



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:18 PM UTC

PDB ID : 6DWZ / pdb_00006dwz
Title : Hermes transposase deletion dimer complex with (C/G) DNA
Authors : Dyda, F.; Hickman, A.B.
Deposited on : 2018-06-28
Resolution : 3.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

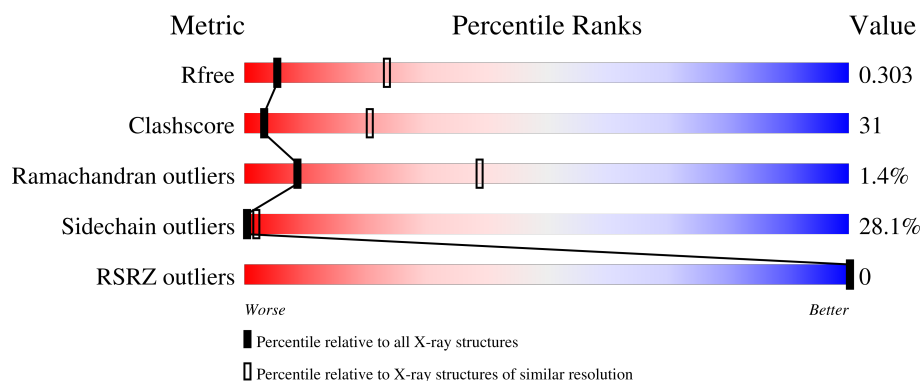
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	517	
1	E	517	
2	B	15	
2	F	15	
3	C	26	

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Mol	Chain	Length	Quality of chain
3	G	26	19% 77% .
4	D	7	29% 71%
4	H	7	29% 71%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9578 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 Hermes transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3832	2454	647	713	18			
1	E	476	Total	C	N	O	S	0	0	0
			3832	2454	647	713	18			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLY	-	expression tag	UNP Q25438
A	77	SER	-	expression tag	UNP Q25438
A	78	HIS	-	expression tag	UNP Q25438
A	79	MET	-	expression tag	UNP Q25438
A	128	GLY	LYS	conflict	UNP Q25438
A	?	-	ASP	deletion	UNP Q25438
A	?	-	ILE	deletion	UNP Q25438
A	?	-	SER	deletion	UNP Q25438
A	?	-	THR	deletion	UNP Q25438
A	?	-	THR	deletion	UNP Q25438
A	?	-	SER	deletion	UNP Q25438
A	?	-	PHE	deletion	UNP Q25438
A	?	-	PHE	deletion	UNP Q25438
A	?	-	PHE	deletion	UNP Q25438
A	?	-	PRO	deletion	UNP Q25438
A	?	-	GLN	deletion	UNP Q25438
A	?	-	LEU	deletion	UNP Q25438
A	?	-	THR	deletion	UNP Q25438
A	?	-	GLN	deletion	UNP Q25438
A	?	-	ASN	deletion	UNP Q25438
A	?	-	ASN	deletion	UNP Q25438
A	?	-	SER	deletion	UNP Q25438
A	?	-	ARG	deletion	UNP Q25438
A	?	-	GLU	deletion	UNP Q25438
A	?	-	PRO	deletion	UNP Q25438

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Chain	Residue	Modelled	Actual	Comment	Reference
A	519	SER	CYS	engineered mutation	UNP Q25438
E	76	GLY	-	expression tag	UNP Q25438
E	77	SER	-	expression tag	UNP Q25438
E	78	HIS	-	expression tag	UNP Q25438
E	79	MET	-	expression tag	UNP Q25438
E	128	GLY	LYS	conflict	UNP Q25438
E	?	-	ASP	deletion	UNP Q25438
E	?	-	ILE	deletion	UNP Q25438
E	?	-	SER	deletion	UNP Q25438
E	?	-	THR	deletion	UNP Q25438
E	?	-	THR	deletion	UNP Q25438
E	?	-	SER	deletion	UNP Q25438
E	?	-	PHE	deletion	UNP Q25438
E	?	-	PHE	deletion	UNP Q25438
E	?	-	PHE	deletion	UNP Q25438
E	?	-	PRO	deletion	UNP Q25438
E	?	-	GLN	deletion	UNP Q25438
E	?	-	LEU	deletion	UNP Q25438
E	?	-	THR	deletion	UNP Q25438
E	?	-	GLN	deletion	UNP Q25438
E	?	-	ASN	deletion	UNP Q25438
E	?	-	ASN	deletion	UNP Q25438
E	?	-	SER	deletion	UNP Q25438
E	?	-	ARG	deletion	UNP Q25438
E	?	-	GLU	deletion	UNP Q25438
E	?	-	PRO	deletion	UNP Q25438
E	519	SER	CYS	engineered mutation	UNP Q25438

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			309	147	69	79	14			
2	F	15	Total	C	N	O	P	0	0	0
			309	147	69	79	14			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			506	244	80	158	24			

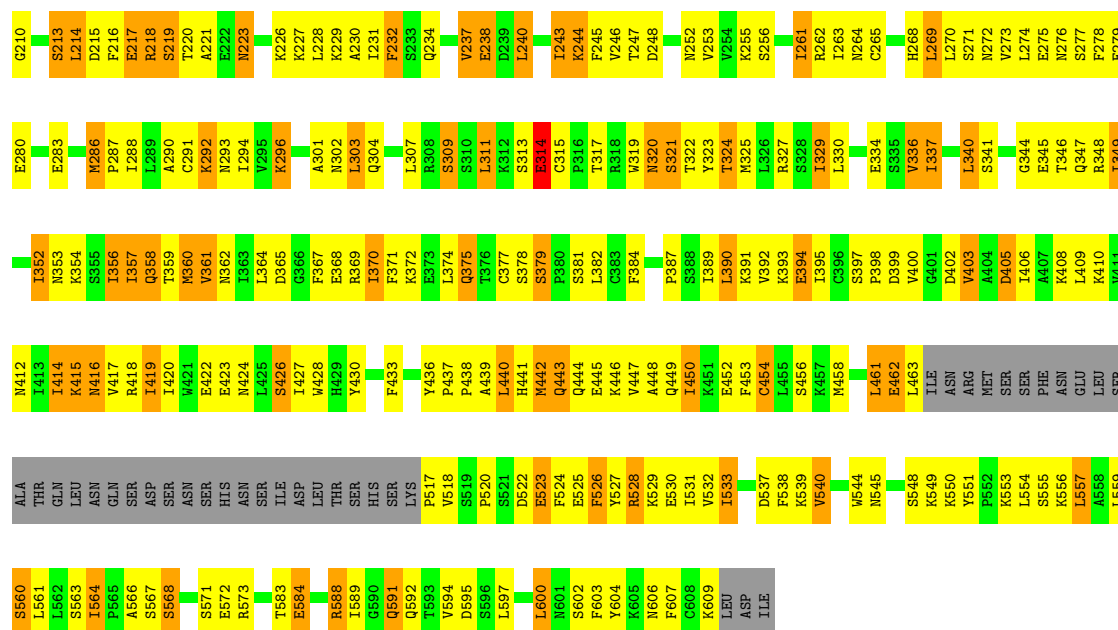
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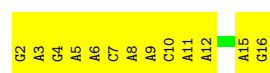
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	25	Total 506	C 244	N 80	O 158	P 24	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*CP*GP*TP*GP*AP*C)-3').

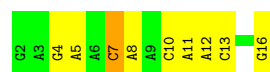
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total 142	C 68	N 28	O 40	P 6	0	0	0
4	H	7	Total 142	C 68	N 28	O 40	P 6	0	0	0



- Molecule 2: DNA (5'-D(*GP*AP*GP*AP*AP*CP*AP*AP*CP*AP*AP*CP*AP*AP*G)-3')



- Molecule 2: DNA (5'-D(*GP*AP*GP*AP*AP*CP*AP*AP*CP*AP*AP*CP*AP*AP*G)-3')



- Molecule 3: DNA (26-MER)

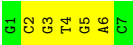


- Molecule 3: DNA (26-MER)



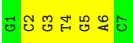
- Molecule 4: DNA (5'-D(*GP*CP*GP*TP*GP*AP*C)-3')

Chain D:  29% 71%

 G1 C2 G3 T4 G5 A6 G7

- Molecule 4: DNA (5'-D(*GP*CP*GP*TP*GP*AP*C)-3')

Chain H:  29% 71%

 G1 C2 G3 T4 G5 A6 G7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.38Å 121.11Å 132.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 3.20 29.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.51-3.20) 98.9 (29.51-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.203 , 0.298 0.206 , 0.303	Depositor DCC
R_{free} test set	935 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	82.4	Xtrriage
Anisotropy	0.471	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9578	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1324e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.64	0/3905	0.92	3/5268 (0.1%)
1	E	0.64	0/3905	0.97	5/5268 (0.1%)
2	B	1.05	0/350	1.15	0/538
2	F	1.04	0/350	1.14	1/538 (0.2%)
3	C	0.90	0/563	1.11	0/868
3	G	1.03	0/563	1.09	0/868
4	D	0.91	0/159	0.87	0/244
4	H	0.90	0/159	0.90	0/244
All	All	0.73	0/9954	0.98	9/13836 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	E	0	4
All	All	0	8

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	ASP	CA-C-N	-7.30	111.39	123.37
1	E	184	ASP	C-N-CA	-7.30	111.39	123.37
1	A	137	VAL	CB-CA-C	6.37	122.46	110.94
1	A	137	VAL	N-CA-CB	-6.31	102.48	112.07
1	E	378	SER	CA-C-N	6.14	136.79	121.80
1	E	378	SER	C-N-CA	6.14	136.79	121.80
2	F	7	DC	C1'-O4'-C4'	-5.74	101.08	109.70
1	A	394	GLU	CA-CB-CG	-5.73	102.65	114.10
1	E	314	GLU	N-CA-C	-5.02	101.78	109.76

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLU	Peptide
1	A	318	ARG	Peptide
1	A	444	GLN	Peptide
1	A	445	GLU	Peptide
1	E	217	GLU	Peptide
1	E	302	ASN	Peptide
1	E	320	ASN	Peptide
1	E	400	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3832	0	3903	239	0
1	E	3832	0	3903	264	0
2	B	309	0	167	20	0
2	F	309	0	167	14	0
3	C	506	0	288	27	0
3	G	506	0	288	32	0
4	D	142	0	80	10	0
4	H	142	0	80	8	0
All	All	9578	0	8876	554	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (554) 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)
2:B:16:DG:H1	3:C:1:DC:H42	1.17	0.92
1:A:288:ILE:HD11	1:A:360:MET:HE1	1.52	0.90
4:D:5:DG:H2''	4:D:6:DA:H5''	1.54	0.89
1:E:412:ASN:O	1:E:416:ASN:ND2	2.04	0.88
1:E:341:SER:HA	1:E:346:THR:HB	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:DA:N6	4:D:4:DT:O4	2.07	0.86
2:F:8:DA:H5'	2:F:8:DA:C8	2.11	0.86
2:F:4:DG:H5''	2:F:4:DG:H8	1.41	0.85
2:F:4:DG:H5''	2:F:4:DG:C8	2.13	0.84
1:E:262:ARG:NH2	1:E:264:ASN:OD1	2.11	0.84
1:A:285:ASN:HA	1:A:288:ILE:HD12	1.61	0.82
1:E:162:ILE:HD13	1:E:607:PHE:HE2	1.42	0.82
1:E:255:LYS:HD3	3:G:22:DA:H5'	1.62	0.81
1:A:137:VAL:HG23	1:A:140:LEU:HD23	1.63	0.81
1:E:203:GLU:OE1	1:E:205:ARG:NH1	2.15	0.80
1:A:341:SER:HA	1:A:346:THR:HB	1.62	0.80
4:H:5:DG:H2''	4:H:6:DA:H5''	1.62	0.79
1:A:359:THR:O	1:A:363:ILE:HG12	1.83	0.78
1:E:416:ASN:ND2	1:E:416:ASN:H	1.79	0.78
4:H:2:DC:H1'	4:H:3:DG:H5'	1.66	0.77
1:E:150:LYS:O	1:E:153:SER:N	2.18	0.77
1:A:95:ILE:HG22	1:E:150:LYS:HD2	1.67	0.77
1:A:304:GLN:HG2	1:A:307:LEU:HD12	1.67	0.76
1:E:416:ASN:HA	1:E:419:ILE:HG12	1.66	0.76
3:C:5:DT:H2'	3:C:6:DT:C6	2.20	0.76
3:C:8:DT:H1'	3:C:9:DT:H5'	1.66	0.76
1:E:330:LEU:HD13	1:E:357:ILE:HG22	1.67	0.75
3:G:7:DG:H2'	3:G:8:DT:H71	1.68	0.74
1:E:264:ASN:HD22	1:E:424:ASN:HB3	1.52	0.73
1:A:170:VAL:HA	1:A:175:ALA:HB2	1.69	0.72
2:B:15:DA:H2''	2:B:16:DG:C8	2.25	0.72
3:C:24:DG:N2	4:D:2:DC:O2	2.18	0.72
1:E:176:SER:HB2	1:E:197:HIS:HB2	1.70	0.72
1:E:304:GLN:OE1	1:E:311:LEU:N	2.23	0.72
1:E:330:LEU:HD22	1:E:361:VAL:HG11	1.71	0.72
1:E:416:ASN:H	1:E:416:ASN:HD22	1.37	0.71
1:A:270:LEU:HD23	1:A:371:PHE:CZ	2.24	0.71
1:A:247:THR:HG23	1:A:248:ASP:O	1.91	0.71
2:B:4:DG:C8	2:B:4:DG:H5''	2.25	0.71
3:G:7:DG:H2''	3:G:8:DT:H5'	1.73	0.70
1:E:420:ILE:O	1:E:424:ASN:ND2	2.22	0.70
3:G:21:DC:H42	4:H:5:DG:H1	1.37	0.70
1:A:84:LYS:HD3	1:E:131:TYR:HB3	1.72	0.70
3:G:5:DT:H2''	3:G:6:DT:O5'	1.92	0.69
1:E:371:PHE:O	1:E:375:GLN:HG2	1.92	0.69
1:E:426:SER:HG	1:E:428:TRP:HD1	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:VAL:HG13	1:A:311:LEU:HB3	1.75	0.68
3:G:23:DC:H2''	3:G:24:DG:H5''	1.73	0.68
1:E:232:PHE:HD1	1:E:240:LEU:HD13	1.59	0.68
1:E:526:PHE:HB3	1:E:551:TYR:HE2	1.57	0.68
1:E:119:ASP:OD1	1:E:119:ASP:N	2.25	0.68
1:A:97:LYS:HG3	1:E:120:MET:HA	1.75	0.68
1:A:530:GLU:OE2	1:A:551:TYR:OH	2.12	0.68
1:E:387:PRO:HA	1:E:390:LEU:HG	1.77	0.67
1:E:167:LYS:HE3	1:E:237:VAL:HG13	1.76	0.67
2:B:4:DG:H5''	2:B:4:DG:H8	1.58	0.67
3:C:23:DC:H2''	3:C:24:DG:C8	2.28	0.67
1:E:416:ASN:HB3	1:E:420:ILE:HG13	1.76	0.67
3:G:23:DC:H2''	3:G:24:DG:C8	2.31	0.66
1:A:109:PHE:CE1	1:E:148:SER:HB2	2.31	0.66
1:E:170:VAL:HG11	1:E:237:VAL:HG11	1.77	0.66
1:A:196:LEU:HB3	1:A:207:LEU:HD21	1.78	0.65
1:A:441:HIS:C	1:A:443:GLN:H	2.02	0.65
1:A:125:ILE:HG21	1:E:135:VAL:HG21	1.78	0.65
1:E:323:TYR:CE2	1:E:365:ASP:HA	2.32	0.65
4:H:2:DC:H1'	4:H:3:DG:C5'	2.26	0.65
3:G:22:DA:H2'	3:G:23:DC:C6	2.32	0.65
1:E:393:LYS:O	1:E:397:SER:N	2.29	0.64
1:E:247:THR:HG22	1:E:262:ARG:HE	1.62	0.64
1:E:525:GLU:HA	1:E:528:ARG:HB2	1.79	0.64
1:A:255:LYS:HA	1:A:258:ALA:HB2	1.79	0.64
1:E:304:GLN:HA	1:E:307:LEU:HD12	1.79	0.64
1:E:527:TYR:O	1:E:530:GLU:N	2.20	0.64
1:E:223:ASN:O	1:E:227:LYS:HG2	1.98	0.64
1:E:226:LYS:HG2	1:E:227:LYS:HD2	1.80	0.64
1:A:231:ILE:HA	1:A:234:GLN:OE1	1.97	0.63
1:E:532:VAL:HG12	1:E:533:ILE:O	1.98	0.63
3:C:7:DG:H2''	3:C:8:DT:H71	1.79	0.63
1:E:248:ASP:HB3	1:E:268:HIS:CE1	2.33	0.63
1:A:223:ASN:O	1:A:227:LYS:HG2	1.98	0.63
1:A:92:LYS:HE3	3:C:6:DT:OP1	1.99	0.63
1:A:229:LYS:HD2	1:A:240:LEU:HD21	1.80	0.63
1:E:444:GLN:HB2	1:E:446:LYS:HG2	1.79	0.63
2:F:10:DC:H2''	2:F:11:DA:O4'	1.99	0.62
1:E:118:ILE:O	1:E:121:ILE:N	2.32	0.62
1:A:320:ASN:C	1:A:322:THR:N	2.58	0.62
3:C:13:DC:H2'	3:C:14:DT:C6	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:SER:O	1:E:172:LYS:HB2	1.98	0.62
1:E:551:TYR:O	1:E:555:SER:N	2.30	0.62
1:A:213:SER:HB2	1:A:215:ASP:H	1.64	0.62
1:A:307:LEU:HB3	1:A:309:SER:O	2.00	0.61
1:A:325:MET:HG2	1:A:329:ILE:HD12	1.82	0.61
4:D:3:DG:H1'	4:D:4:DT:H5'	1.82	0.61
1:A:350:VAL:HG23	1:A:351:HIS:H	1.65	0.61
1:E:161:LEU:HD22	1:E:162:ILE:HG12	1.82	0.61
1:E:278:PHE:CE1	1:E:360:MET:HE1	2.36	0.61
1:E:278:PHE:HE1	1:E:360:MET:HE1	1.65	0.61
1:E:162:ILE:HD13	1:E:607:PHE:CE2	2.30	0.61
1:E:137:VAL:HG23	1:E:138:GLU:OE1	2.00	0.61
1:E:245:PHE:HB2	1:E:261:ILE:O	2.00	0.61
1:E:426:SER:HG	1:E:428:TRP:CD1	2.18	0.61
1:E:138:GLU:OE1	1:E:138:GLU:N	2.28	0.61
1:E:545:ASN:HA	1:E:548:SER:HB3	1.82	0.61
3:G:24:DG:H2''	3:G:25:DC:H5''	1.83	0.61
1:A:593:THR:O	1:A:597:LEU:HB2	2.00	0.61
1:A:142:PRO:HG3	1:E:95:ILE:HG22	1.81	0.61
1:A:447:VAL:HA	1:A:450:ILE:HB	1.83	0.60
1:E:214:LEU:HD12	1:E:227:LYS:HG3	1.83	0.60
1:E:124:PHE:O	1:E:127:VAL:HG12	2.00	0.60
1:E:173:ASP:O	1:E:244:LYS:NZ	2.24	0.60
1:A:601:ASN:O	1:A:605:LYS:HG3	2.02	0.60
1:A:244:LYS:HA	1:A:261:ILE:HB	1.84	0.60
1:A:538:PHE:HD1	1:A:539:LYS:N	1.99	0.60
1:A:435:PHE:HE1	1:A:557:LEU:HB3	1.67	0.60
1:A:441:HIS:O	1:A:443:GLN:N	2.34	0.60
4:D:6:DA:H5''	4:D:6:DA:H8	1.64	0.60
1:E:462:GLU:OE1	1:E:462:GLU:HA	2.02	0.60
1:A:396:CYS:HA	1:A:410:LYS:HD3	1.83	0.60
1:E:247:THR:HG23	1:E:248:ASP:O	2.02	0.60
1:A:518:VAL:HG11	1:A:552:PRO:HD2	1.84	0.59
1:E:403:VAL:HG13	1:E:406:ILE:CD1	2.32	0.59
2:F:8:DA:H5'	2:F:8:DA:H8	1.63	0.59
1:E:447:VAL:HA	1:E:450:ILE:HB	1.84	0.59
3:G:2:DT:H2'	3:G:3:DT:C6	2.37	0.59
1:A:162:ILE:HG21	1:A:607:PHE:HE2	1.68	0.59
1:A:382:LEU:HA	1:A:566:ALA:HB2	1.85	0.59
1:A:379:SER:HB2	1:A:380:PRO:HD2	1.85	0.59
1:E:183:THR:HB	1:E:190:ASN:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LEU:O	1:A:560:SER:N	2.36	0.59
1:A:390:LEU:HA	1:A:393:LYS:HG3	1.84	0.58
1:E:97:LYS:O	1:E:100:GLN:HB2	2.03	0.58
1:E:384:PHE:C	1:E:387:PRO:HD2	2.28	0.58
1:A:158:LYS:HB3	1:A:603:PHE:CE1	2.38	0.58
1:E:349:ILE:HG13	1:E:349:ILE:O	2.03	0.58
1:A:356:ILE:O	1:A:360:MET:HG3	2.03	0.58
1:A:444:GLN:HB2	1:A:446:LYS:H	1.67	0.58
1:A:443:GLN:NE2	1:A:444:GLN:O	2.36	0.58
1:A:112:VAL:HG11	1:E:147:LEU:HD11	1.85	0.58
1:E:416:ASN:ND2	1:E:416:ASN:N	2.50	0.58
1:A:159:LYS:HG2	1:A:599:PHE:CZ	2.39	0.58
1:E:189:ARG:HG3	1:E:216:PHE:CZ	2.39	0.58
1:A:411:VAL:HA	1:A:414:ILE:HG12	1.85	0.57
1:A:265:CYS:HG	1:A:268:HIS:HD1	1.51	0.57
1:A:309:SER:CB	1:A:332:ASN:HD21	2.17	0.57
1:A:319:TRP:O	1:A:320:ASN:C	2.47	0.57
1:A:388:SER:O	1:A:392:VAL:HG23	2.04	0.57
1:E:186:TYR:HE1	1:E:584:GLU:HG3	1.69	0.57
1:A:154:ASP:O	1:A:158:LYS:HG3	2.04	0.57
1:E:353:ASN:HB3	1:E:356:ILE:HB	1.86	0.57
1:A:391:LYS:O	1:A:395:ILE:HG12	2.05	0.57
1:E:403:VAL:HG13	1:E:406:ILE:HD12	1.85	0.57
1:E:209:LEU:HD12	1:E:232:PHE:CE2	2.40	0.57
1:E:544:TRP:CZ3	1:E:555:SER:HA	2.40	0.57
1:E:556:LYS:HA	1:E:559:LEU:HD22	1.85	0.57
1:A:442:MET:O	1:A:442:MET:HG3	2.05	0.56
1:A:86:VAL:HG23	1:A:90:CYS:HB3	1.87	0.56
1:A:346:THR:O	1:A:349:ILE:HG22	2.04	0.56
1:E:178:THR:HG22	1:E:571:SER:OG	2.04	0.56
1:E:286:MET:HE3	1:E:287:PRO:HD3	1.88	0.56
1:E:314:GLU:HA	1:E:321:SER:HB2	1.87	0.56
1:A:411:VAL:HG13	1:A:414:ILE:HD11	1.87	0.56
1:A:135:VAL:HG13	1:E:84:LYS:HB2	1.88	0.56
1:E:358:GLN:O	1:E:358:GLN:NE2	2.39	0.56
1:A:412:ASN:HA	1:A:415:LYS:NZ	2.20	0.56
3:C:23:DC:H2"	3:C:24:DG:H5"	1.87	0.56
1:E:293:ASN:HA	1:E:296:LYS:HG2	1.88	0.56
1:A:136:ASN:O	1:A:136:ASN:ND2	2.39	0.56
1:E:97:LYS:HA	1:E:100:GLN:HG3	1.88	0.56
1:A:387:PRO:HA	1:A:390:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:DT:H2''	3:C:7:DG:H5'	1.88	0.56
1:A:403:VAL:HG12	1:A:406:ILE:HD12	1.88	0.55
1:A:115:SER:O	1:A:115:SER:OG	2.25	0.55
1:A:137:VAL:HA	1:A:140:LEU:HB3	1.89	0.55
1:E:555:SER:O	1:E:559:LEU:HD13	2.05	0.55
1:E:255:LYS:HD2	3:G:23:DC:P	2.46	0.55
1:E:271:SER:O	1:E:275:GLU:N	2.37	0.55
1:A:126:LYS:HB2	1:E:133:GLU:HG3	1.88	0.55
1:A:303:LEU:O	1:A:304:GLN:HB2	2.06	0.55
1:E:453:PHE:O	1:E:456:SER:N	2.37	0.55
1:E:548:SER:C	1:E:550:LYS:H	2.14	0.55
1:E:357:ILE:HA	1:E:360:MET:HG3	1.89	0.55
2:B:16:DG:N2	3:C:1:DC:N3	2.37	0.55
1:E:213:SER:HG	1:E:215:ASP:H	1.54	0.55
3:G:9:DT:H1'	3:G:10:DG:H5'	1.89	0.55
1:A:254:VAL:HG22	1:A:262:ARG:HH12	1.72	0.55
1:E:529:LYS:O	1:E:531:ILE:HG12	2.07	0.54
1:A:109:PHE:O	1:A:112:VAL:HG22	2.07	0.54
1:A:151:VAL:HG11	1:A:597:LEU:HD22	1.89	0.54
1:A:244:LYS:HB3	1:A:263:ILE:HD11	1.88	0.54
1:A:412:ASN:HA	1:A:415:LYS:HZ2	1.72	0.54
1:E:248:ASP:HB3	1:E:268:HIS:ND1	2.22	0.54
1:E:320:ASN:C	1:E:322:THR:N	2.65	0.54
1:A:162:ILE:HG21	1:A:607:PHE:CE2	2.42	0.54
1:E:367:PHE:HA	1:E:370:ILE:HG13	1.90	0.54
2:F:4:DG:H2''	2:F:5:DA:O4'	2.07	0.54
1:A:248:ASP:HB3	1:A:268:HIS:CE1	2.43	0.54
1:A:284:LEU:O	1:A:287:PRO:HD2	2.08	0.54
1:A:282:PRO:HA	1:A:285:ASN:HB3	1.89	0.54
1:E:198:TYR:C	1:E:198:TYR:HD1	2.16	0.54
1:E:219:SER:O	1:E:219:SER:OG	2.25	0.53
1:A:101:TRP:CD1	1:E:117:PHE:HB2	2.43	0.53
1:A:381:SER:HB2	1:A:566:ALA:HB3	1.90	0.53
4:D:6:DA:H5''	4:D:6:DA:C8	2.43	0.53
1:A:213:SER:C	1:A:215:ASP:H	2.16	0.53
1:E:452:GLU:O	1:E:456:SER:HB2	2.08	0.53
1:A:125:ILE:O	1:E:128:GLY:HA3	2.08	0.53
3:C:7:DG:C2'	3:C:8:DT:H71	2.39	0.53
1:E:147:LEU:O	1:E:151:VAL:HB	2.09	0.53
1:E:334:GLU:H	1:E:334:GLU:CD	2.17	0.53
1:A:581:ILE:HD12	1:A:586:ARG:HH12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:SER:O	1:E:344:GLY:N	2.30	0.53
3:C:24:DG:H2''	3:C:25:DC:O4'	2.09	0.53
4:D:6:DA:H8	4:D:6:DA:C5'	2.21	0.53
1:A:104:ARG:HH11	1:E:116:GLY:HA2	1.73	0.53
4:D:2:DC:H2''	4:D:3:DG:C8	2.44	0.52
1:A:101:TRP:NE1	1:E:117:PHE:HB2	2.25	0.52
1:A:451:LYS:HG3	1:A:524:PHE:CE1	2.45	0.52
1:E:303:LEU:O	1:E:304:GLN:HB2	2.10	0.52
1:A:93:GLU:HB3	1:E:123:PHE:CE1	2.45	0.52
1:E:205:ARG:HD2	1:E:606:ASN:HB3	1.91	0.52
2:F:10:DC:N4	3:G:7:DG:H1	2.08	0.52
1:A:143:SER:OG	1:A:145:ILE:HG22	2.09	0.52
1:A:292:LYS:HD2	1:A:314:GLU:OE1	2.10	0.52
1:A:370:ILE:O	1:A:374:LEU:HB2	2.09	0.52
1:A:306:ARG:HD2	1:A:339:ILE:HD13	1.92	0.51
1:E:545:ASN:O	1:E:548:SER:OG	2.21	0.51
1:A:125:ILE:HG22	1:E:128:GLY:HA2	1.93	0.51
2:B:2:DG:H2''	2:B:3:DA:C8	2.45	0.51
1:E:198:TYR:C	1:E:198:TYR:CD1	2.89	0.51
1:E:323:TYR:C	1:E:323:TYR:CD1	2.89	0.51
1:A:441:HIS:C	1:A:443:GLN:N	2.67	0.51
1:E:209:LEU:HD12	1:E:232:PHE:HE2	1.74	0.51
1:A:526:PHE:HB3	1:A:551:TYR:HE2	1.74	0.51
1:A:306:ARG:O	1:A:307:LEU:HG	2.11	0.51
1:A:227:LYS:O	1:A:230:ALA:HB3	2.10	0.51
1:E:454:CYS:O	1:E:458:MET:HB2	2.09	0.51
2:F:5:DA:H61	3:G:12:DT:H3	1.57	0.51
1:E:114:GLY:O	1:E:117:PHE:HB3	2.10	0.51
1:E:322:THR:HA	1:E:325:MET:HE2	1.92	0.51
1:E:375:GLN:O	1:E:573:ARG:NH2	2.44	0.51
1:A:384:PHE:C	1:A:387:PRO:HD2	2.36	0.51
1:A:399:ASP:OD1	1:A:400:VAL:N	2.45	0.50
1:A:543:TRP:O	1:A:547:ASN:HB2	2.10	0.50
1:A:105:ASP:OD1	1:E:114:GLY:HA3	2.12	0.50
1:E:288:ILE:O	1:E:291:CYS:HB2	2.11	0.50
2:F:10:DC:H42	3:G:7:DG:H1	1.59	0.50
1:E:218:ARG:HB2	3:G:21:DC:OP1	2.12	0.50
1:E:231:ILE:O	1:E:234:GLN:HG3	2.11	0.50
1:E:315:CYS:SG	3:G:17:DG:OP2	2.70	0.50
1:E:389:ILE:O	1:E:392:VAL:HB	2.12	0.50
1:E:213:SER:OG	1:E:215:ASP:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:LYS:O	1:E:94:ALA:N	2.42	0.50
1:E:337:ILE:HG23	1:E:349:ILE:HD13	1.93	0.50
1:E:530:GLU:O	1:E:531:ILE:HD13	2.11	0.50
1:E:321:SER:HA	1:E:324:THR:HG23	1.94	0.50
1:E:273:VAL:HG13	1:E:416:ASN:HB2	1.94	0.49
1:A:330:LEU:HD22	1:A:361:VAL:HG11	1.94	0.49
1:E:382:LEU:HA	1:E:566:ALA:HB2	1.94	0.49
1:A:581:ILE:O	1:A:583:THR:HG23	2.13	0.49
1:A:345:GLU:OE2	1:A:348:ARG:NE	2.45	0.49
1:A:434:PHE:HE2	1:A:527:TYR:CD2	2.30	0.49
1:E:126:LYS:O	1:E:130:GLU:HG2	2.13	0.49
1:E:199:HIS:O	1:E:203:GLU:HB2	2.13	0.49
1:E:220:THR:HB	3:G:22:DA:OP1	2.13	0.49
1:E:377:CYS:HB2	1:E:573:ARG:HH12	1.78	0.49
1:A:104:ARG:NH1	1:E:116:GLY:HA2	2.28	0.49
2:B:7:DC:H2''	2:B:8:DA:N7	2.27	0.49
1:E:415:LYS:HG2	1:E:419:ILE:HD13	1.95	0.49
1:A:270:LEU:HD23	1:A:371:PHE:CE1	2.48	0.49
1:A:525:GLU:HA	1:A:528:ARG:HG3	1.95	0.49
2:B:10:DC:H2''	2:B:11:DA:H5'	1.94	0.49
1:E:144:PRO:HA	1:E:147:LEU:HD12	1.94	0.49
1:E:229:LYS:HZ3	1:E:238:GLU:C	2.20	0.49
1:E:336:VAL:O	1:E:340:LEU:HB2	2.12	0.49
1:E:556:LYS:O	1:E:559:LEU:HB2	2.12	0.49
1:A:96:GLU:HB2	1:E:150:LYS:HZ1	1.78	0.49
1:A:222:GLU:OE2	1:A:222:GLU:N	2.45	0.49
1:E:358:GLN:HE22	1:E:362:ASN:CG	2.21	0.49
1:A:128:GLY:HA3	1:E:125:ILE:O	2.13	0.48
2:B:9:DA:H2''	2:B:10:DC:O4'	2.13	0.48
3:C:21:DC:H42	4:D:5:DG:H1	1.60	0.48
3:C:12:DT:H1'	1:E:588:ARG:HH21	1.78	0.48
1:E:276:ASN:O	1:E:279:GLU:N	2.46	0.48
1:A:268:HIS:O	1:A:269:LEU:C	2.56	0.48
1:A:315:CYS:SG	3:C:16:DT:H3'	2.53	0.48
1:A:434:PHE:CD1	1:A:450:ILE:HG21	2.48	0.48
2:B:16:DG:H1	3:C:1:DC:N4	1.98	0.48
3:C:1:DC:H2''	3:C:2:DT:OP2	2.12	0.48
1:E:273:VAL:HA	1:E:420:ILE:HD12	1.96	0.48
1:A:382:LEU:CA	1:A:566:ALA:HB2	2.43	0.48
1:A:435:PHE:CE1	1:A:557:LEU:HB3	2.48	0.48
1:E:174:GLY:HA2	1:E:560:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TYR:HB2	1:A:364:LEU:HB3	1.96	0.48
1:E:180:ASP:OD1	1:E:181:LEU:N	2.35	0.48
1:A:155:ALA:HA	1:A:600:LEU:HD21	1.96	0.48
1:A:224:ILE:CD1	1:A:252:ASN:HB3	2.44	0.48
1:E:264:ASN:ND2	1:E:424:ASN:HB3	2.27	0.47
1:A:107:ARG:HB3	1:A:108:PRO:HD2	1.97	0.47
1:A:337:ILE:HG23	1:A:349:ILE:HG12	1.96	0.47
3:C:9:DT:H1'	3:C:10:DG:H5'	1.96	0.47
1:A:176:SER:O	1:A:196:LEU:HD12	2.15	0.47
1:A:254:VAL:HA	1:A:262:ARG:NH1	2.28	0.47
2:B:6:DA:O3'	1:E:589:ILE:HA	2.14	0.47
1:E:458:MET:HE3	1:E:553:LYS:HB3	1.96	0.47
1:A:109:PHE:O	1:A:111:ALA:N	2.48	0.47
1:A:131:TYR:CE2	1:E:86:VAL:HA	2.49	0.47
1:A:228:LEU:HA	1:A:231:ILE:HD12	1.96	0.47
1:A:262:ARG:NH2	1:A:264:ASN:OD1	2.46	0.47
1:A:287:PRO:O	1:A:290:ALA:N	2.48	0.47
1:A:413:ILE:O	1:A:414:ILE:C	2.58	0.47
1:E:210:GLY:HA3	1:E:231:ILE:HD13	1.97	0.47
1:E:290:ALA:O	1:E:294:ILE:HG12	2.14	0.47
1:E:349:ILE:HG13	1:E:352:ILE:HG23	1.97	0.47
1:E:357:ILE:HA	1:E:357:ILE:HD12	1.75	0.47
1:E:417:VAL:O	1:E:422:GLU:HG3	2.15	0.47
1:E:441:HIS:C	1:E:443:GLN:H	2.23	0.47
1:A:538:PHE:CD1	1:A:538:PHE:C	2.91	0.47
1:E:319:TRP:O	1:E:320:ASN:C	2.57	0.47
1:E:278:PHE:CE1	1:E:288:ILE:HD11	2.49	0.47
1:E:358:GLN:HE21	1:E:358:GLN:C	2.23	0.47
3:G:21:DC:N4	4:H:5:DG:H1	2.10	0.47
1:A:167:LYS:HE3	1:A:236:ASN:O	2.15	0.47
1:A:278:PHE:CZ	1:A:409:LEU:HD21	2.50	0.47
1:A:426:SER:OG	1:A:427:ILE:N	2.48	0.47
1:E:549:LYS:N	1:E:555:SER:OG	2.45	0.47
3:G:12:DT:H2'	3:G:13:DC:C6	2.50	0.47
1:A:270:LEU:HD13	1:A:421:TRP:CZ3	2.50	0.46
1:A:446:LYS:O	1:A:450:ILE:HG13	2.14	0.46
1:E:221:ALA:HB1	1:E:256:SER:HA	1.97	0.46
1:E:337:ILE:H	1:E:337:ILE:HG13	1.43	0.46
1:E:440:LEU:H	1:E:440:LEU:HG	1.49	0.46
1:A:170:VAL:HA	1:A:175:ALA:CB	2.41	0.46
1:A:268:HIS:O	1:A:271:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PHE:O	1:A:388:SER:OG	2.18	0.46
1:E:410:LYS:O	1:E:414:ILE:HG12	2.15	0.46
3:C:2:DT:H2''	3:C:3:DT:OP2	2.14	0.46
1:A:128:GLY:HA2	1:E:125:ILE:HG22	1.98	0.46
1:A:273:VAL:HA	1:A:420:ILE:HD12	1.98	0.46
1:A:367:PHE:HA	1:A:370:ILE:HG13	1.97	0.46
1:E:243:ILE:HB	1:E:245:PHE:CE1	2.49	0.46
1:A:95:ILE:HG22	1:E:150:LYS:HE3	1.98	0.46
1:A:320:ASN:O	1:A:323:TYR:N	2.39	0.46
1:E:520:PRO:O	1:E:523:GLU:HG3	2.16	0.46
1:E:426:SER:OG	1:E:428:TRP:HD1	1.96	0.46
1:A:309:SER:HB3	1:A:332:ASN:HD21	1.81	0.46
2:B:4:DG:H2''	2:B:5:DA:O5'	2.15	0.46
1:E:137:VAL:O	1:E:140:LEU:HB3	2.16	0.46
1:E:153:SER:HA	1:E:156:LYS:HG3	1.98	0.46
1:E:162:ILE:HG22	1:E:165:GLU:HB3	1.98	0.46
1:E:390:LEU:O	1:E:394:GLU:HG2	2.16	0.46
1:E:537:ASP:OD1	1:E:537:ASP:N	2.48	0.46
1:A:357:ILE:O	1:A:360:MET:N	2.48	0.46
1:A:538:PHE:HD1	1:A:538:PHE:C	2.24	0.46
1:A:551:TYR:HB3	1:A:554:LEU:HB2	1.98	0.46
1:E:544:TRP:CE3	1:E:555:SER:HA	2.50	0.46
1:A:245:PHE:CD1	1:A:257:LEU:HD13	2.51	0.46
1:E:323:TYR:C	1:E:323:TYR:HD1	2.23	0.46
1:A:155:ALA:O	1:A:159:LYS:HG3	2.16	0.45
1:A:390:LEU:H	1:A:390:LEU:HG	1.38	0.45
2:B:2:DG:H2''	2:B:3:DA:H8	1.79	0.45
1:E:304:GLN:HA	1:E:307:LEU:CD1	2.45	0.45
1:A:121:ILE:HG13	1:E:124:PHE:HE1	1.80	0.45
1:A:354:LYS:O	1:A:357:ILE:HB	2.16	0.45
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.80	0.45
1:E:436:TYR:HA	1:E:437:PRO:HD3	1.75	0.45
3:G:13:DC:H2'	3:G:14:DT:C6	2.50	0.45
1:A:278:PHE:CE2	1:A:409:LEU:HD21	2.52	0.45
3:C:5:DT:H2'	3:C:6:DT:H6	1.76	0.45
1:E:247:THR:CG2	1:E:262:ARG:HE	2.28	0.45
1:E:286:MET:HE2	1:E:286:MET:HB3	1.68	0.45
2:F:10:DC:N3	3:G:7:DG:N2	2.61	0.45
4:H:4:DT:H2'	4:H:5:DG:C8	2.51	0.45
1:A:134:HIS:O	1:E:84:LYS:HG3	2.17	0.45
1:A:147:LEU:HA	1:A:147:LEU:HD23	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PHE:CG	1:A:257:LEU:HD13	2.52	0.45
1:A:377:CYS:SG	1:A:573:ARG:NH2	2.90	0.45
1:E:81:ARG:CZ	1:E:81:ARG:HB2	2.46	0.45
1:E:262:ARG:CZ	1:E:262:ARG:HB3	2.46	0.45
1:E:461:LEU:HD23	1:E:463:LEU:HD11	1.98	0.45
1:E:522:ASP:O	1:E:525:GLU:N	2.50	0.45
1:A:136:ASN:HD21	1:A:139:GLU:HG3	1.82	0.45
1:E:109:PHE:O	1:E:111:ALA:N	2.50	0.45
1:E:405:ASP:OD2	1:E:405:ASP:N	2.40	0.45
1:A:307:LEU:HD22	1:A:332:ASN:HB3	1.99	0.45
1:A:95:ILE:HG22	1:E:150:LYS:CD	2.41	0.45
1:A:545:ASN:HB3	1:A:546:LEU:HD12	1.99	0.45
3:C:5:DT:H6	3:C:5:DT:OP2	2.00	0.45
1:E:394:GLU:HG2	1:E:394:GLU:H	1.21	0.45
4:D:6:DA:C8	4:D:6:DA:C5'	3.00	0.44
1:E:137:VAL:O	1:E:140:LEU:N	2.47	0.44
1:E:307:LEU:HB3	1:E:309:SER:O	2.17	0.44
3:G:17:DG:N2	3:G:18:DG:H22	2.14	0.44
1:A:160:ALA:HA	1:A:163:SER:HB3	1.99	0.44
1:A:191:PHE:HB3	1:A:211:LEU:HD11	1.99	0.44
1:A:451:LYS:HA	1:A:524:PHE:CE1	2.51	0.44
1:E:185:ASN:HA	1:E:188:LYS:HD2	1.99	0.44
1:E:416:ASN:HA	1:E:419:ILE:CG1	2.42	0.44
1:A:413:ILE:O	1:A:416:ASN:N	2.51	0.44
1:A:459:GLU:H	1:A:459:GLU:HG3	1.38	0.44
1:A:593:THR:HG22	1:A:597:LEU:HD23	1.99	0.44
2:B:4:DG:H2''	2:B:5:DA:O4'	2.17	0.44
2:F:12:DA:H2''	2:F:13:DC:O4'	2.17	0.44
3:G:22:DA:H2'	3:G:23:DC:H6	1.82	0.44
1:A:159:LYS:HG2	1:A:599:PHE:CE1	2.53	0.44
1:E:146:THR:HG23	1:E:149:ARG:HH21	1.83	0.44
1:E:441:HIS:O	1:E:443:GLN:N	2.51	0.44
2:F:7:DC:H2'	2:F:8:DA:N7	2.33	0.44
1:A:557:LEU:O	1:A:558:ALA:C	2.59	0.44
1:E:291:CYS:HB3	1:E:329:ILE:HD13	1.99	0.44
1:E:430:TYR:HD2	1:E:442:MET:HE1	1.83	0.44
3:G:17:DG:H2''	3:G:18:DG:C5	2.52	0.44
1:A:131:TYR:O	1:E:84:LYS:HD2	2.18	0.44
2:B:12:DA:H61	3:C:5:DT:H3	1.66	0.44
1:E:554:LEU:O	1:E:557:LEU:N	2.37	0.44
1:A:166:ILE:O	1:A:170:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:HE2	1:A:428:TRP:CH2	2.53	0.44
1:A:162:ILE:HG12	1:A:603:PHE:HE1	1.83	0.43
1:A:548:SER:C	1:A:550:LYS:H	2.25	0.43
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.46	0.43
2:B:6:DA:H2''	2:B:7:DC:O4'	2.18	0.43
1:E:415:LYS:HG2	1:E:419:ILE:CD1	2.48	0.43
1:A:213:SER:C	1:A:215:ASP:N	2.72	0.43
1:E:276:ASN:O	1:E:277:SER:C	2.61	0.43
1:E:391:LYS:HA	1:E:394:GLU:HG3	2.01	0.43
1:E:591:GLN:H	1:E:591:GLN:HG2	1.31	0.43
1:A:434:PHE:HD1	1:A:450:ILE:HD13	1.82	0.43
1:E:177:ALA:HA	1:E:195:THR:O	2.18	0.43
1:E:185:ASN:HA	1:E:188:LYS:CD	2.48	0.43
1:E:437:PRO:C	1:E:439:ALA:H	2.26	0.43
1:A:291:CYS:SG	1:A:329:ILE:HD13	2.59	0.43
1:E:444:GLN:HB3	1:E:445:GLU:OE1	2.19	0.43
1:E:560:SER:O	1:E:564:ILE:HD12	2.19	0.43
1:E:186:TYR:CE1	1:E:584:GLU:HG3	2.53	0.43
1:E:544:TRP:HZ3	1:E:555:SER:HA	1.82	0.43
1:E:600:LEU:HD23	1:E:600:LEU:H	1.84	0.43
1:A:526:PHE:HB3	1:A:551:TYR:CE2	2.54	0.43
3:G:16:DT:H4'	3:G:16:DT:OP1	2.19	0.43
2:B:6:DA:H2''	2:B:7:DC:O5'	2.19	0.43
3:G:7:DG:H2'	3:G:8:DT:C6	2.54	0.43
1:A:345:GLU:OE1	1:A:345:GLU:HA	2.19	0.43
1:A:415:LYS:HG2	1:A:419:ILE:HD13	2.01	0.43
1:A:451:LYS:HG3	1:A:524:PHE:CZ	2.54	0.43
1:E:397:SER:HA	1:E:398:PRO:HD3	1.90	0.43
3:C:4:DG:C8	3:C:5:DT:H72	2.54	0.43
1:E:382:LEU:HD22	1:E:564:ILE:CG2	2.49	0.43
1:E:538:PHE:CD1	1:E:539:LYS:N	2.87	0.43
1:A:83:LEU:HD23	1:E:134:HIS:HB3	2.01	0.42
1:A:179:ILE:HG22	1:A:194:VAL:HG13	2.00	0.42
1:A:264:ASN:HD22	1:A:424:ASN:HB3	1.84	0.42
2:B:10:DC:H2''	2:B:11:DA:C5'	2.48	0.42
1:A:114:GLY:HA3	1:E:105:ASP:OD1	2.19	0.42
1:A:244:LYS:H	1:A:244:LYS:HD2	1.84	0.42
1:A:278:PHE:HE1	1:A:360:MET:CE	2.31	0.42
1:A:444:GLN:HB2	1:A:446:LYS:HG2	2.01	0.42
2:B:16:DG:H8	2:B:16:DG:OP2	2.02	0.42
1:A:86:VAL:HA	1:E:131:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:436:TYR:CD2	1:E:438:PRO:HD2	2.54	0.42
1:A:180:ASP:OD1	1:A:181:LEU:N	2.48	0.42
1:A:607:PHE:CD1	1:A:607:PHE:N	2.87	0.42
1:E:436:TYR:CD1	1:E:540:VAL:HG11	2.55	0.42
1:A:399:ASP:HB3	1:A:402:ASP:OD1	2.20	0.42
1:E:408:LYS:O	1:E:412:ASN:HB2	2.19	0.42
1:E:557:LEU:HA	1:E:557:LEU:HD23	1.62	0.42
1:A:83:LEU:CD2	1:E:134:HIS:HB3	2.49	0.42
1:A:289:LEU:HD13	1:A:289:LEU:HA	1.90	0.42
1:A:345:GLU:O	1:A:347:GLN:N	2.52	0.42
1:A:561:LEU:O	1:A:564:ILE:HB	2.20	0.42
1:E:130:GLU:HG2	1:E:130:GLU:H	1.60	0.42
1:A:200:GLU:O	1:A:203:GLU:HB2	2.20	0.42
1:A:445:GLU:CD	1:A:445:GLU:H	2.28	0.42
1:E:303:LEU:HD13	1:E:303:LEU:N	2.34	0.42
1:A:357:ILE:HG22	1:A:358:GLN:N	2.34	0.42
1:A:409:LEU:HD12	1:A:413:ILE:HG13	2.02	0.42
4:H:2:DC:H2"	4:H:3:DG:OP2	2.20	0.42
1:A:145:ILE:O	1:A:149:ARG:HG3	2.20	0.42
1:A:179:ILE:HD12	1:A:192:LEU:HD11	2.01	0.42
1:A:234:GLN:HE21	1:A:234:GLN:HB2	1.57	0.42
1:A:542:GLU:O	1:A:546:LEU:HD13	2.18	0.42
1:E:384:PHE:O	1:E:387:PRO:HD2	2.20	0.42
1:E:416:ASN:CB	1:E:420:ILE:HG13	2.48	0.42
1:E:568:SER:O	1:E:571:SER:HB2	2.20	0.42
1:A:270:LEU:O	1:A:273:VAL:HB	2.20	0.41
1:E:303:LEU:O	1:E:304:GLN:CB	2.68	0.41
1:A:235:PHE:CD1	1:A:235:PHE:N	2.87	0.41
1:A:406:ILE:O	1:A:407:ALA:C	2.63	0.41
1:E:325:MET:HE2	1:E:325:MET:HB3	1.58	0.41
1:E:345:GLU:HB3	1:E:348:ARG:HD2	2.03	0.41
1:E:392:VAL:O	1:E:395:ILE:HB	2.20	0.41
1:A:309:SER:HB2	1:A:332:ASN:HD21	1.82	0.41
1:E:205:ARG:HD2	1:E:607:PHE:CE1	2.55	0.41
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.77	0.41
1:A:320:ASN:C	1:A:322:THR:H	2.28	0.41
1:E:589:ILE:HG12	1:E:594:VAL:HG23	2.02	0.41
1:E:276:ASN:HB3	1:E:280:GLU:OE1	2.20	0.41
1:E:588:ARG:HD2	1:E:588:ARG:HA	1.33	0.41
1:A:118:ILE:HG22	1:A:119:ASP:OD1	2.20	0.41
1:A:283:GLU:OE1	1:A:408:LYS:NZ	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:524:PHE:O	1:E:528:ARG:N	2.37	0.41
1:E:527:TYR:O	1:E:528:ARG:C	2.63	0.41
1:E:548:SER:C	1:E:550:LYS:N	2.79	0.41
1:A:122:LYS:CE	1:E:137:VAL:HG21	2.51	0.41
1:A:125:ILE:HG23	1:E:127:VAL:HG13	2.03	0.41
1:A:205:ARG:HD2	1:A:205:ARG:N	2.35	0.41
1:A:272:ASN:HA	1:A:275:GLU:OE2	2.20	0.41
1:A:304:GLN:OE1	1:A:311:LEU:N	2.54	0.41
1:E:120:MET:HB3	1:E:120:MET:HE3	1.61	0.41
1:E:137:VAL:HG23	1:E:138:GLU:CD	2.45	0.41
1:E:269:LEU:O	1:E:273:VAL:HG23	2.20	0.41
1:E:399:ASP:HB3	1:E:402:ASP:CG	2.46	0.41
1:E:600:LEU:HD23	1:E:600:LEU:N	2.35	0.41
2:F:5:DA:N6	3:G:12:DT:H3	2.18	0.41
1:A:121:ILE:HG13	1:E:124:PHE:CE1	2.56	0.41
1:A:340:LEU:HD13	1:A:340:LEU:HA	1.79	0.41
3:C:6:DT:C2'	3:C:7:DG:H5'	2.50	0.41
1:E:527:TYR:HD1	1:E:530:GLU:HG3	1.85	0.41
4:H:4:DT:C2'	4:H:5:DG:C8	3.03	0.41
1:A:112:VAL:HG23	1:E:144:PRO:HD3	2.02	0.41
1:E:190:ASN:OD1	1:E:190:ASN:N	2.54	0.41
1:E:245:PHE:O	1:E:263:ILE:N	2.47	0.41
1:E:450:ILE:O	1:E:453:PHE:HB3	2.21	0.41
3:G:25:DC:H5''	3:G:25:DC:H6	1.85	0.41
1:A:369:ARG:O	1:A:373:GLU:HG3	2.21	0.41
1:E:301:ALA:HB3	1:E:303:LEU:HD22	2.03	0.41
1:A:252:ASN:HB2	1:A:253:VAL:H	1.61	0.40
1:E:269:LEU:O	1:E:272:ASN:HB2	2.21	0.40
1:A:113:SER:OG	1:E:144:PRO:HG3	2.21	0.40
1:A:207:LEU:HB3	1:A:606:ASN:OD1	2.21	0.40
1:A:224:ILE:HB	1:A:256:SER:OG	2.21	0.40
1:A:532:VAL:HG12	1:A:533:ILE:N	2.35	0.40
2:F:16:DG:N2	3:G:1:DC:N3	2.65	0.40
3:G:12:DT:H2''	3:G:13:DC:O4'	2.21	0.40
1:A:116:GLY:O	1:A:120:MET:HB2	2.20	0.40
1:A:167:LYS:O	1:A:170:VAL:HG13	2.21	0.40
1:A:306:ARG:H	1:A:306:ARG:HG3	1.37	0.40
1:A:359:THR:O	1:A:362:ASN:HB2	2.22	0.40
1:E:292:LYS:NZ	1:E:314:GLU:HG2	2.36	0.40
3:G:24:DG:H5''	3:G:24:DG:C8	2.57	0.40
1:A:183:THR:HA	1:A:189:ARG:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:CYS:SG	1:A:268:HIS:ND1	2.88	0.40
1:A:320:ASN:HB3	1:A:322:THR:HB	2.04	0.40
1:A:348:ARG:C	1:A:350:VAL:H	2.27	0.40
1:A:435:PHE:HD1	1:A:558:ALA:HA	1.85	0.40
2:B:7:DC:H42	3:C:10:DG:H1	1.70	0.40
1:E:98:CYS:O	1:E:101:TRP:HB3	2.22	0.40
1:E:123:PHE:CD2	1:E:123:PHE:C	3.00	0.40
1:E:205:ARG:HD2	1:E:607:PHE:HE1	1.85	0.40
1:E:227:LYS:O	1:E:230:ALA:HB3	2.21	0.40
1:E:389:ILE:HG22	1:E:393:LYS:HE2	2.02	0.40
1:E:603:PHE:HD2	1:E:604:TYR:CD2	2.40	0.40
1:A:325:MET:CG	1:A:329:ILE:HD12	2.50	0.40
1:A:388:SER:O	1:A:391:LYS:HB3	2.22	0.40
1:A:534:LEU:H	1:A:534:LEU:HG	1.62	0.40
1:E:368:GLU:HG3	1:E:372:LYS:HE3	2.02	0.40
1:E:433:PHE:HD1	1:E:433:PHE:HA	1.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	472/517 (91%)	412 (87%)	52 (11%)	8 (2%)	7	35
1	E	472/517 (91%)	410 (87%)	57 (12%)	5 (1%)	11	43
All	All	944/1034 (91%)	822 (87%)	109 (12%)	13 (1%)	9	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	379	SER
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	320	ASN
1	A	157	GLU
1	A	200	GLU
1	A	352	ILE
1	E	448	ALA
1	E	518	VAL
1	E	200	GLU
1	E	443	GLN
1	A	350	VAL
1	A	518	VAL
1	A	95	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/475 (92%)	321 (74%)	115 (26%)	0	3
1	E	436/475 (92%)	306 (70%)	130 (30%)	0	1
All	All	872/950 (92%)	627 (72%)	245 (28%)	0	2

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	83	LEU
1	A	86	VAL
1	A	92	LYS
1	A	93	GLU
1	A	97	LYS
1	A	102	VAL
1	A	110	SER
1	A	112	VAL
1	A	115	SER
1	A	118	ILE
1	A	120	MET

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Mol	Chain	Res	Type
1	A	121	ILE
1	A	122	LYS
1	A	125	ILE
1	A	126	LYS
1	A	135	VAL
1	A	136	ASN
1	A	143	SER
1	A	150	LYS
1	A	154	ASP
1	A	161	LEU
1	A	168	SER
1	A	170	VAL
1	A	172	LYS
1	A	179	ILE
1	A	188	LYS
1	A	194	VAL
1	A	199	HIS
1	A	202	ASN
1	A	205	ARG
1	A	206	ASP
1	A	208	ILE
1	A	209	LEU
1	A	213	SER
1	A	219	SER
1	A	223	ASN
1	A	227	LYS
1	A	228	LEU
1	A	229	LYS
1	A	234	GLN
1	A	240	LEU
1	A	243	ILE
1	A	244	LYS
1	A	246	VAL
1	A	254	VAL
1	A	256	SER
1	A	266	SER
1	A	275	GLU
1	A	279	GLU
1	A	289	LEU
1	A	295	VAL
1	A	296	LYS
1	A	303	LEU

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Mol	Chain	Res	Type
1	A	306	ARG
1	A	309	SER
1	A	314	GLU
1	A	318	ARG
1	A	329	ILE
1	A	337	ILE
1	A	340	LEU
1	A	345	GLU
1	A	356	ILE
1	A	357	ILE
1	A	359	THR
1	A	361	VAL
1	A	364	LEU
1	A	370	ILE
1	A	374	LEU
1	A	376	THR
1	A	377	CYS
1	A	379	SER
1	A	381	SER
1	A	390	LEU
1	A	392	VAL
1	A	395	ILE
1	A	400	VAL
1	A	408	LYS
1	A	409	LEU
1	A	415	LYS
1	A	418	ARG
1	A	419	ILE
1	A	423	GLU
1	A	426	SER
1	A	440	LEU
1	A	442	MET
1	A	447	VAL
1	A	451	LYS
1	A	459	GLU
1	A	461	LEU
1	A	462	GLU
1	A	519	SER
1	A	521	SER
1	A	522	ASP
1	A	523	GLU
1	A	526	PHE

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Mol	Chain	Res	Type
1	A	533	ILE
1	A	534	LEU
1	A	535	SER
1	A	537	ASP
1	A	538	PHE
1	A	540	VAL
1	A	542	GLU
1	A	547	ASN
1	A	549	LYS
1	A	554	LEU
1	A	561	LEU
1	A	572	GLU
1	A	580	ASN
1	A	583	THR
1	A	585	LYS
1	A	591	GLN
1	A	597	LEU
1	A	602	SER
1	A	609	LYS
1	E	89	ASP
1	E	92	LYS
1	E	95	ILE
1	E	97	LYS
1	E	102	VAL
1	E	112	VAL
1	E	118	ILE
1	E	119	ASP
1	E	120	MET
1	E	121	ILE
1	E	125	ILE
1	E	127	VAL
1	E	130	GLU
1	E	135	VAL
1	E	137	VAL
1	E	146	THR
1	E	149	ARG
1	E	151	VAL
1	E	154	ASP
1	E	157	GLU
1	E	173	ASP
1	E	176	SER
1	E	179	ILE

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Mol	Chain	Res	Type
1	E	181	LEU
1	E	183	THR
1	E	198	TYR
1	E	200	GLU
1	E	201	ASN
1	E	202	ASN
1	E	206	ASP
1	E	209	LEU
1	E	213	SER
1	E	214	LEU
1	E	217	GLU
1	E	218	ARG
1	E	219	SER
1	E	223	ASN
1	E	228	LEU
1	E	232	PHE
1	E	237	VAL
1	E	238	GLU
1	E	240	LEU
1	E	243	ILE
1	E	244	LYS
1	E	246	VAL
1	E	252	ASN
1	E	253	VAL
1	E	261	ILE
1	E	265	CYS
1	E	269	LEU
1	E	270	LEU
1	E	274	LEU
1	E	283	GLU
1	E	286	MET
1	E	292	LYS
1	E	296	LYS
1	E	303	LEU
1	E	309	SER
1	E	311	LEU
1	E	313	SER
1	E	314	GLU
1	E	317	THR
1	E	321	SER
1	E	324	THR
1	E	327	ARG

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Mol	Chain	Res	Type
1	E	329	ILE
1	E	336	VAL
1	E	337	ILE
1	E	340	LEU
1	E	347	GLN
1	E	349	ILE
1	E	352	ILE
1	E	354	LYS
1	E	356	ILE
1	E	357	ILE
1	E	358	GLN
1	E	359	THR
1	E	360	MET
1	E	361	VAL
1	E	364	LEU
1	E	369	ARG
1	E	370	ILE
1	E	374	LEU
1	E	375	GLN
1	E	379	SER
1	E	381	SER
1	E	390	LEU
1	E	394	GLU
1	E	403	VAL
1	E	405	ASP
1	E	409	LEU
1	E	414	ILE
1	E	415	LYS
1	E	416	ASN
1	E	418	ARG
1	E	419	ILE
1	E	423	GLU
1	E	426	SER
1	E	427	ILE
1	E	440	LEU
1	E	442	MET
1	E	449	GLN
1	E	450	ILE
1	E	454	CYS
1	E	461	LEU
1	E	462	GLU
1	E	517	PRO

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Mol	Chain	Res	Type
1	E	523	GLU
1	E	526	PHE
1	E	528	ARG
1	E	533	ILE
1	E	540	VAL
1	E	557	LEU
1	E	560	SER
1	E	561	LEU
1	E	563	SER
1	E	564	ILE
1	E	567	SER
1	E	568	SER
1	E	572	GLU
1	E	583	THR
1	E	584	GLU
1	E	588	ARG
1	E	591	GLN
1	E	592	GLN
1	E	595	ASP
1	E	597	LEU
1	E	600	LEU
1	E	602	SER
1	E	609	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	234	GLN
1	A	260	ASN
1	A	276	ASN
1	A	285	ASN
1	A	305	HIS
1	A	332	ASN
1	A	347	GLN
1	A	424	ASN
1	A	601	ASN
1	E	234	GLN
1	E	236	ASN
1	E	305	HIS
1	E	320	ASN
1	E	358	GLN

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Mol	Chain	Res	Type
1	E	416	ASN
1	E	449	GLN
1	E	591	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

There are no chain breaks in this entry.

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	476/517 (92%)	-0.57	0 100 100	41, 81, 131, 157	0
1	E	476/517 (92%)	-0.53	0 100 100	37, 83, 132, 193	0
2	B	15/15 (100%)	-0.51	0 100 100	37, 57, 92, 111	0
2	F	15/15 (100%)	-0.51	0 100 100	39, 59, 84, 90	0
3	C	25/26 (96%)	-0.57	0 100 100	38, 69, 96, 127	0
3	G	25/26 (96%)	-0.47	0 100 100	40, 68, 92, 119	0
4	D	7/7 (100%)	-0.72	0 100 100	53, 55, 77, 81	0
4	H	7/7 (100%)	-0.28	0 100 100	49, 52, 98, 108	0
All	All	1046/1130 (92%)	-0.55	0 100 100	37, 80, 131, 193	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.