



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 PM GMT

PDB ID : 4GOP
Title : Structure and Conformational Change of a Replication Protein A Heterotrimer Bound to ssDNA
Authors : Pavletich, N.P.; Jie, F.
Deposited on : 2012-08-20
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

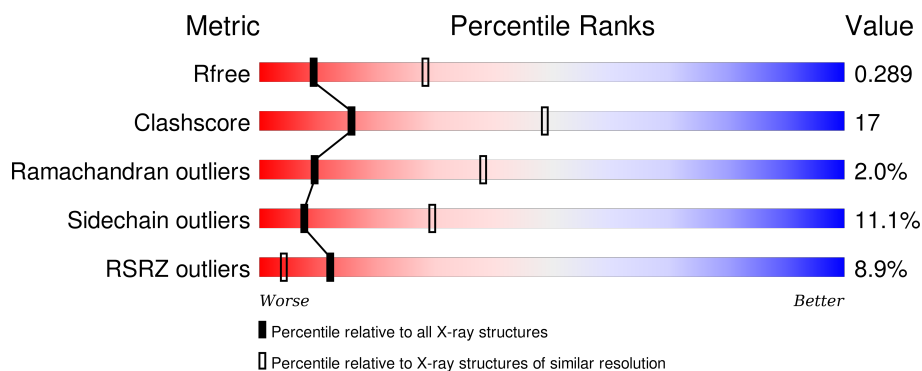
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	114	<div> <div>4%</div> <div>51% 35% 7% 5%</div> </div>
1	X	114	<div> <div>4%</div> <div>53% 32% 9% 5%</div> </div>
2	B	136	<div> <div>7%</div> <div>55% 31% 10%</div> </div>
2	Y	136	<div> <div>4%</div> <div>49% 35% 5% 10%</div> </div>
3	C	444	<div> <div>9%</div> <div>64% 30%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Z	444	<div><div></div><div>10%</div><div>62%</div><div>31%</div><div>5%</div><div></div></div>
4	K	32	<div><div></div><div>28%</div><div>16%</div><div>44%</div><div>19%</div><div>22%</div><div></div></div>
4	L	32	<div><div></div><div>22%</div><div>34%</div><div>19%</div><div>9%</div><div>38%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11350 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			809	505	132	168	4			
1	X	108	Total	C	N	O	S	0	0	0
			809	505	132	168	4			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	0	0
			978	609	186	181	2			
2	Y	122	Total	C	N	O	S	0	0	0
			978	609	186	181	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	VAL	ALA	CONFLICT	UNP Q4PBD4
Y	173	VAL	ALA	CONFLICT	UNP Q4PBD4

- Molecule 3 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	433	Total	C	N	O	S	0	0	0
			3437	2144	600	675	18			
3	Z	433	Total	C	N	O	S	0	0	0
			3437	2144	600	675	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	314	GLN	THR	CONFLICT	UNP Q4P407
Z	314	GLN	THR	CONFLICT	UNP Q4P407

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	25	Total 500	C 250	N 50	O 175	P 25	0	0	0
4	L	20	Total 400	C 200	N 40	O 140	P 20	0	0	0

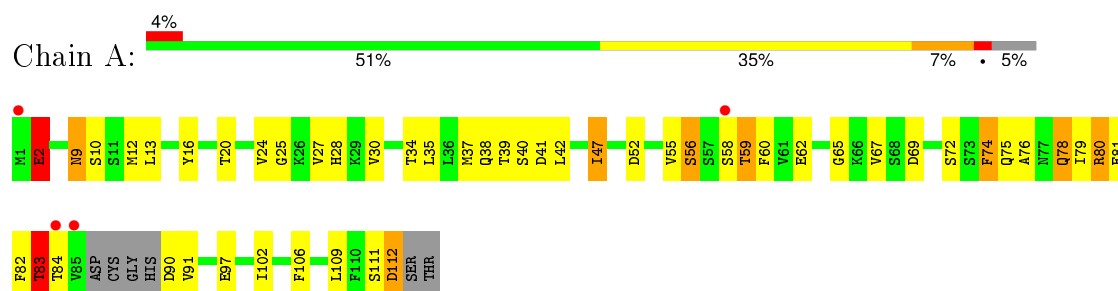
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Z	1	Total 1	Zn 1	0	0
5	C	1	Total 1	Zn 1	0	0

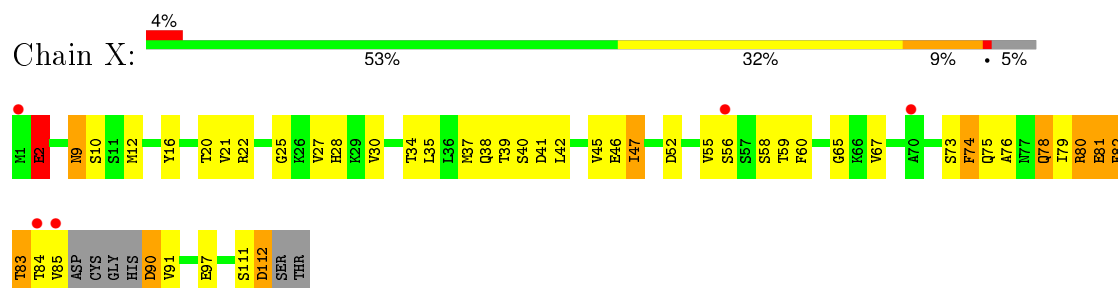
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

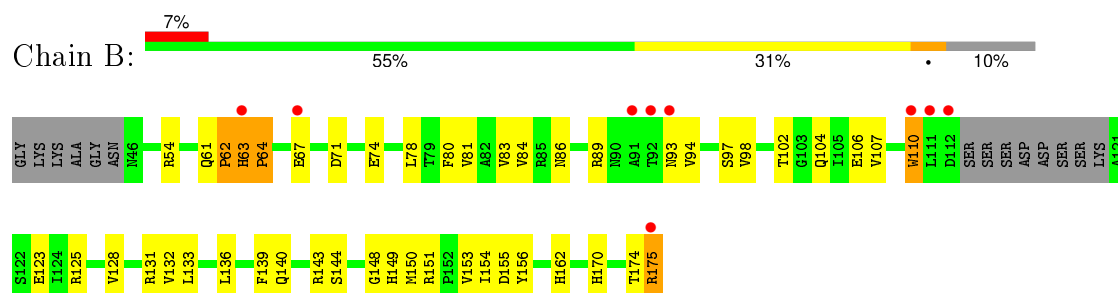
- Molecule 1: Putative uncharacterized protein



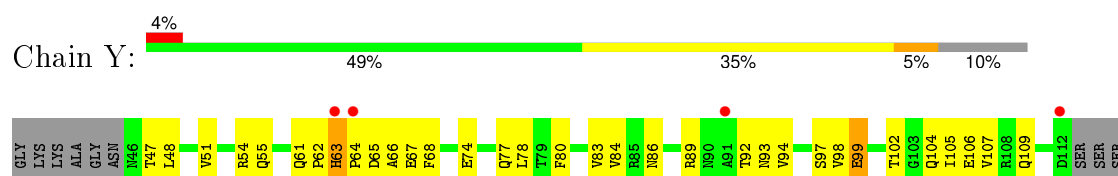
- Molecule 1: Putative uncharacterized protein

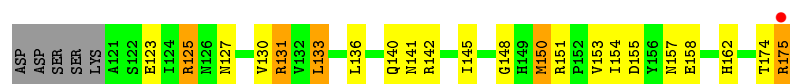


- Molecule 2: Putative uncharacterized protein

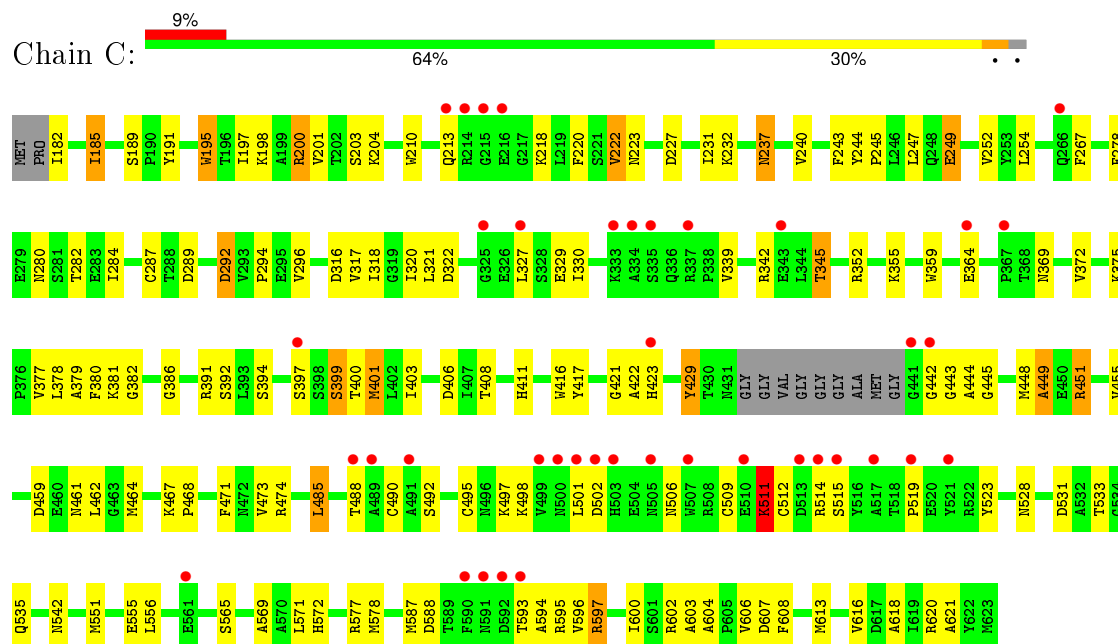


- Molecule 2: Putative uncharacterized protein

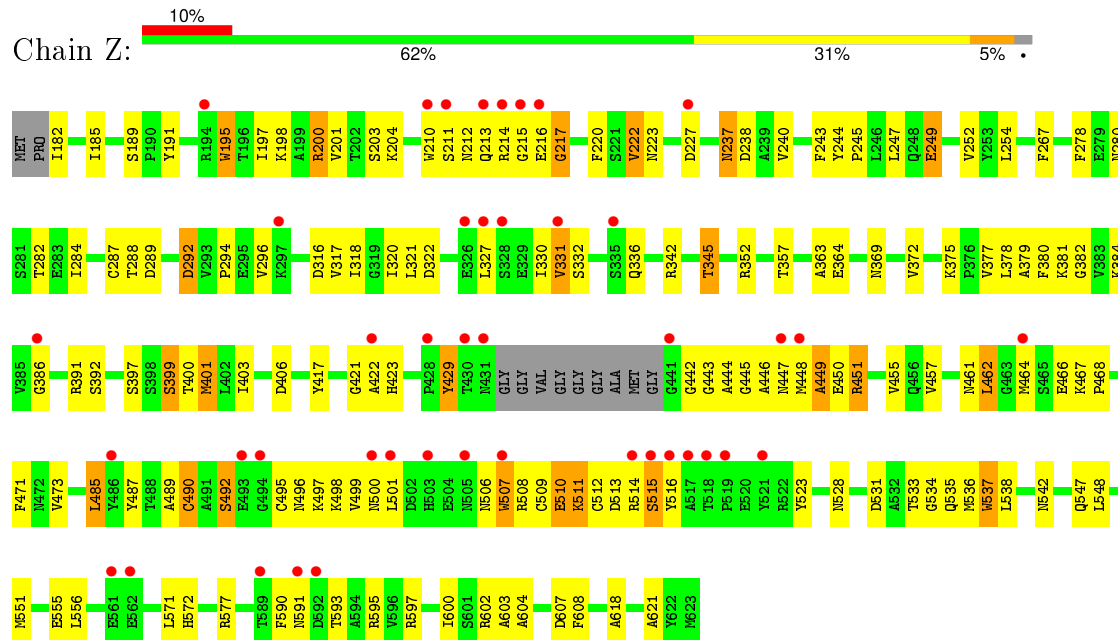




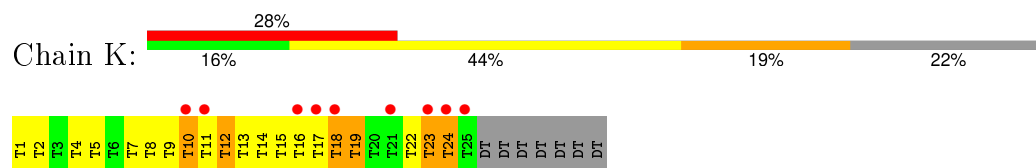
- Molecule 3: Putative uncharacterized protein



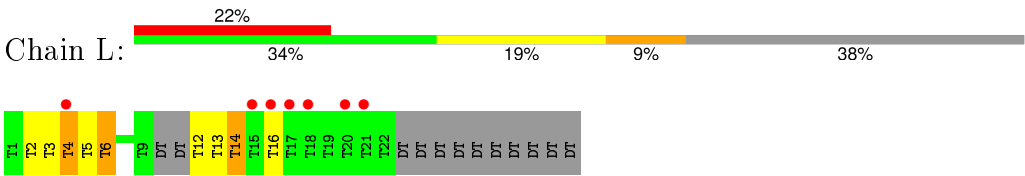
- Molecule 3: Putative uncharacterized protein



- Molecule 4: DNA (25-MER)



● Molecule 4: DNA (25-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.10Å 93.80Å 120.50Å 90.00° 110.90° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 34.23 – 3.07	Depositor EDS
% Data completeness (in resolution range)	85.5 (20.00-3.10) 83.8 (34.23-3.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.82 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.242 , 0.286 0.243 , 0.289	Depositor DCC
R_{free} test set	1629 reflections (5.74%)	DCC
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 32477 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11350	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	0/818	0.78	1/1111 (0.1%)
1	X	0.58	0/818	0.75	0/1111
2	B	0.54	1/994 (0.1%)	0.70	0/1348
2	Y	0.58	0/994	0.72	0/1348
3	C	0.51	4/3502 (0.1%)	0.67	1/4732 (0.0%)
3	Z	0.53	3/3502 (0.1%)	0.67	1/4732 (0.0%)
4	K	0.31	0/549	1.06	8/846 (0.9%)
4	L	0.31	0/438	0.96	4/672 (0.6%)
All	All	0.52	8/11615 (0.1%)	0.73	15/15900 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	195	TRP	CD2-CE2	5.72	1.48	1.41
2	B	110	TRP	CD2-CE2	5.30	1.47	1.41
3	Z	537	TRP	CD2-CE2	5.27	1.47	1.41
3	Z	507	TRP	CD2-CE2	5.19	1.47	1.41
3	C	359	TRP	CD2-CE2	5.17	1.47	1.41
3	C	195	TRP	CD2-CE2	5.16	1.47	1.41
3	C	210	TRP	CD2-CE2	5.14	1.47	1.41
3	C	416	TRP	CD2-CE2	5.06	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	11	DT	P-O3'-C3'	9.31	130.88	119.70
4	K	24	DT	P-O3'-C3'	7.71	128.95	119.70
4	L	4	DT	P-O3'-C3'	7.29	128.45	119.70
4	K	10	DT	P-O3'-C3'	7.10	128.22	119.70
4	K	12	DT	P-O3'-C3'	6.83	127.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	19	DT	P-O3'-C3'	6.83	127.89	119.70
4	K	8	DT	P-O3'-C3'	6.26	127.21	119.70
3	Z	442	GLY	N-CA-C	6.16	128.51	113.10
4	K	18	DT	P-O3'-C3'	5.94	126.83	119.70
4	L	14	DT	P-O3'-C3'	5.83	126.70	119.70
3	C	442	GLY	N-CA-C	5.79	127.58	113.10
4	K	23	DT	P-O3'-C3'	5.77	126.63	119.70
4	L	6	DT	P-O3'-C3'	-5.46	113.15	119.70
1	A	109	LEU	CA-CB-CG	5.04	126.88	115.30
4	L	2	DT	P-O3'-C3'	5.04	125.74	119.70

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	809	0	807	51	0
1	X	809	0	807	47	0
2	B	978	0	970	31	0
2	Y	978	0	970	35	0
3	C	3437	0	3315	106	1
3	Z	3437	0	3315	109	1
4	K	500	0	301	23	0
4	L	400	0	242	10	0
5	C	1	0	0	0	0
5	Z	1	0	0	0	0
All	All	11350	0	10727	377	1

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 17.

All (377) 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)
3:Z:495:CYS:SG	3:Z:511:LYS:HD3	1.80	1.22
1:A:76:ALA:HB1	1:A:79:ILE:HD11	1.37	1.06
1:X:76:ALA:HB1	1:X:79:ILE:HD11	1.35	1.06
1:A:62:GLU:HB2	1:A:82:PHE:HZ	1.31	0.93
3:C:492:SER:OG	3:C:512:CYS:SG	2.26	0.93
1:X:9:ASN:HB2	1:X:41:ASP:HB2	1.52	0.91
2:B:62:PRO:O	2:B:64:PRO:HD2	1.73	0.88
3:Z:497:LYS:HD3	3:Z:511:LYS:HD2	1.56	0.85
1:A:9:ASN:HB2	1:A:41:ASP:HB2	1.57	0.85
1:X:83:THR:HG23	1:X:90:ASP:HA	1.62	0.81
3:Z:357:THR:OG1	3:Z:444:ALA:HB3	1.79	0.81
3:C:597:ARG:HD3	4:K:17:DT:O4	1.80	0.81
3:Z:498:LYS:HB2	4:L:14:DT:H5"	1.64	0.80
1:A:80:ARG:HE	1:A:81:GLU:H	1.30	0.80
3:C:352:ARG:HH21	3:C:429:TYR:HA	1.46	0.79
2:Y:62:PRO:O	2:Y:63:HIS:HB2	1.83	0.78
3:Z:501:LEU:HA	3:Z:506:ASN:O	1.85	0.77
3:Z:352:ARG:HH21	3:Z:429:TYR:HA	1.47	0.77
3:C:200:ARG:HB3	3:C:252:VAL:HG22	1.67	0.76
3:Z:590:PHE:CZ	4:L:16:DT:H2'	2.21	0.74
1:A:62:GLU:HB2	1:A:82:PHE:CZ	2.20	0.74
1:A:82:PHE:CE2	2:B:156:TYR:CD1	2.76	0.73
2:B:139:PHE:HD1	2:B:140:GLN:HE21	1.36	0.73
3:C:375:LYS:HG2	3:C:417:TYR:CE2	2.23	0.73
3:Z:509:CYS:SG	3:Z:511:LYS:HB3	2.29	0.72
1:X:80:ARG:HE	1:X:81:GLU:H	1.35	0.72
2:B:61:GLN:O	2:B:63:HIS:N	2.22	0.71
3:Z:200:ARG:HB3	3:Z:252:VAL:HG22	1.72	0.71
3:Z:375:LYS:HG2	3:Z:417:TYR:CE2	2.26	0.71
1:X:38:GLN:HE21	1:X:42:LEU:HD22	1.55	0.71
1:A:78:GLN:HE21	1:A:79:ILE:H	1.40	0.70
3:Z:369:ASN:HB3	3:Z:403:ILE:CD1	2.21	0.70
2:B:133:LEU:HB3	2:B:149:HIS:HB2	1.74	0.70
1:X:78:GLN:HE21	1:X:79:ILE:H	1.40	0.70
1:A:38:GLN:HE21	1:A:42:LEU:HD22	1.56	0.69
3:C:397:SER:HB3	4:K:5:DT:H3	1.57	0.69
3:C:369:ASN:HB3	3:C:403:ILE:CD1	2.22	0.69
3:C:392:SER:HB2	3:C:445:GLY:H	1.57	0.69
1:X:80:ARG:NH1	2:Y:127:ASN:O	2.25	0.69
2:Y:109:GLN:HE22	2:Y:150:MET:HB2	1.59	0.68
2:B:154:ILE:HD12	3:C:608:PHE:HE1	1.59	0.67
3:C:320:ILE:HD13	3:C:377:VAL:HG22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:148:GLY:O	3:Z:572:HIS:NE2	2.27	0.67
1:X:84:THR:HG22	1:X:85:VAL:N	2.09	0.66
3:Z:382:GLY:O	3:Z:399:SER:OG	2.13	0.66
3:C:329:GLU:HA	3:C:339:VAL:O	1.96	0.66
1:X:10:SER:H	1:X:39:THR:HG21	1.60	0.66
1:X:10:SER:N	1:X:39:THR:HG21	2.10	0.66
3:C:201:VAL:HG13	3:C:222:VAL:HG22	1.78	0.66
3:Z:495:CYS:SG	3:Z:511:LYS:CD	2.72	0.65
2:B:80:PHE:HA	2:B:162:HIS:CE1	2.32	0.65
4:K:4:DT:H2'	4:K:5:DT:H72	1.77	0.65
1:X:27:VAL:HG13	1:X:35:LEU:HD11	1.77	0.65
2:Y:86:ASN:HB3	2:Y:97:SER:HB3	1.79	0.64
2:B:86:ASN:HB3	2:B:97:SER:HB3	1.78	0.64
1:X:9:ASN:HD22	1:X:9:ASN:C	2.00	0.64
3:C:182:ILE:O	3:C:182:ILE:HG22	1.98	0.64
3:Z:320:ILE:HD13	3:Z:377:VAL:HG22	1.79	0.64
1:A:10:SER:N	1:A:39:THR:HG21	2.12	0.64
1:X:60:PHE:HD1	1:X:83:THR:HG1	1.46	0.64
1:A:10:SER:H	1:A:39:THR:HG21	1.62	0.64
3:Z:378:LEU:HD23	3:Z:403:ILE:HA	1.78	0.64
2:B:54:ARG:HD2	2:B:102:THR:O	1.98	0.64
1:X:20:THR:HA	1:X:65:GLY:O	1.98	0.63
2:Y:151:ARG:HH11	3:Z:577:ARG:HG2	1.63	0.63
2:Y:125:ARG:HH11	2:Y:125:ARG:HB2	1.63	0.63
1:A:13:LEU:HD13	1:A:72:SER:HA	1.80	0.63
1:A:27:VAL:HG13	1:A:35:LEU:HD11	1.81	0.63
3:C:495:CYS:SG	3:C:511:LYS:HD2	2.39	0.63
4:K:12:DT:H2''	4:K:13:DT:OP2	1.97	0.62
3:Z:451:ARG:CB	3:Z:451:ARG:HH11	2.12	0.62
3:Z:369:ASN:HB3	3:Z:403:ILE:HD13	1.81	0.62
3:C:528:ASN:HD21	3:C:535:GLN:HE21	1.47	0.62
3:Z:528:ASN:HD21	3:Z:535:GLN:HE21	1.48	0.62
2:Y:155:ASP:OD2	2:Y:155:ASP:C	2.37	0.62
2:B:136:LEU:HD11	2:B:143:ARG:HD3	1.81	0.61
3:C:378:LEU:HD23	3:C:403:ILE:HA	1.82	0.61
3:C:421:GLY:C	3:C:423:HIS:H	2.02	0.61
2:B:139:PHE:HD1	2:B:140:GLN:NE2	1.98	0.61
1:X:25:GLY:HA3	1:X:37:MET:HG3	1.82	0.61
3:C:244:TYR:HB3	3:C:245:PRO:HD3	1.83	0.60
3:Z:397:SER:HB3	4:L:5:DT:H3	1.66	0.60
2:Y:105:ILE:HD13	2:Y:145:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:84:THR:HG22	1:X:85:VAL:H	1.65	0.60
3:Z:292:ASP:N	3:Z:292:ASP:OD1	2.34	0.60
3:C:490:CYS:SG	3:C:492:SER:OG	2.59	0.60
2:B:174:THR:O	2:B:175:ARG:HB2	2.01	0.60
3:Z:602:ARG:HH21	3:Z:604:ALA:HB2	1.66	0.59
3:C:204:LYS:N	3:C:249:GLU:OE1	2.35	0.59
1:A:9:ASN:C	1:A:9:ASN:HD22	2.05	0.59
3:C:327:LEU:HD11	3:C:364:GLU:HG2	1.83	0.59
3:C:382:GLY:O	3:C:399:SER:OG	2.17	0.59
1:X:76:ALA:CB	1:X:79:ILE:HD11	2.23	0.58
1:A:80:ARG:NE	1:A:81:GLU:H	1.98	0.58
2:B:71:ASP:OD2	2:B:170:HIS:HD2	1.86	0.58
1:X:25:GLY:HA3	1:X:37:MET:CG	2.33	0.58
2:B:155:ASP:OD2	2:B:155:ASP:C	2.42	0.58
3:Z:514:ARG:NH1	3:Z:515:SER:O	2.37	0.58
3:C:369:ASN:HB3	3:C:403:ILE:HD13	1.86	0.57
3:Z:327:LEU:HD11	3:Z:364:GLU:HG2	1.86	0.57
3:C:375:LYS:HG2	3:C:417:TYR:HE2	1.67	0.57
1:X:111:SER:OG	1:X:112:ASP:N	2.35	0.57
3:Z:421:GLY:C	3:Z:423:HIS:H	2.05	0.57
1:X:22:ARG:NH2	2:Y:99:GLU:OE2	2.37	0.57
1:X:38:GLN:NE2	1:X:42:LEU:HD22	2.20	0.57
3:C:514:ARG:NH1	3:C:515:SER:O	2.38	0.57
3:C:327:LEU:HD12	3:C:342:ARG:HH12	1.70	0.56
3:Z:204:LYS:N	3:Z:249:GLU:OE1	2.38	0.56
3:Z:461:ASN:HB3	3:Z:464:MET:HG3	1.87	0.56
1:A:38:GLN:NE2	1:A:42:LEU:HD22	2.20	0.56
3:Z:195:TRP:HZ3	3:Z:197:ILE:HG12	1.70	0.56
1:X:80:ARG:HE	1:X:81:GLU:N	2.00	0.56
3:Z:182:ILE:O	3:Z:182:ILE:HG22	2.05	0.56
3:Z:375:LYS:HG2	3:Z:417:TYR:HE2	1.70	0.56
1:A:20:THR:HA	1:A:65:GLY:O	2.06	0.56
2:Y:154:ILE:HD12	3:Z:608:PHE:HE1	1.70	0.56
3:C:501:LEU:HA	3:C:506:ASN:O	2.05	0.55
3:C:292:ASP:N	3:C:292:ASP:OD1	2.39	0.55
2:Y:54:ARG:HD2	2:Y:102:THR:O	2.05	0.55
2:Y:62:PRO:O	2:Y:63:HIS:CB	2.54	0.55
2:B:78:LEU:HD12	2:B:78:LEU:C	2.27	0.55
2:Y:109:GLN:NE2	2:Y:150:MET:HB2	2.21	0.55
3:C:471:PHE:CD1	3:C:473:VAL:HG23	2.41	0.55
3:Z:267:PHE:HA	4:L:5:DT:H73	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:384:LYS:NZ	4:L:6:DT:OP2	2.40	0.55
2:Y:80:PHE:HA	2:Y:162:HIS:CE1	2.42	0.54
3:C:602:ARG:HH21	3:C:604:ALA:HB2	1.71	0.54
3:C:461:ASN:HB3	3:C:464:MET:HG3	1.88	0.54
3:Z:490:CYS:HB3	3:Z:495:CYS:HB3	1.88	0.54
3:C:200:ARG:NH1	3:C:294:PRO:O	2.39	0.54
1:X:30:VAL:HG22	1:X:35:LEU:HD12	1.88	0.54
3:Z:448:MET:O	3:Z:449:ALA:CB	2.56	0.54
3:C:595:ARG:HH11	4:K:17:DT:H73	1.73	0.53
3:C:451:ARG:CB	3:C:451:ARG:HH11	2.20	0.53
2:Y:89:ARG:HG3	2:Y:94:VAL:HG22	1.90	0.53
3:Z:369:ASN:O	3:Z:372:VAL:HB	2.09	0.53
3:C:267:PHE:HE2	4:K:4:DT:H5"	1.73	0.53
3:Z:380:PHE:HA	3:Z:400:THR:O	2.08	0.53
3:C:471:PHE:CE1	3:C:473:VAL:CG2	2.91	0.53
1:A:39:THR:HG22	1:A:40:SER:N	2.24	0.53
3:C:380:PHE:HA	3:C:400:THR:O	2.09	0.53
3:Z:267:PHE:HA	4:L:5:DT:C7	2.38	0.53
3:C:195:TRP:HZ3	3:C:197:ILE:HG12	1.74	0.53
1:A:25:GLY:HA3	1:A:37:MET:HG3	1.90	0.53
1:X:30:VAL:HG22	1:X:35:LEU:CD1	2.39	0.53
2:Y:174:THR:O	2:Y:175:ARG:HB2	2.08	0.53
3:C:352:ARG:NH2	3:C:429:TYR:HA	2.21	0.53
3:Z:448:MET:O	3:Z:449:ALA:HB2	2.10	0.52
3:Z:451:ARG:HB2	3:Z:451:ARG:HH11	1.74	0.52
3:Z:492:SER:HB2	3:Z:512:CYS:SG	2.49	0.52
3:C:448:MET:O	3:C:449:ALA:CB	2.57	0.52
3:Z:471:PHE:CE1	3:Z:473:VAL:CG2	2.92	0.52
3:C:448:MET:O	3:C:449:ALA:HB2	2.10	0.52
3:C:488:THR:HB	3:C:519:PRO:HB2	1.91	0.52
1:A:80:ARG:HH12	2:B:128:VAL:HG22	1.75	0.51
1:X:40:SER:HB2	1:X:97:GLU:HB2	1.92	0.51
1:A:80:ARG:HE	1:A:81:GLU:N	2.03	0.51
3:Z:267:PHE:CE2	4:L:4:DT:H5"	2.46	0.51
1:A:83:THR:HG23	1:A:90:ASP:N	2.26	0.51
3:C:471:PHE:CE1	3:C:473:VAL:HG23	2.45	0.51
3:Z:318:ILE:HD12	3:Z:379:ALA:HB2	1.93	0.51
3:Z:210:TRP:CD1	3:Z:210:TRP:C	2.84	0.51
3:Z:471:PHE:CD1	3:Z:473:VAL:HG23	2.46	0.51
2:Y:61:GLN:HG3	2:Y:66:ALA:O	2.11	0.51
3:Z:244:TYR:HB3	3:Z:245:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:HB2	1:A:97:GLU:HB2	1.92	0.50
1:A:78:GLN:HE21	1:A:79:ILE:N	2.07	0.50
3:C:391:ARG:HB2	3:C:429:TYR:CE2	2.46	0.50
4:K:22:DT:H4'	4:K:23:DT:OP1	2.11	0.50
3:Z:201:VAL:HG13	3:Z:222:VAL:HG22	1.93	0.50
3:C:278:PHE:CD1	3:C:282:THR:HG21	2.46	0.50
3:Z:509:CYS:SG	3:Z:511:LYS:CB	2.99	0.50
3:Z:455:VAL:HB	3:Z:533:THR:HB	1.93	0.50
2:Y:130:VAL:HG21	2:Y:150:MET:HE3	1.94	0.50
3:Z:203:SER:OG	3:Z:223:ASN:HB2	2.12	0.50
3:Z:499:VAL:CG2	3:Z:507:TRP:HB3	2.42	0.50
2:Y:155:ASP:O	2:Y:155:ASP:OD2	2.29	0.50
1:X:2:GLU:HA	1:X:2:GLU:OE1	2.11	0.50
1:X:84:THR:CG2	1:X:85:VAL:N	2.74	0.50
3:Z:490:CYS:SG	3:Z:509:CYS:HB3	2.51	0.49
1:X:84:THR:CG2	1:X:85:VAL:H	2.24	0.49
1:A:80:ARG:NH1	2:B:128:VAL:HG22	2.27	0.49
3:C:394:SER:HB2	3:C:445:GLY:HA3	1.94	0.49
1:A:65:GLY:HA3	1:A:74:PHE:CE2	2.46	0.49
2:B:151:ARG:HD2	3:C:577:ARG:NH1	2.27	0.49
4:K:15:DT:H2''	4:K:16:DT:O5'	2.12	0.49
2:B:148:GLY:O	3:C:572:HIS:NE2	2.45	0.49
1:X:78:GLN:HE21	1:X:79:ILE:N	2.06	0.49
1:X:60:PHE:HB2	1:X:83:THR:OG1	2.13	0.49
3:Z:352:ARG:NH2	3:Z:429:TYR:HA	2.23	0.49
3:Z:497:LYS:HB3	3:Z:509:CYS:SG	2.53	0.49
3:Z:200:ARG:NH1	3:Z:294:PRO:O	2.43	0.49
1:A:82:PHE:CD2	2:B:156:TYR:HB2	2.47	0.49
3:C:200:ARG:HG3	3:C:200:ARG:O	2.11	0.49
2:Y:47:THR:HG22	3:Z:534:GLY:HA2	1.93	0.49
3:C:455:VAL:O	3:C:459:ASP:HB2	2.12	0.49
2:B:110:TRP:HH2	4:K:24:DT:O2	1.94	0.49
2:Y:125:ARG:NH1	2:Y:125:ARG:HB2	2.26	0.49
1:X:39:THR:HG22	1:X:40:SER:N	2.28	0.49
2:B:89:ARG:HG3	2:B:94:VAL:HG22	1.94	0.48
1:X:78:GLN:CA	1:X:78:GLN:HE21	2.26	0.48
3:C:204:LYS:NZ	3:C:244:TYR:O	2.46	0.48
2:B:63:HIS:O	2:B:64:PRO:C	2.52	0.48
3:C:498:LYS:HB2	4:K:14:DT:H5''	1.95	0.48
3:Z:451:ARG:CG	3:Z:451:ARG:HH11	2.26	0.48
3:C:379:ALA:O	3:C:401:MET:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:321:LEU:HB2	3:C:378:LEU:HD12	1.95	0.48
1:A:55:VAL:O	1:A:56:SER:C	2.51	0.48
1:A:111:SER:OG	1:A:112:ASP:N	2.47	0.48
1:A:76:ALA:CB	1:A:79:ILE:HD11	2.27	0.48
1:A:80:ARG:HE	1:A:80:ARG:HA	1.77	0.48
3:C:531:ASP:C	3:C:531:ASP:OD1	2.52	0.48
3:C:451:ARG:HB2	3:C:451:ARG:HH11	1.79	0.48
1:A:47:ILE:HG23	1:A:74:PHE:HB3	1.96	0.48
3:C:471:PHE:HE1	3:C:473:VAL:CG2	2.27	0.48
3:C:455:VAL:HB	3:C:533:THR:HB	1.95	0.48
3:C:220:PHE:HD2	3:C:240:VAL:HG22	1.79	0.48
3:Z:514:ARG:HD3	3:Z:516:TYR:CZ	2.49	0.48
1:X:16:TYR:O	1:X:67:VAL:HB	2.14	0.48
3:C:322:ASP:HB3	3:C:345:THR:HB	1.96	0.48
3:Z:384:LYS:HE3	3:Z:445:GLY:O	2.13	0.47
2:B:110:TRP:CH2	4:K:24:DT:O2	2.67	0.47
3:Z:210:TRP:CD1	3:Z:210:TRP:O	2.68	0.47
3:C:523:TYR:H	3:C:542:ASN:HD22	1.62	0.47
2:Y:68:PHE:CE1	2:Y:136:LEU:HG	2.49	0.47
2:Y:92:THR:OG1	2:Y:93:ASN:ND2	2.42	0.47
3:C:467:LYS:HE3	4:K:9:DT:OP2	2.14	0.47
3:C:203:SER:OG	3:C:223:ASN:HB2	2.14	0.47
3:Z:342:ARG:NH1	3:Z:363:ALA:O	2.48	0.47
3:C:578:MET:HG2	3:C:606:VAL:HG21	1.96	0.47
3:C:618:ALA:O	3:C:621:ALA:HB3	2.14	0.47
1:A:10:SER:HB3	1:A:39:THR:OG1	2.14	0.47
3:Z:327:LEU:HD12	3:Z:342:ARG:HH12	1.79	0.47
3:Z:471:PHE:CE1	3:Z:473:VAL:HG23	2.50	0.47
1:X:27:VAL:CG1	1:X:35:LEU:HD11	2.45	0.47
1:A:30:VAL:HG22	1:A:35:LEU:HD12	1.96	0.47
1:A:60:PHE:HD1	1:A:83:THR:HG1	1.61	0.47
2:B:83:VAL:HG12	2:B:84:VAL:N	2.29	0.47
1:X:83:THR:HG22	1:X:84:THR:H	1.80	0.47
2:Y:151:ARG:HD2	3:Z:577:ARG:NH1	2.30	0.47
3:Z:379:ALA:O	3:Z:401:MET:HA	2.16	0.46
2:Y:78:LEU:HD12	2:Y:78:LEU:C	2.35	0.46
3:C:392:SER:CB	3:C:445:GLY:H	2.26	0.46
3:C:509:CYS:SG	3:C:511:LYS:HB3	2.55	0.46
3:C:451:ARG:HH21	3:C:474:ARG:NH2	2.13	0.46
3:C:369:ASN:O	3:C:372:VAL:HB	2.15	0.46
3:Z:447:ASN:HB2	3:Z:450:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:331:VAL:HG13	3:Z:336:GLN:O	2.16	0.46
1:A:78:GLN:C	1:A:79:ILE:HD12	2.35	0.46
1:X:10:SER:HB3	1:X:39:THR:OG1	2.14	0.46
1:A:27:VAL:CG1	1:A:35:LEU:HD11	2.45	0.46
4:L:3:DT:H2''	4:L:4:DT:O5'	2.16	0.46
1:A:2:GLU:HA	1:A:2:GLU:OE1	2.16	0.46
3:Z:217:GLY:HA2	3:Z:237:ASN:OD1	2.16	0.46
3:C:204:LYS:NZ	3:C:247:LEU:O	2.30	0.46
1:A:62:GLU:CB	1:A:82:PHE:CZ	2.95	0.46
3:C:443:GLY:HA2	4:K:7:DT:O2	2.16	0.45
1:A:78:GLN:CA	1:A:78:GLN:HE21	2.28	0.45
3:Z:590:PHE:CD1	3:Z:591:ASN:N	2.84	0.45
3:Z:471:PHE:HE1	3:Z:473:VAL:CG2	2.28	0.45
1:A:59:THR:HB	1:A:83:THR:OG1	2.16	0.45
3:C:490:CYS:SG	3:C:492:SER:CB	3.05	0.45
3:C:497:LYS:HB3	3:C:509:CYS:SG	2.56	0.45
3:Z:538:LEU:HD13	3:Z:600:ILE:HG12	1.98	0.45
3:Z:510:GLU:HG2	3:Z:510:GLU:H	1.59	0.45
1:A:30:VAL:HG22	1:A:35:LEU:CD1	2.46	0.45
3:C:243:PHE:CD1	3:C:284:ILE:HD12	2.52	0.45
3:Z:547:GLN:NE2	3:Z:603:ALA:O	2.49	0.45
1:X:82:PHE:CD1	1:X:91:VAL:HG21	2.52	0.45
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.17	0.45
1:X:25:GLY:HA2	1:X:38:GLN:O	2.16	0.45
3:C:355:LYS:HB3	3:C:444:ALA:CB	2.47	0.45
3:C:485:LEU:HD11	3:C:571:LEU:HD21	2.00	0.45
3:C:327:LEU:HD12	3:C:364:GLU:HA	2.00	0.44
3:Z:467:LYS:HA	3:Z:468:PRO:HD2	1.88	0.44
3:C:247:LEU:HD21	3:C:284:ILE:HD13	1.99	0.44
3:C:607:ASP:OD1	3:C:607:ASP:C	2.55	0.44
1:X:55:VAL:O	1:X:56:SER:C	2.55	0.44
1:X:21:VAL:CG2	1:X:74:PHE:HZ	2.31	0.44
3:C:551:MET:HG2	3:C:555:GLU:HB2	1.98	0.44
3:C:490:CYS:SG	3:C:492:SER:HB2	2.58	0.44
4:K:4:DT:H2'	4:K:5:DT:C7	2.46	0.44
2:B:86:ASN:HB3	2:B:97:SER:CB	2.46	0.44
3:Z:471:PHE:HE1	3:Z:473:VAL:HG21	1.83	0.44
3:C:613:MET:O	3:C:616:VAL:HB	2.18	0.44
3:Z:220:PHE:HD2	3:Z:240:VAL:HG22	1.83	0.44
3:Z:391:ARG:HB2	3:Z:429:TYR:CE2	2.53	0.44
3:Z:498:LYS:HD3	3:Z:500:ASN:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLY:O	1:A:60:PHE:HA	2.18	0.44
3:C:565:SER:O	3:C:569:ALA:HB2	2.18	0.44
2:Y:131:ARG:HD3	2:Y:158:GLU:OE2	2.18	0.43
3:C:588:ASP:O	3:C:594:ALA:HA	2.18	0.43
3:C:278:PHE:HD1	3:C:282:THR:HG21	1.83	0.43
2:Y:48:LEU:HA	2:Y:77:GLN:O	2.18	0.43
4:K:1:DT:H2''	4:K:2:DT:H5''	2.00	0.43
1:A:25:GLY:HA3	1:A:37:MET:CG	2.48	0.43
4:K:22:DT:H2''	4:K:23:DT:C4	2.54	0.43
3:Z:189:SER:HB2	3:Z:191:TYR:HD2	1.83	0.43
2:B:81:VAL:HG22	2:B:131:ARG:HD2	2.00	0.43
2:Y:83:VAL:HG12	2:Y:84:VAL:N	2.32	0.43
3:Z:327:LEU:HD12	3:Z:364:GLU:HA	1.99	0.43
1:A:83:THR:CG2	1:A:90:ASP:N	2.81	0.43
3:C:355:LYS:HB3	3:C:444:ALA:HB1	2.00	0.43
3:C:408:THR:O	3:C:411:HIS:HB2	2.19	0.43
3:Z:509:CYS:SG	3:Z:511:LYS:N	2.91	0.43
1:X:9:ASN:ND2	1:X:9:ASN:C	2.71	0.43
3:Z:590:PHE:CD1	3:Z:591:ASN:HB2	2.54	0.43
3:C:218:LYS:HG3	3:C:237:ASN:HA	2.01	0.43
3:Z:322:ASP:HB3	3:Z:345:THR:HB	2.00	0.43
3:Z:386:GLY:O	3:Z:392:SER:N	2.52	0.43
3:Z:247:LEU:HD21	3:Z:284:ILE:HD13	2.01	0.43
1:A:24:VAL:HG13	1:A:82:PHE:HE1	1.84	0.43
4:L:13:DT:H2'	4:L:14:DT:H72	2.00	0.43
3:C:232:LYS:NZ	3:C:267:PHE:O	2.52	0.43
3:C:386:GLY:O	3:C:392:SER:N	2.52	0.43
3:C:330:ILE:O	3:C:339:VAL:N	2.26	0.43
1:X:65:GLY:HA3	1:X:74:PHE:CE2	2.53	0.43
2:Y:48:LEU:HD11	2:Y:133:LEU:HD11	2.00	0.43
3:Z:523:TYR:H	3:Z:542:ASN:HD22	1.66	0.42
3:Z:243:PHE:CD1	3:Z:284:ILE:HD12	2.54	0.42
3:Z:214:ARG:HG3	3:Z:215:GLY:H	1.83	0.42
1:X:78:GLN:HA	1:X:78:GLN:NE2	2.34	0.42
2:Y:151:ARG:NH1	3:Z:577:ARG:HG2	2.32	0.42
3:C:616:VAL:O	3:C:620:ARG:HG2	2.19	0.42
3:Z:551:MET:HG2	3:Z:555:GLU:HB2	2.00	0.42
1:A:102:ILE:O	1:A:106:PHE:HD1	2.02	0.42
3:Z:499:VAL:HG12	3:Z:509:CYS:HB2	2.02	0.42
3:C:471:PHE:CD1	3:C:473:VAL:CG2	3.02	0.42
1:A:16:TYR:O	1:A:67:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:18:DT:H4'	4:K:19:DT:OP2	2.19	0.42
3:Z:321:LEU:HB2	3:Z:378:LEU:HD12	2.01	0.42
3:Z:471:PHE:CD1	3:Z:473:VAL:CG2	3.02	0.42
2:Y:63:HIS:O	2:Y:65:ASP:N	2.53	0.42
1:X:47:ILE:HG23	1:X:74:PHE:HB3	2.01	0.42
1:A:60:PHE:CD1	1:A:91:VAL:HB	2.55	0.42
3:Z:531:ASP:OD1	3:Z:531:ASP:C	2.57	0.42
1:A:65:GLY:HA3	1:A:74:PHE:HE2	1.84	0.41
2:B:93:ASN:HB3	2:B:110:TRP:CE3	2.55	0.41
3:Z:607:ASP:OD1	3:Z:607:ASP:C	2.58	0.41
3:Z:443:GLY:O	3:Z:446:ALA:HB3	2.19	0.41
3:C:451:ARG:HH21	3:C:474:ARG:HH22	1.68	0.41
3:C:587:MET:CE	3:C:594:ALA:HB1	2.50	0.41
3:Z:278:PHE:CD1	3:Z:282:THR:HG21	2.54	0.41
4:K:14:DT:H2''	4:K:15:DT:H5''	2.03	0.41
3:C:421:GLY:C	3:C:423:HIS:N	2.70	0.41
3:Z:536:MET:HG2	3:Z:537:TRP:N	2.35	0.41
3:C:220:PHE:CD2	3:C:240:VAL:HG22	2.55	0.41
3:C:600:ILE:HG21	3:C:603:ALA:HB2	2.03	0.41
1:X:45:VAL:HG12	1:X:46:GLU:N	2.35	0.41
3:C:523:TYR:HB2	3:C:542:ASN:HA	2.02	0.41
3:Z:485:LEU:HD11	3:Z:571:LEU:HD21	2.02	0.41
2:B:132:VAL:HG22	2:B:150:MET:HG3	2.02	0.41
3:Z:204:LYS:NZ	3:Z:244:TYR:O	2.53	0.41
3:C:267:PHE:CE2	4:K:4:DT:H5''	2.55	0.41
2:B:110:TRP:HB2	4:K:22:DT:OP1	2.20	0.41
3:Z:332:SER:OG	3:Z:336:GLN:N	2.54	0.41
3:Z:496:ASN:HD22	4:L:12:DT:H2''	1.86	0.41
3:Z:618:ALA:O	3:Z:621:ALA:HB3	2.20	0.41
3:C:597:ARG:NH2	4:K:14:DT:O4	2.53	0.41
3:C:467:LYS:HA	3:C:468:PRO:HD2	1.84	0.41
3:C:189:SER:HB2	3:C:191:TYR:HD2	1.86	0.41
1:X:39:THR:HG22	1:X:40:SER:H	1.85	0.41
2:B:155:ASP:O	2:B:155:ASP:OD2	2.38	0.41
2:Y:84:VAL:O	2:Y:127:ASN:N	2.47	0.40
4:K:12:DT:H1'	4:K:13:DT:O5'	2.21	0.40
1:X:60:PHE:HD1	1:X:83:THR:OG1	2.02	0.40
3:C:471:PHE:HE1	3:C:473:VAL:HG21	1.86	0.40
3:Z:378:LEU:HD21	3:Z:403:ILE:HG12	2.03	0.40
1:A:39:THR:HG22	1:A:40:SER:H	1.86	0.40
2:Y:68:PHE:CG	2:Y:136:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:457:VAL:HA	3:Z:462:LEU:HD22	2.03	0.40
4:K:10:DT:H6	4:K:10:DT:OP2	2.04	0.40
3:C:185:ILE:HG12	3:C:231:ILE:HG22	2.02	0.40
3:C:318:ILE:HD12	3:C:379:ALA:HB2	2.04	0.40
2:Y:51:VAL:HA	2:Y:55:GLN:OE1	2.21	0.40
3:Z:487:TYR:CE1	3:Z:489:ALA:HB2	2.57	0.40
3:Z:238:ASP:OD2	3:Z:238:ASP:N	2.55	0.40

All (1) 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)
3:C:596:VAL:N	3:Z:466:GLU:OE2[4_444]	2.05	0.15

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	104/114 (91%)	89 (86%)	12 (12%)	3 (3%)	6	29
1	X	104/114 (91%)	88 (85%)	15 (14%)	1 (1%)	19	58
2	B	118/136 (87%)	103 (87%)	12 (10%)	3 (2%)	7	32
2	Y	118/136 (87%)	104 (88%)	11 (9%)	3 (2%)	7	32
3	C	429/444 (97%)	384 (90%)	39 (9%)	6 (1%)	14	48
3	Z	429/444 (97%)	379 (88%)	40 (9%)	10 (2%)	8	35
All	All	1302/1388 (94%)	1147 (88%)	129 (10%)	26 (2%)	9	38

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU

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Mol	Chain	Res	Type
1	A	83	THR
2	B	63	HIS
2	B	64	PRO
3	C	449	ALA
2	Y	63	HIS
2	Y	64	PRO
3	Z	449	ALA
3	Z	511	LYS
3	C	237	ASN
1	X	2	GLU
2	Y	157	ASN
3	Z	237	ASN
3	Z	212	ASN
3	Z	217	GLY
1	A	56	SER
3	C	422	ALA
3	C	511	LYS
3	Z	422	ALA
3	C	502	ASP
3	Z	331	VAL
3	Z	593	THR
3	Z	513	ASP
3	C	296	VAL
2	B	62	PRO
3	Z	296	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	96/101 (95%)	79 (82%)	17 (18%)	2	10
1	X	96/101 (95%)	77 (80%)	19 (20%)	1	7
2	B	107/118 (91%)	96 (90%)	11 (10%)	9	32
2	Y	107/118 (91%)	90 (84%)	17 (16%)	3	13
3	C	370/374 (99%)	343 (93%)	27 (7%)	17	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Z	370/374 (99%)	334 (90%)	36 (10%)	10	36
All	All	1146/1186 (97%)	1019 (89%)	127 (11%)	8	29

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	ASN
1	A	12	MET
1	A	28	HIS
1	A	34	THR
1	A	47	ILE
1	A	52	ASP
1	A	58	SER
1	A	59	THR
1	A	69	ASP
1	A	74	PHE
1	A	75	GLN
1	A	78	GLN
1	A	80	ARG
1	A	83	THR
1	A	84	THR
1	A	112	ASP
2	B	67	GLU
2	B	74	GLU
2	B	98	VAL
2	B	104	GLN
2	B	106	GLU
2	B	107	VAL
2	B	123	GLU
2	B	125	ARG
2	B	144	SER
2	B	153	VAL
2	B	175	ARG
3	C	185	ILE
3	C	198	LYS
3	C	200	ARG
3	C	213	GLN
3	C	222	VAL
3	C	227	ASP
3	C	249	GLU
3	C	254	LEU

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Mol	Chain	Res	Type
3	C	280	ASN
3	C	287	CYS
3	C	289	ASP
3	C	292	ASP
3	C	316	ASP
3	C	317	VAL
3	C	345	THR
3	C	381	LYS
3	C	399	SER
3	C	401	MET
3	C	406	ASP
3	C	429	TYR
3	C	451	ARG
3	C	462	LEU
3	C	485	LEU
3	C	511	LYS
3	C	556	LEU
3	C	593	THR
3	C	597	ARG
1	X	2	GLU
1	X	9	ASN
1	X	12	MET
1	X	28	HIS
1	X	34	THR
1	X	47	ILE
1	X	52	ASP
1	X	58	SER
1	X	59	THR
1	X	73	SER
1	X	74	PHE
1	X	75	GLN
1	X	78	GLN
1	X	80	ARG
1	X	81	GLU
1	X	82	PHE
1	X	83	THR
1	X	90	ASP
1	X	112	ASP
2	Y	67	GLU
2	Y	74	GLU
2	Y	98	VAL
2	Y	99	GLU

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Mol	Chain	Res	Type
2	Y	104	GLN
2	Y	106	GLU
2	Y	107	VAL
2	Y	123	GLU
2	Y	125	ARG
2	Y	131	ARG
2	Y	133	LEU
2	Y	140	GLN
2	Y	141	ASN
2	Y	142	ARG
2	Y	150	MET
2	Y	153	VAL
2	Y	175	ARG
3	Z	185	ILE
3	Z	198	LYS
3	Z	200	ARG
3	Z	211	SER
3	Z	213	GLN
3	Z	216	GLU
3	Z	222	VAL
3	Z	227	ASP
3	Z	249	GLU
3	Z	254	LEU
3	Z	280	ASN
3	Z	287	CYS
3	Z	288	THR
3	Z	289	ASP
3	Z	292	ASP
3	Z	316	ASP
3	Z	317	VAL
3	Z	330	ILE
3	Z	345	THR
3	Z	381	LYS
3	Z	399	SER
3	Z	401	MET
3	Z	406	ASP
3	Z	429	TYR
3	Z	451	ARG
3	Z	462	LEU
3	Z	485	LEU
3	Z	490	CYS
3	Z	492	SER

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Mol	Chain	Res	Type
3	Z	508	ARG
3	Z	510	GLU
3	Z	515	SER
3	Z	548	LEU
3	Z	556	LEU
3	Z	595	ARG
3	Z	597	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	15	GLN
1	A	38	GLN
1	A	44	ASN
1	A	78	GLN
1	A	101	GLN
2	B	104	GLN
2	B	109	GLN
2	B	140	GLN
2	B	170	HIS
3	C	261	ASN
3	C	280	ASN
3	C	506	ASN
3	C	528	ASN
3	C	542	ASN
3	C	547	GLN
3	C	557	HIS
3	C	582	ASN
1	X	9	ASN
1	X	15	GLN
1	X	38	GLN
1	X	44	ASN
1	X	78	GLN
1	X	101	GLN
2	Y	77	GLN
2	Y	104	GLN
2	Y	109	GLN
2	Y	140	GLN
2	Y	149	HIS
2	Y	170	HIS
3	Z	261	ASN

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Mol	Chain	Res	Type
3	Z	280	ASN
3	Z	500	ASN
3	Z	528	ASN
3	Z	542	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	108/114 (94%)	0.13	4 (3%)	45	22	31, 61, 99, 121	0
1	X	108/114 (94%)	0.13	5 (4%)	36	17	29, 55, 93, 114	0
2	B	122/136 (89%)	0.21	9 (7%)	17	6	34, 62, 126, 165	0
2	Y	122/136 (89%)	0.18	5 (4%)	41	19	33, 57, 109, 135	0
3	C	433/444 (97%)	0.43	40 (9%)	11	4	36, 86, 152, 175	0
3	Z	433/444 (97%)	0.45	43 (9%)	9	3	32, 84, 146, 186	0
4	K	25/32 (78%)	1.85	9 (36%)	0	0	119, 166, 208, 221	0
4	L	20/32 (62%)	1.73	7 (35%)	0	0	107, 175, 239, 245	0
All	All	1371/1452 (94%)	0.39	122 (8%)	12	4	29, 76, 154, 245	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	518	THR	9.7
3	C	517	ALA	8.8
2	Y	112	ASP	7.8
3	C	441	GLY	6.4
3	C	515	SER	6.4
3	Z	591	ASN	6.2
3	C	591	ASN	5.9
1	A	1	MET	5.9
3	Z	441	GLY	5.9
3	C	503	HIS	5.8
1	A	85	VAL	5.8
3	C	335	SER	5.6
3	C	510	GLU	5.4
4	L	17	DT	5.4
2	Y	91	ALA	5.3
3	Z	213	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	X	70	ALA	5.3
3	Z	517	ALA	5.0
3	Z	503	HIS	4.8
3	C	500	ASN	4.7
4	K	24	DT	4.7
4	K	10	DT	4.6
3	C	334	ALA	4.6
3	Z	507	TRP	4.4
3	C	592	ASP	4.3
3	Z	428	PRO	4.3
3	C	215	GLY	4.2
3	Z	501	LEU	4.2
4	L	16	DT	4.1
1	A	84	THR	4.1
1	A	58	SER	4.0
3	Z	514	ARG	3.9
4	L	20	DT	3.9
2	B	112	ASP	3.8
3	C	213	GLN	3.8
4	L	21	DT	3.8
2	B	92	THR	3.7
3	C	327	LEU	3.7
3	Z	494	GLY	3.7
2	B	91	ALA	3.6
3	Z	448	MET	3.6
3	C	214	ARG	3.6
3	C	423	HIS	3.5
3	Z	327	LEU	3.5
4	K	17	DT	3.5
4	K	11	DT	3.5
4	K	16	DT	3.5
3	Z	216	GLU	3.5
3	Z	331	VAL	3.5
1	X	1	MET	3.4
3	C	442	GLY	3.4
3	Z	493	GLU	3.3
3	Z	447	ASN	3.3
3	C	514	ARG	3.3
3	Z	326	GLU	3.3
4	K	23	DT	3.3
3	Z	464	MET	3.3
3	Z	561	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	502	ASP	3.1
3	Z	211	SER	3.1
3	C	507	TRP	3.1
3	Z	431	ASN	3.1
3	Z	589	THR	3.0
3	Z	592	ASP	3.0
3	C	343	GLU	3.0
1	X	56	SER	3.0
3	C	499	VAL	3.0
3	C	521	TYR	2.9
3	C	501	LEU	2.9
1	X	85	VAL	2.9
4	L	15	DT	2.9
3	Z	505	ASN	2.8
2	B	67	GLU	2.7
4	K	25	DT	2.7
3	C	489	ALA	2.7
3	Z	335	SER	2.7
3	Z	430	THR	2.7
3	Z	422	ALA	2.6
3	C	561	GLU	2.5
3	C	325	GLY	2.5
3	C	513	ASP	2.5
3	C	593	THR	2.4
2	B	110	TRP	2.4
4	L	18	DT	2.4
3	Z	214	ARG	2.4
3	Z	515	SER	2.4
2	Y	63	HIS	2.4
3	C	491	ALA	2.4
3	C	266	GLN	2.4
3	Z	215	GLY	2.3
3	Z	519	PRO	2.3
3	Z	500	ASN	2.3
3	C	337	ARG	2.3
1	X	84	THR	2.3
3	C	397	SER	2.3
3	Z	516	TYR	2.3
3	C	505	ASN	2.3
2	B	93	ASN	2.2
2	B	111	LEU	2.2
2	B	175	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	Z	521	TYR	2.2
3	Z	227	ASP	2.2
2	Y	175	ARG	2.2
4	K	21	DT	2.2
3	Z	386	GLY	2.2
3	Z	194	ARG	2.1
3	C	519	PRO	2.1
3	Z	328	SER	2.1
4	K	18	DT	2.1
3	Z	210	TRP	2.1
4	L	4	DT	2.1
3	Z	562	GLU	2.1
3	C	488	THR	2.1
3	C	590	PHE	2.1
3	Z	486	TYR	2.1
2	B	63	HIS	2.1
3	Z	297	LYS	2.1
3	C	367	PRO	2.1
3	C	333	LYS	2.1
3	C	216	GLU	2.0
3	C	364	GLU	2.0
2	Y	64	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ZN	C	701	1/1	0.96	0.18	-0.78	136,136,136,136	0
5	ZN	Z	701	1/1	0.80	0.15	-1.29	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.