Worldwide PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 02:37 am BST

PDB ID	:	5K98
Title	:	Structure of HipA-HipB-O2-O3 complex
Authors	:	Schumacher, M.
Deposited on	:	2016-05-31
Resolution	:	3.99 Å(reported)

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

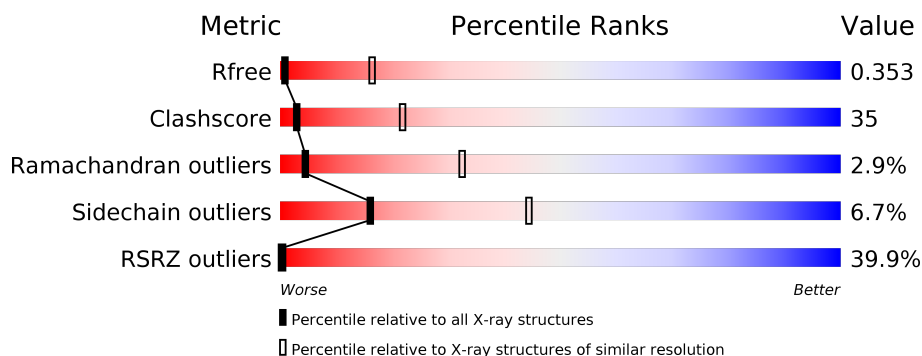|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.99 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	Percentile Ranks	Value
Rfree		0.353
Clashscore		35
Ramachandran outliers		2.9%
Sidechain outliers		6.7%
RSRZ outliers		39.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	448	37% / 48% 40% · · 8%
1	D	448	38% / 49% 38% · · 8%
2	B	91	25% / 34% 37% 7% 22%
2	P	91	24% / 36% 33% 9% 22%
3	T	23	57% / 13% 65% 22%
4	E	23	52% / 22% 35% 43%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8605 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 Serine/threonine-protein kinase HipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total 3270	C 2098	N 570	O 590	S 12	0	0	0
1	D	414	Total 3270	C 2098	N 570	O 590	S 12	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P23874
A	-6	HIS	-	expression tag	UNP P23874
A	-5	HIS	-	expression tag	UNP P23874
A	-4	HIS	-	expression tag	UNP P23874
A	-3	HIS	-	expression tag	UNP P23874
A	-2	HIS	-	expression tag	UNP P23874
A	-1	HIS	-	expression tag	UNP P23874
A	0	SER	-	expression tag	UNP P23874
A	1	ARG	-	expression tag	UNP P23874
A	309	GLN	ASP	engineered mutation	UNP P23874
D	-7	MET	-	initiating methionine	UNP P23874
D	-6	HIS	-	expression tag	UNP P23874
D	-5	HIS	-	expression tag	UNP P23874
D	-4	HIS	-	expression tag	UNP P23874
D	-3	HIS	-	expression tag	UNP P23874
D	-2	HIS	-	expression tag	UNP P23874
D	-1	HIS	-	expression tag	UNP P23874
D	0	SER	-	expression tag	UNP P23874
D	1	ARG	-	expression tag	UNP P23874
D	309	GLN	ASP	engineered mutation	UNP P23874

- Molecule 2 is a protein called Antitoxin HipB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total 564	C 358	N 95	O 108	S 3	0	0	0
2	P	71	Total 564	C 358	N 95	O 108	S 3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP M9IJX7
B	-1	SER	-	expression tag	UNP M9IJX7
B	0	HIS	-	expression tag	UNP M9IJX7
P	-2	GLY	-	expression tag	UNP M9IJX7
P	-1	SER	-	expression tag	UNP M9IJX7
P	0	HIS	-	expression tag	UNP M9IJX7

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*CP*CP*CP*TP*AP*TP*CP*CP*CP* CP*TP*TP*AP*AP*GP*GP*GP*GP*AP*TP*AP*G)-3').

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	23	Total 465	C 223	N 83	O 137	P 22	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*TP*AP*TP*CP*CP*CP*CP*TP*TP* AP*AP*GP*GP*GP*GP*AP*TP*AP*GP*GP*GP*A)-3').

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	23	Total 472	C 225	N 90	O 135	P 22	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Serine/threonine-protein kinase HipA
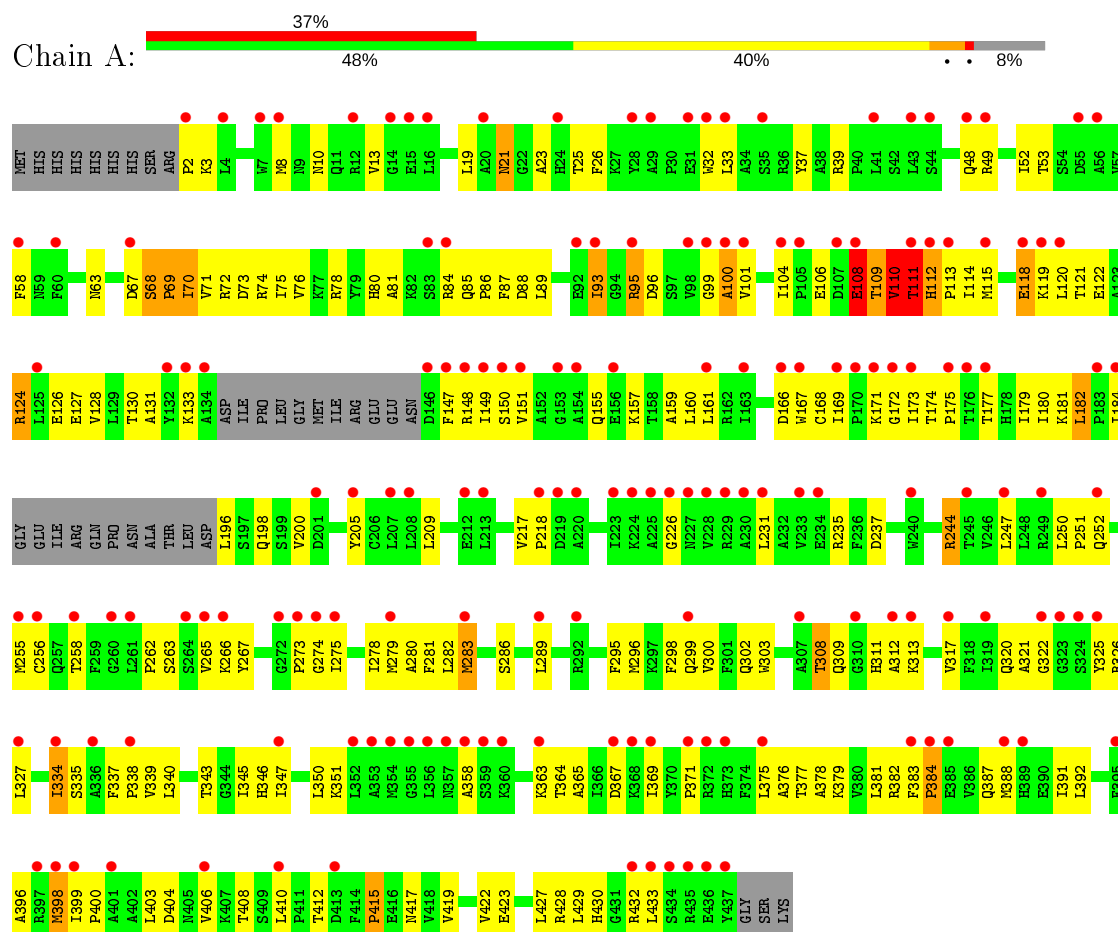
- Molecule 1: Serine/threonine-protein kinase HipA
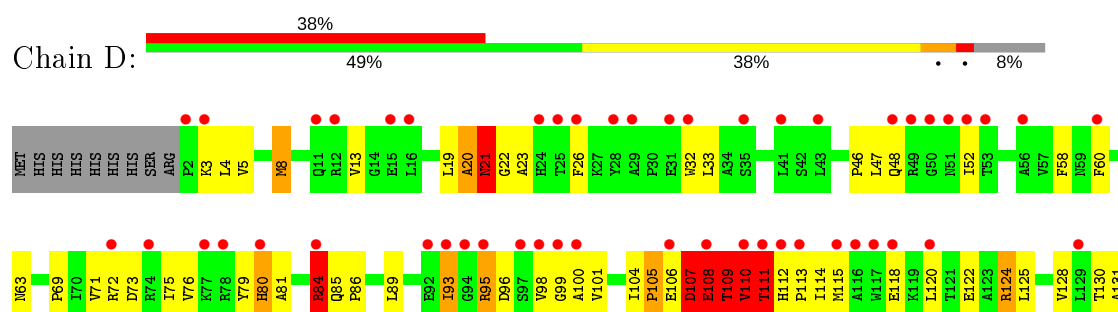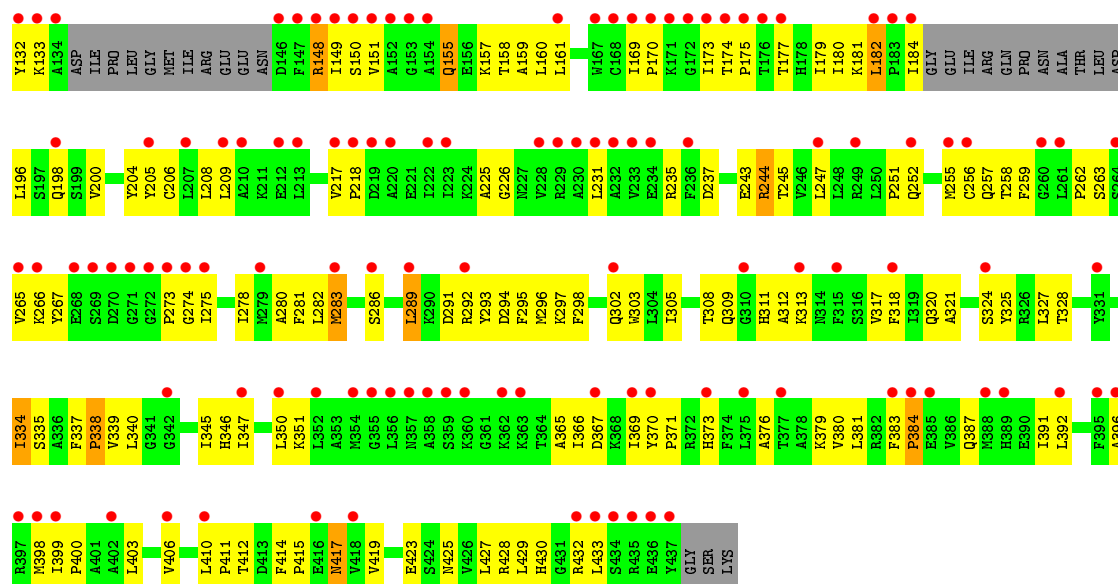
- Molecule 2: Antitoxin HipB

Chain B:

- Molecule 2: Antitoxin HipB
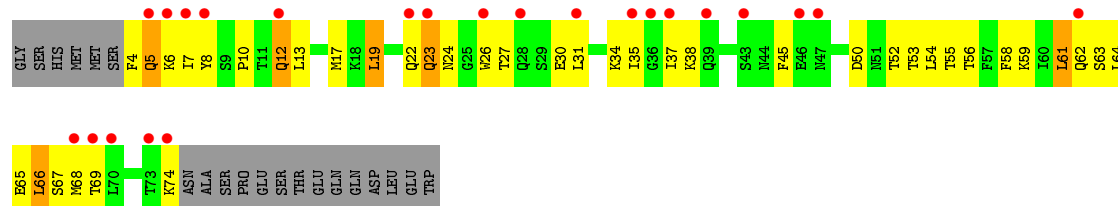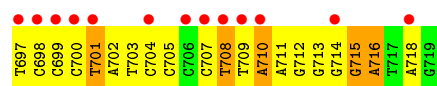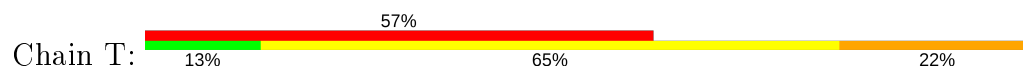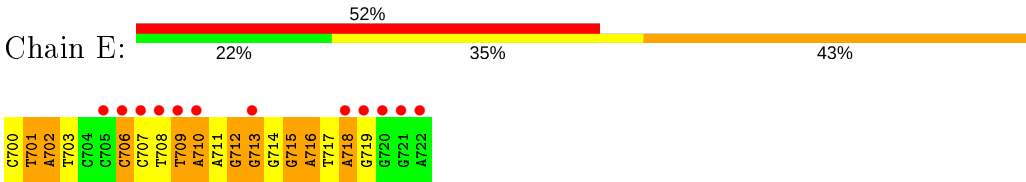
Chain P:
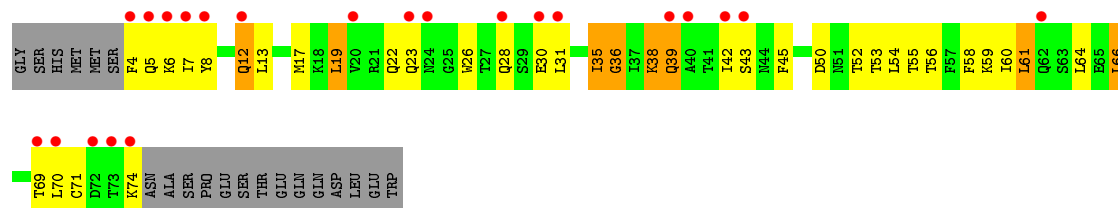
- Molecule 3: DNA (5'-D(*TP*CP*CP*CP*TP*AP*TP*CP*CP*CP*CP*TP*TP*AP*AP*GP* GP*GP*GP*AP*TP*AP*G)-3')

Chain T:

- Molecule 4: DNA (5'-D(*CP*TP*AP*TP*CP*CP*CP*CP*TP*TP*AP*AP*GP*GP*GP*GP *AP*TP*AP*GP*GP*GP*A)-3')

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	214.04Å 146.83Å 53.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.08 – 3.99 121.08 – 3.99	Depositor EDS
% Data completeness (in resolution range)	92.2 (121.08-3.99) 92.4 (121.08-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.97 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.350 , 0.375 0.327 , 0.353	Depositor DCC
R_{free} test set	1405 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	120.1	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 108.1	EDS
L-test for twinning[2]	$<|L|> = 0.36, <L^2> = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	8605	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6243e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.91	8/3343 (0.2%)	0.73	7/4530 (0.2%)
1	D	0.67	9/3343 (0.3%)	0.75	11/4530 (0.2%)
2	B	0.54	0/572	0.65	0/771
2	P	0.48	0/572	0.65	1/771 (0.1%)
3	T	1.02	1/520 (0.2%)	1.56	8/800 (1.0%)
4	E	1.00	3/530 (0.6%)	1.98	21/817 (2.6%)
All	All	0.79	21/8880 (0.2%)	0.94	48/12219 (0.4%)

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	A	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	VAL	CA-CB	30.12	2.18	1.54
1	A	110	VAL	CB-CG1	28.62	2.12	1.52
1	D	109	THR	CA-CB	15.28	1.93	1.53
1	D	107	ASP	CB-CG	11.98	1.76	1.51
1	D	109	THR	CA-C	10.09	1.79	1.52
1	A	111	THR	N-CA	9.89	1.66	1.46
1	A	110	VAL	CA-C	7.55	1.72	1.52
1	D	283	MET	CG-SD	6.92	1.99	1.81
1	D	398	MET	CG-SD	6.64	1.98	1.81
1	A	283	MET	CG-SD	6.37	1.97	1.81
3	T	708	DT	C1'-N1	6.30	1.57	1.49
1	D	107	ASP	CA-CB	6.16	1.67	1.53
1	D	110	VAL	CA-C	6.07	1.68	1.52
1	A	398	MET	CG-SD	5.91	1.96	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	715	DG	N7-C5	5.65	1.42	1.39
4	E	713	DG	N3-C4	5.38	1.39	1.35
1	D	108	GLU	CB-CG	5.25	1.62	1.52
1	A	111	THR	CA-CB	5.20	1.66	1.53
4	E	702	DA	C3'-O3'	-5.16	1.37	1.44
1	D	107	ASP	CA-C	5.07	1.66	1.52
1	A	112	HIS	N-CA	5.07	1.56	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	713	DG	O4'-C1'-N9	23.20	124.24	108.00
4	E	715	DG	O4'-C1'-N9	16.66	119.66	108.00
1	A	111	THR	N-CA-CB	15.95	140.61	110.30
3	T	708	DT	O4'-C1'-N1	11.79	116.25	108.00
1	D	109	THR	CA-CB-CG2	10.08	126.51	112.40
4	E	716	DA	O4'-C1'-N9	9.63	114.74	108.00
4	E	713	DG	N3-C4-C5	-9.54	123.83	128.60
1	D	84	ARG	NE-CZ-NH1	-9.43	115.59	120.30
1	D	109	THR	O-C-N	-9.37	107.70	122.70
1	A	110	VAL	CA-CB-CG1	9.27	124.80	110.90
1	A	110	VAL	CB-CA-C	9.03	128.56	111.40
4	E	710	DA	O4'-C1'-N9	8.29	113.80	108.00
1	D	107	ASP	CB-CG-OD1	8.18	125.66	118.30
1	D	107	ASP	CB-CA-C	8.04	126.48	110.40
4	E	712	DG	O4'-C1'-N9	7.90	113.53	108.00
2	P	38	LYS	CD-CE-NZ	7.69	129.38	111.70
3	T	716	DA	O4'-C1'-N9	7.56	113.30	108.00
3	T	715	DG	O4'-C1'-N9	7.10	112.97	108.00
4	E	709	DT	O4'-C1'-N1	7.07	112.95	108.00
3	T	701	DT	O4'-C1'-C2'	-7.04	100.27	105.90
4	E	715	DG	C4-C5-N7	-7.01	108.00	110.80
1	D	110	VAL	N-CA-C	6.95	129.77	111.00
4	E	713	DG	C8-N9-C4	-6.84	103.66	106.40
4	E	715	DG	N9-C4-C5	6.74	108.09	105.40
4	E	718	DA	O4'-C1'-N9	6.52	112.56	108.00
1	A	111	THR	N-CA-C	-6.15	94.39	111.00
1	A	70	ILE	CB-CA-C	-6.04	99.52	111.60
4	E	713	DG	O4'-C4'-C3'	5.93	109.56	106.00
4	E	713	DG	N3-C4-N9	5.85	129.51	126.00
4	E	715	DG	N7-C8-N9	5.75	115.97	113.10
3	T	708	DT	C6-N1-C2	-5.74	118.43	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	706	DC	O4'-C1'-N1	5.74	112.02	108.00
4	E	715	DG	C8-N9-C4	-5.73	104.11	106.40
1	A	111	THR	CA-CB-OG1	5.59	120.74	109.00
3	T	697	DT	O4'-C1'-N1	5.59	111.91	108.00
4	E	713	DG	C4'-C3'-C2'	-5.56	98.10	103.10
3	T	708	DT	N3-C4-O4	5.54	123.22	119.90
1	D	109	THR	CB-CA-C	5.53	126.52	111.60
1	D	108	GLU	C-N-CA	-5.41	108.19	121.70
4	E	713	DG	O4'-C1'-C2'	-5.30	101.66	105.90
1	D	107	ASP	OD1-CG-OD2	-5.29	113.24	123.30
4	E	715	DG	C5-C6-O6	5.26	131.75	128.60
1	D	110	VAL	CB-CA-C	-5.15	101.61	111.40
1	A	68	SER	N-CA-CB	-5.14	102.78	110.50
4	E	701	DT	O4'-C1'-C2'	-5.13	101.79	105.90
4	E	701	DT	C1'-O4'-C4'	-5.08	105.02	110.10
3	T	710	DA	O4'-C1'-N9	5.04	111.53	108.00
1	D	111	THR	N-CA-CB	5.04	119.88	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	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	3270	0	3313	236	10
1	D	3270	0	3313	214	10
2	B	564	0	574	52	0
2	P	564	0	574	48	0
3	T	465	0	261	37	0
4	E	472	0	260	55	0
All	All	8605	0	8295	582	10

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 35.

All (582) 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:109:THR:C	1:D:109:THR:CA	1.79	1.51
1:D:107:ASP:CB	1:D:107:ASP:CG	1.76	1.50
1:D:109:THR:CA	1:D:109:THR:CB	1.93	1.42
1:A:110:VAL:CB	1:A:110:VAL:CG1	2.12	1.27
1:A:68:SER:OG	1:A:70:ILE:HD12	1.31	1.25
1:A:112:HIS:CG	1:A:173:ILE:HG23	1.71	1.22
1:A:110:VAL:CB	1:A:110:VAL:CA	2.18	1.22
2:B:38:LYS:HD2	4:E:715:DG:C6	1.76	1.19
1:A:118:GLU:HB2	1:A:171:LYS:HE3	1.24	1.17
1:D:110:VAL:HG12	1:D:110:VAL:O	1.35	1.13
1:D:104:ILE:HG22	1:D:108:GLU:HB3	1.31	1.11
1:D:110:VAL:HG11	1:D:112:HIS:CE1	1.87	1.08
1:D:124:ARG:HH11	1:D:124:ARG:HB3	0.95	1.07
1:D:148:ARG:HG3	1:D:148:ARG:HH11	1.18	1.04
1:D:206:CYS:SG	1:D:305:ILE:HD12	1.97	1.03
1:A:95:ARG:NE	1:A:112:HIS:HE1	1.58	1.01
1:A:95:ARG:CD	1:A:112:HIS:CE1	2.45	1.00
1:A:110:VAL:CB	1:A:110:VAL:HA	1.92	0.99
1:D:106:GLU:O	1:D:107:ASP:C	2.02	0.96
1:D:124:ARG:NH1	1:D:124:ARG:HB3	1.80	0.95
2:P:39:GLN:HE22	4:E:702:DA:H62	1.06	0.95
1:A:112:HIS:HB2	1:A:173:ILE:HG12	1.48	0.94
1:A:345:ILE:H	1:A:345:ILE:HD12	1.33	0.94
1:A:95:ARG:NE	1:A:112:HIS:CE1	2.36	0.93
1:A:95:ARG:HD3	1:A:112:HIS:ND1	1.84	0.93
1:D:345:ILE:H	1:D:345:ILE:HD12	1.33	0.92
1:A:68:SER:HG	1:A:70:ILE:HD12	1.34	0.91
1:D:20:ALA:O	1:D:22:GLY:N	2.03	0.91
1:A:112:HIS:CD2	1:A:173:ILE:HG23	2.05	0.90
1:A:429:LEU:HD23	1:A:432:ARG:HH12	1.34	0.90
1:A:112:HIS:CB	1:A:173:ILE:HG23	2.02	0.90
1:A:118:GLU:HB2	1:A:171:LYS:CE	2.01	0.89
1:D:110:VAL:HG11	1:D:112:HIS:NE2	1.86	0.89
1:D:105:PRO:HB2	1:D:108:GLU:HB2	1.54	0.89
1:D:110:VAL:O	1:D:112:HIS:N	2.06	0.89
3:T:713:DG:H2"	2:P:38:LYS:HD3	1.54	0.88
1:D:399:ILE:HB	1:D:430:HIS:HD2	1.38	0.87
1:D:106:GLU:O	1:D:107:ASP:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:707:DC:H2"	4:E:708:DT:H5'	1.54	0.87
3:T:700:DC:H42	4:E:719:DG:H1	1.22	0.87
1:D:399:ILE:HB	1:D:430:HIS:CD2	2.09	0.87
1:A:399:ILE:HB	1:A:430:HIS:HD2	1.40	0.85
1:D:429:LEU:HD23	1:D:432:ARG:HH12	1.41	0.85
1:A:99:GLY:HA2	1:A:252:GLN:HG2	1.55	0.85
2:B:38:LYS:HD2	4:E:715:DG:C5	2.11	0.85
1:D:124:ARG:HH11	1:D:124:ARG:CB	1.86	0.85
1:A:63:ASN:OD1	1:A:263:SER:HB3	1.76	0.85
2:B:27:THR:OG1	2:B:30:GLU:HG2	1.78	0.83
1:D:104:ILE:HG22	1:D:108:GLU:CB	2.07	0.83
4:E:709:DT:H1'	4:E:710:DA:H5'	1.59	0.83
2:B:38:LYS:HE2	4:E:713:DG:H2"	1.60	0.83
1:A:399:ILE:HB	1:A:430:HIS:CD2	2.13	0.83
1:D:96:ASP:HB3	1:D:149:ILE:HG23	1.59	0.83
1:D:428:ARG:HH11	1:D:428:ARG:HG2	1.42	0.83
1:A:112:HIS:CB	1:A:173:ILE:N	2.42	0.82
1:A:95:ARG:HD3	1:A:112:HIS:HD1	1.43	0.82
1:A:112:HIS:HB3	1:A:173:ILE:N	1.95	0.82
1:D:110:VAL:O	1:D:111:THR:C	2.19	0.81
2:B:38:LYS:HE2	4:E:713:DG:C2'	2.10	0.81
1:A:429:LEU:HD23	1:A:432:ARG:NH1	1.94	0.81
1:A:403:LEU:HD13	1:A:423:GLU:HG3	1.63	0.81
4:E:706:DC:H1'	4:E:707:DC:H5'	1.60	0.81
1:A:112:HIS:HB2	1:A:173:ILE:HG23	1.62	0.80
1:D:99:GLY:HA2	1:D:252:GLN:HG2	1.64	0.80
2:B:38:LYS:CE	4:E:713:DG:H2"	2.11	0.80
3:T:704:DC:O2	4:E:716:DA:H2	1.65	0.79
1:A:119:LYS:HA	1:A:168:CYS:SG	2.22	0.79
1:A:200:VAL:HG13	1:A:231:LEU:HB2	1.65	0.79
1:A:124:ARG:HH11	1:A:124:ARG:HB3	1.48	0.78
3:T:702:DA:N1	4:E:718:DA:H2	1.82	0.78
3:T:705:DC:C4	4:E:714:DG:O6	2.36	0.78
1:A:76:VAL:HG13	1:A:81:ALA:HB3	1.64	0.77
1:A:95:ARG:HD3	1:A:112:HIS:CE1	2.16	0.77
1:A:112:HIS:HB3	1:A:172:GLY:CA	2.15	0.77
1:D:110:VAL:O	1:D:110:VAL:CG1	2.21	0.77
3:T:702:DA:H2"	3:T:703:DT:H5"	1.66	0.77
1:D:109:THR:HB	1:D:109:THR:CA	2.14	0.77
3:T:698:DC:H2"	3:T:699:DC:C5	2.20	0.77
3:T:712:DG:H4'	3:T:713:DG:H5'	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:HA	1:D:283:MET:HE1	1.66	0.76
1:D:169:ILE:HG23	1:D:170:PRO:HD2	1.69	0.75
1:D:109:THR:O	1:D:110:VAL:HB	1.86	0.75
1:A:112:HIS:HB2	1:A:173:ILE:CG1	2.17	0.74
1:D:105:PRO:CB	1:D:108:GLU:HB2	2.17	0.74
1:D:383:PHE:CD1	1:D:384:PRO:HD2	2.23	0.74
1:A:151:VAL:HG12	1:A:157:LYS:HE3	1.69	0.74
1:A:49:ARG:HD2	2:B:23:GLN:HG2	1.70	0.74
2:B:7:ILE:HG23	2:B:12:GLN:HG2	1.70	0.74
2:P:39:GLN:NE2	4:E:702:DA:H62	1.85	0.74
1:D:20:ALA:C	1:D:22:GLY:H	1.91	0.73
1:D:69:PRO:HA	1:D:72:ARG:HG3	1.70	0.73
1:A:95:ARG:HD2	1:A:148:ARG:HB2	1.71	0.73
1:A:112:HIS:CB	1:A:173:ILE:H	2.02	0.72
1:D:72:ARG:O	1:D:76:VAL:HG23	1.90	0.72
2:B:10:PRO:HG2	2:B:50:ASP:OD1	1.89	0.72
1:D:76:VAL:HG22	1:D:89:LEU:HD21	1.71	0.72
1:D:392:LEU:HD22	1:D:433:LEU:HD21	1.72	0.71
1:A:21:ASN:HD21	1:A:23:ALA:CB	2.03	0.71
1:D:204:TYR:CZ	1:D:208:LEU:HD11	2.24	0.71
1:D:109:THR:O	1:D:110:VAL:CB	2.36	0.71
1:A:69:PRO:O	1:A:72:ARG:HB2	1.90	0.71
1:A:339:VAL:O	1:A:339:VAL:HG12	1.91	0.70
1:D:76:VAL:HG13	1:D:81:ALA:HB3	1.72	0.70
1:A:111:THR:HG21	1:A:114:ILE:HD11	1.74	0.70
1:D:109:THR:C	1:D:109:THR:HA	2.08	0.69
2:B:38:LYS:CD	4:E:713:DG:H2"	2.22	0.69
1:A:399:ILE:CB	1:A:430:HIS:HD2	2.06	0.69
1:A:95:ARG:HG2	1:A:112:HIS:CE1	2.28	0.69
1:A:85:GLN:HE21	1:A:86:PRO:HD2	1.59	0.69
1:A:21:ASN:HD21	1:A:23:ALA:HB3	1.58	0.68
1:D:120:LEU:HD22	1:D:124:ARG:NH1	2.09	0.68
1:D:384:PRO:HG2	1:D:387:GLN:NE2	2.08	0.68
1:A:298:PHE:O	1:A:302:GLN:HG3	1.93	0.68
1:A:71:VAL:O	1:A:75:ILE:HD13	1.94	0.68
1:D:148:ARG:HH11	1:D:148:ARG:CG	2.03	0.68
1:A:111:THR:HG23	1:A:112:HIS:N	2.08	0.68
1:D:76:VAL:HG21	1:D:84:ARG:HG3	1.76	0.68
3:T:701:DT:O2	3:T:702:DA:C5	2.46	0.68
1:A:280:ALA:O	1:A:283:MET:HB2	1.94	0.68
1:A:71:VAL:O	1:A:74:ARG:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ARG:HG3	1:D:148:ARG:NH1	1.98	0.67
1:D:71:VAL:O	1:D:75:ILE:HD13	1.95	0.67
1:D:5:VAL:HG23	1:D:106:GLU:HA	1.76	0.67
1:D:286:SER:HA	2:P:8:TYR:CE2	2.29	0.67
1:A:428:ARG:HG2	1:A:428:ARG:HH11	1.60	0.67
1:D:76:VAL:HG21	1:D:84:ARG:CG	2.26	0.66
1:D:58:PHE:CE1	1:D:86:PRO:HG2	2.30	0.66
1:A:112:HIS:HB2	1:A:173:ILE:CG2	2.24	0.66
1:A:96:ASP:HB3	1:A:149:ILE:HG23	1.78	0.66
2:P:6:LYS:NZ	2:P:74:LYS:HE3	2.10	0.66
1:A:95:ARG:CG	1:A:112:HIS:CE1	2.78	0.66
1:A:161:LEU:HD12	1:A:177:THR:HG23	1.77	0.66
2:B:56:THR:OG1	4:E:712:DG:H5"	1.96	0.66
2:B:55:THR:O	2:B:59:LYS:HG3	1.96	0.66
1:D:179:ILE:HD11	1:D:235:ARG:CZ	2.26	0.65
1:A:112:HIS:CD2	1:A:173:ILE:CG2	2.79	0.65
1:D:26:PHE:O	1:D:52:ILE:HG12	1.97	0.65
3:T:704:DC:O2	4:E:716:DA:C2	2.49	0.65
2:B:17:MET:SD	2:B:45:PHE:CZ	2.89	0.64
1:A:112:HIS:HB2	1:A:173:ILE:N	2.12	0.64
1:A:13:VAL:HG13	1:A:32:TRP:CE2	2.33	0.64
1:A:383:PHE:CD1	1:A:384:PRO:HD2	2.32	0.64
2:B:37:ILE:HB	4:E:713:DG:OP2	1.97	0.64
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.61	0.64
1:D:399:ILE:CB	1:D:430:HIS:HD2	2.08	0.63
2:P:19:LEU:CD2	2:P:23:GLN:HG3	2.29	0.63
1:A:111:THR:CG2	1:A:112:HIS:N	2.59	0.63
3:T:716:DA:H61	4:E:703:DT:H3	1.46	0.63
2:P:35:ILE:HG13	2:P:36:GLY:H	1.63	0.63
2:P:6:LYS:HZ1	2:P:74:LYS:HE3	1.63	0.63
2:B:17:MET:SD	2:B:45:PHE:HZ	2.21	0.63
1:D:429:LEU:HD23	1:D:432:ARG:NH1	2.12	0.63
1:A:175:PRO:HB2	1:A:247:LEU:HD23	1.81	0.63
1:A:112:HIS:HB2	1:A:173:ILE:CB	2.30	0.62
1:D:3:LYS:O	1:D:106:GLU:N	2.32	0.62
1:A:112:HIS:HB3	1:A:173:ILE:H	1.60	0.62
1:D:182:LEU:H	1:D:182:LEU:HD22	1.64	0.62
1:D:345:ILE:N	1:D:345:ILE:HD12	2.12	0.62
2:B:38:LYS:HG3	4:E:713:DG:C2'	2.30	0.62
1:A:112:HIS:CG	1:A:173:ILE:CG2	2.67	0.62
1:D:345:ILE:H	1:D:345:ILE:CD1	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:55:THR:O	2:P:59:LYS:HG3	2.00	0.62
1:A:119:LYS:HG3	1:A:166:ASP:CB	2.30	0.62
1:D:95:ARG:HB2	1:D:148:ARG:O	1.99	0.62
1:A:115:MET:CE	1:A:174:THR:HG23	2.30	0.61
1:D:179:ILE:HG12	1:D:235:ARG:HG2	1.83	0.61
1:A:68:SER:HB3	1:A:71:VAL:HG23	1.82	0.61
1:A:110:VAL:CA	1:A:110:VAL:HB	2.27	0.61
1:D:151:VAL:HG12	1:D:157:LYS:HE3	1.82	0.61
2:B:59:LYS:HA	1:D:283:MET:CE	2.29	0.61
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.63	0.61
2:B:64:LEU:O	2:B:66:LEU:HD13	2.00	0.61
1:A:75:ILE:HG22	1:A:89:LEU:HD22	1.83	0.61
1:A:205:TYR:HD1	1:A:410:LEU:HD21	1.65	0.61
1:D:175:PRO:HB2	1:D:247:LEU:HD23	1.81	0.61
4:E:712:DG:C6	4:E:713:DG:C2	2.89	0.61
1:A:159:ALA:O	1:A:160:LEU:HD23	2.00	0.60
1:A:274:GLY:O	1:A:278:ILE:HG12	2.01	0.60
1:A:256:CYS:SG	1:A:313:LYS:HG3	2.42	0.60
2:P:64:LEU:O	2:P:66:LEU:HD13	2.00	0.60
1:A:13:VAL:HG13	1:A:32:TRP:NE1	2.16	0.60
2:B:52:THR:HB	2:P:54:LEU:HD12	1.83	0.60
1:A:382:ARG:HD3	3:T:714:DG:OP1	2.01	0.60
1:D:21:ASN:HD22	1:D:22:GLY:N	1.98	0.60
1:A:120:LEU:HD22	1:A:124:ARG:HH11	1.66	0.60
1:A:110:VAL:O	1:A:111:THR:O	2.20	0.60
2:B:38:LYS:CD	4:E:715:DG:C6	2.70	0.60
1:D:281:PHE:HE2	1:D:317:VAL:HG11	1.66	0.59
1:A:320:GLN:OE1	1:A:326:ARG:HG2	2.02	0.59
1:D:21:ASN:HD22	1:D:21:ASN:C	2.05	0.59
1:A:184:ILE:HD12	1:A:196:LEU:HB2	1.84	0.59
2:P:7:ILE:HG23	2:P:12:GLN:HG2	1.83	0.59
1:D:303:TRP:HE1	1:D:369:ILE:HB	1.67	0.59
1:A:58:PHE:CE1	1:A:86:PRO:HG2	2.38	0.59
1:A:21:ASN:ND2	1:A:23:ALA:CB	2.65	0.59
2:B:26:TRP:HA	2:B:30:GLU:OE1	2.03	0.58
1:D:108:GLU:HG3	1:D:110:VAL:CG2	2.33	0.58
3:T:718:DA:H2	4:E:702:DA:C2	2.21	0.58
3:T:715:DG:O6	2:P:38:LYS:NZ	2.31	0.58
1:A:72:ARG:O	1:A:76:VAL:HG23	2.03	0.58
1:D:110:VAL:CG1	1:D:112:HIS:CE1	2.77	0.58
3:T:712:DG:H2"	3:T:713:DG:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ASN:OD1	1:D:263:SER:HB3	2.03	0.58
1:A:89:LEU:O	1:A:93:ILE:HD13	2.03	0.58
2:B:38:LYS:HE2	4:E:713:DG:C8	2.39	0.58
1:A:112:HIS:O	1:A:113:PRO:C	2.38	0.58
1:A:339:VAL:O	1:A:345:ILE:HB	2.04	0.58
1:D:159:ALA:O	1:D:160:LEU:HD23	2.03	0.58
1:D:347:ILE:HG13	1:D:367:ASP:HB2	1.86	0.58
1:D:19:LEU:HD12	1:D:23:ALA:HB3	1.85	0.58
3:T:711:DA:N1	4:E:710:DA:H5"	2.19	0.58
1:A:10:ASN:HD21	1:A:173:ILE:HD12	1.69	0.58
1:A:345:ILE:CD1	1:A:345:ILE:H	2.09	0.58
1:A:217:VAL:HB	1:A:218:PRO:HD2	1.85	0.58
1:D:370:TYR:CD2	1:D:432:ARG:HD3	2.39	0.58
1:D:48:GLN:HB2	2:P:22:GLN:HE22	1.68	0.58
1:A:48:GLN:HB2	2:B:22:GLN:HE22	1.68	0.57
1:D:157:LYS:HD3	1:D:181:LYS:HE2	1.86	0.57
1:A:112:HIS:HB2	1:A:173:ILE:H	1.68	0.57
1:D:21:ASN:HD21	1:D:23:ALA:HB3	1.69	0.57
1:D:303:TRP:NE1	1:D:369:ILE:HB	2.20	0.57
1:A:19:LEU:HB2	1:A:23:ALA:HB3	1.87	0.57
1:A:387:GLN:O	1:A:391:ILE:HG13	2.04	0.57
1:A:112:HIS:HB3	1:A:172:GLY:C	2.25	0.57
2:P:17:MET:SD	2:P:45:PHE:CZ	2.98	0.57
1:A:85:GLN:HB2	1:A:88:ASP:OD2	2.04	0.57
1:A:322:GLY:HA2	2:B:5:GLN:NE2	2.20	0.56
1:A:108:GLU:HG3	1:A:110:VAL:HG23	1.86	0.56
1:A:104:ILE:CD1	1:A:112:HIS:NE2	2.69	0.56
3:T:712:DG:H2"	3:T:713:DG:N7	2.19	0.56
2:B:69:THR:OG1	2:P:4:PHE:HB3	2.05	0.56
1:D:124:ARG:O	1:D:128:VAL:HG23	2.05	0.56
4:E:702:DA:H2"	4:E:703:DT:H71	1.88	0.56
1:A:179:ILE:HD11	1:A:235:ARG:CZ	2.35	0.56
4:E:707:DC:H2"	4:E:708:DT:C5'	2.33	0.56
1:D:298:PHE:O	1:D:302:GLN:HG3	2.06	0.56
1:D:308:THR:HG22	1:D:351:LYS:O	2.06	0.56
1:A:108:GLU:O	1:A:109:THR:C	2.42	0.56
1:A:75:ILE:CG2	1:A:89:LEU:HD22	2.36	0.56
1:D:339:VAL:O	1:D:345:ILE:HB	2.06	0.55
1:A:161:LEU:CD1	1:A:177:THR:HG23	2.36	0.55
2:P:17:MET:SD	2:P:45:PHE:HZ	2.30	0.55
4:E:714:DG:H2"	4:E:715:DG:O4'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:39:GLN:HE22	4:E:702:DA:N6	1.89	0.55
3:T:718:DA:C2	4:E:702:DA:C2	2.94	0.55
1:A:21:ASN:ND2	1:A:23:ALA:HB2	2.21	0.55
1:D:337:PHE:C	1:D:339:VAL:H	2.08	0.55
1:A:399:ILE:HG22	1:A:400:PRO:N	2.19	0.55
1:D:200:VAL:HG13	1:D:231:LEU:HB2	1.89	0.55
1:A:281:PHE:CZ	1:A:325:TYR:CE2	2.95	0.55
1:A:26:PHE:O	1:A:52:ILE:HG12	2.07	0.55
1:A:130:THR:HA	1:A:133:LYS:NZ	2.22	0.55
1:D:347:ILE:HD12	1:D:350:LEU:HD12	1.89	0.55
1:A:85:GLN:NE2	1:A:86:PRO:HD2	2.21	0.55
1:D:282:LEU:HD21	1:D:327:LEU:HD13	1.88	0.55
1:A:308:THR:HG22	1:A:351:LYS:O	2.07	0.54
1:D:115:MET:HE2	1:D:174:THR:HG23	1.89	0.54
4:E:717:DT:O2	4:E:718:DA:C2	2.60	0.54
1:A:19:LEU:HB2	1:A:21:ASN:HD21	1.72	0.54
1:A:384:PRO:HG2	1:A:387:GLN:NE2	2.22	0.54
1:D:130:THR:HA	1:D:133:LYS:NZ	2.22	0.54
1:A:347:ILE:HD12	1:A:350:LEU:HD12	1.88	0.54
1:D:370:TYR:H	1:D:373:HIS:HD1	1.55	0.54
4:E:712:DG:C5	4:E:713:DG:C4	2.95	0.54
1:D:339:VAL:HG12	1:D:339:VAL:O	2.07	0.54
1:D:428:ARG:NH1	1:D:428:ARG:HG2	2.16	0.54
2:B:35:ILE:HG23	2:B:63:SER:HB3	1.87	0.54
1:D:104:ILE:HG22	1:D:108:GLU:CG	2.38	0.54
1:D:427:LEU:HA	1:D:430:HIS:HB3	1.90	0.54
1:D:85:GLN:HE21	1:D:86:PRO:HD2	1.71	0.54
1:A:112:HIS:HB3	1:A:172:GLY:HA3	1.87	0.54
4:E:702:DA:C2'	4:E:703:DT:H71	2.38	0.54
1:A:303:TRP:NE1	1:A:369:ILE:HB	2.23	0.54
1:A:93:ILE:H	1:A:93:ILE:HD13	1.72	0.54
1:D:198:GLN:HE22	1:D:415:PRO:HB3	1.74	0.53
1:D:52:ILE:HD13	1:D:52:ILE:N	2.22	0.53
3:T:713:DG:C4	3:T:714:DG:N7	2.77	0.53
2:B:54:LEU:O	2:B:58:PHE:HD1	1.90	0.53
1:D:206:CYS:HG	1:D:305:ILE:HD12	1.73	0.53
3:T:702:DA:C2'	3:T:703:DT:H5"	2.35	0.53
1:A:104:ILE:HD12	1:A:112:HIS:NE2	2.22	0.53
1:A:278:ILE:HG21	1:A:295:PHE:CE1	2.42	0.53
2:B:35:ILE:HG21	2:B:59:LYS:O	2.09	0.53
1:D:71:VAL:O	1:D:75:ILE:CD1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HG3	1:A:166:ASP:HB3	1.89	0.53
1:D:104:ILE:CG2	1:D:108:GLU:HG2	2.38	0.53
2:B:6:LYS:HZ1	2:B:74:LYS:HG3	1.73	0.53
4:E:700:DC:H2"	4:E:701:DT:O5'	2.08	0.53
1:A:19:LEU:HD12	1:A:23:ALA:HB3	1.91	0.53
1:A:120:LEU:HD22	1:A:124:ARG:HB3	1.92	0.52
1:A:182:LEU:HD22	1:A:182:LEU:H	1.73	0.52
1:A:345:ILE:N	1:A:345:ILE:HD12	2.14	0.52
1:D:85:GLN:NE2	1:D:86:PRO:HD2	2.24	0.52
2:P:58:PHE:HA	2:P:61:LEU:HB2	1.91	0.52
1:D:410:LEU:HD13	1:D:419:VAL:HG22	1.90	0.52
1:D:108:GLU:HG3	1:D:110:VAL:HG23	1.90	0.52
1:D:291:ASP:O	1:D:292:ARG:C	2.48	0.52
2:P:19:LEU:HD22	2:P:23:GLN:HG3	1.91	0.52
1:A:95:ARG:HE	1:A:112:HIS:HE1	1.52	0.52
1:D:243:GLU:CB	1:D:245:THR:HG23	2.40	0.52
1:A:19:LEU:HB2	1:A:21:ASN:ND2	2.25	0.52
1:D:237:ASP:HB3	1:D:252:GLN:OE1	2.10	0.52
1:D:21:ASN:ND2	1:D:23:ALA:H	2.07	0.52
2:P:53:THR:HG22	2:P:55:THR:H	1.75	0.52
1:D:370:TYR:CE2	1:D:432:ARG:HD3	2.45	0.51
2:B:35:ILE:CG2	2:B:63:SER:HB3	2.40	0.51
2:B:69:THR:HG22	2:P:69:THR:HG23	1.92	0.51
1:D:96:ASP:CB	1:D:149:ILE:HG23	2.37	0.51
1:A:209:LEU:HA	1:A:406:VAL:HG21	1.91	0.51
4:E:716:DA:H2"	4:E:717:DT:H5'	1.93	0.51
2:P:53:THR:HG22	2:P:54:LEU:N	2.25	0.51
4:E:717:DT:C2	4:E:718:DA:C6	2.98	0.51
1:A:399:ILE:CB	1:A:430:HIS:CD2	2.87	0.51
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.76	0.51
1:D:205:TYR:HD1	1:D:410:LEU:HD21	1.75	0.51
2:B:38:LYS:CG	4:E:713:DG:H2"	2.41	0.51
2:P:7:ILE:HG23	2:P:12:GLN:CG	2.40	0.51
1:D:255:MET:HB2	1:D:312:ALA:O	2.10	0.50
1:D:79:TYR:O	1:D:80:HIS:C	2.49	0.50
1:A:275:ILE:HG22	1:A:381:LEU:HD11	1.93	0.50
1:D:19:LEU:HB2	1:D:21:ASN:HD21	1.76	0.50
1:D:110:VAL:CG1	1:D:112:HIS:NE2	2.66	0.50
1:D:295:PHE:O	1:D:296:MET:C	2.49	0.50
1:D:320:GLN:O	1:D:321:ALA:C	2.50	0.50
1:D:428:ARG:HH11	1:D:428:ARG:CG	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:CZ	1:A:148:ARG:HG3	2.41	0.50
2:B:31:LEU:O	2:B:35:ILE:HG12	2.12	0.50
2:B:61:LEU:HD21	2:P:70:LEU:HD22	1.92	0.50
1:A:255:MET:HB2	1:A:312:ALA:O	2.12	0.50
1:A:347:ILE:HG13	1:A:367:ASP:HB2	1.93	0.50
1:A:33:LEU:HD11	1:A:48:GLN:O	2.10	0.50
1:D:376:ALA:O	1:D:379:LYS:HB2	2.12	0.50
1:A:175:PRO:HG2	1:A:247:LEU:HB3	1.94	0.50
1:A:428:ARG:HG2	1:A:428:ARG:NH1	2.26	0.50
1:D:380:VAL:HG23	1:D:381:LEU:N	2.27	0.50
1:D:387:GLN:O	1:D:391:ILE:HG13	2.11	0.50
4:E:718:DA:H2'	4:E:718:DA:OP2	2.12	0.50
2:B:7:ILE:HG23	2:B:12:GLN:CG	2.42	0.49
1:A:337:PHE:C	1:A:339:VAL:H	2.15	0.49
1:D:104:ILE:O	1:D:105:PRO:O	2.29	0.49
1:D:169:ILE:CG2	1:D:170:PRO:HD2	2.42	0.49
1:D:161:LEU:CD1	1:D:177:THR:HG23	2.42	0.49
1:D:33:LEU:HD11	1:D:48:GLN:O	2.12	0.49
1:D:371:PRO:HB3	1:D:392:LEU:HD13	1.95	0.49
1:A:100:ALA:HB3	1:A:251:PRO:HA	1.95	0.49
1:D:262:PRO:O	1:D:265:VAL:HG22	2.12	0.49
1:A:198:GLN:HE22	1:A:415:PRO:HB3	1.78	0.49
1:D:21:ASN:ND2	1:D:23:ALA:CB	2.76	0.49
2:P:6:LYS:NZ	2:P:74:LYS:HG3	2.28	0.49
3:T:703:DT:H1'	3:T:704:DC:H5'	1.94	0.49
1:A:376:ALA:O	1:A:379:LYS:HB2	2.13	0.49
1:A:375:LEU:HD23	1:A:388:MET:HG2	1.94	0.49
1:D:125:LEU:HD23	1:D:225:ALA:HB2	1.93	0.49
1:D:149:ILE:HG22	1:D:150:SER:H	1.78	0.49
1:D:266:LYS:HD2	1:D:311:HIS:CD2	2.47	0.49
1:A:179:ILE:HG12	1:A:235:ARG:HG2	1.94	0.48
1:A:151:VAL:CG1	1:A:157:LYS:HE3	2.41	0.48
1:A:237:ASP:HB3	1:A:252:GLN:OE1	2.13	0.48
1:A:182:LEU:N	1:A:182:LEU:HD13	2.28	0.48
1:A:275:ILE:CG2	1:A:381:LEU:HD11	2.43	0.48
1:A:404:ASP:O	1:A:408:THR:HG23	2.14	0.48
1:A:384:PRO:HB2	1:A:387:GLN:HB2	1.95	0.48
1:A:340:LEU:HD23	1:A:345:ILE:HG22	1.96	0.48
1:D:161:LEU:HD12	1:D:177:THR:HG23	1.94	0.48
1:D:115:MET:CE	1:D:174:THR:HG23	2.43	0.48
2:P:42:ILE:HD13	2:P:60:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:CD2	1:A:432:ARG:HH12	2.17	0.48
1:D:280:ALA:O	1:D:283:MET:HB2	2.14	0.48
1:D:318:PHE:CD1	1:D:328:THR:HG22	2.49	0.48
2:P:53:THR:CG2	2:P:54:LEU:N	2.76	0.48
4:E:712:DG:O6	4:E:713:DG:C2	2.67	0.48
2:B:17:MET:HG3	2:P:70:LEU:HD11	1.94	0.48
1:D:309:GLN:HG3	1:D:334:ILE:CG2	2.44	0.48
1:D:148:ARG:NH1	1:D:148:ARG:CG	2.69	0.47
1:D:93:ILE:HG12	1:D:93:ILE:O	2.13	0.47
2:P:31:LEU:O	2:P:35:ILE:HG12	2.14	0.47
1:A:303:TRP:HE1	1:A:369:ILE:HB	1.78	0.47
1:D:104:ILE:HG22	1:D:108:GLU:HG2	1.96	0.47
1:D:209:LEU:HA	1:D:406:VAL:HG21	1.97	0.47
1:A:358:ALA:HB2	1:A:363:LYS:H	1.78	0.47
1:D:414:PHE:CD2	1:D:415:PRO:HD2	2.50	0.47
1:D:414:PHE:CG	1:D:415:PRO:HD2	2.50	0.47
1:D:399:ILE:CB	1:D:430:HIS:CD2	2.88	0.47
1:D:46:PRO:O	1:D:47:LEU:C	2.53	0.47
3:T:705:DC:N4	4:E:714:DG:O6	2.47	0.47
1:A:115:MET:HE2	1:A:174:THR:HG23	1.95	0.47
1:A:3:LYS:HD2	1:A:106:GLU:OE1	2.15	0.47
2:B:19:LEU:CD2	2:B:23:GLN:HG3	2.45	0.47
2:B:38:LYS:HG3	4:E:713:DG:H2"	1.95	0.47
2:P:56:THR:O	2:P:59:LYS:HB2	2.15	0.47
3:T:710:DA:H5"	4:E:711:DA:C2	2.49	0.47
1:A:429:LEU:CD2	1:A:432:ARG:NH1	2.72	0.47
3:T:708:DT:H3	4:E:712:DG:H22	1.62	0.47
3:T:703:DT:H2"	3:T:704:DC:OP2	2.14	0.47
1:A:351:LYS:HD2	1:A:365:ALA:HA	1.97	0.47
1:A:300:VAL:O	1:A:303:TRP:HB3	2.15	0.47
1:A:392:LEU:HD22	1:A:433:LEU:HD21	1.97	0.47
1:A:68:SER:HB3	1:A:71:VAL:CG2	2.45	0.47
1:D:108:GLU:HG3	1:D:110:VAL:HG21	1.97	0.47
1:D:309:GLN:HG3	1:D:334:ILE:HG23	1.97	0.47
1:D:256:CYS:SG	1:D:313:LYS:HG3	2.55	0.46
1:D:60:PHE:CE1	1:D:257:GLN:NE2	2.83	0.46
2:P:26:TRP:HA	2:P:30:GLU:OE1	2.15	0.46
1:A:371:PRO:HB3	1:A:392:LEU:HD13	1.97	0.46
1:D:337:PHE:O	1:D:339:VAL:N	2.49	0.46
1:D:399:ILE:HG22	1:D:400:PRO:N	2.31	0.46
4:E:702:DA:H2"	4:E:703:DT:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD12	2:P:52:THR:HB	1.97	0.46
2:B:53:THR:HG22	2:B:55:THR:H	1.80	0.46
1:D:311:HIS:CE1	1:D:313:LYS:HB2	2.51	0.46
1:D:396:ALA:O	1:D:430:HIS:NE2	2.47	0.46
2:B:6:LYS:NZ	2:B:74:LYS:HG3	2.30	0.46
4:E:717:DT:O2	4:E:718:DA:N1	2.49	0.46
1:A:375:LEU:HD23	1:A:388:MET:CG	2.45	0.46
1:D:182:LEU:N	1:D:182:LEU:HD22	2.30	0.46
1:D:184:ILE:HD12	1:D:196:LEU:HB2	1.98	0.46
1:D:204:TYR:CE2	1:D:208:LEU:HD11	2.51	0.46
1:A:110:VAL:O	1:A:111:THR:C	2.54	0.46
1:A:382:ARG:CD	3:T:714:DG:OP1	2.63	0.46
1:A:399:ILE:HG22	1:A:400:PRO:CD	2.46	0.46
2:B:22:GLN:C	2:B:24:ASN:H	2.19	0.46
1:A:273:PRO:HD2	1:A:312:ALA:HB2	1.98	0.46
1:A:76:VAL:HG22	1:A:89:LEU:HD21	1.97	0.46
1:D:109:THR:HA	1:D:109:THR:CB	2.27	0.45
1:D:114:ILE:HD13	1:D:173:ILE:HD11	1.97	0.45
1:A:25:THR:HG22	1:A:53:THR:HG22	1.99	0.45
1:D:158:THR:OG1	1:D:159:ALA:N	2.49	0.45
1:A:396:ALA:O	1:A:430:HIS:NE2	2.48	0.45
1:D:370:TYR:CZ	1:D:432:ARG:NE	2.83	0.45
1:A:115:MET:CE	1:A:115:MET:HA	2.47	0.45
1:A:99:GLY:O	1:A:250:LEU:O	2.34	0.45
1:A:296:MET:O	1:A:299:GLN:N	2.50	0.45
1:A:2:PRO:O	1:A:87:PHE:HZ	2.00	0.45
1:D:13:VAL:HG13	1:D:32:TRP:CE2	2.52	0.45
1:D:21:ASN:HD21	1:D:23:ALA:CB	2.29	0.45
1:D:410:LEU:HD13	1:D:419:VAL:CG2	2.46	0.45
3:T:714:DG:OP2	3:T:714:DG:H3'	2.17	0.45
1:A:68:SER:HG	1:A:70:ILE:CD1	2.17	0.45
1:D:274:GLY:O	1:D:278:ILE:HG12	2.17	0.45
1:D:293:TYR:O	1:D:294:ASP:C	2.55	0.45
1:D:297:LYS:HG3	1:D:391:ILE:HG23	1.99	0.45
1:A:126:GLU:O	1:A:130:THR:HG23	2.17	0.45
1:A:126:GLU:OE2	1:A:226:GLY:HA3	2.17	0.45
1:A:37:TYR:HB3	1:A:39:ARG:HH21	1.82	0.45
1:D:100:ALA:HB3	1:D:251:PRO:HA	1.98	0.45
1:D:104:ILE:O	1:D:105:PRO:C	2.55	0.45
4:E:707:DC:C2'	4:E:708:DT:H5'	2.37	0.45
2:P:55:THR:O	2:P:56:THR:C	2.52	0.45

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:O	1:A:147:PHE:CD1	2.70	0.44
1:A:351:LYS:CD	1:A:365:ALA:HA	2.47	0.44
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.89	0.44
4:E:712:DG:N7	4:E:713:DG:C5	2.84	0.44
3:T:709:DT:H2"	3:T:710:DA:O5'	2.17	0.44
1:A:427:LEU:HA	1:A:430:HIS:HB3	1.98	0.44
1:D:157:LYS:CD	1:D:181:LYS:HE2	2.48	0.44
3:T:712:DG:OP1	2:P:53:THR:N	2.34	0.44
1:A:110:VAL:C	1:A:111:THR:O	2.53	0.44
1:A:104:ILE:HD11	1:A:112:HIS:NE2	2.32	0.44
1:D:410:LEU:CD1	1:D:419:VAL:HG22	2.47	0.44
2:P:54:LEU:O	2:P:58:PHE:HD1	1.99	0.44
1:A:130:THR:HA	1:A:133:LYS:CE	2.48	0.44
1:A:429:LEU:O	1:A:432:ARG:HB2	2.17	0.44
1:A:262:PRO:O	1:A:265:VAL:HG22	2.18	0.44
4:E:708:DT:H1'	4:E:709:DT:C4	2.52	0.44
1:A:410:LEU:HD13	1:A:419:VAL:HG22	1.99	0.44
1:A:430:HIS:ND1	1:A:430:HIS:C	2.71	0.44
1:D:320:GLN:HB2	1:D:324:SER:HB2	1.99	0.44
1:A:118:GLU:HB2	1:A:171:LYS:NZ	2.31	0.44
1:A:283:MET:HE1	2:P:59:LYS:HA	1.99	0.44
1:D:273:PRO:HD2	1:D:312:ALA:HB2	1.99	0.44
1:D:340:LEU:HD23	1:D:345:ILE:HG22	1.99	0.44
1:D:425:ASN:HD22	1:D:425:ASN:H	1.66	0.44
1:A:320:GLN:O	1:A:321:ALA:C	2.57	0.44
1:D:8:MET:HE3	1:D:101:VAL:HG12	2.00	0.44
1:D:110:VAL:CG1	1:D:112:HIS:CD2	3.01	0.44
1:A:100:ALA:CB	1:A:251:PRO:HA	2.48	0.43
1:D:243:GLU:O	1:D:245:THR:HG23	2.17	0.43
4:E:700:DC:C5	4:E:701:DT:H73	2.53	0.43
2:P:6:LYS:HZ1	2:P:74:LYS:HG3	1.83	0.43
1:D:98:VAL:HG12	1:D:99:GLY:N	2.33	0.43
1:D:160:LEU:HG	1:D:180:ILE:HD12	2.00	0.43
1:D:258:THR:HG22	1:D:259:PHE:CD2	2.53	0.43
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.29	0.43
1:A:266:LYS:HD2	1:A:311:HIS:CD2	2.53	0.43
1:A:337:PHE:O	1:A:339:VAL:N	2.51	0.43
1:D:120:LEU:HD22	1:D:124:ARG:HH11	1.81	0.43
1:A:95:ARG:NH2	1:A:148:ARG:NH1	2.67	0.43
1:D:266:LYS:HD2	1:D:311:HIS:CE1	2.53	0.43
1:D:98:VAL:HG12	1:D:99:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:717:DT:C2	4:E:718:DA:N1	2.86	0.43
1:A:124:ARG:O	1:A:128:VAL:HG23	2.19	0.43
2:B:38:LYS:HD2	4:E:715:DG:N1	2.27	0.43
1:A:52:ILE:N	1:A:52:ILE:HD13	2.33	0.43
1:A:21:ASN:N	1:A:21:ASN:ND2	2.67	0.43
1:A:182:LEU:HD22	1:A:182:LEU:N	2.34	0.43
1:A:279:MET:HG3	1:A:381:LEU:HD13	2.00	0.43
1:D:21:ASN:ND2	1:D:23:ALA:N	2.67	0.43
1:D:337:PHE:C	1:D:339:VAL:N	2.72	0.42
1:D:337:PHE:N	1:D:338:PRO:CD	2.82	0.42
1:A:120:LEU:HD11	1:A:169:ILE:HG13	2.01	0.42
1:A:149:ILE:HG22	1:A:150:SER:H	1.83	0.42
1:A:120:LEU:HB2	1:A:167:TRP:O	2.20	0.42
2:B:65:GLU:O	2:B:66:LEU:HD12	2.18	0.42
1:D:217:VAL:HB	1:D:218:PRO:HD2	2.01	0.42
2:B:38:LYS:CG	4:E:713:DG:C2'	2.96	0.42
2:P:38:LYS:HB2	2:P:38:LYS:HE2	1.35	0.42
1:A:112:HIS:O	1:A:114:ILE:N	2.53	0.42
1:A:296:MET:O	1:A:299:GLN:HB2	2.19	0.42
2:B:62:GLN:NE2	2:P:8:TYR:HB3	2.35	0.42
3:T:701:DT:C2	3:T:702:DA:C5	3.07	0.42
1:A:84:ARG:HE	1:A:84:ARG:HB2	1.69	0.42
1:D:120:LEU:HD11	1:D:169:ILE:HG13	2.02	0.42
1:A:127:GLU:O	1:A:131:ALA:HB2	2.20	0.42
1:A:343:THR:OG1	1:A:345:ILE:HD13	2.19	0.42
1:D:155:GLN:HG2	1:D:184:ILE:HG12	2.02	0.42
1:D:428:ARG:NH1	1:D:428:ARG:CG	2.79	0.42
3:T:707:DC:H42	4:E:713:DG:H21	1.68	0.42
1:A:96:ASP:OD2	1:A:175:PRO:HA	2.19	0.42
1:A:309:GLN:HG3	1:A:334:ILE:HG23	2.01	0.42
1:A:334:ILE:HG12	1:A:335:SER:N	2.34	0.42
1:A:398:MET:O	1:A:399:ILE:C	2.56	0.42
3:T:712:DG:P	2:P:53:THR:H	2.42	0.42
1:A:75:ILE:HG22	1:A:89:LEU:CD2	2.50	0.42
1:D:275:ILE:CG2	1:D:381:LEU:HD11	2.50	0.42
1:D:334:ILE:HG12	1:D:335:SER:N	2.34	0.42
1:D:403:LEU:HD13	1:D:423:GLU:HG3	2.01	0.42
1:A:282:LEU:HD21	1:A:327:LEU:HD13	2.01	0.41
1:D:13:VAL:HG13	1:D:32:TRP:NE1	2.34	0.41
3:T:705:DC:N3	4:E:714:DG:O6	2.52	0.41
2:P:39:GLN:HE21	2:P:39:GLN:HB3	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:NE	3:T:714:DG:OP1	2.53	0.41
1:A:89:LEU:O	1:A:93:ILE:CD1	2.68	0.41
1:D:21:ASN:HD22	1:D:23:ALA:H	1.66	0.41
1:D:410:LEU:HA	1:D:411:PRO:HD2	1.89	0.41
3:T:712:DG:C4'	3:T:713:DG:H5'	2.43	0.41
1:A:205:TYR:HE2	1:A:422:VAL:HG11	1.84	0.41
1:D:160:LEU:HB2	1:D:180:ILE:HD11	2.02	0.41
1:D:351:LYS:CD	1:D:365:ALA:HA	2.49	0.41
2:P:28:GLN:OE1	2:P:43:SER:HB2	2.20	0.41
2:P:58:PHE:O	2:P:59:LYS:C	2.56	0.41
1:D:266:LYS:HE2	1:D:267:TYR:HE1	1.85	0.41
1:D:76:VAL:HG21	1:D:84:ARG:HG2	2.00	0.41
1:D:128:VAL:O	1:D:131:ALA:HB3	2.20	0.41
1:D:281:PHE:CZ	1:D:325:TYR:CE2	3.08	0.41
1:A:157:LYS:HD3	1:A:181:LYS:HE2	2.02	0.41
1:D:266:LYS:HD2	1:D:311:HIS:CG	2.56	0.41
2:B:68:MET:HE3	2:B:68:MET:HB2	1.95	0.41
1:D:180:ILE:HA	1:D:231:LEU:O	2.20	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.73	0.41
1:A:286:SER:HA	2:B:8:TYR:CE2	2.56	0.41
1:D:120:LEU:HD21	1:D:169:ILE:HD12	2.02	0.41
3:T:714:DG:N7	2:P:38:LYS:NZ	2.63	0.41
1:A:120:LEU:HD22	1:A:124:ARG:NH1	2.35	0.41
1:A:205:TYR:CD1	1:A:410:LEU:HD21	2.52	0.41
2:B:34:LYS:HE2	1:D:289:LEU:HD23	2.02	0.41
1:D:149:ILE:HG22	1:D:150:SER:N	2.36	0.41
4:E:712:DG:C5	4:E:713:DG:C5	3.09	0.41
1:A:108:GLU:C	1:A:110:VAL:N	2.74	0.41
1:A:13:VAL:HG13	1:A:32:TRP:CD1	2.55	0.41
1:A:295:PHE:O	1:A:296:MET:C	2.57	0.40
1:A:205:TYR:CE2	1:A:422:VAL:HG11	2.55	0.40
1:A:70:ILE:HG13	1:A:70:ILE:H	1.57	0.40
1:D:182:LEU:N	1:D:182:LEU:HD13	2.36	0.40
2:P:60:ILE:O	2:P:64:LEU:HG	2.20	0.40
2:B:67:SER:N	2:P:71:CYS:O	2.51	0.40
1:A:174:THR:HA	1:A:175:PRO:HD3	1.86	0.40
1:A:196:LEU:N	1:A:196:LEU:HD22	2.36	0.40
1:A:281:PHE:HE2	1:A:317:VAL:HG11	1.86	0.40
1:A:85:GLN:HE21	1:A:86:PRO:CD	2.32	0.40
1:D:366:ILE:HG22	1:D:367:ASP:N	2.34	0.40
3:T:712:DG:OP2	2:P:52:THR:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HA	1:A:231:LEU:O	2.21	0.40
1:A:266:LYS:HE2	1:A:267:TYR:HE1	1.86	0.40
2:B:34:LYS:HE2	1:D:289:LEU:CD2	2.51	0.40
1:D:4:LEU:HD23	1:D:105:PRO:HA	2.02	0.40
1:A:337:PHE:C	1:A:339:VAL:N	2.74	0.40
1:A:377:THR:O	1:A:378:ALA:C	2.58	0.40
1:A:399:ILE:CB	1:A:400:PRO:HD3	2.51	0.40
1:A:121:THR:H	1:A:124:ARG:HB2	1.87	0.40
1:A:112:HIS:CB	1:A:173:ILE:HG12	2.35	0.40
1:D:21:ASN:HD22	1:D:23:ALA:N	2.19	0.40
1:D:337:PHE:HB2	1:D:338:PRO:HD3	2.03	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:CB	1:D:109:THR:C[3_456]	1.68	0.52
1:A:110:VAL:CA	1:D:110:VAL:N[3_456]	1.94	0.26
1:A:110:VAL:CG1	1:D:109:THR:O[3_456]	1.95	0.25
1:A:110:VAL:O	1:D:110:VAL:N[3_456]	2.00	0.20
1:A:110:VAL:CB	1:D:110:VAL:N[3_456]	2.09	0.11
1:A:110:VAL:C	1:D:110:VAL:N[3_456]	2.10	0.10
1:A:67:ASP:O	1:D:84:ARG:NH1[3_455]	2.15	0.05
1:A:340:LEU:O	1:D:417:ASN:OD1[4_465]	2.15	0.05
1:A:110:VAL:CB	1:D:109:THR:CA[3_456]	2.15	0.05
1:A:110:VAL:CG1	1:D:109:THR:C[3_456]	2.18	0.02

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/448 (91%)	353 (86%)	45 (11%)	10 (2%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	408/448 (91%)	353 (86%)	41 (10%)	14 (3%)	3	30
2	B	69/91 (76%)	63 (91%)	5 (7%)	1 (1%)	11	46
2	P	69/91 (76%)	63 (91%)	3 (4%)	3 (4%)	2	25
All	All	954/1078 (88%)	832 (87%)	94 (10%)	28 (3%)	4	32

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	108	GLU
1	A	110	VAL
1	D	20	ALA
1	D	21	ASN
1	D	95	ARG
1	D	108	GLU
1	A	78	ARG
1	A	80	HIS
1	D	80	HIS
1	D	110	VAL
1	D	111	THR
1	A	100	ALA
2	B	23	GLN
1	D	105	PRO
1	A	384	PRO
1	D	113	PRO
1	A	415	PRO
1	D	109	THR
1	D	132	TYR
1	D	384	PRO
2	P	36	GLY
2	P	50	ASP
1	A	109	THR
1	D	338	PRO
1	A	338	PRO
1	D	226	GLY
2	P	35	ILE

5.3.2 Protein sidechains (i)

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	351/382 (92%)	328 (93%)	23 (7%)	16	45
1	D	351/382 (92%)	332 (95%)	19 (5%)	22	50
2	B	64/83 (77%)	57 (89%)	7 (11%)	6	26
2	P	64/83 (77%)	57 (89%)	7 (11%)	6	26
All	All	830/930 (89%)	774 (93%)	56 (7%)	16	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	21	ASN
1	A	69	PRO
1	A	73	ASP
1	A	93	ILE
1	A	101	VAL
1	A	108	GLU
1	A	110	VAL
1	A	111	THR
1	A	118	GLU
1	A	122	GLU
1	A	124	ARG
1	A	155	GLN
1	A	182	LEU
1	A	244	ARG
1	A	258	THR
1	A	289	LEU
1	A	308	THR
1	A	334	ILE
1	A	346	HIS
1	A	364	THR
1	A	412	THR
1	A	417	ASN
2	B	4	PHE
2	B	5	GLN
2	B	12	GLN
2	B	13	LEU
2	B	19	LEU

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Mol	Chain	Res	Type
2	B	61	LEU
2	B	66	LEU
1	D	8	MET
1	D	21	ASN
1	D	73	ASP
1	D	84	ARG
1	D	93	ILE
1	D	107	ASP
1	D	108	GLU
1	D	118	GLU
1	D	122	GLU
1	D	124	ARG
1	D	148	ARG
1	D	155	GLN
1	D	182	LEU
1	D	244	ARG
1	D	289	LEU
1	D	334	ILE
1	D	346	HIS
1	D	412	THR
1	D	417	ASN
2	P	5	GLN
2	P	12	GLN
2	P	13	LEU
2	P	19	LEU
2	P	39	GLN
2	P	61	LEU
2	P	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	21	ASN
1	A	85	GLN
1	A	198	GLN
1	A	227	ASN
1	A	357	ASN
1	A	387	GLN
2	B	5	GLN
2	B	12	GLN
2	B	22	GLN

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Mol	Chain	Res	Type
2	B	39	GLN
1	D	10	ASN
1	D	21	ASN
1	D	85	GLN
1	D	198	GLN
1	D	216	ASN
1	D	387	GLN
1	D	417	ASN
1	D	425	ASN
2	P	5	GLN
2	P	12	GLN
2	P	22	GLN
2	P	39	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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, 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	414/448 (92%)	2.11	166 (40%)	0	0	155, 179, 191, 199	0
1	D	414/448 (92%)	2.06	169 (40%)	0	0	157, 179, 191, 206	0
2	B	71/91 (78%)	1.56	23 (32%)	0	0	162, 176, 183, 185	0
2	P	71/91 (78%)	1.66	22 (30%)	0	0	158, 175, 187, 190	0
3	T	23/23 (100%)	2.27	13 (56%)	0	0	168, 186, 195, 198	0
4	E	23/23 (100%)	2.91	12 (52%)	0	0	166, 191, 196, 204	0
All	All	1016/1124 (90%)	2.04	405 (39%)	0	0	155, 179, 191, 206	0

All (405) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	20.9
1	D	273	PRO	13.1
1	D	230	ALA	11.9
1	A	229	ARG	11.7
1	D	146	ASP	10.7
1	A	100	ALA	10.6
1	D	229	ARG	10.6
1	A	149	ILE	10.2
1	A	273	PRO	10.2
2	P	73	THR	10.1
1	A	146	ASP	10.0
1	A	148	ARG	9.4
1	A	132	TYR	8.9
1	D	175	PRO	8.8
2	B	8	TYR	8.7
1	A	112	HIS	8.6
1	D	151	VAL	8.3
1	A	434	SER	8.2
1	D	218	PRO	8.2

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Mol	Chain	Res	Type	RSRZ
4	E	707	DC	7.9
4	E	710	DA	7.9
1	D	147	PHE	7.9
1	A	84	ARG	7.8
1	D	183	PRO	7.7
1	A	147	PHE	7.7
1	A	225	ALA	7.7
2	P	74	LYS	7.7
4	E	720	DG	7.4
1	D	219	ASP	7.3
1	A	437	TYR	7.3
1	D	231	LEU	7.2
1	D	49	ARG	7.2
1	A	255	MET	7.1
1	D	149	ILE	7.1
1	D	150	SER	7.1
1	D	434	SER	7.1
1	A	355	GLY	7.0
1	D	272	GLY	7.0
1	A	12	ARG	6.9
1	A	2	PRO	6.9
2	P	5	GLN	6.9
1	D	220	ALA	6.8
1	A	228	VAL	6.7
2	P	72	ASP	6.5
1	A	83	SER	6.4
1	D	359	SER	6.3
1	A	118	GLU	6.3
1	A	107	ASP	6.3
1	A	134	ALA	6.3
1	A	120	LEU	6.2
2	B	73	THR	6.2
1	A	98	VAL	6.2
1	D	395	PHE	6.1
1	A	67	ASP	5.9
1	D	223	ILE	5.9
1	D	397	ARG	5.9
1	D	111	THR	5.8
1	D	134	ALA	5.7
1	A	183	PRO	5.6
1	D	112	HIS	5.6
1	A	223	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	16	LEU	5.6
1	D	249	ARG	5.6
1	A	113	PRO	5.6
2	P	6	LYS	5.6
1	D	270	ASP	5.5
1	D	31	GLU	5.5
4	E	706	DC	5.4
1	A	265	VAL	5.4
2	B	68	MET	5.4
1	D	383	PHE	5.4
1	A	111	THR	5.4
1	A	220	ALA	5.3
2	P	23	GLN	5.3
1	D	2	PRO	5.3
1	D	99	GLY	5.3
1	D	15	GLU	5.3
1	D	24	HIS	5.3
1	A	15	GLU	5.2
1	A	383	PHE	5.2
1	A	167	TRP	5.2
1	A	105	PRO	5.2
1	D	118	GLU	5.2
1	A	435	ARG	5.1
1	D	176	THR	5.1
1	D	148	ARG	5.1
1	A	433	LEU	5.1
1	D	129	LEU	5.0
1	A	31	GLU	5.0
1	D	117	TRP	5.0
1	D	435	ARG	5.0
1	A	49	ARG	4.9
1	D	213	LEU	4.9
1	D	358	ALA	4.9
1	D	170	PRO	4.9
2	B	6	LYS	4.8
1	D	437	TYR	4.8
1	A	363	LYS	4.8
1	D	385	GLU	4.7
1	D	433	LEU	4.7
1	A	256	CYS	4.7
1	A	176	THR	4.7
4	E	708	DT	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	50	GLY	4.7
1	D	78	ARG	4.7
1	A	150	SER	4.6
1	A	406	VAL	4.6
1	D	132	TYR	4.6
1	D	367	ASP	4.6
1	D	313	LYS	4.6
1	D	115	MET	4.6
1	D	396	ALA	4.6
1	A	357	ASN	4.6
1	D	356	LEU	4.5
1	A	398	MET	4.5
2	B	5	GLN	4.5
1	D	120	LEU	4.5
1	D	271	GLY	4.5
2	B	62	GLN	4.5
1	A	101	VAL	4.5
1	A	354	MET	4.5
1	A	108	GLU	4.4
1	D	52	ILE	4.4
1	A	28	TYR	4.4
1	A	175	PRO	4.4
1	A	172	GLY	4.4
1	D	171	LYS	4.3
1	D	60	PHE	4.3
1	A	60	PHE	4.3
1	D	355	GLY	4.3
1	D	212	GLU	4.3
1	D	173	ILE	4.2
1	D	153	GLY	4.2
1	A	324	SER	4.2
1	A	93	ILE	4.2
1	D	363	LYS	4.2
2	B	74	LYS	4.2
1	D	265	VAL	4.2
1	D	410	LEU	4.2
1	D	174	THR	4.1
1	D	95	ARG	4.1
1	D	360	LYS	4.1
2	P	4	PHE	4.1
1	D	279	MET	4.1
1	D	286	SER	4.1

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Mol	Chain	Res	Type	RSRZ
3	T	708	DT	4.1
1	A	413	ASP	4.1
1	A	399	ILE	4.1
2	B	7	ILE	4.1
1	A	274	GLY	4.0
1	D	110	VAL	4.0
1	A	207	LEU	4.0
1	A	313	LYS	4.0
2	B	46	GLU	4.0
1	A	356	LEU	4.0
1	D	283	MET	4.0
1	D	324	SER	4.0
1	A	119	LYS	4.0
1	D	168	CYS	4.0
1	D	377	THR	3.9
1	D	26	PHE	3.9
1	A	385	GLU	3.9
1	D	154	ALA	3.9
1	A	173	ILE	3.9
1	A	224	LYS	3.9
1	D	261	LEU	3.9
1	A	245	THR	3.8
1	D	373	HIS	3.8
2	P	62	GLN	3.8
1	D	315	PHE	3.8
1	A	272	GLY	3.8
1	A	371	PRO	3.7
1	D	357	ASN	3.7
1	D	32	TRP	3.7
3	T	710	DA	3.7
1	D	16	LEU	3.7
2	B	69	THR	3.7
1	D	399	ILE	3.7
3	T	707	DC	3.6
1	A	171	LYS	3.6
1	A	161	LEU	3.6
1	A	219	ASP	3.6
1	D	388	MET	3.6
2	B	37	ILE	3.6
1	D	116	ALA	3.6
3	T	709	DT	3.5
1	A	151	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	44	SER	3.5
2	P	8	TYR	3.5
1	A	347	ILE	3.5
1	A	133	LYS	3.5
2	B	28	GLN	3.5
2	B	70	LEU	3.5
1	D	398	MET	3.4
1	D	384	PRO	3.4
4	E	719	DG	3.4
1	A	395	PHE	3.4
1	D	12	ARG	3.4
1	D	275	ILE	3.4
1	D	217	VAL	3.4
1	A	43	LEU	3.4
1	A	227	ASN	3.4
1	D	11	GLN	3.4
1	D	106	GLU	3.4
1	A	358	ALA	3.3
1	A	41	LEU	3.3
1	A	218	PRO	3.3
1	A	360	LYS	3.3
1	A	247	LEU	3.3
3	T	699	DC	3.3
1	D	184	ILE	3.3
1	D	228	VAL	3.3
1	D	98	VAL	3.3
2	P	69	THR	3.3
1	D	97	SER	3.3
1	D	255	MET	3.3
4	E	705	DC	3.3
2	P	39	GLN	3.3
1	A	261	LEU	3.2
1	A	436	GLU	3.2
3	T	698	DC	3.2
1	A	373	HIS	3.2
1	A	310	GLY	3.2
1	A	389	HIS	3.2
1	D	342	GLY	3.2
1	A	384	PRO	3.2
2	P	7	ILE	3.1
1	D	41	LEU	3.1
1	A	4	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	P	28	GLN	3.1
1	D	113	PRO	3.1
1	A	260	GLY	3.1
4	E	718	DA	3.1
1	D	389	HIS	3.1
1	D	108	GLU	3.1
3	T	697	DT	3.1
1	D	369	ILE	3.1
1	A	184	ILE	3.1
1	D	352	LEU	3.1
1	A	312	ALA	3.0
1	D	161	LEU	3.0
1	D	167	TRP	3.0
1	D	94	GLY	3.0
1	A	240	TRP	3.0
2	B	39	GLN	3.0
1	A	169	ILE	3.0
1	A	353	ALA	2.9
1	D	172	GLY	2.9
1	A	319	ILE	2.9
1	D	169	ILE	2.9
1	A	166	ASP	2.9
1	A	154	ALA	2.9
1	A	323	GLY	2.9
1	D	233	VAL	2.9
2	P	20	VAL	2.9
1	A	33	LEU	2.9
3	T	700	DC	2.9
1	A	367	ASP	2.9
1	D	43	LEU	2.9
1	A	115	MET	2.8
1	A	359	SER	2.8
1	A	289	LEU	2.8
1	A	401	ALA	2.8
1	D	256	CYS	2.8
1	A	368	LYS	2.8
1	A	24	HIS	2.8
2	P	31	LEU	2.8
1	D	48	GLN	2.8
1	A	14	GLY	2.8
2	P	40	ALA	2.8
1	D	51	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	25	THR	2.7
1	A	283	MET	2.7
1	A	249	ARG	2.7
1	A	177	THR	2.7
1	A	170	PRO	2.7
1	A	230	ALA	2.7
1	D	432	ARG	2.7
2	B	35	ILE	2.7
1	A	156	GLU	2.7
3	T	706	DC	2.7
1	D	177	THR	2.7
1	D	436	GLU	2.7
1	A	322	GLY	2.7
1	D	93	ILE	2.7
4	E	709	DT	2.7
1	D	74	ARG	2.7
2	P	12	GLN	2.7
1	A	104	ILE	2.6
1	A	292	ARG	2.6
1	A	29	ALA	2.6
1	A	432	ARG	2.6
1	A	275	ILE	2.6
1	D	236	PHE	2.6
1	D	260	GLY	2.6
1	D	198	GLN	2.6
2	P	70	LEU	2.6
4	E	721	DG	2.6
1	A	233	VAL	2.6
2	B	23	GLN	2.6
4	E	722	DA	2.6
1	D	84	ARG	2.6
2	P	30	GLU	2.6
1	A	397	ARG	2.6
1	A	95	ARG	2.6
1	A	352	LEU	2.6
2	B	43	SER	2.6
1	A	55	ASP	2.6
1	A	212	GLU	2.6
1	D	247	LEU	2.6
1	D	234	GLU	2.5
1	D	266	LYS	2.5
1	D	100	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	289	LEU	2.5
2	B	47	ASN	2.5
1	D	205	TYR	2.5
1	D	152	ALA	2.5
1	A	163	ILE	2.5
1	D	392	LEU	2.5
1	A	372	ARG	2.5
1	A	201	ASP	2.5
1	D	133	LYS	2.5
1	D	53	THR	2.5
1	A	266	LYS	2.5
1	A	369	ILE	2.5
1	D	418	VAL	2.5
1	A	338	PRO	2.5
1	D	209	LEU	2.4
1	D	182	LEU	2.4
1	A	279	MET	2.4
1	A	153	GLY	2.4
1	A	56	ALA	2.4
1	D	354	MET	2.4
1	D	347	ILE	2.4
2	B	31	LEU	2.4
1	A	234	GLU	2.4
1	A	264	SER	2.4
1	D	222	ILE	2.3
1	A	58	PHE	2.3
1	D	264	SER	2.3
1	D	331	TYR	2.3
1	A	208	LEU	2.3
1	D	350	LEU	2.3
1	D	292	ARG	2.3
2	P	24	ASN	2.3
2	P	43	SER	2.3
1	A	325	TYR	2.3
1	D	92	GLU	2.3
3	T	701	DT	2.3
1	A	35	SER	2.3
1	D	310	GLY	2.3
3	T	704	DC	2.3
1	A	205	TYR	2.3
1	D	274	GLY	2.3
1	D	29	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	26	TRP	2.3
2	B	22	GLN	2.3
1	A	32	TRP	2.3
1	D	406	VAL	2.3
1	D	232	ALA	2.2
1	D	72	ARG	2.2
1	D	269	SER	2.2
1	D	268	GLU	2.2
1	A	388	MET	2.2
1	A	336	ALA	2.2
1	A	317	VAL	2.2
1	D	252	GLN	2.2
1	D	362	LYS	2.2
1	A	226	GLY	2.2
1	D	318	PHE	2.2
1	D	56	ALA	2.2
2	B	12	GLN	2.2
1	A	20	ALA	2.2
3	T	714	DG	2.2
1	D	35	SER	2.2
1	D	210	ALA	2.2
1	A	410	LEU	2.2
1	A	334	ILE	2.2
1	D	77	LYS	2.2
1	D	207	LEU	2.2
1	D	375	LEU	2.2
1	A	48	GLN	2.2
1	D	28	TYR	2.2
2	P	42	ILE	2.2
1	A	252	GLN	2.1
1	A	375	LEU	2.1
1	A	7	TRP	2.1
1	A	299	GLN	2.1
1	A	327	LEU	2.1
3	T	718	DA	2.1
1	D	416	GLU	2.1
4	E	713	DG	2.1
1	A	213	LEU	2.1
1	A	92	GLU	2.1
1	D	3	LYS	2.1
1	A	8	MET	2.1
1	A	231	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	370	TYR	2.1
1	D	402	ALA	2.1
1	A	258	THR	2.1
1	A	125	LEU	2.1
1	A	307	ALA	2.0
1	D	80	HIS	2.0
1	D	302	GLN	2.0
2	B	36	GLY	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 carbohydrates 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.