



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 06:49 PM EDT

PDB ID : 2IS1  
Title : Crystal structure of UvrD-DNA-SO4 complex  
Authors : Yang, W.; Lee, J.Y.  
Deposited on : unknown  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

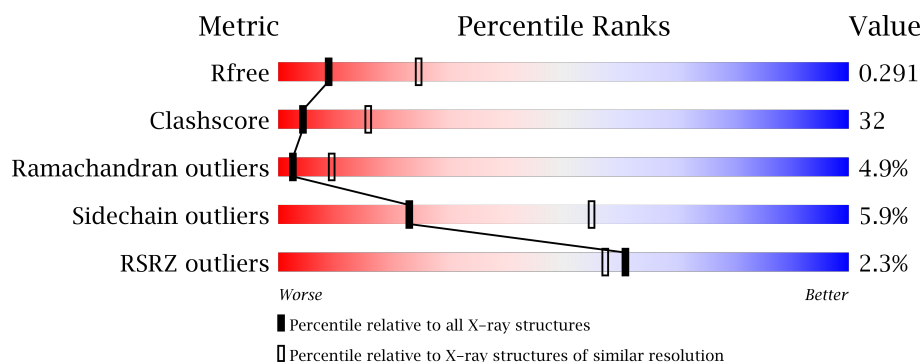
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	17	<div> <div>6%</div> <div>18% 65% 12% 6%</div> </div>
1	E	17	<div> <div>24% 65% 12%</div> </div>
2	D	10	<div> <div>10% 90%</div> </div>
2	F	10	<div> <div>20% 80%</div> </div>
3	A	680	<div> <div>56% 37% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	680	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	686	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10896 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 DNA chain called 5'-D(\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	16	Total	C	N	O	P	0	0	0
			323	157	50	101	15			
1	E	15	Total	C	N	O	P	0	0	0
			300	147	48	92	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	0	0	0
			201	96	39	57	9			
2	F	10	Total	C	N	O	P	0	0	0
			200	96	39	56	9			

- Molecule 3 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	649	Total	C	N	O	S	0	0	0
			5058	3175	920	940	23			
3	B	624	Total	C	N	O	S	0	0	0
			4727	2967	848	889	23			

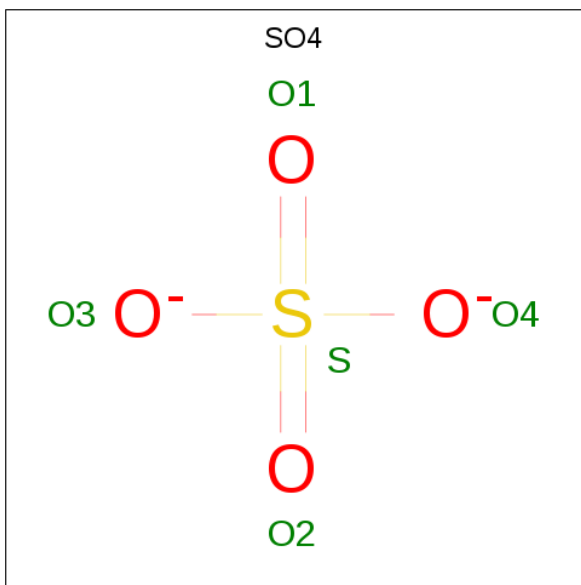
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	ENGINEERED	UNP P03018
B	399	VAL	ALA	ENGINEERED	UNP P03018

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Hg 2 2	0	0
4	A	3	Total Hg 3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	40	Total	O	0	0
			40	40		
7	B	15	Total	O	0	0
			15	15		

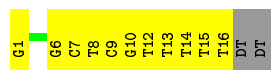
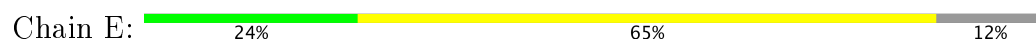
### 3 Residue-property plots [i](#)

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.

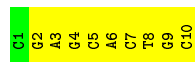
- Molecule 1: 5'-D(\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3',



- Molecule 1: 5'-D(\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3',



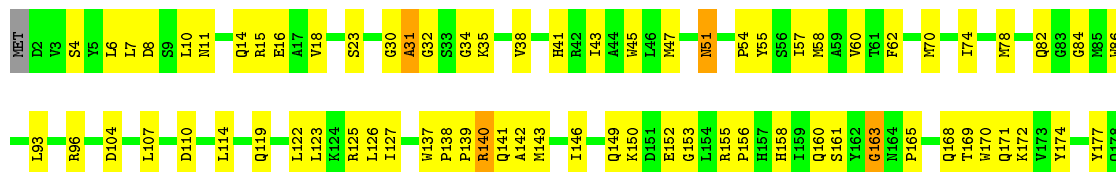
- Molecule 2: 5'-D(\*CP\*GP\*AP\*GP\*CP\*AP\*CP\*TP\*GP\*C)-3'

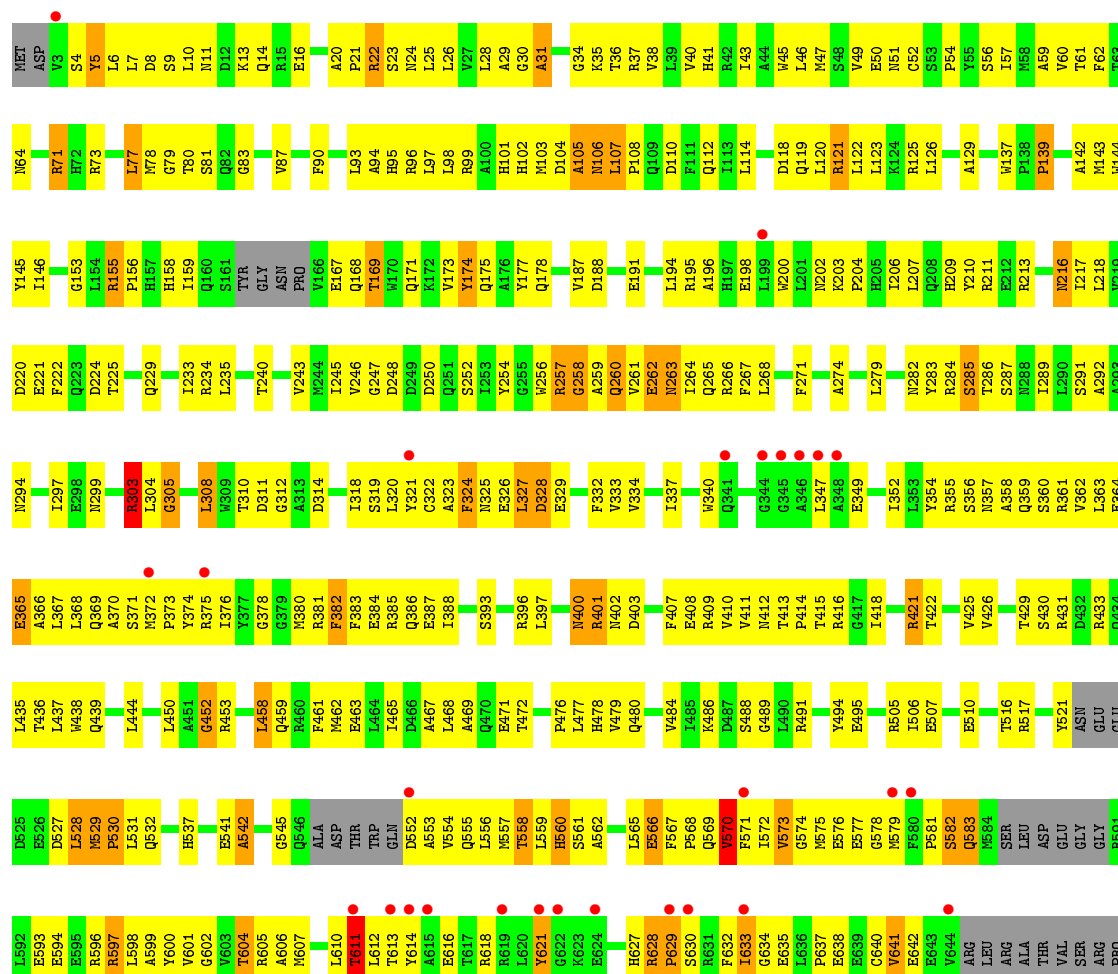


- Molecule 2: 5'-D(\*CP\*GP\*AP\*GP\*CP\*AP\*CP\*TP\*GP\*C)-3'



- Molecule 3: DNA helicase II







VAL
SER
HIS
GLN
ARG
MET
GLY
THR
PRO
MET
VAL
GLU
ASN
ASP
SER
GLY
TYR
LYS
LEU
GLY
GLN
ARG
VAL
ARG
HIS
ALA
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.45Å 94.49Å 136.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.76 – 2.90 47.62 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.76-2.90) 92.3 (47.62-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.236 , 0.295 0.233 , 0.291	Depositor DCC
$R_{free}$ test set	4334 reflections (11.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, HG

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	C	0.63	0/359	0.99	3/553 (0.5%)
1	E	0.47	0/333	0.76	0/511
2	D	0.42	0/225	0.68	0/345
2	F	0.40	0/224	0.68	0/343
3	A	0.44	0/5153	0.68	1/6979 (0.0%)
3	B	0.43	0/4811	0.66	1/6529 (0.0%)
All	All	0.45	0/11105	0.68	5/15260 (0.0%)

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	C	1	0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	DT	O5'-P-OP1	-6.12	100.19	105.70
3	B	105	ALA	N-CA-C	-5.92	95.01	111.00
1	C	11	DT	O4'-C1'-N1	5.55	111.88	108.00
3	A	653	PRO	N-CA-CB	5.40	109.78	103.30
1	C	11	DT	N1-C1'-C2'	5.19	122.47	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	11	DT	C1'

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	323	0	186	21	0
1	E	300	0	176	20	0
2	D	201	0	113	15	0
2	F	200	0	111	11	0
3	A	5058	0	4857	220	0
3	B	4727	0	4410	384	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	A	10	0	0	2	0
5	B	5	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	2	0
7	A	40	0	0	0	0
7	B	15	0	0	0	0
All	All	10896	0	9869	662	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 32.

All (662) 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:E:12:DT:H3'	1:E:13:DT:C5'	1.70	1.21
1:E:12:DT:C3'	1:E:13:DT:H5''	1.75	1.17
1:C:11:DT:H3'	1:C:12:DT:C5'	1.72	1.16
1:C:11:DT:C3'	1:C:12:DT:H5''	1.75	1.15
3:A:23:SER:HA	3:A:242:LYS:HD2	1.15	1.10
3:A:140:ARG:HH11	3:A:140:ARG:HB2	1.21	1.06
2:F:6:DA:H2''	2:F:7:DC:H5'	1.36	1.03
3:B:155:ARG:HB3	3:B:156:PRO:HD2	1.37	1.02
3:B:367:LEU:HD13	3:B:374:TYR:HB3	1.44	0.99
3:B:217:ILE:HB	3:B:243:VAL:HG12	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:326:GLU:OE1	3:A:618:ARG:HA	1.65	0.96
3:A:140:ARG:HB2	3:A:140:ARG:NH1	1.81	0.95
3:A:287:SER:HB3	3:A:314:ASP:HA	1.46	0.95
3:B:472:THR:HG23	3:B:480:GLN:HE21	1.34	0.93
1:E:13:DT:H2''	1:E:14:DT:H5'	1.51	0.93
3:B:282:ASN:HD21	3:B:285:SER:H	1.16	0.92
3:B:468:LEU:O	3:B:472:THR:HG22	1.68	0.91
1:E:12:DT:H3'	1:E:13:DT:H5''	0.92	0.91
1:C:14:DT:H2''	1:C:15:DT:OP2	1.71	0.90
3:B:576:GLU:HA	3:B:630:SER:N	1.88	0.89
3:A:23:SER:HA	3:A:242:LYS:CD	2.02	0.88
3:B:575:MET:HB3	3:B:614:TYR:HB3	1.54	0.87
3:B:299:ASN:ND2	3:B:635:GLU:HG2	1.88	0.87
3:B:310:THR:HG22	3:B:312:GLY:H	1.39	0.87
3:B:318:ILE:HG12	3:B:641:VAL:HA	1.56	0.86
1:C:3:DA:H2''	1:C:4:DG:H5''	1.57	0.86
1:C:9:DC:H2''	1:C:10:DG:C8	2.10	0.86
2:D:2:DG:H2''	2:D:3:DA:N7	1.91	0.86
1:E:9:DC:H2''	1:E:10:DG:C8	2.12	0.85
3:A:47:MET:HE1	3:A:54:PRO:HB3	1.59	0.84
3:B:632:PHE:HA	3:B:635:GLU:OE2	1.78	0.82
3:B:155:ARG:HB3	3:B:156:PRO:CD	2.10	0.81
3:B:382:PHE:O	3:B:385:ARG:HG2	1.80	0.81
3:B:34:GLY:HA2	6:B:684:GOL:H32	1.63	0.81
3:A:155:ARG:H	3:A:158:HIS:HD2	1.27	0.80
3:B:572:ILE:HB	3:B:612:LEU:HD22	1.62	0.80
3:B:633:ILE:HG12	3:B:633:ILE:O	1.81	0.80
3:B:477:LEU:HG	3:B:516:THR:HG23	1.63	0.80
3:B:36:THR:HB	3:B:73:ARG:HH12	1.46	0.80
3:B:22:ARG:NH2	3:B:52:CYS:SG	2.52	0.79
3:B:292:ALA:HA	3:B:637:PRO:HD2	1.63	0.79
3:B:299:ASN:HD21	3:B:635:GLU:HG2	1.45	0.78
3:B:5:TYR:HD2	3:B:5:TYR:H	1.31	0.78
3:A:217:ILE:HB	3:A:243:VAL:HG12	1.65	0.78
3:B:396:ARG:HD2	3:B:403:ASP:OD2	1.84	0.78
3:B:322:CYS:HA	3:B:614:TYR:O	1.84	0.77
3:B:95:HIS:CE1	3:B:99:ARG:HE	2.01	0.77
3:A:155:ARG:HB3	3:A:156:PRO:HD2	1.64	0.77
1:C:12:DT:H2''	1:C:13:DT:O5'	1.85	0.77
3:A:468:LEU:O	3:A:472:THR:HG22	1.85	0.76
3:B:110:ASP:OD1	3:B:532:GLN:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:31:ALA:HB2	3:B:308:LEU:HD13	1.65	0.76
3:B:153:GLY:HA2	3:B:194:LEU:HD11	1.67	0.75
3:A:194:LEU:O	3:A:198:GLU:HG3	1.86	0.75
3:B:472:THR:CG2	3:B:480:GLN:HE21	2.00	0.74
3:B:292:ALA:HA	3:B:637:PRO:CD	2.17	0.74
3:B:252:SER:OG	3:B:261:VAL:HG22	1.87	0.74
3:B:47:MET:HE3	3:B:57:ILE:HD12	1.68	0.74
3:B:297:ILE:HG12	3:B:303:ARG:HH21	1.53	0.74
3:B:402:ASN:HB3	3:B:436:THR:HG21	1.70	0.74
3:A:55:TYR:HA	3:A:84:GLY:O	1.88	0.74
3:A:321:TYR:CE2	3:A:323:ALA:HB2	2.23	0.73
3:B:245:ILE:O	3:B:245:ILE:HG13	1.87	0.73
3:A:10:LEU:HD13	3:A:18:VAL:HG21	1.69	0.73
3:A:35:LYS:HE2	3:A:221:GLU:OE2	1.87	0.73
3:B:638:GLU:CD	3:B:638:GLU:H	1.92	0.73
3:B:287:SER:HB2	3:B:314:ASP:HA	1.71	0.72
3:A:631:ARG:HG3	3:A:635:GLU:OE2	1.89	0.72
3:A:114:LEU:HD11	3:A:186:LEU:HD13	1.71	0.72
3:A:155:ARG:H	3:A:158:HIS:CD2	2.06	0.71
3:B:320:LEU:HD22	3:B:633:ILE:HD11	1.71	0.71
3:A:467:ALA:O	3:A:471:GLU:HG3	1.91	0.71
1:C:9:DC:H2''	1:C:10:DG:N7	2.05	0.71
3:A:599:ALA:O	3:A:603:VAL:HG23	1.92	0.70
3:B:354:TYR:O	3:B:558:THR:HA	1.91	0.70
3:B:333:VAL:O	3:B:337:ILE:HG13	1.91	0.70
3:B:11:ASN:CG	3:B:14:GLN:HG3	2.11	0.70
3:B:562:ALA:O	3:B:565:LEU:HD12	1.91	0.70
3:B:621:TYR:HD1	3:B:621:TYR:O	1.75	0.69
3:B:400:ASN:ND2	3:B:402:ASN:H	1.91	0.69
3:B:537:HIS:NE2	3:B:541:GLU:HG3	2.07	0.69
3:A:86:TRP:CH2	3:A:96:ARG:HD3	2.28	0.69
2:D:4:DG:H1'	2:D:5:DC:H5'	1.72	0.69
3:A:23:SER:CA	3:A:242:LYS:HD2	2.08	0.69
1:E:6:DG:OP1	1:E:6:DG:H4'	1.93	0.69
3:A:637:PRO:HB2	3:A:640:CYS:SG	2.33	0.68
3:A:114:LEU:HD13	3:A:186:LEU:HB3	1.76	0.68
3:B:11:ASN:OD1	3:B:14:GLN:HG3	1.93	0.68
1:C:3:DA:C2'	1:C:4:DG:H5''	2.24	0.68
3:B:575:MET:HB2	3:B:613:THR:O	1.93	0.67
3:A:78:MET:CE	3:A:82:GLN:HE21	2.07	0.67
3:B:112:GLN:CD	3:B:396:ARG:HD3	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:DA:C2'	2:F:7:DC:H5'	2.18	0.67
1:E:8:DT:C2'	1:E:9:DC:H5''	2.24	0.67
3:B:477:LEU:HG	3:B:516:THR:CG2	2.25	0.67
3:B:347:LEU:HB3	3:B:554:VAL:HG23	1.77	0.67
3:B:355:ARG:HG3	3:B:355:ARG:HH11	1.60	0.66
3:B:494:TYR:C	3:B:506:ILE:HD11	2.15	0.66
3:B:308:LEU:HD11	3:B:600:TYR:OH	1.95	0.66
3:B:637:PRO:HG2	3:B:640:CYS:SG	2.36	0.66
3:A:60:VAL:HG22	3:A:93:LEU:HD12	1.78	0.66
3:A:78:MET:HE2	3:A:82:GLN:HE21	1.60	0.66
3:B:575:MET:CE	3:B:612:LEU:HD13	2.26	0.66
3:B:601:VAL:O	3:B:605:ARG:HG2	1.95	0.66
3:A:477:LEU:HD23	3:A:516:THR:HG23	1.78	0.65
3:B:203:LYS:HB2	3:B:206:ILE:HD11	1.79	0.65
3:A:374:TYR:HA	3:A:553:ALA:HB1	1.78	0.65
3:B:326:GLU:HB3	3:B:618:ARG:HA	1.78	0.65
3:B:637:PRO:CG	3:B:640:CYS:SG	2.84	0.65
3:B:575:MET:HG2	3:B:612:LEU:HB3	1.78	0.65
3:B:386:GLN:HG2	3:B:505:ARG:NH1	2.12	0.65
2:D:6:DA:H2''	2:D:7:DC:O5'	1.94	0.65
3:B:155:ARG:HB2	3:B:158:HIS:CD2	2.32	0.65
3:A:169:THR:O	3:A:172:LYS:HB2	1.97	0.64
3:A:325:ASN:HD21	3:A:327:LEU:HD12	1.62	0.64
1:C:3:DA:H2''	1:C:4:DG:C5'	2.28	0.64
3:B:268:LEU:HD23	3:B:274:ALA:HB1	1.78	0.64
3:B:11:ASN:HB3	3:B:283:TYR:OH	1.98	0.64
3:B:334:VAL:HG13	3:B:372:MET:CE	2.27	0.64
3:A:282:ASN:HB3	3:A:290:LEU:HD11	1.80	0.64
3:B:380:MET:HG3	3:B:385:ARG:NH1	2.13	0.64
3:B:421:ARG:O	3:B:425:VAL:HG23	1.98	0.64
3:B:153:GLY:HA2	3:B:194:LEU:CD1	2.29	0.63
3:B:31:ALA:CB	3:B:308:LEU:HD13	2.29	0.63
3:B:367:LEU:HD13	3:B:374:TYR:CB	2.25	0.63
2:D:8:DT:H2''	2:D:9:DG:C8	2.32	0.63
3:B:581:PRO:HD3	3:B:632:PHE:CE2	2.34	0.63
3:A:480:GLN:O	3:A:484:VAL:HG23	1.99	0.63
3:A:442:ARG:O	3:A:446:GLN:HG3	1.99	0.62
3:A:494:TYR:CE2	3:A:505:ARG:HD3	2.34	0.62
3:B:297:ILE:CG1	3:B:303:ARG:HH21	2.11	0.62
3:A:472:THR:CG2	3:A:480:GLN:HE21	2.12	0.62
3:B:146:ILE:HG23	3:B:174:TYR:CD1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:521:TYR:CB	3:B:528:LEU:HD11	2.30	0.62
3:B:36:THR:O	3:B:40:VAL:HG13	2.00	0.62
3:B:234:ARG:HH11	3:B:234:ARG:HG3	1.63	0.62
3:A:321:TYR:HE2	3:A:323:ALA:HB2	1.64	0.62
3:B:491:ARG:O	3:B:495:GLU:HB2	1.99	0.62
1:E:6:DG:H2'	1:E:7:DC:C5	2.34	0.62
3:B:467:ALA:O	3:B:471:GLU:HG3	2.00	0.62
3:B:383:PHE:HD1	3:B:542:ALA:HA	1.65	0.62
3:B:570:VAL:HG11	3:B:606:ALA:HA	1.81	0.62
3:A:645:ARG:HG3	3:A:646:LEU:N	2.15	0.62
1:E:14:DT:P	3:B:558:THR:HG21	2.39	0.62
3:A:11:ASN:O	3:A:15:ARG:HG3	2.00	0.61
3:B:101:HIS:HB3	3:B:104:ASP:OD2	1.99	0.61
1:E:8:DT:C3'	1:E:9:DC:H5''	2.30	0.61
1:C:12:DT:H2''	1:C:13:DT:C5'	2.29	0.61
3:A:481:THR:O	3:A:485:ILE:HG13	2.00	0.61
3:A:562:ALA:HA	3:A:565:LEU:HD12	1.83	0.61
3:B:506:ILE:O	3:B:510:GLU:HG3	2.01	0.61
3:B:320:LEU:HD22	3:B:633:ILE:CD1	2.30	0.61
3:B:570:VAL:O	3:B:570:VAL:HG22	2.00	0.61
3:A:327:LEU:HD23	3:A:362:VAL:HG13	1.82	0.61
1:C:10:DG:H5''	1:C:10:DG:H8	1.65	0.61
3:A:364:GLU:CD	3:A:376:ILE:HD11	2.22	0.60
3:A:573:VAL:CG1	3:A:574:GLY:N	2.63	0.60
3:B:155:ARG:HB2	3:B:158:HIS:HD2	1.64	0.60
3:B:282:ASN:HD21	3:B:285:SER:N	1.94	0.60
3:B:560:HIS:C	3:B:562:ALA:H	2.04	0.60
3:A:152:GLU:OE1	3:A:227:ASN:ND2	2.34	0.60
3:A:226:ASN:OD1	3:A:229:GLN:HG3	2.01	0.60
3:B:541:GLU:O	3:B:542:ALA:HB2	2.02	0.60
3:A:138:PRO:HG2	3:A:141:GLN:CB	2.31	0.60
3:B:250:ASP:O	3:B:597:ARG:HD2	2.00	0.60
3:B:263:ASN:HA	3:B:266:ARG:HB3	1.83	0.60
3:B:468:LEU:HD22	3:B:484:VAL:HG22	1.81	0.60
3:B:598:LEU:O	3:B:602:GLY:N	2.35	0.60
3:A:82:GLN:HA	3:A:82:GLN:OE1	2.02	0.60
3:B:323:ALA:HB1	3:B:328:ASP:HB3	1.83	0.60
3:B:284:ARG:HG3	3:B:566:GLU:OE1	2.02	0.60
3:B:594:GLU:HA	3:B:597:ARG:HG3	1.83	0.60
3:A:196:ALA:O	3:A:199:LEU:HB3	2.01	0.60
3:B:35:LYS:HB2	3:B:246:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:334:VAL:HG13	3:B:372:MET:HE1	1.84	0.60
3:B:200:TRP:HB3	3:B:207:LEU:HD22	1.84	0.60
3:A:374:TYR:CA	3:A:553:ALA:HB1	2.30	0.59
3:B:22:ARG:HG3	3:B:50:GLU:OE1	2.01	0.59
3:A:262:GLU:O	3:A:264:ILE:N	2.34	0.59
3:A:355:ARG:HD3	3:A:580:PHE:CD2	2.37	0.59
3:B:355:ARG:NH1	3:B:355:ARG:HG3	2.16	0.59
2:D:8:DT:OP1	2:D:8:DT:H4'	2.02	0.59
3:A:575:MET:HB3	3:A:633:ILE:HD11	1.83	0.59
3:A:568:PRO:N	3:A:607:MET:HE3	2.17	0.59
2:F:2:DG:H2"	2:F:3:DA:C8	2.37	0.59
3:B:287:SER:CB	3:B:314:ASP:HA	2.32	0.59
3:B:337:ILE:O	3:B:340:TRP:HB3	2.03	0.59
3:B:472:THR:HG23	3:B:480:GLN:NE2	2.11	0.58
3:A:416:ARG:HG3	3:A:418:ILE:HD13	1.84	0.58
3:A:491:ARG:O	3:A:495:GLU:HB2	2.02	0.58
3:B:381:ARG:HB3	3:B:542:ALA:HB1	1.85	0.58
3:B:303:ARG:NH1	3:B:305:GLY:HA2	2.18	0.58
3:B:77:LEU:O	3:B:78:MET:HG2	2.02	0.58
3:A:150:LYS:C	3:A:152:GLU:H	2.07	0.58
3:A:477:LEU:CD2	3:A:516:THR:HG23	2.33	0.58
3:A:639:GLU:H	3:A:639:GLU:CD	2.06	0.58
3:A:218:LEU:HD23	3:A:244:MET:HE2	1.84	0.58
3:B:572:ILE:HB	3:B:612:LEU:CD2	2.33	0.58
3:B:630:SER:O	3:B:633:ILE:CG2	2.52	0.58
3:B:347:LEU:HB3	3:B:554:VAL:CG2	2.33	0.58
3:A:537:HIS:ND1	3:A:541:GLU:HG3	2.19	0.58
3:B:222:PHE:O	3:B:225:THR:HG23	2.04	0.58
3:A:522:ASN:O	3:A:526:GLU:N	2.37	0.57
3:B:386:GLN:HG2	3:B:505:ARG:HH12	1.68	0.57
3:B:146:ILE:HG23	3:B:174:TYR:HD1	1.69	0.57
3:B:125:ARG:HD2	3:B:408:GLU:CD	2.25	0.57
3:B:422:THR:O	3:B:426:VAL:HG23	2.04	0.57
3:B:632:PHE:C	3:B:634:GLY:H	2.08	0.57
3:A:10:LEU:CD1	3:A:18:VAL:HG21	2.34	0.57
3:B:429:THR:O	3:B:433:ARG:HG2	2.04	0.57
3:A:300:ASN:OD1	3:A:596:ARG:HD2	2.05	0.57
3:B:321:TYR:HB3	3:B:613:THR:HG22	1.86	0.57
3:B:575:MET:SD	3:B:612:LEU:HD13	2.45	0.57
3:B:621:TYR:CD1	3:B:621:TYR:O	2.57	0.57
1:C:11:DT:H3'	1:C:12:DT:H5"	0.80	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:LYS:O	3:B:206:ILE:HG12	2.05	0.57
3:B:436:THR:OG1	3:B:439:GLN:HG3	2.04	0.57
3:B:478:HIS:CG	3:B:517:ARG:HG3	2.40	0.57
2:F:5:DC:H2"	2:F:6:DA:C8	2.40	0.57
3:A:325:ASN:HA	3:A:617:THR:O	2.05	0.57
3:B:597:ARG:O	3:B:601:VAL:HG23	2.05	0.57
1:E:9:DC:H2"	1:E:10:DG:N7	2.19	0.57
3:A:187:VAL:HG13	3:A:191:GLU:CG	2.35	0.56
3:A:292:ALA:HB1	3:A:636:LEU:HD22	1.86	0.56
3:A:381:ARG:CB	3:A:542:ALA:HB1	2.34	0.56
1:E:8:DT:H2"	1:E:9:DC:H5"	1.86	0.56
3:A:70:MET:O	3:A:74:ILE:HG13	2.04	0.56
3:B:282:ASN:ND2	3:B:285:SER:H	1.97	0.56
3:B:637:PRO:HG2	3:B:640:CYS:HB2	1.85	0.56
3:B:71:ARG:HH11	3:B:71:ARG:HG2	1.69	0.56
2:D:2:DG:H2"	2:D:3:DA:C8	2.39	0.56
3:A:320:LEU:HG	3:A:641:VAL:HG13	1.87	0.56
3:B:630:SER:HB3	3:B:633:ILE:HG22	1.87	0.56
3:B:187:VAL:HG13	3:B:191:GLU:CG	2.35	0.56
3:A:31:ALA:H	3:A:308:LEU:HD21	1.70	0.56
3:A:355:ARG:HH11	3:A:355:ARG:HG3	1.70	0.56
3:A:625:VAL:HG12	3:A:626:TYR:N	2.20	0.56
3:B:284:ARG:NH1	3:B:566:GLU:HB3	2.21	0.56
3:B:367:LEU:HB3	3:B:372:MET:O	2.05	0.56
3:B:119:GLN:NE2	3:B:143:MET:HG3	2.20	0.56
3:A:284:ARG:HG3	3:A:284:ARG:HH11	1.70	0.56
3:A:329:GLU:CD	3:A:573:VAL:HG13	2.26	0.56
3:A:297:ILE:HB	3:A:600:TYR:CD1	2.40	0.56
3:B:254:TYR:O	3:B:259:ALA:HB3	2.05	0.56
3:B:107:LEU:HB2	3:B:108:PRO:HD2	1.88	0.56
3:A:601:VAL:O	3:A:605:ARG:HG2	2.06	0.56
3:B:593:GLU:O	3:B:597:ARG:HG2	2.05	0.56
3:A:284:ARG:HG3	3:A:566:GLU:OE1	2.06	0.56
3:B:79:GLY:O	3:B:80:THR:C	2.43	0.55
3:A:305:GLY:O	3:A:306:LYS:HB3	2.05	0.55
3:A:296:LEU:HD11	3:A:596:ARG:HG3	1.86	0.55
3:B:47:MET:CE	3:B:54:PRO:HA	2.36	0.55
3:B:310:THR:HG22	3:B:311:ASP:N	2.21	0.55
3:A:248:ASP:CG	3:A:306:LYS:HZ3	2.10	0.55
3:B:191:GLU:OE2	3:B:195:ARG:HD3	2.06	0.55
3:A:38:VAL:HG21	3:A:279:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:575:MET:O	3:B:614:TYR:CB	2.55	0.55
3:B:188:ASP:OD1	3:B:191:GLU:HB2	2.06	0.55
3:B:23:SER:O	3:B:25:LEU:HG	2.06	0.55
3:A:127:ILE:HD12	3:A:139:PRO:HG3	1.88	0.55
3:B:47:MET:HE3	3:B:57:ILE:CD1	2.37	0.55
3:A:472:THR:HG23	3:A:480:GLN:HE21	1.71	0.55
3:B:352:ILE:O	3:B:556:LEU:HA	2.06	0.54
3:A:438:TRP:CE2	3:A:462:MET:HE2	2.42	0.54
3:B:234:ARG:NH1	3:B:234:ARG:HG3	2.21	0.54
3:B:355:ARG:HH12	3:B:560:HIS:HE1	1.53	0.54
3:B:367:LEU:HD23	3:B:372:MET:CE	2.38	0.54
3:A:385:ARG:HH11	3:A:385:ARG:HG2	1.72	0.54
3:B:575:MET:O	3:B:614:TYR:HB3	2.07	0.54
3:B:529:MET:O	3:B:531:LEU:N	2.41	0.54
3:A:327:LEU:HD23	3:A:362:VAL:CG1	2.37	0.54
1:E:16:DT:OP1	3:B:64:ASN:N	2.28	0.54
3:A:401:ARG:HH12	3:A:469:ALA:CB	2.20	0.54
3:B:477:LEU:CG	3:B:516:THR:HG23	2.35	0.54
1:C:15:DT:H2''	1:C:16:DT:O5'	2.07	0.54
1:C:15:DT:H3'	1:C:15:DT:OP1	2.08	0.54
3:B:507:GLU:HA	3:B:510:GLU:OE1	2.08	0.53
3:A:184:ALA:HB1	3:A:402:ASN:O	2.08	0.53
3:A:568:PRO:CD	3:A:607:MET:HE3	2.38	0.53
3:B:400:ASN:C	3:B:400:ASN:HD22	2.11	0.53
3:B:401:ARG:HH22	3:B:469:ALA:CB	2.21	0.53
3:B:202:ASN:O	3:B:204:PRO:HD3	2.08	0.53
3:B:560:HIS:O	3:B:562:ALA:N	2.42	0.53
3:B:159:ILE:HG13	3:B:171:GLN:HG3	1.90	0.53
3:B:142:ALA:O	3:B:146:ILE:HG13	2.09	0.53
3:B:36:THR:HB	3:B:73:ARG:NH1	2.21	0.53
3:B:411:VAL:HA	3:B:461:PHE:CZ	2.44	0.53
3:B:376:ILE:N	3:B:376:ILE:HD12	2.23	0.53
1:E:12:DT:C2'	1:E:13:DT:H5''	2.39	0.53
3:B:364:GLU:HA	3:B:367:LEU:HD12	1.91	0.53
3:B:381:ARG:HB2	3:B:384:GLU:OE2	2.08	0.52
3:B:30:GLY:O	3:B:31:ALA:O	2.27	0.52
2:F:9:DG:H5''	3:A:419:GLY:H	1.74	0.52
3:B:102:HIS:O	3:B:105:ALA:O	2.28	0.52
3:B:194:LEU:O	3:B:198:GLU:HG3	2.09	0.52
3:B:229:GLN:O	3:B:233:ILE:HG13	2.09	0.52
3:A:477:LEU:HG	3:A:516:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:110:ASP:CG	3:A:532:GLN:HG2	2.30	0.52
3:A:477:LEU:CG	3:A:516:THR:HG23	2.40	0.52
3:B:349:GLU:HB3	3:B:568:PRO:HD2	1.92	0.52
3:B:452:GLY:O	3:B:453:ARG:C	2.48	0.52
3:A:245:ILE:HG13	3:A:245:ILE:O	2.08	0.52
3:B:224:ASP:HA	3:B:259:ALA:HB1	1.91	0.52
3:B:412:ASN:ND2	3:B:416:ARG:H	2.08	0.52
3:B:576:GLU:HA	3:B:630:SER:H	1.68	0.52
1:E:13:DT:OP2	3:B:357:ASN:HB2	2.09	0.51
3:B:114:LEU:HD22	3:B:118:ASP:HB3	1.93	0.51
3:B:596:ARG:O	3:B:599:ALA:N	2.43	0.51
3:B:202:ASN:C	3:B:204:PRO:HD3	2.30	0.51
3:B:334:VAL:O	3:B:337:ILE:N	2.42	0.51
3:B:393:SER:OG	3:B:409:ARG:HD3	2.10	0.51
3:A:163:GLY:O	3:A:165:PRO:HD3	2.11	0.51
3:B:188:ASP:O	3:B:191:GLU:HB3	2.10	0.51
3:B:630:SER:O	3:B:633:ILE:HG23	2.10	0.51
3:B:494:TYR:O	3:B:506:ILE:HD11	2.10	0.51
3:B:90:PHE:CZ	3:B:233:ILE:HD11	2.46	0.51
3:B:107:LEU:CB	3:B:108:PRO:HD2	2.41	0.51
3:B:21:PRO:O	3:B:22:ARG:C	2.49	0.51
3:A:47:MET:HE3	3:A:54:PRO:HD3	1.92	0.51
3:B:47:MET:SD	3:B:78:MET:CE	2.99	0.51
3:B:329:GLU:OE2	3:B:573:VAL:HG22	2.12	0.50
3:A:11:ASN:OD1	3:A:14:GLN:HG3	2.10	0.50
3:B:633:ILE:CG1	3:B:633:ILE:O	2.58	0.50
3:A:605:ARG:NH2	5:A:684:SO4:O1	2.45	0.50
3:A:644:VAL:HG12	3:A:645:ARG:N	2.26	0.50
3:B:282:ASN:ND2	3:B:284:ARG:H	2.09	0.50
3:B:385:ARG:HG3	3:B:388:ILE:HD12	1.94	0.50
3:B:347:LEU:HD12	3:B:552:ASP:O	2.11	0.50
3:B:218:LEU:HD12	3:B:218:LEU:N	2.27	0.50
3:B:367:LEU:HD23	3:B:372:MET:HE3	1.94	0.50
3:A:122:LEU:O	3:A:126:LEU:HG	2.12	0.50
3:B:260:GLN:HE21	3:B:260:GLN:CA	2.25	0.50
3:B:416:ARG:HG3	3:B:418:ILE:HD12	1.94	0.50
3:B:178:GLN:NE2	3:B:178:GLN:HA	2.26	0.50
3:B:95:HIS:HE1	3:B:99:ARG:HE	1.58	0.50
3:A:294:ASN:O	3:A:297:ILE:HG22	2.12	0.49
3:A:477:LEU:HG	3:A:516:THR:CG2	2.42	0.49
3:A:110:ASP:CG	3:A:532:GLN:HE21	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:652:ARG:O	3:A:653:PRO:O	2.30	0.49
3:B:120:LEU:HD13	3:B:143:MET:CE	2.43	0.49
3:A:385:ARG:NH1	3:A:385:ARG:HG2	2.26	0.49
3:A:320:LEU:HD13	3:A:633:ILE:CG2	2.43	0.49
3:B:327:LEU:O	3:B:328:ASP:C	2.50	0.49
3:B:597:ARG:O	3:B:600:TYR:HB3	2.12	0.49
1:C:10:DG:H5''	1:C:10:DG:C8	2.47	0.49
3:B:129:ALA:HB1	3:B:431:ARG:CD	2.41	0.49
3:B:322:CYS:SG	3:B:616:GLU:HG2	2.53	0.49
3:A:325:ASN:ND2	3:A:327:LEU:HD12	2.27	0.49
3:A:153:GLY:HA2	3:A:194:LEU:HD13	1.95	0.49
3:B:90:PHE:CD1	3:B:229:GLN:NE2	2.81	0.49
3:B:537:HIS:CE1	3:B:541:GLU:HG3	2.48	0.49
3:A:7:LEU:HD11	3:A:45:TRP:CZ3	2.48	0.49
3:B:571:PHE:CD1	3:B:611:THR:HG23	2.48	0.49
3:A:11:ASN:CG	3:A:14:GLN:HG3	2.33	0.49
3:A:459:GLN:O	3:A:463:GLU:HG3	2.13	0.49
3:A:568:PRO:HA	3:A:607:MET:HB2	1.93	0.49
3:B:45:TRP:O	3:B:47:MET:N	2.45	0.49
3:B:528:LEU:HD23	3:B:529:MET:N	2.28	0.49
3:A:416:ARG:HG3	3:A:418:ILE:CD1	2.42	0.49
3:A:537:HIS:CE1	3:A:541:GLU:HG3	2.48	0.48
3:B:324:PHE:CD2	3:B:325:ASN:OD1	2.66	0.48
3:A:47:MET:CE	3:A:54:PRO:HB3	2.35	0.48
3:B:576:GLU:HA	3:B:630:SER:CA	2.43	0.48
2:F:1:DC:O2	3:B:621:TYR:HB2	2.13	0.48
3:B:299:ASN:CG	3:B:635:GLU:HG2	2.34	0.48
1:E:8:DT:H2''	1:E:9:DC:O4'	2.12	0.48
3:A:410:VAL:HA	3:A:413:THR:HB	1.94	0.48
3:A:575:MET:CB	3:A:633:ILE:HD11	2.43	0.48
3:A:641:VAL:HG12	3:A:642:GLU:N	2.28	0.48
3:B:139:PRO:O	3:B:142:ALA:HB3	2.12	0.48
3:B:358:ALA:O	3:B:360:SER:N	2.41	0.48
3:B:29:ALA:O	3:B:248:ASP:HB2	2.14	0.48
3:B:325:ASN:ND2	3:B:328:ASP:H	2.11	0.48
3:A:494:TYR:CD2	3:A:505:ARG:HD3	2.48	0.48
3:B:566:GLU:HA	3:B:605:ARG:O	2.14	0.48
3:A:4:SER:HB3	3:A:8:ASP:OD2	2.14	0.48
3:B:38:VAL:HG21	3:B:279:LEU:HD11	1.95	0.48
3:B:458:LEU:O	3:B:461:PHE:HB3	2.14	0.48
3:B:554:VAL:O	3:B:554:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:DT:H2''	1:C:6:DG:C8	2.49	0.48
3:A:110:ASP:OD1	3:A:532:GLN:HG2	2.14	0.48
3:A:323:ALA:HB1	3:A:328:ASP:HB3	1.95	0.48
3:A:472:THR:HG23	3:A:480:GLN:NE2	2.28	0.48
3:A:78:MET:CE	3:A:82:GLN:NE2	2.75	0.48
3:B:267:PHE:O	3:B:271:PHE:HD1	1.96	0.48
3:B:354:TYR:HD1	3:B:356:SER:O	1.97	0.48
3:B:557:MET:HG3	3:B:558:THR:O	2.14	0.48
3:B:596:ARG:O	3:B:599:ALA:HB3	2.13	0.48
3:B:637:PRO:HG2	3:B:640:CYS:CB	2.43	0.48
3:A:631:ARG:O	3:A:635:GLU:HG3	2.13	0.47
3:B:528:LEU:HD23	3:B:529:MET:H	1.79	0.47
3:A:521:TYR:O	3:A:522:ASN:CB	2.61	0.47
3:A:60:VAL:HG22	3:A:93:LEU:CD1	2.42	0.47
3:B:47:MET:CE	3:B:54:PRO:HG3	2.44	0.47
3:A:7:LEU:HD11	3:A:45:TRP:CH2	2.48	0.47
3:B:129:ALA:HB1	3:B:431:ARG:HD2	1.96	0.47
3:B:486:LYS:HG3	3:B:491:ARG:NH1	2.30	0.47
3:B:630:SER:O	3:B:633:ILE:HG22	2.14	0.47
3:B:137:TRP:HH2	3:B:169:THR:HG1	1.52	0.47
3:B:310:THR:HG22	3:B:312:GLY:N	2.19	0.47
3:B:325:ASN:ND2	3:B:327:LEU:CB	2.78	0.47
3:B:478:HIS:CD2	3:B:517:ARG:HG3	2.50	0.47
3:B:97:LEU:O	3:B:99:ARG:N	2.47	0.47
2:D:10:DC:H2'	1:E:1:DG:H1'	1.95	0.47
3:A:207:LEU:O	3:A:207:LEU:HD12	2.14	0.47
3:A:472:THR:HG21	3:A:480:GLN:HE21	1.80	0.47
3:A:492:THR:O	3:A:496:GLN:HG2	2.14	0.47
3:B:31:ALA:HB2	3:B:308:LEU:CD1	2.42	0.47
3:B:364:GLU:C	3:B:366:ALA:N	2.67	0.47
3:B:299:ASN:ND2	3:B:635:GLU:CG	2.72	0.47
3:B:360:SER:O	3:B:363:LEU:N	2.37	0.47
3:B:578:GLY:HA2	3:B:582:SER:O	2.15	0.47
3:A:355:ARG:NH1	3:A:355:ARG:HG3	2.30	0.47
3:B:7:LEU:O	3:B:9:SER:N	2.47	0.47
3:A:170:TRP:O	3:A:171:GLN:C	2.53	0.47
3:A:200:TRP:CZ3	3:A:236:LEU:HB2	2.50	0.47
3:A:47:MET:CE	3:A:54:PRO:HD3	2.45	0.47
3:A:641:VAL:CG1	3:A:642:GLU:N	2.77	0.47
3:A:472:THR:OG1	3:A:480:GLN:HG3	2.15	0.47
3:A:590:GLY:C	3:A:592:LEU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:400:ASN:C	3:B:400:ASN:ND2	2.68	0.47
3:B:438:TRP:CE2	3:B:462:MET:HE2	2.49	0.47
3:B:319:SER:HB3	3:B:611:THR:HB	1.97	0.47
1:E:6:DG:H2'	1:E:7:DC:C6	2.50	0.47
3:B:299:ASN:HD21	3:B:635:GLU:CG	2.19	0.47
2:D:10:DC:OP1	3:B:415:THR:HB	2.15	0.47
3:B:541:GLU:O	3:B:542:ALA:CB	2.62	0.47
3:B:578:GLY:HA2	3:B:583:GLN:CB	2.44	0.47
3:B:576:GLU:CA	3:B:630:SER:HB2	2.44	0.47
3:A:32:GLY:H	3:A:282:ASN:ND2	2.13	0.47
3:A:47:MET:O	3:A:51:ASN:HA	2.14	0.47
3:B:30:GLY:O	3:B:31:ALA:C	2.53	0.47
3:B:476:PRO:HB2	3:B:479:VAL:HG23	1.97	0.47
3:B:60:VAL:HG22	3:B:93:LEU:CD1	2.44	0.47
3:B:121:ARG:HG2	3:B:121:ARG:HH11	1.80	0.46
3:B:573:VAL:HG13	3:B:574:GLY:N	2.30	0.46
3:A:30:GLY:HA2	3:A:306:LYS:HZ2	1.80	0.46
3:A:590:GLY:C	3:A:592:LEU:N	2.69	0.46
1:E:15:DT:H6	1:E:15:DT:OP2	1.99	0.46
3:A:187:VAL:HG13	3:A:191:GLU:HG2	1.97	0.46
1:E:13:DT:H2''	1:E:14:DT:C5'	2.36	0.46
3:A:475:MET:SD	3:A:479:VAL:HG12	2.55	0.46
3:B:16:GLU:O	3:B:20:ALA:HB2	2.15	0.46
3:B:284:ARG:NH2	3:B:605:ARG:HH21	2.14	0.46
3:B:400:ASN:HD22	3:B:401:ARG:N	2.14	0.46
3:B:560:HIS:C	3:B:562:ALA:N	2.68	0.46
3:B:581:PRO:O	3:B:583:GLN:N	2.49	0.46
3:B:56:SER:HA	3:B:213:ARG:O	2.15	0.46
3:B:261:VAL:O	3:B:264:ILE:HG22	2.14	0.46
3:B:628:ARG:HH21	3:B:628:ARG:HG3	1.80	0.46
3:B:62:PHE:HZ	3:B:225:THR:HG22	1.81	0.46
3:A:11:ASN:ND2	3:A:14:GLN:HG3	2.31	0.46
3:A:337:ILE:O	3:A:340:TRP:HB3	2.15	0.46
3:A:605:ARG:HG2	3:A:605:ARG:HH11	1.79	0.46
3:A:625:VAL:CG1	3:A:626:TYR:N	2.79	0.46
2:D:8:DT:H2'	2:D:9:DG:N7	2.31	0.46
3:B:326:GLU:HG3	3:B:327:LEU:N	2.30	0.46
3:B:610:LEU:HD12	3:B:611:THR:H	1.81	0.46
1:C:12:DT:OP1	1:C:13:DT:O4	2.34	0.46
2:D:4:DG:H1'	2:D:5:DC:C5'	2.43	0.46
3:B:234:ARG:O	3:B:234:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:383:PHE:CD1	3:B:542:ALA:HA	2.48	0.46
3:B:577:GLU:HB2	3:B:628:ARG:CD	2.45	0.46
3:B:294:ASN:HD21	3:B:308:LEU:H	1.63	0.46
3:B:582:SER:O	3:B:583:GLN:CB	2.64	0.46
3:A:30:GLY:HA2	3:A:306:LYS:NZ	2.31	0.46
3:B:334:VAL:HA	3:B:372:MET:HE1	1.97	0.46
3:B:581:PRO:C	3:B:583:GLN:H	2.19	0.46
3:B:355:ARG:HH12	3:B:560:HIS:CE1	2.34	0.45
1:C:4:DG:H2'	1:C:5:DT:H72	1.97	0.45
3:A:620:LEU:O	3:A:621:TYR:C	2.55	0.45
3:B:95:HIS:HE1	3:B:99:ARG:HH21	1.63	0.45
3:B:7:LEU:C	3:B:9:SER:H	2.19	0.45
2:F:7:DC:H2''	2:F:8:DT:OP2	2.17	0.45
3:A:107:LEU:HD23	3:A:195:ARG:NH2	2.31	0.45
3:A:34:GLY:HA2	5:A:685:SO4:O1	2.17	0.45
3:B:11:ASN:ND2	3:B:14:GLN:HG3	2.30	0.45
3:B:575:MET:CB	3:B:614:TYR:HB3	2.38	0.45
3:B:90:PHE:HZ	3:B:233:ILE:HD11	1.80	0.45
3:B:450:LEU:HD11	3:B:458:LEU:HD12	1.98	0.45
3:B:529:MET:HA	3:B:530:PRO:HD2	1.64	0.45
3:B:34:GLY:CA	6:B:684:GOL:H32	2.41	0.45
3:A:289:ILE:HD13	3:A:606:ALA:HB3	1.97	0.45
3:A:123:LEU:O	3:A:127:ILE:HG13	2.16	0.45
3:B:43:ILE:HG23	3:B:57:ILE:HD13	1.98	0.45
3:B:600:TYR:O	3:B:604:THR:OG1	2.32	0.45
3:A:506:ILE:O	3:A:510:GLU:HG3	2.17	0.45
3:B:110:ASP:CG	3:B:532:GLN:HG2	2.36	0.45
3:B:368:LEU:O	3:B:369:GLN:C	2.53	0.45
3:B:570:VAL:CG1	3:B:606:ALA:HA	2.45	0.45
3:B:575:MET:CG	3:B:612:LEU:HB3	2.45	0.45
3:A:573:VAL:HG13	3:A:574:GLY:N	2.32	0.45
3:B:528:LEU:HD21	3:B:530:PRO:HD3	1.99	0.45
3:B:570:VAL:CG2	3:B:570:VAL:O	2.65	0.45
3:A:137:TRP:CH2	3:A:169:THR:HG21	2.52	0.44
3:A:621:TYR:HD1	3:A:621:TYR:O	1.99	0.44
3:A:86:TRP:CZ3	3:A:96:ARG:HD3	2.53	0.44
3:B:360:SER:O	3:B:361:ARG:C	2.55	0.44
3:B:581:PRO:C	3:B:583:GLN:N	2.70	0.44
3:B:570:VAL:O	3:B:610:LEU:HD12	2.17	0.44
3:A:359:GLN:NE2	3:A:574:GLY:HA3	2.32	0.44
3:A:618:ARG:HD2	3:A:620:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:ALA:O	3:A:146:ILE:HG13	2.17	0.44
3:A:138:PRO:HA	3:A:139:PRO:HD3	1.95	0.44
3:A:43:ILE:HG23	3:A:57:ILE:HD13	1.98	0.44
3:A:86:TRP:CZ2	3:A:96:ARG:HD3	2.52	0.44
3:B:156:PRO:HA	3:B:159:ILE:HD11	2.00	0.44
3:B:220:ASP:OD1	3:B:221:GLU:N	2.48	0.44
3:B:575:MET:SD	3:B:612:LEU:HB3	2.58	0.44
3:A:122:LEU:HD23	3:A:177:TYR:CE1	2.51	0.44
3:A:321:TYR:HB3	3:A:613:THR:HG22	2.00	0.44
3:B:123:LEU:HD23	3:B:142:ALA:HB3	1.99	0.44
3:B:26:LEU:HD23	3:B:268:LEU:HD11	2.00	0.44
3:A:287:SER:CB	3:A:314:ASP:HA	2.34	0.44
3:B:159:ILE:CG1	3:B:171:GLN:HG3	2.47	0.44
3:B:327:LEU:O	3:B:329:GLU:N	2.51	0.44
3:B:367:LEU:CD2	3:B:372:MET:HE3	2.47	0.44
3:A:329:GLU:OE2	3:A:573:VAL:HG13	2.18	0.44
3:B:373:PRO:O	3:B:553:ALA:HA	2.18	0.44
3:B:576:GLU:HB3	3:B:629:PRO:HA	2.00	0.44
3:A:423:LEU:HD22	3:A:427:ARG:NH1	2.33	0.44
3:B:381:ARG:CB	3:B:542:ALA:HB1	2.47	0.44
3:B:57:ILE:HG12	3:B:216:ASN:HD21	1.82	0.43
3:B:478:HIS:N	3:B:516:THR:HG22	2.33	0.43
1:C:8:DT:C2'	1:C:9:DC:O4'	2.66	0.43
3:A:556:LEU:N	3:A:556:LEU:HD12	2.33	0.43
3:B:374:TYR:HD1	3:B:376:ILE:HD12	1.84	0.43
3:B:429:THR:OG1	3:B:444:LEU:HD21	2.19	0.43
3:B:537:HIS:CD2	3:B:541:GLU:HG3	2.53	0.43
3:B:627:HIS:HA	3:B:628:ARG:NH2	2.33	0.43
3:A:123:LEU:HA	3:A:123:LEU:HD23	1.81	0.43
3:B:401:ARG:HG3	3:B:438:TRP:CE2	2.53	0.43
3:A:150:LYS:C	3:A:152:GLU:N	2.70	0.43
3:A:153:GLY:HA2	3:A:194:LEU:CD1	2.48	0.43
3:A:388:ILE:O	3:A:392:LEU:HG	2.18	0.43
3:B:10:LEU:HB3	3:B:14:GLN:HB2	2.00	0.43
3:B:45:TRP:C	3:B:47:MET:H	2.22	0.43
3:B:575:MET:HE2	3:B:612:LEU:HD13	1.98	0.43
2:D:4:DG:H2''	2:D:5:DC:O5'	2.17	0.43
3:A:402:ASN:HB3	3:A:436:THR:HG21	2.01	0.43
3:A:555:GLN:C	3:A:556:LEU:HD12	2.38	0.43
3:B:10:LEU:CD2	3:B:37:ARG:HD3	2.48	0.43
3:B:28:LEU:HA	3:B:247:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:410:VAL:HA	3:B:413:THR:HB	2.01	0.43
3:A:16:GLU:HG2	3:A:277:ILE:HD13	2.00	0.43
3:A:58:MET:HE3	3:A:60:VAL:HG21	1.99	0.43
3:B:435:LEU:HB3	3:B:439:GLN:HB2	2.00	0.43
2:F:8:DT:H2'	3:A:421:ARG:NH1	2.34	0.43
3:B:386:GLN:HG3	3:B:387:GLU:N	2.34	0.43
3:B:486:LYS:CG	3:B:491:ARG:NH1	2.82	0.43
3:B:572:ILE:HG22	3:B:573:VAL:N	2.33	0.43
2:D:5:DC:H2''	2:D:6:DA:C8	2.54	0.43
3:A:397:LEU:HD13	3:A:465:ILE:CD1	2.49	0.43
3:A:320:LEU:HD13	3:A:633:ILE:HG23	2.01	0.43
3:A:78:MET:HE3	3:A:82:GLN:NE2	2.33	0.43
3:A:486:LYS:HE2	3:A:491:ARG:NH1	2.33	0.42
3:A:593:GLU:O	3:A:597:ARG:HG3	2.19	0.42
3:A:250:ASP:O	3:A:597:ARG:HD2	2.19	0.42
3:B:329:GLU:O	3:B:332:PHE:HB3	2.18	0.42
3:B:364:GLU:O	3:B:365:GLU:C	2.56	0.42
3:B:532:GLN:N	3:B:532:GLN:OE1	2.39	0.42
3:B:7:LEU:C	3:B:9:SER:N	2.72	0.42
1:C:10:DG:H2'	3:A:621:TYR:CZ	2.53	0.42
3:A:573:VAL:HG12	3:A:574:GLY:N	2.35	0.42
3:B:103:MET:HA	3:B:103:MET:CE	2.49	0.42
3:B:211:ARG:NH2	3:B:235:LEU:O	2.50	0.42
1:C:12:DT:H2''	1:C:13:DT:H5'	1.98	0.42
2:F:5:DC:H2''	2:F:6:DA:N7	2.34	0.42
3:A:394:TYR:CZ	3:A:488:SER:HB2	2.55	0.42
3:A:218:LEU:HA	3:A:244:MET:O	2.19	0.42
3:A:104:ASP:HB3	3:A:203:LYS:HD3	2.02	0.42
3:A:440:ALA:O	3:A:444:LEU:HG	2.19	0.42
3:A:569:GLN:NE2	3:A:609:LYS:HB3	2.35	0.42
3:B:94:ALA:HB1	3:B:196:ALA:HB2	2.01	0.42
3:B:257:ARG:HG2	3:B:258:GLY:N	2.34	0.42
3:B:291:SER:OG	3:B:292:ALA:N	2.53	0.42
3:B:45:TRP:CE2	3:B:49:VAL:HG11	2.55	0.42
3:B:484:VAL:O	3:B:488:SER:HB3	2.20	0.42
3:B:576:GLU:HA	3:B:630:SER:HB2	2.00	0.42
3:A:283:TYR:CD1	3:A:283:TYR:N	2.87	0.42
3:B:340:TRP:HZ2	3:B:349:GLU:OE1	2.03	0.42
3:B:628:ARG:H	3:B:628:ARG:HD2	1.84	0.42
3:B:122:LEU:O	3:B:126:LEU:HG	2.20	0.42
3:B:416:ARG:HG3	3:B:418:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:59:ALA:HB3	3:B:87:VAL:HG22	2.01	0.42
3:A:380:MET:HG3	3:A:385:ARG:NH1	2.34	0.42
3:B:256:TRP:O	3:B:257:ARG:C	2.57	0.42
3:A:62:PHE:HZ	3:A:225:THR:HG22	1.84	0.42
3:B:207:LEU:HD12	3:B:207:LEU:O	2.20	0.42
3:B:430:SER:OG	3:B:435:LEU:O	2.30	0.42
3:A:6:LEU:O	3:A:41:HIS:HD2	2.03	0.42
3:B:304:LEU:O	3:B:305:GLY:O	2.38	0.42
3:B:284:ARG:NH1	3:B:566:GLU:OE1	2.53	0.42
3:A:35:LYS:NZ	3:A:220:ASP:OD2	2.47	0.41
3:A:501:LYS:HE3	3:A:505:ARG:NH1	2.35	0.41
3:B:144:TRP:O	3:B:145:TYR:C	2.58	0.41
3:B:303:ARG:HG3	3:B:303:ARG:HH11	1.85	0.41
3:B:562:ALA:C	3:B:565:LEU:HD12	2.40	0.41
3:A:165:PRO:HA	3:A:168:GLN:CB	2.50	0.41
3:A:445:LEU:HA	3:A:445:LEU:HD23	1.86	0.41
3:B:414:PRO:HG2	3:B:489:GLY:HA3	2.02	0.41
3:A:119:GLN:NE2	3:A:143:MET:HG3	2.35	0.41
3:A:201:LEU:HD23	3:A:235:LEU:HD11	2.01	0.41
3:B:13:LYS:HB3	3:B:279:LEU:HD23	2.02	0.41
3:B:334:VAL:HG13	3:B:372:MET:HE2	2.01	0.41
3:B:560:HIS:ND1	3:B:560:HIS:N	2.52	0.41
3:B:326:GLU:CB	3:B:618:ARG:HA	2.50	0.41
3:A:568:PRO:HD3	3:A:607:MET:CE	2.51	0.41
3:A:618:ARG:HG3	3:A:620:LEU:HG	2.03	0.41
3:B:5:TYR:CD2	3:B:5:TYR:N	2.77	0.41
3:A:204:PRO:O	3:A:208:GLN:HB2	2.20	0.41
3:A:421:ARG:HG3	3:A:421:ARG:HH11	1.85	0.41
3:B:194:LEU:HD12	3:B:194:LEU:HA	1.84	0.41
3:B:45:TRP:C	3:B:47:MET:N	2.72	0.41
3:A:326:GLU:HB3	3:A:618:ARG:NH1	2.35	0.41
3:A:573:VAL:HG13	3:A:574:GLY:H	1.86	0.41
3:B:167:GLU:C	3:B:169:THR:H	2.24	0.41
3:B:173:VAL:O	3:B:175:GLN:N	2.54	0.41
3:B:325:ASN:HD22	3:B:327:LEU:CB	2.34	0.41
3:B:367:LEU:HD23	3:B:372:MET:HE2	2.03	0.41
3:A:414:PRO:HA	3:A:493:MET:CE	2.50	0.41
3:B:200:TRP:HE1	3:B:210:TYR:HD2	1.68	0.41
3:B:328:ASP:O	3:B:329:GLU:C	2.58	0.41
3:B:125:ARG:NH1	3:B:437:LEU:HD11	2.36	0.41
3:B:187:VAL:HG13	3:B:191:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:206:ILE:O	3:B:209:HIS:HB3	2.20	0.41
3:B:397:LEU:HD13	3:B:465:ILE:CD1	2.50	0.41
3:B:596:ARG:O	3:B:600:TYR:N	2.47	0.41
3:B:286:THR:HG23	3:B:607:MET:O	2.21	0.41
3:B:79:GLY:C	3:B:81:SER:N	2.71	0.41
3:A:58:MET:HA	3:A:86:TRP:O	2.21	0.41
3:B:137:TRP:CH2	3:B:169:THR:OG1	2.67	0.41
3:B:256:TRP:N	3:B:256:TRP:CD1	2.89	0.41
3:B:380:MET:HG3	3:B:385:ARG:HH11	1.83	0.41
3:B:559:LEU:O	3:B:562:ALA:HB3	2.21	0.41
3:B:57:ILE:HG12	3:B:216:ASN:ND2	2.35	0.41
3:A:284:ARG:NH1	3:A:284:ARG:HG3	2.34	0.41
3:A:335:ASN:ND2	3:A:338:LYS:NZ	2.69	0.41
3:B:321:TYR:CE2	3:B:323:ALA:HB2	2.55	0.41
3:B:6:LEU:O	3:B:41:HIS:HD2	2.03	0.41
3:B:577:GLU:C	3:B:579:MET:H	2.24	0.41
2:F:2:DG:H2''	2:F:3:DA:N7	2.36	0.41
3:B:106:ASN:HA	3:B:106:ASN:HD22	1.62	0.41
3:B:354:TYR:CD1	3:B:356:SER:O	2.72	0.41
2:D:8:DT:C2'	2:D:9:DG:C8	3.03	0.41
3:A:248:ASP:CG	3:A:306:LYS:NZ	2.74	0.40
3:A:267:PHE:O	3:A:271:PHE:HD1	2.03	0.40
2:F:1:DC:H2'	2:F:2:DG:C8	2.57	0.40
3:A:340:TRP:CD1	3:A:350:CYS:SG	3.15	0.40
3:A:568:PRO:CD	3:A:607:MET:CE	2.99	0.40
3:B:286:THR:OG1	3:B:289:ILE:HG13	2.21	0.40
3:B:121:ARG:HG2	3:B:121:ARG:NH1	2.36	0.40
3:A:520:SER:O	3:A:521:TYR:O	2.39	0.40
3:B:262:GLU:O	3:B:265:GLN:CG	2.69	0.40
3:B:596:ARG:O	3:B:597:ARG:C	2.59	0.40
2:D:5:DC:H1'	2:D:6:DA:C8	2.56	0.40
3:B:123:LEU:HD11	3:B:177:TYR:CD1	2.57	0.40
3:B:246:VAL:HG12	3:B:247:GLY:N	2.37	0.40
3:B:297:ILE:HG13	3:B:303:ARG:HE	1.86	0.40
3:B:374:TYR:CD1	3:B:376:ILE:CD1	3.04	0.40
3:B:459:GLN:O	3:B:463:GLU:HG3	2.21	0.40
2:D:8:DT:C2'	2:D:9:DG:N7	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	645/680 (95%)	575 (89%)	52 (8%)	18 (3%)	6	22
3	B	614/680 (90%)	471 (77%)	99 (16%)	44 (7%)	1	3
All	All	1259/1360 (93%)	1046 (83%)	151 (12%)	62 (5%)	2	9

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	263	ASN
3	A	303	ARG
3	A	521	TYR
3	A	547	ALA
3	A	583	GLN
3	B	31	ALA
3	B	303	ARG
3	B	305	GLY
3	B	359	GLN
3	B	371	SER
3	B	527	ASP
3	B	530	PRO
3	B	542	ALA
3	A	306	LYS
3	A	324	PHE
3	A	499	GLY
3	A	621	TYR
3	B	77	LEU
3	B	98	LEU
3	B	452	GLY
3	B	545	GLY
3	B	561	SER
3	B	583	GLN
3	B	642	GLU
3	A	161	SER

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Mol	Chain	Res	Type
3	A	587	ASP
3	B	8	ASP
3	B	22	ARG
3	B	46	LEU
3	B	257	ARG
3	B	263	ASN
3	B	328	ASP
3	B	370	ALA
3	B	555	GLN
3	B	582	SER
3	B	611	THR
3	A	163	GLY
3	A	380	MET
3	A	471	GLU
3	A	590	GLY
3	B	4	SER
3	B	24	ASN
3	B	168	GLN
3	B	174	TYR
3	B	258	GLY
3	B	285	SER
3	B	375	ARG
3	B	382	PHE
3	B	633	ILE
3	A	31	ALA
3	A	452	GLY
3	A	588	GLU
3	B	155	ARG
3	B	407	PHE
3	B	327	LEU
3	B	566	GLU
3	B	139	PRO
3	B	378	GLY
3	B	570	VAL
3	B	641	VAL
3	B	83	GLY
3	B	629	PRO

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	502/574 (88%)	481 (96%)	21 (4%)	34	69
3	B	450/574 (78%)	415 (92%)	35 (8%)	15	39
All	All	952/1148 (83%)	896 (94%)	56 (6%)	23	55

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

Mol	Chain	Res	Type
3	A	51	ASN
3	A	125	ARG
3	A	140	ARG
3	A	149	GLN
3	A	160	GLN
3	A	174	TYR
3	A	179	GLU
3	A	203	LYS
3	A	208	GLN
3	A	235	LEU
3	A	262	GLU
3	A	275	GLU
3	A	285	SER
3	A	291	SER
3	A	298	GLU
3	A	319	SER
3	A	431	ARG
3	A	439	GLN
3	A	577	GLU
3	A	594	GLU
3	A	639	GLU
3	B	5	TYR
3	B	51	ASN
3	B	61	THR
3	B	71	ARG
3	B	96	ARG
3	B	106	ASN
3	B	107	LEU
3	B	121	ARG
3	B	169	THR
3	B	216	ASN

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Mol	Chain	Res	Type
3	B	240	THR
3	B	260	GLN
3	B	262	GLU
3	B	303	ARG
3	B	308	LEU
3	B	324	PHE
3	B	362	VAL
3	B	365	GLU
3	B	400	ASN
3	B	401	ARG
3	B	421	ARG
3	B	458	LEU
3	B	528	LEU
3	B	529	MET
3	B	558	THR
3	B	560	HIS
3	B	567	PHE
3	B	569	GLN
3	B	570	VAL
3	B	573	VAL
3	B	597	ARG
3	B	604	THR
3	B	611	THR
3	B	621	TYR
3	B	628	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	41	HIS
3	A	82	GLN
3	A	102	HIS
3	A	119	GLN
3	A	147	ASN
3	A	149	GLN
3	A	158	HIS
3	A	178	GLN
3	A	227	ASN
3	A	335	ASN
3	A	386	GLN
3	A	480	GLN
3	A	551	GLN

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Mol	Chain	Res	Type
3	A	555	GLN
3	B	24	ASN
3	B	51	ASN
3	B	64	ASN
3	B	72	HIS
3	B	95	HIS
3	B	102	HIS
3	B	106	ASN
3	B	119	GLN
3	B	147	ASN
3	B	158	HIS
3	B	178	GLN
3	B	197	HIS
3	B	216	ASN
3	B	227	ASN
3	B	260	GLN
3	B	263	ASN
3	B	281	GLN
3	B	282	ASN
3	B	299	ASN
3	B	325	ASN
3	B	341	GLN
3	B	400	ASN
3	B	412	ASN
3	B	446	GLN
3	B	480	GLN
3	B	569	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z  > 2$
5	SO4	A	684	-	4,4,4	0.33	0	6,6,6	0.11	0
5	SO4	A	685	-	4,4,4	0.45	0	6,6,6	0.20	0
6	GOL	A	686	-	5,5,5	0.52	0	5,5,5	0.29	0
5	SO4	B	683	-	4,4,4	0.32	0	6,6,6	0.22	0
6	GOL	B	684	-	5,5,5	0.39	0	5,5,5	0.17	0

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
5	SO4	A	684	-	-	0/0/0/0	0/0/0/0
5	SO4	A	685	-	-	0/0/0/0	0/0/0/0
6	GOL	A	686	-	-	0/4/4/4	0/0/0/0
5	SO4	B	683	-	-	0/0/0/0	0/0/0/0
6	GOL	B	684	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	684	SO4	1	0
5	A	685	SO4	1	0
6	B	684	GOL	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	16/17 (94%)	0.33	1 (6%) 21 16	35, 68, 116, 117	0
1	E	15/17 (88%)	0.03	0 100 100	39, 78, 115, 124	0
2	D	10/10 (100%)	0.27	0 100 100	32, 85, 101, 103	0
2	F	10/10 (100%)	0.26	0 100 100	34, 64, 107, 108	0
3	A	649/680 (95%)	-0.17	3 (0%) 90 90	18, 43, 75, 95	0
3	B	624/680 (91%)	0.19	27 (4%) 36 31	21, 68, 96, 109	0
All	All	1324/1414 (93%)	0.01	31 (2%) 61 57	18, 53, 93, 124	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	633	ILE	4.7
3	A	587	ASP	4.7
3	B	630	SER	4.6
3	B	613	THR	4.2
3	B	579	MET	4.0
3	B	624	GLU	3.4
3	B	621	TYR	3.4
3	B	372	MET	3.3
3	A	620	LEU	3.1
3	B	344	GLY	3.1
3	B	341	GLN	3.0
3	A	545	GLY	2.8
3	B	3	VAL	2.7
3	B	348	ALA	2.7
3	B	580	PHE	2.6
3	B	611	THR	2.6
3	B	375	ARG	2.6
3	B	321	TYR	2.5
3	B	614	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	347	LEU	2.5
3	B	619	ARG	2.4
3	B	571	PHE	2.3
3	B	345	GLY	2.3
3	B	629	PRO	2.3
3	B	615	ALA	2.2
3	B	552	ASP	2.2
3	B	199	LEU	2.1
1	C	11	DT	2.1
3	B	622	GLY	2.1
3	B	644	VAL	2.1
3	B	346	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	A	686	6/6	0.68	0.33	7.62	71,73,73,73	0
5	SO4	A	685	5/5	0.93	0.20	1.24	56,56,59,60	0
5	SO4	B	683	5/5	0.94	0.22	0.41	56,57,58,58	0
5	SO4	A	684	5/5	0.99	0.16	-0.67	44,45,46,47	0
4	HG	A	683	1/1	0.96	0.11	-2.52	107,107,107,107	1
4	HG	B	682	1/1	0.95	0.11	-	113,113,113,113	1
6	GOL	B	684	6/6	0.95	0.21	-	46,46,48,48	0
4	HG	A	681	1/1	0.94	0.11	-	84,84,84,84	1
4	HG	B	681	1/1	0.85	0.08	-	127,127,127,127	1
4	HG	A	682	1/1	0.99	0.09	-	75,75,75,75	1

## 6.5 Other polymers

There are no such residues in this entry.