Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 03:38 pm BST

PDB ID	:	2XCR
Title	:	The 3.5A crystal structure of the catalytic core (B'A' region) of Staphylococcus aureus DNA Gyrase complexed with GSK299423 and DNA
Authors	:	Bax, B.D.; Chan, P.F.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.W.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.F.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on	:	2010-04-25
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

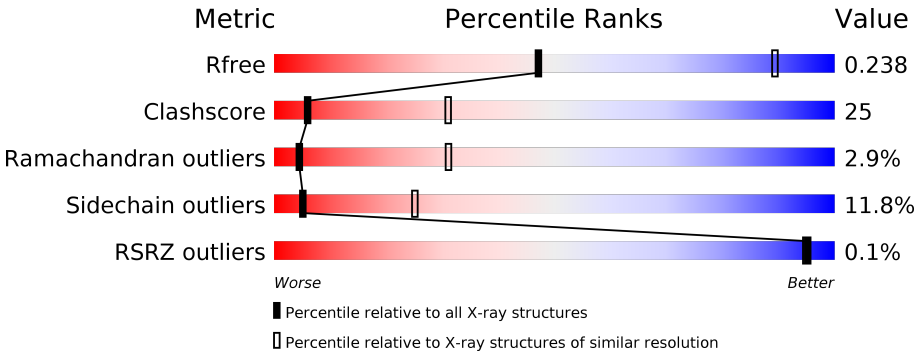
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	B	726	53% 39% 7%
1	D	726	55% 37% 7%
1	S	726	51% 40% 8%
1	U	726	53% 37% 8%
2	E	20	25% 55% 20%

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Mol	Chain	Length	Quality of chain
2	F	20	45% 30% 25%
3	V	20	5% 55% 40%
3	W	20	15% 55% 20% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24495 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	718	Total	C	N	O	S	0	0	0
			5689	3556	1018	1090	25			
1	D	719	Total	C	N	O	S	0	0	0
			5692	3556	1021	1090	25			
1	S	718	Total	C	N	O	S	0	0	0
			5694	3561	1022	1086	25			
1	U	717	Total	C	N	O	S	0	0	0
			5689	3558	1020	1086	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	expression tag	UNP Q99XG5
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5
D	409	MET	-	expression tag	UNP Q99XG5
D	1123	PHE	TYR	engineered mutation	UNP Q99XG5
S	409	MET	-	expression tag	UNP Q99XG5
S	1123	PHE	TYR	engineered mutation	UNP Q99XG5
U	409	MET	-	expression tag	UNP Q99XG5
U	1123	PHE	TYR	engineered mutation	UNP Q99XG5

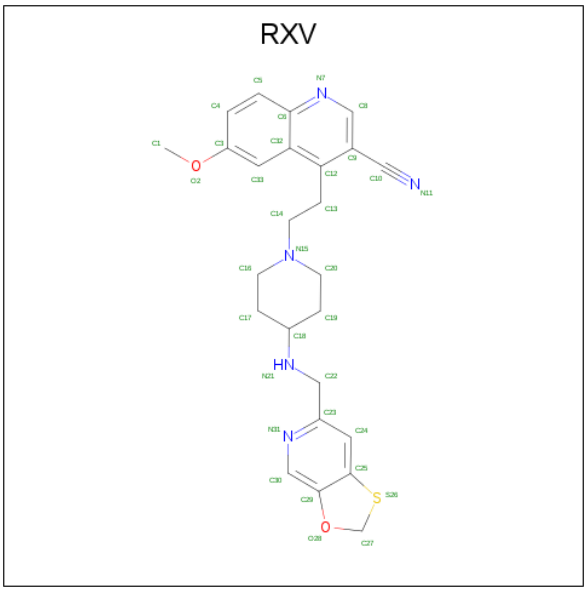
- Molecule 2 is a DNA chain called 5'-D(*5UA*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			
2	F	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
3	W	18	Total	C	N	O	P	0	0	0
			369	173	70	108	18			

- Molecule 4 is 6-METHOXY-4-(2-{4-[([1,3]OXATHIOLO[5,4-C]PYRIDIN-6-YLMETHYL) AMINO]PIPERIDIN-1-YL}ETHYL)QUINOLINE-3-CARBONITRILE (three-letter code: RXV) (formula: $C_{25}H_{27}N_5O_2S$).



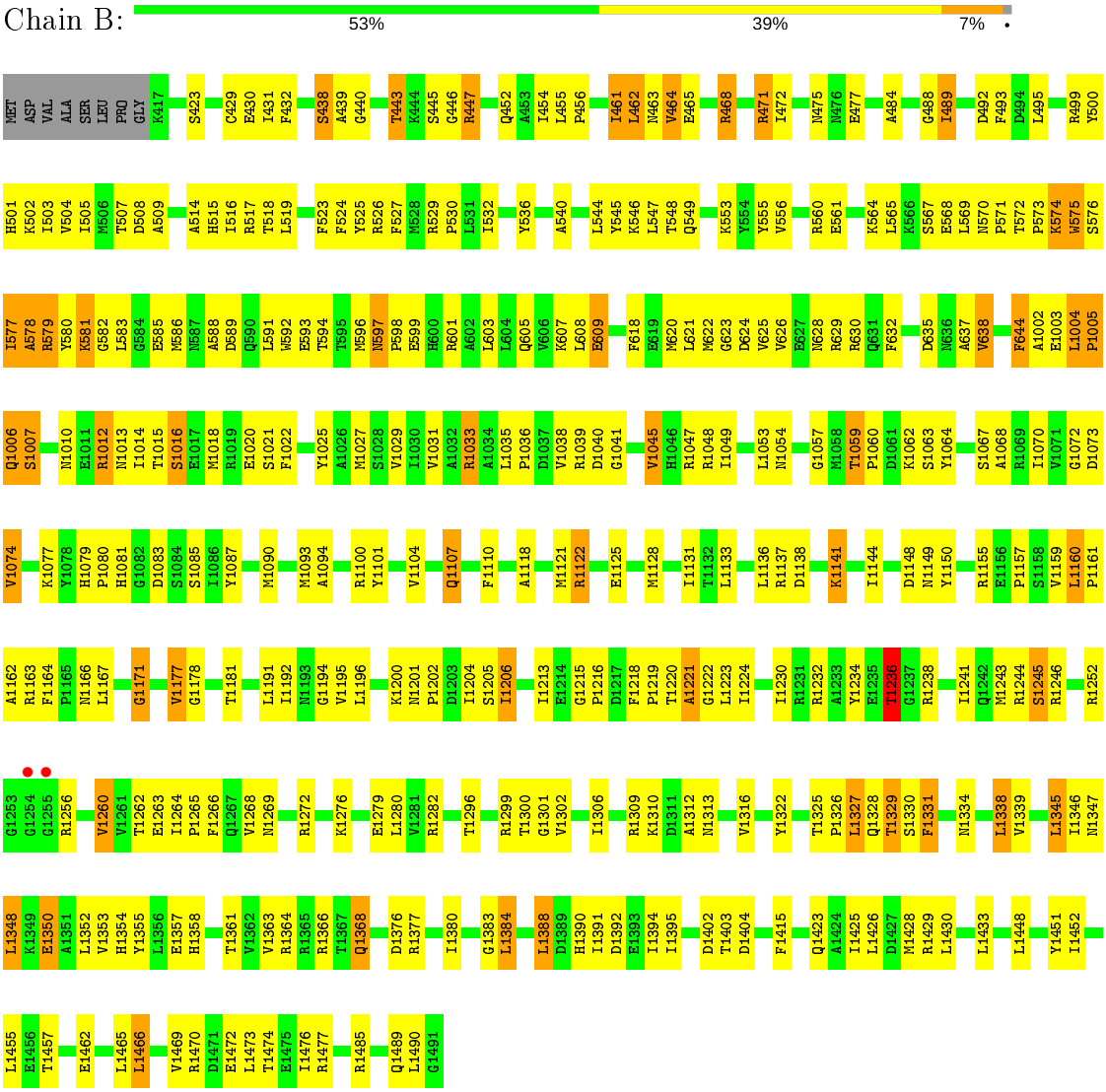
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	1
			66	50	10	4	2		
4	W	1	Total	C	N	O	S	0	1
			66	50	10	4	2		

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 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.

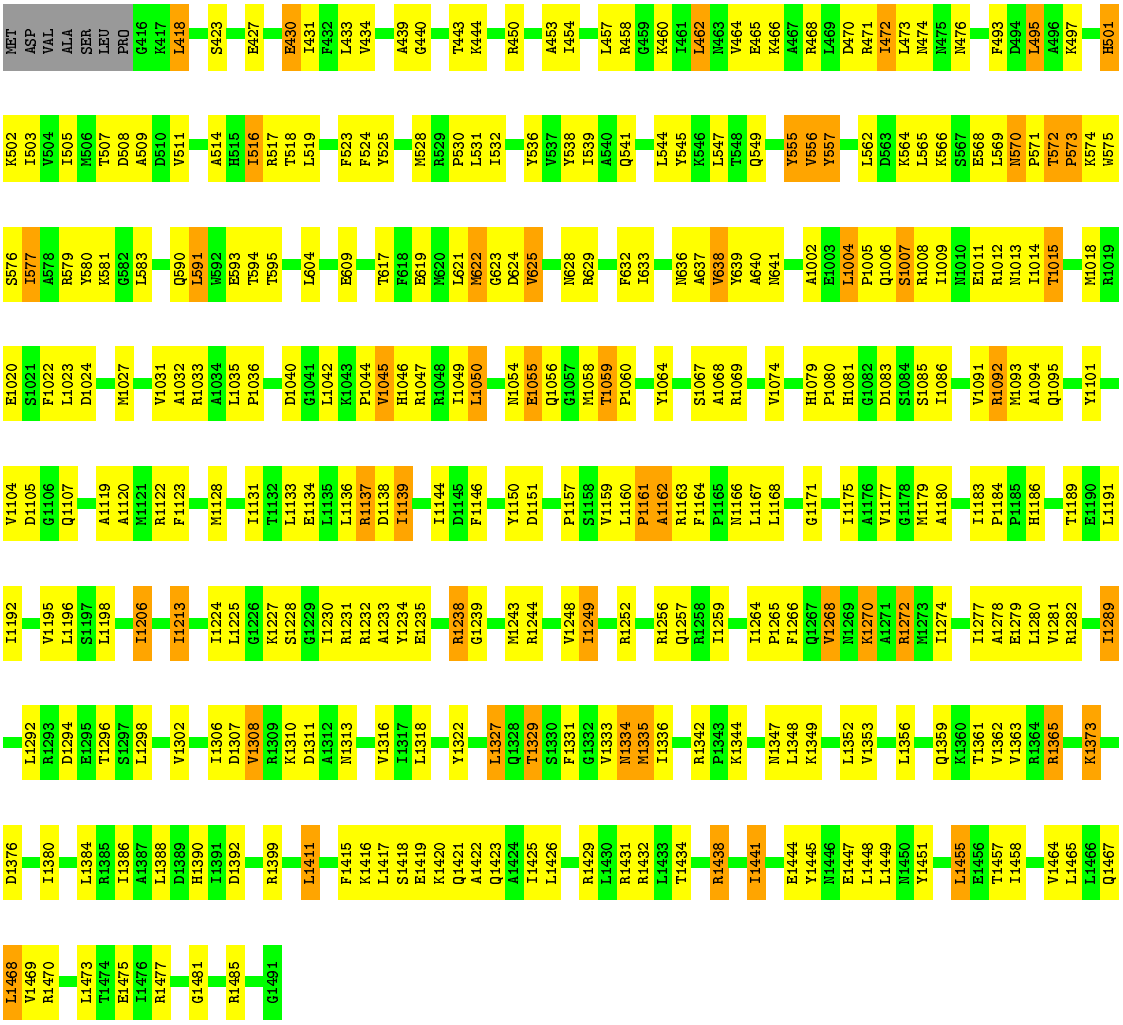
- Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain B:



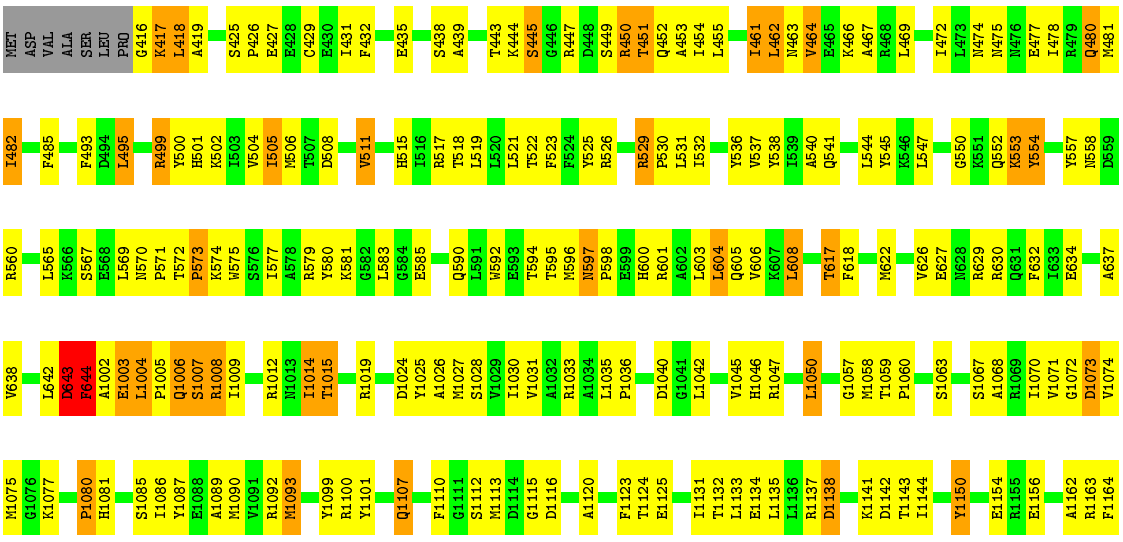
- Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

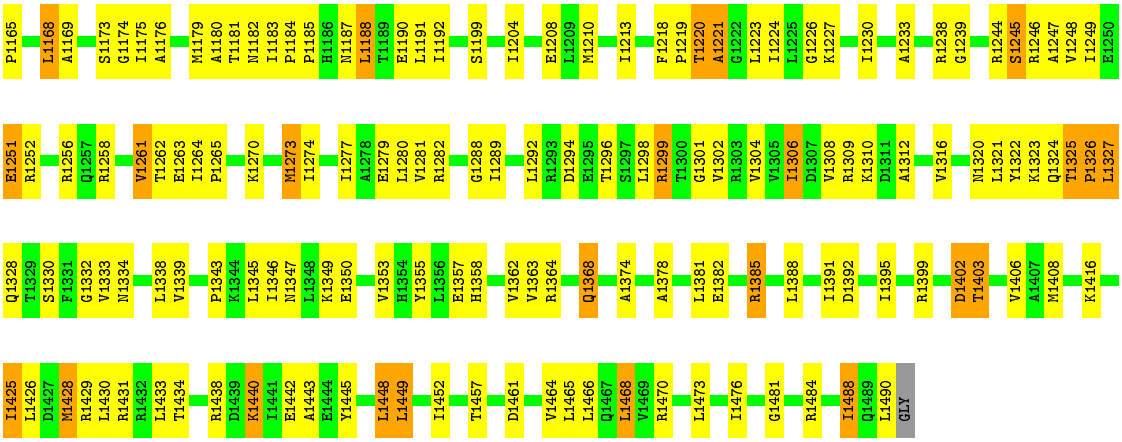
Chain D:



• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

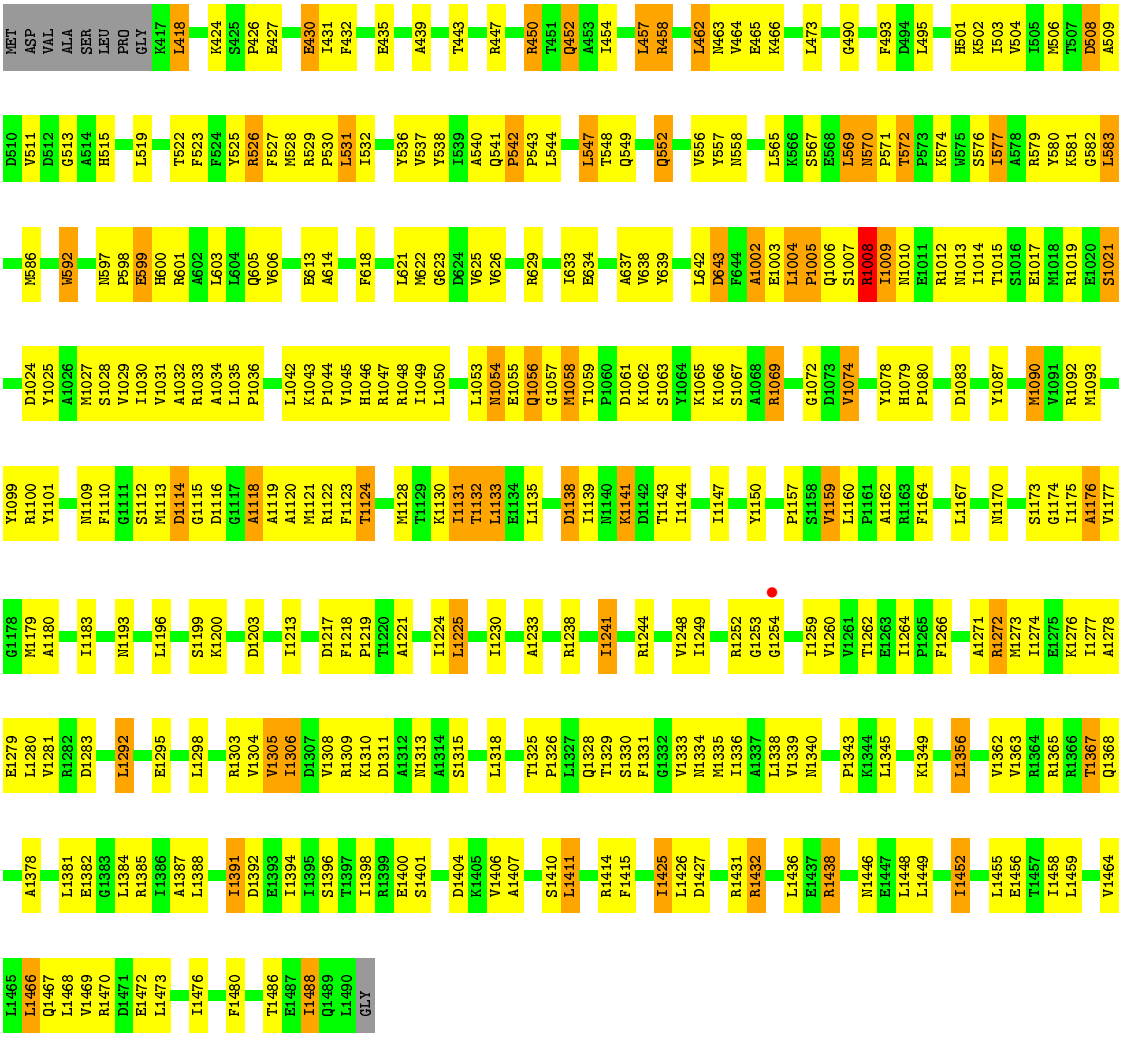
Chain S:





• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain U:



• Molecule 2: 5'-D(*5UA*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*TP)-3'

Chain E:

• Molecule 2: 5'-D(*5UA*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*TP)-3'

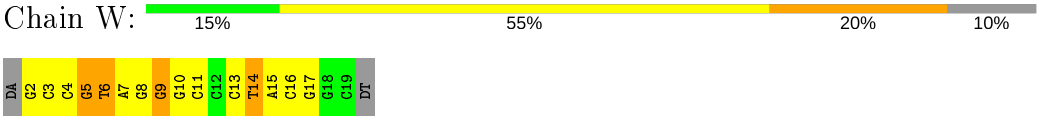
Chain F:

• Molecule 3: 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*TP)-3'

Chain V:

• Molecule 3: 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*TP)-3'

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.26Å 165.38Å 308.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.99 – 3.50 23.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.5 (23.99-3.50) 84.6 (23.99-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.258 0.176 , 0.238	Depositor DCC
R_{free} test set	2505 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	1.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	None for NONE	Depositor
Outliers	1 of 62227 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24495	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5UA, RXV

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	B	0.40	0/5772	0.63	0/7784
1	D	0.42	0/5775	0.63	0/7792
1	S	0.43	0/5777	0.66	1/7789 (0.0%)
1	U	0.42	0/5772	0.64	0/7785
2	E	0.85	0/435	1.86	10/669 (1.5%)
2	F	0.84	0/435	1.70	9/669 (1.3%)
3	V	0.90	0/459	1.84	14/706 (2.0%)
3	W	0.94	1/413 (0.2%)	1.84	13/635 (2.0%)
All	All	0.47	1/24838 (0.0%)	0.80	47/33829 (0.1%)

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	S	0	1
1	U	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	14	DT	C1'-N1	5.28	1.56	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	8	DG	O4'-C1'-N9	-15.90	96.87	108.00
3	W	14	DT	O4'-C1'-N1	11.09	115.76	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	16	DC	O4'-C4'-C3'	-10.56	99.66	106.00
3	V	16	DC	O4'-C4'-C3'	-10.33	99.80	106.00
2	E	10	DG	O4'-C1'-N9	10.29	115.20	108.00
2	F	10	DG	O4'-C1'-N9	9.75	114.82	108.00
2	F	8	DG	O4'-C1'-N9	-9.37	101.44	108.00
2	E	7	DA	O4'-C4'-C3'	-9.13	100.52	106.00
3	V	16	DC	O4'-C1'-N1	8.98	114.29	108.00
3	V	14	DT	O4'-C1'-N1	8.96	114.27	108.00
3	W	9	DG	O4'-C4'-C3'	-8.86	100.69	106.00
3	V	6	DT	O4'-C1'-N1	8.74	114.12	108.00
3	V	17	DG	O4'-C1'-N9	-8.61	101.97	108.00
2	E	8	DG	P-O5'-C5'	-8.43	107.41	120.90
3	W	7	DA	O4'-C1'-N9	8.29	113.80	108.00
2	F	11	DC	O4'-C1'-N1	8.24	113.77	108.00
2	E	9	DG	O4'-C1'-N9	7.96	113.57	108.00
2	E	9	DG	C8-N9-C4	-7.93	103.23	106.40
2	F	19	DC	O4'-C1'-N1	7.55	113.29	108.00
3	V	12	DC	O4'-C1'-N1	7.51	113.26	108.00
2	E	9	DG	O4'-C4'-C3'	-7.23	101.61	104.50
2	F	9	DG	C4'-C3'-C2'	-7.12	96.69	103.10
3	W	13	DC	O4'-C1'-N1	6.88	112.82	108.00
3	V	1	DA	P-O3'-C3'	6.82	127.88	119.70
3	V	9	DG	O4'-C4'-C3'	-6.53	101.89	104.50
2	F	7	DA	O4'-C4'-C3'	-6.50	101.90	104.50
3	V	14	DT	N3-C4-O4	6.38	123.73	119.90
3	W	6	DT	N3-C4-O4	6.37	123.72	119.90
2	E	14	DT	C4'-C3'-C2'	-6.31	97.42	103.10
2	E	8	DG	C4'-C3'-C2'	-6.23	97.50	103.10
2	F	9	DG	O4'-C4'-C3'	-6.16	102.04	104.50
3	W	2	DG	P-O3'-C3'	6.07	126.98	119.70
3	W	5	DG	C3'-C2'-C1'	-5.92	95.40	102.50
3	V	15	DA	O4'-C1'-N9	5.79	112.05	108.00
3	V	11	DC	O4'-C4'-C3'	-5.67	102.23	104.50
3	V	11	DC	O4'-C1'-N1	5.60	111.92	108.00
3	V	16	DC	C1'-O4'-C4'	-5.60	104.50	110.10
1	S	1473	LEU	CA-CB-CG	5.54	128.05	115.30
3	W	17	DG	N1-C6-O6	5.36	123.11	119.90
3	W	14	DT	C6-N1-C2	-5.28	118.66	121.30
3	W	5	DG	O4'-C1'-N9	5.28	111.69	108.00
3	W	6	DT	C5-C4-O4	-5.25	121.22	124.90
2	E	14	DT	N3-C4-O4	5.14	122.98	119.90
3	V	12	DC	O4'-C1'-C2'	5.09	109.98	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	8	DG	P-O3'-C3'	5.07	125.78	119.70
2	F	19	DC	C1'-O4'-C4'	-5.04	105.06	110.10
3	W	5	DG	C1'-O4'-C4'	-5.00	105.10	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	572	THR	Peptide
1	U	572	THR	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	B	5689	0	5712	310	0
1	D	5692	0	5704	271	0
1	S	5694	0	5731	296	0
1	U	5689	0	5721	296	0
2	E	410	0	225	24	0
2	F	410	0	225	19	0
3	V	410	0	224	26	0
3	W	369	0	201	16	0
4	E	66	0	54	9	0
4	W	66	0	54	12	0
All	All	24495	0	23851	1204	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 25.

All (1204) 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:439:ALA:HB1	1:D:583:LEU:HB2	1.27	1.14
1:B:468:ARG:HG3	1:B:468:ARG:HH21	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HG2	1:B:471:ARG:HH11	0.92	1.08
1:S:1005:PRO:HA	1:S:1006:GLN:CB	1.85	1.07
1:S:1003:GLU:HA	1:S:1004:LEU:HB3	1.12	1.05
1:U:1002:ALA:HB3	1:U:1003:GLU:HA	1.38	1.04
1:D:1272:ARG:HH11	1:D:1272:ARG:HG2	1.13	1.04
1:U:1432:ARG:NH1	1:U:1432:ARG:HG3	1.61	1.04
1:B:630:ARG:HG2	1:B:630:ARG:HH11	1.14	1.03
1:U:1432:ARG:CG	1:U:1432:ARG:HH11	1.74	1.01
2:E:2:DG:H2"	2:E:3:DC:O5'	1.59	1.00
1:B:1122:ARG:HB3	1:B:1122:ARG:HH11	1.24	1.00
1:D:1279:GLU:HG2	1:D:1282:ARG:NH1	1.78	0.99
1:S:1003:GLU:HA	1:S:1004:LEU:CB	1.91	0.99
1:U:1432:ARG:HG3	1:U:1432:ARG:HH11	0.82	0.98
1:S:1003:GLU:CA	1:S:1004:LEU:HB3	1.93	0.98
1:B:471:ARG:CG	1:B:471:ARG:HH11	1.76	0.98
4:E:1021[A]:RXV:H141	4:E:1021[A]:RXV:H33	1.45	0.97
1:B:515:HIS:HD2	1:B:1025:TYR:CE2	1.82	0.96
1:B:468:ARG:HH21	1:B:468:ARG:CG	1.76	0.96
1:D:1388:LEU:HD13	1:D:1438:ARG:HG3	1.46	0.96
1:B:1325:THR:HB	1:B:1326:PRO:HD3	1.48	0.95
1:B:439:ALA:HB1	1:B:583:LEU:HB2	1.46	0.95
4:W:1020[B]:RXV:H33	4:W:1020[B]:RXV:H142	1.46	0.95
1:S:1247:ALA:HB2	1:S:1261:VAL:HG13	1.47	0.94
1:B:1243:MET:CE	1:B:1331:PHE:HB2	1.98	0.94
1:D:1139:ILE:HD12	1:D:1161:PRO:HD3	1.50	0.93
1:B:471:ARG:NH1	1:B:471:ARG:HG2	1.72	0.93
1:S:1002:ALA:HA	1:S:1003:GLU:O	1.68	0.93
1:S:1299:ARG:HD2	1:S:1299:ARG:H	1.34	0.93
1:S:1245:SER:HB3	1:S:1264:ILE:HA	1.47	0.93
1:B:580:TYR:HD2	1:B:586:MET:HG2	1.34	0.93
1:S:1273:MET:HG3	1:S:1326:PRO:HG2	1.51	0.91
1:D:1079:HIS:CD2	1:D:1081:HIS:HD2	1.89	0.91
1:S:1325:THR:HB	1:S:1326:PRO:HD2	1.53	0.89
1:U:1200:LYS:HG3	1:U:1470:ARG:HH21	1.34	0.89
1:D:1184:PRO:HG3	1:D:1331:PHE:CE2	2.08	0.88
2:E:12:DC:H2"	2:E:13:DC:H5"	1.55	0.88
1:U:548:THR:HB	1:U:576:SER:HB3	1.54	0.87
1:B:1309:ARG:NH2	1:B:1312:ALA:HB2	1.89	0.87
1:B:1054:ASN:HB2	1:B:1136:LEU:HD13	1.53	0.87
1:D:1080:PRO:HG3	1:D:1150:TYR:CG	2.09	0.86
2:E:12:DC:C2'	2:E:13:DC:H5"	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1230:ILE:HG13	1:U:1241:ILE:HD11	1.57	0.86
1:U:1272:ARG:CG	1:U:1272:ARG:HH11	1.89	0.86
1:B:630:ARG:HG2	1:B:630:ARG:NH1	1.90	0.85
1:D:622:MET:HE2	1:D:622:MET:HA	1.59	0.85
1:D:1272:ARG:HG2	1:D:1272:ARG:NH1	1.92	0.84
1:S:1325:THR:HB	1:S:1326:PRO:CD	2.06	0.84
1:S:1067:SER:HA	1:S:1070:ILE:HD12	1.58	0.84
1:B:1122:ARG:HH11	1:B:1122:ARG:CB	1.91	0.84
1:B:1361:THR:HG23	1:B:1364:ARG:HH12	1.42	0.84
1:B:1040:ASP:O	1:B:1166:ASN:HB3	1.78	0.83
1:U:1394:ILE:O	1:U:1398:ILE:HD12	1.78	0.83
1:D:1279:GLU:HG2	1:D:1282:ARG:HH11	1.40	0.83
1:B:1122:ARG:HB3	1:B:1122:ARG:NH1	1.93	0.83
1:U:1002:ALA:CB	1:U:1003:GLU:HA	2.07	0.83
1:D:1119:ALA:HB1	1:D:1123:PHE:HD1	1.44	0.83
4:W:1020[B]:RXV:C33	4:W:1020[B]:RXV:H142	2.08	0.83
1:U:1003:GLU:O	1:U:1004:LEU:HB2	1.79	0.82
1:B:1218:PHE:HD1	1:B:1266:PHE:HB2	1.44	0.81
1:U:1144:ILE:HD12	1:U:1157:PRO:HB3	1.62	0.81
1:U:515:HIS:CE1	1:U:519:LEU:HD11	2.15	0.81
1:S:1143:THR:HB	1:S:1362:VAL:HG13	1.61	0.81
1:B:1309:ARG:HH22	1:B:1312:ALA:HB2	1.42	0.81
1:U:1175:ILE:HD12	3:W:5:DG:C2	2.16	0.81
1:D:564:LYS:O	1:D:568:GLU:HG3	1.81	0.81
1:D:547:LEU:CD1	1:D:575:TRP:HB3	2.11	0.80
1:S:540:ALA:HA	1:S:603:LEU:CD2	2.10	0.80
1:D:1049:ILE:HA	1:D:1074:VAL:HG21	1.63	0.80
1:B:438:SER:HB2	2:E:10:DG:OP1	1.82	0.80
1:U:1048:ARG:HD3	1:U:1078:TYR:HB3	1.63	0.80
1:B:1243:MET:HE2	1:B:1331:PHE:HB2	1.62	0.80
1:B:1325:THR:HB	1:B:1326:PRO:CD	2.11	0.79
1:S:499:ARG:HH11	1:S:499:ARG:HG3	1.46	0.79
1:B:464:VAL:HG21	1:B:527:PHE:HE1	1.46	0.79
1:B:580:TYR:CD2	1:B:586:MET:HG2	2.18	0.79
1:B:1010:ASN:ND2	1:U:1010:ASN:HD21	1.81	0.79
1:D:1119:ALA:HB1	1:D:1123:PHE:CD1	2.17	0.78
1:B:468:ARG:HG3	1:B:468:ARG:NH2	1.88	0.78
1:U:1144:ILE:CD1	1:U:1157:PRO:HB3	2.14	0.78
1:B:565:LEU:HB2	1:U:1004:LEU:HD12	1.64	0.78
1:B:515:HIS:CD2	1:B:1025:TYR:CE2	2.69	0.78
1:B:1090:MET:HA	1:B:1093:MET:HE3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1047:ARG:HG3	1:B:1160:LEU:HD11	1.66	0.77
1:B:1206:ILE:HD13	1:B:1206:ILE:H	1.49	0.77
1:U:450:ARG:HG3	1:U:450:ARG:HH21	1.48	0.77
1:D:1206:ILE:HG21	1:D:1235:GLU:HG2	1.66	0.77
1:U:509:ALA:O	1:U:544:LEU:HD13	1.85	0.77
1:U:1200:LYS:HG3	1:U:1470:ARG:NH2	2.00	0.77
1:D:1206:ILE:HG21	1:D:1235:GLU:CG	2.15	0.76
1:D:544:LEU:HD23	1:D:545:TYR:CE1	2.21	0.76
1:D:591:LEU:O	1:D:591:LEU:HG	1.86	0.76
1:S:552:GLN:HB3	1:S:554:TYR:HE1	1.50	0.76
1:S:1093:MET:HA	1:S:1099:TYR:CD1	2.20	0.75
1:D:1386:ILE:O	1:D:1390:HIS:HB2	1.87	0.75
1:S:552:GLN:HB3	1:S:554:TYR:CE1	2.20	0.75
1:S:1002:ALA:HA	1:S:1003:GLU:C	2.08	0.75
1:B:525:TYR:HA	1:B:532:ILE:HD11	1.69	0.74
1:U:1446:ASN:HA	1:U:1449:LEU:HD12	1.67	0.74
1:U:1388:LEU:HD13	1:U:1438:ARG:HG2	1.69	0.74
1:U:439:ALA:HB1	1:U:583:LEU:HD12	1.67	0.74
1:D:495:LEU:HG	1:D:495:LEU:O	1.87	0.74
1:S:1035:LEU:CD2	1:S:1036:PRO:HD3	2.17	0.74
1:U:538:TYR:CE2	1:U:605:GLN:HG3	2.23	0.74
2:E:6:DT:H2"	2:E:7:DA:O5'	1.87	0.73
1:U:1005:PRO:HA	1:U:1006:GLN:C	2.09	0.73
1:D:466:LYS:HE2	1:D:623:GLY:O	1.87	0.73
1:S:1402:ASP:O	1:U:1436:LEU:HB2	1.89	0.73
1:D:458:ARG:NH2	2:F:11:DC:H5"	2.04	0.73
1:B:1469:VAL:O	1:B:1473:LEU:HG	1.88	0.72
1:D:1079:HIS:CD2	1:D:1081:HIS:CD2	2.74	0.72
1:S:1363:VAL:HG12	1:S:1465:LEU:HD11	1.70	0.72
1:S:1107:GLN:HG2	1:S:1125:GLU:HG3	1.72	0.72
1:B:556:VAL:HG13	1:B:561:GLU:HB2	1.70	0.72
1:D:549:GLN:HG2	1:D:573:PRO:HB2	1.72	0.72
1:U:1004:LEU:O	1:U:1006:GLN:HB3	1.89	0.72
1:U:447:ARG:HD3	1:U:454:ILE:HD11	1.71	0.72
1:D:1027:MET:O	1:D:1031:VAL:HG22	1.89	0.72
1:B:1448:LEU:O	1:B:1452:ILE:HG13	1.89	0.72
1:D:1296:THR:HG23	1:D:1302:VAL:HA	1.70	0.71
1:D:547:LEU:HD11	1:D:575:TRP:HB3	1.72	0.71
1:D:640:ALA:HB3	1:D:641:ASN:HA	1.70	0.71
1:U:1356:LEU:O	1:U:1356:LEU:HD12	1.90	0.71
1:B:1243:MET:HE3	1:B:1331:PHE:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1195:VAL:CG2	1:D:1352:LEU:HD22	2.20	0.71
1:S:455:LEU:O	1:S:455:LEU:HG	1.90	0.71
1:U:1042:LEU:HB3	1:U:1046:HIS:HB2	1.72	0.71
1:B:1013:ASN:HB3	1:B:1016:SER:HB2	1.73	0.71
3:V:10:DG:H2"	3:V:11:DC:H5"	1.71	0.71
4:E:1021[A]:RXV:H141	4:E:1021[A]:RXV:C33	2.21	0.70
1:S:1135:LEU:HG	1:S:1164:PHE:CE2	2.27	0.70
1:S:1199:SER:HB2	1:S:1466:LEU:HD11	1.73	0.70
1:B:626:VAL:HG21	2:F:17:DG:H3'	1.73	0.70
1:U:1042:LEU:HD12	1:U:1047:ARG:HG3	1.74	0.70
1:B:430:GLU:OE2	1:B:452:GLN:HG2	1.92	0.70
1:B:1469:VAL:HG12	1:B:1473:LEU:HD11	1.73	0.70
1:U:1272:ARG:HH11	1:U:1272:ARG:HG2	1.56	0.70
1:S:522:THR:HA	1:S:618:PHE:HE2	1.56	0.70
1:B:1178:GLY:H	2:F:17:DG:H5"	1.56	0.69
1:U:1048:ARG:HD2	1:U:1079:HIS:HB2	1.72	0.69
1:D:1011:GLU:HG2	1:D:1012:ARG:H	1.56	0.69
1:S:1273:MET:HG3	1:S:1326:PRO:CG	2.19	0.69
1:B:575:TRP:N	1:B:575:TRP:CD1	2.59	0.69
1:U:1090:MET:HA	1:U:1093:MET:CE	2.22	0.69
1:U:450:ARG:CG	1:U:450:ARG:HH21	2.05	0.69
1:U:1310:LYS:O	1:U:1311:ASP:HB2	1.93	0.69
1:B:1004:LEU:CB	1:B:1005:PRO:CD	2.71	0.69
1:B:1218:PHE:CD1	1:B:1266:PHE:HB2	2.28	0.69
1:D:1179:MET:O	2:E:17:DG:H4'	1.91	0.69
1:B:630:ARG:CG	1:B:630:ARG:HH11	2.00	0.69
1:S:1218:PHE:HE2	1:S:1224:ILE:HD11	1.56	0.68
1:S:1326:PRO:O	1:S:1328:GLN:N	2.27	0.68
1:U:565:LEU:O	1:U:569:LEU:HD12	1.93	0.68
1:B:1004:LEU:O	1:B:1006:GLN:HG3	1.94	0.68
1:D:1050:LEU:HD21	1:D:1093:MET:SD	2.34	0.68
1:S:1026:ALA:O	1:S:1030:ILE:HG12	1.94	0.68
1:S:1274:ILE:HG22	1:S:1292:LEU:HD21	1.75	0.68
1:B:1325:THR:CB	1:B:1326:PRO:HD3	2.24	0.68
1:D:1232:ARG:HD2	1:D:1239:GLY:HA2	1.76	0.68
1:S:418:LEU:HD12	1:S:454:ILE:O	1.94	0.68
1:D:524:PHE:O	1:D:528:MET:HB2	1.94	0.67
1:D:622:MET:HA	1:D:622:MET:CE	2.23	0.67
1:D:1363:VAL:HG21	1:D:1469:VAL:HG22	1.76	0.67
1:B:1010:ASN:HD21	1:U:1010:ASN:HD21	1.41	0.67
1:D:565:LEU:O	1:D:565:LEU:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1381:LEU:O	1:U:1385:ARG:HG3	1.94	0.67
1:B:505:ILE:HD11	1:B:524:PHE:HE1	1.60	0.67
2:E:2:DG:C2'	2:E:3:DC:O5'	2.40	0.67
1:U:515:HIS:O	1:U:519:LEU:HD12	1.95	0.67
1:B:1264:ILE:HB	1:B:1265:PRO:CD	2.25	0.67
1:U:1008:ARG:O	1:U:1009:ILE:HG13	1.95	0.66
4:W:1020[A]:RXV:H142	4:W:1020[A]:RXV:H33	1.77	0.66
2:E:8:DG:C2'	2:E:9:DG:O5'	2.44	0.66
1:U:1045:VAL:HG12	1:U:1079:HIS:HE1	1.60	0.66
1:U:1199:SER:HB2	1:U:1466:LEU:HD11	1.74	0.66
1:D:1094:ALA:HB2	1:D:1104:VAL:HB	1.75	0.66
1:D:1274:ILE:CG2	1:D:1292:LEU:HD21	2.25	0.66
1:B:1390:HIS:O	1:B:1394:ILE:HG12	1.96	0.66
1:D:1139:ILE:HD12	1:D:1161:PRO:CD	2.24	0.66
1:B:1426:LEU:HB3	1:D:1431:ARG:HB3	1.76	0.66
1:D:1056:GLN:HB2	1:D:1058:MET:HG3	1.77	0.66
1:S:1252:ARG:NH2	1:S:1256:ARG:HE	1.94	0.66
1:D:1059:THR:HB	1:D:1060:PRO:CD	2.26	0.66
1:S:495:LEU:HG	1:S:495:LEU:O	1.94	0.66
1:S:606:VAL:CG1	1:S:1014:ILE:HG13	2.26	0.66
1:U:1120:ALA:HB3	1:U:1123:PHE:CD1	2.31	0.66
1:B:1053:LEU:HD21	1:B:1070:ILE:HD13	1.77	0.65
1:U:1090:MET:HA	1:U:1093:MET:HE2	1.79	0.65
1:B:1054:ASN:HB2	1:B:1136:LEU:CD1	2.27	0.65
1:B:1094:ALA:HB2	1:B:1104:VAL:CG1	2.27	0.65
1:B:1313:ASN:O	1:B:1316:VAL:HG12	1.97	0.65
1:D:579:ARG:HG2	1:D:580:TYR:H	1.61	0.65
1:S:1120:ALA:HB3	1:S:1123:PHE:HD1	1.60	0.65
1:S:570:ASN:N	1:S:571:PRO:CD	2.60	0.65
1:B:556:VAL:HG22	1:U:1004:LEU:HD13	1.79	0.65
1:B:1402:ASP:O	1:D:1434:THR:HB	1.97	0.65
1:B:556:VAL:HG13	1:B:561:GLU:CB	2.27	0.65
1:S:1218:PHE:CE2	1:S:1224:ILE:HD11	2.32	0.65
1:D:1189:THR:HG23	1:D:1477:ARG:HD2	1.78	0.65
1:U:570:ASN:CB	1:U:571:PRO:HD3	2.27	0.65
1:S:1042:LEU:HD22	1:S:1046:HIS:HB2	1.78	0.64
1:B:1325:THR:CB	1:B:1326:PRO:CD	2.73	0.64
1:S:1238:ARG:HA	1:S:1333:VAL:O	1.97	0.64
3:V:11:DC:H1'	3:V:12:DC:H5'	1.80	0.64
1:U:1048:ARG:HD3	1:U:1078:TYR:CB	2.27	0.64
1:B:489:ILE:HD13	1:B:489:ILE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LYS:N	1:B:1141:LYS:HD2	2.12	0.64
1:B:468:ARG:NH2	1:B:468:ARG:CG	2.46	0.64
1:D:464:VAL:HG21	1:D:523:PHE:HA	1.79	0.64
1:U:443:THR:HG22	1:U:454:ILE:HD13	1.79	0.64
1:D:1270:LYS:O	1:D:1274:ILE:HG13	1.98	0.64
1:S:590:GLN:O	1:S:594:THR:HG23	1.97	0.64
1:B:1391:ILE:HG21	1:D:1399:ARG:CZ	2.27	0.64
1:S:601:ARG:HH12	1:S:603:LEU:HD12	1.63	0.64
1:U:1177:VAL:HG22	3:V:16:DC:H4'	1.80	0.64
1:S:1135:LEU:CD2	1:S:1162:ALA:HA	2.28	0.64
1:S:505:ILE:HG21	1:S:517:ARG:HG2	1.80	0.64
1:U:579:ARG:HG3	1:U:580:TYR:N	2.13	0.64
1:D:1059:THR:HG22	1:D:1133:LEU:HD21	1.80	0.63
1:D:1272:ARG:CG	1:D:1272:ARG:HH11	1.98	0.63
2:E:8:DG:H2'	2:E:9:DG:O5'	1.98	0.63
1:S:1135:LEU:HD23	1:S:1162:ALA:HA	1.79	0.63
1:S:1445:TYR:CD1	1:S:1449:LEU:HD11	2.34	0.63
1:S:461:ILE:HG23	1:S:462:LEU:N	2.13	0.63
1:U:1241:ILE:HG22	1:U:1331:PHE:HB3	1.80	0.63
1:B:1068:ALA:HB1	4:E:1021[A]:RXV:S26	2.38	0.63
1:D:1080:PRO:HG3	1:D:1150:TYR:CD1	2.32	0.63
1:D:1104:VAL:HG12	1:D:1105:ASP:N	2.12	0.63
1:S:1035:LEU:HD23	1:S:1036:PRO:HD3	1.80	0.63
3:V:18:DG:H2"	3:V:19:DC:O5'	1.97	0.63
1:D:572:THR:N	1:D:573:PRO:CD	2.62	0.63
1:U:1054:ASN:HB2	1:U:1128:MET:CE	2.29	0.63
1:B:1191:LEU:O	1:B:1195:VAL:HG23	1.98	0.63
1:S:525:TYR:CE1	1:S:529:ARG:HD2	2.33	0.63
1:S:606:VAL:HG11	1:S:1014:ILE:HG13	1.80	0.63
1:B:1178:GLY:N	2:F:17:DG:H5"	2.13	0.63
1:S:1347:ASN:OD1	1:S:1350:GLU:HG3	1.98	0.63
1:B:1361:THR:HG23	1:B:1364:ARG:NH1	2.13	0.63
1:S:1252:ARG:HH22	1:S:1256:ARG:HE	1.45	0.63
1:U:447:ARG:HD3	1:U:454:ILE:CD1	2.29	0.63
1:B:439:ALA:CB	1:B:583:LEU:HB2	2.25	0.62
1:S:1134:GLU:O	1:S:1163:ARG:HG2	1.99	0.62
1:S:597:ASN:HD22	1:S:598:PRO:N	1.97	0.62
1:U:1143:THR:HB	1:U:1362:VAL:HG13	1.80	0.62
1:B:501:HIS:HA	1:B:536:TYR:CD1	2.34	0.62
1:S:643:ASP:O	1:S:1002:ALA:N	2.32	0.62
1:U:1384:LEU:HD23	1:U:1425:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1130:LYS:O	1:U:1133:LEU:HB2	1.99	0.62
1:D:1225:LEU:HD21	1:D:1244:ARG:HG3	1.81	0.62
1:B:1005:PRO:HG2	1:U:565:LEU:HD13	1.81	0.62
1:S:1005:PRO:CA	1:S:1006:GLN:CB	2.70	0.62
1:S:597:ASN:HD22	1:S:598:PRO:CD	2.13	0.62
1:B:430:GLU:HB3	1:B:502:LYS:HB2	1.82	0.62
1:B:488:GLY:C	1:B:489:ILE:HD13	2.20	0.62
1:D:1014:ILE:HG23	1:D:1015:THR:N	2.15	0.62
1:D:458:ARG:NH2	2:F:11:DC:C5'	2.62	0.62
1:S:604:LEU:N	1:S:604:LEU:HD23	2.14	0.62
1:U:1368:GLN:HG3	1:U:1459:LEU:HD21	1.81	0.62
1:U:1174:GLY:O	1:U:1180:ALA:HB1	2.00	0.62
1:B:515:HIS:CD2	1:B:1025:TYR:CZ	2.88	0.62
1:S:447:ARG:HD3	1:S:454:ILE:HD11	1.80	0.62
1:U:1219:PRO:HD2	1:U:1266:PHE:CE1	2.35	0.62
1:U:1313:ASN:ND2	1:U:1315:SER:HB2	2.15	0.62
1:D:1074:VAL:HG12	1:D:1086:ILE:HD13	1.82	0.62
1:S:1388:LEU:HD23	1:S:1391:ILE:HD13	1.82	0.62
1:B:589:ASP:HB3	1:D:1298:LEU:HD21	1.81	0.61
1:D:547:LEU:HD11	1:D:575:TRP:CG	2.34	0.61
1:D:622:MET:HE1	1:D:1022:PHE:HE1	1.63	0.61
1:S:1468:LEU:HD12	1:S:1468:LEU:O	1.99	0.61
1:U:431:ILE:HG23	1:U:503:ILE:HA	1.81	0.61
2:F:8:DG:H2'	2:F:9:DG:O4'	1.99	0.61
1:U:511:VAL:HG11	1:U:1028:SER:HB2	1.82	0.61
1:B:509:ALA:HB3	1:B:544:LEU:HD13	1.81	0.61
1:D:1272:ARG:CG	1:D:1272:ARG:NH1	2.61	0.61
1:B:1148:ASP:OD1	1:B:1155:ARG:NH1	2.34	0.61
1:S:1080:PRO:HB3	1:S:1150:TYR:CD1	2.35	0.61
1:S:502:LYS:HG2	1:S:538:TYR:HE1	1.64	0.61
1:U:1031:VAL:HG23	1:U:1032:ALA:H	1.66	0.61
1:U:1278:ALA:HB2	1:U:1292:LEU:HD22	1.83	0.61
1:B:1366:ARG:O	1:B:1366:ARG:HG2	2.00	0.61
1:S:499:ARG:CG	1:S:499:ARG:HH11	2.14	0.61
1:S:540:ALA:HA	1:S:603:LEU:HD23	1.82	0.61
1:U:1388:LEU:CD1	1:U:1438:ARG:HG2	2.30	0.60
1:B:464:VAL:HG21	1:B:527:PHE:CE1	2.32	0.60
1:D:1092:ARG:HA	1:D:1095:GLN:HE21	1.66	0.60
1:U:1055:GLU:HG3	1:U:1078:TYR:OH	2.01	0.60
1:U:1058:MET:CE	1:U:1065:LYS:HG3	2.31	0.60
1:U:1054:ASN:HB2	1:U:1128:MET:HE1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:ALA:CB	1:D:583:LEU:HB2	2.18	0.60
1:S:1175:ILE:HD12	3:V:5:DG:C2	2.36	0.60
1:S:1448:LEU:O	1:S:1452:ILE:HG13	2.01	0.60
1:B:1430:LEU:HA	1:B:1433:LEU:HD12	1.83	0.60
1:S:1035:LEU:HD22	1:S:1036:PRO:HD3	1.83	0.60
1:S:1438:ARG:HD2	1:S:1438:ARG:O	2.02	0.60
1:S:522:THR:HA	1:S:618:PHE:CE2	2.37	0.60
1:U:457:LEU:N	1:U:457:LEU:HD23	2.15	0.60
1:S:592:TRP:HA	1:S:596:MET:HB2	1.84	0.59
1:B:1346:ILE:HB	1:B:1350:GLU:HG3	1.84	0.59
1:S:1385:ARG:NH2	1:S:1442:GLU:OE1	2.34	0.59
1:U:1176:ALA:HB3	1:U:1179:MET:O	2.01	0.59
1:B:555:TYR:HE1	1:B:594:THR:HG21	1.66	0.59
2:E:11:DC:C2	4:E:1021[A]:RXV:N7	2.71	0.59
1:D:1177:VAL:HG22	2:E:16:DC:H4'	1.84	0.59
1:B:556:VAL:CG1	1:B:561:GLU:HB2	2.33	0.59
1:D:572:THR:H	1:D:573:PRO:HD3	1.66	0.59
1:D:1175:ILE:HD12	2:E:17:DG:N3	2.17	0.59
1:B:1054:ASN:CB	1:B:1136:LEU:HD13	2.29	0.59
1:B:1138:ASP:HA	1:B:1141:LYS:HD3	1.84	0.59
1:B:1230:ILE:HG12	1:B:1241:ILE:HD12	1.84	0.59
1:D:431:ILE:HA	1:D:453:ALA:O	2.02	0.59
1:D:562:LEU:HD23	1:D:566:LYS:HG3	1.85	0.59
1:S:1227:LYS:HA	1:S:1230:ILE:HD13	1.85	0.59
1:S:502:LYS:HG2	1:S:538:TYR:CE1	2.37	0.59
1:B:1027:MET:O	1:B:1031:VAL:HG22	2.02	0.59
1:D:1101:TYR:HB3	1:D:1131:ILE:HD13	1.84	0.59
1:S:1075:MET:HE1	4:W:1020[A]:RXV:H30	1.84	0.59
1:B:547:LEU:HD21	1:B:575:TRP:CE3	2.38	0.59
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.38	0.59
1:D:544:LEU:HD23	1:D:545:TYR:HE1	1.66	0.59
3:V:10:DG:H2"	3:V:11:DC:C5'	2.33	0.59
1:B:1053:LEU:HD21	1:B:1070:ILE:HG21	1.85	0.59
1:B:1245:SER:OG	1:B:1327:LEU:HD12	2.02	0.59
1:U:1272:ARG:HG3	1:U:1272:ARG:HH11	1.65	0.59
1:B:1353:VAL:O	1:B:1357:GLU:HG2	2.03	0.58
1:D:557:TYR:CD1	1:D:557:TYR:N	2.70	0.58
1:D:1256:ARG:HB3	1:D:1310:LYS:HB3	1.85	0.58
1:S:1262:THR:O	1:S:1302:VAL:HB	2.03	0.58
1:B:529:ARG:N	1:B:530:PRO:HD2	2.17	0.58
1:U:601:ARG:HD2	1:U:603:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1045:VAL:HG23	1:D:1079:HIS:CE1	2.39	0.58
1:D:621:LEU:HD21	1:D:632:PHE:CE1	2.38	0.58
1:D:427:GLU:HG3	1:D:501:HIS:CD2	2.39	0.58
1:U:1407:ALA:O	1:U:1411:LEU:HD12	2.02	0.58
1:D:1167:LEU:HD11	1:D:1183:ILE:HD12	1.84	0.58
1:S:1187:ASN:HD22	1:S:1484:ARG:HA	1.69	0.58
1:B:1079:HIS:NE2	1:B:1081:HIS:HD2	2.02	0.58
1:D:1195:VAL:HG23	1:D:1352:LEU:HD22	1.84	0.57
1:U:1003:GLU:O	1:U:1004:LEU:CB	2.50	0.57
1:U:1131:ILE:HB	1:U:1480:PHE:CE1	2.39	0.57
1:U:457:LEU:O	1:U:458:ARG:HG2	2.04	0.57
1:B:1160:LEU:HD12	1:B:1160:LEU:N	2.19	0.57
1:S:416:GLY:O	1:S:417:LYS:HB3	2.03	0.57
1:B:1329:THR:HG22	1:B:1330:SER:H	1.70	0.57
3:V:11:DC:C2	4:W:1020[A]:RXV:N7	2.72	0.57
1:U:1448:LEU:O	1:U:1452:ILE:HG12	2.04	0.57
1:B:1161:PRO:O	1:B:1163:ARG:HD2	2.05	0.57
1:B:1347:ASN:OD1	1:B:1350:GLU:HG2	2.05	0.57
1:U:435:GLU:OE2	1:U:508:ASP:HB2	2.04	0.57
1:U:528:MET:HB3	1:U:531:LEU:HB2	1.86	0.57
3:W:10:DG:H2"	3:W:11:DC:H5"	1.85	0.57
4:W:1020[B]:RXV:H33	4:W:1020[B]:RXV:C14	2.21	0.57
1:S:1279:GLU:HG3	1:S:1282:ARG:HH22	1.70	0.57
1:U:1049:ILE:HG12	1:U:1074:VAL:HG11	1.87	0.57
1:S:1080:PRO:HB3	1:S:1150:TYR:CE1	2.40	0.57
1:S:439:ALA:HB1	1:S:583:LEU:HD12	1.86	0.57
1:U:1025:TYR:HE2	1:U:1177:VAL:HG21	1.68	0.57
1:U:522:THR:OG1	1:U:622:MET:HG3	2.04	0.57
1:D:1265:PRO:O	1:D:1268:VAL:HG22	2.05	0.57
1:S:1251:GLU:H	1:S:1251:GLU:CD	2.05	0.57
1:S:544:LEU:HD23	1:S:558:ASN:HA	1.86	0.57
1:D:1232:ARG:HG2	1:D:1238:ARG:O	2.05	0.56
1:S:1107:GLN:O	1:S:1107:GLN:HG3	2.05	0.56
1:U:1277:ILE:O	1:U:1281:VAL:HG23	2.05	0.56
1:U:556:VAL:HG12	1:U:557:TYR:N	2.20	0.56
1:B:1090:MET:HA	1:B:1093:MET:CE	2.36	0.56
1:D:1186:HIS:HB2	1:D:1191:LEU:HD11	1.85	0.56
1:D:509:ALA:HB1	1:D:544:LEU:HB2	1.86	0.56
1:S:1143:THR:HB	1:S:1362:VAL:CG1	2.35	0.56
1:B:462:LEU:HD21	1:B:472:ILE:HG12	1.86	0.56
1:U:1114:ASP:OD2	1:U:1271:ALA:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1131:ILE:HD13	1:U:1132:THR:N	2.20	0.56
1:S:1402:ASP:HB2	1:U:1436:LEU:HD13	1.87	0.56
3:W:14:DT:H2"	3:W:15:DA:H5'	1.86	0.56
1:B:1083:ASP:C	1:B:1085:SER:H	2.08	0.56
1:U:1295:GLU:HB2	1:U:1303:ARG:HG2	1.88	0.56
1:U:431:ILE:CG2	1:U:503:ILE:HG13	2.35	0.56
3:V:18:DG:H1	3:W:3:DC:H42	1.54	0.56
1:B:1035:LEU:HB2	1:B:1338:LEU:CD1	2.35	0.56
1:B:580:TYR:HD2	1:B:586:MET:CG	2.10	0.56
1:B:638:VAL:O	1:B:638:VAL:HG12	2.03	0.56
1:S:1074:VAL:O	1:S:1074:VAL:CG1	2.54	0.56
1:B:465:GLU:HG3	1:B:622:MET:HB2	1.87	0.56
1:B:585:GLU:HG2	1:B:585:GLU:O	2.05	0.56
1:D:547:LEU:HD11	1:D:575:TRP:CB	2.35	0.56
1:S:1073:ASP:OD2	1:S:1077:LYS:HD2	2.05	0.56
1:U:463:ASN:ND2	1:U:466:LYS:HE3	2.21	0.56
1:B:630:ARG:NH1	1:B:630:ARG:CG	2.64	0.56
1:S:1007:SER:O	1:S:1009:ILE:N	2.39	0.56
1:S:1107:GLN:HG2	1:S:1125:GLU:CG	2.35	0.56
1:U:642:LEU:O	1:U:643:ASP:HB2	2.05	0.56
1:B:1064:TYR:CE2	1:B:1107:GLN:HB2	2.41	0.56
1:U:1109:ASN:O	1:U:1118:ALA:HB1	2.06	0.56
1:B:1230:ILE:HG12	1:B:1241:ILE:CD1	2.35	0.56
1:S:1042:LEU:HD22	1:S:1046:HIS:CB	2.36	0.56
1:S:450:ARG:HG3	1:S:451:THR:HG22	1.88	0.56
1:S:541:GLN:CD	1:S:604:LEU:HD21	2.26	0.56
1:D:1438:ARG:HA	1:D:1441:ILE:HD11	1.88	0.56
1:S:1110:PHE:HE1	1:S:1124:THR:HB	1.70	0.56
1:S:637:ALA:HB1	1:S:1027:MET:SD	2.46	0.56
1:U:1029:VAL:HG22	1:U:1033:ARG:HD2	1.88	0.56
1:U:1087:TYR:CG	1:U:1121:MET:HE2	2.41	0.56
1:B:1216:PRO:HB2	1:B:1218:PHE:HE2	1.71	0.55
1:B:505:ILE:HD11	1:B:524:PHE:CE1	2.41	0.55
1:D:1249:ILE:HG23	1:D:1259:ILE:HG12	1.88	0.55
1:S:1252:ARG:HB2	1:S:1258:ARG:HH11	1.71	0.55
1:U:1313:ASN:HD21	1:U:1315:SER:HB2	1.70	0.55
1:U:1183:ILE:N	1:U:1183:ILE:HD12	2.21	0.55
1:B:578:ALA:O	1:B:579:ARG:HB3	2.06	0.55
1:D:1007:SER:O	1:D:1009:ILE:N	2.38	0.55
1:D:1274:ILE:HG22	1:D:1292:LEU:HD21	1.87	0.55
1:S:1188:LEU:O	1:S:1192:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1292:LEU:CD1	1:S:1306:ILE:HG23	2.36	0.55
1:U:1025:TYR:CE2	1:U:1177:VAL:HG21	2.41	0.55
1:U:1339:VAL:O	1:U:1340:ASN:HB3	2.06	0.55
3:V:1:DA:H2"	3:V:2:DG:O5'	2.05	0.55
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	1.87	0.55
1:B:461:ILE:HD11	1:B:477:GLU:OE1	2.06	0.55
1:D:640:ALA:HB3	1:D:641:ASN:CA	2.34	0.55
1:U:1135:LEU:CD2	1:U:1162:ALA:HA	2.36	0.55
1:B:1309:ARG:HG2	1:B:1310:LYS:H	1.70	0.55
1:D:1388:LEU:HD12	1:D:1441:ILE:HD11	1.86	0.55
1:D:511:VAL:O	1:D:514:ALA:HB3	2.06	0.55
1:U:511:VAL:HG11	1:U:1028:SER:CB	2.36	0.55
1:B:1238:ARG:HH22	2:F:19:DC:P	2.29	0.55
1:B:1472:GLU:O	1:B:1476:ILE:HG12	2.06	0.55
1:U:1401:SER:HB3	1:U:1406:VAL:HG13	1.88	0.55
1:D:1054:ASN:HA	1:D:1128:MET:CE	2.37	0.55
1:D:1422:ALA:O	1:D:1426:LEU:HG	2.07	0.55
1:S:1210:MET:HA	1:S:1213:ILE:O	2.07	0.55
1:S:517:ARG:O	1:S:521:LEU:HG	2.07	0.55
1:S:617:THR:HG21	1:S:1015:THR:HG23	1.89	0.55
1:U:1120:ALA:HB3	1:U:1123:PHE:HD1	1.67	0.55
1:S:1277:ILE:CD1	1:S:1321:LEU:HD22	2.37	0.54
1:U:1183:ILE:HG13	1:U:1335:MET:HG2	1.89	0.54
1:B:1049:ILE:HD13	1:B:1090:MET:HB2	1.88	0.54
1:B:1234:TYR:CD1	1:B:1348:LEU:HD22	2.42	0.54
1:B:464:VAL:CG2	1:B:527:PHE:HE1	2.16	0.54
2:E:11:DC:H2"	2:E:12:DC:H5"	1.88	0.54
1:S:1316:VAL:O	1:S:1320:ASN:HB2	2.06	0.54
1:S:570:ASN:N	1:S:571:PRO:HD3	2.21	0.54
1:U:1049:ILE:HD13	1:U:1090:MET:HB3	1.89	0.54
1:U:1218:PHE:HB3	1:U:1266:PHE:HD1	1.73	0.54
3:V:14:DT:H2'	3:V:15:DA:H8	1.72	0.54
1:B:1264:ILE:HB	1:B:1265:PRO:HD2	1.89	0.54
1:S:1031:VAL:HA	1:S:1338:LEU:HD11	1.89	0.54
1:S:501:HIS:HA	1:S:536:TYR:CD1	2.42	0.54
1:S:554:TYR:N	1:S:554:TYR:CD1	2.72	0.54
1:B:447:ARG:NH2	1:B:452:GLN:O	2.40	0.54
1:D:549:GLN:OE1	1:D:569:LEU:HD22	2.08	0.54
1:S:1281:VAL:HG21	1:S:1289:ILE:HG21	1.89	0.54
1:S:467:ALA:HB3	1:S:472:ILE:HD11	1.89	0.54
1:S:529:ARG:N	1:S:530:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:544:LEU:O	1:S:544:LEU:HD12	2.07	0.54
1:U:1446:ASN:HA	1:U:1449:LEU:CD1	2.37	0.54
1:S:525:TYR:CD1	1:S:529:ARG:HD2	2.42	0.54
1:U:1045:VAL:HG12	1:U:1079:HIS:CE1	2.42	0.54
1:U:1110:PHE:CE1	1:U:1124:THR:HB	2.43	0.54
1:D:1011:GLU:HG2	1:D:1012:ARG:N	2.22	0.54
2:E:13:DC:H6	2:E:13:DC:C5'	2.21	0.54
1:D:458:ARG:HH22	2:F:11:DC:C5'	2.20	0.54
1:U:1391:ILE:HG23	1:U:1392:ASP:H	1.72	0.54
1:U:1414:ARG:HB3	1:U:1415:PHE:CD1	2.42	0.54
1:B:1230:ILE:HA	1:B:1241:ILE:HD11	1.90	0.54
1:B:547:LEU:CD2	1:B:577:ILE:HB	2.38	0.54
1:B:644:PHE:CG	1:B:1002:ALA:N	2.76	0.54
1:S:1144:ILE:HD12	1:S:1144:ILE:O	2.07	0.54
1:U:1425:ILE:HG22	1:U:1426:LEU:HD23	1.90	0.54
1:D:1373:LYS:HD3	1:D:1373:LYS:N	2.22	0.54
1:S:1292:LEU:HD12	1:S:1306:ILE:HG23	1.90	0.54
1:B:564:LYS:O	1:B:568:GLU:HG2	2.08	0.53
1:S:1168:LEU:O	1:S:1185:PRO:HA	2.09	0.53
1:U:1080:PRO:HG3	1:U:1150:TYR:CD1	2.43	0.53
1:U:529:ARG:N	1:U:530:PRO:CD	2.71	0.53
1:B:1260:VAL:O	1:B:1260:VAL:HG12	2.07	0.53
1:D:619:GLU:HG2	1:D:619:GLU:O	2.07	0.53
1:S:1169:ALA:O	1:S:1185:PRO:HB3	2.09	0.53
1:U:1175:ILE:HD12	3:W:5:DG:N1	2.24	0.53
1:S:1042:LEU:HD13	1:S:1047:ARG:HB2	1.90	0.53
1:S:1430:LEU:HD23	1:S:1433:LEU:HD12	1.91	0.53
1:U:1090:MET:HA	1:U:1093:MET:HE3	1.89	0.53
1:D:470:ASP:HA	1:D:473:LEU:HD12	1.91	0.53
1:U:1002:ALA:CB	1:U:1003:GLU:CA	2.84	0.53
1:U:432:PHE:CE2	1:U:504:VAL:HG11	2.44	0.53
1:B:465:GLU:HG3	1:B:622:MET:CB	2.39	0.53
1:S:581:LYS:HB3	1:S:585:GLU:OE2	2.08	0.53
1:U:457:LEU:C	1:U:458:ARG:HG2	2.29	0.53
3:W:8:DG:H2'	3:W:9:DG:O4'	2.08	0.53
1:B:1040:ASP:OD2	1:B:1159:VAL:HG23	2.09	0.53
1:D:1259:ILE:HB	1:D:1306:ILE:HD12	1.91	0.53
1:U:1224:ILE:HG13	1:U:1488:ILE:HG22	1.91	0.53
1:U:1113:MET:SD	1:U:1264:ILE:HD11	2.49	0.53
3:W:14:DT:C2'	3:W:15:DA:H5'	2.39	0.53
1:D:1431:ARG:HH12	1:D:1432:ARG:HD3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:MET:HE1	1:D:1022:PHE:CE1	2.42	0.53
1:S:417:LYS:HG2	1:S:480:GLN:OE1	2.09	0.53
1:U:418:LEU:C	1:U:418:LEU:HD23	2.29	0.53
1:B:547:LEU:HD22	1:B:577:ILE:HB	1.91	0.53
1:D:1376:ASP:O	1:D:1380:ILE:HG12	2.08	0.53
1:D:625:VAL:HB	1:D:628:ASN:HB2	1.90	0.53
1:U:431:ILE:HG21	1:U:503:ILE:HG13	1.91	0.53
1:U:430:GLU:HB3	1:U:502:LYS:HB2	1.91	0.53
1:B:1204:ILE:HG13	1:B:1205:SER:N	2.25	0.52
1:B:1363:VAL:HG21	1:B:1469:VAL:HG22	1.91	0.52
1:U:1042:LEU:CD1	1:U:1160:LEU:HD12	2.39	0.52
1:S:1299:ARG:NH1	1:U:592:TRP:CD2	2.77	0.52
1:U:493:PHE:HE1	1:U:528:MET:HG2	1.74	0.52
1:D:1451:TYR:CE1	1:D:1455:LEU:HD21	2.45	0.52
1:D:465:GLU:HB3	1:D:622:MET:O	2.10	0.52
1:D:503:ILE:HD13	1:D:531:LEU:HD11	1.90	0.52
2:E:11:DC:N4	4:E:1021[B]:RXV:H13C	2.25	0.52
1:S:464:VAL:HG21	1:S:523:PHE:HA	1.90	0.52
1:S:505:ILE:CG2	1:S:517:ARG:HG2	2.39	0.52
1:D:1167:LEU:O	1:D:1171:GLY:HA2	2.10	0.52
1:S:1006:GLN:O	1:S:1007:SER:C	2.48	0.52
1:S:443:THR:HG22	1:S:454:ILE:CD1	2.40	0.52
1:U:1043:LYS:HG3	1:U:1046:HIS:CE1	2.45	0.52
1:S:1299:ARG:NH1	1:U:592:TRP:CD1	2.78	0.52
1:B:464:VAL:HG11	1:B:523:PHE:HB2	1.92	0.52
1:D:434:VAL:HG21	1:D:440:GLY:CA	2.39	0.52
1:S:1249:ILE:HD12	1:S:1249:ILE:N	2.25	0.52
1:U:1027:MET:O	1:U:1031:VAL:HG22	2.10	0.52
1:D:1281:VAL:HG13	1:D:1289:ILE:HG13	1.91	0.52
1:D:549:GLN:HG2	1:D:573:PRO:CB	2.40	0.52
1:S:1015:THR:O	1:S:1019:ARG:HG3	2.09	0.52
1:B:501:HIS:CD2	1:B:536:TYR:HE1	2.28	0.52
1:U:537:VAL:HG12	1:U:606:VAL:CG2	2.40	0.52
1:U:1043:LYS:HE2	3:W:6:DT:O5'	2.09	0.52
1:B:565:LEU:HD12	1:B:565:LEU:O	2.09	0.52
1:D:1234:TYR:CD1	1:D:1348:LEU:HB2	2.45	0.52
1:D:1419:GLU:O	1:D:1423:GLN:HB2	2.09	0.52
1:S:1137:ARG:O	1:S:1138:ASP:HB2	2.10	0.52
1:U:493:PHE:CE2	1:U:530:PRO:HB2	2.45	0.52
1:B:516:ILE:O	1:B:517:ARG:C	2.47	0.52
1:D:1264:ILE:HB	1:D:1265:PRO:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1233:ALA:HB2	1:S:1239:GLY:HA3	1.92	0.52
1:S:1256:ARG:HG2	1:S:1310:LYS:HG2	1.92	0.52
1:S:644:PHE:CD1	1:S:644:PHE:N	2.77	0.52
1:U:1100:ARG:HG3	1:U:1101:TYR:CE2	2.45	0.52
1:U:1378:ALA:O	1:U:1382:GLU:HG3	2.10	0.52
1:B:1269:ASN:HB3	1:B:1272:ARG:HB3	1.91	0.51
1:B:461:ILE:O	1:B:519:LEU:HD13	2.10	0.51
1:S:1057:GLY:O	1:S:1059:THR:HG23	2.10	0.51
1:S:579:ARG:HG3	1:S:580:TYR:N	2.25	0.51
1:U:1452:ILE:O	1:U:1456:GLU:HB2	2.11	0.51
1:U:1367:THR:HB	1:U:1459:LEU:HD23	1.91	0.51
1:D:1079:HIS:CE1	2:F:7:DA:OP1	2.63	0.51
1:S:1030:ILE:HG22	1:S:1343:PRO:HG3	1.92	0.51
1:U:1414:ARG:HB3	1:U:1415:PHE:HD1	1.75	0.51
1:B:1079:HIS:CD2	1:B:1081:HIS:HD2	2.28	0.51
1:S:644:PHE:HD1	1:S:644:PHE:N	2.08	0.51
1:U:1336:ILE:HG13	1:U:1345:LEU:HD13	1.93	0.51
1:B:1059:THR:HB	1:B:1060:PRO:CD	2.41	0.51
1:B:462:LEU:HB3	1:B:475:ASN:HD22	1.75	0.51
1:D:622:MET:CA	1:D:622:MET:CE	2.89	0.51
1:S:1120:ALA:HB3	1:S:1123:PHE:CD1	2.44	0.51
1:B:607:LYS:HE3	1:U:600:HIS:CE1	2.46	0.51
1:B:1110:PHE:HA	1:B:1118:ALA:CB	2.41	0.51
1:S:1252:ARG:HB2	1:S:1258:ARG:NH1	2.25	0.51
1:B:1276:LYS:O	1:B:1280:LEU:HG	2.10	0.51
3:V:13:DC:H42	3:W:8:DG:H1	1.57	0.51
1:B:1094:ALA:HB2	1:B:1104:VAL:HG12	1.92	0.51
1:S:432:PHE:CE2	1:S:504:VAL:HG11	2.46	0.51
3:W:10:DG:H2'	4:W:1020[B]:RXV:N11	2.26	0.51
1:B:569:LEU:HD23	1:B:569:LEU:N	2.24	0.51
1:S:1385:ARG:HB3	1:S:1438:ARG:HH12	1.76	0.51
1:U:1055:GLU:C	1:U:1057:GLY:H	2.14	0.51
1:U:1219:PRO:HD2	1:U:1266:PHE:HE1	1.76	0.51
1:B:1004:LEU:O	1:B:1006:GLN:N	2.44	0.50
1:B:1059:THR:HG22	1:B:1133:LEU:HD21	1.93	0.50
1:U:1013:ASN:HD22	1:U:1014:ILE:N	2.10	0.50
1:U:1238:ARG:HA	1:U:1333:VAL:O	2.11	0.50
1:B:569:LEU:C	1:B:571:PRO:HD2	2.31	0.50
1:D:1081:HIS:HB3	2:F:8:DG:P	2.51	0.50
1:D:434:VAL:HG21	1:D:440:GLY:HA2	1.92	0.50
1:B:1068:ALA:HB1	4:E:1021[B]:RXV:O28	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1034:ALA:C	1:U:1035:LEU:HD23	2.31	0.50
1:U:1384:LEU:HD23	1:U:1425:ILE:CD1	2.41	0.50
1:S:554:TYR:HD2	1:S:565:LEU:HD21	1.77	0.50
1:U:1014:ILE:O	1:U:1014:ILE:HG13	2.10	0.50
1:B:592:TRP:HA	1:B:596:MET:HB2	1.93	0.50
1:D:430:GLU:HB3	1:D:502:LYS:HB2	1.92	0.50
1:U:1100:ARG:NH1	1:U:1101:TYR:CZ	2.80	0.50
1:U:626:VAL:HG11	3:V:18:DG:OP2	2.12	0.50
1:B:581:LYS:O	1:B:581:LYS:HG3	2.11	0.50
1:D:1161:PRO:O	1:D:1163:ARG:HD2	2.11	0.50
1:S:1220:THR:O	1:S:1221:ALA:HB3	2.11	0.50
1:S:1349:LYS:O	1:S:1353:VAL:HG23	2.11	0.50
1:B:1246:ARG:HH11	1:B:1246:ARG:HG3	1.76	0.50
1:B:1376:ASP:O	1:B:1380:ILE:HG12	2.11	0.50
1:S:1430:LEU:HD23	1:S:1433:LEU:CD1	2.42	0.50
1:U:1093:MET:HA	1:U:1099:TYR:CD1	2.46	0.50
1:B:570:ASN:N	1:B:571:PRO:HD2	2.27	0.50
1:D:544:LEU:O	1:D:545:TYR:CG	2.65	0.50
1:S:1449:LEU:H	1:S:1449:LEU:HD12	1.76	0.50
1:U:1135:LEU:HD22	1:U:1162:ALA:HA	1.94	0.50
1:D:1184:PRO:HG3	1:D:1331:PHE:HE2	1.74	0.50
1:D:418:LEU:HD13	1:D:418:LEU:O	2.12	0.50
1:D:629:ARG:O	1:D:633:ILE:HD12	2.12	0.50
1:S:525:TYR:O	1:S:525:TYR:CG	2.65	0.50
1:U:1472:GLU:O	1:U:1476:ILE:HG13	2.11	0.50
1:B:443:THR:HB	1:B:454:ILE:HD13	1.93	0.50
1:D:1180:ALA:O	1:D:1336:ILE:HD12	2.12	0.50
1:D:1278:ALA:O	1:D:1282:ARG:HG3	2.11	0.50
1:S:1245:SER:CB	1:S:1264:ILE:HA	2.31	0.50
1:U:1143:THR:CB	1:U:1362:VAL:HG13	2.42	0.50
1:U:638:VAL:HG12	1:U:638:VAL:O	2.12	0.50
1:D:1380:ILE:O	1:D:1384:LEU:HG	2.12	0.49
1:U:1017:GLU:O	1:U:1021:SER:HB2	2.12	0.49
1:U:464:VAL:HG21	1:U:523:PHE:HA	1.94	0.49
1:B:1110:PHE:HA	1:B:1118:ALA:HB2	1.94	0.49
1:D:1274:ILE:HG23	1:D:1292:LEU:HD21	1.93	0.49
1:S:1112:SER:OG	1:S:1116:ASP:HB2	2.11	0.49
1:S:515:HIS:HB2	1:S:1025:TYR:CD1	2.47	0.49
1:B:1384:LEU:O	1:B:1388:LEU:HD23	2.12	0.49
2:F:1:5UA:C6'	2:F:1:5UA:H3'	2.42	0.49
1:U:1469:VAL:O	1:U:1473:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LYS:O	1:B:546:LYS:HG2	2.12	0.49
1:B:609:GLU:OE1	1:B:609:GLU:HA	2.11	0.49
1:D:1006:GLN:O	1:D:1007:SER:C	2.50	0.49
1:D:1045:VAL:CG1	1:D:1046:HIS:N	2.75	0.49
1:D:1195:VAL:HG22	1:D:1352:LEU:HD22	1.93	0.49
1:B:578:ALA:O	1:B:579:ARG:CB	2.61	0.49
1:U:1279:GLU:O	1:U:1283:ASP:HB2	2.13	0.49
1:B:1101:TYR:HB3	1:B:1131:ILE:CD1	2.42	0.49
1:S:426:PRO:O	1:S:501:HIS:CD2	2.66	0.49
1:B:440:GLY:HA2	1:B:443:THR:OG1	2.12	0.49
1:B:471:ARG:CG	1:B:471:ARG:NH1	2.46	0.49
1:B:572:THR:N	1:B:573:PRO:HD3	2.28	0.49
1:D:1388:LEU:HD12	1:D:1441:ILE:CD1	2.43	0.49
1:U:579:ARG:HG3	1:U:580:TYR:H	1.77	0.49
1:S:554:TYR:N	1:S:554:TYR:HD1	2.11	0.49
1:U:1005:PRO:HA	1:U:1007:SER:N	2.27	0.49
1:S:499:ARG:NH1	1:S:499:ARG:CG	2.76	0.49
1:U:1058:MET:HE1	1:U:1065:LYS:HG3	1.95	0.49
1:S:1299:ARG:NH1	1:U:592:TRP:CG	2.81	0.48
1:U:1387:ALA:HB3	1:U:1425:ILE:HD11	1.94	0.48
1:B:1246:ARG:HB3	1:B:1263:GLU:HB2	1.95	0.48
1:D:556:VAL:C	1:D:557:TYR:CD1	2.87	0.48
1:S:1442:GLU:HA	1:S:1445:TYR:CB	2.43	0.48
1:U:621:LEU:O	1:U:629:ARG:HD3	2.12	0.48
1:B:1296:THR:HG23	1:B:1301:GLY:O	2.13	0.48
1:D:1104:VAL:CG1	1:D:1105:ASP:N	2.76	0.48
1:D:1144:ILE:HD13	1:D:1159:VAL:O	2.12	0.48
1:D:1388:LEU:CD1	1:D:1438:ARG:HG3	2.32	0.48
1:U:1047:ARG:HD3	1:U:1159:VAL:HA	1.95	0.48
1:D:531:LEU:O	1:D:536:TYR:HB2	2.14	0.48
2:E:13:DC:C2	2:F:9:DG:N2	2.81	0.48
1:S:1131:ILE:O	1:S:1131:ILE:HG13	2.12	0.48
1:U:463:ASN:HD21	1:U:466:LYS:HE3	1.78	0.48
3:W:11:DC:C2	4:W:1020[B]:RXV:C8	2.97	0.48
1:S:1035:LEU:HD22	1:S:1036:PRO:CD	2.43	0.48
1:U:1092:ARG:NH1	3:W:5:DG:OP1	2.46	0.48
3:W:11:DC:C2	4:W:1020[A]:RXV:C4	2.97	0.48
1:B:605:GLN:HE22	1:U:599:GLU:HB3	1.78	0.48
1:D:1055:GLU:HA	1:D:1055:GLU:OE2	2.13	0.48
1:D:1159:VAL:HG22	1:D:1160:LEU:N	2.29	0.48
1:D:1277:ILE:O	1:D:1281:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1361:THR:O	1:D:1365:ARG:HG2	2.14	0.48
1:S:1123:PHE:HE2	1:U:582:GLY:HA3	1.77	0.48
1:B:1391:ILE:O	1:B:1395:ILE:HD13	2.13	0.48
1:B:493:PHE:HE2	1:B:495:LEU:HB2	1.78	0.48
1:D:468:ARG:HH21	1:D:471:ARG:HD3	1.79	0.48
1:D:503:ILE:HD12	1:D:503:ILE:N	2.28	0.48
1:S:1176:ALA:HB3	1:S:1179:MET:O	2.13	0.48
1:S:1280:LEU:HD11	1:S:1324:GLN:HB3	1.96	0.48
1:S:1382:GLU:HA	1:S:1385:ARG:HD2	1.95	0.48
1:U:519:LEU:HD21	3:V:15:DA:H4'	1.96	0.48
1:B:1059:THR:HB	1:B:1060:PRO:HD2	1.95	0.48
1:B:555:TYR:CE1	1:B:594:THR:HG21	2.47	0.48
1:D:1023:LEU:O	1:D:1027:MET:HG2	2.14	0.48
1:D:1091:VAL:HG12	1:D:1095:GLN:NE2	2.29	0.48
1:D:525:TYR:HA	1:D:532:ILE:HD11	1.95	0.48
1:D:549:GLN:HE22	1:D:569:LEU:HB3	1.79	0.48
1:S:1226:GLY:O	1:S:1230:ILE:HD13	2.14	0.48
1:D:639:TYR:CD1	1:D:1342:ARG:HG2	2.49	0.47
4:E:1021[B]:RXV:H202	4:E:1021[B]:RXV:H131	1.28	0.47
1:S:1239:GLY:O	1:S:1333:VAL:HB	2.14	0.47
1:S:1445:TYR:CE1	1:S:1449:LEU:HD11	2.49	0.47
1:S:466:LYS:HG3	1:S:622:MET:O	2.14	0.47
1:S:626:VAL:O	1:S:629:ARG:N	2.44	0.47
1:U:431:ILE:CG2	1:U:503:ILE:HA	2.44	0.47
1:U:1123:PHE:HZ	3:V:9:DG:OP1	1.96	0.47
1:D:1160:LEU:C	1:D:1162:ALA:H	2.17	0.47
1:D:565:LEU:HD11	1:D:569:LEU:CD1	2.44	0.47
1:S:501:HIS:HA	1:S:536:TYR:CE1	2.50	0.47
1:S:575:TRP:CD1	1:S:575:TRP:N	2.80	0.47
1:U:1113:MET:O	1:U:1115:GLY:N	2.47	0.47
1:U:424:LYS:O	1:U:426:PRO:HD3	2.15	0.47
1:D:507:THR:HG21	1:D:516:ILE:CG2	2.44	0.47
1:S:1426:LEU:HB3	1:U:1431:ARG:HB3	1.96	0.47
1:U:1009:ILE:O	1:U:1009:ILE:HG22	2.13	0.47
1:D:622:MET:CE	1:D:1022:PHE:CE1	2.98	0.47
1:U:1467:GLN:O	1:U:1470:ARG:HB2	2.15	0.47
1:U:450:ARG:NH2	1:U:450:ARG:CG	2.69	0.47
1:B:1167:LEU:O	1:B:1171:GLY:HA2	2.14	0.47
1:D:1014:ILE:CG2	1:D:1015:THR:N	2.76	0.47
1:D:1234:TYR:HD1	1:D:1348:LEU:HB2	1.77	0.47
1:D:1388:LEU:HD13	1:D:1438:ARG:CG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1080:PRO:HD2	1:S:1081:HIS:CD2	2.50	0.47
1:S:1346:ILE:O	1:S:1346:ILE:HG13	2.13	0.47
1:U:1260:VAL:HG22	1:U:1305:VAL:CG2	2.44	0.47
1:B:1029:VAL:HA	1:B:1033:ARG:HB3	1.96	0.47
1:B:1222:GLY:C	1:B:1223:LEU:HD12	2.35	0.47
1:B:544:LEU:O	1:B:545:TYR:CD1	2.67	0.47
1:D:458:ARG:HH21	2:F:11:DC:H5"	1.76	0.47
1:U:570:ASN:O	1:U:572:THR:N	2.47	0.47
1:B:514:ALA:O	1:B:518:THR:HG23	2.15	0.47
1:D:1074:VAL:CG1	1:D:1086:ILE:HD13	2.45	0.47
1:U:529:ARG:N	1:U:530:PRO:HD3	2.30	0.47
3:V:11:DC:C2	4:W:1020[A]:RXV:C8	2.98	0.47
1:B:462:LEU:HB3	1:B:475:ASN:ND2	2.30	0.47
1:D:1040:ASP:CG	1:D:1047:ARG:HH21	2.19	0.47
1:S:1030:ILE:HG21	1:S:1343:PRO:HG2	1.96	0.47
1:U:537:VAL:HG12	1:U:606:VAL:HG21	1.97	0.47
1:U:557:TYR:O	1:U:558:ASN:HB3	2.14	0.47
1:U:549:GLN:OE1	1:U:569:LEU:HD22	2.15	0.47
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.80	0.47
1:S:1245:SER:HB2	1:S:1263:GLU:O	2.15	0.47
1:S:1378:ALA:O	1:S:1382:GLU:HG3	2.15	0.47
1:S:557:TYR:O	1:S:558:ASN:HB3	2.15	0.47
1:U:1100:ARG:HH11	1:U:1100:ARG:HG3	1.80	0.47
1:U:1225:LEU:HD21	1:U:1244:ARG:HD2	1.97	0.47
1:U:465:GLU:HG2	1:U:623:GLY:HA2	1.95	0.47
3:V:15:DA:H2"	3:V:16:DC:C6	2.49	0.47
1:B:608:LEU:HD13	1:B:1014:ILE:HG21	1.96	0.47
1:D:1164:PHE:O	1:D:1166:ASN:N	2.47	0.47
1:S:1072:GLY:O	1:U:1069:ARG:HB2	2.15	0.47
1:U:1292:LEU:HB2	1:U:1306:ILE:HG22	1.97	0.47
1:B:1053:LEU:CD2	1:B:1070:ILE:HG21	2.46	0.46
1:B:1164:PHE:HA	1:B:1355:TYR:OH	2.15	0.46
1:B:515:HIS:HB2	1:B:1025:TYR:CD1	2.50	0.46
1:D:1080:PRO:HG3	1:D:1150:TYR:CD2	2.47	0.46
1:D:1310:LYS:O	1:D:1311:ASP:HB3	2.14	0.46
1:D:505:ILE:HD11	1:D:524:PHE:HE2	1.80	0.46
1:S:1040:ASP:HB3	1:S:1162:ALA:HB2	1.96	0.46
1:S:1168:LEU:HB2	1:S:1191:LEU:HD11	1.96	0.46
1:S:1238:ARG:HG3	1:S:1345:LEU:HD21	1.97	0.46
1:U:1410:SER:O	1:U:1414:ARG:HB2	2.15	0.46
1:U:1458:ILE:HG12	1:U:1464:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1173:SER:OG	3:W:5:DG:H5'	2.14	0.46
1:B:1040:ASP:OD1	1:B:1041:GLY:N	2.48	0.46
1:B:632:PHE:C	1:B:632:PHE:CD2	2.88	0.46
1:D:1040:ASP:HB2	1:D:1162:ALA:HB2	1.97	0.46
1:S:431:ILE:HA	1:S:453:ALA:O	2.16	0.46
1:S:540:ALA:HB1	1:S:595:THR:CG2	2.45	0.46
1:D:1064:TYR:CD1	1:D:1107:GLN:HB2	2.51	0.46
1:D:427:GLU:HG3	1:D:501:HIS:NE2	2.30	0.46
1:D:516:ILE:HG22	1:D:517:ARG:N	2.30	0.46
1:S:1100:ARG:NH1	1:S:1101:TYR:CE1	2.83	0.46
1:S:1204:ILE:HG13	1:S:1208:GLU:CD	2.36	0.46
1:S:1445:TYR:O	1:S:1448:LEU:HB2	2.15	0.46
1:U:1183:ILE:HD11	1:U:1335:MET:HA	1.97	0.46
1:U:1363:VAL:HG21	1:U:1469:VAL:HG22	1.97	0.46
1:B:1049:ILE:HA	1:B:1074:VAL:HG21	1.97	0.46
1:B:509:ALA:CB	1:B:544:LEU:HD13	2.45	0.46
1:D:518:THR:HB	1:D:1018:MET:CE	2.46	0.46
1:D:1137:ARG:HG2	1:D:1163:ARG:HG3	1.98	0.46
1:S:1182:ASN:HB3	1:S:1332:GLY:O	2.15	0.46
1:S:1445:TYR:CE1	1:S:1449:LEU:HD21	2.50	0.46
1:S:435:GLU:OE1	1:S:508:ASP:OD2	2.32	0.46
1:U:1128:MET:HG2	1:U:1132:THR:HG21	1.97	0.46
1:U:1144:ILE:HD11	1:U:1157:PRO:HB3	1.92	0.46
1:B:1031:VAL:HA	1:B:1338:LEU:HD21	1.98	0.46
1:D:1318:LEU:HG	1:D:1322:TYR:CE2	2.50	0.46
1:D:1448:LEU:HD12	1:D:1448:LEU:HA	1.76	0.46
1:D:555:TYR:HE1	1:D:594:THR:HG21	1.81	0.46
1:S:1190:GLU:O	1:S:1213:ILE:HG12	2.15	0.46
1:S:1358:HIS:O	1:S:1362:VAL:HG23	2.16	0.46
1:S:1488:ILE:H	1:S:1488:ILE:HD12	1.80	0.46
1:U:527:PHE:O	1:U:528:MET:HG3	2.13	0.46
3:V:13:DC:N4	3:W:8:DG:H1	2.13	0.46
1:B:1391:ILE:HG23	1:B:1392:ASP:H	1.80	0.46
1:B:1451:TYR:O	1:B:1455:LEU:HG	2.15	0.46
1:D:1458:ILE:HD13	1:D:1468:LEU:HD22	1.97	0.46
1:S:1113:MET:C	1:S:1115:GLY:H	2.19	0.46
1:S:1442:GLU:HA	1:S:1445:TYR:HB3	1.97	0.46
1:S:627:GLU:HA	1:S:627:GLU:OE1	2.16	0.46
1:U:511:VAL:HG21	1:U:1028:SER:OG	2.16	0.46
1:U:1056:GLN:HB3	1:U:1058:MET:HE3	1.96	0.46
1:U:1113:MET:C	1:U:1115:GLY:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1273:MET:HG3	1:U:1326:PRO:HB2	1.97	0.46
1:U:556:VAL:CG1	1:U:557:TYR:N	2.79	0.46
1:B:445:SER:HB3	1:B:588:ALA:HB1	1.97	0.46
1:D:1137:ARG:O	1:D:1138:ASP:HB2	2.16	0.46
1:D:1477:ARG:O	1:D:1481:GLY:HA3	2.15	0.46
3:V:14:DT:H2'	3:V:15:DA:C8	2.50	0.46
1:B:1062:LYS:HD3	1:B:1062:LYS:HA	1.68	0.46
1:B:565:LEU:C	1:B:567:SER:H	2.18	0.46
1:D:1234:TYR:O	1:D:1347:ASN:HB2	2.16	0.46
1:D:632:PHE:C	1:D:632:PHE:CD2	2.89	0.46
1:S:1288:GLY:HA2	1:S:1309:ARG:HB2	1.96	0.46
1:S:462:LEU:HD12	1:S:463:ASN:N	2.31	0.46
1:S:571:PRO:C	1:S:573:PRO:HD3	2.35	0.46
1:S:601:ARG:NH1	1:S:603:LEU:HD12	2.30	0.46
1:U:577:ILE:HG12	1:U:577:ILE:O	2.15	0.46
1:S:581:LYS:NZ	3:V:8:DG:OP1	2.48	0.46
1:D:1146:PHE:CE2	1:D:1157:PRO:HB3	2.50	0.46
1:D:1313:ASN:OD1	1:D:1316:VAL:HG23	2.16	0.46
1:D:549:GLN:HG2	1:D:573:PRO:HG2	1.98	0.46
1:S:1395:ILE:O	1:S:1399:ARG:HG3	2.15	0.46
1:S:526:ARG:HA	1:S:526:ARG:HD3	1.58	0.46
1:B:1073:ASP:O	1:B:1077:LYS:HB2	2.15	0.46
1:B:465:GLU:OE2	1:B:526:ARG:NH2	2.49	0.46
1:B:505:ILE:HG22	1:B:505:ILE:O	2.16	0.46
1:D:541:GLN:CD	1:D:604:LEU:HD11	2.37	0.46
1:S:1270:LYS:O	1:S:1274:ILE:HG13	2.16	0.46
1:S:1274:ILE:HG22	1:S:1292:LEU:CD2	2.45	0.46
1:U:547:LEU:C	1:U:547:LEU:HD12	2.36	0.46
3:V:11:DC:H2"	3:V:12:DC:OP2	2.16	0.46
1:B:1196:LEU:O	1:B:1200:LYS:HG3	2.16	0.45
1:B:1201:ASN:HD21	1:B:1204:ILE:HA	1.81	0.45
1:D:1444:GLU:HA	1:D:1447:GLU:HB2	1.97	0.45
1:S:515:HIS:HB2	1:S:1025:TYR:CG	2.50	0.45
1:S:1381:LEU:HD23	1:S:1381:LEU:HA	1.61	0.45
1:S:475:ASN:C	1:S:475:ASN:OD1	2.53	0.45
1:B:1107:GLN:HG2	1:B:1125:GLU:OE1	2.16	0.45
1:D:1068:ALA:HB1	4:E:1021[B]:RXV:S26	2.56	0.45
1:D:1281:VAL:CG1	1:D:1289:ILE:HG13	2.46	0.45
1:U:597:ASN:OD1	1:U:598:PRO:HD2	2.15	0.45
4:W:1020[A]:RXV:H142	4:W:1020[A]:RXV:C33	2.45	0.45
1:B:547:LEU:HD21	1:B:575:TRP:HE3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:LYS:HE3	2:E:16:DC:OP2	2.16	0.45
1:D:516:ILE:HA	1:D:519:LEU:HD12	1.99	0.45
1:D:565:LEU:HD11	1:D:569:LEU:HD12	1.99	0.45
1:S:1322:TYR:O	1:S:1328:GLN:HB3	2.16	0.45
1:U:1034:ALA:O	1:U:1035:LEU:HD23	2.17	0.45
1:U:1277:ILE:HG12	1:U:1325:THR:HG21	1.98	0.45
1:U:525:TYR:HD2	1:U:526:ARG:HG2	1.80	0.45
1:S:1187:ASN:ND2	1:S:1484:ARG:HA	2.32	0.45
1:S:481:MET:O	1:S:482:ILE:C	2.54	0.45
1:S:506:MET:HG3	1:S:540:ALA:HB3	1.99	0.45
1:S:1068:ALA:O	1:U:1072:GLY:HA3	2.16	0.45
1:U:556:VAL:HG12	1:U:557:TYR:H	1.81	0.45
1:U:570:ASN:CB	1:U:571:PRO:CD	2.94	0.45
1:U:540:ALA:HA	1:U:603:LEU:HD23	1.98	0.45
1:B:1048:ARG:HD2	1:B:1079:HIS:ND1	2.31	0.45
1:B:1080:PRO:HG3	1:B:1150:TYR:CG	2.52	0.45
1:B:1234:TYR:CE1	1:B:1348:LEU:HD22	2.52	0.45
1:D:1027:MET:HE2	1:D:1027:MET:HB3	1.78	0.45
1:D:1042:LEU:HA	1:D:1042:LEU:HD23	1.72	0.45
1:D:1445:TYR:CE2	1:D:1449:LEU:HD11	2.51	0.45
1:D:1467:GLN:O	1:D:1470:ARG:HB2	2.16	0.45
1:D:569:LEU:O	1:D:571:PRO:HD3	2.16	0.45
1:D:624:ASP:OD1	1:D:624:ASP:N	2.50	0.45
1:S:469:LEU:HD22	1:S:469:LEU:O	2.17	0.45
1:S:493:PHE:CE2	1:S:495:LEU:HB2	2.51	0.45
1:U:1112:SER:OG	1:U:1116:ASP:HB2	2.16	0.45
1:B:574:LYS:C	1:B:575:TRP:HD1	2.19	0.45
1:D:1163:ARG:HA	1:D:1359:GLN:HE22	1.82	0.45
1:U:1193:ASN:HA	1:U:1196:LEU:HD12	1.99	0.45
1:U:1143:THR:HA	1:U:1365:ARG:HE	1.81	0.45
1:B:1244:ARG:HD2	1:B:1322:TYR:CZ	2.52	0.45
1:B:1279:GLU:HA	1:B:1282:ARG:NH1	2.32	0.45
1:B:565:LEU:HB2	1:U:1004:LEU:CD1	2.41	0.45
1:S:1174:GLY:O	1:S:1180:ALA:HB1	2.17	0.45
1:U:1066:LYS:O	1:U:1067:SER:C	2.54	0.45
1:B:1216:PRO:HB2	1:B:1218:PHE:CE2	2.52	0.45
1:D:1243:MET:HB2	1:D:1329:THR:O	2.17	0.45
1:B:1045:VAL:HG11	2:E:6:DT:O3'	2.17	0.45
1:S:1165:PRO:HG3	1:S:1355:TYR:CE1	2.52	0.45
1:U:1219:PRO:HD2	1:U:1266:PHE:CD1	2.52	0.45
1:B:1177:VAL:HG13	2:F:16:DC:H4'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:493:PHE:CE1	1:U:528:MET:HG2	2.51	0.45
1:B:1035:LEU:HB2	1:B:1338:LEU:HD11	1.99	0.45
1:B:1236:THR:HB	1:B:1238:ARG:H	1.83	0.45
1:B:1243:MET:O	1:B:1328:GLN:HA	2.17	0.45
1:B:601:ARG:HG3	1:B:603:LEU:HG	1.99	0.45
1:D:1191:LEU:HD23	1:D:1213:ILE:HD12	1.99	0.45
1:B:561:GLU:HB3	1:U:1004:LEU:HD21	1.97	0.45
1:U:1253:GLY:HA2	1:U:1254:GLY:HA2	1.54	0.45
1:B:597:ASN:O	1:B:599:GLU:N	2.50	0.44
1:D:1333:VAL:HG12	1:D:1334:ASN:N	2.33	0.44
1:D:1334:ASN:O	1:D:1336:ILE:N	2.50	0.44
1:D:555:TYR:CE1	1:D:594:THR:HG21	2.52	0.44
1:S:1326:PRO:HB2	1:S:1327:LEU:H	1.57	0.44
1:S:1030:ILE:CG2	1:S:1343:PRO:HG3	2.47	0.44
1:S:1403:THR:OG1	1:S:1406:VAL:HG23	2.17	0.44
1:S:461:ILE:HG22	1:S:519:LEU:HB3	1.98	0.44
1:U:1135:LEU:HA	1:U:1162:ALA:HA	1.99	0.44
1:D:1060:PRO:CG	1:D:1133:LEU:HD11	2.48	0.44
1:S:438:SER:HB3	1:U:1119:ALA:HB1	1.99	0.44
1:S:538:TYR:CE2	1:S:605:GLN:HB2	2.52	0.44
1:U:1458:ILE:HG12	1:U:1464:VAL:HG12	1.98	0.44
1:B:1012:ARG:NH2	1:B:1020:GLU:OE2	2.50	0.44
1:B:1402:ASP:CG	1:B:1403:THR:H	2.21	0.44
1:D:1020:GLU:O	1:D:1024:ASP:HB3	2.17	0.44
1:S:1364:ARG:HG2	1:S:1368:GLN:HE22	1.82	0.44
1:S:1429:ARG:NH1	1:U:1427:ASP:O	2.49	0.44
1:U:597:ASN:O	1:U:601:ARG:HG2	2.17	0.44
1:B:1345:LEU:HD12	1:B:1346:ILE:N	2.33	0.44
1:B:579:ARG:C	1:B:580:TYR:CD1	2.90	0.44
1:B:624:ASP:N	1:B:624:ASP:OD1	2.49	0.44
1:D:1196:LEU:HA	1:D:1196:LEU:HD23	1.69	0.44
1:D:1349:LYS:O	1:D:1353:VAL:HG23	2.18	0.44
1:D:1423:GLN:C	1:D:1425:ILE:H	2.21	0.44
1:S:426:PRO:C	1:S:501:HIS:CD2	2.91	0.44
1:U:1298:LEU:HD12	1:U:1298:LEU:HA	1.73	0.44
1:B:432:PHE:N	1:B:432:PHE:CD1	2.85	0.44
1:B:445:SER:HB3	1:B:588:ALA:CB	2.47	0.44
1:B:621:LEU:HA	1:B:629:ARG:HD3	1.98	0.44
1:D:1167:LEU:HD12	1:D:1167:LEU:O	2.17	0.44
1:S:1045:VAL:HG13	1:S:1046:HIS:H	1.81	0.44
1:S:1223:LEU:HB2	1:S:1244:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1054:ASN:HB2	1:D:1136:LEU:CD1	2.48	0.44
1:D:1415:PHE:O	1:D:1417:LEU:HG	2.17	0.44
1:U:549:GLN:HB3	1:U:552:GLN:HG3	1.99	0.44
1:U:579:ARG:CG	1:U:580:TYR:N	2.79	0.44
1:B:1206:ILE:HD13	1:B:1206:ILE:N	2.26	0.44
1:B:423:SER:HB3	1:B:429:CYS:SG	2.58	0.44
1:D:640:ALA:CB	1:D:641:ASN:HA	2.38	0.44
1:S:1003:GLU:CB	1:S:1004:LEU:HB3	2.47	0.44
1:S:1308:VAL:HG12	1:S:1312:ALA:HB3	2.00	0.44
1:S:432:PHE:HE1	1:S:452:GLN:HB3	1.83	0.44
1:S:469:LEU:HD13	1:S:469:LEU:C	2.38	0.44
1:U:1274:ILE:HG23	1:U:1292:LEU:HD21	2.00	0.44
1:U:1329:THR:HG22	1:U:1330:SER:N	2.33	0.44
1:B:1022:PHE:O	1:B:1025:TYR:HB3	2.17	0.44
4:E:1021[A]:RXV:C4	2:F:11:DC:C2	3.01	0.44
1:D:1179:MET:C	2:E:17:DG:H4'	2.38	0.44
1:S:1135:LEU:HD22	1:S:1162:ALA:HA	2.00	0.44
1:S:1353:VAL:O	1:S:1357:GLU:HB2	2.17	0.44
1:S:418:LEU:HD11	1:S:453:ALA:HB1	2.00	0.44
1:U:1131:ILE:HD13	1:U:1131:ILE:C	2.38	0.44
1:U:1272:ARG:NH1	1:U:1272:ARG:HG2	2.25	0.44
1:U:633:ILE:HG22	1:U:634:GLU:N	2.32	0.44
1:B:1428:MET:HG2	1:B:1429:ARG:N	2.33	0.44
1:D:1045:VAL:HG13	1:D:1046:HIS:N	2.33	0.44
1:D:505:ILE:HD11	1:D:524:PHE:CE2	2.53	0.44
2:E:10:DG:H2'	2:E:10:DG:O5'	2.18	0.44
1:S:1298:LEU:H	1:S:1299:ARG:HH21	1.66	0.44
1:S:1425:ILE:HG22	1:S:1426:LEU:N	2.33	0.44
1:U:1391:ILE:HG23	1:U:1392:ASP:N	2.33	0.44
1:U:447:ARG:HD2	1:U:452:GLN:O	2.18	0.44
1:B:1339:VAL:HG11	1:B:1354:HIS:CE1	2.53	0.43
1:B:1350:GLU:HG2	1:B:1350:GLU:H	1.62	0.43
2:E:6:DT:C2	2:E:7:DA:C8	3.05	0.43
1:S:1381:LEU:O	1:S:1385:ARG:HG2	2.18	0.43
1:U:1349:LYS:O	1:U:1349:LYS:HG2	2.16	0.43
1:D:1196:LEU:HD22	1:D:1470:ARG:HG2	2.00	0.43
1:D:549:GLN:CG	1:D:573:PRO:HG2	2.48	0.43
1:U:1042:LEU:HD22	1:U:1046:HIS:HB3	1.99	0.43
1:U:1213:ILE:HD12	1:U:1213:ILE:N	2.33	0.43
1:B:1035:LEU:HA	1:B:1036:PRO:HD3	1.71	0.43
1:B:1059:THR:CB	1:B:1060:PRO:CD	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1466:LEU:HD11	1:B:1470:ARG:NH2	2.33	0.43
1:B:446:GLY:O	1:B:592:TRP:CE3	2.71	0.43
1:D:1136:LEU:HD22	1:D:1160:LEU:HD22	1.99	0.43
1:S:1071:VAL:HG22	1:S:1086:ILE:HG22	2.00	0.43
1:S:1030:ILE:HD13	1:S:1176:ALA:HB1	2.01	0.43
1:S:553:LYS:C	1:S:554:TYR:HD1	2.21	0.43
1:U:418:LEU:HD23	1:U:418:LEU:O	2.18	0.43
1:U:542:PRO:HA	1:U:543:PRO:HD3	1.83	0.43
1:B:464:VAL:HG23	1:B:464:VAL:O	2.18	0.43
1:S:1245:SER:OG	1:S:1327:LEU:HG	2.17	0.43
1:S:462:LEU:HD23	1:S:475:ASN:HD22	1.83	0.43
1:U:462:LEU:HD12	1:U:462:LEU:HA	1.57	0.43
1:B:484:ALA:O	1:B:499:ARG:HG3	2.19	0.43
1:D:1004:LEU:HG	1:D:1005:PRO:HA	2.01	0.43
1:D:1032:ALA:C	1:D:1044:PRO:HG2	2.38	0.43
1:S:1042:LEU:HA	1:S:1042:LEU:HD23	1.79	0.43
1:S:1246:ARG:HB3	1:S:1263:GLU:HB2	1.99	0.43
1:U:1015:THR:HG22	1:U:1019:ARG:HG3	2.00	0.43
1:U:1042:LEU:HD11	1:U:1160:LEU:HD12	2.00	0.43
1:B:1220:THR:O	1:B:1221:ALA:HB3	2.18	0.43
1:B:586:MET:SD	1:B:591:LEU:CD1	3.07	0.43
1:S:1087:TYR:O	1:S:1090:MET:N	2.52	0.43
1:S:1173:SER:HA	1:S:1181:THR:O	2.19	0.43
1:U:1308:VAL:HG12	1:U:1309:ARG:O	2.19	0.43
1:B:1038:VAL:O	1:B:1038:VAL:HG22	2.17	0.43
1:D:1252:ARG:NH1	1:D:1256:ARG:HE	2.16	0.43
1:D:1411:LEU:HD12	1:D:1422:ALA:CB	2.48	0.43
1:S:431:ILE:HD13	1:S:485:PHE:HE1	1.84	0.43
1:U:556:VAL:CG1	1:U:557:TYR:H	2.31	0.43
1:U:597:ASN:HA	1:U:598:PRO:HD3	1.87	0.43
1:U:606:VAL:HG11	1:U:1014:ILE:CD1	2.48	0.43
1:B:1144:ILE:C	1:B:1144:ILE:HD12	2.39	0.43
1:B:1039:ARG:HB3	1:B:1358:HIS:CD2	2.54	0.43
1:B:508:ASP:OD2	1:B:582:GLY:HA2	2.19	0.43
1:D:1134:GLU:O	1:D:1163:ARG:HG2	2.19	0.43
1:D:1230:ILE:O	1:D:1233:ALA:HB3	2.19	0.43
1:D:431:ILE:HG23	1:D:431:ILE:O	2.17	0.43
1:S:1428:MET:HG2	1:S:1429:ARG:N	2.34	0.43
1:S:429:CYS:HB3	1:S:500:TYR:HD2	1.83	0.43
1:B:1137:ARG:O	1:B:1138:ASP:HB2	2.18	0.43
1:B:509:ALA:C	1:B:544:LEU:HD13	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:HD13	1:B:548:THR:N	2.34	0.43
1:D:555:TYR:O	1:D:556:VAL:HG23	2.19	0.43
1:S:1093:MET:CA	1:S:1099:TYR:CD1	2.99	0.43
1:U:1466:LEU:O	1:U:1470:ARG:HG3	2.18	0.43
1:B:1072:GLY:O	1:D:1069:ARG:HA	2.19	0.43
1:D:545:TYR:HD2	1:D:577:ILE:HD11	1.82	0.43
1:S:1141:LYS:O	1:S:1142:ASP:C	2.56	0.43
1:U:1099:TYR:HD2	1:U:1170:ASN:ND2	2.17	0.43
1:B:1364:ARG:HG2	1:B:1368:GLN:HE22	1.84	0.42
1:D:1080:PRO:O	1:D:1081:HIS:CG	2.72	0.42
1:D:1359:GLN:O	1:D:1362:VAL:HG12	2.19	0.42
1:U:1135:LEU:HD23	1:U:1162:ALA:HA	2.00	0.42
3:V:17:DG:H2"	3:V:18:DG:O5'	2.19	0.42
1:B:1064:TYR:CD2	1:B:1107:GLN:HB2	2.54	0.42
1:B:1201:ASN:HA	1:B:1202:PRO:HD3	1.91	0.42
1:B:1246:ARG:NH1	1:B:1246:ARG:HG3	2.34	0.42
1:B:1345:LEU:C	1:B:1345:LEU:HD12	2.39	0.42
1:B:503:ILE:HD12	1:B:503:ILE:N	2.34	0.42
1:B:443:THR:HG22	1:B:596:MET:HE1	2.00	0.42
1:D:1079:HIS:NE2	1:D:1081:HIS:CD2	2.87	0.42
1:D:1270:LYS:HE2	1:D:1296:THR:OG1	2.19	0.42
1:D:1457:THR:HG22	1:D:1464:VAL:HG11	2.01	0.42
1:S:1107:GLN:CG	1:S:1125:GLU:HG3	2.46	0.42
1:S:1461:ASP:HB3	1:S:1464:VAL:HG23	2.00	0.42
1:B:1035:LEU:HB2	1:B:1338:LEU:HD12	2.01	0.42
1:B:1057:GLY:O	1:B:1059:THR:N	2.51	0.42
1:B:1194:GLY:HA3	1:B:1213:ILE:HD11	2.00	0.42
1:B:579:ARG:C	1:B:580:TYR:HD1	2.22	0.42
1:D:544:LEU:O	1:D:545:TYR:CD1	2.72	0.42
1:U:1110:PHE:HA	1:U:1118:ALA:CB	2.49	0.42
1:U:1276:LYS:O	1:U:1280:LEU:HG	2.19	0.42
1:B:504:VAL:CG1	1:B:540:ALA:HB2	2.49	0.42
1:S:444:LYS:HA	1:S:454:ILE:CD1	2.49	0.42
1:S:450:ARG:CG	1:S:451:THR:HG22	2.50	0.42
1:B:461:ILE:HA	1:B:461:ILE:HD13	1.63	0.42
1:D:555:TYR:N	1:D:555:TYR:CD2	2.87	0.42
1:S:1042:LEU:HB2	1:S:1047:ARG:NH2	2.34	0.42
1:S:1382:GLU:HG2	1:S:1445:TYR:HE2	1.84	0.42
1:S:532:ILE:HA	1:S:537:VAL:HG23	2.01	0.42
1:U:1249:ILE:HD11	1:U:1318:LEU:HD22	2.02	0.42
1:B:1159:VAL:HG22	1:B:1160:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1417:LEU:HB3	1:D:1421:GLN:HB3	2.01	0.42
2:F:13:DC:C2'	2:F:14:DT:O5'	2.68	0.42
1:S:1035:LEU:HD23	1:S:1035:LEU:HA	1.71	0.42
1:S:565:LEU:O	1:S:569:LEU:HD12	2.20	0.42
1:U:443:THR:HG22	1:U:454:ILE:CD1	2.47	0.42
1:B:1368:GLN:HE21	1:B:1368:GLN:HB2	1.65	0.42
1:D:1233:ALA:HA	1:D:1238:ARG:O	2.20	0.42
1:S:608:LEU:HA	1:S:608:LEU:HD13	1.78	0.42
1:U:1004:LEU:N	1:U:1005:PRO:CD	2.83	0.42
1:U:1233:ALA:HB1	1:U:1333:VAL:HG11	2.01	0.42
1:B:1087:TYR:CD1	1:B:1090:MET:HE2	2.55	0.42
1:B:1192:ILE:HD12	1:B:1477:ARG:HB2	2.01	0.42
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.50	0.42
1:B:493:PHE:CE2	1:B:530:PRO:HG2	2.54	0.42
1:B:553:LYS:HB3	1:B:553:LYS:HE2	1.91	0.42
1:D:1004:LEU:HA	1:D:1005:PRO:HA	1.76	0.42
1:D:1060:PRO:HG2	1:D:1133:LEU:HD11	2.01	0.42
1:D:1465:LEU:C	1:D:1465:LEU:HD23	2.40	0.42
1:S:597:ASN:HD22	1:S:598:PRO:HD2	1.84	0.42
1:U:1100:ARG:NH2	1:U:1217:ASP:OD2	2.43	0.42
3:V:4:DC:C2'	3:V:5:DG:H5'	2.49	0.42
1:B:618:PHE:CE2	1:B:1018:MET:CE	3.03	0.42
1:B:1391:ILE:HG23	1:B:1392:ASP:N	2.34	0.42
1:B:499:ARG:HH11	1:B:499:ARG:HG3	1.84	0.42
1:D:1040:ASP:OD1	1:D:1047:ARG:NH2	2.53	0.42
1:D:440:GLY:O	1:D:444:LYS:HG3	2.20	0.42
1:D:572:THR:H	1:D:573:PRO:CD	2.25	0.42
1:S:522:THR:O	1:S:522:THR:HG22	2.20	0.42
1:U:515:HIS:ND1	1:U:519:LEU:HD11	2.34	0.42
3:V:20:DT:H6	3:V:20:DT:H5"	1.85	0.42
1:B:501:HIS:HA	1:B:536:TYR:HD1	1.82	0.42
1:S:1050:LEU:HD23	1:S:1050:LEU:N	2.35	0.42
1:U:1056:GLN:HB2	1:U:1058:MET:SD	2.59	0.42
1:U:1233:ALA:O	1:U:1335:MET:HE2	2.19	0.42
1:U:637:ALA:HB1	1:U:639:TYR:CE1	2.55	0.42
3:V:8:DG:H2'	3:V:9:DG:O4'	2.20	0.42
1:B:1083:ASP:C	1:B:1085:SER:N	2.72	0.41
1:B:565:LEU:CD1	1:B:569:LEU:HG	2.50	0.41
1:D:609:GLU:HA	1:D:609:GLU:OE1	2.20	0.41
1:S:1183:ILE:HA	1:S:1184:PRO:HD3	1.83	0.41
1:S:544:LEU:HG	1:S:545:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1138:ASP:HA	1:U:1141:LYS:HD3	2.02	0.41
1:B:1195:VAL:HG22	1:B:1352:LEU:HD13	2.01	0.41
1:B:583:LEU:HD22	1:B:591:LEU:HD11	2.02	0.41
1:B:586:MET:SD	1:B:591:LEU:HD13	2.59	0.41
1:D:458:ARG:NH2	2:F:11:DC:H5'	2.35	0.41
1:S:1385:ARG:HB3	1:S:1438:ARG:NH1	2.35	0.41
1:S:464:VAL:HG12	1:S:472:ILE:HD13	2.02	0.41
1:S:522:THR:HG23	1:S:618:PHE:HD2	1.85	0.41
1:B:565:LEU:CB	1:U:1004:LEU:HD12	2.42	0.41
1:D:1183:ILE:HA	1:D:1184:PRO:HD3	1.78	0.41
1:D:1257:GLN:H	1:D:1308:VAL:HG12	1.84	0.41
1:D:539:ILE:HG22	1:D:539:ILE:O	2.20	0.41
1:D:595:THR:HG22	1:D:595:THR:O	2.18	0.41
1:S:1204:ILE:HG23	1:S:1204:ILE:O	2.20	0.41
1:S:1466:LEU:HD21	1:S:1470:ARG:HH21	1.85	0.41
1:S:601:ARG:NH1	1:S:603:LEU:CD1	2.83	0.41
1:B:1064:TYR:HB3	1:B:1125:GLU:CB	2.50	0.41
1:B:623:GLY:O	1:B:629:ARG:NH1	2.53	0.41
1:D:1050:LEU:N	1:D:1050:LEU:HD23	2.36	0.41
1:D:1136:LEU:HD23	1:D:1136:LEU:N	2.36	0.41
1:D:1192:ILE:CG2	1:D:1473:LEU:HB3	2.51	0.41
2:E:13:DC:N3	2:F:9:DG:N2	2.67	0.41
1:S:1002:ALA:CA	1:S:1003:GLU:C	2.85	0.41
1:S:1374:ALA:HB1	1:S:1452:ILE:HD11	2.01	0.41
1:U:606:VAL:HG11	1:U:1014:ILE:HD13	2.02	0.41
1:U:1135:LEU:HD21	1:U:1164:PHE:CE2	2.55	0.41
1:U:432:PHE:HE2	1:U:504:VAL:HG11	1.84	0.41
1:U:508:ASP:O	1:U:513:GLY:HA3	2.21	0.41
1:U:543:PRO:HD2	1:U:586:MET:CE	2.49	0.41
1:D:1191:LEU:HD23	1:D:1213:ILE:CD1	2.50	0.41
1:D:562:LEU:HD22	1:D:566:LYS:HE2	2.03	0.41
1:S:529:ARG:HG3	1:S:529:ARG:O	2.19	0.41
1:U:581:LYS:HE2	1:U:1080:PRO:O	2.21	0.41
1:U:614:ALA:O	1:U:618:PHE:HD1	2.03	0.41
1:B:507:THR:HG21	1:B:516:ILE:CG2	2.51	0.41
1:D:1104:VAL:HG12	1:D:1105:ASP:H	1.86	0.41
1:D:433:LEU:HD11	1:D:503:ILE:CG2	2.50	0.41
1:D:460:LYS:HA	1:D:516:ILE:HD11	2.03	0.41
1:S:1289:ILE:HG22	1:S:1289:ILE:O	2.20	0.41
1:S:445:SER:O	1:U:1298:LEU:HD13	2.21	0.41
1:U:1135:LEU:HA	1:U:1135:LEU:HD23	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1233:ALA:HA	1:U:1238:ARG:O	2.20	0.41
1:U:541:GLN:HA	1:U:542:PRO:HD3	1.82	0.41
1:B:1252:ARG:HG2	1:B:1252:ARG:O	2.19	0.41
1:B:1272:ARG:O	1:B:1276:LYS:HG3	2.21	0.41
1:B:1377:ARG:O	1:B:1380:ILE:HB	2.21	0.41
1:B:431:ILE:HD11	1:B:455:LEU:HB2	2.02	0.41
1:B:461:ILE:HG23	1:B:462:LEU:N	2.35	0.41
1:B:570:ASN:N	1:B:571:PRO:CD	2.84	0.41
1:B:549:GLN:CG	1:B:573:PRO:HD2	2.50	0.41
1:D:1289:ILE:H	1:D:1289:ILE:HG12	1.34	0.41
1:D:1327:LEU:HA	1:D:1327:LEU:HD13	1.78	0.41
1:D:462:LEU:HD21	1:D:472:ILE:HG23	2.02	0.41
1:D:545:TYR:CE2	1:D:579:ARG:HG3	2.56	0.41
1:S:1040:ASP:CG	1:S:1047:ARG:HH21	2.24	0.41
1:S:601:ARG:HH11	1:S:603:LEU:HG	1.86	0.41
1:U:1015:THR:O	1:U:1019:ARG:HG3	2.21	0.41
1:U:1394:ILE:HG12	1:U:1394:ILE:H	1.71	0.41
1:U:506:MET:HB2	1:U:540:ALA:HB3	2.03	0.41
1:D:1168:LEU:HD23	1:D:1168:LEU:HA	1.89	0.41
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.55	0.41
2:E:20:DT:N3	2:F:1:5UA:N1	2.69	0.41
1:S:1060:PRO:HD2	1:S:1133:LEU:HD11	2.02	0.41
1:S:1296:THR:HG23	1:S:1301:GLY:C	2.41	0.41
1:B:1215:GLY:HA2	1:B:1234:TYR:OH	2.20	0.41
1:D:570:ASN:O	1:D:573:PRO:HD3	2.21	0.41
1:S:419:ALA:O	1:S:447:ARG:NH2	2.49	0.41
1:S:455:LEU:CG	1:S:455:LEU:O	2.60	0.41
1:S:632:PHE:C	1:S:632:PHE:CD2	2.94	0.41
1:U:1031:VAL:O	1:U:1338:LEU:HD11	2.20	0.41
1:U:503:ILE:N	1:U:536:TYR:O	2.49	0.41
1:B:514:ALA:HB1	1:B:1021:SER:HB3	2.02	0.41
1:B:1101:TYR:HB3	1:B:1131:ILE:HD13	2.02	0.41
1:B:1265:PRO:HB2	1:B:1268:VAL:HG21	2.03	0.41
1:B:1348:LEU:O	1:B:1348:LEU:HD12	2.21	0.41
1:B:509:ALA:HB3	1:B:544:LEU:CD1	2.51	0.41
1:D:1007:SER:C	1:D:1009:ILE:H	2.23	0.41
1:S:531:LEU:O	1:S:536:TYR:HB2	2.20	0.41
1:U:1200:LYS:HB2	1:U:1200:LYS:HE3	1.82	0.41
1:U:1308:VAL:HG12	1:U:1309:ARG:N	2.35	0.41
1:U:536:TYR:N	1:U:536:TYR:CD1	2.89	0.41
3:V:3:DC:H5"	3:V:3:DC:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:LEU:CB	1:B:1005:PRO:HD2	2.47	0.41
1:B:1490:LEU:H	1:B:1490:LEU:HD12	1.85	0.41
1:D:1227:LYS:O	1:D:1231:ARG:HB2	2.21	0.41
1:D:1335:MET:HE3	1:D:1347:ASN:HA	2.02	0.41
2:E:1:5UA:H3'	2:E:2:DG:P	2.61	0.41
1:U:1367:THR:HG22	1:U:1455:LEU:HD22	2.02	0.41
1:B:1265:PRO:HB2	1:B:1268:VAL:CG2	2.51	0.40
1:B:455:LEU:HA	1:B:456:PRO:HD2	1.80	0.40
1:B:625:VAL:HG11	1:B:628:ASN:ND2	2.36	0.40
1:D:1035:LEU:HA	1:D:1036:PRO:HD2	1.81	0.40
1:D:1198:LEU:HD23	1:D:1356:LEU:HD22	2.01	0.40
1:S:1085:SER:O	1:S:1089:ALA:HB2	2.21	0.40
1:S:1218:PHE:HA	1:S:1219:PRO:HD3	1.86	0.40
1:B:1060:PRO:HG3	1:B:1128:MET:HB3	2.04	0.40
1:D:1333:VAL:CG1	1:D:1334:ASN:N	2.84	0.40
1:D:457:LEU:O	1:D:458:ARG:HG3	2.21	0.40
1:S:1273:MET:HB3	1:S:1273:MET:HE2	2.00	0.40
1:S:1440:LYS:HA	1:S:1443:ALA:HB3	2.03	0.40
1:S:477:GLU:O	1:S:478:ILE:C	2.59	0.40
1:U:1008:ARG:HG2	1:U:1008:ARG:H	1.39	0.40
1:U:1031:VAL:HG23	1:U:1032:ALA:N	2.35	0.40
1:U:1035:LEU:HA	1:U:1036:PRO:HD3	1.67	0.40
1:U:1053:LEU:O	1:U:1055:GLU:N	2.54	0.40
1:U:1143:THR:HA	1:U:1365:ARG:NE	2.37	0.40
1:B:1309:ARG:CZ	1:B:1312:ALA:HB2	2.49	0.40
1:B:1383:GLY:O	1:B:1425:ILE:HD11	2.21	0.40
1:B:585:GLU:CG	1:B:585:GLU:O	2.69	0.40
1:D:557:TYR:N	1:D:557:TYR:HD1	2.18	0.40
1:D:549:GLN:HG2	1:D:573:PRO:CG	2.52	0.40
1:U:1030:ILE:HG22	1:U:1343:PRO:HG3	2.04	0.40
1:U:427:GLU:HA	1:U:501:HIS:CG	2.56	0.40
1:U:571:PRO:O	1:U:572:THR:C	2.58	0.40
3:V:13:DC:C5	3:V:14:DT:C7	3.04	0.40
1:B:1160:LEU:CD1	1:B:1160:LEU:N	2.85	0.40
1:D:443:THR:HG22	1:D:454:ILE:HD11	2.04	0.40
1:S:1086:ILE:O	1:S:1089:ALA:HB3	2.21	0.40
1:S:1245:SER:CB	1:S:1263:GLU:O	2.69	0.40
1:S:1264:ILE:HB	1:S:1265:PRO:CD	2.50	0.40
1:S:1274:ILE:HD11	1:S:1294:ASP:OD2	2.21	0.40
1:U:537:VAL:O	1:U:606:VAL:HG23	2.21	0.40
3:W:4:DC:C2'	3:W:5:DG:O5'	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:GLU:HA	1:B:1004:LEU:CB	2.49	0.40
1:B:1100:ARG:NH1	1:B:1485:ARG:CZ	2.84	0.40
1:B:1218:PHE:N	1:B:1218:PHE:CD2	2.89	0.40
1:B:1326:PRO:C	1:B:1328:GLN:N	2.75	0.40
1:B:1448:LEU:HD23	1:B:1448:LEU:HA	1.89	0.40
1:B:430:GLU:HA	1:B:500:TYR:HB3	2.04	0.40
1:B:637:ALA:O	1:B:638:VAL:HG23	2.21	0.40
1:S:1169:ALA:N	1:S:1191:LEU:HD11	2.37	0.40
1:S:1322:TYR:HB3	1:S:1328:GLN:HB2	2.03	0.40
1:S:511:VAL:HG21	1:S:1028:SER:OG	2.22	0.40
1:S:630:ARG:NH1	1:S:634:GLU:OE2	2.51	0.40
1:U:1049:ILE:O	1:U:1053:LEU:HG	2.21	0.40
4:W:1020[A]:RXV:H202	4:W:1020[A]:RXV:H132	1.80	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	B	716/726 (99%)	596 (83%)	102 (14%)	18 (2%)	5	34
1	D	717/726 (99%)	599 (84%)	97 (14%)	21 (3%)	4	31
1	S	716/726 (99%)	598 (84%)	95 (13%)	23 (3%)	4	29
1	U	715/726 (98%)	607 (85%)	86 (12%)	22 (3%)	4	30
All	All	2864/2904 (99%)	2400 (84%)	380 (13%)	84 (3%)	4	31

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	ARG
1	B	644	PHE

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Mol	Chain	Res	Type
1	B	1004	LEU
1	B	1005	PRO
1	B	1007	SER
1	B	1162	ALA
1	D	637	ALA
1	D	1002	ALA
1	D	1008	ARG
1	D	1162	ALA
1	D	1335	MET
1	D	1418	SER
1	S	644	PHE
1	S	1003	GLU
1	S	1006	GLN
1	S	1007	SER
1	S	1008	ARG
1	S	1327	LEU
1	U	570	ASN
1	U	574	LYS
1	U	1002	ALA
1	U	1004	LEU
1	U	1008	ARG
1	U	1114	ASP
1	U	1391	ILE
1	B	463	ASN
1	B	1149	ASN
1	D	581	LYS
1	D	593	GLU
1	D	1007	SER
1	S	482	ILE
1	S	574	LYS
1	S	1033	ARG
1	S	1221	ALA
1	S	1326	PRO
1	S	1481	GLY
1	U	490	GLY
1	U	508	ASP
1	U	577	ILE
1	U	1054	ASN
1	U	1124	THR
1	D	1120	ALA
1	D	1266	PHE
1	S	417	LYS

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Mol	Chain	Res	Type
1	S	1004	LEU
1	S	1138	ASP
1	S	1416	LYS
1	U	552	GLN
1	U	1056	GLN
1	U	1118	ALA
1	U	1176	ALA
1	B	578	ALA
1	B	638	VAL
1	B	1063	SER
1	B	1221	ALA
1	B	1236	THR
1	D	638	VAL
1	S	643	ASP
1	U	643	ASP
1	U	1009	ILE
1	B	574	LYS
1	B	1033	ARG
1	B	1171	GLY
1	D	508	ASP
1	D	574	LYS
1	D	1033	ARG
1	D	1416	LYS
1	S	550	GLY
1	S	1063	SER
1	S	1325	THR
1	U	1221	ALA
1	D	1161	PRO
1	S	1080	PRO
1	U	1005	PRO
1	U	1074	VAL
1	B	1157	PRO
1	U	542	PRO
1	B	1219	PRO
1	D	570	ASN
1	D	573	PRO
1	D	1004	LEU
1	S	573	PRO
1	D	572	THR
1	S	505	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	B	611/624 (98%)	543 (89%)	68 (11%)	6 28
1	D	610/624 (98%)	541 (89%)	69 (11%)	6 27
1	S	611/624 (98%)	531 (87%)	80 (13%)	4 21
1	U	611/624 (98%)	539 (88%)	72 (12%)	5 25
All	All	2443/2496 (98%)	2154 (88%)	289 (12%)	5 25

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	438	SER
1	B	443	THR
1	B	447	ARG
1	B	461	ILE
1	B	462	LEU
1	B	464	VAL
1	B	468	ARG
1	B	471	ARG
1	B	489	ILE
1	B	492	ASP
1	B	560	ARG
1	B	575	TRP
1	B	576	SER
1	B	577	ILE
1	B	581	LYS
1	B	593	GLU
1	B	597	ASN
1	B	609	GLU
1	B	620	MET
1	B	635	ASP
1	B	1006	GLN
1	B	1007	SER
1	B	1012	ARG
1	B	1015	THR

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Mol	Chain	Res	Type
1	B	1016	SER
1	B	1045	VAL
1	B	1059	THR
1	B	1067	SER
1	B	1074	VAL
1	B	1107	GLN
1	B	1121	MET
1	B	1122	ARG
1	B	1141	LYS
1	B	1160	LEU
1	B	1177	VAL
1	B	1181	THR
1	B	1206	ILE
1	B	1224	ILE
1	B	1232	ARG
1	B	1236	THR
1	B	1245	SER
1	B	1256	ARG
1	B	1260	VAL
1	B	1262	THR
1	B	1299	ARG
1	B	1300	THR
1	B	1302	VAL
1	B	1306	ILE
1	B	1327	LEU
1	B	1329	THR
1	B	1331	PHE
1	B	1334	ASN
1	B	1338	LEU
1	B	1345	LEU
1	B	1348	LEU
1	B	1350	GLU
1	B	1368	GLN
1	B	1384	LEU
1	B	1388	LEU
1	B	1404	ASP
1	B	1415	PHE
1	B	1423	GLN
1	B	1457	THR
1	B	1462	GLU
1	B	1465	LEU
1	B	1466	LEU

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Mol	Chain	Res	Type
1	B	1474	THR
1	B	1489	GLN
1	D	418	LEU
1	D	423	SER
1	D	430	GLU
1	D	450	ARG
1	D	462	LEU
1	D	472	ILE
1	D	474	ASN
1	D	476	ASN
1	D	495	LEU
1	D	497	LYS
1	D	501	HIS
1	D	516	ILE
1	D	555	TYR
1	D	556	VAL
1	D	557	TYR
1	D	576	SER
1	D	577	ILE
1	D	590	GLN
1	D	591	LEU
1	D	617	THR
1	D	622	MET
1	D	625	VAL
1	D	636	ASN
1	D	638	VAL
1	D	1013	ASN
1	D	1015	THR
1	D	1045	VAL
1	D	1050	LEU
1	D	1055	GLU
1	D	1059	THR
1	D	1067	SER
1	D	1083	ASP
1	D	1085	SER
1	D	1092	ARG
1	D	1122	ARG
1	D	1137	ARG
1	D	1139	ILE
1	D	1151	ASP
1	D	1206	ILE
1	D	1213	ILE

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Mol	Chain	Res	Type
1	D	1224	ILE
1	D	1228	SER
1	D	1238	ARG
1	D	1248	VAL
1	D	1249	ILE
1	D	1268	VAL
1	D	1270	LYS
1	D	1272	ARG
1	D	1280	LEU
1	D	1289	ILE
1	D	1294	ASP
1	D	1307	ASP
1	D	1308	VAL
1	D	1327	LEU
1	D	1329	THR
1	D	1334	ASN
1	D	1344	LYS
1	D	1365	ARG
1	D	1373	LYS
1	D	1392	ASP
1	D	1411	LEU
1	D	1420	LYS
1	D	1429	ARG
1	D	1438	ARG
1	D	1441	ILE
1	D	1455	LEU
1	D	1468	LEU
1	D	1475	GLU
1	D	1485	ARG
1	S	418	LEU
1	S	425	SER
1	S	427	GLU
1	S	445	SER
1	S	449	SER
1	S	450	ARG
1	S	451	THR
1	S	461	ILE
1	S	462	LEU
1	S	464	VAL
1	S	474	ASN
1	S	480	GLN
1	S	495	LEU

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Mol	Chain	Res	Type
1	S	499	ARG
1	S	511	VAL
1	S	518	THR
1	S	529	ARG
1	S	547	LEU
1	S	553	LYS
1	S	554	TYR
1	S	560	ARG
1	S	567	SER
1	S	577	ILE
1	S	597	ASN
1	S	600	HIS
1	S	604	LEU
1	S	608	LEU
1	S	617	THR
1	S	638	VAL
1	S	642	LEU
1	S	643	ASP
1	S	644	PHE
1	S	1008	ARG
1	S	1012	ARG
1	S	1014	ILE
1	S	1015	THR
1	S	1024	ASP
1	S	1050	LEU
1	S	1058	MET
1	S	1073	ASP
1	S	1092	ARG
1	S	1093	MET
1	S	1107	GLN
1	S	1132	THR
1	S	1150	TYR
1	S	1154	GLU
1	S	1156	GLU
1	S	1168	LEU
1	S	1188	LEU
1	S	1220	THR
1	S	1245	SER
1	S	1248	VAL
1	S	1251	GLU
1	S	1261	VAL
1	S	1273	MET

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Mol	Chain	Res	Type
1	S	1299	ARG
1	S	1304	VAL
1	S	1306	ILE
1	S	1323	LYS
1	S	1330	SER
1	S	1334	ASN
1	S	1339	VAL
1	S	1368	GLN
1	S	1385	ARG
1	S	1392	ASP
1	S	1402	ASP
1	S	1403	THR
1	S	1408	MET
1	S	1425	ILE
1	S	1428	MET
1	S	1431	ARG
1	S	1434	THR
1	S	1440	LYS
1	S	1448	LEU
1	S	1449	LEU
1	S	1457	THR
1	S	1468	LEU
1	S	1476	ILE
1	S	1488	ILE
1	S	1490	LEU
1	U	418	LEU
1	U	430	GLU
1	U	450	ARG
1	U	452	GLN
1	U	457	LEU
1	U	458	ARG
1	U	462	LEU
1	U	473	LEU
1	U	495	LEU
1	U	526	ARG
1	U	531	LEU
1	U	532	ILE
1	U	547	LEU
1	U	567	SER
1	U	569	LEU
1	U	583	LEU
1	U	592	TRP

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Mol	Chain	Res	Type
1	U	599	GLU
1	U	613	GLU
1	U	625	VAL
1	U	1008	ARG
1	U	1012	ARG
1	U	1021	SER
1	U	1024	ASP
1	U	1044	PRO
1	U	1050	LEU
1	U	1058	MET
1	U	1059	THR
1	U	1061	ASP
1	U	1062	LYS
1	U	1063	SER
1	U	1069	ARG
1	U	1083	ASP
1	U	1090	MET
1	U	1122	ARG
1	U	1131	ILE
1	U	1132	THR
1	U	1133	LEU
1	U	1138	ASP
1	U	1139	ILE
1	U	1141	LYS
1	U	1147	ILE
1	U	1159	VAL
1	U	1167	LEU
1	U	1203	ASP
1	U	1225	LEU
1	U	1241	ILE
1	U	1248	VAL
1	U	1252	ARG
1	U	1259	ILE
1	U	1262	THR
1	U	1272	ARG
1	U	1292	LEU
1	U	1304	VAL
1	U	1305	VAL
1	U	1306	ILE
1	U	1328	GLN
1	U	1334	ASN
1	U	1356	LEU

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Mol	Chain	Res	Type
1	U	1367	THR
1	U	1396	SER
1	U	1400	GLU
1	U	1404	ASP
1	U	1411	LEU
1	U	1425	ILE
1	U	1432	ARG
1	U	1438	ARG
1	U	1452	ILE
1	U	1466	LEU
1	U	1468	LEU
1	U	1486	THR
1	U	1488	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	474	ASN
1	B	501	HIS
1	B	515	HIS
1	B	549	GLN
1	B	597	ASN
1	B	605	GLN
1	B	636	ASN
1	B	1010	ASN
1	B	1046	HIS
1	B	1081	HIS
1	B	1334	ASN
1	B	1354	HIS
1	B	1368	GLN
1	B	1423	GLN
1	D	476	ASN
1	D	605	GLN
1	D	1013	ASN
1	D	1046	HIS
1	D	1079	HIS
1	D	1081	HIS
1	D	1095	GLN
1	D	1201	ASN
1	D	1359	GLN
1	D	1368	GLN
1	S	474	ASN

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Mol	Chain	Res	Type
1	S	501	HIS
1	S	597	ASN
1	S	600	HIS
1	S	605	GLN
1	S	1056	GLN
1	S	1081	HIS
1	S	1107	GLN
1	S	1109	ASN
1	S	1187	ASN
1	S	1334	ASN
1	S	1368	GLN
1	S	1412	GLN
1	S	1450	ASN
1	U	476	ASN
1	U	587	ASN
1	U	600	HIS
1	U	616	GLN
1	U	1013	ASN
1	U	1081	HIS
1	U	1313	ASN
1	U	1334	ASN
1	U	1358	HIS
1	U	1368	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	5UA	F	1	-	18,23,23	2.71	2 (11%)	18,33,33	2.76	4 (22%)
2	5UA	E	1	-	18,23,23	2.73	2 (11%)	18,33,33	2.79	4 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5UA	F	1	-	-	1/3/21/21	0/3/3/3
2	5UA	E	1	-	-	2/3/21/21	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	5UA	C2-N3	8.92	1.46	1.32
2	F	1	5UA	C2-N3	8.78	1.46	1.32
2	F	1	5UA	C2-N1	6.74	1.46	1.33
2	E	1	5UA	C2-N1	6.67	1.46	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	5UA	N3-C2-N1	-9.39	114.00	128.68
2	E	1	5UA	N3-C2-N1	-9.11	114.44	128.68
2	E	1	5UA	C5'-O5'-C6'	5.51	122.71	117.46
2	F	1	5UA	C5'-O5'-C6'	4.64	121.88	117.46
2	F	1	5UA	C4-C5-N7	-3.39	105.86	109.40
2	E	1	5UA	C4-C5-N7	-3.37	105.88	109.40
2	F	1	5UA	C2-N1-C6	3.14	124.12	118.75
2	E	1	5UA	C2-N1-C6	2.91	123.73	118.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	5UA	C3'-C4'-C5'-O5'
2	E	1	5UA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	F	1	5UA	C4'-C5'-O5'-C6'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	5UA	2	0
2	E	1	5UA	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	RXV	E	1021[B]	-	36,37,37	2.47	5 (13%)	45,51,51	1.86	13 (28%)
4	RXV	W	1020[A]	-	36,37,37	2.38	5 (13%)	45,51,51	1.61	10 (22%)
4	RXV	E	1021[A]	-	36,37,37	2.55	5 (13%)	45,51,51	3.03	16 (35%)
4	RXV	W	1020[B]	-	36,37,37	2.27	6 (16%)	45,51,51	1.98	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RXV	E	1021[B]	-	-	3/14/30/30	0/5/5/5
4	RXV	W	1020[A]	-	-	6/14/30/30	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RXV	E	1021[A]	-	-	6/14/30/30	0/5/5/5
4	RXV	W	1020[B]	-	-	6/14/30/30	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1021[A]	RXV	C9-C10	-11.77	1.26	1.44
4	E	1021[B]	RXV	C9-C10	-10.10	1.29	1.44
4	W	1020[B]	RXV	C9-C10	-9.68	1.29	1.44
4	W	1020[A]	RXV	C9-C10	-9.46	1.30	1.44
4	W	1020[A]	RXV	C25-S26	-7.10	1.68	1.76
4	E	1021[B]	RXV	C8-C9	-6.76	1.31	1.40
4	W	1020[B]	RXV	C25-S26	-6.74	1.69	1.76
4	E	1021[B]	RXV	C25-S26	-6.35	1.69	1.76
4	E	1021[A]	RXV	C25-S26	-5.87	1.70	1.76
4	W	1020[A]	RXV	C8-C9	-5.26	1.33	1.40
4	E	1021[A]	RXV	C9-C12	-4.72	1.35	1.41
4	E	1021[A]	RXV	C8-N7	3.23	1.37	1.31
4	E	1021[A]	RXV	C8-C9	2.83	1.44	1.40
4	W	1020[B]	RXV	C8-N7	2.79	1.36	1.31
4	W	1020[B]	RXV	C12-C32	-2.60	1.38	1.43
4	E	1021[B]	RXV	C33-C32	-2.44	1.37	1.42
4	E	1021[B]	RXV	C12-C32	-2.27	1.39	1.43
4	W	1020[B]	RXV	C29-C25	-2.22	1.36	1.40
4	W	1020[B]	RXV	C33-C32	-2.18	1.37	1.42
4	W	1020[A]	RXV	C13-C12	2.11	1.55	1.52
4	W	1020[A]	RXV	C29-C25	-2.07	1.36	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1021[A]	RXV	C9-C8-N7	-12.15	116.65	125.68
4	E	1021[B]	RXV	C22-N21-C18	7.31	124.60	114.14
4	W	1020[B]	RXV	C9-C8-N7	-7.22	120.31	125.68
4	E	1021[A]	RXV	C8-N7-C6	6.23	124.41	116.91
4	E	1021[A]	RXV	C9-C10-N11	-6.00	167.99	177.88
4	E	1021[A]	RXV	C22-N21-C18	5.39	121.85	114.14
4	W	1020[B]	RXV	C22-N21-C18	5.09	121.41	114.14
4	W	1020[B]	RXV	C9-C10-N11	-4.99	169.66	177.88
4	E	1021[A]	RXV	C32-C6-N7	-4.86	117.65	122.83
4	E	1021[A]	RXV	C4-C5-C6	-4.68	114.95	120.84
4	E	1021[A]	RXV	C5-C6-C32	4.14	123.87	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	1020[A]	RXV	C8-N7-C6	3.98	121.70	116.91
4	E	1021[B]	RXV	C27-O28-C29	3.46	113.45	106.68
4	E	1021[A]	RXV	C27-O28-C29	3.38	113.29	106.68
4	W	1020[A]	RXV	C27-O28-C29	3.36	113.25	106.68
4	E	1021[A]	RXV	C30-N31-C23	3.33	122.10	117.82
4	W	1020[A]	RXV	C9-C8-N7	-3.31	123.22	125.68
4	W	1020[B]	RXV	C27-O28-C29	3.30	113.14	106.68
4	W	1020[A]	RXV	C32-C6-N7	-3.23	119.39	122.83
4	E	1021[B]	RXV	C32-C6-N7	-3.16	119.46	122.83
4	E	1021[A]	RXV	C5-C4-C3	3.03	124.24	120.17
4	E	1021[B]	RXV	C30-N31-C23	2.98	121.64	117.82
4	W	1020[B]	RXV	C30-N31-C23	2.92	121.57	117.82
4	W	1020[A]	RXV	C22-N21-C18	2.71	118.02	114.14
4	W	1020[A]	RXV	C22-C23-N31	2.69	121.47	116.20
4	E	1021[A]	RXV	C13-C12-C32	2.61	123.79	119.36
4	W	1020[A]	RXV	C30-N31-C23	2.58	121.13	117.82
4	E	1021[A]	RXV	C12-C32-C6	2.58	121.37	118.31
4	E	1021[B]	RXV	C13-C14-N15	-2.55	104.21	114.38
4	W	1020[A]	RXV	C29-C30-N31	-2.52	118.80	122.66
4	W	1020[B]	RXV	C29-C30-N31	-2.51	118.81	122.66
4	W	1020[B]	RXV	C17-C16-N15	-2.49	107.25	111.11
4	E	1021[A]	RXV	C29-C30-N31	-2.48	118.85	122.66
4	E	1021[B]	RXV	O2-C3-C33	-2.37	117.96	124.43
4	E	1021[B]	RXV	C9-C12-C32	-2.31	117.44	119.42
4	W	1020[B]	RXV	C8-N7-C6	2.30	119.68	116.91
4	E	1021[B]	RXV	C29-C30-N31	-2.26	119.20	122.66
4	E	1021[A]	RXV	C8-C9-C10	2.22	123.72	119.10
4	E	1021[A]	RXV	C4-C3-C33	-2.21	117.84	120.81
4	W	1020[A]	RXV	O2-C3-C33	-2.19	118.45	124.43
4	E	1021[B]	RXV	C22-C23-N31	2.17	120.46	116.20
4	E	1021[B]	RXV	C8-N7-C6	2.15	119.50	116.91
4	E	1021[B]	RXV	C14-N15-C20	-2.14	105.75	111.23
4	E	1021[B]	RXV	C9-C10-N11	-2.14	174.36	177.88
4	E	1021[B]	RXV	C13-C12-C32	2.13	122.99	119.36
4	E	1021[A]	RXV	C19-C20-N15	-2.02	107.97	111.11
4	W	1020[A]	RXV	C9-C12-C32	-2.02	117.68	119.42

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	W	1020[A]	RXV	N11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	W	1020[A]	RXV	C9-C12-C13-C14
4	E	1021[A]	RXV	C9-C12-C13-C14
4	E	1021[A]	RXV	C19-C18-N21-C22
4	W	1020[B]	RXV	C9-C12-C13-C14
4	W	1020[B]	RXV	C19-C18-N21-C22
4	E	1021[A]	RXV	C13-C14-N15-C16
4	W	1020[A]	RXV	C13-C14-N15-C20
4	E	1021[B]	RXV	C23-C22-N21-C18
4	E	1021[B]	RXV	C13-C14-N15-C20
4	E	1021[A]	RXV	C23-C22-N21-C18
4	E	1021[A]	RXV	C13-C14-N15-C20
4	W	1020[A]	RXV	C13-C14-N15-C16
4	E	1021[A]	RXV	C32-C12-C13-C14
4	W	1020[B]	RXV	C32-C12-C13-C14
4	W	1020[B]	RXV	C23-C22-N21-C18
4	W	1020[A]	RXV	N11-C10-C9-C12
4	W	1020[A]	RXV	C19-C18-N21-C22
4	W	1020[B]	RXV	C17-C18-N21-C22
4	E	1021[B]	RXV	N11-C10-C9-C8
4	W	1020[B]	RXV	N21-C22-C23-N31

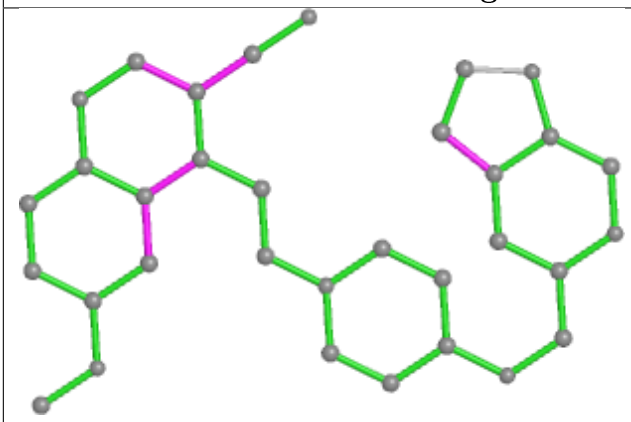
There are no ring outliers.

4 monomers are involved in 21 short contacts:

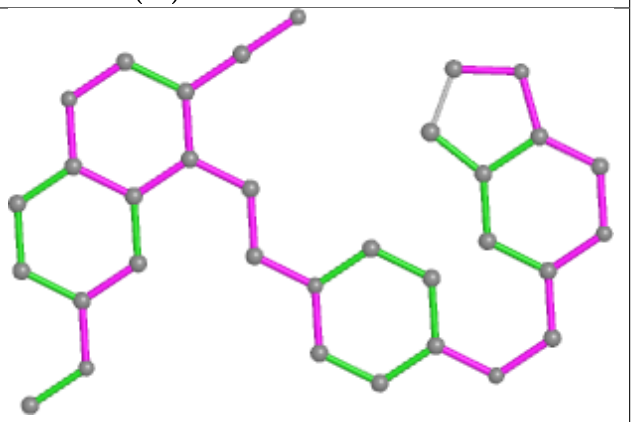
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1021[B]	RXV	4	0
4	W	1020[A]	RXV	7	0
4	E	1021[A]	RXV	5	0
4	W	1020[B]	RXV	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

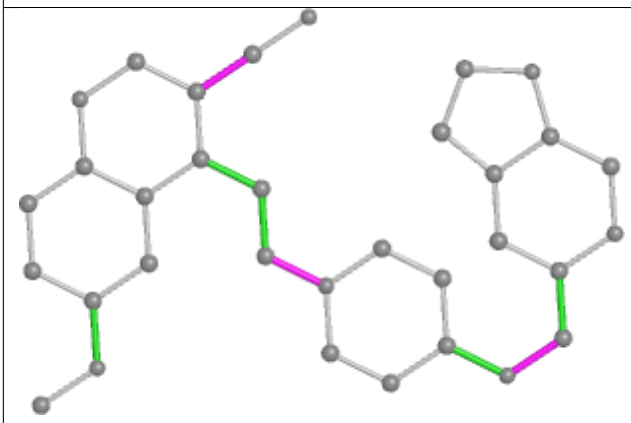
Ligand RXV E 1021 (B)



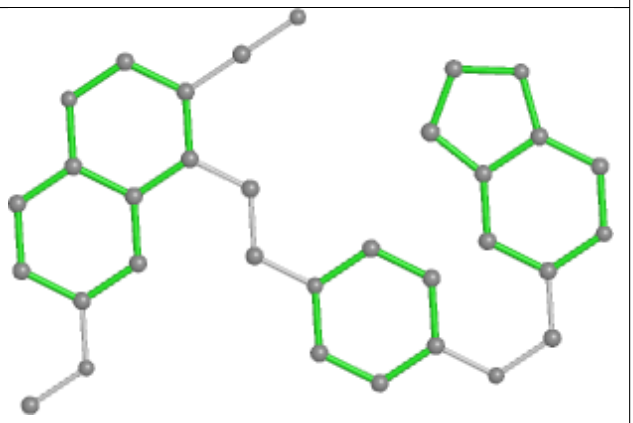
Bond lengths



Bond angles

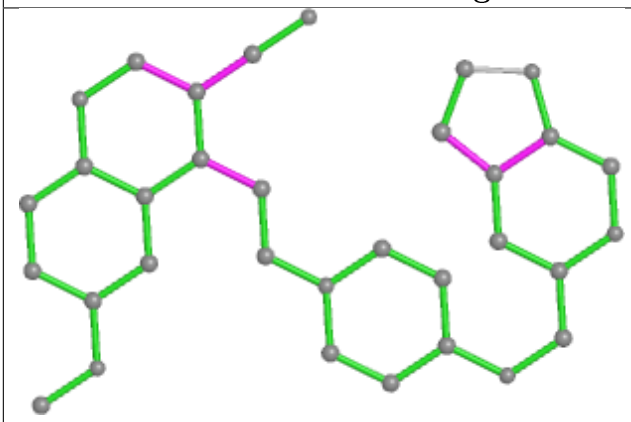


Torsions

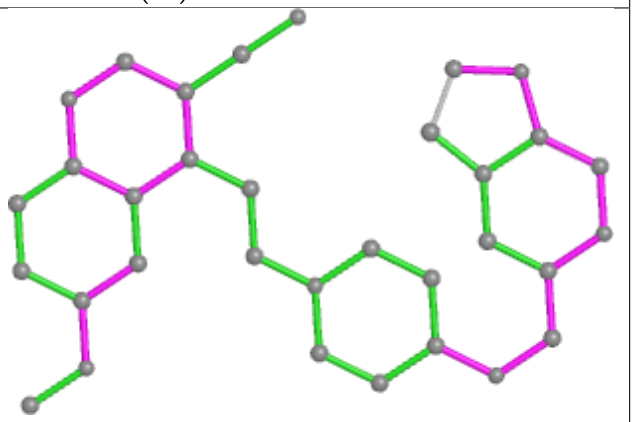


Rings

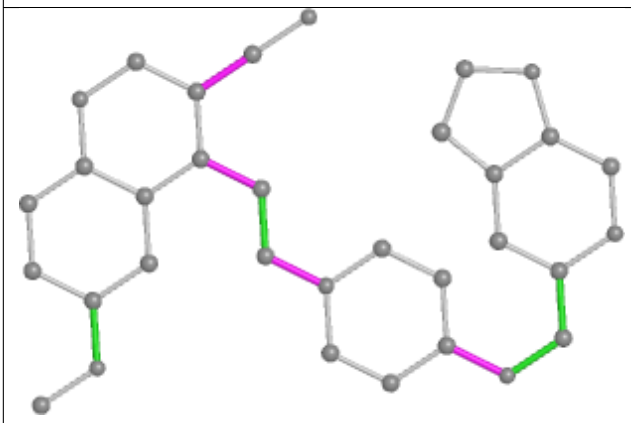
Ligand RXV W 1020 (A)



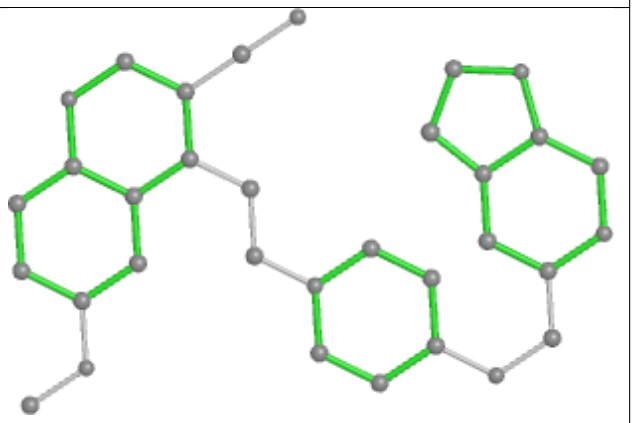
Bond lengths



Bond angles

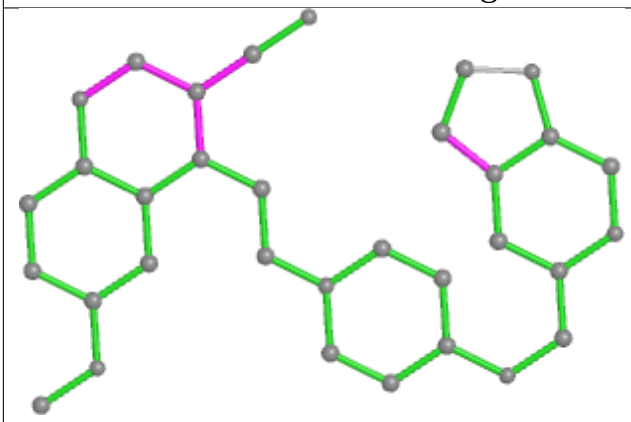


Torsions

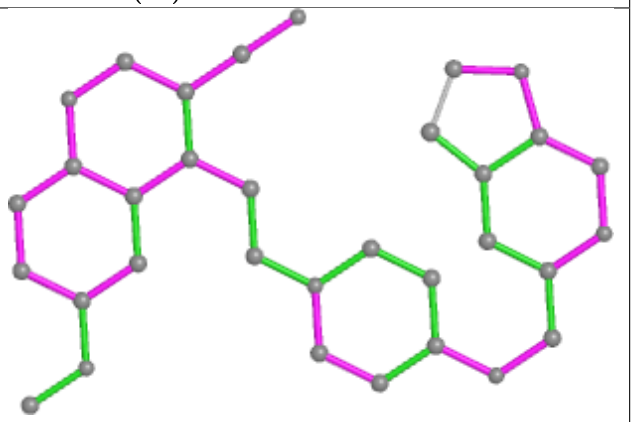


Rings

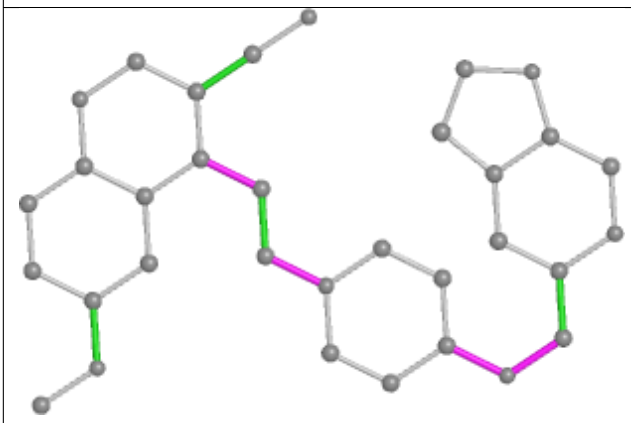
Ligand RXV E 1021 (A)



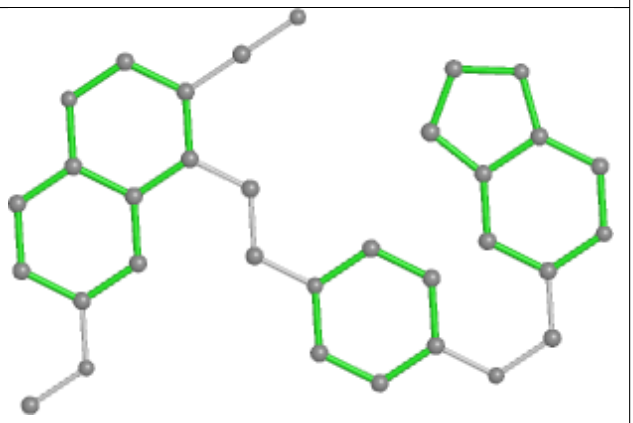
Bond lengths



Bond angles

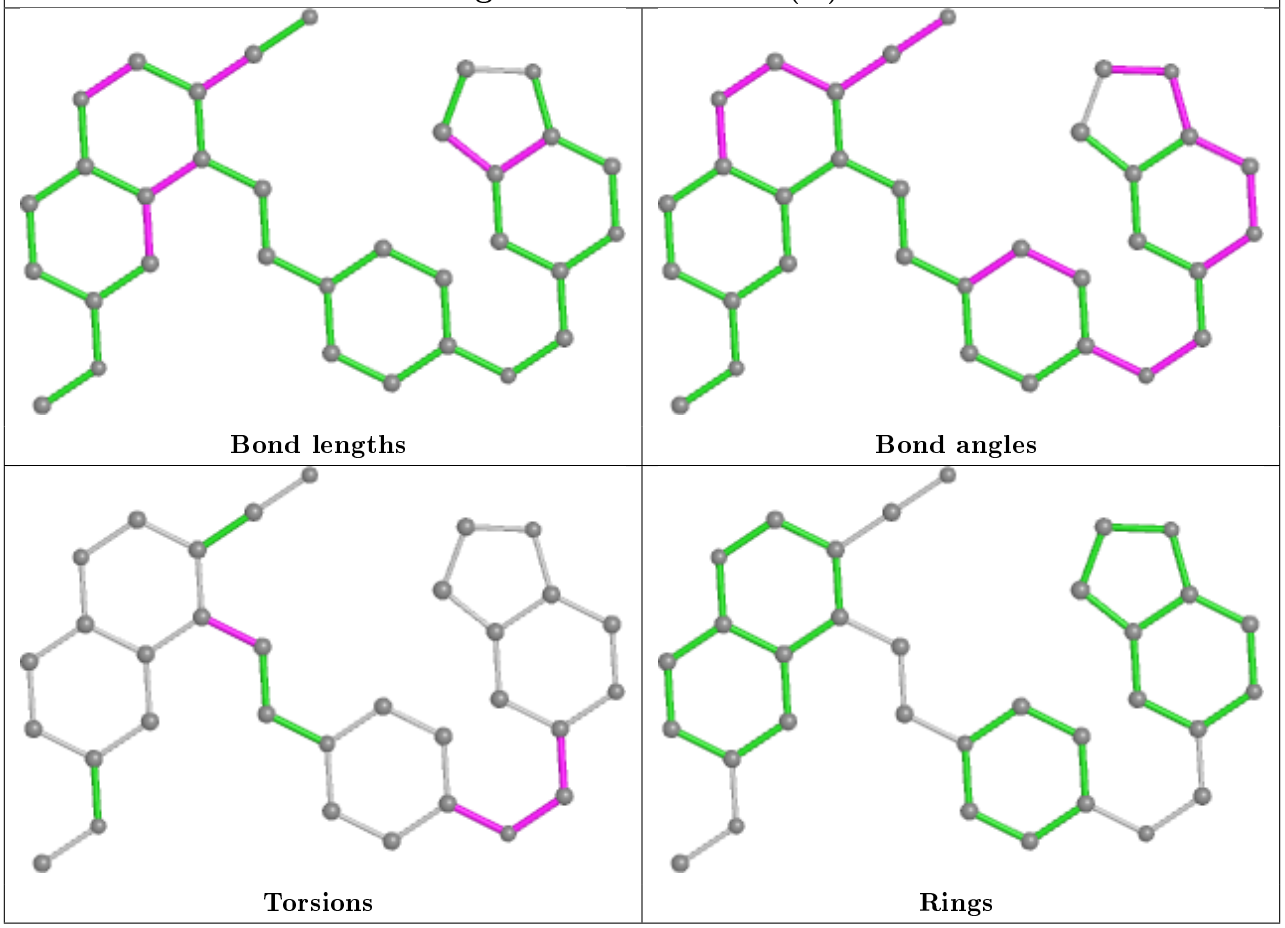


Torsions



Rings

Ligand RXV W 1020 (B)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1:5UA	O3'	2:DG	P	3.52
1	F	1:5UA	O3'	2:DG	P	3.24

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, 95^{th} 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	B	718/726 (98%)	-0.67	2 (0%) 94 91	78, 126, 188, 218	0
1	D	719/726 (99%)	-0.68	0 100 100	63, 111, 184, 221	0
1	S	718/726 (98%)	-0.73	0 100 100	64, 116, 171, 203	0
1	U	717/726 (98%)	-0.72	1 (0%) 95 95	64, 123, 171, 222	0
2	E	19/20 (95%)	-0.48	0 100 100	103, 115, 196, 218	0
2	F	19/20 (95%)	-0.53	0 100 100	97, 112, 188, 193	0
3	V	20/20 (100%)	-0.33	0 100 100	91, 116, 209, 268	0
3	W	18/20 (90%)	-0.43	0 100 100	100, 119, 173, 202	0
All	All	2948/2984 (98%)	-0.69	3 (0%) 95 95	63, 120, 181, 268	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1254	GLY	2.6
1	B	1255	GLY	2.3
1	U	1254	GLY	2.1

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

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	5UA	F	1	21/21	0.89	0.42	220,235,239,241	0
2	5UA	E	1	21/21	0.89	0.29	193,198,206,208	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

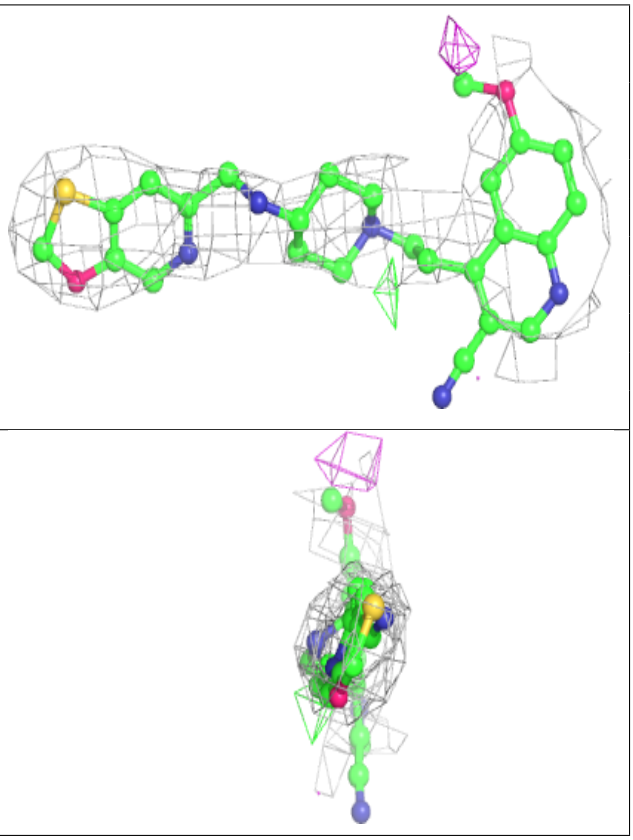
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	RXV	E	1021[B]	33/33	0.88	0.29	110,128,143,146	33
4	RXV	E	1021[A]	33/33	0.88	0.29	111,129,144,148	33
4	RXV	W	1020[A]	33/33	0.94	0.20	100,108,111,111	33
4	RXV	W	1020[B]	33/33	0.94	0.20	100,108,110,110	33

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

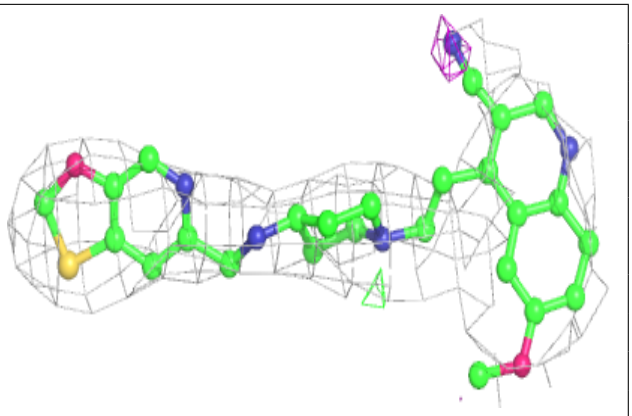
Electron density around RXV E 1021 (B):

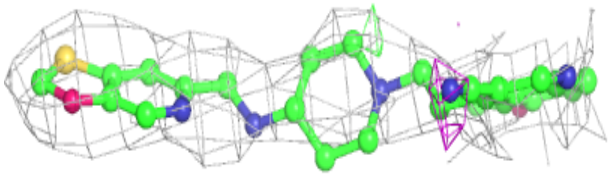
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

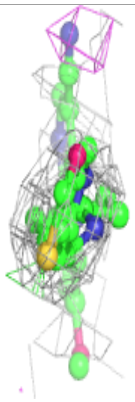


Electron density around RXV E 1021 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

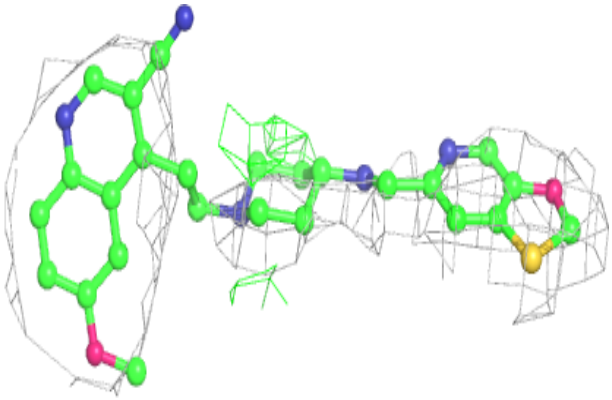


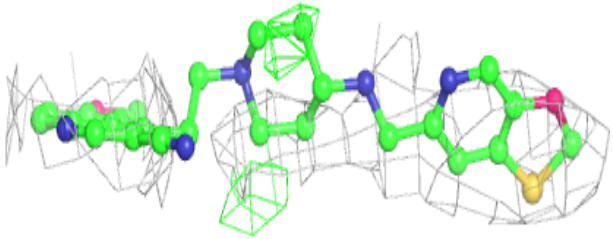


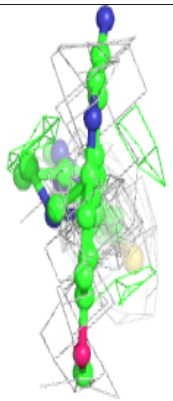


Electron density around RXV W 1020 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

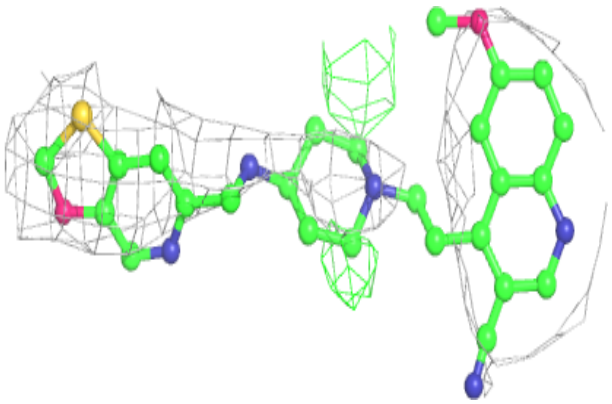


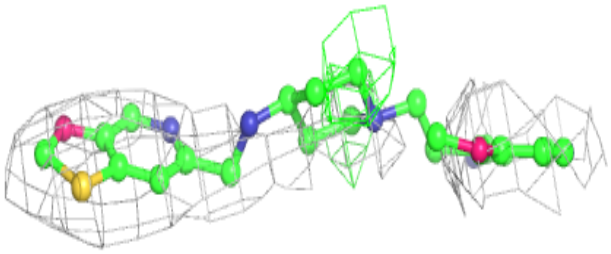


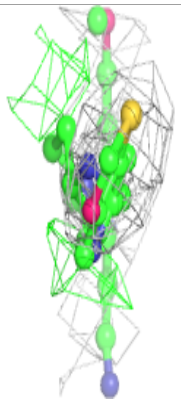


Electron density around RXV W 1020 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.