SG	1:I:166:ARG:NH1	2.88	0.44
1:I:272:THR:HG22	1:I:276:MET:HE3	2.00	0.44
1:J:102:MET:HE1	1:J:110:ILE:HG22	2.00	0.44
1:K:98:LEU:HD13	1:K:114:TYR:HE1	1.83	0.43
1:K:173:TYR:O	1:K:177:THR:HG23	2.18	0.43
1:B:164:GLN:HA	1:B:343:ARG:HG2	2.00	0.43
1:C:369:LEU:HA	1:C:372:GLU:HB3	1.99	0.43
1:I:107:ASP:HB3	1:I:110:ILE:HG12	2.00	0.43
1:I:120:ARG:HA	1:I:123:ILE:HD12	2.00	0.43
1:I:286:TYR:HD1	1:I:317:VAL:HG23	1.83	0.43
1:I:369:LEU:HD22	1:I:390:TYR:HE1	1.82	0.43
1:L:116:LEU:O	1:L:119:THR:HB	2.18	0.43
1:B:236:ALA:O	1:B:240:THR:OG1	2.36	0.43
1:J:272:THR:O	1:J:276:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:THR:O	1:A:123:ILE:HG13	2.18	0.43
1:C:325:GLU:CD	1:C:325:GLU:H	2.26	0.43
1:H:86:LEU:HG	1:H:124:MET:HE2	2.01	0.43
1:L:92:GLU:OE2	1:L:125:LYS:NZ	2.51	0.43
1:G:111:ILE:HG22	1:G:115:LYS:NZ	2.33	0.43
1:I:354:LEU:HD23	1:I:354:LEU:H	1.83	0.43
1:J:84:VAL:HG22	1:J:120:ARG:HH12	1.84	0.43
1:C:80:LEU:HD13	1:C:117:LEU:HD11	2.01	0.43
1:C:209:ILE:HG23	1:C:235:ILE:HD13	1.99	0.43
1:F:278:SER:OG	1:F:313:GLU:OE1	2.31	0.43
1:G:328:ARG:HA	1:G:331:ILE:HG22	2.00	0.43
1:I:116:LEU:O	1:I:119:THR:HB	2.18	0.43
1:K:115:LYS:HD3	1:K:138:LEU:HD21	2.01	0.43
1:C:413:VAL:O	1:C:417:MET:HG2	2.19	0.43
1:D:229:ILE:O	1:D:233:ILE:HG13	2.18	0.43
1:E:74:GLY:O	1:E:78:GLU:HG2	2.18	0.43
1:E:409:TYR:O	1:E:413:VAL:HG13	2.19	0.43
1:G:106:LEU:HA	1:G:111:ILE:HD11	2.00	0.43
1:G:405:GLU:C	1:G:407:ASN:H	2.27	0.43
1:J:296:SER:O	1:J:300:GLN:HG3	2.18	0.43
1:A:126:ARG:HA	1:A:126:ARG:HD3	1.87	0.43
1:A:406:SER:O	1:A:408:ARG:N	2.52	0.43
1:C:131:LEU:HD23	1:C:160:LEU:HD23	1.99	0.43
1:C:236:ALA:O	1:C:240:THR:HG23	2.19	0.43
1:C:401:SER:OG	1:C:402:ARG:N	2.52	0.43
1:D:345:ASN:O	1:D:348:LEU:HB3	2.18	0.43
1:F:374:ILE:H	1:F:375:PRO:HD3	1.84	0.43
1:G:229:ILE:O	1:G:233:ILE:HG13	2.18	0.43
1:I:135:LEU:HD12	1:I:160:LEU:HD22	2.00	0.43
1:B:113:TYR:O	1:B:117:LEU:HG	2.18	0.43
1:D:178:GLU:O	1:D:182:LYS:HG2	2.18	0.43
1:H:131:LEU:HD23	1:H:160:LEU:HD13	2.01	0.43
1:C:291:LYS:NZ	1:C:295:ASP:OD1	2.49	0.42
1:D:281:TYR:HE1	1:D:320:LYS:HG3	1.85	0.42
1:E:314:MET:HA	1:E:317:VAL:HG12	2.00	0.42
1:F:264:ASP:OD1	1:F:264:ASP:N	2.51	0.42
1:F:269:LEU:HB3	1:F:299:LEU:HD13	2.00	0.42
1:F:308:LEU:HD23	1:F:347:LYS:HB3	2.01	0.42
1:H:222:GLU:HG3	1:H:224:LYS:HG2	2.00	0.42
1:K:146:SER:HB2	1:K:149:GLN:HG3	2.00	0.42
1:I:356:TYR:HB3	1:I:365:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:CE2	1:A:188:GLU:HG3	2.55	0.42
1:L:218:GLY:O	1:L:222:GLU:HG2	2.20	0.42
1:C:349:TYR:HB3	1:C:372:GLU:OE1	2.19	0.42
1:E:366:LYS:NZ	1:E:370:GLU:OE2	2.48	0.42
1:H:407:ASN:HA	1:H:410:TYR:HD2	1.83	0.42
1:I:387:LYS:O	1:I:391:VAL:HG22	2.20	0.42
1:K:174:LEU:HB3	1:K:195:ILE:HG12	2.01	0.42
1:D:353:MET:HE1	1:D:390:TYR:CE2	2.54	0.42
1:L:224:LYS:O	1:L:228:ILE:HG13	2.20	0.42
1:L:272:THR:O	1:L:276:MET:HG3	2.19	0.42
1:B:120:ARG:HE	1:B:120:ARG:HB2	1.69	0.42
1:E:155:TYR:O	1:E:159:LEU:HG	2.19	0.42
1:H:237:VAL:O	1:H:240:THR:OG1	2.29	0.42
1:I:309:ASP:OD2	2:U:25:SER:N	2.52	0.42
1:J:66:ARG:HD2	1:J:69:GLU:HG3	2.01	0.42
1:L:331:ILE:HD12	1:L:359:PHE:HE2	1.84	0.42
1:A:413:VAL:O	1:A:417:MET:HG2	2.19	0.42
1:B:347:LYS:HD2	1:B:350:LEU:HD21	2.02	0.42
1:D:355:ARG:NH2	1:D:360:GLU:OE2	2.53	0.42
1:E:286:TYR:HB2	1:E:321:LEU:HD21	2.02	0.42
1:J:226:ARG:O	1:J:229:ILE:HG22	2.19	0.42
1:K:123:ILE:HD11	2:W:30:ILE:HD11	2.00	0.42
1:L:165:TYR:CZ	1:L:305:LEU:HB2	2.54	0.42
1:L:200:THR:HG21	1:L:234:LEU:HD22	2.01	0.42
1:I:229:ILE:HD13	1:I:268:LEU:HD13	2.01	0.42
1:K:256:LEU:HD22	1:K:276:MET:HE1	2.02	0.42
1:K:273:LEU:HD22	1:K:292:TYR:HD1	1.84	0.42
1:A:286:TYR:HB3	1:A:317:VAL:HG13	2.02	0.42
1:B:177:THR:HG22	1:B:191:LEU:HD11	2.01	0.42
1:E:341:GLU:HG2	1:E:343:ARG:HH11	1.85	0.42
1:F:229:ILE:HD13	1:F:268:LEU:HD13	2.00	0.42
1:G:205:HIS:HB3	1:G:208:ALA:H	1.85	0.42
1:J:398:SER:HB3	1:J:405:GLU:HB2	2.02	0.42
1:L:116:LEU:HD23	1:L:152:LEU:HB2	2.01	0.42
1:B:316:LEU:HA	1:B:319:ILE:HG12	2.02	0.42
1:C:293:TYR:OH	1:C:313:GLU:HB3	2.19	0.42
1:D:121:TYR:CZ	1:D:125:LYS:HD2	2.55	0.42
1:H:226:ARG:NH1	1:H:230:ASN:OD1	2.50	0.42
1:A:74:GLY:O	1:A:78:GLU:HG2	2.19	0.41
1:A:342:GLU:O	1:A:345:ASN:ND2	2.53	0.41
1:B:239:TYR:HD1	1:B:251:MET:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HA	1:B:311:ILE:HG22	2.01	0.41
1:H:146:SER:HB3	1:H:149:GLN:HG3	2.02	0.41
1:B:362:ALA:O	1:B:366:LYS:NZ	2.50	0.41
1:C:106:LEU:HA	1:C:111:ILE:HD11	2.02	0.41
1:D:122:LEU:HD22	1:D:131:LEU:HB2	2.02	0.41
1:H:150:LYS:O	1:H:154:MET:HG2	2.20	0.41
1:K:79:TRP:HE1	1:K:117:LEU:HD23	1.85	0.41
1:K:98:LEU:HD13	1:K:114:TYR:CE1	2.55	0.41
1:B:229:ILE:O	1:B:233:ILE:HG13	2.19	0.41
1:E:168:LYS:HD3	1:E:377:TYR:HD1	1.85	0.41
1:G:360:GLU:HG2	1:G:363:LYS:HD3	2.01	0.41
1:I:141:VAL:HG22	1:I:144:LYS:HB3	2.02	0.41
1:C:366:LYS:H	1:C:366:LYS:HG2	1.62	0.41
1:G:178:GLU:HA	1:G:191:LEU:HD21	2.02	0.41
1:K:192:TYR:HD1	1:K:211:PHE:HD1	1.68	0.41
1:K:314:MET:HG2	1:K:330:LEU:HD13	2.03	0.41
1:E:341:GLU:HB3	1:E:344:PHE:CE2	2.56	0.41
1:F:69:GLU:O	1:F:71:ASP:N	2.52	0.41
1:H:249:LEU:HG	1:H:279:ILE:HG21	2.01	0.41
1:L:314:MET:O	1:L:317:VAL:HG22	2.19	0.41
1:L:411:ARG:HA	1:L:414:ILE:HG22	2.03	0.41
1:B:302:GLN:HB3	1:B:303:ILE:H	1.56	0.41
1:C:120:ARG:O	1:C:123:ILE:HG13	2.21	0.41
1:E:209:ILE:HD11	1:E:238:SER:HB3	2.02	0.41
1:B:395:GLU:O	1:B:399:SER:OG	2.34	0.41
1:D:225:PHE:HA	1:D:228:ILE:HD12	2.01	0.41
1:L:231:CYS:O	1:L:235:ILE:HG12	2.21	0.41
1:L:307:TYR:O	1:L:310:THR:OG1	2.38	0.41
1:A:142:TYR:HA	1:A:145:TYR:CD2	2.56	0.41
1:A:406:SER:HB2	1:D:403:PHE:CZ	2.56	0.41
1:B:206:HIS:CD2	1:C:242:LYS:HD3	2.56	0.41
1:C:412:LEU:HD13	1:C:416:LEU:HD23	2.03	0.41
1:E:242:LYS:HG2	1:H:206:HIS:CE1	2.56	0.41
1:H:135:LEU:HD13	1:H:157:ARG:HD2	2.02	0.41
1:J:242:LYS:HA	1:J:242:LYS:HD3	1.88	0.41
1:K:171:LEU:HD11	1:K:199:TYR:CZ	2.55	0.41
1:L:78:GLU:OE2	1:L:90:GLN:NE2	2.53	0.41
1:B:161:CYS:SG	1:B:169:ASP:HB3	2.61	0.41
1:B:192:TYR:HD1	1:B:211:PHE:CD1	2.36	0.41
1:B:338:ALA:HB3	1:B:348:LEU:HD13	2.02	0.41
1:C:228:ILE:O	1:C:232:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:LEU:HD13	1:G:131:LEU:HA	2.03	0.41
1:H:157:ARG:NH1	1:H:160:LEU:HD23	2.36	0.41
1:I:395:GLU:HG2	1:I:406:SER:HB3	2.03	0.41
1:K:319:ILE:HG23	1:K:358:TYR:HE1	1.86	0.41
1:K:319:ILE:HD13	1:K:319:ILE:HA	1.95	0.41
1:L:119:THR:O	1:L:123:ILE:HG13	2.21	0.41
1:L:216:LEU:HD11	1:L:228:ILE:HG23	2.02	0.41
1:C:286:TYR:HB3	1:C:317:VAL:HG23	2.03	0.41
1:C:319:ILE:HD12	1:C:358:TYR:CE2	2.56	0.41
1:E:409:TYR:O	1:E:412:LEU:HB3	2.21	0.41
1:F:312:TYR:HD1	1:F:351:LEU:HD23	1.86	0.41
1:G:123:ILE:HD13	1:G:159:LEU:HD12	2.02	0.41
1:I:203:ASP:C	1:I:205:HIS:H	2.28	0.41
1:K:226:ARG:O	1:K:229:ILE:HG22	2.21	0.41
1:B:164:GLN:O	1:B:166:ARG:N	2.54	0.40
1:F:143:LYS:HD3	1:F:143:LYS:HA	1.92	0.40
1:G:304:ASP:H	1:G:307:TYR:HB3	1.85	0.40
1:C:284:GLY:HA2	1:C:286:TYR:CZ	2.57	0.40
1:D:409:TYR:O	1:D:413:VAL:HG23	2.21	0.40
1:F:216:LEU:HD12	1:F:216:LEU:HA	1.90	0.40
1:H:119:THR:O	1:H:123:ILE:HG13	2.21	0.40
1:K:252:TYR:O	1:K:256:LEU:HB2	2.20	0.40
1:K:255:ILE:HD11	1:K:272:THR:OG1	2.22	0.40
1:L:90:GLN:HG3	1:L:93:ARG:HH21	1.87	0.40
1:L:123:ILE:HD13	1:L:159:LEU:HD12	2.03	0.40
1:D:150:LYS:O	1:D:154:MET:HG2	2.21	0.40
1:E:146:SER:O	1:E:149:GLN:N	2.49	0.40
1:E:229:ILE:O	1:E:233:ILE:HG13	2.21	0.40
1:I:203:ASP:HB3	1:I:204:ILE:HD12	2.04	0.40
1:I:204:ILE:HG13	1:I:241:GLU:HB3	2.02	0.40
1:K:88:LYS:HA	1:K:91:VAL:HG22	2.02	0.40
1:K:251:MET:O	1:K:255:ILE:HG23	2.21	0.40
1:K:264:ASP:OD1	1:K:264:ASP:N	2.54	0.40
1:L:353:MET:HG3	1:L:390:TYR:CE1	2.56	0.40
1:L:355:ARG:HD2	1:L:359:PHE:HB2	2.03	0.40
1:E:363:LYS:HB3	1:E:364:ASP:OD1	2.21	0.40
1:I:314:MET:HE2	1:I:314:MET:HB3	1.96	0.40
1:I:414:ILE:HA	1:I:417:MET:HG2	2.03	0.40
1:K:233:ILE:HD11	1:K:255:ILE:HD13	2.03	0.40
1:A:390:TYR:CE1	1:A:394:ALA:HB2	2.57	0.40
1:D:312:TYR:CE1	1:D:354:LEU:HD22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:GLY:HA2	2:Q:31:VAL:HG11	2.03	0.40
1:J:228:ILE:O	1:J:232:GLN:HG2	2.21	0.40
1:K:347:LYS:O	1:K:351:LEU:HG	2.22	0.40
2:T:27:LYS:HA	2:T:28:PRO:HD3	1.97	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	339/372 (91%)	323 (95%)	13 (4%)	3 (1%)	14	47
1	B	338/372 (91%)	313 (93%)	21 (6%)	4 (1%)	10	42
1	C	336/372 (90%)	314 (94%)	19 (6%)	3 (1%)	14	47
1	D	338/372 (91%)	316 (94%)	20 (6%)	2 (1%)	21	56
1	E	335/372 (90%)	312 (93%)	20 (6%)	3 (1%)	14	47
1	F	337/372 (91%)	315 (94%)	20 (6%)	2 (1%)	21	56
1	G	341/372 (92%)	323 (95%)	14 (4%)	4 (1%)	10	42
1	H	339/372 (91%)	322 (95%)	13 (4%)	4 (1%)	10	42
1	I	340/372 (91%)	325 (96%)	13 (4%)	2 (1%)	21	56
1	J	343/372 (92%)	326 (95%)	16 (5%)	1 (0%)	36	68
1	K	336/372 (90%)	308 (92%)	24 (7%)	4 (1%)	10	42
1	L	342/372 (92%)	326 (95%)	14 (4%)	2 (1%)	21	56
2	M	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	N	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	O	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	P	6/8 (75%)	5 (83%)	1 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	R	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	S	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	T	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	U	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	V	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	W	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
2	X	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	4136/4560 (91%)	3879 (94%)	223 (5%)	34 (1%)	16	50

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ILE
1	B	166	ARG
1	F	373	ALA
1	G	142	TYR
1	H	105	VAL
1	H	342	GLU
1	A	407	ASN
1	B	165	TYR
1	C	361	GLU
1	E	104	HIS
1	J	204	ILE
1	A	301	LYS
1	C	323	GLU
1	D	203	ASP
1	H	106	LEU
1	H	203	ASP
1	I	204	ILE
1	C	108	PHE
1	D	342	GLU
1	E	203	ASP
1	F	374	ILE
1	G	361	GLU
1	K	108	PHE
1	K	203	ASP
1	K	205	HIS
1	L	70	GLU

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Mol	Chain	Res	Type
1	G	301	LYS
1	G	395	GLU
1	I	362	ALA
1	B	203	ASP
1	L	374	ILE
1	K	204	ILE
1	E	204	ILE
1	B	243	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/335 (92%)	302 (98%)	7 (2%)	44	70
1	B	308/335 (92%)	294 (96%)	14 (4%)	24	58
1	C	306/335 (91%)	287 (94%)	19 (6%)	16	49
1	D	308/335 (92%)	298 (97%)	10 (3%)	34	65
1	E	305/335 (91%)	300 (98%)	5 (2%)	55	75
1	F	307/335 (92%)	301 (98%)	6 (2%)	48	72
1	G	311/335 (93%)	296 (95%)	15 (5%)	23	56
1	H	309/335 (92%)	300 (97%)	9 (3%)	37	67
1	I	310/335 (92%)	306 (99%)	4 (1%)	61	78
1	J	313/335 (93%)	305 (97%)	8 (3%)	40	69
1	K	306/335 (91%)	292 (95%)	14 (5%)	24	58
1	L	312/335 (93%)	305 (98%)	7 (2%)	45	71
2	M	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	N	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	O	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	P	7/7 (100%)	7 (100%)	0	100	100
2	Q	7/7 (100%)	6 (86%)	1 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	S	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	T	7/7 (100%)	7 (100%)	0	100	100
2	U	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	V	7/7 (100%)	6 (86%)	1 (14%)	3	16
2	W	7/7 (100%)	7 (100%)	0	100	100
2	X	7/7 (100%)	6 (86%)	1 (14%)	3	16
All	All	3788/4104 (92%)	3658 (97%)	130 (3%)	32	64

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	141	VAL
1	A	267	VAL
1	A	288	GLN
1	A	330	LEU
1	A	340	GLN
1	A	391	VAL
1	B	76	LEU
1	B	98	LEU
1	B	120	ARG
1	B	131	LEU
1	B	189	THR
1	B	201	HIS
1	B	202	LEU
1	B	206	HIS
1	B	320	LYS
1	B	321	LEU
1	B	323	GLU
1	B	354	LEU
1	B	374	ILE
1	B	388	LYS
1	C	105	VAL
1	C	123	ILE
1	C	151	LEU
1	C	159	LEU
1	C	160	LEU
1	C	204	ILE
1	C	207	LEU

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Mol	Chain	Res	Type
1	C	212	VAL
1	C	249	LEU
1	C	267	VAL
1	C	311	ILE
1	C	314	MET
1	C	320	LYS
1	C	321	LEU
1	C	324	LEU
1	C	351	LEU
1	C	366	LYS
1	C	377	TYR
1	C	412	LEU
1	D	105	VAL
1	D	122	LEU
1	D	138	LEU
1	D	206	HIS
1	D	249	LEU
1	D	303	ILE
1	D	347	LYS
1	D	348	LEU
1	D	351	LEU
1	D	355	ARG
1	E	72	VAL
1	E	141	VAL
1	E	160	LEU
1	E	163	LEU
1	E	364	ASP
1	F	141	VAL
1	F	204	ILE
1	F	267	VAL
1	F	320	LYS
1	F	391	VAL
1	F	409	TYR
1	G	72	VAL
1	G	86	LEU
1	G	91	VAL
1	G	92	GLU
1	G	102	MET
1	G	119	THR
1	G	122	LEU
1	G	124	MET
1	G	141	VAL

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Mol	Chain	Res	Type
1	G	160	LEU
1	G	204	ILE
1	G	205	HIS
1	G	212	VAL
1	G	303	ILE
1	G	354	LEU
1	H	105	VAL
1	H	106	LEU
1	H	119	THR
1	H	152	LEU
1	H	267	VAL
1	H	349	TYR
1	H	371	ASN
1	H	374	ILE
1	H	386	LEU
1	I	98	LEU
1	I	109	GLU
1	I	234	LEU
1	I	361	GLU
1	J	103	LYS
1	J	122	LEU
1	J	235	ILE
1	J	335	ILE
1	J	350	LEU
1	J	352	LEU
1	J	353	MET
1	J	389	VAL
1	K	106	LEU
1	K	107	ASP
1	K	108	PHE
1	K	109	GLU
1	K	113	TYR
1	K	206	HIS
1	K	212	VAL
1	K	255	ILE
1	K	294	LEU
1	K	305	LEU
1	K	311	ILE
1	K	374	ILE
1	K	403	PHE
1	K	414	ILE
1	L	119	THR

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Mol	Chain	Res	Type
1	L	160	LEU
1	L	267	VAL
1	L	317	VAL
1	L	396	HIS
1	L	397	PHE
1	L	406	SER
2	M	25	SER
2	M	27	LYS
2	N	27	LYS
2	N	31	VAL
2	O	30	ILE
2	Q	31	VAL
2	R	31	VAL
2	S	30	ILE
2	S	31	VAL
2	U	27	LYS
2	V	31	VAL
2	X	27	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	104	HIS
1	A	345	ASN
1	B	90	GLN
1	B	112	ASN
1	B	187	HIS
1	B	288	GLN
1	B	302	GLN
1	D	85	HIS
1	D	112	ASN
1	D	396	HIS
1	E	149	GLN
1	E	194	ASN
1	F	230	ASN
1	G	187	HIS
1	H	99	GLN
1	H	184	GLN
1	I	306	ASN
1	J	213	ASN
1	J	244	GLN

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Mol	Chain	Res	Type
1	J	287	GLN
1	J	396	HIS
1	K	194	ASN
1	K	407	ASN
1	L	90	GLN
1	L	230	ASN
1	L	244	GLN
1	L	300	GLN
1	L	418	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	343/372 (92%)	0.13	4 (1%) 76 58	27, 72, 144, 152	0
1	B	342/372 (91%)	0.60	24 (7%) 22 14	36, 90, 143, 162	0
1	C	340/372 (91%)	0.13	6 (1%) 67 48	28, 69, 151, 163	0
1	D	342/372 (91%)	0.01	4 (1%) 76 58	31, 67, 147, 157	0
1	E	339/372 (91%)	0.31	13 (3%) 44 27	18, 76, 149, 159	0
1	F	341/372 (91%)	-0.13	4 (1%) 76 58	15, 52, 131, 155	0
1	G	345/372 (92%)	0.03	5 (1%) 73 54	16, 62, 135, 152	0
1	H	343/372 (92%)	0.11	10 (2%) 53 35	19, 79, 147, 157	0
1	I	344/372 (92%)	-0.19	2 (0%) 85 73	9, 44, 128, 145	0
1	J	347/372 (93%)	-0.09	4 (1%) 76 58	11, 51, 135, 146	0
1	K	340/372 (91%)	0.25	6 (1%) 67 48	13, 72, 134, 146	0
1	L	346/372 (93%)	-0.15	5 (1%) 73 54	18, 52, 135, 147	0
2	M	8/8 (100%)	0.12	0 100 100	46, 54, 66, 68	0
2	N	8/8 (100%)	0.53	0 100 100	57, 61, 65, 72	0
2	O	8/8 (100%)	-0.36	0 100 100	43, 46, 73, 81	0
2	P	8/8 (100%)	0.32	0 100 100	39, 42, 52, 69	0
2	Q	8/8 (100%)	-0.09	0 100 100	40, 44, 63, 63	0
2	R	8/8 (100%)	-0.07	0 100 100	17, 23, 42, 45	0
2	S	8/8 (100%)	-0.02	1 (12%) 8 6	23, 32, 47, 52	0
2	T	8/8 (100%)	0.01	0 100 100	36, 47, 53, 74	0
2	U	8/8 (100%)	-0.18	0 100 100	19, 27, 31, 36	0
2	V	8/8 (100%)	-0.04	0 100 100	22, 28, 40, 47	0
2	W	8/8 (100%)	0.25	0 100 100	31, 40, 47, 54	0
2	X	8/8 (100%)	-0.67	0 100 100	21, 25, 36, 38	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4208/4560 (92%)	0.08	88 (2%) 63 43	9, 66, 141, 163	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	LEU	5.5
1	E	80	LEU	5.1
1	E	98	LEU	4.9
1	F	410	TYR	4.6
1	E	102	MET	4.1
1	J	394	ALA	3.6
1	J	388	LYS	3.6
1	E	116	LEU	3.6
1	K	390	TYR	3.5
1	H	106	LEU	3.5
1	B	113	TYR	3.3
1	I	410	TYR	3.2
1	L	100	GLY	3.2
1	C	414	ILE	3.2
1	G	376	LEU	3.1
1	E	123	ILE	3.1
1	H	104	HIS	3.1
1	C	235	ILE	3.0
1	C	279	ILE	3.0
1	B	68	VAL	3.0
1	C	391	VAL	3.0
1	B	131	LEU	3.0
1	B	138	LEU	3.0
1	L	393	LEU	3.0
1	E	94	ILE	2.9
1	B	344	PHE	2.9
1	B	170	GLY	2.8
1	H	390	TYR	2.8
1	K	123	ILE	2.8
1	C	238	SER	2.8
1	K	98	LEU	2.8
2	S	32	GLY	2.7
1	B	311	ILE	2.7
1	D	207	LEU	2.7
1	K	376	LEU	2.7
1	G	365	TYR	2.7
1	B	303	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	158	GLY	2.7
1	H	135	LEU	2.6
1	A	238	SER	2.6
1	A	266	ASP	2.6
1	C	369	LEU	2.6
1	D	177	THR	2.6
1	B	128	ILE	2.5
1	K	77	ASP	2.5
1	K	389	VAL	2.5
1	H	105	VAL	2.5
1	B	83	LEU	2.5
1	E	72	VAL	2.5
1	A	327	ALA	2.4
1	E	114	TYR	2.4
1	E	148	PHE	2.4
1	E	76	LEU	2.4
1	B	123	ILE	2.4
1	F	389	VAL	2.4
1	B	105	VAL	2.4
1	B	112	ASN	2.3
1	E	390	TYR	2.3
1	L	386	LEU	2.3
1	B	118	TYR	2.3
1	B	200	THR	2.3
1	D	390	TYR	2.3
1	J	376	LEU	2.2
1	H	391	VAL	2.2
1	A	317	VAL	2.2
1	B	149	GLN	2.2
1	G	128	ILE	2.2
1	F	318	CYS	2.2
1	E	413	VAL	2.1
1	H	114	TYR	2.1
1	H	98	LEU	2.1
1	L	395	GLU	2.1
1	J	204	ILE	2.1
1	B	135	LEU	2.1
1	G	352	LEU	2.1
1	B	376	LEU	2.1
1	L	390	TYR	2.1
1	B	289	ALA	2.1
1	G	392	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	410	TYR	2.1
1	H	395	GLU	2.1
1	I	403	PHE	2.1
1	B	400	LEU	2.0
1	B	189	THR	2.0
1	B	281	TYR	2.0
1	B	162	CYS	2.0
1	D	313	GLU	2.0
1	F	204	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.