Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 07:29 PM EDT

PDB ID	:	4E5Z
Title	:	Damaged DNA induced UV-damaged DNA-binding protein (UV-DDB) dimerization and its roles in chromatinized DNA repair
Authors	:	Yeh, J.I.; Du, S.
Deposited on	:	2012-03-15
Resolution	:	3.22 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

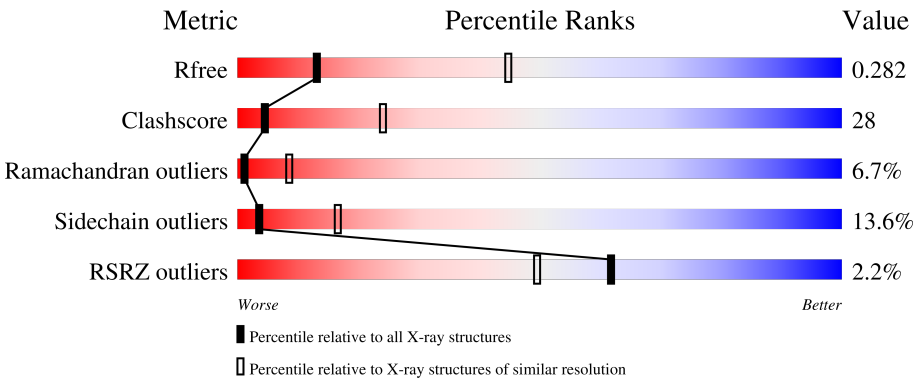
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	1150	2%; 51%, 37%, 11%
2	B	436	2%; 35%, 44%, 10%, 8%
3	F	24	58%, 33%, 8%
4	G	24	29%, 54%, 17%

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
4	3DR	G	11	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1140	8851	5596	1497	1712	46	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q16531
A	-8	HIS	-	expression tag	UNP Q16531
A	-7	HIS	-	expression tag	UNP Q16531
A	-6	HIS	-	expression tag	UNP Q16531
A	-5	HIS	-	expression tag	UNP Q16531
A	-4	HIS	-	expression tag	UNP Q16531
A	-3	HIS	-	expression tag	UNP Q16531
A	-2	HIS	-	expression tag	UNP Q16531
A	-1	HIS	-	expression tag	UNP Q16531
A	0	HIS	-	expression tag	UNP Q16531
A	1	HIS	-	expression tag	UNP Q16531

- Molecule 2 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	402	3157	2001	570	566	20	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	expression tag	UNP Q92466
B	-6	ASP	-	expression tag	UNP Q92466
B	-5	TYR	-	expression tag	UNP Q92466
B	-4	LYS	-	expression tag	UNP Q92466
B	-3	ASP	-	expression tag	UNP Q92466

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ASP	-	expression tag	UNP Q92466
B	-1	ASP	-	expression tag	UNP Q92466
B	0	ASP	-	expression tag	UNP Q92466
B	1	LYS	-	expression tag	UNP Q92466
B	420	GLU	-	expression tag	UNP Q92466

- Molecule 3 is a DNA chain called AP24 DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	24	497	236	91	146	24	0	0	0

- Molecule 4 is a DNA chain called AP24 DNA complementary strand.

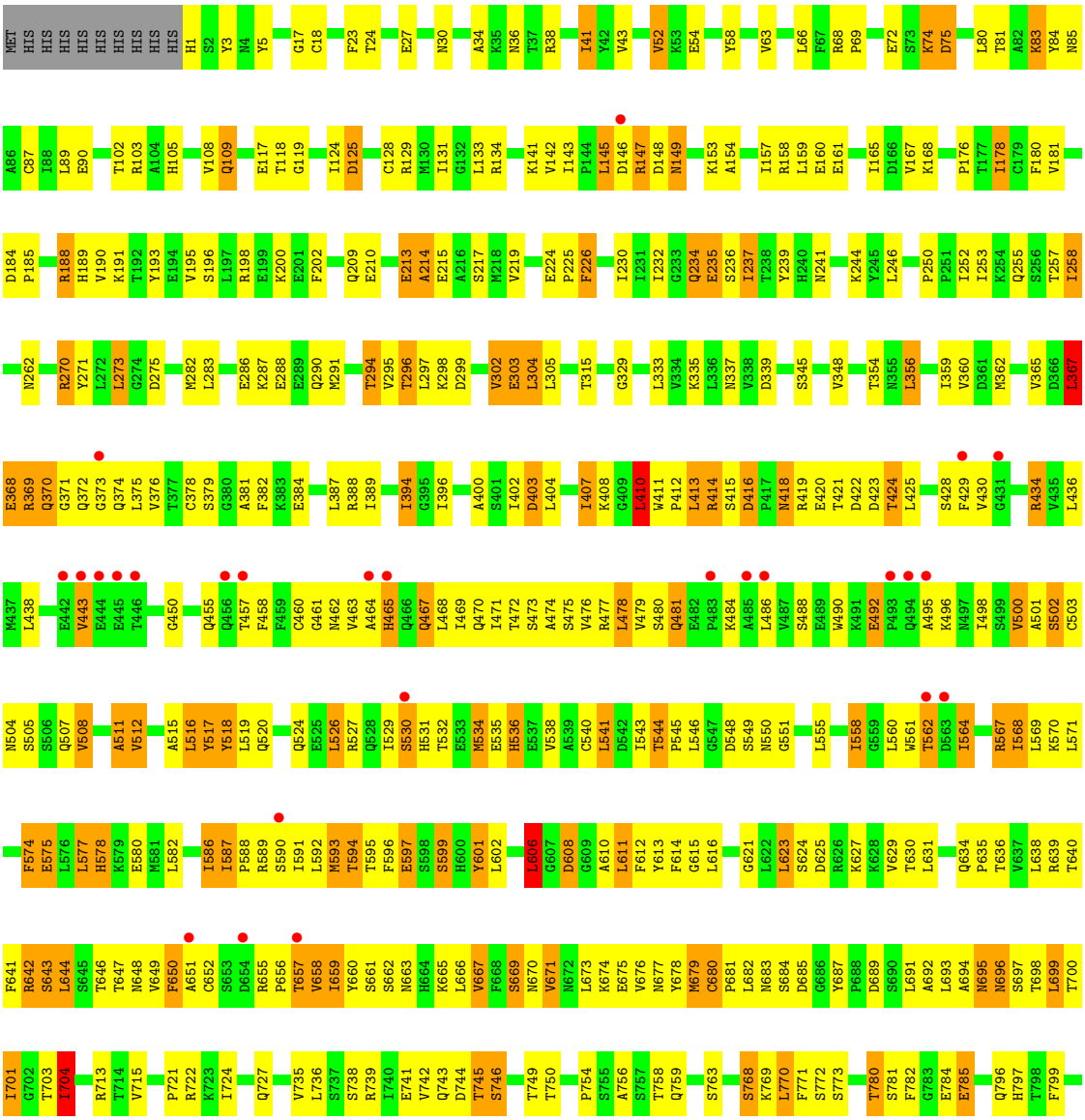
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	G	24	480	228	86	142	24	0	0	0

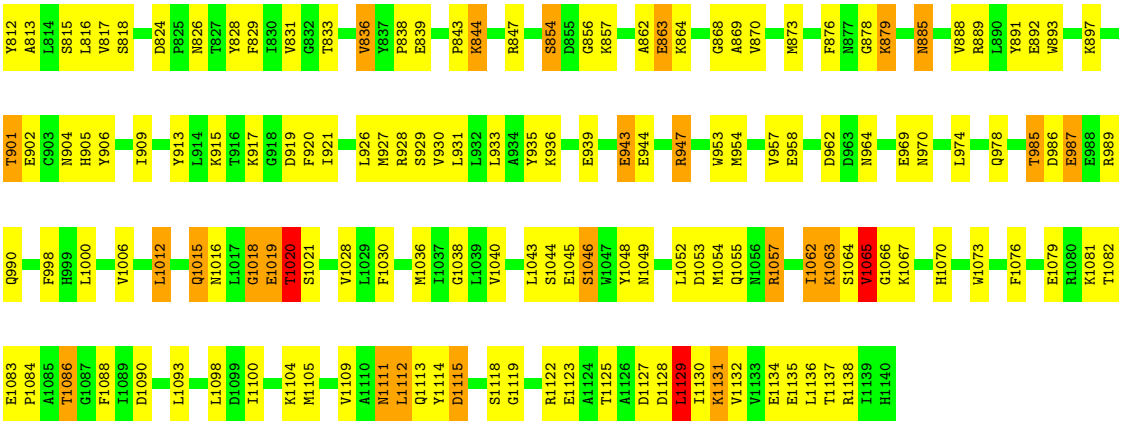
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA damage-binding protein 1

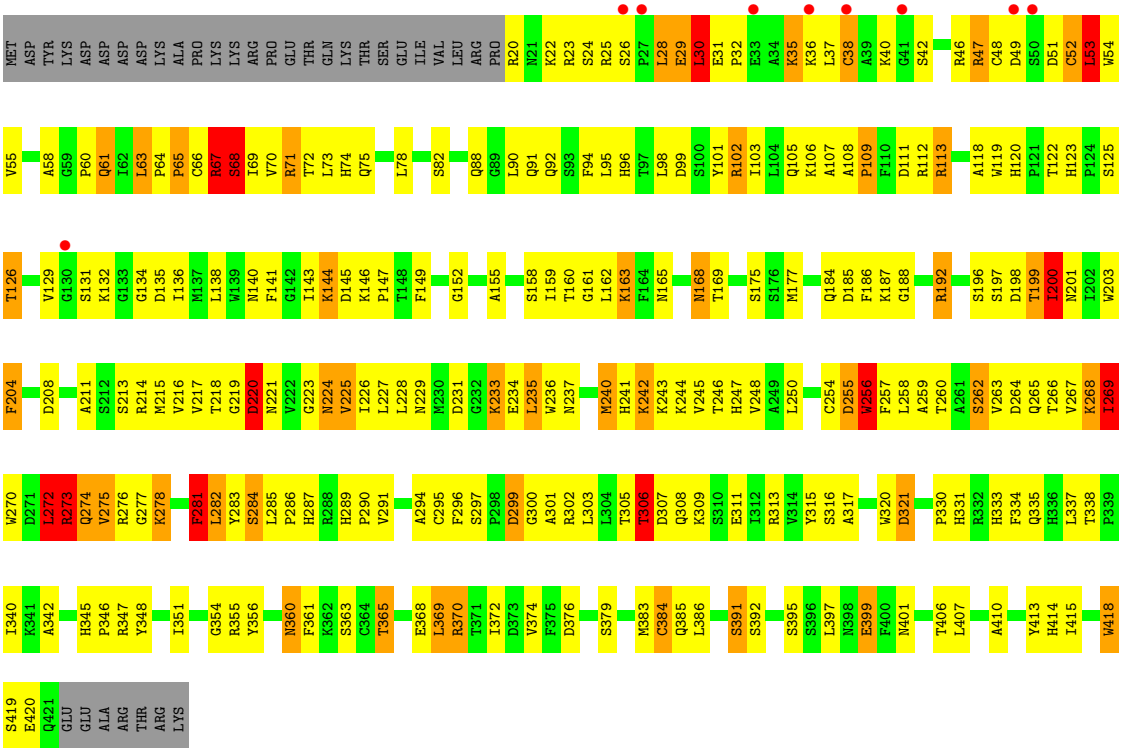
Chain A: 2% 51% 37% 11%





• Molecule 2: DNA damage-binding protein 2

Chain B:

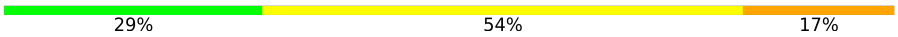


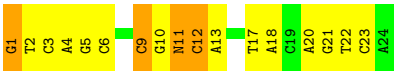
• Molecule 3: AP24 DNA strand

Chain F:

• Molecule 4: AP24 DNA complementary strand

Chain G:




G1
T2
C3
A4
G5
C6
C9
G10
N11
C12
A13
T17
A18
C19
A20
G21
T22
C23
A24

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	72.42Å 76.50Å 389.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 3.22 41.09 – 3.22	Depositor EDS
% Data completeness (in resolution range)	93.6 (41.09-3.22) 93.7 (41.09-3.22)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.73 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8_1069, REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.284 0.231 , 0.282	Depositor DCC
R_{free} test set	1690 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	109.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.05 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12985	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.34	0/9013	0.62	6/12220 (0.0%)
2	B	0.42	2/3244 (0.1%)	0.75	9/4404 (0.2%)
3	F	0.66	1/557 (0.2%)	1.22	4/857 (0.5%)
4	G	0.88	3/524 (0.6%)	1.24	3/801 (0.4%)
All	All	0.41	6/13338 (0.0%)	0.73	22/18282 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	9	DC	O3'-P	12.42	1.76	1.61
3	F	1	DT	OP3-P	-10.76	1.48	1.61
4	G	1	DG	OP3-P	-10.69	1.48	1.61
2	B	256	TRP	CG-CD1	7.70	1.47	1.36
2	B	256	TRP	CG-CD2	-6.40	1.32	1.43
4	G	12	DC	O3'-P	-5.64	1.54	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	9	DC	P-O3'-C3'	-13.46	103.54	119.70
2	B	273	ARG	CG-CD-NE	-9.08	92.73	111.80
4	G	1	DG	OP1-P-OP2	-8.30	107.15	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	DT	OP1-P-OP2	-8.11	107.43	119.60
2	B	256	TRP	CA-CB-CG	7.59	128.12	113.70
3	F	11	DA	O4'-C4'-C3'	-7.34	101.56	104.50
2	B	273	ARG	CD-NE-CZ	6.79	133.11	123.60
2	B	272	LEU	CA-CB-CG	6.78	130.89	115.30
2	B	240	MET	CG-SD-CE	-6.63	89.59	100.20
4	G	9	DC	OP2-P-O3'	6.61	119.74	105.20
1	A	410	LEU	CA-CB-CG	6.55	130.36	115.30
2	B	67	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	1129	LEU	CA-CB-CG	5.52	128.00	115.30
2	B	273	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	B	240	MET	CA-CB-CG	-5.28	104.32	113.30
1	A	367	LEU	CA-CB-CG	5.21	127.29	115.30
3	F	12	DT	N3-C4-O4	5.18	123.01	119.90
3	F	12	DT	O4'-C1'-N1	5.18	111.63	108.00
2	B	68	SER	N-CA-C	-5.15	97.09	111.00
1	A	606	LEU	N-CA-C	5.09	124.75	111.00
1	A	526	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	A	480	SER	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	28	LEU	Peptide
2	B	29	GLU	Peptide
2	B	63	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8851	0	8754	487	1
2	B	3157	0	3126	210	1
3	F	497	0	272	12	0
4	G	480	0	267	33	0
All	All	12985	0	12419	722	2

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 28.

All (722) 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)
4:G:9:DC:H2"	4:G:10:DG:C8	1.73	1.23
1:A:508:VAL:HG13	1:A:519:LEU:HD22	1.44	0.99
1:A:224:GLU:HA	1:A:226:PHE:H	1.34	0.93
2:B:67:ARG:HA	2:B:67:ARG:HE	1.29	0.93
1:A:372:GLN:HB2	1:A:374:GLN:HE22	1.32	0.93
1:A:693:LEU:HB3	1:A:700:THR:HB	1.50	0.92
4:G:9:DC:H2"	4:G:10:DG:H8	1.33	0.91
1:A:234:GLN:O	1:A:236:SER:N	2.03	0.91
4:G:9:DC:C2'	4:G:10:DG:C8	2.53	0.91
1:A:394:ILE:HD12	1:A:671:VAL:HG13	1.56	0.88
1:A:467:GLN:HE22	1:A:478:LEU:HG	1.37	0.86
2:B:204:PHE:HA	2:B:220:ASP:HA	1.57	0.86
1:A:414:ARG:NH1	1:A:421:THR:OG1	2.09	0.86
1:A:287:LYS:O	1:A:298:LYS:NZ	2.08	0.85
2:B:58:ALA:HA	2:B:61:GLN:HE21	1.42	0.85
2:B:268:LYS:HA	2:B:284:SER:HA	1.58	0.85
2:B:199:THR:OG1	2:B:200:ILE:N	2.08	0.84
2:B:345:HIS:ND1	2:B:346:PRO:O	2.10	0.84
4:G:10:DG:H8	4:G:10:DG:O5'	1.61	0.83
2:B:112:ARG:CZ	4:G:11:3DR:OP1	2.27	0.83
1:A:1054:MET:HA	1:A:1057:ARG:HD2	1.59	0.82
1:A:129:ARG:HH12	1:A:176:PRO:HB3	1.45	0.82
1:A:463:VAL:HG11	1:A:469:ILE:HG13	1.61	0.81
1:A:684:SER:HB2	1:A:687:TYR:HB2	1.62	0.80
2:B:112:ARG:NH1	4:G:11:3DR:OP1	2.14	0.80
2:B:276:ARG:O	2:B:278:LYS:N	2.15	0.80
1:A:367:LEU:HD12	1:A:367:LEU:H	1.46	0.79
1:A:413:LEU:O	1:A:423:ASP:N	2.14	0.79
1:A:650:PHE:HA	1:A:658:VAL:HA	1.62	0.79
1:A:1111:ASN:O	1:A:1114:TYR:N	2.14	0.79
2:B:273:ARG:HD3	2:B:274:GLN:HG2	1.65	0.79
1:A:270:ARG:HH12	1:A:283:LEU:H	1.29	0.79
1:A:414:ARG:HH11	1:A:422:ASP:N	1.81	0.78
1:A:460:CYS:SG	1:A:461:GLY:N	2.54	0.78
2:B:67:ARG:HA	2:B:67:ARG:NE	1.91	0.78
1:A:696:ASN:OD1	1:A:696:ASN:N	2.14	0.77
1:A:642:ARG:NH1	1:A:643:SER:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HB	1:A:659:ILE:HG23	1.66	0.77
1:A:58:TYR:O	1:A:83:LYS:NZ	2.18	0.77
1:A:1062:ILE:HB	1:A:1064:SER:H	1.50	0.76
3:F:16:DG:C2	4:G:10:DG:N2	2.53	0.76
1:A:290:GLN:H	1:A:294:THR:HG1	1.30	0.76
1:A:655:ARG:HB3	1:A:670:ASN:HD21	1.50	0.76
1:A:41:ILE:HD11	1:A:52:VAL:HG22	1.66	0.76
4:G:10:DG:H2"	4:G:11:3DR:OP2	1.85	0.76
1:A:534:MET:SD	1:A:567:ARG:NH2	2.55	0.75
1:A:1053:ASP:OD1	1:A:1057:ARG:NH1	2.20	0.75
2:B:247:HIS:HD2	2:B:294:ALA:H	1.34	0.75
1:A:270:ARG:HB2	1:A:270:ARG:HH11	1.50	0.75
1:A:414:ARG:HB2	1:A:422:ASP:HA	1.69	0.75
1:A:847:ARG:NH1	1:A:863:GLU:OE1	2.18	0.75
1:A:500:VAL:HG11	1:A:538:VAL:HG23	1.68	0.75
2:B:236:TRP:HZ2	2:B:240:MET:HE1	1.51	0.75
1:A:288:GLU:OE1	1:A:296:THR:OG1	2.06	0.74
3:F:16:DG:N2	4:G:10:DG:C2	2.56	0.73
1:A:915:LYS:NZ	1:A:958:GLU:OE1	2.20	0.73
2:B:243:LYS:HG3	2:B:263:VAL:HG13	1.70	0.73
1:A:410:LEU:HD23	1:A:694:ALA:HB2	1.70	0.73
1:A:869:ALA:H	1:A:885:ASN:HD22	1.36	0.73
2:B:48:CYS:SG	2:B:49:ASP:N	2.60	0.73
2:B:24:SER:OG	2:B:36:LYS:NZ	2.22	0.73
1:A:124:ILE:HG23	1:A:131:ILE:HG12	1.71	0.73
1:A:743:GLN:HG3	1:A:745:THR:H	1.54	0.73
1:A:467:GLN:NE2	1:A:478:LEU:HG	2.04	0.72
1:A:838:PRO:HA	2:B:67:ARG:CD	2.19	0.72
2:B:129:VAL:HG11	2:B:415:ILE:HD11	1.71	0.72
1:A:550:ASN:N	1:A:551:GLY:HA2	2.04	0.72
2:B:244:LYS:O	2:B:262:SER:OG	2.07	0.72
3:F:19:DG:N2	4:G:6:DC:N3	2.38	0.72
1:A:564:ILE:HG23	1:A:588:PRO:HD3	1.72	0.72
1:A:68:ARG:NH1	1:A:69:PRO:O	2.22	0.71
1:A:642:ARG:O	1:A:648:ASN:ND2	2.24	0.71
1:A:670:ASN:OD1	1:A:671:VAL:N	2.24	0.71
2:B:267:VAL:HG23	2:B:287:HIS:HE1	1.56	0.70
2:B:360:ASN:OD1	2:B:360:ASN:N	2.24	0.70
1:A:419:ARG:NH1	1:A:685:ASP:OD1	2.25	0.69
1:A:931:LEU:HD22	1:A:947:ARG:HH12	1.57	0.69
2:B:233:LYS:HE3	2:B:235:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ARG:HG3	2:B:276:ARG:HH11	1.57	0.69
1:A:224:GLU:HA	1:A:226:PHE:N	2.06	0.69
2:B:203:TRP:O	2:B:221:ASN:ND2	2.25	0.69
4:G:9:DC:C2'	4:G:10:DG:N7	2.56	0.69
2:B:65:PRO:O	2:B:67:ARG:NH2	2.23	0.69
2:B:211:ALA:O	2:B:214:ARG:NH1	2.26	0.69
2:B:265:GLN:O	2:B:287:HIS:N	2.26	0.68
1:A:741:GLU:HG3	1:A:749:THR:HB	1.75	0.68
1:A:176:PRO:HB2	1:A:195:VAL:HG13	1.75	0.68
1:A:724:ILE:HG22	1:A:735:VAL:HG22	1.75	0.68
2:B:365:THR:O	2:B:365:THR:OG1	2.09	0.68
1:A:470:GLN:OE1	1:A:477:ARG:NH2	2.27	0.68
2:B:258:LEU:HD22	2:B:259:ALA:H	1.57	0.68
2:B:263:VAL:HG23	2:B:290:PRO:HB3	1.76	0.68
1:A:592:LEU:HD23	1:A:638:LEU:HD13	1.76	0.68
1:A:1127:ASP:HA	1:A:1130:ILE:HG12	1.76	0.68
2:B:363:SER:OG	2:B:368:GLU:OE2	2.11	0.68
2:B:245:VAL:HA	2:B:262:SER:HB2	1.76	0.67
1:A:770:LEU:O	1:A:772:SER:HA	1.93	0.67
1:A:1081:LYS:HZ1	1:A:1082:THR:H	1.42	0.67
2:B:216:VAL:HG22	2:B:228:LEU:HB2	1.76	0.67
1:A:477:ARG:HH11	1:A:486:LEU:HD11	1.60	0.67
2:B:120:HIS:CE1	2:B:169:THR:HG21	2.30	0.67
1:A:102:THR:HG21	1:A:1066:GLY:H	1.58	0.67
1:A:290:GLN:N	1:A:294:THR:OG1	2.22	0.67
1:A:90:GLU:OE1	1:A:103:ARG:NE	2.28	0.67
2:B:236:TRP:CZ2	2:B:240:MET:HE1	2.29	0.66
2:B:51:ASP:OD1	2:B:52:CYS:N	2.28	0.66
2:B:126:THR:HG22	2:B:140:ASN:HD22	1.59	0.66
2:B:63:LEU:O	2:B:65:PRO:HD3	1.95	0.66
2:B:184:GLN:NE2	2:B:188:GLY:O	2.29	0.66
1:A:722:ARG:NH1	1:A:738:SER:OG	2.27	0.66
1:A:367:LEU:HD13	1:A:375:LEU:HD22	1.77	0.66
1:A:400:ALA:HB3	1:A:701:ILE:HD11	1.78	0.66
1:A:455:GLN:NE2	1:A:472:THR:OG1	2.28	0.65
2:B:242:LYS:O	2:B:243:LYS:HG2	1.96	0.65
1:A:904:ASN:ND2	1:A:906:TYR:OH	2.29	0.65
1:A:520:GLN:NE2	1:A:527:ARG:O	2.16	0.65
1:A:985:THR:OG1	1:A:986:ASP:N	2.27	0.65
1:A:569:LEU:HD13	1:A:574:PHE:HD1	1.61	0.65
2:B:120:HIS:HE1	2:B:122:THR:HB	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:GLN:NE2	1:A:1016:ASN:O	2.30	0.64
1:A:1118:SER:O	1:A:1122:ARG:NH1	2.30	0.64
1:A:578:HIS:NE2	1:A:621:GLY:O	2.29	0.64
1:A:736:LEU:HD13	1:A:816:LEU:HD22	1.80	0.64
3:F:20:DC:H42	4:G:5:DG:H1	1.46	0.64
1:A:369:ARG:O	1:A:371:GLY:N	2.30	0.64
2:B:267:VAL:HG23	2:B:287:HIS:CE1	2.32	0.64
2:B:185:ASP:OD1	2:B:186:PHE:N	2.31	0.64
1:A:928:ARG:O	1:A:947:ARG:NH2	2.28	0.63
2:B:306:THR:HG21	2:B:342:ALA:HB3	1.81	0.63
2:B:220:ASP:OD2	2:B:224:ASN:ND2	2.31	0.63
1:A:593:MET:HA	1:A:602:LEU:HA	1.80	0.63
2:B:51:ASP:HA	2:B:54:TRP:CZ2	2.34	0.63
1:A:403:ASP:OD1	1:A:403:ASP:N	2.28	0.63
1:A:302:VAL:O	1:A:304:LEU:N	2.28	0.62
1:A:838:PRO:HA	2:B:67:ARG:HD3	1.81	0.62
2:B:203:TRP:H	2:B:221:ASN:HD21	1.47	0.62
1:A:72:GLU:HG3	1:A:74:LYS:H	1.63	0.62
1:A:119:GLY:O	1:A:134:ARG:NH2	2.32	0.62
1:A:270:ARG:HH12	1:A:283:LEU:N	1.97	0.62
2:B:247:HIS:CD2	2:B:294:ALA:H	2.17	0.62
1:A:230:ILE:HD11	1:A:237:ILE:HD11	1.81	0.62
1:A:1115:ASP:OD1	1:A:1115:ASP:N	2.32	0.62
1:A:418:ASN:OD1	1:A:418:ASN:N	2.33	0.62
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.34	0.62
2:B:99:ASP:HA	2:B:102:ARG:HE	1.65	0.62
2:B:228:LEU:HG	2:B:233:LYS:O	2.00	0.62
1:A:146:ASP:HB2	1:A:148:ASP:O	1.99	0.62
1:A:1083:GLU:HG3	1:A:1084:PRO:HD2	1.80	0.62
4:G:10:DG:C2'	4:G:11:3DR:OP2	2.47	0.62
1:A:677:ASN:HD21	1:A:696:ASN:CG	2.02	0.62
2:B:28:LEU:HA	2:B:29:GLU:HB3	1.81	0.62
2:B:129:VAL:HG21	2:B:415:ILE:HG13	1.81	0.62
2:B:67:ARG:HB3	2:B:71:ARG:HH11	1.64	0.61
1:A:425:LEU:HD11	1:A:436:LEU:HD22	1.82	0.61
1:A:472:THR:OG1	1:A:473:SER:N	2.33	0.61
1:A:507:GLN:OE1	1:A:518:TYR:OH	2.16	0.61
1:A:675:GLU:O	1:A:695:ASN:ND2	2.34	0.61
1:A:1100:ILE:CD1	1:A:1105:MET:HG2	2.31	0.61
1:A:974:LEU:HD11	1:A:1000:LEU:HD22	1.83	0.61
3:F:16:DG:H2'	3:F:17:DA:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:GLY:N	1:A:625:ASP:OD1	2.34	0.61
1:A:541:LEU:HG	1:A:558:ILE:HG22	1.82	0.60
1:A:656:PRO:O	1:A:671:VAL:HG23	2.00	0.60
1:A:213:GLU:OE2	1:A:236:SER:OG	2.15	0.60
1:A:878:GLY:O	1:A:879:LYS:NZ	2.21	0.60
1:A:577:LEU:HD13	1:A:578:HIS:CD2	2.36	0.60
1:A:758:THR:OG1	1:A:759:GLN:OE1	2.18	0.60
2:B:123:HIS:HB3	2:B:126:THR:HG23	1.83	0.60
1:A:457:THR:HA	1:A:472:THR:HA	1.83	0.59
1:A:601:TYR:HE2	1:A:613:TYR:HB2	1.66	0.59
1:A:414:ARG:HG3	1:A:423:ASP:HB2	1.83	0.59
2:B:334:PHE:HB3	2:B:337:LEU:HB3	1.83	0.59
2:B:255:ASP:O	2:B:257:PHE:N	2.35	0.59
2:B:346:PRO:O	2:B:348:TYR:N	2.32	0.59
3:F:1:DT:H2"	3:F:2:DG:C8	2.38	0.59
2:B:68:SER:HB3	2:B:71:ARG:NH1	2.17	0.59
1:A:239:TYR:HB3	1:A:246:LEU:HB3	1.84	0.59
1:A:1135:GLU:HA	1:A:1138:ARG:CZ	2.33	0.59
1:A:693:LEU:HD12	1:A:694:ALA:H	1.67	0.59
1:A:1128:ASP:O	1:A:1132:VAL:N	2.36	0.59
1:A:531:HIS:CG	1:A:532:THR:H	2.21	0.58
2:B:268:LYS:O	2:B:269:ILE:HG13	2.04	0.58
1:A:255:GLN:OE1	1:A:255:GLN:N	2.35	0.58
1:A:24:THR:H	1:A:30:ASN:ND2	2.02	0.58
1:A:414:ARG:HD2	1:A:421:THR:C	2.24	0.58
1:A:472:THR:HG23	1:A:475:SER:H	1.69	0.58
1:A:423:ASP:OD1	1:A:424:THR:N	2.27	0.58
2:B:196:SER:O	2:B:198:ASP:N	2.36	0.58
2:B:273:ARG:CD	2:B:274:GLN:HG2	2.33	0.58
1:A:408:LYS:HA	1:A:678:TYR:CE2	2.38	0.58
1:A:168:LYS:HG2	1:A:219:VAL:HG13	1.86	0.58
1:A:673:LEU:H	1:A:673:LEU:HD12	1.69	0.58
2:B:38:CYS:O	2:B:42:SER:N	2.22	0.58
4:G:10:DG:C8	4:G:10:DG:O5'	2.52	0.58
1:A:149:ASN:HD22	1:A:153:LYS:HB3	1.69	0.57
1:A:1057:ARG:NH1	1:A:1114:TYR:OH	2.36	0.57
2:B:131:SER:H	2:B:159:ILE:HD12	1.69	0.57
2:B:308:GLN:HG2	2:B:333:HIS:HB2	1.86	0.57
1:A:408:LYS:O	1:A:428:SER:OG	2.21	0.57
1:A:481:GLN:O	1:A:484:LYS:N	2.37	0.57
1:A:519:LEU:HD23	1:A:520:GLN:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:VAL:HB	1:A:905:HIS:HB3	1.86	0.57
1:A:756:ALA:O	1:A:758:THR:N	2.38	0.57
1:A:414:ARG:HE	1:A:419:ARG:NH2	2.02	0.57
1:A:519:LEU:HG	1:A:526:LEU:HD11	1.86	0.57
1:A:588:PRO:O	1:A:589:ARG:NH1	2.34	0.57
3:F:16:DG:C2	4:G:10:DG:C2	2.92	0.57
2:B:272:LEU:HD12	2:B:273:ARG:H	1.70	0.57
2:B:419:SER:OG	2:B:420:GLU:N	2.37	0.57
1:A:695:ASN:HB2	1:A:698:THR:O	2.05	0.57
1:A:516:LEU:C	1:A:518:TYR:H	2.07	0.57
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	1.85	0.57
1:A:105:HIS:CD2	1:A:1067:LYS:HB2	2.40	0.56
1:A:504:ASN:ND2	1:A:551:GLY:O	2.38	0.56
1:A:467:GLN:HG3	1:A:468:LEU:N	2.18	0.56
1:A:414:ARG:HD3	1:A:421:THR:HG23	1.88	0.56
1:A:889:ARG:HD2	1:A:891:TYR:CE2	2.40	0.56
2:B:48:CYS:N	2:B:52:CYS:SG	2.78	0.56
2:B:203:TRP:H	2:B:221:ASN:ND2	2.03	0.56
2:B:123:HIS:HD2	2:B:125:SER:H	1.52	0.56
1:A:1109:VAL:HG12	1:A:1129:LEU:HD11	1.88	0.56
1:A:379:SER:HB3	1:A:721:PRO:HG2	1.88	0.56
1:A:570:LYS:NZ	1:A:571:LEU:O	2.38	0.56
2:B:250:LEU:HD23	2:B:258:LEU:HD23	1.88	0.56
2:B:269:ILE:HD11	2:B:282:LEU:HB2	1.86	0.56
1:A:594:THR:HG21	1:A:649:VAL:HG22	1.88	0.56
2:B:135:ASP:OD1	2:B:152:GLY:N	2.25	0.56
1:A:191:LYS:HD3	1:A:209:GLN:HG3	1.87	0.55
1:A:414:ARG:HG3	1:A:423:ASP:CB	2.35	0.55
1:A:478:LEU:HD13	1:A:490:TRP:HH2	1.72	0.55
1:A:471:ILE:HG23	1:A:476:VAL:HA	1.89	0.55
1:A:824:ASP:OD2	1:A:828:TYR:OH	2.10	0.55
2:B:58:ALA:HA	2:B:61:GLN:NE2	2.17	0.55
1:A:188:ARG:HG2	1:A:188:ARG:HH11	1.71	0.55
1:A:365:VAL:HG13	1:A:367:LEU:HD11	1.88	0.55
1:A:490:TRP:CE2	1:A:526:LEU:HB2	2.41	0.55
1:A:864:LYS:HE2	1:A:891:TYR:CE1	2.42	0.55
1:A:639:ARG:HH11	1:A:681:PRO:HD3	1.70	0.55
2:B:53:LEU:HB2	2:B:54:TRP:HA	1.88	0.55
2:B:227:LEU:H	2:B:236:TRP:HB3	1.72	0.55
1:A:425:LEU:HG	1:A:436:LEU:HB2	1.89	0.55
2:B:112:ARG:NH1	4:G:11:3DR:P	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:HG12	2:B:283:TYR:HB2	1.87	0.55
1:A:658:VAL:HG13	1:A:669:SER:O	2.07	0.55
1:A:1045:GLU:O	1:A:1049:ASN:ND2	2.36	0.55
1:A:518:TYR:OH	1:A:571:LEU:HD21	2.07	0.55
2:B:158:SER:O	2:B:177:MET:N	2.35	0.55
1:A:1130:ILE:HG13	1:A:1131:LYS:N	2.22	0.54
2:B:132:LYS:HA	2:B:158:SER:HA	1.89	0.54
2:B:302:ARG:HD3	2:B:316:SER:HA	1.88	0.54
4:G:12:DC:H5"	4:G:12:DC:H6	1.73	0.54
1:A:549:SER:H	1:A:550:ASN:HA	1.73	0.54
1:A:679:MET:SD	1:A:693:LEU:HB2	2.47	0.54
2:B:120:HIS:CE1	2:B:122:THR:HB	2.41	0.54
2:B:262:SER:OG	2:B:263:VAL:N	2.39	0.54
1:A:780:THR:HB	1:A:782:PHE:H	1.72	0.54
1:A:68:ARG:NE	1:A:72:GLU:O	2.41	0.54
2:B:20:ARG:HG3	2:B:40:LYS:HD2	1.90	0.54
2:B:98:LEU:HA	2:B:101:TYR:CD2	2.43	0.54
1:A:612:PHE:HE2	1:A:614:PHE:CD2	2.26	0.53
1:A:436:LEU:HB3	1:A:443:VAL:HG12	1.88	0.53
1:A:467:GLN:NE2	1:A:479:VAL:H	2.06	0.53
1:A:985:THR:O	1:A:989:ARG:NE	2.41	0.53
1:A:1105:MET:O	1:A:1109:VAL:HG22	2.09	0.53
1:A:1129:LEU:HA	1:A:1132:VAL:HG22	1.90	0.53
1:A:926:LEU:O	1:A:953:TRP:HD1	1.92	0.53
1:A:1128:ASP:OD1	1:A:1131:LYS:NZ	2.26	0.53
2:B:94:PHE:O	2:B:96:HIS:N	2.34	0.53
1:A:985:THR:OG1	1:A:987:GLU:N	2.42	0.53
1:A:270:ARG:HB2	1:A:270:ARG:NH1	2.22	0.53
1:A:703:THR:O	1:A:704:ILE:HG22	2.09	0.53
1:A:165:ILE:HB	1:A:181:VAL:HG13	1.90	0.53
1:A:232:ILE:HG21	1:A:258:ILE:HD12	1.91	0.53
1:A:627:LYS:HD2	1:A:1130:ILE:HD12	1.89	0.53
1:A:404:LEU:N	1:A:697:SER:O	2.30	0.53
1:A:642:ARG:HH12	1:A:644:LEU:C	2.12	0.53
1:A:754:PRO:HB2	1:A:759:GLN:HE22	1.74	0.52
1:A:943:GLU:N	1:A:943:GLU:OE1	2.41	0.52
1:A:677:ASN:ND2	1:A:696:ASN:OD1	2.37	0.52
1:A:414:ARG:CD	1:A:421:THR:HG23	2.40	0.52
1:A:473:SER:HA	1:A:498:ILE:HB	1.91	0.52
1:A:501:ALA:O	1:A:502:SER:HB2	2.10	0.52
2:B:123:HIS:CD2	2:B:125:SER:H	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:16:DG:N2	4:G:10:DG:N3	2.58	0.52
2:B:372:ILE:HB	2:B:386:LEU:HB2	1.91	0.52
1:A:507:GLN:HG3	1:A:520:GLN:HA	1.90	0.52
1:A:1111:ASN:OD1	1:A:1111:ASN:N	2.39	0.52
2:B:67:ARG:HE	2:B:67:ARG:CA	2.13	0.52
1:A:3:TYR:HB3	1:A:1048:TYR:HB2	1.91	0.52
2:B:53:LEU:HB2	2:B:54:TRP:CA	2.40	0.52
2:B:407:LEU:HB3	2:B:418:TRP:HB2	1.92	0.52
1:A:414:ARG:HD2	1:A:422:ASP:N	2.24	0.52
1:A:502:SER:OG	1:A:543:ILE:HG12	2.09	0.52
1:A:516:LEU:O	1:A:518:TYR:N	2.37	0.52
1:A:639:ARG:NE	1:A:650:PHE:HZ	2.07	0.52
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.45	0.52
2:B:307:ASP:OD1	2:B:308:GLN:N	2.38	0.52
1:A:117:GLU:OE2	2:B:82:SER:OG	2.24	0.52
1:A:520:GLN:HG2	1:A:529:ILE:HG12	1.91	0.52
2:B:101:TYR:O	2:B:103:ILE:N	2.43	0.52
2:B:208:ASP:O	2:B:217:VAL:HG12	2.10	0.52
1:A:414:ARG:HH21	1:A:419:ARG:HH22	1.57	0.52
1:A:492:GLU:OE2	1:A:496:LYS:N	2.27	0.52
1:A:465:HIS:ND1	1:A:465:HIS:O	2.40	0.51
1:A:722:ARG:NH2	1:A:812:TYR:OH	2.36	0.51
1:A:414:ARG:NE	1:A:423:ASP:HB2	2.25	0.51
1:A:519:LEU:CD2	1:A:526:LEU:HD11	2.40	0.51
1:A:84:TYR:HD1	1:A:109:GLN:HE21	1.59	0.51
1:A:568:ILE:HG13	1:A:577:LEU:HD11	1.92	0.51
1:A:677:ASN:OD1	1:A:695:ASN:HA	2.09	0.51
2:B:66:CYS:HB3	2:B:92:GLN:HE22	1.75	0.51
1:A:902:GLU:OE2	1:A:935:TYR:OH	2.29	0.51
2:B:126:THR:HB	2:B:140:ASN:HB2	1.91	0.51
2:B:287:HIS:HD2	2:B:313:ARG:NH1	2.07	0.51
1:A:374:GLN:O	1:A:1012:LEU:HD12	2.10	0.51
1:A:536:HIS:CD2	1:A:562:THR:HG1	2.29	0.51
3:F:2:DG:H2'	3:F:3:DA:C8	2.46	0.51
1:A:404:LEU:HD21	1:A:407:ILE:HG23	1.93	0.51
1:A:381:ALA:HA	1:A:721:PRO:HD2	1.92	0.51
1:A:423:ASP:CG	1:A:438:LEU:HB3	2.32	0.51
1:A:558:ILE:HD11	1:A:567:ARG:HB2	1.93	0.51
1:A:796:GLN:HE21	1:A:797:HIS:CE1	2.29	0.51
1:A:836:VAL:HB	2:B:71:ARG:NH2	2.25	0.51
1:A:368:GLU:C	1:A:370:GLN:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ARG:NH1	1:A:680:CYS:HA	2.26	0.51
1:A:683:ASN:ND2	1:A:689:ASP:OD1	2.44	0.51
1:A:869:ALA:H	1:A:885:ASN:ND2	2.07	0.51
1:A:1111:ASN:C	1:A:1113:GLN:N	2.63	0.51
2:B:132:LYS:NZ	4:G:12:DC:OP1	2.43	0.51
1:A:258:ILE:HA	1:A:275:ASP:HA	1.93	0.51
1:A:650:PHE:CA	1:A:658:VAL:HA	2.37	0.51
1:A:836:VAL:HB	2:B:71:ARG:HH22	1.76	0.50
1:A:1081:LYS:NZ	1:A:1082:THR:H	2.08	0.50
2:B:131:SER:OG	2:B:134:GLY:N	2.44	0.50
1:A:5:TYR:OH	1:A:1136:LEU:HD23	2.11	0.50
1:A:133:LEU:HB2	1:A:141:LYS:HB2	1.92	0.50
1:A:627:LYS:HD2	1:A:1130:ILE:CD1	2.41	0.50
1:A:651:ALA:HB3	1:A:657:THR:HG23	1.93	0.50
1:A:423:ASP:CG	1:A:424:THR:H	2.07	0.50
1:A:502:SER:HB2	1:A:541:LEU:HB3	1.92	0.50
1:A:889:ARG:HG3	1:A:904:ASN:OD1	2.11	0.50
4:G:1:DG:N2	4:G:2:DT:O2	2.42	0.50
1:A:1111:ASN:C	1:A:1113:GLN:H	2.14	0.50
4:G:13:DA:H8	4:G:13:DA:H5'	1.75	0.50
1:A:824:ASP:OD1	1:A:826:ASN:ND2	2.40	0.50
1:A:198:ARG:C	1:A:200:LYS:H	2.15	0.50
1:A:596:PHE:O	1:A:599:SER:OG	2.15	0.50
1:A:739:ARG:NH1	1:A:741:GLU:OE1	2.44	0.50
1:A:367:LEU:O	1:A:369:ARG:N	2.45	0.50
1:A:634:GLN:NE2	1:A:675:GLU:OE2	2.45	0.50
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.94	0.50
1:A:517:TYR:N	1:A:532:THR:OG1	2.45	0.50
1:A:639:ARG:NH2	1:A:679:MET:HG2	2.27	0.50
2:B:376:ASP:HB3	2:B:379:SER:OG	2.12	0.50
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.94	0.49
1:A:838:PRO:HA	2:B:67:ARG:HD2	1.94	0.49
1:A:470:GLN:O	1:A:477:ARG:HB3	2.13	0.49
1:A:602:LEU:HD23	1:A:616:LEU:HD21	1.94	0.49
1:A:741:GLU:HG3	1:A:749:THR:CB	2.42	0.49
2:B:259:ALA:HA	2:B:269:ILE:HA	1.94	0.49
1:A:1125:THR:HA	1:A:1128:ASP:CB	2.42	0.49
2:B:248:VAL:HG13	2:B:260:THR:HG22	1.93	0.49
1:A:1020:THR:HA	1:A:1021:SER:C	2.33	0.49
1:A:416:ASP:N	1:A:416:ASP:OD1	2.46	0.49
1:A:550:ASN:H	1:A:551:GLY:HA2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:SER:O	2:B:196:SER:OG	2.25	0.49
2:B:236:TRP:CH2	2:B:272:LEU:HB2	2.48	0.49
4:G:9:DC:H2'	4:G:10:DG:N7	2.28	0.49
1:A:24:THR:H	1:A:30:ASN:HD21	1.61	0.48
1:A:812:TYR:HB2	1:A:836:VAL:CG2	2.43	0.48
1:A:1125:THR:HA	1:A:1128:ASP:HB3	1.96	0.48
1:A:23:PHE:HB2	1:A:66:LEU:HD21	1.94	0.48
1:A:519:LEU:CG	1:A:526:LEU:HD11	2.43	0.48
1:A:650:PHE:HB3	1:A:658:VAL:HB	1.95	0.48
1:A:586:ILE:HD13	1:A:586:ILE:H	1.78	0.48
1:A:613:TYR:OH	1:A:627:LYS:HD3	2.14	0.48
2:B:241:HIS:HE1	2:B:262:SER:HB3	1.78	0.48
1:A:639:ARG:NE	1:A:650:PHE:CZ	2.82	0.48
1:A:157:ILE:HD11	1:A:202:PHE:CE2	2.49	0.48
1:A:909:ILE:HG21	1:A:927:MET:HG3	1.95	0.48
1:A:1111:ASN:O	1:A:1113:GLN:N	2.46	0.48
2:B:354:GLY:HA3	2:B:395:SER:O	2.13	0.48
1:A:511:ALA:HA	1:A:516:LEU:HA	1.95	0.48
1:A:889:ARG:HD3	1:A:901:THR:HB	1.95	0.48
2:B:64:PRO:C	2:B:67:ARG:NH2	2.67	0.48
2:B:263:VAL:HG23	2:B:290:PRO:CB	2.44	0.48
1:A:555:LEU:HD22	1:A:593:MET:SD	2.54	0.48
1:A:929:SER:HA	1:A:954:MET:HE1	1.95	0.48
1:A:1063:LYS:O	1:A:1065:VAL:N	2.39	0.48
2:B:69:ILE:O	2:B:72:THR:N	2.46	0.48
4:G:9:DC:C4	4:G:10:DG:C6	3.02	0.48
1:A:558:ILE:HG13	1:A:567:ARG:CZ	2.43	0.47
1:A:650:PHE:HB2	1:A:657:THR:O	2.14	0.47
2:B:254:CYS:SG	2:B:257:PHE:HB2	2.53	0.47
1:A:167:VAL:HG23	1:A:180:PHE:HB3	1.97	0.47
1:A:209:GLN:OE1	1:A:209:GLN:N	2.47	0.47
1:A:768:SER:HA	1:A:769:LYS:CB	2.44	0.47
1:A:1128:ASP:O	1:A:1132:VAL:HG13	2.14	0.47
2:B:281:PHE:O	2:B:283:TYR:N	2.45	0.47
1:A:396:ILE:HG22	1:A:704:ILE:HA	1.96	0.47
1:A:661:SER:HA	1:A:666:LEU:HA	1.96	0.47
2:B:71:ARG:O	2:B:75:GLN:HG2	2.14	0.47
1:A:634:GLN:HG2	1:A:635:PRO:HD2	1.97	0.47
1:A:817:VAL:HG23	1:A:873:MET:HG3	1.95	0.47
1:A:1131:LYS:O	1:A:1134:GLU:HG2	2.15	0.47
2:B:36:LYS:NZ	2:B:40:LYS:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ILE:C	2:B:145:ASP:H	2.18	0.47
2:B:276:ARG:HG3	2:B:276:ARG:NH1	2.27	0.47
1:A:498:ILE:HG13	1:A:512:VAL:HG12	1.96	0.47
1:A:577:LEU:HD12	1:A:578:HIS:H	1.78	0.47
2:B:138:LEU:HB2	2:B:186:PHE:CD1	2.48	0.47
1:A:258:ILE:HG13	1:A:273:LEU:HB3	1.96	0.47
1:A:660:TYR:HB2	1:A:667:VAL:HG13	1.97	0.47
2:B:306:THR:CG2	2:B:342:ALA:HB3	2.45	0.47
1:A:81:THR:OG1	1:A:85:ASN:HB2	2.15	0.47
1:A:879:LYS:HG3	1:A:892:GLU:HA	1.96	0.47
1:A:964:ASN:CG	1:A:978:GLN:HE21	2.17	0.47
1:A:998:PHE:HB2	1:A:1088:PHE:CD2	2.49	0.47
2:B:269:ILE:HG13	2:B:270:TRP:H	1.80	0.47
2:B:309:LYS:HD2	2:B:309:LYS:HA	1.71	0.47
1:A:252:ILE:H	1:A:252:ILE:HG13	1.53	0.47
1:A:414:ARG:HH11	1:A:422:ASP:H	1.60	0.47
1:A:558:ILE:HG13	1:A:567:ARG:NE	2.30	0.47
2:B:30:LEU:HD13	2:B:30:LEU:HA	1.64	0.47
2:B:155:ALA:HA	4:G:11:3DR:H5'	1.95	0.47
2:B:266:THR:HG22	2:B:286:PRO:HA	1.96	0.47
2:B:305:THR:HG21	2:B:315:TYR:HE2	1.80	0.47
1:A:450:GLY:O	1:A:477:ARG:NH1	2.48	0.47
1:A:658:VAL:HG21	1:A:660:TYR:CZ	2.50	0.47
1:A:879:LYS:HE3	1:A:892:GLU:HG3	1.96	0.47
2:B:125:SER:OG	2:B:140:ASN:ND2	2.48	0.47
1:A:118:THR:HG1	1:A:134:ARG:HH22	1.63	0.46
1:A:286:GLU:HG3	1:A:298:LYS:HG3	1.95	0.46
1:A:526:LEU:HA	1:A:526:LEU:HD12	1.56	0.46
1:A:655:ARG:HB3	1:A:670:ASN:ND2	2.24	0.46
1:A:784:GLU:CG	1:A:785:GLU:H	2.28	0.46
2:B:29:GLU:O	2:B:30:LEU:HB2	2.15	0.46
1:A:568:ILE:O	1:A:577:LEU:HD11	2.15	0.46
1:A:610:ALA:HA	1:A:630:THR:HA	1.97	0.46
1:A:611:LEU:HD21	1:A:631:LEU:HD23	1.98	0.46
1:A:931:LEU:HD11	1:A:944:GLU:HG3	1.96	0.46
2:B:391:SER:O	2:B:391:SER:OG	2.31	0.46
1:A:889:ARG:NH1	1:A:891:TYR:OH	2.48	0.46
2:B:108:ALA:HA	2:B:109:PRO:HD3	1.74	0.46
2:B:287:HIS:ND1	2:B:291:VAL:HG11	2.30	0.46
1:A:879:LYS:NZ	1:A:879:LYS:HA	2.31	0.46
2:B:397:LEU:HB2	2:B:410:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:10:DG:O3'	4:G:11:3DR:O3'	2.33	0.46
1:A:74:LYS:HD2	1:A:74:LYS:HA	1.30	0.46
1:A:410:LEU:HD12	1:A:411:TRP:N	2.30	0.46
1:A:530:SER:OG	1:A:531:HIS:N	2.49	0.46
1:A:936:LYS:HB3	1:A:939:GLU:OE1	2.16	0.46
1:A:676:VAL:HG23	1:A:693:LEU:HD13	1.97	0.46
2:B:113:ARG:HH22	2:B:338:THR:H	1.63	0.46
2:B:158:SER:HB3	2:B:177:MET:HB2	1.97	0.46
4:G:9:DC:C2	4:G:10:DG:C5	3.04	0.46
4:G:13:DA:H5'	4:G:13:DA:C8	2.49	0.46
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	1.97	0.46
1:A:458:PHE:CE1	1:A:501:ALA:HB1	2.51	0.46
1:A:639:ARG:NH1	1:A:681:PRO:HD3	2.31	0.46
1:A:1136:LEU:O	1:A:1138:ARG:N	2.49	0.46
2:B:414:HIS:O	2:B:415:ILE:HD13	2.16	0.46
1:A:41:ILE:HD12	1:A:52:VAL:HG13	1.96	0.46
1:A:58:TYR:HB3	1:A:1073:TRP:CB	2.46	0.46
1:A:478:LEU:HD21	1:A:524:GLN:HA	1.97	0.46
1:A:943:GLU:N	1:A:943:GLU:CD	2.70	0.46
1:A:407:ILE:HD12	1:A:678:TYR:HD2	1.81	0.46
4:G:22:DT:H2'	4:G:23:DC:C6	2.50	0.46
1:A:561:TRP:CD1	1:A:587:ILE:HG21	2.51	0.45
1:A:838:PRO:HB2	1:A:839:GLU:OE2	2.16	0.45
2:B:95:LEU:HA	2:B:98:LEU:HB3	1.97	0.45
2:B:241:HIS:HD2	2:B:242:LYS:O	1.99	0.45
3:F:19:DG:H1	4:G:6:DC:H42	1.62	0.45
4:G:3:DC:H2'	4:G:4:DA:C8	2.52	0.45
1:A:727:GLN:HB2	1:A:829:PHE:CZ	2.51	0.45
2:B:299:ASP:OD1	2:B:300:GLY:N	2.49	0.45
2:B:397:LEU:HD12	2:B:410:ALA:HB3	1.99	0.45
1:A:178:ILE:HG22	1:A:193:TYR:HB2	1.97	0.45
1:A:414:ARG:HH12	1:A:684:SER:HA	1.80	0.45
2:B:69:ILE:O	2:B:71:ARG:N	2.49	0.45
2:B:99:ASP:CG	2:B:102:ARG:HH21	2.19	0.45
2:B:218:THR:HB	2:B:226:ILE:HD11	1.97	0.45
1:A:83:LYS:H	1:A:83:LYS:HG3	1.61	0.45
1:A:545:PRO:O	1:A:550:ASN:ND2	2.49	0.45
2:B:163:LYS:HA	2:B:163:LYS:HD3	1.55	0.45
2:B:370:ARG:NE	2:B:392:SER:O	2.49	0.45
1:A:414:ARG:HH21	1:A:419:ARG:NH2	2.15	0.45
1:A:905:HIS:CE1	1:A:933:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:PRO:O	2:B:67:ARG:NH2	2.49	0.45
2:B:223:GLY:HA2	2:B:245:VAL:HG23	1.97	0.45
1:A:404:LEU:HD21	1:A:429:PHE:HE1	1.80	0.45
1:A:680:CYS:O	1:A:691:LEU:HD12	2.16	0.45
2:B:112:ARG:NH2	4:G:11:3DR:OP1	2.48	0.45
2:B:219:GLY:HA2	2:B:225:VAL:HB	1.97	0.45
2:B:335:GLN:OE1	3:F:13:DG:N2	2.49	0.45
3:F:12:DT:H2"	3:F:13:DG:N7	2.31	0.45
1:A:58:TYR:HB3	1:A:1073:TRP:CG	2.52	0.45
1:A:356:LEU:HD12	1:A:388:ARG:HG3	1.99	0.45
1:A:964:ASN:OD1	1:A:978:GLN:NE2	2.49	0.45
2:B:351:ILE:O	2:B:374:VAL:HA	2.17	0.45
1:A:129:ARG:C	1:A:145:LEU:HG	2.37	0.45
1:A:575:GLU:HG2	1:A:575:GLU:O	2.15	0.45
1:A:1057:ARG:HH21	1:A:1112:LEU:CB	2.30	0.45
2:B:60:PRO:HA	2:B:63:LEU:HB2	1.97	0.45
2:B:90:LEU:HD12	2:B:90:LEU:HA	1.82	0.45
1:A:128:CYS:O	1:A:145:LEU:HD11	2.16	0.45
1:A:149:ASN:OD1	1:A:149:ASN:N	2.47	0.45
1:A:586:ILE:HG21	1:A:608:ASP:OD1	2.16	0.45
1:A:614:PHE:HB3	1:A:616:LEU:HD12	1.99	0.45
1:A:226:PHE:CE1	1:A:297:LEU:HG	2.51	0.44
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.81	0.44
1:A:414:ARG:HB2	1:A:421:THR:O	2.17	0.44
1:A:515:ALA:HA	1:A:534:MET:HG2	1.98	0.44
1:A:614:PHE:CE1	1:A:623:LEU:HB3	2.52	0.44
1:A:639:ARG:NH1	1:A:641:PHE:CE2	2.85	0.44
1:A:815:SER:HB2	1:A:873:MET:HG2	1.99	0.44
1:A:492:GLU:OE2	1:A:495:ALA:N	2.50	0.44
1:A:936:LYS:HB3	1:A:939:GLU:CD	2.37	0.44
1:A:1128:ASP:O	1:A:1131:LYS:N	2.51	0.44
2:B:384:CYS:SG	2:B:385:GLN:N	2.89	0.44
1:A:679:MET:HG3	1:A:691:LEU:HD11	1.98	0.44
1:A:1100:ILE:HD13	1:A:1105:MET:HG2	1.98	0.44
2:B:160:THR:O	2:B:175:SER:HB2	2.17	0.44
1:A:360:VAL:HG22	1:A:379:SER:HB2	2.00	0.44
1:A:465:HIS:HE1	1:A:467:GLN:OE1	2.01	0.44
2:B:216:VAL:CG2	2:B:228:LEU:HB2	2.44	0.44
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.99	0.44
1:A:246:LEU:HD21	1:A:299:ASP:N	2.32	0.44
1:A:359:ILE:HG23	1:A:378:CYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:ASP:C	1:A:746:SER:H	2.21	0.44
1:A:913:TYR:CE2	1:A:954:MET:HG3	2.52	0.44
2:B:69:ILE:HG22	2:B:73:LEU:HG	2.00	0.44
2:B:255:ASP:CG	2:B:256:TRP:H	2.12	0.44
1:A:17:GLY:H	1:A:34:ALA:HB3	1.82	0.44
1:A:27:GLU:H	1:A:27:GLU:CD	2.19	0.44
1:A:408:LYS:HG3	1:A:428:SER:OG	2.18	0.44
1:A:613:TYR:HE2	1:A:629:VAL:HG13	1.82	0.44
1:A:656:PRO:HG3	1:A:676:VAL:HG12	2.00	0.44
2:B:273:ARG:HG3	2:B:274:GLN:N	2.32	0.44
1:A:68:ARG:HD3	1:A:74:LYS:O	2.17	0.44
1:A:378:CYS:SG	1:A:388:ARG:HB2	2.57	0.44
1:A:657:THR:HA	1:A:670:ASN:HA	1.99	0.44
1:A:412:PRO:O	1:A:461:GLY:HA2	2.16	0.44
1:A:784:GLU:HG3	1:A:785:GLU:H	1.82	0.44
1:A:1129:LEU:HA	1:A:1132:VAL:HG13	1.99	0.44
2:B:245:VAL:HA	2:B:262:SER:CB	2.44	0.44
1:A:387:LEU:HB2	1:A:715:VAL:HG13	2.00	0.44
1:A:813:ALA:HA	1:A:833:THR:HG22	2.00	0.44
1:A:935:TYR:CG	1:A:936:LYS:N	2.85	0.44
2:B:113:ARG:NH2	2:B:338:THR:H	2.16	0.44
2:B:119:TRP:NE1	2:B:399:GLU:O	2.48	0.44
2:B:317:ALA:HA	2:B:320:TRP:CE2	2.53	0.44
1:A:471:ILE:HG23	1:A:476:VAL:HG13	2.00	0.43
1:A:535:GLU:O	1:A:536:HIS:ND1	2.51	0.43
1:A:262:ASN:CG	1:A:315:THR:HA	2.39	0.43
1:A:373:GLY:O	1:A:374:GLN:HB2	2.19	0.43
1:A:477:ARG:NH1	1:A:486:LEU:HD11	2.30	0.43
1:A:515:ALA:O	1:A:516:LEU:HD12	2.18	0.43
1:A:516:LEU:HD11	1:A:541:LEU:HD11	1.99	0.43
1:A:1076:PHE:N	1:A:1083:GLU:O	2.51	0.43
2:B:270:TRP:NE1	2:B:281:PHE:HB3	2.32	0.43
2:B:331:HIS:HB2	2:B:340:ILE:HD12	2.00	0.43
1:A:467:GLN:HE21	1:A:479:VAL:H	1.66	0.43
1:A:727:GLN:OE1	1:A:818:SER:OG	2.24	0.43
2:B:131:SER:HG	2:B:134:GLY:H	1.62	0.43
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.18	0.43
1:A:434:ARG:HH21	1:A:436:LEU:CD2	2.31	0.43
1:A:455:GLN:NE2	1:A:474:ALA:HB3	2.34	0.43
1:A:545:PRO:HG2	1:A:550:ASN:H	1.81	0.43
1:A:642:ARG:NH1	1:A:644:LEU:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ILE:HG12	1:A:928:ARG:NH1	2.33	0.43
1:A:1053:ASP:OD1	1:A:1054:MET:N	2.51	0.43
1:A:1070:HIS:HE1	1:A:1090:ASP:OD2	2.01	0.43
1:A:545:PRO:CG	1:A:550:ASN:H	2.32	0.43
2:B:317:ALA:HA	2:B:320:TRP:CZ2	2.54	0.43
2:B:321:ASP:OD1	2:B:321:ASP:N	2.35	0.43
1:A:1:HIS:C	1:A:978:GLN:HE22	2.21	0.43
1:A:614:PHE:HB3	1:A:616:LEU:CD1	2.49	0.43
1:A:826:ASN:HB2	1:A:828:TYR:CZ	2.53	0.43
2:B:143:ILE:O	2:B:144:LYS:HG2	2.19	0.43
2:B:307:ASP:O	2:B:331:HIS:NE2	2.51	0.43
1:A:161:GLU:OE1	1:A:161:GLU:N	2.52	0.43
1:A:250:PRO:HG2	1:A:253:ILE:HG12	2.01	0.43
1:A:612:PHE:HE2	1:A:614:PHE:CE2	2.37	0.43
1:A:920:PHE:O	1:A:921:ILE:HD13	2.19	0.43
1:A:682:LEU:HD22	1:A:692:ALA:HB2	2.01	0.43
2:B:236:TRP:CZ3	2:B:272:LEU:HB2	2.53	0.43
1:A:396:ILE:HD11	1:A:673:LEU:CG	2.49	0.43
1:A:921:ILE:HB	1:A:933:LEU:HB2	2.01	0.43
2:B:265:GLN:HG2	2:B:289:HIS:C	2.39	0.43
1:A:518:TYR:CE2	1:A:529:ILE:HG13	2.54	0.42
1:A:917:LYS:HE3	1:A:962:ASP:OD1	2.19	0.42
2:B:105:GLN:C	2:B:106:LYS:HD2	2.39	0.42
4:G:20:DA:H2'	4:G:21:DG:C8	2.54	0.42
1:A:246:LEU:HD21	1:A:299:ASP:H	1.85	0.42
1:A:372:GLN:HE22	1:A:655:ARG:HH12	1.67	0.42
1:A:414:ARG:HD2	1:A:422:ASP:CA	2.49	0.42
1:A:490:TRP:CD2	1:A:526:LEU:HD22	2.54	0.42
1:A:544:THR:HA	1:A:545:PRO:HD3	1.81	0.42
1:A:844:LYS:O	1:A:868:GLY:N	2.52	0.42
1:A:864:LYS:HE3	1:A:864:LYS:HB3	1.70	0.42
1:A:909:ILE:CG2	1:A:927:MET:HG3	2.49	0.42
2:B:20:ARG:HH21	2:B:47:ARG:HD3	1.83	0.42
2:B:165:ASN:ND2	2:B:168:ASN:H	2.17	0.42
1:A:407:ILE:H	1:A:407:ILE:HG13	1.49	0.42
1:A:677:ASN:HB2	1:A:678:TYR:H	1.57	0.42
1:A:408:LYS:HZ2	1:A:430:VAL:HA	1.84	0.42
2:B:74:HIS:O	2:B:78:LEU:HG	2.19	0.42
1:A:38:ARG:NE	1:A:54:GLU:OE2	2.51	0.42
1:A:158:ARG:NE	1:A:160:GLU:OE2	2.52	0.42
1:A:190:VAL:HG12	1:A:210:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:GLU:C	1:A:599:SER:H	2.23	0.42
1:A:824:ASP:OD2	1:A:897:LYS:HE3	2.19	0.42
2:B:46:ARG:O	2:B:48:CYS:HA	2.19	0.42
2:B:135:ASP:HB3	2:B:149:PHE:CZ	2.54	0.42
1:A:570:LYS:HA	1:A:570:LYS:HD2	1.84	0.42
1:A:335:LYS:NZ	1:A:337:ASN:ND2	2.67	0.42
1:A:587:ILE:HD13	1:A:589:ARG:NH2	2.34	0.42
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.66	0.42
2:B:67:ARG:HB3	2:B:71:ARG:NH1	2.32	0.42
1:A:87:CYS:SG	1:A:89:LEU:HD11	2.60	0.42
1:A:500:VAL:O	1:A:511:ALA:HB3	2.19	0.42
1:A:843:PRO:O	1:A:844:LYS:HD2	2.20	0.42
1:A:879:LYS:NZ	1:A:893:TRP:H	2.18	0.42
1:A:969:GLU:HG2	1:A:970:ASN:H	1.84	0.42
2:B:111:ASP:HA	2:B:413:TYR:CE2	2.54	0.42
2:B:215:MET:SD	2:B:233:LYS:NZ	2.91	0.42
2:B:273:ARG:CG	2:B:274:GLN:N	2.83	0.42
1:A:362:MET:HA	1:A:724:ILE:HD11	2.02	0.42
1:A:389:ILE:HB	1:A:713:ARG:HB3	2.02	0.42
1:A:549:SER:N	1:A:550:ASN:HA	2.34	0.42
2:B:107:ALA:HA	2:B:415:ILE:O	2.20	0.42
2:B:120:HIS:CE1	2:B:123:HIS:H	2.38	0.42
1:A:234:GLN:OE1	1:A:234:GLN:N	2.52	0.42
1:A:282:MET:SD	1:A:305:LEU:HD11	2.59	0.42
1:A:413:LEU:HD11	1:A:424:THR:HB	2.01	0.42
2:B:68:SER:HB3	2:B:71:ARG:HH11	1.85	0.42
2:B:290:PRO:HB2	2:B:308:GLN:CD	2.40	0.42
1:A:270:ARG:NH2	1:A:271:TYR:O	2.53	0.41
1:A:335:LYS:HB3	1:A:335:LYS:HZ2	1.84	0.41
1:A:518:TYR:HE2	1:A:529:ILE:HG13	1.85	0.41
1:A:531:HIS:CG	1:A:532:THR:N	2.88	0.41
1:A:1109:VAL:HB	1:A:1123:GLU:OE1	2.20	0.41
2:B:88:GLN:HA	2:B:91:GLN:HE21	1.85	0.41
2:B:233:LYS:HG3	2:B:235:LEU:HG	2.02	0.41
1:A:467:GLN:HE22	1:A:478:LEU:CG	2.21	0.41
1:A:516:LEU:C	1:A:518:TYR:N	2.73	0.41
1:A:1018:GLY:HA2	1:A:1019:GLU:HA	1.56	0.41
2:B:109:PRO:HB3	2:B:414:HIS:ND1	2.35	0.41
2:B:330:PRO:CG	2:B:355:ARG:HE	2.34	0.41
1:A:184:ASP:OD1	1:A:189:HIS:NE2	2.48	0.41
1:A:354:THR:HG23	1:A:388:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ILE:HG22	1:A:582:LEU:HD21	2.03	0.41
1:A:612:PHE:CE2	1:A:614:PHE:CE2	3.09	0.41
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.20	0.41
1:A:241:ASN:HD21	1:A:244:LYS:HB3	1.86	0.41
1:A:273:LEU:HD22	1:A:283:LEU:HB2	2.01	0.41
1:A:394:ILE:H	1:A:394:ILE:HG13	1.68	0.41
1:A:519:LEU:HD21	1:A:526:LEU:HD11	2.01	0.41
1:A:659:ILE:HA	1:A:667:VAL:O	2.19	0.41
1:A:694:ALA:O	1:A:695:ASN:O	2.38	0.41
1:A:698:THR:OG1	1:A:699:LEU:N	2.54	0.41
1:A:128:CYS:C	1:A:145:LEU:HD21	2.40	0.41
1:A:213:GLU:HG3	1:A:214:ALA:H	1.85	0.41
1:A:408:LYS:NZ	1:A:430:VAL:HA	2.36	0.41
1:A:558:ILE:HD13	1:A:558:ILE:N	2.35	0.41
2:B:346:PRO:C	2:B:348:TYR:H	2.23	0.41
1:A:165:ILE:HG21	1:A:217:SER:HA	2.02	0.41
2:B:113:ARG:HH22	2:B:337:LEU:HA	1.85	0.41
1:A:108:VAL:HG21	1:A:154:ALA:HB3	2.03	0.41
1:A:129:ARG:HH12	1:A:176:PRO:CB	2.24	0.41
1:A:402:ILE:HB	1:A:699:LEU:CD2	2.50	0.41
1:A:567:ARG:NH1	1:A:569:LEU:HD11	2.34	0.41
1:A:693:LEU:HD21	1:A:695:ASN:HD21	1.85	0.41
2:B:240:MET:O	2:B:241:HIS:HB3	2.21	0.41
2:B:241:HIS:ND1	2:B:268:LYS:HE2	2.36	0.41
2:B:415:ILE:HD13	2:B:415:ILE:HA	1.87	0.41
1:A:508:VAL:O	1:A:519:LEU:HB3	2.21	0.41
1:A:662:SER:N	1:A:665:LYS:O	2.48	0.41
2:B:229:ASN:HB3	2:B:231:ASP:H	1.84	0.41
2:B:236:TRP:HE1	2:B:240:MET:HE3	1.86	0.41
2:B:269:ILE:O	2:B:270:TRP:HB2	2.21	0.41
1:A:68:ARG:CZ	1:A:72:GLU:O	2.69	0.41
1:A:146:ASP:O	1:A:147:ARG:C	2.58	0.41
1:A:372:GLN:NE2	1:A:655:ARG:HH12	2.19	0.41
1:A:419:ARG:HG2	1:A:421:THR:CG2	2.51	0.41
1:A:548:ASP:OD1	1:A:549:SER:N	2.48	0.41
1:A:648:ASN:HB3	1:A:660:TYR:HE1	1.86	0.41
1:A:1028:VAL:HB	1:A:1040:VAL:HB	2.01	0.41
2:B:25:ARG:HG3	2:B:25:ARG:O	2.21	0.41
2:B:118:ALA:HB2	2:B:162:LEU:O	2.20	0.41
2:B:146:LYS:HA	2:B:147:PRO:HD3	1.81	0.41
2:B:255:ASP:C	2:B:257:PHE:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:LEU:H	2:B:369:LEU:HG	1.39	0.41
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.87	0.41
1:A:624:SER:OG	1:A:625:ASP:N	2.53	0.41
1:A:657:THR:OG1	1:A:658:VAL:N	2.53	0.41
1:A:699:LEU:HD12	1:A:700:THR:N	2.36	0.41
2:B:31:GLU:OE2	2:B:32:PRO:HA	2.20	0.41
1:A:601:TYR:CE2	1:A:613:TYR:HB2	2.51	0.40
2:B:401:ASN:ND2	2:B:406:THR:HG22	2.36	0.40
4:G:17:DT:H2'	4:G:18:DA:O4'	2.21	0.40
1:A:184:ASP:HB2	1:A:185:PRO:HD2	2.03	0.40
1:A:854:SER:O	1:A:857:LYS:HG2	2.21	0.40
1:A:876:PHE:O	1:A:879:LYS:HB2	2.22	0.40
1:A:1053:ASP:CG	1:A:1057:ARG:HH12	2.23	0.40
1:A:1079:GLU:CD	1:A:1079:GLU:H	2.24	0.40
2:B:246:THR:H	2:B:262:SER:HB2	1.86	0.40
1:A:614:PHE:HD1	1:A:624:SER:O	2.04	0.40
1:A:189:HIS:HB3	1:A:210:GLU:O	2.21	0.40
1:A:636:THR:HA	1:A:652:CYS:O	2.21	0.40
1:A:1109:VAL:HA	1:A:1112:LEU:CB	2.50	0.40
1:A:1125:THR:O	1:A:1129:LEU:HD13	2.22	0.40
2:B:53:LEU:CB	2:B:54:TRP:HA	2.51	0.40
2:B:199:THR:HG1	2:B:200:ILE:H	1.58	0.40
1:A:43:VAL:HG23	1:A:52:VAL:HG11	2.03	0.40
1:A:389:ILE:HD11	1:A:799:PHE:CE1	2.57	0.40
1:A:536:HIS:CE1	1:A:562:THR:HG1	2.36	0.40
1:A:1015:GLN:HE21	1:A:1016:ASN:H	1.69	0.40
1:A:1134:GLU:HG3	1:A:1138:ARG:NH1	2.37	0.40
2:B:95:LEU:HD13	2:B:383:MET:HB3	2.02	0.40
2:B:223:GLY:HA3	2:B:241:HIS:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:OD2	1:A:1046:SER:OG[1_455]	2.16	0.04
2:B:42:SER:OG	2:B:187:LYS:O[1_455]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1138/1150 (99%)	932 (82%)	142 (12%)	64 (6%)	2 13
2	B	400/436 (92%)	301 (75%)	60 (15%)	39 (10%)	0 3
All	All	1538/1586 (97%)	1233 (80%)	202 (13%)	103 (7%)	1 8

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	A	295	VAL
1	A	303	GLU
1	A	370	GLN
1	A	502	SER
1	A	518	TYR
1	A	546	LEU
1	A	575	GLU
1	A	606	LEU
1	A	640	THR
1	A	644	LEU
1	A	647	THR
1	A	650	PHE
1	A	695	ASN
1	A	771	PHE
1	A	1065	VAL
1	A	1137	THR
2	B	22	LYS
2	B	26	SER
2	B	30	LEU
2	B	47	ARG
2	B	65	PRO
2	B	197	SER
2	B	256	TRP
2	B	264	ASP

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Mol	Chain	Res	Type
2	B	277	GLY
2	B	306	THR
2	B	311	GLU
1	A	214	ALA
1	A	226	PHE
1	A	424	THR
1	A	481	GLN
1	A	512	VAL
1	A	540	CYS
1	A	663	ASN
1	A	674	LYS
1	A	701	ILE
1	A	704	ILE
1	A	742	VAL
1	A	750	THR
1	A	856	GLY
1	A	1112	LEU
1	A	1119	GLY
2	B	52	CYS
2	B	53	LEU
2	B	102	ARG
2	B	113	ARG
2	B	269	ILE
2	B	274	GLN
2	B	278	LYS
2	B	281	PHE
2	B	399	GLU
1	A	234	GLN
1	A	345	SER
1	A	368	GLU
1	A	413	LEU
1	A	488	SER
1	A	511	ALA
1	A	580	GLU
1	A	643	SER
1	A	1086	THR
2	B	68	SER
2	B	192	ARG
2	B	201	ASN
2	B	220	ASP
2	B	237	ASN
2	B	255	ASP

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Mol	Chain	Res	Type
2	B	282	LEU
2	B	301	ALA
2	B	303	LEU
1	A	36	ASN
1	A	225	PRO
1	A	464	ALA
1	A	534	MET
1	A	536	HIS
1	A	590	SER
2	B	70	VAL
2	B	144	LYS
2	B	200	ILE
2	B	275	VAL
2	B	347	ARG
1	A	75	ASP
1	A	213	GLU
1	A	304	LEU
1	A	367	LEU
1	A	517	TYR
1	A	544	THR
1	A	574	PHE
1	A	785	GLU
1	A	862	ALA
1	A	863	GLU
1	A	1020	THR
1	A	1115	ASP
2	B	35	LYS
2	B	109	PRO
2	B	161	GLY
2	B	233	LYS
2	B	284	SER
1	A	109	GLN
1	A	369	ARG
1	A	564	ILE
1	A	1018	GLY
1	A	125	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	980/1009 (97%)	849 (87%)	131 (13%)	4 17
2	B	347/380 (91%)	297 (86%)	50 (14%)	3 14
All	All	1327/1389 (96%)	1146 (86%)	181 (14%)	3 16

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	41	ILE
1	A	52	VAL
1	A	74	LYS
1	A	75	ASP
1	A	83	LYS
1	A	125	ASP
1	A	142	VAL
1	A	145	LEU
1	A	147	ARG
1	A	149	ASN
1	A	159	LEU
1	A	178	ILE
1	A	188	ARG
1	A	196	SER
1	A	215	GLU
1	A	235	GLU
1	A	237	ILE
1	A	257	THR
1	A	258	ILE
1	A	270	ARG
1	A	273	LEU
1	A	291	MET
1	A	294	THR
1	A	296	THR
1	A	302	VAL
1	A	303	GLU
1	A	348	VAL
1	A	356	LEU
1	A	367	LEU
1	A	376	VAL
1	A	382	PHE
1	A	394	ILE

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Mol	Chain	Res	Type
1	A	403	ASP
1	A	407	ILE
1	A	410	LEU
1	A	414	ARG
1	A	415	SER
1	A	416	ASP
1	A	418	ASN
1	A	420	GLU
1	A	434	ARG
1	A	443	VAL
1	A	462	ASN
1	A	465	HIS
1	A	467	GLN
1	A	478	LEU
1	A	492	GLU
1	A	500	VAL
1	A	503	CYS
1	A	505	SER
1	A	508	VAL
1	A	516	LEU
1	A	530	SER
1	A	541	LEU
1	A	558	ILE
1	A	560	LEU
1	A	562	THR
1	A	567	ARG
1	A	568	ILE
1	A	577	LEU
1	A	578	HIS
1	A	586	ILE
1	A	587	ILE
1	A	591	ILE
1	A	593	MET
1	A	594	THR
1	A	595	THR
1	A	597	GLU
1	A	599	SER
1	A	601	TYR
1	A	606	LEU
1	A	608	ASP
1	A	611	LEU
1	A	623	LEU

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Mol	Chain	Res	Type
1	A	642	ARG
1	A	646	THR
1	A	657	THR
1	A	658	VAL
1	A	659	ILE
1	A	667	VAL
1	A	669	SER
1	A	671	VAL
1	A	679	MET
1	A	680	CYS
1	A	696	ASN
1	A	699	LEU
1	A	704	ILE
1	A	745	THR
1	A	746	SER
1	A	763	SER
1	A	768	SER
1	A	770	LEU
1	A	773	SER
1	A	780	THR
1	A	781	SER
1	A	831	VAL
1	A	836	VAL
1	A	844	LYS
1	A	854	SER
1	A	870	VAL
1	A	879	LYS
1	A	885	ASN
1	A	901	THR
1	A	919	ASP
1	A	930	VAL
1	A	943	GLU
1	A	947	ARG
1	A	957	VAL
1	A	985	THR
1	A	987	GLU
1	A	990	GLN
1	A	1006	VAL
1	A	1012	LEU
1	A	1015	GLN
1	A	1019	GLU
1	A	1020	THR

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Mol	Chain	Res	Type
1	A	1036	MET
1	A	1043	LEU
1	A	1044	SER
1	A	1046	SER
1	A	1057	ARG
1	A	1062	ILE
1	A	1063	LYS
1	A	1065	VAL
1	A	1086	THR
1	A	1098	LEU
1	A	1104	LYS
1	A	1111	ASN
1	A	1129	LEU
1	A	1131	LYS
2	B	23	ARG
2	B	30	LEU
2	B	35	LYS
2	B	37	LEU
2	B	38	CYS
2	B	53	LEU
2	B	55	VAL
2	B	61	GLN
2	B	67	ARG
2	B	71	ARG
2	B	126	THR
2	B	136	ILE
2	B	141	PHE
2	B	163	LYS
2	B	168	ASN
2	B	192	ARG
2	B	199	THR
2	B	200	ILE
2	B	204	PHE
2	B	213	SER
2	B	220	ASP
2	B	224	ASN
2	B	225	VAL
2	B	234	GLU
2	B	235	LEU
2	B	242	LYS
2	B	256	TRP
2	B	262	SER

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Mol	Chain	Res	Type
2	B	268	LYS
2	B	269	ILE
2	B	272	LEU
2	B	273	ARG
2	B	275	VAL
2	B	281	PHE
2	B	285	LEU
2	B	295	CYS
2	B	296	PHE
2	B	297	SER
2	B	299	ASP
2	B	306	THR
2	B	321	ASP
2	B	356	TYR
2	B	360	ASN
2	B	361	PHE
2	B	365	THR
2	B	369	LEU
2	B	370	ARG
2	B	384	CYS
2	B	391	SER
2	B	418	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	183	GLN
1	A	240	HIS
1	A	337	ASN
1	A	343	GLN
1	A	374	GLN
1	A	455	GLN
1	A	465	HIS
1	A	467	GLN
1	A	677	ASN
1	A	695	ASN
1	A	797	HIS
1	A	803	HIS
1	A	885	ASN
1	A	904	ASN
1	A	978	GLN

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Mol	Chain	Res	Type
1	A	999	HIS
1	A	1015	GLN
1	A	1055	GLN
1	A	1070	HIS
1	A	1077	HIS
2	B	61	GLN
2	B	91	GLN
2	B	92	GLN
2	B	105	GLN
2	B	123	HIS
2	B	140	ASN
2	B	165	ASN
2	B	168	ASN
2	B	221	ASN
2	B	224	ASN
2	B	247	HIS
2	B	287	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	3DR	G	11	4	8,11,12	3.10	3 (37%)	9,14,17	1.52	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3DR	G	11	4	-	2/3/15/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	11	3DR	C2'-C3'	-7.31	1.39	1.52
4	G	11	3DR	O4'-C4'	-3.21	1.39	1.44
4	G	11	3DR	O5'-C5'	-2.05	1.39	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	11	3DR	O5'-C5'-C4'	2.56	117.71	108.99
4	G	11	3DR	C1'-C2'-C3'	2.40	105.92	103.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	11	3DR	C4'-C5'-O5'-P
4	G	11	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	11	3DR	8	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	G	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	11:3DR	O3'	12:DC	P	2.90
1	G	9:DC	O3'	10:DG	P	1.76

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1140/1150 (99%)	-0.66	26 (2%) 60 48	29, 73, 182, 360	0
2	B	402/436 (92%)	-0.63	9 (2%) 62 49	36, 69, 176, 276	0
3	F	24/24 (100%)	-0.86	0 100 100	60, 93, 120, 138	0
4	G	23/24 (95%)	-0.74	0 100 100	64, 95, 133, 165	0
All	All	1589/1634 (97%)	-0.66	35 (2%) 62 49	29, 73, 180, 360	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	26	SER	9.7
2	B	27	PRO	7.2
1	A	651	ALA	5.6
1	A	464	ALA	4.9
1	A	445	GLU	4.7
2	B	36	LYS	4.6
1	A	443	VAL	4.4
2	B	130	GLY	4.4
2	B	33	GLU	4.0
1	A	483	PRO	3.8
1	A	465	HIS	3.5
1	A	530	SER	3.5
1	A	457	THR	3.2
1	A	657	THR	3.2
1	A	493	PRO	3.1
2	B	41	GLY	3.1
1	A	373	GLY	3.1
1	A	654	ASP	3.0
1	A	431	GLY	3.0
1	A	495	ALA	2.9
1	A	494	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	486	LEU	2.9
1	A	446	THR	2.8
1	A	442	GLU	2.7
2	B	50	SER	2.6
1	A	590	SER	2.4
1	A	562	THR	2.4
2	B	38	CYS	2.4
1	A	444	GLU	2.4
1	A	456	GLN	2.4
1	A	146	ASP	2.3
1	A	485	ALA	2.2
1	A	429	PHE	2.2
2	B	49	ASP	2.1
1	A	563	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	3DR	G	11	11/12	0.78	0.21	71,109,126,187	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.