



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:44 AM GMT

PDB ID : 2IS2  
Title : Crystal structure of UvrD-DNA binary complex  
Authors : Yang, W.; Lee, J.Y.  
Deposited on : 2006-10-16  
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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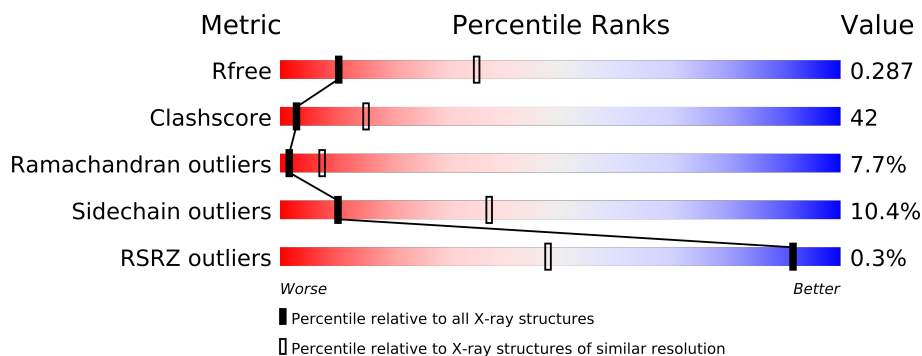
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	35	
1	D	35	
2	A	680	
2	B	680	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11505 atoms, of which 0 are hydrogen and 0 are deuterium.

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 33-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	33	Total	C	N	O	P	0	0	0
			673	321	120	200	32			
1	D	33	Total	C	N	O	P	0	0	0
			673	321	120	200	32			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	642	Total	C	N	O	S	0	0	0
			5076	3180	924	946	26			
2	B	642	Total	C	N	O	S	0	0	0
			5060	3169	923	942	26			

There are 2 discrepancies between the modelled and reference sequences:

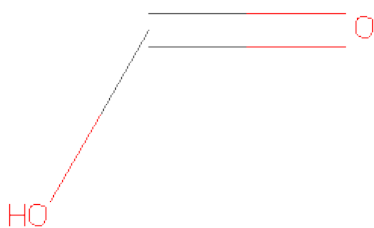
Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	ENGINEERED	UNP P03018
B	399	VAL	ALA	ENGINEERED	UNP P03018

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total 14	O 14	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: 33-MER

Chain C:



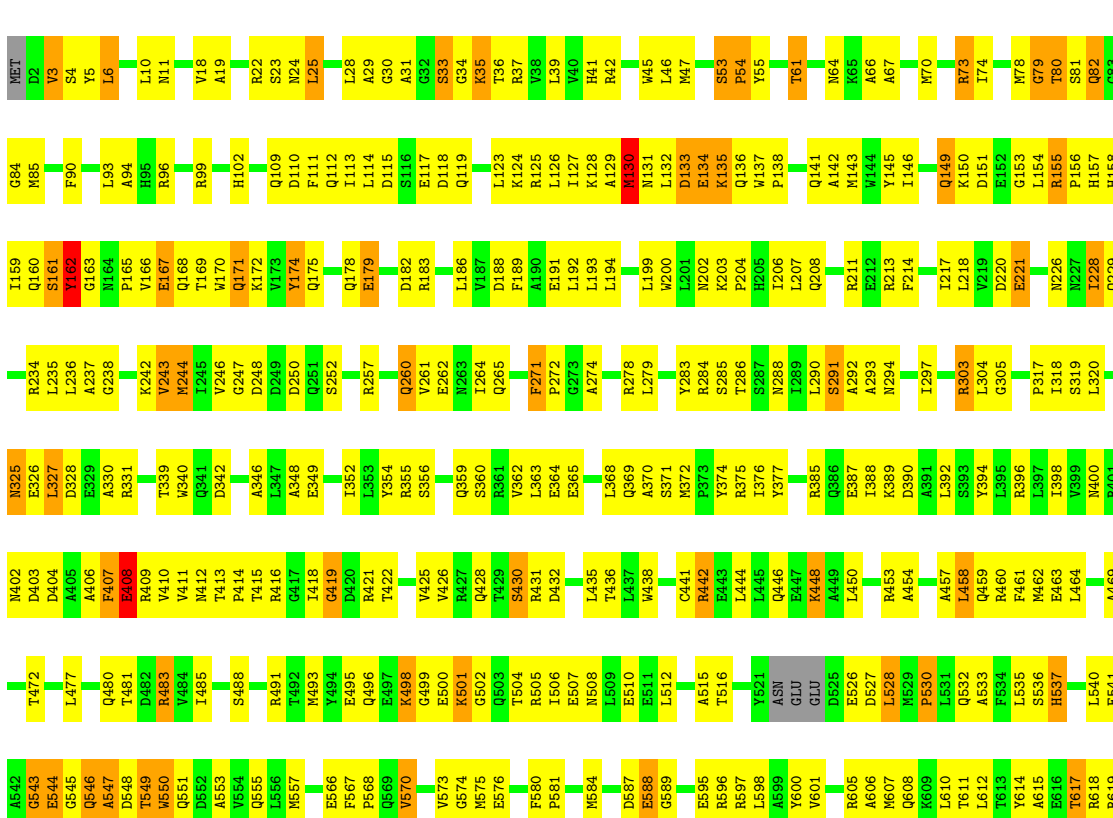
- Molecule 1: 33-MER

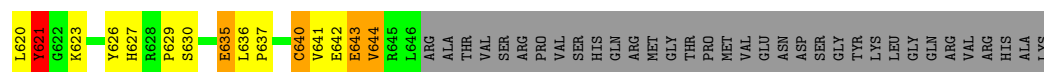
Chain D:



- Molecule 2: DNA helicase II

Chain A:





• Molecule 2: DNA helicase II

Chain B:

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.60Å 105.97Å 295.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.00 49.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.7 (29.75-3.00) 83.6 (49.48-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.283 0.242 , 0.287	Depositor DCC
$R_{free}$ test set	3600 reflections (10.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 37435 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.51	0/753	0.80	0/1161
1	D	0.49	0/753	0.75	0/1161
2	A	0.49	1/5170 (0.0%)	0.73	0/6993
2	B	0.37	1/5154 (0.0%)	0.65	0/6972
All	All	0.44	2/11830 (0.0%)	0.70	0/16287

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
2	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	162	TYR	CB-CG	-6.50	1.41	1.51
2	B	162	TYR	CB-CG	-6.36	1.42	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	621	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	673	0	374	42	0
1	D	673	0	374	57	0
2	A	5076	0	4944	338	0
2	B	5060	0	4908	529	0
3	A	6	0	8	4	0
4	A	3	0	1	1	0
5	A	14	0	0	0	0
All	All	11505	0	10609	933	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

All (933) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:19:DG:H2"	1:D:20:DC:H5"	1.32	1.09
2:B:155:ARG:HG3	2:B:156:PRO:HD2	1.14	1.08
2:B:261:VAL:HG21	2:B:597:ARG:HH21	1.24	1.01
2:B:7:LEU:HD11	2:B:45:TRP:HZ3	1.21	0.99
2:A:288:ASN:ND2	2:A:317:PRO:HA	1.78	0.98
2:B:112:GLN:HE21	2:B:113:ILE:H	1.04	0.98
2:B:400:ASN:HD21	2:B:402:ASN:HB2	1.24	0.96
2:A:161:SER:O	2:A:162:TYR:CG	2.18	0.96
2:A:203:LYS:O	2:A:206:ILE:HG12	1.67	0.94
2:A:73:ARG:HH11	2:A:73:ARG:HG2	1.32	0.93
2:A:325:ASN:C	2:A:325:ASN:HD22	1.72	0.93
2:A:284:ARG:HD3	2:A:566:GLU:HB3	1.51	0.93
2:A:161:SER:HB3	2:A:168:GLN:HE21	1.34	0.93
2:B:320:LEU:HD11	2:B:633:ILE:HG21	1.51	0.92
2:B:155:ARG:CG	2:B:156:PRO:HD2	2.01	0.91
2:B:285:SER:HB3	2:B:606:ALA:O	1.71	0.90
2:A:284:ARG:HG3	2:A:566:GLU:OE1	1.73	0.88
1:C:14:DC:HI'	2:B:453:ARG:HH21	1.37	0.88
2:B:475:MET:HE3	2:B:479:VAL:HG12	1.55	0.87
2:B:7:LEU:HD11	2:B:45:TRP:CZ3	2.07	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:162:TYR:C	2:B:164:ASN:H	1.77	0.87
2:B:79:GLY:O	2:B:80:THR:HG23	1.76	0.86
2:B:23:SER:HA	2:B:242:LYS:HG3	1.55	0.85
2:B:349:GLU:HB3	2:B:568:PRO:HG2	1.58	0.85
1:D:19:DG:C2'	1:D:20:DC:H5''	2.06	0.85
2:A:217:ILE:HB	2:A:243:VAL:HB	1.56	0.85
2:B:453:ARG:NH1	2:B:453:ARG:HB2	1.91	0.84
2:B:112:GLN:HG2	2:B:396:ARG:HH11	1.40	0.84
2:B:261:VAL:HG21	2:B:597:ARG:NH2	1.92	0.84
2:B:453:ARG:HH11	2:B:453:ARG:HB2	1.40	0.84
2:B:575:MET:HB2	2:B:613:THR:O	1.77	0.84
2:B:61:THR:HG22	2:B:62:PHE:H	1.41	0.83
2:B:154:LEU:HD22	2:B:158:HIS:HB3	1.61	0.83
2:B:112:GLN:HE21	2:B:113:ILE:N	1.76	0.83
2:A:643:GLU:HG3	2:A:644:VAL:H	1.42	0.83
2:B:43:ILE:HD12	2:B:74:ILE:HD12	1.60	0.82
1:D:22:DG:H2''	1:D:23:DT:OP2	1.77	0.82
2:B:246:VAL:HG12	2:B:247:GLY:H	1.45	0.82
2:B:360:SER:HA	2:B:363:LEU:HD12	1.63	0.81
2:B:300:ASN:HB2	2:B:303:ARG:HD3	1.62	0.81
2:B:472:THR:HA	2:B:475:MET:SD	2.21	0.81
2:B:252:SER:OG	2:B:261:VAL:HG22	1.81	0.81
2:A:42:ARG:HG2	2:A:244:MET:CE	2.11	0.81
2:B:401:ARG:HH22	2:B:469:ALA:HB2	1.46	0.80
2:B:300:ASN:OD1	2:B:596:ARG:HD2	1.81	0.80
2:B:322:CYS:HG	2:B:614:TYR:HE1	1.30	0.80
1:C:2:DG:H2''	1:C:3:DA:OP2	1.81	0.80
2:A:504:THR:HG22	2:A:508:ASN:HD21	1.46	0.80
2:A:78:MET:O	2:A:80:THR:N	2.15	0.79
2:B:112:GLN:OE1	2:B:396:ARG:HD3	1.82	0.79
2:A:414:PRO:HA	2:A:493:MET:CE	2.12	0.79
2:B:44:ALA:HB2	2:B:77:LEU:HD23	1.63	0.79
1:D:7:DC:H2'	1:D:8:DT:H72	1.63	0.79
2:A:285:SER:HB3	2:A:606:ALA:O	1.81	0.79
1:D:23:DT:H2''	1:D:24:DG:O4'	1.83	0.79
2:A:138:PRO:HG2	2:A:141:GLN:HB3	1.64	0.79
2:B:396:ARG:HD2	2:B:403:ASP:OD2	1.83	0.78
2:A:131:ASN:OD1	2:A:132:LEU:N	2.17	0.78
1:C:6:DA:H2''	1:C:7:DC:O5'	1.81	0.78
2:B:288:ASN:HD21	2:B:317:PRO:HA	1.48	0.78
2:A:42:ARG:HG2	2:A:244:MET:HE1	1.64	0.78
2:B:475:MET:CE	2:B:479:VAL:HG12	2.14	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:323:ALA:HB1	2:B:328:ASP:HB3	1.66	0.77
2:B:112:GLN:NE2	2:B:113:ILE:H	1.81	0.77
2:B:42:ARG:O	2:B:46:LEU:HG	1.84	0.77
1:C:14:DC:H1'	2:B:453:ARG:NH2	2.00	0.77
2:B:26:LEU:HD12	2:B:27:VAL:H	1.48	0.76
2:B:504:THR:HG22	2:B:508:ASN:ND2	2.00	0.76
2:B:436:THR:OG1	2:B:439:GLN:HG3	1.86	0.76
1:C:18:DT:H2''	1:C:19:DG:H5'	1.68	0.76
2:B:341:GLN:NE2	2:B:347:LEU:HD11	2.00	0.76
2:A:112:GLN:HE21	2:A:113:ILE:N	1.83	0.76
2:A:252:SER:OG	2:A:261:VAL:HG22	1.85	0.76
2:B:156:PRO:HD3	2:B:174:TYR:HE1	1.50	0.75
2:B:597:ARG:O	2:B:601:VAL:HG23	1.87	0.75
2:A:119:GLN:HE21	2:A:143:MET:CE	1.99	0.75
2:B:618:ARG:HH11	2:B:618:ARG:HB2	1.51	0.75
2:B:570:VAL:HG11	2:B:606:ALA:HA	1.69	0.75
2:A:288:ASN:OD1	2:A:640:CYS:HB3	1.87	0.75
2:B:400:ASN:ND2	2:B:402:ASN:H	1.84	0.75
2:A:73:ARG:HG2	2:A:73:ARG:NH1	2.00	0.74
2:A:30:GLY:O	2:A:31:ALA:HB3	1.86	0.74
2:A:200:TRP:HB3	2:A:207:LEU:HD13	1.69	0.74
2:B:346:ALA:HB3	2:B:349:GLU:CD	2.08	0.74
2:B:353:LEU:HB3	2:B:559:LEU:CD2	2.18	0.74
2:A:64:ASN:ND2	2:A:541:GLU:HB3	2.03	0.74
2:A:637:PRO:HB2	2:A:640:CYS:SG	2.28	0.73
2:B:113:ILE:H	2:B:113:ILE:HD12	1.53	0.73
2:B:129:ALA:HB1	2:B:431:ARG:HD2	1.69	0.73
2:B:381:ARG:HD3	2:B:543:GLY:H	1.53	0.73
2:A:644:VAL:HG12	2:A:644:VAL:O	1.86	0.73
2:B:26:LEU:HD12	2:B:27:VAL:N	2.04	0.73
2:B:504:THR:HG22	2:B:508:ASN:HD21	1.54	0.73
2:B:263:ASN:HA	2:B:266:ARG:HB3	1.71	0.73
2:A:288:ASN:HD21	2:A:317:PRO:HA	1.49	0.72
2:A:346:ALA:HB3	2:A:349:GLU:HG3	1.70	0.72
2:A:112:GLN:HG2	2:A:396:ARG:HH11	1.54	0.72
1:C:11:DA:H2''	1:C:12:DC:C5'	2.19	0.72
2:B:472:THR:O	2:B:475:MET:HB2	1.90	0.72
2:B:321:TYR:HE2	2:B:323:ALA:HB2	1.54	0.72
1:D:7:DC:H2''	1:D:8:DT:C6	2.25	0.72
2:A:188:ASP:OD2	2:A:191:GLU:HB2	1.90	0.72
2:A:325:ASN:ND2	2:A:328:ASP:H	1.88	0.71
2:B:554:VAL:HG12	2:B:555:GLN:N	2.04	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:54:PRO:HA	2:B:57:ILE:HD13	1.71	0.71
1:D:24:DG:OP1	1:D:24:DG:H4'	1.89	0.71
2:A:134:GLU:O	2:A:136:GLN:N	2.23	0.71
2:B:501:LYS:HE3	2:B:505:ARG:HH12	1.55	0.71
2:B:569:GLN:HG3	2:B:571:PHE:CE2	2.25	0.71
2:B:43:ILE:CG2	2:B:57:ILE:HG21	2.20	0.71
2:B:468:LEU:HD21	2:B:487:ASP:HB3	1.73	0.70
2:B:509:LEU:O	2:B:512:LEU:HB3	1.91	0.70
2:B:23:SER:HA	2:B:242:LYS:CG	2.21	0.70
2:B:468:LEU:O	2:B:472:THR:HG22	1.91	0.70
2:A:549:THR:O	2:A:551:GLN:N	2.19	0.70
2:A:643:GLU:HG3	2:A:644:VAL:N	2.05	0.70
2:B:554:VAL:HG12	2:B:555:GLN:H	1.56	0.70
2:B:388:ILE:HG13	2:B:512:LEU:HD22	1.73	0.70
2:B:498:LYS:HB2	2:B:501:LYS:HB2	1.74	0.70
1:C:14:DC:C1'	2:B:453:ARG:HH21	2.04	0.69
2:A:161:SER:HB3	2:A:168:GLN:NE2	2.05	0.69
2:A:28:LEU:HD22	2:A:304:LEU:HD12	1.72	0.69
1:D:7:DC:H2'	1:D:8:DT:C7	2.21	0.69
2:B:550:TRP:O	2:B:551:GLN:C	2.31	0.69
2:B:106:ASN:O	2:B:107:LEU:HD23	1.93	0.69
2:B:234:ARG:HG3	2:B:235:LEU:N	2.08	0.69
2:A:325:ASN:HD21	2:A:327:LEU:HB2	1.56	0.69
2:B:380:MET:HG3	2:B:385:ARG:NH2	2.08	0.69
2:B:298:GLU:HG3	2:B:303:ARG:HH21	1.56	0.68
2:B:288:ASN:ND2	2:B:317:PRO:HA	2.08	0.68
2:B:603:VAL:C	2:B:605:ARG:H	1.94	0.68
2:A:414:PRO:HA	2:A:493:MET:HE1	1.74	0.68
1:D:10:DC:H2'	1:D:11:DA:C8	2.28	0.68
2:A:110:ASP:OD1	2:A:532:GLN:HG2	1.94	0.68
2:B:478:HIS:CD2	2:B:517:ARG:HE	2.12	0.68
2:B:162:TYR:C	2:B:164:ASN:N	2.48	0.68
2:B:383:PHE:CD1	2:B:538:ALA:HA	2.29	0.68
2:B:601:VAL:O	2:B:605:ARG:HG2	1.93	0.68
2:B:571:PHE:C	2:B:572:ILE:HD12	2.15	0.67
2:B:353:LEU:HB3	2:B:559:LEU:HD23	1.76	0.67
2:A:325:ASN:C	2:A:325:ASN:ND2	2.47	0.67
2:A:568:PRO:N	2:A:607:MET:HE3	2.10	0.67
2:B:58:MET:HB2	2:B:214:PHE:CD1	2.29	0.67
2:A:413:THR:HA	2:A:414:PRO:C	2.13	0.67
2:A:610:LEU:HD12	2:A:611:THR:N	2.09	0.67
2:A:472:THR:HG21	2:A:480:GLN:HG3	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:333:VAL:HG13	2:B:571:PHE:CE1	2.29	0.67
1:C:18:DT:OP1	2:A:422:THR:OG1	2.08	0.66
1:D:1:DC:H6	1:D:1:DC:HO5'	1.43	0.66
1:C:11:DA:H2''	1:C:12:DC:H5'	1.75	0.66
2:A:189:PHE:HA	2:A:192:LEU:HD12	1.76	0.66
2:B:638:GLU:O	2:B:638:GLU:HG2	1.95	0.66
2:B:326:GLU:OE2	2:B:327:LEU:HD22	1.95	0.66
2:B:569:GLN:HG3	2:B:571:PHE:HE2	1.60	0.66
2:B:382:PHE:HD2	2:B:383:PHE:CD2	2.13	0.66
2:B:10:LEU:CD1	2:B:18:VAL:HG21	2.25	0.66
2:A:138:PRO:HG2	2:A:141:GLN:CB	2.24	0.66
2:B:349:GLU:HB3	2:B:568:PRO:CG	2.25	0.66
2:A:601:VAL:O	2:A:605:ARG:HG2	1.96	0.66
2:A:165:PRO:HA	2:A:168:GLN:HB2	1.77	0.65
1:D:19:DG:H2''	1:D:20:DC:C5'	2.18	0.65
2:B:398:ILE:HA	2:B:401:ARG:HH21	1.61	0.65
2:B:457:ALA:HA	2:B:460:ARG:NH1	2.11	0.65
2:B:472:THR:HG23	2:B:480:GLN:HE21	1.61	0.65
2:B:475:MET:HE3	2:B:479:VAL:CG1	2.25	0.65
2:B:347:LEU:HD12	2:B:552:ASP:OD2	1.96	0.65
2:A:150:LYS:NZ	2:A:178:GLN:HE22	1.95	0.65
1:C:17:DG:H8	2:A:421:ARG:NH1	1.95	0.65
2:A:355:ARG:NH2	2:A:595:GLU:OE2	2.22	0.65
2:B:549:THR:O	2:B:551:GLN:N	2.30	0.65
2:A:112:GLN:CG	2:A:396:ARG:HH11	2.10	0.65
2:B:220:ASP:OD1	2:B:221:GLU:N	2.30	0.65
2:A:326:GLU:OE1	2:A:618:ARG:HA	1.97	0.64
2:B:380:MET:HG3	2:B:385:ARG:HH22	1.62	0.64
1:D:18:DT:H5'	2:B:419:GLY:HA3	1.79	0.64
2:B:341:GLN:HE21	2:B:347:LEU:HD11	1.59	0.64
1:D:17:DG:H3'	2:B:421:ARG:HD2	1.78	0.64
2:B:453:ARG:HH11	2:B:453:ARG:CB	2.09	0.64
2:B:356:SER:OG	2:B:359:GLN:HG3	1.96	0.64
2:B:570:VAL:CG1	2:B:606:ALA:HA	2.28	0.64
2:A:142:ALA:O	2:A:146:ILE:HG13	1.97	0.64
2:A:284:ARG:HD3	2:A:566:GLU:CB	2.26	0.64
2:B:39:LEU:CD2	2:B:218:LEU:HD23	2.28	0.64
2:B:403:ASP:HB3	2:B:406:ALA:HB3	1.79	0.64
2:B:258:GLY:O	2:B:260:GLN:NE2	2.31	0.63
2:A:290:LEU:O	2:A:293:ALA:HB3	1.98	0.63
2:B:621:TYR:O	2:B:621:TYR:HD1	1.80	0.63
2:B:89:THR:O	2:B:93:LEU:HG	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:4:SER:HB3	2:B:7:LEU:HD12	1.81	0.63
2:B:129:ALA:HB1	2:B:431:ARG:CD	2.29	0.63
2:B:113:ILE:N	2:B:113:ILE:HD12	2.12	0.63
2:B:396:ARG:HG2	2:B:535:LEU:HD13	1.81	0.63
2:A:119:GLN:HE21	2:A:143:MET:HE2	1.62	0.63
1:D:29:DT:H5'	1:D:29:DT:O2	1.99	0.63
2:A:431:ARG:HH11	2:A:431:ARG:HG3	1.62	0.63
2:B:582:SER:OG	2:B:585:SER:HB3	1.98	0.63
2:A:288:ASN:O	2:A:291:SER:HB3	1.99	0.63
2:A:288:ASN:HD22	2:A:317:PRO:HA	1.60	0.63
2:B:23:SER:CA	2:B:242:LYS:HG3	2.28	0.63
2:B:246:VAL:HG12	2:B:247:GLY:N	2.11	0.63
2:A:491:ARG:O	2:A:495:GLU:HG3	1.99	0.63
2:B:610:LEU:HD12	2:B:611:THR:N	2.15	0.62
2:B:222:PHE:O	2:B:225:THR:HG23	1.99	0.62
2:B:325:ASN:H	2:B:325:ASN:HD22	1.45	0.62
2:A:457:ALA:HA	2:A:460:ARG:NH2	2.14	0.62
2:B:341:GLN:CD	2:B:347:LEU:HD21	2.20	0.62
2:B:182:ASP:O	2:B:185:GLY:N	2.31	0.62
1:C:17:DG:H1'	1:C:18:DT:H5''	1.81	0.62
1:D:6:DA:H2'	1:D:7:DC:C6	2.35	0.62
1:C:27:DC:H1'	1:C:28:DG:C8	2.35	0.62
2:B:483:ARG:HG2	2:B:483:ARG:HH11	1.64	0.62
2:B:10:LEU:HD11	2:B:18:VAL:HG21	1.82	0.62
2:B:247:GLY:O	2:B:248:ASP:HB2	2.00	0.61
2:B:36:THR:O	2:B:40:VAL:HG23	2.00	0.61
2:B:641:VAL:HG12	2:B:642:GLU:N	2.15	0.61
2:A:53:SER:O	2:A:55:TYR:N	2.33	0.61
2:B:262:GLU:O	2:B:264:ILE:N	2.34	0.61
2:A:412:ASN:O	2:A:415:THR:HA	2.00	0.61
1:D:17:DG:H2''	1:D:18:DT:O5'	1.99	0.61
2:A:156:PRO:HD3	2:A:174:TYR:HE1	1.64	0.61
2:B:340:TRP:CD1	2:B:345:GLY:HA3	2.36	0.61
2:B:320:LEU:HD11	2:B:633:ILE:CG2	2.30	0.61
2:B:146:ILE:HG23	2:B:174:TYR:CE2	2.35	0.61
2:B:39:LEU:HD22	2:B:218:LEU:HD23	1.82	0.61
2:A:133:ASP:O	2:A:135:LYS:N	2.34	0.61
2:B:321:TYR:CE2	2:B:323:ALA:HB2	2.35	0.61
2:B:70:MET:O	2:B:74:ILE:HG12	2.00	0.61
2:B:280:GLU:HB3	2:B:307:LYS:O	2.00	0.61
2:A:129:ALA:C	2:A:130:MET:HG3	2.21	0.61
2:B:546:GLN:O	2:B:548:ASP:N	2.34	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:16:DA:H2''	1:D:17:DG:C5'	2.31	0.60
2:B:161:SER:O	2:B:162:TYR:CG	2.54	0.60
2:B:383:PHE:CE1	2:B:538:ALA:HA	2.36	0.60
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.13	0.60
2:A:37:ARG:NH1	3:A:681:GOL:H2	2.15	0.60
2:B:122:LEU:HD12	2:B:122:LEU:O	2.01	0.60
2:A:39:LEU:HD21	2:A:246:VAL:HG21	1.83	0.60
2:B:155:ARG:HG3	2:B:156:PRO:CD	2.09	0.60
2:B:412:ASN:HB2	2:B:418:ILE:HB	1.84	0.60
1:C:6:DA:C2'	1:C:7:DC:O5'	2.50	0.60
2:B:347:LEU:N	2:B:552:ASP:OD2	2.34	0.60
2:A:573:VAL:HG13	2:A:574:GLY:N	2.17	0.60
2:B:23:SER:O	2:B:25:LEU:HD23	2.01	0.60
2:B:501:LYS:CE	2:B:505:ARG:HH12	2.14	0.60
2:A:156:PRO:HD3	2:A:174:TYR:CE1	2.36	0.60
2:B:12:ASP:O	2:B:16:GLU:N	2.30	0.60
2:B:326:GLU:HB3	2:B:618:ARG:HH12	1.66	0.60
2:B:161:SER:O	2:B:162:TYR:CB	2.49	0.60
2:A:6:LEU:HD12	2:A:45:TRP:HE3	1.66	0.60
1:C:11:DA:HI'	1:C:12:DC:H5''	1.84	0.60
2:A:236:LEU:HD12	2:A:236:LEU:O	2.01	0.60
2:A:42:ARG:HG2	2:A:244:MET:HE3	1.84	0.60
2:B:152:GLU:OE2	2:B:227:ASN:ND2	2.34	0.60
2:B:112:GLN:HB3	2:B:186:LEU:CD2	2.32	0.60
2:B:107:LEU:HD21	2:B:195:ARG:HE	1.66	0.59
2:A:459:GLN:O	2:A:463:GLU:HG3	2.01	0.59
2:B:150:LYS:HE2	2:B:178:GLN:HE22	1.66	0.59
2:A:162:TYR:O	2:A:162:TYR:CG	2.56	0.59
2:B:253:ILE:CD1	2:B:253:ILE:H	2.15	0.59
2:B:226:ASN:OD1	2:B:229:GLN:HG3	2.01	0.59
2:A:70:MET:O	2:A:74:ILE:HG13	2.03	0.59
2:B:398:ILE:HG23	2:B:469:ALA:HA	1.85	0.59
1:C:17:DG:H2'	2:A:421:ARG:HD2	1.84	0.59
2:A:28:LEU:HD12	2:A:247:GLY:O	2.03	0.59
2:B:165:PRO:HA	2:B:168:GLN:HB2	1.84	0.59
2:B:491:ARG:O	2:B:495:GLU:HG3	2.03	0.59
2:B:253:ILE:HD13	2:B:253:ILE:H	1.68	0.59
2:A:319:SER:C	2:A:320:LEU:HD23	2.22	0.59
2:A:414:PRO:HA	2:A:493:MET:HE3	1.83	0.59
1:D:18:DT:H5'	2:B:419:GLY:CA	2.33	0.58
2:A:23:SER:HA	2:A:242:LYS:HG3	1.83	0.58
2:A:325:ASN:HA	2:A:617:THR:O	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:504:THR:HG22	2:A:508:ASN:ND2	2.18	0.58
2:B:226:ASN:OD1	2:B:228:ILE:HG22	2.04	0.58
2:B:400:ASN:HD21	2:B:402:ASN:CB	2.08	0.58
2:A:119:GLN:HE21	2:A:143:MET:HE3	1.66	0.58
2:A:290:LEU:O	2:A:294:ASN:ND2	2.36	0.58
2:B:351:ALA:HA	2:B:555:GLN:O	2.03	0.58
2:B:333:VAL:HG11	2:B:352:ILE:HD12	1.85	0.58
2:A:134:GLU:C	2:A:136:GLN:H	2.07	0.58
2:A:601:VAL:O	2:A:605:ARG:NH1	2.35	0.58
2:B:571:PHE:CD2	2:B:571:PHE:N	2.72	0.58
2:B:142:ALA:HB2	2:B:170:TRP:HZ3	1.67	0.58
1:D:17:DG:H5'	2:B:421:ARG:NH1	2.18	0.58
2:A:643:GLU:O	2:A:644:VAL:HG23	2.02	0.58
2:A:368:LEU:O	2:A:370:ALA:N	2.36	0.58
2:A:543:GLY:O	2:A:544:GLU:CB	2.52	0.58
2:B:329:GLU:CD	2:B:573:VAL:HG13	2.24	0.57
1:D:17:DG:H5'	2:B:421:ARG:HH11	1.69	0.57
2:B:557:MET:HG3	2:B:558:THR:O	2.04	0.57
2:A:112:GLN:HG2	2:A:396:ARG:NH1	2.18	0.57
2:A:10:LEU:HD11	2:A:18:VAL:HG21	1.85	0.57
2:B:603:VAL:HG23	2:B:610:LEU:HD21	1.86	0.57
1:C:7:DC:H2''	1:C:8:DT:OP2	2.05	0.57
2:B:230:TYR:HB2	2:B:263:ASN:ND2	2.19	0.57
1:C:12:DC:C6	1:C:13:DT:H72	2.40	0.57
2:B:461:PHE:CZ	2:B:465:ILE:HD11	2.40	0.57
1:C:18:DT:C2'	1:C:19:DG:H5'	2.35	0.57
2:B:421:ARG:O	2:B:425:VAL:HG23	2.04	0.57
2:B:569:GLN:HE22	2:B:609:LYS:HB3	1.70	0.57
2:A:217:ILE:C	2:A:218:LEU:HD12	2.24	0.57
2:A:53:SER:C	2:A:55:TYR:H	2.06	0.57
2:A:149:GLN:HG3	2:A:154:LEU:HB2	1.87	0.57
1:D:16:DA:H2''	1:D:17:DG:H5'	1.86	0.57
1:D:18:DT:H5'	2:B:419:GLY:N	2.20	0.57
2:A:568:PRO:HA	2:A:607:MET:HB2	1.87	0.57
2:B:104:ASP:HB3	2:B:203:LYS:HG3	1.85	0.57
2:A:506:ILE:O	2:A:510:GLU:HG3	2.05	0.57
2:B:483:ARG:NH1	2:B:483:ARG:HG2	2.20	0.57
2:A:374:TYR:HA	2:A:553:ALA:HB1	1.85	0.57
2:B:140:ARG:HG3	2:B:140:ARG:HH11	1.69	0.57
2:A:30:GLY:O	2:A:31:ALA:CB	2.52	0.57
2:A:325:ASN:ND2	2:A:327:LEU:HB2	2.18	0.56
2:A:112:GLN:HE21	2:A:113:ILE:H	1.50	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:298:GLU:HG3	2:B:303:ARG:NH2	2.20	0.56
2:B:543:GLY:O	2:B:544:GLU:CB	2.53	0.56
2:A:260:GLN:HA	2:A:260:GLN:HE21	1.70	0.56
2:B:154:LEU:HD23	2:B:158:HIS:HD2	1.70	0.56
2:B:550:TRP:O	2:B:552:ASP:N	2.38	0.56
2:A:119:GLN:NE2	2:A:143:MET:HE2	2.20	0.56
2:A:262:GLU:OE1	2:A:262:GLU:N	2.21	0.56
2:B:597:ARG:O	2:B:600:TYR:HB3	2.05	0.56
2:B:579:MET:HE2	2:B:618:ARG:NE	2.21	0.56
2:A:325:ASN:ND2	2:A:327:LEU:N	2.53	0.56
2:B:483:ARG:O	2:B:486:LYS:N	2.38	0.56
2:B:292:ALA:HA	2:B:637:PRO:HD2	1.88	0.56
2:B:337:ILE:HD12	2:B:350:CYS:SG	2.45	0.56
2:B:329:GLU:OE2	2:B:573:VAL:HG13	2.06	0.55
2:B:114:LEU:CD1	2:B:186:LEU:HD13	2.36	0.55
2:B:412:ASN:O	2:B:413:THR:HG23	2.05	0.55
2:B:161:SER:O	2:B:162:TYR:HB3	2.06	0.55
2:B:614:TYR:CE1	2:B:629:PRO:HG3	2.41	0.55
2:A:154:LEU:O	2:A:155:ARG:CB	2.54	0.55
2:B:284:ARG:HG3	2:B:284:ARG:HH11	1.71	0.55
2:B:410:VAL:HA	2:B:413:THR:OG1	2.05	0.55
2:B:299:ASN:HD21	2:B:635:GLU:HB3	1.71	0.55
2:B:198:GLU:O	2:B:202:ASN:ND2	2.39	0.55
1:C:11:DA:C2'	1:C:12:DC:H5''	2.36	0.55
2:A:402:ASN:HB3	2:A:436:THR:HG21	1.88	0.55
1:D:18:DT:H2''	1:D:19:DG:O5'	2.06	0.55
2:B:7:LEU:O	2:B:9:SER:N	2.39	0.55
2:A:349:GLU:HB3	2:A:568:PRO:HD2	1.89	0.55
2:A:80:THR:HG22	2:A:81:SER:H	1.71	0.55
2:A:199:LEU:HG	2:A:206:ILE:CD1	2.37	0.55
2:A:573:VAL:CG1	2:A:574:GLY:N	2.69	0.55
1:D:11:DA:H2''	1:D:12:DC:H5'	1.89	0.55
2:A:349:GLU:HB3	2:A:568:PRO:HG2	1.89	0.55
2:A:154:LEU:O	2:A:155:ARG:HB2	2.06	0.55
2:A:292:ALA:HB1	2:A:636:LEU:HD22	1.88	0.55
2:A:202:ASN:O	2:A:204:PRO:HD3	2.07	0.55
1:D:28:DG:H4'	1:D:28:DG:OP1	2.06	0.55
1:D:20:DC:H2''	1:D:21:DA:C8	2.42	0.55
1:C:33:DT:H3'	2:A:540:LEU:O	2.07	0.55
2:B:368:LEU:HD21	2:B:374:TYR:HE2	1.71	0.55
2:A:394:TYR:CE2	2:A:488:SER:HB2	2.42	0.55
2:A:403:ASP:HB3	2:A:406:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:348:ALA:HA	2:A:553:ALA:O	2.07	0.55
2:B:341:GLN:NE2	2:B:347:LEU:HD21	2.21	0.54
2:A:394:TYR:O	2:A:398:ILE:HG13	2.07	0.54
2:A:125:ARG:NE	2:A:408:GLU:OE1	2.40	0.54
2:B:495:GLU:HA	2:B:506:ILE:HD11	1.90	0.54
2:A:619:ARG:HG3	2:A:623:LYS:O	2.07	0.54
2:B:350:CYS:O	2:B:351:ALA:HB2	2.07	0.54
2:B:35:LYS:HE2	2:B:221:GLU:OE2	2.07	0.54
2:B:32:GLY:O	2:B:283:TYR:HD1	1.91	0.54
2:A:360:SER:O	2:A:364:GLU:HG3	2.07	0.54
2:B:603:VAL:C	2:B:605:ARG:N	2.61	0.54
2:B:325:ASN:HD22	2:B:325:ASN:N	2.05	0.54
2:A:394:TYR:CE1	2:A:410:VAL:HB	2.43	0.54
2:A:137:TRP:CZ3	2:A:169:THR:HB	2.43	0.54
2:B:61:THR:HB	2:B:67:ALA:HB2	1.89	0.54
1:C:2:DG:H4'	2:B:361:ARG:NH1	2.23	0.54
1:C:17:DG:H2''	1:C:18:DT:H5'	1.89	0.54
2:A:567:PHE:O	2:A:607:MET:HG3	2.08	0.54
2:B:150:LYS:HE2	2:B:178:GLN:NE2	2.22	0.54
2:B:44:ALA:CB	2:B:77:LEU:HD23	2.37	0.54
1:D:32:DT:H2''	1:D:33:DT:C6	2.42	0.54
2:B:172:LYS:O	2:B:175:GLN:HB3	2.07	0.54
2:A:576:GLU:OE2	2:A:627:HIS:HD2	1.90	0.54
2:B:49:VAL:C	2:B:51:ASN:H	2.11	0.54
2:B:618:ARG:HH11	2:B:618:ARG:CB	2.19	0.54
2:B:61:THR:HG22	2:B:62:PHE:N	2.15	0.54
2:B:27:VAL:O	2:B:29:ALA:N	2.41	0.54
2:B:112:GLN:HB3	2:B:186:LEU:HD23	1.88	0.53
2:B:398:ILE:HA	2:B:401:ARG:NH2	2.22	0.53
2:A:81:SER:O	2:A:82:GLN:HB2	2.08	0.53
2:B:326:GLU:HA	2:B:329:GLU:HB3	1.89	0.53
2:B:570:VAL:C	2:B:571:PHE:CD2	2.82	0.53
1:D:25:DC:H2''	1:D:26:DT:OP2	2.08	0.53
2:B:381:ARG:HB3	2:B:543:GLY:N	2.23	0.53
2:B:203:LYS:N	2:B:204:PRO:HD3	2.23	0.53
2:B:606:ALA:HB2	2:B:610:LEU:HD22	1.91	0.53
2:A:153:GLY:HA2	2:A:194:LEU:HD13	1.90	0.53
2:B:642:GLU:HG2	2:B:643:GLU:O	2.09	0.53
2:A:442:ARG:NH1	2:A:442:ARG:HG2	2.22	0.53
2:A:202:ASN:C	2:A:204:PRO:HD3	2.29	0.53
2:A:30:GLY:N	2:A:33:SER:OG	2.41	0.53
2:A:400:ASN:HD21	2:A:402:ASN:HB2	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:149:GLN:HG3	2:B:154:LEU:HB2	1.89	0.53
2:B:298:GLU:CG	2:B:303:ARG:HH21	2.21	0.53
2:A:53:SER:C	2:A:55:TYR:N	2.62	0.53
2:B:376:ILE:HG22	2:B:377:TYR:N	2.24	0.53
2:B:556:LEU:N	2:B:556:LEU:HD12	2.24	0.53
2:B:458:LEU:O	2:B:461:PHE:HB3	2.09	0.53
2:B:436:THR:HG1	2:B:439:GLN:HG3	1.74	0.53
1:D:32:DT:H3'	2:B:381:ARG:HH22	1.74	0.53
2:B:109:GLN:NE2	2:B:528:LEU:HD23	2.23	0.53
2:A:54:PRO:O	2:A:85:MET:HA	2.10	0.52
2:B:385:ARG:HG2	2:B:385:ARG:HH21	1.74	0.52
2:B:396:ARG:HB3	2:B:403:ASP:OD2	2.10	0.52
2:A:158:HIS:O	2:A:160:GLN:N	2.43	0.52
2:B:554:VAL:CG1	2:B:555:GLN:H	2.23	0.52
2:B:407:PHE:O	2:B:409:ARG:N	2.41	0.52
2:A:264:ILE:CG2	2:A:265:GLN:N	2.71	0.52
2:B:443:GLU:O	2:B:447:GLU:HG3	2.10	0.52
2:B:352:ILE:C	2:B:353:LEU:HD23	2.30	0.52
2:B:244:MET:HG2	2:B:245:ILE:N	2.25	0.52
1:C:5:DC:H2''	1:C:6:DA:C8	2.45	0.52
2:B:435:LEU:HB3	2:B:439:GLN:HB2	1.91	0.52
2:A:156:PRO:HG2	2:A:157:HIS:H	1.75	0.52
2:B:340:TRP:O	2:B:345:GLY:HA3	2.09	0.52
2:B:253:ILE:HD13	2:B:253:ILE:N	2.25	0.52
2:B:470:GLN:O	2:B:472:THR:N	2.43	0.52
2:A:80:THR:HG22	2:A:81:SER:N	2.24	0.52
1:D:32:DT:C4	2:B:257:ARG:HD2	2.45	0.52
2:B:265:GLN:NE2	2:B:269:ASN:OD1	2.43	0.52
2:B:643:GLU:HG3	2:B:644:VAL:H	1.74	0.52
2:B:601:VAL:HG12	2:B:605:ARG:NH1	2.25	0.52
2:B:438:TRP:HZ3	2:B:465:ILE:HD12	1.75	0.52
2:B:107:LEU:HD21	2:B:195:ARG:NE	2.24	0.52
2:B:621:TYR:O	2:B:621:TYR:CD1	2.63	0.52
2:A:126:LEU:O	2:A:127:ILE:C	2.48	0.52
2:B:294:ASN:HA	2:B:297:ILE:HG22	1.92	0.52
2:A:339:THR:O	2:A:342:ASP:N	2.43	0.52
2:B:472:THR:CG2	2:B:480:GLN:HE21	2.23	0.52
2:B:61:THR:HG21	2:B:66:ALA:HB3	1.92	0.52
2:A:642:GLU:HG2	2:A:643:GLU:O	2.09	0.52
2:A:5:TYR:CZ	2:A:6:LEU:HD21	2.45	0.52
2:A:446:GLN:C	2:A:448:LYS:H	2.12	0.52
2:B:306:LYS:HE3	2:B:600:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:128:LYS:C	2:B:130:MET:H	2.13	0.51
2:B:156:PRO:HG2	2:B:157:HIS:H	1.74	0.51
2:B:571:PHE:N	2:B:571:PHE:HD2	2.07	0.51
2:A:264:ILE:HG23	2:A:265:GLN:N	2.25	0.51
2:B:34:GLY:O	2:B:37:ARG:HB3	2.10	0.51
2:A:385:ARG:HH21	2:A:385:ARG:HG2	1.74	0.51
2:A:193:LEU:CD1	2:A:229:GLN:HE21	2.24	0.51
2:B:618:ARG:O	2:B:618:ARG:HG3	2.11	0.51
2:B:207:LEU:O	2:B:211:ARG:HG3	2.10	0.51
2:A:318:ILE:HD12	2:A:318:ILE:N	2.25	0.51
2:A:320:LEU:O	2:A:644:VAL:HB	2.10	0.51
1:D:7:DC:C2'	1:D:8:DT:C6	2.93	0.51
2:B:420:ASP:OD2	2:B:420:ASP:N	2.35	0.51
1:C:11:DA:H2''	1:C:12:DC:H5''	1.88	0.51
2:B:112:GLN:HG2	2:B:396:ARG:NH1	2.18	0.51
2:A:442:ARG:HG2	2:A:442:ARG:HH11	1.75	0.51
2:B:577:GLU:O	2:B:627:HIS:HB3	2.11	0.51
1:C:30:DT:H2''	1:C:31:DG:H5'	1.92	0.51
2:A:161:SER:OG	2:A:162:TYR:N	2.42	0.51
2:B:224:ASP:HA	2:B:259:ALA:HB1	1.91	0.51
2:B:554:VAL:CG1	2:B:555:GLN:N	2.73	0.51
2:A:252:SER:H	2:A:597:ARG:HD2	1.76	0.51
2:B:492:THR:HG22	2:B:493:MET:N	2.26	0.51
2:B:292:ALA:HB1	2:B:636:LEU:HD22	1.92	0.51
2:B:156:PRO:HD3	2:B:174:TYR:CE1	2.39	0.50
2:B:634:GLY:C	2:B:636:LEU:H	2.14	0.50
2:B:411:VAL:HG13	2:B:412:ASN:N	2.26	0.50
2:B:414:PRO:HA	2:B:493:MET:CE	2.41	0.50
1:C:8:DT:H2''	1:C:9:DG:C8	2.46	0.50
2:A:119:GLN:NE2	2:A:143:MET:CE	2.74	0.50
2:B:385:ARG:HG2	2:B:385:ARG:NH2	2.25	0.50
2:B:531:LEU:O	2:B:534:PHE:N	2.44	0.50
2:A:99:ARG:HD3	2:A:111:PHE:CE2	2.46	0.50
2:A:411:VAL:HG13	2:A:412:ASN:N	2.26	0.50
2:B:150:LYS:CE	2:B:178:GLN:HE22	2.24	0.50
2:B:30:GLY:O	2:B:31:ALA:HB2	2.10	0.50
1:C:32:DT:C4	2:A:257:ARG:HD2	2.46	0.50
2:B:382:PHE:HA	2:B:385:ARG:HD2	1.92	0.50
2:B:49:VAL:O	2:B:51:ASN:N	2.44	0.50
2:B:389:LYS:HB2	2:B:409:ARG:NH2	2.26	0.50
2:B:603:VAL:O	2:B:605:ARG:N	2.44	0.50
2:B:401:ARG:HG2	2:B:438:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:642:GLU:O	2:A:643:GLU:O	2.30	0.50
2:B:12:ASP:HA	2:B:15:ARG:HD3	1.93	0.50
2:A:220:ASP:O	2:A:221:GLU:C	2.50	0.50
2:B:114:LEU:HD13	2:B:186:LEU:HB3	1.92	0.50
2:B:39:LEU:O	2:B:43:ILE:HG13	2.12	0.50
2:B:610:LEU:HD12	2:B:610:LEU:C	2.32	0.50
2:B:360:SER:O	2:B:364:GLU:HG3	2.12	0.50
1:D:1:DC:C2	2:A:621:TYR:HB2	2.47	0.50
2:B:368:LEU:C	2:B:370:ALA:H	2.15	0.50
2:A:596:ARG:NH1	2:A:635:GLU:OE1	2.45	0.50
2:B:579:MET:HE2	2:B:618:ARG:HE	1.77	0.50
2:A:36:THR:HG22	2:A:73:ARG:HH21	1.75	0.50
2:B:631:ARG:O	2:B:635:GLU:HG3	2.12	0.50
2:B:10:LEU:HD13	2:B:18:VAL:HG21	1.93	0.50
1:D:6:DA:H2'	1:D:7:DC:H6	1.76	0.50
2:A:102:HIS:CD2	2:A:109:GLN:HB2	2.47	0.50
2:B:401:ARG:NH2	2:B:469:ALA:HB2	2.21	0.49
1:D:16:DA:H2''	2:B:421:ARG:NH1	2.27	0.49
1:C:18:DT:O5'	2:A:419:GLY:HA3	2.12	0.49
2:B:501:LYS:HE3	2:B:505:ARG:NH1	2.25	0.49
2:B:264:ILE:CG2	2:B:265:GLN:N	2.75	0.49
2:B:382:PHE:HD2	2:B:383:PHE:HD2	1.60	0.49
2:A:416:ARG:HB2	2:A:418:ILE:CD1	2.41	0.49
2:A:425:VAL:HG11	2:A:450:LEU:HD21	1.95	0.49
2:A:352:ILE:HG21	2:A:363:LEU:HD13	1.95	0.49
2:B:39:LEU:HD11	2:B:246:VAL:HG21	1.93	0.49
2:A:149:GLN:CA	2:A:149:GLN:HE21	2.26	0.49
2:B:644:VAL:HG12	2:B:644:VAL:O	2.13	0.49
2:B:290:LEU:CD1	2:B:310:THR:HB	2.43	0.49
2:B:401:ARG:HG2	2:B:438:TRP:CE2	2.48	0.49
2:B:472:THR:OG1	2:B:480:GLN:HG3	2.13	0.49
1:D:9:DG:H2''	1:D:10:DC:O5'	2.13	0.49
2:A:568:PRO:CD	2:A:607:MET:HE3	2.42	0.49
2:B:370:ALA:O	2:B:371:SER:C	2.51	0.49
2:B:119:GLN:HE22	2:B:147:ASN:HD21	1.60	0.49
2:B:472:THR:CA	2:B:475:MET:SD	2.99	0.48
2:B:154:LEU:HD23	2:B:158:HIS:CD2	2.47	0.48
2:B:596:ARG:HG3	2:B:596:ARG:HH11	1.78	0.48
2:B:223:GLN:OE1	2:B:223:GLN:N	2.40	0.48
2:A:374:TYR:HE1	2:A:376:ILE:HD11	1.77	0.48
2:A:614:TYR:CE1	2:A:629:PRO:HG3	2.48	0.48
2:B:401:ARG:HG2	2:B:438:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:115:ASP:OD1	2:A:389:LYS:NZ	2.37	0.48
2:B:609:LYS:HG3	2:B:610:LEU:N	2.28	0.48
1:C:5:DC:H2''	1:C:6:DA:N7	2.29	0.48
2:A:461:PHE:O	2:A:464:LEU:HB3	2.13	0.48
2:B:68:ALA:HA	2:B:71:ARG:HH12	1.77	0.48
2:B:333:VAL:HG13	2:B:571:PHE:CD1	2.48	0.48
2:A:19:ALA:HA	2:A:45:TRP:CE2	2.49	0.48
2:A:5:TYR:CE1	2:A:6:LEU:CD2	2.97	0.48
2:B:545:GLY:O	2:B:546:GLN:CB	2.62	0.48
2:A:398:ILE:HG23	2:A:469:ALA:HA	1.94	0.48
2:A:172:LYS:O	2:A:175:GLN:HB3	2.14	0.48
2:A:481:THR:O	2:A:485:ILE:HG13	2.13	0.48
2:B:41:HIS:HD1	2:B:77:LEU:HD21	1.78	0.48
2:A:37:ARG:CZ	3:A:681:GOL:H2	2.44	0.48
2:B:394:TYR:O	2:B:398:ILE:HG12	2.13	0.48
2:A:392:LEU:O	2:A:396:ARG:HG3	2.14	0.48
2:B:407:PHE:C	2:B:409:ARG:H	2.17	0.48
2:B:219:VAL:HG21	2:B:233:ILE:HD13	1.96	0.48
2:A:112:GLN:CG	2:A:396:ARG:NH1	2.75	0.48
2:B:339:THR:HG23	2:B:340:TRP:N	2.29	0.48
2:A:614:TYR:CD1	2:A:614:TYR:O	2.66	0.48
2:B:112:GLN:HE21	2:B:113:ILE:HD12	1.77	0.48
1:C:21:DA:H2''	1:C:22:DG:H5'	1.95	0.48
2:A:349:GLU:HB3	2:A:568:PRO:CD	2.44	0.48
2:A:82:GLN:HB3	2:A:85:MET:HE3	1.96	0.48
2:B:505:ARG:HG2	2:B:505:ARG:HH11	1.79	0.48
2:A:483:ARG:NH1	2:A:483:ARG:HG3	2.28	0.48
2:A:235:LEU:C	2:A:237:ALA:H	2.16	0.48
1:D:18:DT:C5'	2:B:419:GLY:HA3	2.42	0.47
2:B:252:SER:CB	2:B:261:VAL:HG22	2.44	0.47
2:B:376:ILE:HD13	2:B:556:LEU:HB2	1.96	0.47
2:A:150:LYS:HZ1	2:A:178:GLN:HE22	1.60	0.47
2:A:431:ARG:NH1	2:A:431:ARG:HG3	2.29	0.47
2:B:11:ASN:ND2	2:B:283:TYR:OH	2.47	0.47
2:A:35:LYS:HE2	2:A:220:ASP:OD1	2.14	0.47
2:B:68:ALA:HA	2:B:71:ARG:NH1	2.29	0.47
2:B:134:GLU:C	2:B:136:GLN:H	2.17	0.47
2:B:250:ASP:HB3	2:B:600:TYR:CE2	2.48	0.47
2:A:349:GLU:O	2:A:568:PRO:HD2	2.13	0.47
2:B:220:ASP:O	2:B:221:GLU:C	2.52	0.47
2:B:336:ARG:O	2:B:339:THR:HG22	2.13	0.47
2:B:570:VAL:C	2:B:571:PHE:HD2	2.18	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:579:MET:HE1	2:B:618:ARG:HD2	1.95	0.47
2:B:400:ASN:ND2	2:B:402:ASN:N	2.58	0.47
2:A:235:LEU:N	2:A:235:LEU:HD23	2.28	0.47
2:B:564:GLY:C	2:B:565:LEU:HD23	2.33	0.47
2:A:438:TRP:CE2	2:A:462:MET:HE3	2.50	0.47
2:A:407:PHE:O	2:A:409:ARG:N	2.47	0.47
2:A:375:ARG:NH1	2:A:548:ASP:CB	2.77	0.47
2:A:385:ARG:NH2	2:A:385:ARG:HG2	2.29	0.47
2:A:271:PHE:N	2:A:271:PHE:CD1	2.83	0.47
2:B:401:ARG:HG2	2:B:438:TRP:CZ2	2.49	0.47
2:A:413:THR:CA	2:A:414:PRO:C	2.81	0.47
2:B:231:ALA:O	2:B:234:ARG:HG2	2.15	0.47
2:A:459:GLN:HE21	2:A:463:GLU:HG2	1.78	0.47
2:B:565:LEU:HD23	2:B:565:LEU:N	2.30	0.47
2:A:272:PRO:C	2:A:274:ALA:N	2.67	0.47
2:A:530:PRO:O	2:A:533:ALA:HB3	2.14	0.47
2:B:506:ILE:O	2:B:510:GLU:HG2	2.15	0.47
2:B:321:TYR:HE2	2:B:323:ALA:CB	2.27	0.47
2:A:325:ASN:ND2	2:A:327:LEU:H	2.13	0.47
2:B:407:PHE:C	2:B:409:ARG:N	2.68	0.47
2:A:214:PHE:HB2	2:A:236:LEU:HD11	1.97	0.47
2:B:454:ALA:O	2:B:457:ALA:N	2.47	0.47
2:A:283:TYR:CZ	3:A:681:GOL:H12	2.50	0.47
2:A:498:LYS:HD3	2:A:498:LYS:H	1.80	0.47
2:B:583:GLN:C	2:B:585:SER:H	2.18	0.46
2:B:354:TYR:CE2	2:B:360:SER:HB3	2.50	0.46
2:A:472:THR:O	2:A:472:THR:HG22	2.15	0.46
2:B:256:TRP:C	2:B:258:GLY:H	2.18	0.46
1:D:17:DG:C3'	2:B:421:ARG:HD2	2.46	0.46
2:B:337:ILE:HD11	2:B:571:PHE:CE2	2.50	0.46
2:A:206:ILE:HG13	2:A:207:LEU:N	2.30	0.46
2:B:164:ASN:CG	2:B:164:ASN:O	2.52	0.46
2:A:134:GLU:C	2:A:136:GLN:N	2.68	0.46
2:B:104:ASP:HA	2:B:203:LYS:NZ	2.30	0.46
2:B:119:GLN:HG2	2:B:143:MET:HE3	1.96	0.46
2:A:272:PRO:C	2:A:274:ALA:H	2.19	0.46
1:C:24:DG:H2''	1:C:25:DC:OP2	2.15	0.46
2:B:205:HIS:CE1	2:B:206:ILE:HG13	2.50	0.46
2:B:601:VAL:HG12	2:B:605:ARG:HH11	1.79	0.46
2:A:199:LEU:HG	2:A:206:ILE:HD11	1.97	0.46
2:A:80:THR:CG2	2:A:81:SER:H	2.25	0.46
1:C:17:DG:C8	2:A:421:ARG:NH1	2.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:286:THR:HG23	2:A:607:MET:O	2.15	0.46
2:B:483:ARG:O	2:B:484:VAL:C	2.54	0.46
2:B:407:PHE:CD2	2:B:407:PHE:C	2.88	0.46
2:B:245:ILE:HG13	2:B:245:ILE:O	2.15	0.46
2:B:331:ARG:HH11	2:B:331:ARG:HG3	1.80	0.46
2:B:157:HIS:O	2:B:157:HIS:CG	2.68	0.46
2:B:401:ARG:HG2	2:B:438:TRP:CD2	2.51	0.46
2:A:546:GLN:O	2:A:547:ALA:C	2.53	0.46
2:A:37:ARG:HG2	2:A:41:HIS:HD2	1.81	0.46
2:A:368:LEU:O	2:A:371:SER:N	2.47	0.46
2:A:34:GLY:HA2	4:A:682:FMT:H	1.97	0.46
2:A:207:LEU:HD21	2:A:211:ARG:NH2	2.30	0.46
2:B:62:PHE:CE1	2:B:90:PHE:HE1	2.34	0.46
2:B:299:ASN:ND2	2:B:635:GLU:HB3	2.31	0.46
2:B:548:ASP:O	2:B:549:THR:C	2.53	0.46
2:A:483:ARG:CG	2:A:483:ARG:HH11	2.28	0.46
2:A:29:ALA:O	2:A:248:ASP:HB2	2.15	0.46
2:B:47:MET:CE	2:B:78:MET:HG2	2.46	0.46
1:D:4:DG:H2"	1:D:5:DC:OP2	2.15	0.46
2:B:420:ASP:O	2:B:421:ARG:C	2.54	0.46
2:B:644:VAL:O	2:B:646:LEU:N	2.41	0.46
2:B:278:ARG:HH11	2:B:278:ARG:HG3	1.81	0.46
2:A:504:THR:O	2:A:507:GLU:HB2	2.16	0.46
2:A:441:CYS:O	2:A:442:ARG:C	2.53	0.46
2:B:373:PRO:HB2	2:B:553:ALA:HB2	1.96	0.46
2:B:286:THR:OG1	2:B:289:ILE:HD13	2.16	0.46
1:D:16:DA:H1'	1:D:17:DG:H5"	1.98	0.46
2:B:329:GLU:O	2:B:333:VAL:HG23	2.16	0.46
2:B:346:ALA:HB3	2:B:349:GLU:OE1	2.16	0.46
2:B:260:GLN:C	2:B:262:GLU:N	2.69	0.46
2:A:154:LEU:O	2:A:155:ARG:HG2	2.16	0.46
2:B:290:LEU:HD12	2:B:310:THR:HB	1.98	0.46
2:A:425:VAL:HG12	2:A:444:LEU:CD1	2.46	0.46
2:A:584:MET:O	2:A:588:GLU:CB	2.64	0.46
2:B:401:ARG:HG2	2:B:438:TRP:CE3	2.51	0.46
2:B:11:ASN:OD1	2:B:11:ASN:O	2.34	0.46
2:A:151:ASP:O	2:A:228:ILE:HB	2.16	0.46
2:A:193:LEU:HD13	2:A:229:GLN:HE21	1.81	0.46
2:B:569:GLN:NE2	2:B:609:LYS:HB3	2.31	0.46
2:B:146:ILE:HG23	2:B:174:TYR:CD2	2.51	0.45
2:B:22:ARG:O	2:B:23:SER:CB	2.64	0.45
2:B:299:ASN:HB2	2:B:596:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:133:ASP:O	2:B:135:LYS:N	2.49	0.45
2:B:353:LEU:HD22	2:B:557:MET:HG2	1.99	0.45
2:B:284:ARG:O	2:B:607:MET:HA	2.15	0.45
2:B:135:LYS:O	2:B:138:PRO:HD3	2.17	0.45
2:A:533:ALA:O	2:A:536:SER:HB3	2.16	0.45
2:A:535:LEU:HD23	2:A:535:LEU:HA	1.76	0.45
2:A:325:ASN:HD22	2:A:328:ASP:H	1.64	0.45
1:C:16:DA:H2''	1:C:17:DG:H5'	1.98	0.45
2:A:114:LEU:CD1	2:A:186:LEU:HD13	2.47	0.45
2:A:570:VAL:HG22	2:A:610:LEU:HD13	1.97	0.45
2:B:156:PRO:CD	2:B:174:TYR:HE1	2.26	0.45
2:B:609:LYS:HG3	2:B:610:LEU:H	1.82	0.45
1:C:6:DA:H2'	1:C:7:DC:C6	2.51	0.45
2:B:264:ILE:HG23	2:B:265:GLN:N	2.32	0.45
2:A:428:GLN:O	2:A:431:ARG:N	2.49	0.45
2:A:446:GLN:C	2:A:448:LYS:N	2.70	0.45
1:D:4:DG:H1'	1:D:5:DC:H5'	1.98	0.45
2:B:92:GLY:O	2:B:95:HIS:HB3	2.17	0.45
2:B:618:ARG:CB	2:B:618:ARG:NH1	2.79	0.45
1:D:33:DT:H4'	2:B:91:HIS:HD2	1.81	0.45
1:D:15:DG:H5'	2:A:453:ARG:HG2	1.98	0.45
2:A:349:GLU:HB3	2:A:568:PRO:CG	2.46	0.45
2:A:457:ALA:CA	2:A:460:ARG:NH2	2.78	0.45
2:B:370:ALA:O	2:B:372:MET:N	2.49	0.45
2:B:43:ILE:HG23	2:B:57:ILE:HG21	1.95	0.45
2:B:57:ILE:HG21	2:B:85:MET:HE2	1.99	0.45
2:A:174:TYR:CD1	2:A:174:TYR:C	2.90	0.45
2:A:175:GLN:HA	2:A:175:GLN:NE2	2.31	0.45
2:A:29:ALA:HA	2:A:279:LEU:HB2	1.99	0.45
2:B:624:GLU:HA	2:B:624:GLU:OE2	2.17	0.45
1:D:16:DA:H2''	2:B:421:ARG:HH12	1.81	0.45
2:A:47:MET:HE1	2:A:78:MET:HG3	1.98	0.45
2:A:457:ALA:HA	2:A:460:ARG:CZ	2.47	0.45
2:A:3:VAL:HG23	2:A:4:SER:N	2.31	0.45
2:B:392:LEU:O	2:B:396:ARG:HG3	2.16	0.45
2:B:397:LEU:HD13	2:B:465:ILE:CD1	2.47	0.45
2:B:24:ASN:O	2:B:25:LEU:HB3	2.17	0.45
2:B:40:VAL:HG21	2:B:73:ARG:HD3	1.97	0.45
2:B:11:ASN:O	2:B:13:LYS:N	2.49	0.45
2:A:149:GLN:CD	2:A:154:LEU:HD12	2.38	0.45
2:B:295:ALA:HB3	2:B:637:PRO:HD3	1.98	0.45
2:A:339:THR:O	2:A:340:TRP:C	2.54	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:127:ILE:HG22	2:B:128:LYS:N	2.31	0.45
2:A:235:LEU:C	2:A:237:ALA:N	2.69	0.45
2:B:378:GLY:O	2:B:379:GLY:O	2.35	0.44
2:B:613:THR:O	2:B:614:TYR:HB3	2.17	0.44
2:A:368:LEU:HD23	2:A:368:LEU:HA	1.73	0.44
2:A:61:THR:HG21	2:A:66:ALA:HB1	1.98	0.44
2:A:326:GLU:OE2	2:A:327:LEU:HD22	2.17	0.44
2:A:118:ASP:OD2	2:A:396:ARG:NH2	2.50	0.44
2:B:134:GLU:O	2:B:136:GLN:N	2.48	0.44
2:B:101:HIS:HB3	2:B:104:ASP:OD2	2.18	0.44
2:A:250:ASP:CG	2:A:303:ARG:HE	2.20	0.44
2:B:576:GLU:N	2:B:630:SER:OG	2.51	0.44
1:D:25:DC:H2''	1:D:26:DT:H72	1.99	0.44
2:B:368:LEU:CD2	2:B:374:TYR:HE2	2.30	0.44
2:B:162:TYR:N	2:B:168:GLN:HE21	2.16	0.44
2:A:134:GLU:O	2:A:136:GLN:HG3	2.18	0.44
2:A:472:THR:HG21	2:A:480:GLN:CG	2.43	0.44
1:D:1:DC:H6	1:D:1:DC:O5'	2.01	0.44
2:B:282:ASN:HB3	2:B:290:LEU:HD11	1.98	0.44
2:A:483:ARG:NH1	2:A:483:ARG:CG	2.80	0.44
2:B:403:ASP:O	2:B:405:ALA:N	2.50	0.44
2:A:114:LEU:HD23	2:A:119:GLN:HB2	1.99	0.44
2:B:91:HIS:CE1	2:B:193:LEU:HD11	2.53	0.44
2:A:428:GLN:HG2	2:A:432:ASP:OD2	2.17	0.44
2:B:236:LEU:HD12	2:B:236:LEU:HA	1.80	0.44
2:A:11:ASN:OD1	2:A:11:ASN:C	2.56	0.44
2:A:546:GLN:O	2:A:548:ASP:N	2.51	0.44
2:A:472:THR:HG23	2:A:480:GLN:HB2	1.98	0.44
2:B:339:THR:CG2	2:B:340:TRP:N	2.81	0.44
2:A:167:GLU:O	2:A:171:GLN:HB2	2.18	0.44
1:C:11:DA:C1'	1:C:12:DC:H5''	2.47	0.43
2:B:605:ARG:NE	2:B:605:ARG:HA	2.33	0.43
2:A:217:ILE:HD11	2:A:236:LEU:HG	2.00	0.43
2:B:39:LEU:HD21	2:B:246:VAL:CG2	2.47	0.43
2:A:5:TYR:CZ	2:A:6:LEU:CD2	3.01	0.43
2:A:394:TYR:CZ	2:A:410:VAL:HB	2.53	0.43
2:B:369:GLN:O	2:B:369:GLN:HG3	2.17	0.43
2:B:155:ARG:HA	2:B:155:ARG:HD3	1.73	0.43
2:B:113:ILE:H	2:B:113:ILE:CD1	2.26	0.43
2:A:133:ASP:O	2:A:134:GLU:C	2.56	0.43
2:B:517:ARG:O	2:B:517:ARG:HG2	2.19	0.43
2:B:641:VAL:CG1	2:B:642:GLU:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:59:ALA:HB3	2:B:87:VAL:HG22	2.00	0.43
2:B:610:LEU:HD11	2:B:612:LEU:HD21	2.01	0.43
2:B:42:ARG:NE	2:B:46:LEU:HD21	2.34	0.43
2:B:386:GLN:NE2	2:B:505:ARG:HH21	2.16	0.43
2:A:149:GLN:HA	2:A:149:GLN:NE2	2.33	0.43
2:A:179:GLU:HB2	2:A:183:ARG:HH12	1.83	0.43
2:B:350:CYS:HA	2:B:569:GLN:O	2.18	0.43
2:A:644:VAL:CG1	2:A:644:VAL:O	2.58	0.43
2:B:39:LEU:HD23	2:B:218:LEU:HD23	1.99	0.43
2:B:127:ILE:HG21	2:B:133:ASP:HB3	2.01	0.43
2:A:24:ASN:O	2:A:274:ALA:HA	2.18	0.43
2:B:579:MET:CE	2:B:618:ARG:HE	2.32	0.43
2:B:512:LEU:O	2:B:512:LEU:HD12	2.19	0.43
2:B:27:VAL:HG12	2:B:27:VAL:O	2.18	0.43
1:D:31:DG:N3	1:D:32:DT:H72	2.33	0.43
2:B:102:HIS:HB2	2:B:107:LEU:O	2.19	0.43
1:C:1:DC:H4'	2:B:619:ARG:NH1	2.34	0.43
2:A:575:MET:C	2:A:630:SER:OG	2.57	0.43
2:A:626:TYR:N	2:A:626:TYR:CD1	2.87	0.43
2:A:550:TRP:O	2:A:550:TRP:CD1	2.72	0.43
2:B:579:MET:O	2:B:582:SER:HA	2.18	0.43
2:A:459:GLN:HE21	2:A:463:GLU:CG	2.32	0.43
2:B:637:PRO:HB2	2:B:640:CYS:SG	2.59	0.43
2:A:84:GLY:O	2:A:213:ARG:NH2	2.51	0.43
2:A:387:GLU:HG2	2:A:388:ILE:HD13	2.00	0.43
2:A:320:LEU:HA	2:A:612:LEU:O	2.18	0.43
2:A:42:ARG:O	2:A:45:TRP:HB3	2.19	0.43
2:A:54:PRO:O	2:A:85:MET:CA	2.67	0.43
2:A:422:THR:O	2:A:426:VAL:HG23	2.19	0.43
2:A:39:LEU:HD21	2:A:246:VAL:CG2	2.49	0.43
2:B:31:ALA:O	2:B:282:ASN:ND2	2.52	0.43
2:A:109:GLN:NE2	2:A:528:LEU:HD23	2.33	0.43
2:B:301:ASN:N	2:B:301:ASN:OD1	2.52	0.43
1:D:18:DT:O3'	2:B:417:GLY:HA2	2.19	0.42
2:B:250:ASP:O	2:B:597:ARG:HB3	2.19	0.42
2:B:403:ASP:O	2:B:406:ALA:N	2.52	0.42
2:A:568:PRO:HB3	2:A:608:GLN:NE2	2.33	0.42
2:B:643:GLU:HG3	2:B:644:VAL:N	2.34	0.42
2:B:150:LYS:CE	2:B:178:GLN:NE2	2.81	0.42
2:A:23:SER:CA	2:A:242:LYS:HG3	2.49	0.42
2:B:156:PRO:O	2:B:171:GLN:NE2	2.52	0.42
2:B:579:MET:CE	2:B:618:ARG:NE	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:24:DG:H2''	1:D:25:DC:C6	2.54	0.42
2:A:567:PHE:C	2:A:607:MET:HG3	2.39	0.42
2:B:325:ASN:HA	2:B:617:THR:O	2.18	0.42
2:B:325:ASN:ND2	2:B:325:ASN:N	2.67	0.42
2:B:513:VAL:O	2:B:514:THR:C	2.58	0.42
2:A:356:SER:OG	2:A:359:GLN:HG3	2.19	0.42
1:D:17:DG:H2'	2:B:421:ARG:HD2	2.01	0.42
2:B:57:ILE:N	2:B:57:ILE:HD12	2.34	0.42
1:D:10:DC:C2'	1:D:11:DA:C8	2.98	0.42
2:B:641:VAL:HG12	2:B:642:GLU:H	1.83	0.42
2:B:139:PRO:O	2:B:142:ALA:HB3	2.20	0.42
1:D:17:DG:H8	2:B:421:ARG:NH1	2.17	0.42
2:B:476:PRO:HG2	2:B:479:VAL:HB	2.01	0.42
2:A:252:SER:CB	2:A:261:VAL:HG22	2.49	0.42
2:B:386:GLN:HG3	2:B:387:GLU:N	2.34	0.42
2:B:234:ARG:HG3	2:B:235:LEU:H	1.83	0.42
2:B:225:THR:HA	2:B:229:GLN:OE1	2.19	0.42
2:A:411:VAL:HG13	2:A:412:ASN:H	1.85	0.42
2:A:93:LEU:O	2:A:94:ALA:C	2.56	0.42
2:B:328:ASP:O	2:B:329:GLU:C	2.57	0.42
2:B:114:LEU:HD11	2:B:186:LEU:HD13	2.00	0.42
2:B:400:ASN:ND2	2:B:402:ASN:HB2	2.09	0.42
2:A:123:LEU:O	2:A:124:LYS:C	2.58	0.42
1:C:6:DA:C2'	1:C:7:DC:C6	3.03	0.42
2:B:506:ILE:O	2:B:509:LEU:HB2	2.20	0.42
2:A:129:ALA:O	2:A:130:MET:HG3	2.18	0.42
2:B:202:ASN:C	2:B:204:PRO:HD3	2.39	0.42
2:A:125:ARG:HE	2:A:408:GLU:CD	2.23	0.42
2:A:226:ASN:OD1	2:A:229:GLN:HB2	2.20	0.42
1:C:14:DC:O2	2:B:453:ARG:NH2	2.52	0.42
1:D:6:DA:OP1	2:A:124:LYS:CE	2.67	0.42
1:C:6:DA:H2'	1:C:7:DC:H6	1.84	0.42
1:D:12:DC:C6	1:D:13:DT:H72	2.55	0.42
2:B:265:GLN:HG3	2:B:269:ASN:HD21	1.85	0.42
2:B:290:LEU:O	2:B:294:ASN:ND2	2.52	0.42
2:B:578:GLY:O	2:B:583:GLN:N	2.53	0.42
2:B:113:ILE:N	2:B:113:ILE:CD1	2.82	0.42
2:B:413:THR:HA	2:B:414:PRO:C	2.40	0.42
2:A:128:LYS:C	2:A:130:MET:H	2.23	0.42
2:B:146:ILE:HG12	2:B:174:TYR:HD2	1.84	0.42
2:B:473:ALA:C	2:B:475:MET:H	2.22	0.42
2:A:642:GLU:C	2:A:643:GLU:O	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:57:ILE:H	2:B:57:ILE:HD12	1.85	0.42
2:B:635:GLU:HG3	2:B:635:GLU:H	1.66	0.42
2:B:619:ARG:HG3	2:B:623:LYS:O	2.20	0.42
2:A:25:LEU:HD23	2:A:25:LEU:N	2.34	0.42
2:A:297:ILE:HB	2:A:600:TYR:CD1	2.54	0.42
2:B:403:ASP:O	2:B:404:ASP:C	2.58	0.42
2:B:382:PHE:O	2:B:384:GLU:N	2.53	0.42
2:B:11:ASN:OD1	2:B:14:GLN:HG3	2.18	0.42
2:A:115:ASP:OD2	2:A:115:ASP:C	2.57	0.42
2:A:390:ASP:OD1	2:A:409:ARG:NE	2.48	0.42
2:B:110:ASP:OD1	2:B:532:GLN:HG2	2.20	0.42
2:A:377:TYR:HB2	2:A:557:MET:HB3	2.02	0.42
2:A:278:ARG:HG3	2:A:278:ARG:HH11	1.85	0.42
2:B:370:ALA:O	2:B:372:MET:HB2	2.20	0.42
2:B:128:LYS:C	2:B:130:MET:N	2.73	0.42
1:D:16:DA:H2''	1:D:17:DG:H5''	2.01	0.41
2:B:353:LEU:HA	2:B:557:MET:O	2.19	0.41
2:A:325:ASN:HD21	2:A:328:ASP:H	1.66	0.41
2:B:79:GLY:O	2:B:80:THR:CG2	2.57	0.41
2:B:153:GLY:CA	2:B:228:ILE:HD12	2.49	0.41
2:B:483:ARG:HD3	2:B:483:ARG:HA	1.81	0.41
2:A:418:ILE:O	2:A:418:ILE:HG22	2.19	0.41
2:B:47:MET:HE1	2:B:78:MET:HG2	2.02	0.41
2:A:327:LEU:HA	2:A:327:LEU:HD13	1.91	0.41
2:A:319:SER:HB2	2:A:644:VAL:HG21	2.02	0.41
2:B:11:ASN:O	2:B:12:ASP:C	2.59	0.41
2:B:389:LYS:HB3	2:B:389:LYS:HE2	1.85	0.41
2:B:576:GLU:HA	2:B:630:SER:N	2.34	0.41
2:B:540:LEU:O	2:B:541:GLU:HB3	2.20	0.41
2:A:330:ALA:O	2:A:331:ARG:C	2.58	0.41
2:B:112:GLN:NE2	2:B:113:ILE:HD12	2.35	0.41
2:B:247:GLY:O	2:B:248:ASP:CB	2.66	0.41
2:A:78:MET:O	2:A:79:GLY:C	2.57	0.41
1:C:6:DA:C2'	1:C:7:DC:H6	2.32	0.41
2:B:325:ASN:H	2:B:325:ASN:ND2	2.17	0.41
2:B:142:ALA:HB2	2:B:170:TRP:CZ3	2.51	0.41
2:A:537:HIS:O	2:A:537:HIS:CG	2.74	0.41
2:B:114:LEU:HD21	2:B:122:LEU:HD23	2.03	0.41
2:B:61:THR:CB	2:B:67:ALA:HB2	2.50	0.41
1:D:10:DC:OP1	1:D:10:DC:H4'	2.20	0.41
2:B:550:TRP:O	2:B:550:TRP:CD1	2.73	0.41
2:A:548:ASP:O	2:A:549:THR:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:418:ILE:H	2:A:418:ILE:HD12	1.84	0.41
2:A:66:ALA:O	2:A:67:ALA:C	2.58	0.41
2:A:598:LEU:HD12	2:A:598:LEU:HA	1.82	0.41
2:B:397:LEU:HA	2:B:400:ASN:O	2.20	0.41
2:A:206:ILE:O	2:A:207:LEU:C	2.57	0.41
2:A:320:LEU:HD23	2:A:320:LEU:N	2.35	0.41
1:C:3:DA:H2'	1:C:3:DA:OP2	2.21	0.41
2:A:505:ARG:HA	2:A:508:ASN:HD22	1.86	0.41
2:B:231:ALA:C	2:B:234:ARG:HG2	2.41	0.41
2:B:227:ASN:OD1	2:B:260:GLN:HG3	2.21	0.41
2:A:283:TYR:CE2	3:A:681:GOL:H12	2.55	0.41
2:B:284:ARG:HD3	2:B:566:GLU:CB	2.50	0.41
2:B:529:MET:HB2	2:B:532:GLN:OE1	2.19	0.41
2:B:306:LYS:CE	2:B:600:TYR:OH	2.69	0.41
2:B:10:LEU:HD21	2:B:41:HIS:CD2	2.55	0.41
2:B:382:PHE:O	2:B:385:ARG:HG3	2.20	0.41
2:A:430:SER:OG	2:A:435:LEU:O	2.31	0.41
2:B:498:LYS:HB3	2:B:499:GLY:H	1.69	0.41
2:B:194:LEU:HD13	2:B:228:ILE:HD11	2.02	0.41
2:B:200:TRP:CH2	2:B:236:LEU:HD13	2.56	0.41
2:A:22:ARG:HE	2:A:22:ARG:HB3	1.36	0.41
2:B:587:ASP:CG	2:B:588:GLU:N	2.73	0.41
1:D:16:DA:C2'	1:D:17:DG:H5''	2.50	0.41
2:B:352:ILE:O	2:B:353:LEU:HD23	2.21	0.41
2:B:406:ALA:O	2:B:410:VAL:HG22	2.20	0.41
2:A:325:ASN:HA	2:A:615:ALA:HB1	2.02	0.41
1:C:17:DG:H5'	2:A:421:ARG:HH11	1.85	0.41
2:B:203:LYS:N	2:B:204:PRO:CD	2.84	0.41
2:B:64:ASN:ND2	2:B:541:GLU:HB3	2.36	0.41
2:A:477:LEU:HG	2:A:516:THR:HB	2.01	0.41
2:B:223:GLN:HB2	2:B:252:SER:HB2	2.02	0.41
2:A:284:ARG:HH11	2:A:566:GLU:HB3	1.86	0.41
2:B:22:ARG:O	2:B:23:SER:HB3	2.20	0.41
2:B:88:GLY:HA3	2:B:93:LEU:HD21	2.03	0.41
2:B:13:LYS:O	2:B:16:GLU:HB3	2.20	0.41
2:A:149:GLN:CA	2:A:149:GLN:NE2	2.83	0.41
2:B:49:VAL:HG12	2:B:50:GLU:N	2.36	0.41
2:A:228:ILE:CG2	2:A:229:GLN:N	2.84	0.41
2:B:187:VAL:CG1	2:B:191:GLU:HG2	2.51	0.41
2:B:412:ASN:OD1	2:B:415:THR:HA	2.21	0.41
2:B:385:ARG:CG	2:B:385:ARG:HH21	2.34	0.41
2:A:126:LEU:HD23	2:A:126:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:55:TYR:CD1	2:B:55:TYR:N	2.89	0.41
2:A:165:PRO:O	2:A:169:THR:N	2.41	0.40
2:B:472:THR:OG1	2:B:480:GLN:HA	2.21	0.40
2:A:82:GLN:HB3	2:A:85:MET:CE	2.51	0.40
2:B:253:ILE:CD1	2:B:253:ILE:N	2.81	0.40
2:B:175:GLN:O	2:B:179:GLU:HG3	2.20	0.40
2:B:556:LEU:O	2:B:557:MET:HB3	2.20	0.40
2:B:61:THR:CG2	2:B:62:PHE:H	2.22	0.40
2:B:85:MET:O	2:B:86:TRP:HD1	2.04	0.40
2:B:211:ARG:HG2	2:B:236:LEU:O	2.20	0.40
2:B:251:GLN:HE21	2:B:251:GLN:HB2	1.66	0.40
2:A:320:LEU:HG	2:A:641:VAL:CG1	2.51	0.40
1:D:32:DT:OP2	1:D:32:DT:H6	2.05	0.40
2:A:188:ASP:OD2	2:A:191:GLU:CB	2.66	0.40
2:B:200:TRP:HB3	2:B:207:LEU:HD22	2.04	0.40
2:B:442:ARG:HD3	2:B:442:ARG:HA	1.82	0.40
2:B:161:SER:OG	2:B:162:TYR:N	2.52	0.40
2:A:28:LEU:CD2	2:A:304:LEU:HD12	2.47	0.40
2:B:319:SER:HA	2:B:642:GLU:O	2.20	0.40
2:A:540:LEU:HD23	2:A:540:LEU:HA	1.79	0.40
2:B:49:VAL:C	2:B:51:ASN:N	2.75	0.40
2:B:254:TYR:O	2:B:259:ALA:HB3	2.21	0.40
2:A:580:PHE:HA	2:A:581:PRO:C	2.41	0.40
2:B:375:ARG:HG3	2:B:375:ARG:O	2.22	0.40
2:A:512:LEU:O	2:A:515:ALA:HB3	2.20	0.40
2:B:472:THR:CG2	2:B:480:GLN:HG3	2.51	0.40
2:A:117:GLU:O	2:A:118:ASP:C	2.59	0.40
2:B:226:ASN:CG	2:B:229:GLN:HG3	2.42	0.40
2:A:387:GLU:HG2	2:A:388:ILE:CD1	2.51	0.40
2:A:145:TYR:CD2	2:A:170:TRP:HB3	2.57	0.40
2:A:454:ALA:O	2:A:458:LEU:HB2	2.22	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	
2	A	638/680 (94%)	516 (81%)	82 (13%)	40 (6%)	2	12
2	B	638/680 (94%)	435 (68%)	145 (23%)	58 (9%)	1	5
All	All	1276/1360 (94%)	951 (74%)	227 (18%)	98 (8%)	1	7

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	79	GLY
2	A	134	GLU
2	A	135	LYS
2	A	155	ARG
2	A	369	GLN
2	A	498	LYS
2	A	543	GLY
2	A	544	GLU
2	A	546	GLN
2	A	547	ALA
2	A	550	TRP
2	A	588	GLU
2	A	643	GLU
2	B	12	ASP
2	B	28	LEU
2	B	31	ALA
2	B	49	VAL
2	B	80	THR
2	B	134	GLU
2	B	162	TYR
2	B	201	LEU
2	B	248	ASP
2	B	263	ASN
2	B	351	ALA
2	B	371	SER
2	B	379	GLY
2	B	383	PHE
2	B	454	ALA
2	B	471	GLU
2	B	498	LYS
2	B	501	LYS
2	B	543	GLY
2	B	544	GLU
2	B	546	GLN
2	B	547	ALA

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Mol	Chain	Res	Type
2	B	550	TRP
2	B	621	TYR
2	A	130	MET
2	A	159	ILE
2	A	238	GLY
2	A	408	GLU
2	A	419	GLY
2	A	502	GLY
2	A	589	GLY
2	A	621	TYR
2	A	635	GLU
2	A	644	VAL
2	B	8	ASP
2	B	50	GLU
2	B	51	ASN
2	B	79	GLY
2	B	131	ASN
2	B	161	SER
2	B	214	PHE
2	B	305	GLY
2	B	347	LEU
2	B	551	GLN
2	B	604	THR
2	A	82	GLN
2	A	162	TYR
2	A	407	PHE
2	A	527	ASP
2	B	23	SER
2	B	272	PRO
2	B	382	PHE
2	B	404	ASP
2	B	408	GLU
2	B	474	ASP
2	B	487	ASP
2	B	541	GLU
2	B	645	ARG
2	A	54	PRO
2	A	80	THR
2	A	163	GLY
2	B	221	GLU
2	B	315	GLY
2	B	473	ALA

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Mol	Chain	Res	Type
2	B	554	VAL
2	B	584	MET
2	B	635	GLU
2	A	90	PHE
2	A	500	GLU
2	A	526	GLU
2	A	530	PRO
2	B	477	LEU
2	B	545	GLY
2	B	629	PRO
2	A	161	SER
2	A	221	GLU
2	A	501	LYS
2	B	407	PHE
2	A	305	GLY
2	A	545	GLY
2	B	644	VAL
2	B	219	VAL
2	A	499	GLY
2	B	156	PRO
2	B	484	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	519/574 (90%)	467 (90%)	52 (10%)	11	39
2	B	513/574 (89%)	458 (89%)	55 (11%)	10	35
All	All	1032/1148 (90%)	925 (90%)	107 (10%)	10	37

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	VAL
2	A	6	LEU
2	A	25	LEU
2	A	33	SER

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Mol	Chain	Res	Type
2	A	35	LYS
2	A	46	LEU
2	A	53	SER
2	A	61	THR
2	A	73	ARG
2	A	96	ARG
2	A	130	MET
2	A	133	ASP
2	A	149	GLN
2	A	166	VAL
2	A	167	GLU
2	A	171	GLN
2	A	174	TYR
2	A	179	GLU
2	A	182	ASP
2	A	208	GLN
2	A	228	ILE
2	A	234	ARG
2	A	243	VAL
2	A	244	MET
2	A	260	GLN
2	A	271	PHE
2	A	291	SER
2	A	303	ARG
2	A	325	ASN
2	A	327	LEU
2	A	354	TYR
2	A	362	VAL
2	A	365	GLU
2	A	372	MET
2	A	404	ASP
2	A	408	GLU
2	A	430	SER
2	A	442	ARG
2	A	448	LYS
2	A	458	LEU
2	A	483	ARG
2	A	496	GLN
2	A	501	LYS
2	A	528	LEU
2	A	537	HIS
2	A	549	THR

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Mol	Chain	Res	Type
2	A	555	GLN
2	A	570	VAL
2	A	587	ASP
2	A	617	THR
2	A	620	LEU
2	A	640	CYS
2	B	25	LEU
2	B	28	LEU
2	B	43	ILE
2	B	78	MET
2	B	96	ARG
2	B	106	ASN
2	B	112	GLN
2	B	116	SER
2	B	127	ILE
2	B	133	ASP
2	B	140	ARG
2	B	149	GLN
2	B	151	ASP
2	B	182	ASP
2	B	201	LEU
2	B	208	GLN
2	B	240	THR
2	B	243	VAL
2	B	251	GLN
2	B	253	ILE
2	B	264	ILE
2	B	269	ASN
2	B	287	SER
2	B	320	LEU
2	B	325	ASN
2	B	347	LEU
2	B	354	TYR
2	B	362	VAL
2	B	365	GLU
2	B	372	MET
2	B	385	ARG
2	B	393	SER
2	B	401	ARG
2	B	404	ASP
2	B	408	GLU
2	B	420	ASP

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Mol	Chain	Res	Type
2	B	444	LEU
2	B	474	ASP
2	B	483	ARG
2	B	492	THR
2	B	536	SER
2	B	555	GLN
2	B	570	VAL
2	B	571	PHE
2	B	579	MET
2	B	580	PHE
2	B	587	ASP
2	B	594	GLU
2	B	597	ARG
2	B	610	LEU
2	B	618	ARG
2	B	621	TYR
2	B	626	TYR
2	B	633	ILE
2	B	639	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	41	HIS
2	A	64	ASN
2	A	109	GLN
2	A	112	GLN
2	A	119	GLN
2	A	149	GLN
2	A	168	GLN
2	A	175	GLN
2	A	178	GLN
2	A	208	GLN
2	A	227	ASN
2	A	229	GLN
2	A	260	GLN
2	A	281	GLN
2	A	325	ASN
2	A	446	GLN
2	A	459	GLN
2	A	480	GLN
2	A	508	ASN

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Mol	Chain	Res	Type
2	A	569	GLN
2	A	583	GLN
2	A	608	GLN
2	A	627	HIS
2	B	11	ASN
2	B	64	ASN
2	B	82	GLN
2	B	91	HIS
2	B	112	GLN
2	B	119	GLN
2	B	141	GLN
2	B	147	ASN
2	B	149	GLN
2	B	168	GLN
2	B	171	GLN
2	B	175	GLN
2	B	178	GLN
2	B	202	ASN
2	B	208	GLN
2	B	251	GLN
2	B	260	GLN
2	B	265	GLN
2	B	269	ASN
2	B	299	ASN
2	B	325	ASN
2	B	341	GLN
2	B	386	GLN
2	B	400	ASN
2	B	478	HIS
2	B	480	GLN
2	B	508	ASN
2	B	569	GLN
2	B	627	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	$\# Z  > 2$
3	GOL	A	681	-	5,5,5	0.40	0	5,5,5	0.11	0
4	FMT	A	682	-	2,2,2	0.90	0	1,1,1	0.60	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
3	GOL	A	681	-	-	0/4/4/4	0/0/0/0
4	FMT	A	682	-	-	0/0/0/0	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.

## 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	33/35 (94%)	-0.44	0	100 100	43, 71, 131, 136	0
1	D	33/35 (94%)	-0.43	0	100 100	48, 84, 132, 137	0
2	A	642/680 (94%)	-0.22	0	100 100	26, 51, 91, 109	0
2	B	642/680 (94%)	0.02	4 (0%)	86 32	59, 101, 127, 149	0
All	All	1350/1430 (94%)	-0.11	4 (0%)	91 48	26, 79, 120, 149	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	320	LEU	2.5
2	B	372	MET	2.3
2	B	612	LEU	2.2
2	B	2	ASP	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMT	A	682	3/3	0.23	1.35	49,49,51,51	0
3	GOL	A	681	6/6	0.19	0.70	53,53,54,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.