



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:41 PM GMT

PDB ID : 3UKH
Title : Crystal structure of udp-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPGALP (non-reduced)
Authors : Van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2011-11-09
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

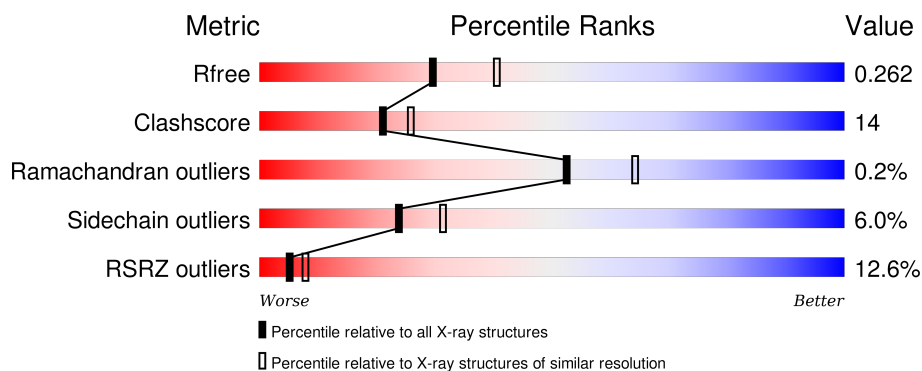
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	519	<div> <div>9%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	B	519	<div> <div>14%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	C	519	<div> <div>13%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>
1	D	519	<div> <div>12%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	E	519	<div> <div>18%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	519	
1	G	519	
1	H	519	

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
3	GDU	A	521	-	-	-	X
3	GDU	B	521	-	-	-	X
3	GDU	C	521	-	-	-	X
3	GDU	D	521	-	-	-	X
3	GDU	E	521	-	-	-	X
3	GDU	F	521	-	-	-	X
3	GDU	G	521	-	-	-	X
3	GDU	H	521	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34881 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	15	0
			4080	2590	699	768	23			
1	B	510	Total	C	N	O	S	0	15	0
			4126	2619	711	774	22			
1	C	511	Total	C	N	O	S	0	42	0
			4270	2713	734	801	22			
1	D	510	Total	C	N	O	S	0	3	0
			4035	2560	694	759	22			
1	E	510	Total	C	N	O	S	0	9	0
			4074	2586	700	767	21			
1	F	504	Total	C	N	O	S	0	8	0
			4026	2554	689	761	22			
1	G	504	Total	C	N	O	S	0	1	0
			3977	2525	680	751	21			
1	H	511	Total	C	N	O	S	0	42	0
			4301	2733	740	807	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
A	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
A	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
A	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
A	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
A	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
B	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
B	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2

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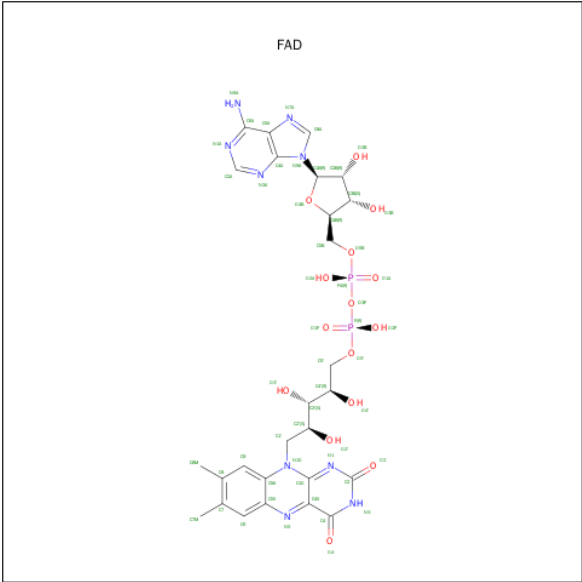
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
B	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
B	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
C	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
C	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
C	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
C	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
C	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
D	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
D	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
D	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
D	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
D	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
E	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
E	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
E	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
E	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
E	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
F	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
F	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
F	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
F	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2

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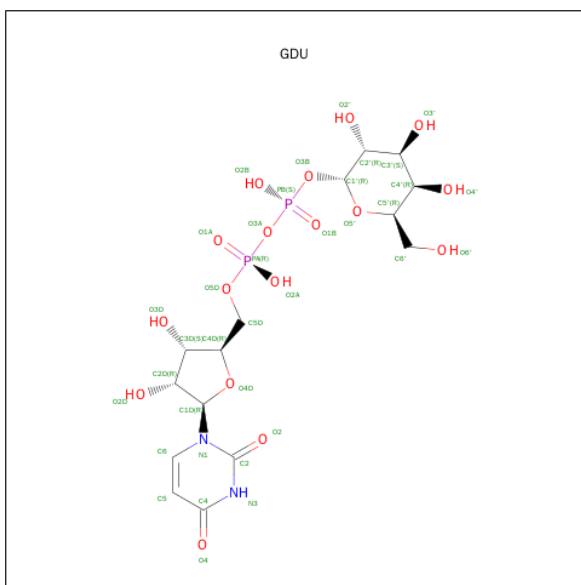
Chain	Residue	Modelled	Actual	Comment	Reference
F	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
F	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
G	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
G	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
G	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
G	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
G	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	511	LEU	-	EXPRESSION TAG	UNP Q4W1X2
H	512	GLU	-	EXPRESSION TAG	UNP Q4W1X2
H	513	LEU	-	EXPRESSION TAG	UNP Q4W1X2
H	514	GLU	-	EXPRESSION TAG	UNP Q4W1X2
H	515	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	516	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	517	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	518	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	519	HIS	-	EXPRESSION TAG	UNP Q4W1X2
H	520	HIS	-	EXPRESSION TAG	UNP Q4W1X2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).

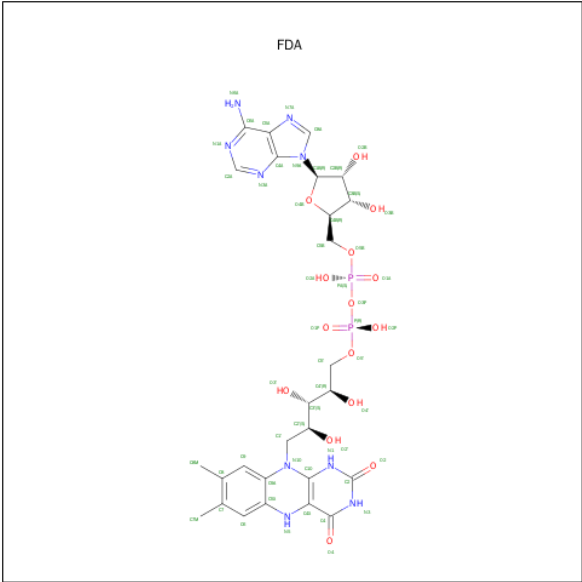


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	F	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	G	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	H	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

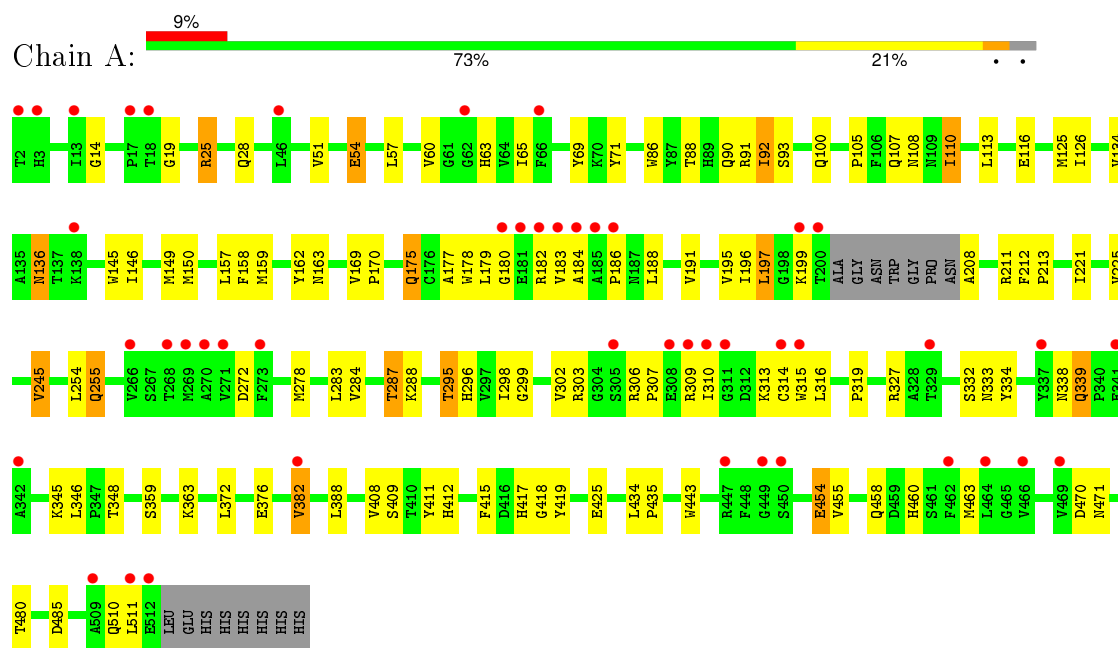
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	207	Total	O	0	0
			207	207		
6	B	180	Total	O	0	0
			180	180		
6	C	150	Total	O	0	0
			150	150		
6	D	172	Total	O	0	0
			172	172		
6	E	137	Total	O	0	0
			137	137		
6	F	126	Total	O	0	0
			126	126		
6	G	156	Total	O	0	0
			156	156		
6	H	150	Total	O	0	0
			150	150		

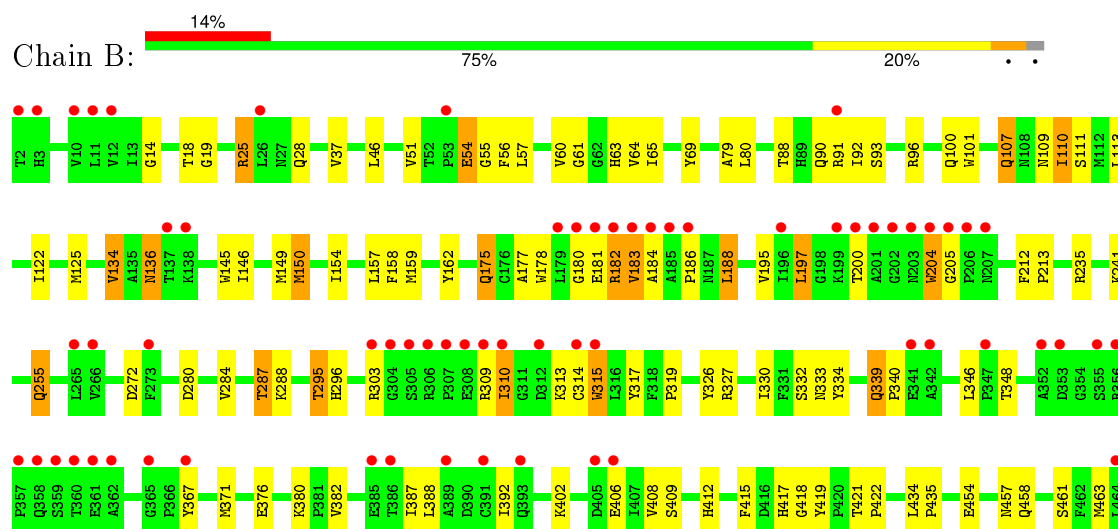
3 Residue-property plots [i](#)

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

• Molecule 1: UDP-galactopyranose mutase

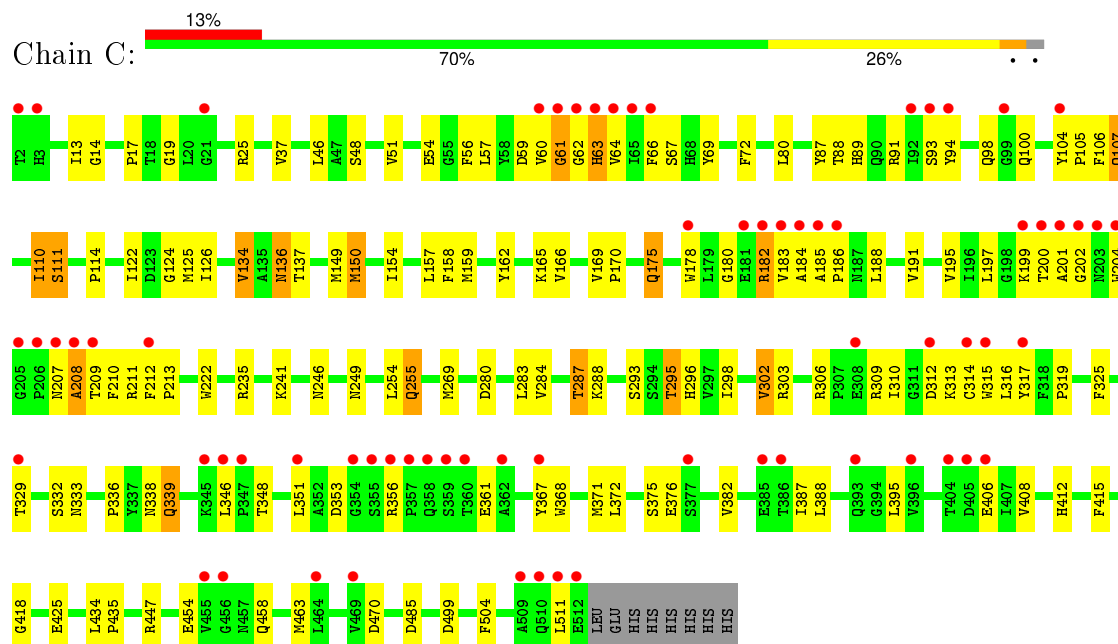


• Molecule 1: UDP-galactopyranose mutase

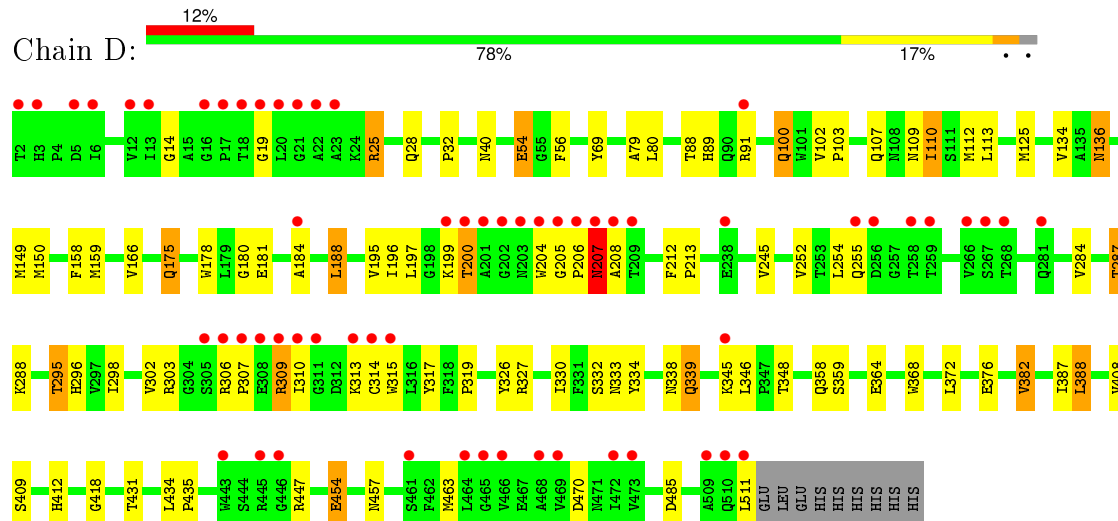




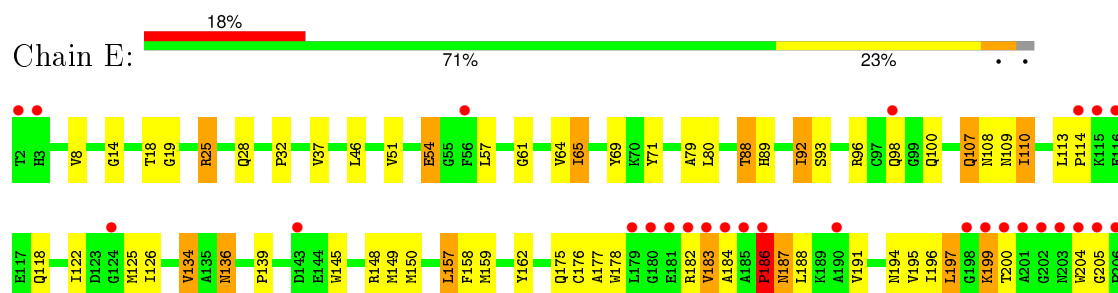
• Molecule 1: UDP-galactopyranose mutase

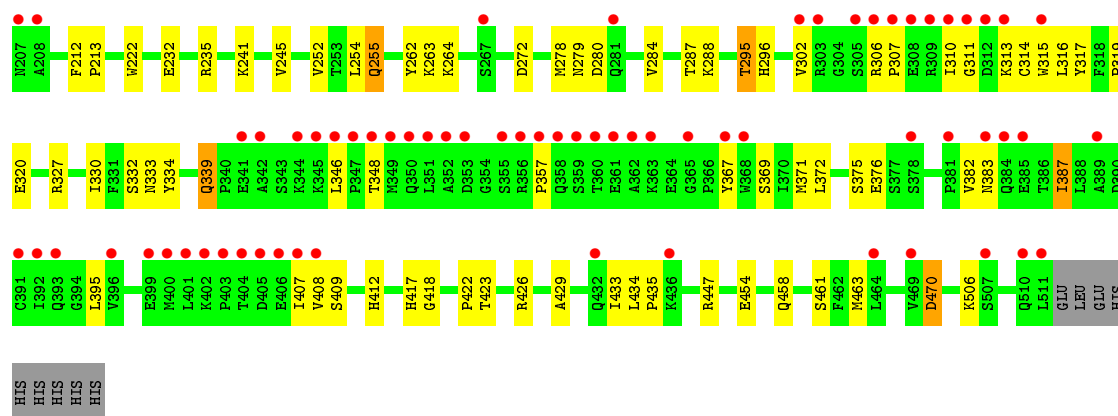


• Molecule 1: UDP-galactopyranose mutase

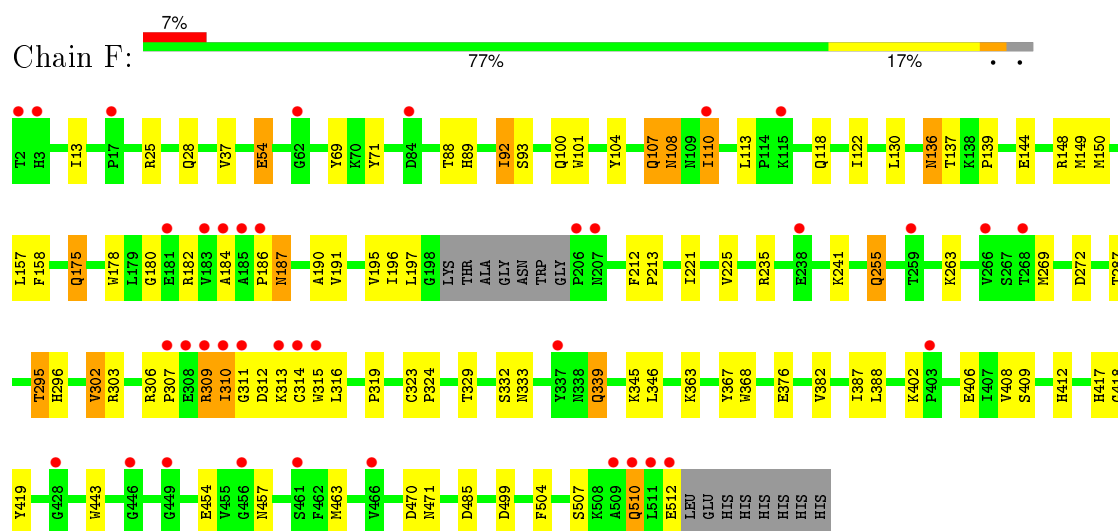


• Molecule 1: UDP-galactopyranose mutase

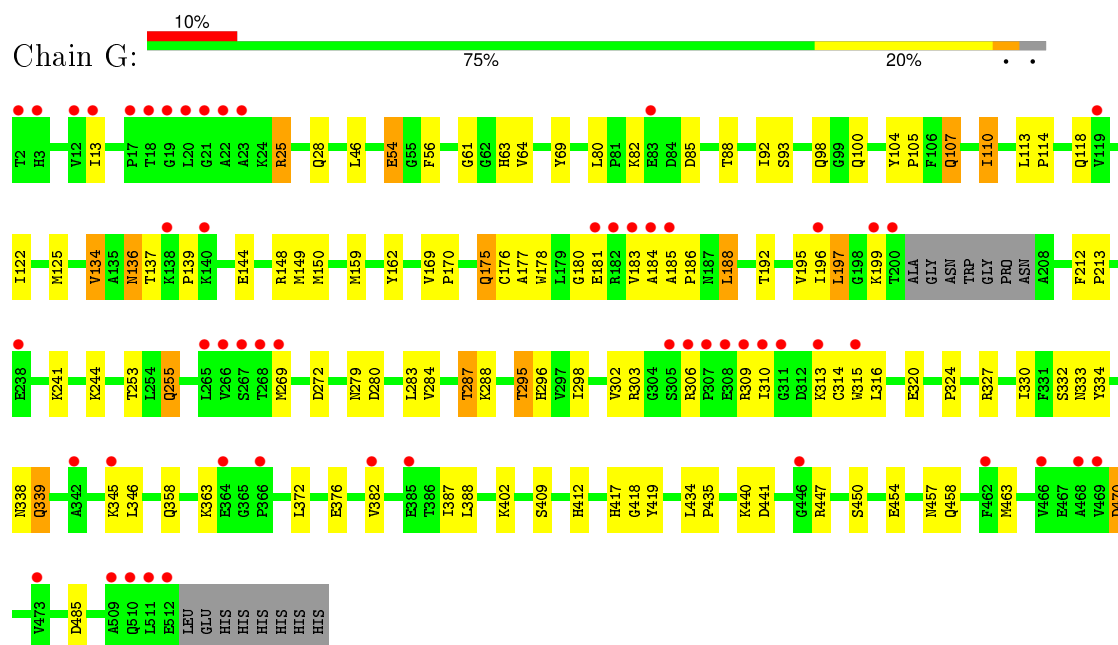




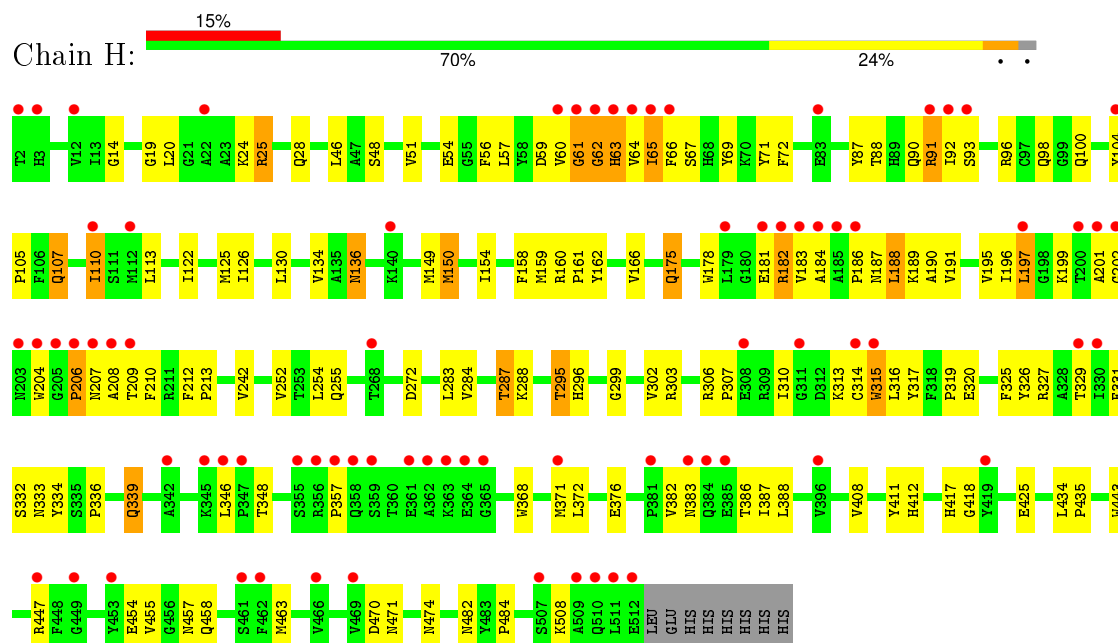
• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase



● Molecule 1: UDP-galactopyranose mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.97 Å 129.26 Å 173.88 Å 89.87° 84.64° 81.21°	Depositor
Resolution (Å)	35.55 – 2.30 35.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.55-2.30) 97.1 (35.55-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.222 , 0.264 0.220 , 0.262	Depositor DCC
R_{free} test set	13334 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 266579 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34881	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FDA, GDU, FAD, CL

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	0.25	0/4180	0.43	0/5680
1	B	0.25	0/4230	0.43	0/5751
1	C	0.25	0/4378	0.43	0/5951
1	D	0.25	0/4136	0.43	0/5621
1	E	0.25	0/4176	0.43	0/5677
1	F	0.24	0/4125	0.42	0/5603
1	G	0.25	0/4074	0.43	0/5534
1	H	0.26	0/4413	0.44	0/6000
All	All	0.25	0/33712	0.43	0/45817

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	E	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	186[B]	PRO	Peptide
1	H	206[A]	PRO	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	4080	0	3999	120	0
1	B	4126	0	4041	123	0
1	C	4270	0	4171	135	0
1	D	4035	0	3951	91	0
1	E	4074	0	3992	130	0
1	F	4026	0	3941	88	0
1	G	3977	0	3899	88	0
1	H	4301	0	4193	154	0
2	A	53	0	30	6	0
2	B	53	0	30	4	0
2	D	53	0	30	2	0
2	E	53	0	30	2	0
2	F	53	0	30	6	0
2	G	53	0	30	4	0
3	A	36	0	22	10	0
3	B	36	0	22	10	0
3	C	36	0	22	7	0
3	D	36	0	22	4	0
3	E	36	0	22	12	0
3	F	36	0	22	3	0
3	G	36	0	22	8	0
3	H	36	0	22	11	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
5	C	53	0	32	6	0
5	H	53	0	32	6	0
6	A	207	0	0	4	0
6	B	180	0	0	13	0
6	C	150	0	0	12	0
6	D	172	0	0	8	0
6	E	137	0	0	7	0
6	F	126	0	0	5	0
6	G	156	0	0	4	0
6	H	150	0	0	4	0
All	All	34881	0	32607	949	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 14.

All (949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104[A]:TYR:O	1:H:202[A]:GLY:HA2	1.68	0.92
1:E:175:GLN:HG2	6:E:820:HOH:O	1.67	0.92
3:B:521:GDU:O1A	6:B:1234:HOH:O	1.88	0.89
1:B:109:ASN:OD1	1:B:200:THR:HG21	1.74	0.88
1:F:296:HIS:HD2	1:F:412:HIS:HE1	1.22	0.87
1:A:455:VAL:HG13	1:A:460:HIS:HB3	1.57	0.86
1:G:296:HIS:HD2	1:G:412:HIS:HE1	1.24	0.86
1:B:162:TYR:HE2	3:B:521:GDU:H3D	1.41	0.85
1:B:54:GLU:HG3	1:B:409:SER:HB2	1.58	0.84
1:F:295:THR:HG23	1:F:418:GLY:HA3	1.56	0.84
1:E:54:GLU:HG3	1:E:409:SER:HB2	1.59	0.84
1:C:211[A]:ARG:O	6:C:833:HOH:O	1.96	0.84
1:E:307:PRO:HB2	1:E:310:ILE:HD13	1.60	0.83
1:D:110:ILE:HG22	1:D:113:LEU:HD12	1.59	0.82
1:F:54:GLU:HG3	1:F:409:SER:HB2	1.59	0.82
1:B:107:GLN:OE1	6:B:1158:HOH:O	1.96	0.82
1:E:149:MET:O	1:E:186[B]:PRO:HG2	1.79	0.82
1:H:104[A]:TYR:HE2	1:H:204[A]:TRP:HB3	1.45	0.82
1:A:455:VAL:O	1:A:455:VAL:HG12	1.80	0.81
1:D:295:THR:HG23	1:D:418:GLY:HA3	1.62	0.81
1:C:149:MET:SD	1:C:184[A]:ALA:HA	2.21	0.81
1:H:91[A]:ARG:HB2	1:H:208[A]:ALA:O	1.80	0.81
5:H:600:FDA:C4	3:H:521:GDU:H2'	2.11	0.80
1:B:204:TRP:HE3	1:B:205:GLY:H	1.26	0.80
1:B:65:ILE:HD11	1:B:315[B]:TRP:HE1	1.45	0.80
1:E:109:ASN:OD1	1:E:200:THR:HG21	1.80	0.80
1:H:91[A]:ARG:HD3	1:H:207[A]:ASN:OD1	1.83	0.79
1:E:182[B]:ARG:HH12	3:E:521:GDU:H3'	1.46	0.79
1:A:178[A]:TRP:HB2	1:A:454:GLU:CG	2.14	0.78
1:C:175:GLN:NE2	1:C:178[A]:TRP:H	1.82	0.77
3:D:521:GDU:O1A	6:D:1241:HOH:O	2.01	0.77
1:A:295:THR:HG23	1:A:418:GLY:HA3	1.67	0.77
1:F:307:PRO:HB2	1:F:310:ILE:HG12	1.66	0.76
1:H:65[A]:ILE:HD12	1:H:207[A]:ASN:HD21	1.50	0.76
1:B:313:LYS:HD2	1:B:313:LYS:H	1.50	0.76
1:B:303:ARG:NH2	1:B:346:LEU:O	2.19	0.76
1:F:296:HIS:HD2	1:F:412:HIS:CE1	2.04	0.76
1:E:313:LYS:HG3	1:E:333:ASN:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:521:GDU:O2'	6:C:995:HOH:O	2.03	0.75
1:A:136:ASN:H	1:A:136:ASN:HD22	1.36	0.74
1:H:105[A]:PRO:HD2	1:H:201[A]:ALA:O	1.88	0.74
1:H:104[A]:TYR:CE2	1:H:204[A]:TRP:HB3	2.23	0.74
1:A:183[B]:VAL:HG22	3:A:521:GDU:H1D	1.68	0.73
1:E:296:HIS:HD2	1:E:412:HIS:HE1	1.35	0.73
1:E:272:ASP:OD2	1:E:417:HIS:HE1	1.72	0.73
1:G:110:ILE:HG22	1:G:113:LEU:HD12	1.71	0.73
1:D:178:TRP:HB2	1:D:454:GLU:CG	2.19	0.73
1:D:296:HIS:HD2	1:D:412:HIS:HE1	1.34	0.73
1:H:175:GLN:NE2	1:H:178[A]:TRP:H	1.85	0.73
1:A:296:HIS:HD2	1:A:412:HIS:HE1	1.37	0.73
1:F:296:HIS:CD2	1:F:412:HIS:HE1	2.05	0.72
3:B:521:GDU:O2'	6:B:645:HOH:O	2.07	0.72
1:E:175:GLN:HG3	1:E:178:TRP:HD1	1.55	0.72
1:B:92:ILE:HG22	1:B:93:SER:N	2.04	0.72
1:D:313:LYS:HG3	1:D:314[A]:CYS:SG	2.30	0.72
3:E:521:GDU:H6	3:E:521:GDU:O1A	1.89	0.72
1:B:296:HIS:HD2	1:B:412:HIS:HE1	1.36	0.71
1:C:93[A]:SER:HB3	1:C:104:TYR:HB2	1.72	0.71
1:C:93[A]:SER:HG	1:C:317:TYR:HE2	1.36	0.71
1:G:296:HIS:HD2	1:G:412:HIS:CE1	2.07	0.71
1:A:197:LEU:HB3	1:A:199:LYS:HG2	1.72	0.71
1:H:296:HIS:HD2	1:H:412:HIS:HE1	1.39	0.71
1:H:63[B]:HIS:ND1	1:H:458:GLN:OE1	2.21	0.71
1:A:110:ILE:HA	1:A:113:LEU:HD12	1.73	0.71
1:B:309:ARG:HG3	1:B:310:ILE:HG13	1.73	0.70
1:F:296:HIS:CE1	1:F:382:VAL:HG21	2.26	0.70
1:B:92:ILE:HG22	1:B:93:SER:H	1.56	0.70
1:G:296:HIS:CD2	1:G:412:HIS:HE1	2.06	0.70
3:E:521:GDU:H5'	3:E:521:GDU:O2A	1.91	0.70
1:C:310:ILE:O	1:C:313:LYS:HG2	1.92	0.70
1:B:482:ASN:ND2	6:B:731:HOH:O	2.08	0.70
2:E:600:FAD:C4	3:E:521:GDU:H2'	2.21	0.70
1:E:136:ASN:H	1:E:136:ASN:HD22	1.39	0.70
2:D:600:FAD:O4'	2:D:600:FAD:O2'	2.06	0.70
1:B:295:THR:CG2	1:B:418:GLY:HA3	2.21	0.69
1:F:136:ASN:H	1:F:136:ASN:HD22	1.40	0.69
1:H:303:ARG:NH2	1:H:346:LEU:O	2.25	0.69
1:F:149:MET:SD	1:F:184:ALA:HA	2.33	0.69
1:B:110:ILE:HA	1:B:113:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:296:HIS:CE1	1:G:382:VAL:HG21	2.27	0.69
1:D:313:LYS:HB3	1:D:333:ASN:HB3	1.75	0.69
1:A:455:VAL:HG11	1:A:480:THR:HG22	1.75	0.68
1:E:183[B]:VAL:HG22	3:E:521:GDU:H1D	1.75	0.68
5:C:600:FDA:N5	3:C:521:GDU:H2'	2.08	0.68
1:G:447:ARG:NH1	6:G:740:HOH:O	2.27	0.68
1:B:309:ARG:NH1	1:B:402:LYS:HE3	2.09	0.68
1:A:178[B]:TRP:HB2	1:A:454:GLU:HG3	1.74	0.68
1:H:457:ASN:OD1	3:H:521:GDU:O3'	2.09	0.68
1:D:136:ASN:HD22	1:D:136:ASN:H	1.42	0.68
1:H:61[B]:GLY:O	1:H:315[B]:TRP:HH2	1.75	0.67
1:E:295:THR:CG2	1:E:418:GLY:HA3	2.24	0.67
1:D:25:ARG:HH21	1:D:28:GLN:HE22	1.41	0.67
3:H:521:GDU:H5'	3:H:521:GDU:O2A	1.93	0.67
1:E:125:MET:HE1	1:E:188:LEU:HD23	1.77	0.67
1:B:146:ILE:HD13	1:B:159:MET:HB3	1.75	0.67
1:F:110:ILE:HD13	1:F:195:VAL:CG2	2.24	0.67
1:G:457:ASN:OD1	3:G:521:GDU:O3'	2.12	0.67
1:D:40:ASN:OD1	6:D:1094:HOH:O	2.13	0.67
1:D:178:TRP:HB2	1:D:454:GLU:HG3	1.77	0.66
1:A:296:HIS:HE1	1:A:376:GLU:OE2	1.78	0.66
1:B:296:HIS:CD2	1:B:412:HIS:HE1	2.12	0.66
1:F:104:TYR:OH	6:F:1237:HOH:O	2.14	0.66
1:B:178[B]:TRP:HB2	1:B:454:GLU:HG3	1.76	0.66
1:F:312[A]:ASP:HA	1:F:333:ASN:OD1	1.95	0.66
1:F:13:ILE:HG21	1:F:269:MET:HE3	1.77	0.66
1:E:178:TRP:HB2	1:E:454:GLU:CG	2.26	0.66
1:B:296:HIS:HD2	1:B:412:HIS:CE1	2.13	0.66
1:D:25:ARG:HH21	1:D:28:GLN:NE2	1.93	0.66
1:C:110:ILE:HD11	1:C:191:VAL:HG13	1.78	0.66
1:C:150:MET:HE3	1:C:159:MET:HG3	1.77	0.66
1:A:92:ILE:HG22	1:A:314[B]:CYS:SG	2.36	0.66
1:F:186[B]:PRO:O	1:F:187[B]:ASN:HB3	1.95	0.65
5:C:600:FDA:C4X	3:C:521:GDU:H2'	2.27	0.65
1:A:306:ARG:HD3	1:A:333:ASN:HD21	1.60	0.65
1:C:182[B]:ARG:HH12	3:C:521:GDU:H4'	1.60	0.65
1:E:196:ILE:HD11	1:G:122:ILE:HG13	1.78	0.65
1:E:182[B]:ARG:NH1	3:E:521:GDU:H3'	2.09	0.65
1:H:64[B]:VAL:HG13	1:H:210:PHE:CD1	2.32	0.65
1:E:54:GLU:HG3	1:E:409:SER:CB	2.27	0.65
2:A:600:FAD:C4	3:A:521:GDU:H2'	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:HIS:HD2	1:C:412:HIS:HE1	1.44	0.64
1:G:125:MET:HE2	1:G:188:LEU:HA	1.79	0.64
1:A:175:GLN:NE2	1:A:178[A]:TRP:H	1.96	0.64
1:B:175:GLN:NE2	1:B:178[A]:TRP:H	1.95	0.64
1:E:98:GLN:N	1:E:320:GLU:OE1	2.16	0.64
1:H:307:PRO:HG2	1:H:310:ILE:HD13	1.79	0.64
1:C:110:ILE:HD12	6:C:1227:HOH:O	1.96	0.64
1:F:499:ASP:OD1	6:F:1277:HOH:O	2.15	0.64
1:C:295:THR:CG2	1:C:418:GLY:HA3	2.28	0.64
1:C:178[B]:TRP:HB2	1:C:454:GLU:HG3	1.79	0.63
1:E:346:LEU:HD13	1:E:408:VAL:HG11	1.80	0.63
1:H:64[A]:VAL:CG2	1:H:458:GLN:HB2	2.28	0.63
3:B:521:GDU:O3'	6:B:602:HOH:O	2.15	0.63
1:B:315[A]:TRP:HZ3	1:B:334:TYR:HH	1.42	0.63
1:H:197:LEU:HB3	1:H:199[A]:LYS:HG3	1.80	0.63
1:H:62[B]:GLY:N	1:H:371:MET:SD	2.71	0.63
1:F:54:GLU:HG3	1:F:409:SER:CB	2.29	0.63
1:E:186[B]:PRO:O	1:E:187:ASN:HB2	1.97	0.63
1:A:443:TRP:HE1	1:A:471:ASN:HD22	1.46	0.63
1:C:182[B]:ARG:NH1	3:C:521:GDU:H4'	2.14	0.63
1:D:205:GLY:HA2	1:D:206:PRO:C	2.17	0.63
1:G:295:THR:CG2	1:G:418:GLY:HA3	2.29	0.63
1:A:125:MET:HE3	1:A:186[A]:PRO:HB2	1.80	0.63
1:H:104[A]:TYR:CD1	1:H:105[A]:PRO:HA	2.33	0.63
1:E:296:HIS:HD2	1:E:412:HIS:CE1	2.17	0.63
1:E:296:HIS:CD2	1:E:412:HIS:HE1	2.16	0.62
1:H:296:HIS:CE1	1:H:382:VAL:HG21	2.34	0.62
1:H:296:HIS:CD2	1:H:412:HIS:HE1	2.17	0.62
1:D:109:ASN:OD1	1:D:200:THR:HG21	1.99	0.62
1:G:197:LEU:HD23	1:G:199:LYS:HE3	1.82	0.62
1:B:25:ARG:HD3	1:B:470:ASP:OD1	2.00	0.62
1:A:54:GLU:HG3	1:A:409:SER:HB2	1.81	0.62
1:H:25:ARG:HH21	1:H:28:GLN:NE2	1.97	0.62
1:H:65[A]:ILE:HB	1:H:207[A]:ASN:OD1	2.00	0.62
1:B:182[A]:ARG:HH11	1:B:182[A]:ARG:CG	2.12	0.62
1:C:241:LYS:HD3	1:C:255:GLN:HG3	1.81	0.62
1:E:367:TYR:HE1	1:E:408:VAL:HG21	1.63	0.62
1:E:222:TRP:HE1	1:E:458:GLN:NE2	1.98	0.62
1:G:125:MET:HE3	1:G:186:PRO:HB2	1.81	0.61
1:C:313:LYS:HB3	1:C:316:LEU:HD21	1.82	0.61
1:G:69:TYR:CD1	1:G:463:MET:HG3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ILE:H	1:F:110:ILE:HD12	1.65	0.61
1:C:59[A]:ASP:C	1:C:61[A]:GLY:H	2.03	0.61
1:C:302:VAL:HG22	1:C:368:TRP:NE1	2.15	0.61
1:G:178:TRP:HB2	1:G:454:GLU:HG3	1.81	0.61
1:A:149:MET:SD	1:A:184[A]:ALA:HA	2.39	0.61
1:C:62[B]:GLY:N	1:C:371:MET:SD	2.73	0.61
1:B:303:ARG:NH1	1:B:406:GLU:OE1	2.34	0.61
1:H:296:HIS:HD2	1:H:412:HIS:CE1	2.19	0.61
1:B:183[B]:VAL:HG22	3:B:521:GDU:H1D	1.80	0.61
1:A:295:THR:CG2	1:A:418:GLY:HA3	2.29	0.61
1:A:296:HIS:HD2	1:A:412:HIS:CE1	2.18	0.61
1:H:474:ASN:ND2	6:H:546:HOH:O	2.32	0.61
1:D:296:HIS:CD2	1:D:412:HIS:HE1	2.18	0.61
1:H:104[A]:TYR:CG	1:H:105[A]:PRO:HA	2.36	0.61
1:E:110:ILE:HG22	1:E:113:LEU:HD12	1.81	0.61
1:D:110:ILE:HD13	1:D:195:VAL:CG2	2.31	0.61
1:F:314[B]:CYS:HB3	1:F:315[B]:TRP:CE3	2.36	0.61
1:F:302:VAL:HG22	1:F:368:TRP:NE1	2.15	0.61
1:A:92:ILE:CG2	1:A:93:SER:N	2.64	0.60
1:D:306:ARG:HD3	1:D:333:ASN:HD21	1.65	0.60
1:B:162:TYR:CE2	3:B:521:GDU:H3D	2.29	0.60
1:E:126:ILE:HA	1:E:188:LEU:HD11	1.83	0.60
1:F:306:ARG:NH1	1:F:312[A]:ASP:HB3	2.16	0.60
1:H:183[B]:VAL:HG22	3:H:521:GDU:H1D	1.83	0.60
1:C:295:THR:HG22	1:C:418:GLY:HA3	1.83	0.60
1:D:158:PHE:HD1	1:D:319:PRO:HG3	1.66	0.60
1:H:66[A]:PHE:CG	1:H:206[A]:PRO:HB2	2.36	0.60
1:E:313:LYS:H	1:E:313:LYS:HD3	1.65	0.60
1:A:105:PRO:HG2	1:A:108:ASN:HB2	1.82	0.60
1:C:149:MET:HE3	1:C:185[B]:ALA:HA	1.84	0.60
1:A:296:HIS:CD2	1:A:412:HIS:HE1	2.19	0.60
1:F:313[A]:LYS:O	1:F:314[A]:CYS:HB3	2.02	0.60
1:A:65:ILE:HD12	3:A:521:GDU:O4'	2.01	0.60
1:H:110:ILE:HD12	1:H:110:ILE:H	1.66	0.60
1:E:175:GLN:HG3	1:E:178:TRP:CD1	2.35	0.60
1:G:296:HIS:HE1	1:G:376:GLU:OE2	1.85	0.60
2:F:600:FAD:C4X	3:F:521:GDU:H2'	2.31	0.60
5:H:600:FDA:C4X	3:H:521:GDU:H2'	2.32	0.59
1:A:455:VAL:O	1:A:455:VAL:CG1	2.50	0.59
1:F:306:ARG:HD3	1:F:311[A]:GLY:O	2.02	0.59
1:B:92:ILE:CG2	1:B:93:SER:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:LYS:N	1:E:313:LYS:HD3	2.18	0.59
1:D:175:GLN:NE2	1:D:178:TRP:H	2.00	0.59
1:B:149:MET:SD	1:B:184[A]:ALA:HA	2.43	0.59
1:H:65[A]:ILE:HB	1:H:207[A]:ASN:CG	2.22	0.59
1:H:91[A]:ARG:HH11	1:H:207[A]:ASN:HB3	1.67	0.59
1:F:107:GLN:CD	1:F:107:GLN:H	2.06	0.59
1:H:136:ASN:HD22	1:H:136:ASN:H	1.50	0.59
1:A:110:ILE:HD13	1:A:195:VAL:CG2	2.33	0.59
1:A:178[B]:TRP:HB2	1:A:454:GLU:CG	2.32	0.59
1:C:296:HIS:HD2	1:C:412:HIS:CE1	2.20	0.59
1:C:303:ARG:NH2	1:C:346:LEU:O	2.35	0.59
1:B:272:ASP:HA	1:B:287:THR:HG21	1.83	0.59
1:E:93:SER:HG	1:E:317:TYR:HE2	1.49	0.59
1:B:313:LYS:HD2	1:B:313:LYS:N	2.17	0.58
1:E:296:HIS:HE1	1:E:376:GLU:OE2	1.86	0.58
1:H:295:THR:CG2	1:H:418:GLY:HA3	2.33	0.58
1:B:284:VAL:O	1:B:288:LYS:HG2	2.03	0.58
1:B:136:ASN:H	1:B:136:ASN:HD22	1.50	0.58
1:H:91[A]:ARG:NH1	1:H:207[A]:ASN:HB3	2.18	0.58
1:H:178[A]:TRP:HB2	1:H:454:GLU:CG	2.32	0.58
1:F:457:ASN:OD1	3:F:521:GDU:O4'	2.20	0.58
1:F:178:TRP:HB2	1:F:454:GLU:HG3	1.85	0.58
1:H:284:VAL:O	1:H:288:LYS:HG2	2.03	0.58
1:D:313:LYS:O	1:D:314[B]:CYS:SG	2.61	0.58
1:F:92:ILE:CG2	1:F:93:SER:N	2.67	0.58
1:A:333:ASN:ND2	6:A:589:HOH:O	2.35	0.58
1:H:110:ILE:HG22	1:H:113:LEU:HD12	1.86	0.58
1:G:332:SER:HA	1:G:339:GLN:HE21	1.69	0.58
1:E:149:MET:SD	1:E:184[A]:ALA:HA	2.43	0.58
1:H:66[A]:PHE:HB2	1:H:207[A]:ASN:N	2.18	0.58
1:D:295:THR:CG2	1:D:418:GLY:HA3	2.34	0.58
1:H:175:GLN:HE22	1:H:178[A]:TRP:H	1.51	0.58
1:G:175:GLN:NE2	1:G:178:TRP:H	2.02	0.58
1:F:175:GLN:NE2	1:F:178:TRP:H	2.01	0.58
1:F:303:ARG:NH1	1:F:406:GLU:OE1	2.37	0.58
1:G:345:LYS:HA	1:G:363:LYS:O	2.04	0.58
1:C:111:SER:O	6:C:1008:HOH:O	2.17	0.58
1:H:326:TYR:CE1	1:H:327:ARG:HG2	2.39	0.57
1:G:110:ILE:HD12	1:G:110:ILE:N	2.18	0.57
1:C:110:ILE:HD12	1:C:110:ILE:H	1.68	0.57
1:A:425:GLU:N	1:A:425:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:SER:HA	1:F:339:GLN:HE21	1.69	0.57
1:E:315[B]:TRP:N	1:E:315[B]:TRP:CD2	2.73	0.57
1:C:499:ASP:OD1	6:C:575:HOH:O	2.17	0.57
1:D:149:MET:SD	1:D:184:ALA:HA	2.44	0.57
1:E:306:ARG:HD3	1:E:333:ASN:HD21	1.69	0.57
1:B:175:GLN:HE21	1:B:177[B]:ALA:H	1.51	0.57
1:F:309:ARG:NH1	1:F:402:LYS:HE3	2.19	0.57
2:F:600:FAD:C4	3:F:521:GDU:H2'	2.34	0.57
1:G:306:ARG:HD3	1:G:333:ASN:HD21	1.69	0.57
1:A:63:HIS:CE1	1:A:334:TYR:HE2	2.23	0.57
1:D:91[A]:ARG:HD3	1:D:208:ALA:HB1	1.87	0.57
1:G:272:ASP:OD2	1:G:417:HIS:HE1	1.87	0.57
1:H:327:ARG:NH2	5:H:600:FDA:H6	2.18	0.57
1:B:315[A]:TRP:CZ3	1:B:334:TYR:OH	2.57	0.57
1:H:346:LEU:HD13	1:H:408:VAL:HG11	1.87	0.57
1:E:434:LEU:HB2	1:E:435:PRO:HD3	1.86	0.57
1:H:482:ASN:ND2	6:H:651:HOH:O	2.16	0.57
1:C:105:PRO:CD	1:C:202[B]:GLY:HA2	2.34	0.57
1:E:25:ARG:HH21	1:E:28:GLN:NE2	2.03	0.57
1:H:327:ARG:NH1	3:H:521:GDU:O5'	2.36	0.57
1:H:296:HIS:HE1	1:H:376:GLU:OE2	1.88	0.57
1:H:65[A]:ILE:HD11	3:H:521:GDU:H6'2	1.87	0.57
1:A:175:GLN:NE2	1:A:177[B]:ALA:H	2.02	0.57
1:B:296:HIS:HE1	1:B:376:GLU:OE2	1.88	0.57
1:F:110:ILE:HG22	1:F:113:LEU:HD12	1.85	0.57
1:G:110:ILE:HD12	1:G:110:ILE:H	1.70	0.57
1:E:295:THR:HG22	1:E:418:GLY:HA3	1.87	0.57
1:C:110:ILE:HD13	1:C:195:VAL:CG2	2.35	0.57
1:E:178:TRP:HB2	1:E:454:GLU:HG3	1.86	0.56
1:C:315[B]:TRP:O	1:C:316:LEU:HD23	2.05	0.56
1:A:345:LYS:HE3	1:E:205:GLY:C	2.25	0.56
1:G:107:GLN:H	1:G:107:GLN:CD	2.08	0.56
1:B:295:THR:HG22	1:B:418:GLY:HA3	1.86	0.56
1:C:91[B]:ARG:HD3	1:C:207[B]:ASN:HB3	1.87	0.56
1:G:283:LEU:O	1:G:287:THR:HB	2.05	0.56
1:A:283:LEU:O	1:A:287:THR:HB	2.05	0.56
1:B:92:ILE:CG2	1:B:93:SER:N	2.69	0.56
1:C:296:HIS:CD2	1:C:412:HIS:HE1	2.21	0.56
1:A:126:ILE:HA	1:A:188[A]:LEU:HD11	1.87	0.56
1:D:204:TRP:CD1	1:D:207:ASN:HA	2.41	0.56
1:A:145:TRP:CH2	1:A:183[B]:VAL:HB	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183[B]:VAL:HG22	3:C:521:GDU:H1D	1.87	0.56
5:C:600:FDA:O2'	5:C:600:FDA:O4'	2.22	0.56
1:G:110:ILE:HD13	1:G:195:VAL:CG2	2.36	0.56
1:C:284:VAL:O	1:C:288:LYS:HG2	2.06	0.56
1:G:98:GLN:N	1:G:320:GLU:OE1	2.30	0.56
1:A:332:SER:HA	1:A:339:GLN:HE21	1.71	0.56
1:E:241:LYS:HD3	1:E:255:GLN:HG3	1.87	0.56
1:E:149:MET:HB3	1:E:150:MET:HE2	1.86	0.56
1:F:178:TRP:HB2	1:F:454:GLU:CG	2.36	0.56
1:A:332:SER:HA	1:A:339:GLN:NE2	2.19	0.56
1:G:178:TRP:HB2	1:G:454:GLU:CG	2.35	0.56
1:H:447:ARG:NH1	6:H:1293:HOH:O	2.25	0.56
1:H:187[B]:ASN:HD21	1:H:189:LYS:HB2	1.71	0.56
1:E:232:GLU:HB3	6:E:1003:HOH:O	2.06	0.56
1:H:110:ILE:HD13	1:H:195:VAL:CG2	2.36	0.56
1:B:434:LEU:HB2	1:B:435:PRO:HD3	1.87	0.56
1:G:69:TYR:CG	1:G:463:MET:HG3	2.41	0.55
1:C:346:LEU:HD13	1:C:408:VAL:HG11	1.88	0.55
1:B:134:VAL:HG22	1:C:134:VAL:HG22	1.87	0.55
1:D:345:LYS:NZ	1:D:364:GLU:OE1	2.38	0.55
1:H:91[A]:ARG:HB2	1:H:208[A]:ALA:C	2.26	0.55
1:C:91[B]:ARG:NH2	1:C:204[B]:TRP:O	2.35	0.55
1:B:178[A]:TRP:HB2	1:B:454:GLU:CG	2.36	0.55
1:A:443:TRP:HE1	1:A:471:ASN:ND2	2.04	0.55
1:B:60:VAL:HB	1:B:415:PHE:CZ	2.42	0.55
1:A:175:GLN:HE22	1:A:178[A]:TRP:H	1.54	0.55
1:H:110:ILE:HD12	1:H:110:ILE:N	2.22	0.55
1:H:443:TRP:HE1	1:H:471:ASN:HD22	1.54	0.55
1:G:192:THR:OG1	6:G:545:HOH:O	2.18	0.55
1:C:212[A]:PHE:CG	1:C:213:PRO:HD2	2.41	0.55
1:D:284:VAL:O	1:D:287:THR:HG22	2.06	0.55
1:D:303:ARG:NH1	6:D:632:HOH:O	2.18	0.55
1:H:105[A]:PRO:HB2	1:H:107:GLN:HE22	1.71	0.55
1:A:175:GLN:NE2	1:A:178[A]:TRP:HD1	2.05	0.55
1:A:110:ILE:H	1:A:110:ILE:HD12	1.72	0.55
1:C:110:ILE:HD13	1:C:195:VAL:HG23	1.87	0.55
1:D:204:TRP:CD1	1:D:207:ASN:HB2	2.41	0.55
1:D:315[B]:TRP:CD2	1:D:315[B]:TRP:N	2.74	0.55
1:A:175:GLN:HE21	1:A:177[B]:ALA:H	1.54	0.55
1:B:54:GLU:HG3	1:B:409:SER:CB	2.33	0.55
1:A:178[A]:TRP:HB2	1:A:454:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLN:HE21	1:C:178[A]:TRP:H	1.51	0.55
1:C:178[A]:TRP:HB2	1:C:454:GLU:CG	2.37	0.55
1:B:55:GLY:O	1:B:340:PRO:HD3	2.07	0.55
1:F:241:LYS:HD3	1:F:255:GLN:HG3	1.89	0.55
1:G:212:PHE:CG	1:G:213:PRO:HD2	2.41	0.54
1:H:327:ARG:HH21	5:H:600:FDA:H6	1.71	0.54
1:D:284:VAL:O	1:D:288:LYS:HG2	2.07	0.54
1:C:332:SER:HA	1:C:339:GLN:HE21	1.72	0.54
1:C:222:TRP:HE1	1:C:458:GLN:NE2	2.05	0.54
2:F:600:FAD:N1	2:F:600:FAD:H2'	2.22	0.54
1:G:180:GLY:HA2	1:G:485:ASP:OD1	2.08	0.54
1:E:65:ILE:HG12	1:E:315[B]:TRP:CZ2	2.42	0.54
1:C:184[B]:ALA:HA	1:C:204[B]:TRP:CZ2	2.42	0.54
1:D:158:PHE:CD1	1:D:319:PRO:HG3	2.41	0.54
1:E:110:ILE:HD12	1:E:110:ILE:H	1.72	0.54
1:B:367:TYR:HE1	1:B:408:VAL:HG21	1.71	0.54
1:H:182[A]:ARG:O	1:H:183[A]:VAL:O	2.26	0.54
1:C:93[A]:SER:OG	1:C:317:TYR:HE2	1.91	0.54
1:D:136:ASN:HD22	1:D:136:ASN:N	2.04	0.54
1:A:178[A]:TRP:HB2	1:A:454:GLU:HG2	1.89	0.53
1:E:313:LYS:O	1:E:314:CYS:HB3	2.07	0.53
1:E:64:VAL:CG2	1:E:458:GLN:HB2	2.38	0.53
1:D:204:TRP:O	1:D:204:TRP:CD2	2.61	0.53
1:C:104:TYR:O	1:C:106:PHE:N	2.41	0.53
1:C:207[B]:ASN:O	1:C:209[B]:THR:N	2.41	0.53
1:A:314[B]:CYS:HB2	1:A:315[B]:TRP:CE3	2.43	0.53
1:B:315[B]:TRP:HZ2	6:B:540:HOH:O	1.90	0.53
1:D:313:LYS:HB3	1:D:333:ASN:CB	2.38	0.53
1:G:303:ARG:NH2	1:G:346:LEU:O	2.31	0.53
1:E:96:ARG:NH1	6:E:1181:HOH:O	2.25	0.53
1:D:180:GLY:HA2	1:D:485:ASP:OD1	2.09	0.53
1:D:296:HIS:HE1	1:D:376:GLU:OE2	1.91	0.53
1:H:158:PHE:CD1	1:H:319:PRO:HG3	2.43	0.53
1:A:303:ARG:NH2	1:A:346:LEU:O	2.40	0.53
1:C:296:HIS:HE1	1:C:376:GLU:OE2	1.91	0.53
1:D:330:ILE:HG12	6:D:920:HOH:O	2.08	0.53
1:C:149:MET:O	1:C:186[A]:PRO:HB3	2.09	0.53
1:A:314[A]:CYS:SG	6:A:735:HOH:O	2.59	0.53
1:B:150:MET:HG2	1:B:154:ILE:HG21	1.89	0.53
1:E:212:PHE:CG	1:E:213:PRO:HD2	2.44	0.53
1:D:447:ARG:NH1	6:D:1066:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:TYR:CE1	1:E:408:VAL:HG21	2.43	0.53
1:F:303:ARG:NH1	6:F:539:HOH:O	2.37	0.53
1:H:92[A]:ILE:HG13	1:H:93[A]:SER:N	2.24	0.52
1:A:182[B]:ARG:HH12	3:A:521:GDU:H3'	1.74	0.52
1:B:178[A]:TRP:HB2	1:B:454:GLU:HG3	1.91	0.52
1:C:178[B]:TRP:HA	1:C:454:GLU:HG2	1.91	0.52
1:G:110:ILE:CD1	1:G:110:ILE:H	2.23	0.52
1:F:89:HIS:HB3	1:F:313[A]:LYS:HD2	1.90	0.52
1:B:25:ARG:HH21	1:B:28:GLN:HE22	1.58	0.52
1:D:447:ARG:NH1	6:D:1294:HOH:O	2.34	0.52
1:F:37:VAL:HG12	1:F:235:ARG:HB3	1.90	0.52
1:B:125:MET:HE3	1:B:186[A]:PRO:HB2	1.91	0.52
1:E:422:PRO:C	6:E:820:HOH:O	2.48	0.52
1:H:25:ARG:HH21	1:H:28:GLN:HE22	1.56	0.52
1:D:149:MET:HB3	1:D:150:MET:HE2	1.90	0.52
1:C:136:ASN:HD22	1:C:136:ASN:H	1.58	0.52
1:B:107:GLN:CD	1:B:107:GLN:H	2.12	0.52
1:H:149:MET:SD	1:H:184[A]:ALA:HA	2.50	0.52
1:H:67[B]:SER:HB2	1:H:72:PHE:CD2	2.45	0.52
1:C:104:TYR:CE2	1:C:204[B]:TRP:HE3	2.27	0.52
1:D:327:ARG:NH1	3:D:521:GDU:O5'	2.43	0.52
1:B:313:LYS:HG3	1:B:333:ASN:HB3	1.92	0.52
1:D:89:HIS:CG	1:D:313:LYS:HE2	2.45	0.52
1:G:162:TYR:HE2	3:G:521:GDU:H5'1	1.74	0.52
1:H:62[B]:GLY:HA2	1:H:331:PHE:CE1	2.45	0.52
1:E:65:ILE:HG12	1:E:315[B]:TRP:CH2	2.45	0.52
1:E:25:ARG:HH21	1:E:28:GLN:HE22	1.56	0.52
1:G:105:PRO:HA	6:G:797:HOH:O	2.10	0.52
1:F:122:ILE:HG13	1:H:196:ILE:HD11	1.92	0.52
1:H:299:GLY:HA3	1:H:411:TYR:HB3	1.92	0.52
1:B:182[A]:ARG:HG3	1:B:182[A]:ARG:HH11	1.74	0.52
1:B:303:ARG:NH1	6:B:828:HOH:O	2.38	0.52
1:E:136:ASN:N	1:E:136:ASN:HD22	2.02	0.52
1:H:93[A]:SER:OG	1:H:317:TYR:HE2	1.92	0.51
1:B:272:ASP:HB3	1:B:287:THR:HG23	1.92	0.51
1:B:419:TYR:HE1	2:B:600:FAD:HM73	1.75	0.51
1:D:110:ILE:HD13	1:D:195:VAL:HG22	1.92	0.51
1:H:178[B]:TRP:HB2	1:H:454:GLU:HG3	1.91	0.51
1:B:93:SER:HG	1:B:317:TYR:HE2	1.58	0.51
1:D:307:PRO:HB3	1:D:309:ARG:HE	1.75	0.51
1:D:54:GLU:HG3	1:D:409:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ILE:HD13	1:F:195:VAL:HG22	1.91	0.51
1:C:69:TYR:CG	1:C:463:MET:HG3	2.46	0.51
1:B:122:ILE:HG13	1:D:196:ILE:HD11	1.91	0.51
1:A:182[B]:ARG:NH1	3:A:521:GDU:H3'	2.25	0.51
1:B:92:ILE:HB	1:B:314:CYS:SG	2.51	0.51
1:F:92:ILE:HG22	1:F:93:SER:N	2.26	0.51
1:E:92:ILE:CG2	1:E:93:SER:N	2.73	0.51
1:C:280:ASP:O	1:C:284:VAL:HG23	2.11	0.51
1:D:296:HIS:HD2	1:D:412:HIS:CE1	2.20	0.51
1:G:162:TYR:CE2	3:G:521:GDU:H5'1	2.45	0.51
1:G:295:THR:HG23	1:G:418:GLY:HA3	1.91	0.51
1:G:284:VAL:O	1:G:288:LYS:HG2	2.11	0.51
1:A:359:SER:HB3	1:E:88:THR:HG23	1.93	0.51
1:A:298:ILE:HB	1:A:372:LEU:CD1	2.40	0.51
1:C:126:ILE:HA	1:C:188[A]:LEU:HD11	1.91	0.51
1:A:65:ILE:HD12	3:A:521:GDU:H6'2	1.92	0.51
1:E:110:ILE:HD13	1:E:195:VAL:CG2	2.40	0.51
1:D:298:ILE:HB	1:D:372:LEU:CD1	2.41	0.51
1:C:283:LEU:O	1:C:287:THR:HB	2.10	0.51
1:F:180:GLY:HA2	1:F:485:ASP:OD1	2.11	0.51
1:D:125:MET:CE	1:D:188:LEU:HA	2.40	0.51
1:C:93[A]:SER:OG	1:C:317:TYR:CE2	2.64	0.51
1:B:204:TRP:HE3	1:B:205:GLY:N	2.04	0.51
1:H:69:TYR:CD1	1:H:463:MET:HG3	2.46	0.51
1:D:110:ILE:N	1:D:110:ILE:HD12	2.27	0.50
1:G:110:ILE:HD13	1:G:195:VAL:HG23	1.94	0.50
1:C:110:ILE:N	1:C:110:ILE:HD12	2.25	0.50
1:H:315[A]:TRP:HZ3	1:H:334:TYR:HH	1.53	0.50
1:C:64[B]:VAL:HG13	1:C:210[B]:PHE:HB2	1.93	0.50
1:H:187[B]:ASN:ND2	1:H:190:ALA:H	2.08	0.50
2:B:600:FAD:C4	3:B:521:GDU:H2'	2.41	0.50
2:G:600:FAD:O4	3:G:521:GDU:H2'	2.11	0.50
1:C:110:ILE:CD1	1:C:110:ILE:H	2.20	0.50
1:B:158:PHE:CD1	1:B:319:PRO:HG3	2.46	0.50
1:B:241:LYS:HD3	1:B:255:GLN:HG3	1.91	0.50
1:B:110:ILE:HD13	1:B:195:VAL:CG2	2.41	0.50
1:F:110:ILE:HD12	1:F:110:ILE:N	2.26	0.50
1:C:199:LYS:HG2	1:C:200:THR:N	2.26	0.50
1:A:145:TRP:HH2	1:A:183[B]:VAL:HB	1.77	0.50
1:D:457:ASN:OD1	3:D:521:GDU:O3'	2.19	0.50
1:H:158:PHE:HD1	1:H:319:PRO:HG3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PHE:HD1	1:B:319:PRO:HG3	1.77	0.50
1:A:310:ILE:O	1:A:313:LYS:HG3	2.12	0.50
1:B:111:SER:HB2	6:B:538:HOH:O	2.11	0.50
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.47	0.50
1:G:25:ARG:HD3	1:G:470:ASP:OD1	2.10	0.50
1:G:309:ARG:NH1	1:G:402:LYS:HG3	2.27	0.50
1:H:14:GLY:O	1:H:19:GLY:HA3	2.10	0.50
1:E:447:ARG:NH1	6:E:601:HOH:O	2.39	0.50
1:B:175:GLN:NE2	1:B:177[B]:ALA:H	2.09	0.50
1:H:283:LEU:O	1:H:287:THR:HB	2.12	0.50
1:A:284:VAL:O	1:A:288:LYS:HG3	2.12	0.50
1:D:332:SER:HA	1:D:339:GLN:HE21	1.77	0.50
1:H:64[A]:VAL:HG22	1:H:458:GLN:HB2	1.92	0.49
1:B:457:ASN:OD1	3:B:521:GDU:O3'	2.20	0.49
1:A:110:ILE:CD1	1:A:110:ILE:H	2.24	0.49
1:A:150:MET:SD	1:A:186[B]:PRO:HG3	2.52	0.49
1:H:162:TYR:CZ	1:H:166:VAL:HG21	2.47	0.49
1:A:51:VAL:HG22	1:A:57:LEU:HG	1.94	0.49
1:E:422:PRO:HA	1:E:426:ARG:HD3	1.94	0.49
1:H:310:ILE:O	1:H:313:LYS:HG3	2.11	0.49
1:A:162:TYR:HE2	3:A:521:GDU:H3D	1.77	0.49
1:A:346:LEU:HD13	1:A:408:VAL:HG11	1.93	0.49
1:A:434:LEU:HB2	1:A:435:PRO:HD3	1.93	0.49
1:E:46:LEU:O	1:E:61:GLY:HA3	2.12	0.49
1:F:158:PHE:CD1	1:F:319:PRO:HG3	2.47	0.49
1:C:89:HIS:HB2	1:C:210[A]:PHE:CE2	2.47	0.49
1:B:93:SER:OG	1:B:317:TYR:HE2	1.95	0.49
1:D:212:PHE:CG	1:D:213:PRO:HD2	2.48	0.49
1:D:159:MET:HE1	3:D:521:GDU:O2	2.13	0.49
1:G:159:MET:HE1	3:G:521:GDU:O2	2.12	0.49
1:E:327:ARG:NH1	3:E:521:GDU:O5'	2.44	0.49
1:A:136:ASN:HD22	1:A:136:ASN:N	1.98	0.49
1:B:348:THR:N	6:B:828:HOH:O	2.45	0.49
1:A:348:THR:N	6:A:631:HOH:O	2.45	0.49
1:F:510:GLN:HE21	1:F:510:GLN:CA	2.26	0.49
1:H:105[A]:PRO:HB2	1:H:107:GLN:NE2	2.28	0.49
1:F:346:LEU:HD13	1:F:408:VAL:HG11	1.94	0.49
1:G:149:MET:HB3	1:G:150:MET:HE2	1.94	0.49
1:H:59[A]:ASP:C	1:H:61[A]:GLY:H	2.16	0.49
1:C:91[B]:ARG:HH11	1:C:207[B]:ASN:HB2	1.78	0.49
1:C:504:PHE:CD2	1:D:32:PRO:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:HIS:ND1	1:E:313:LYS:HE3	2.28	0.48
1:A:110:ILE:N	1:A:110:ILE:HD12	2.28	0.48
1:D:212:PHE:CD2	1:D:213:PRO:HD2	2.48	0.48
1:B:63:HIS:NE2	1:B:315[A]:TRP:CZ3	2.81	0.48
1:C:63[B]:HIS:HE1	5:C:600:FDA:O2'	1.96	0.48
1:F:110:ILE:H	1:F:110:ILE:CD1	2.21	0.48
1:B:272:ASP:N	1:B:272:ASP:OD1	2.46	0.48
1:A:455:VAL:CG1	1:A:460:HIS:HB3	2.36	0.48
1:B:136:ASN:HD22	1:B:136:ASN:N	2.08	0.48
1:C:314:CYS:O	1:C:329:THR:HA	2.12	0.48
1:B:56:PHE:CD1	1:B:339:GLN:HB3	2.48	0.48
2:G:600:FAD:N1	2:G:600:FAD:H2'	2.28	0.48
1:G:13:ILE:HG21	1:G:269:MET:HE3	1.94	0.48
1:H:425:GLU:OE2	1:H:425:GLU:N	2.45	0.48
1:C:125:MET:HE3	1:C:186[A]:PRO:HB2	1.95	0.48
1:G:181:GLU:HG3	1:G:485:ASP:OD2	2.14	0.48
1:H:60[B]:VAL:HG12	1:H:60[B]:VAL:O	2.14	0.48
1:A:92:ILE:HG23	1:A:93:SER:N	2.28	0.48
1:E:110:ILE:H	1:E:110:ILE:CD1	2.25	0.48
1:B:272:ASP:HB3	1:B:287:THR:CG2	2.44	0.48
1:H:295:THR:HB	6:H:1288:HOH:O	2.13	0.48
1:H:150:MET:HG2	1:H:154:ILE:HG21	1.95	0.48
1:G:136:ASN:H	1:G:136:ASN:HD22	1.61	0.48
1:B:182[B]:ARG:HH12	3:B:521:GDU:H4'	1.78	0.48
1:C:175:GLN:NE2	1:C:178[A]:TRP:N	2.57	0.48
1:D:69:TYR:CG	1:D:463:MET:HG3	2.47	0.48
1:B:212:PHE:CG	1:B:213:PRO:HD2	2.49	0.48
1:B:25:ARG:HH21	1:B:28:GLN:NE2	2.12	0.48
1:B:150:MET:HB3	1:B:154:ILE:HB	1.95	0.48
1:G:212:PHE:CD2	1:G:213:PRO:HD2	2.48	0.48
1:E:51:VAL:HG13	1:E:57:LEU:HD12	1.95	0.48
1:C:13:ILE:HG21	1:C:269:MET:HE3	1.96	0.48
1:C:447:ARG:NH1	6:C:995:HOH:O	2.20	0.48
1:F:107:GLN:O	1:F:110:ILE:HD11	2.14	0.48
1:H:51:VAL:HG13	1:H:57:LEU:HD12	1.96	0.48
1:G:314:CYS:HB3	1:G:315[B]:TRP:CE3	2.49	0.48
1:A:92:ILE:HG23	1:A:93:SER:H	1.78	0.48
1:H:150:MET:HE3	1:H:159:MET:HG3	1.95	0.48
1:G:63:HIS:NE2	1:G:315[B]:TRP:CZ3	2.82	0.48
1:F:212:PHE:CG	1:F:213:PRO:HD2	2.48	0.48
1:B:303:ARG:NH2	6:B:828:HOH:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:521:GDU:O2A	3:G:521:GDU:H5'	2.14	0.47
1:H:69:TYR:CG	1:H:463:MET:HG3	2.49	0.47
1:E:159:MET:HE3	1:E:183[B]:VAL:CG1	2.44	0.47
1:E:346:LEU:HD13	1:E:408:VAL:CG1	2.44	0.47
1:B:180[A]:GLY:HA2	1:B:485:ASP:OD1	2.14	0.47
1:C:51:VAL:HG22	1:C:57:LEU:HG	1.96	0.47
1:A:159:MET:HE3	1:A:183[B]:VAL:CG1	2.44	0.47
1:G:447:ARG:NH1	6:G:534:HOH:O	2.33	0.47
1:F:419:TYR:HE1	2:F:600:FAD:HM73	1.78	0.47
1:D:56:PHE:CD1	1:D:339:GLN:HB3	2.49	0.47
1:G:315[B]:TRP:HZ3	1:G:334:TYR:HH	1.61	0.47
1:G:310:ILE:CG2	1:G:330:ILE:HG13	2.44	0.47
1:H:66[A]:PHE:CD2	1:H:206[A]:PRO:HB2	2.48	0.47
1:H:66[A]:PHE:HB2	1:H:207[A]:ASN:CA	2.44	0.47
1:C:178[A]:TRP:O	1:C:454:GLU:HG2	2.15	0.47
1:A:54:GLU:HG3	1:A:409:SER:CB	2.45	0.47
1:A:105:PRO:HA	4:A:522:CL:CL	2.51	0.47
1:B:150:MET:HG2	1:B:154:ILE:CG2	2.45	0.47
1:B:280:ASP:O	1:B:284:VAL:HG23	2.15	0.47
1:D:125:MET:HG3	1:D:150:MET:O	2.15	0.47
1:E:110:ILE:N	1:E:110:ILE:HD12	2.30	0.47
1:C:105:PRO:CG	1:C:202[B]:GLY:HA2	2.45	0.47
1:H:98:GLN:N	1:H:320:GLU:OE1	2.33	0.47
1:H:272:ASP:OD2	1:H:417:HIS:HE1	1.98	0.47
1:E:108:ASN:HB3	1:E:194:ASN:ND2	2.30	0.47
1:E:315[A]:TRP:NE1	3:E:521:GDU:H6'1	2.29	0.47
1:E:125:MET:CE	1:E:186[A]:PRO:HB2	2.45	0.47
1:D:376:GLU:HB2	1:D:382:VAL:HG13	1.97	0.47
1:F:312[A]:ASP:HB2	1:F:313[A]:LYS:NZ	2.29	0.47
1:C:107:GLN:O	1:C:110:ILE:HD11	2.14	0.47
1:C:150:MET:HG2	1:C:154:ILE:HG21	1.96	0.47
1:F:187[B]:ASN:ND2	1:F:190:ALA:H	2.13	0.47
1:G:175:GLN:HE22	1:G:177:ALA:HB3	1.79	0.47
1:C:303:ARG:NH1	6:C:634:HOH:O	2.26	0.47
1:D:315[B]:TRP:CE3	1:D:315[B]:TRP:N	2.83	0.47
1:B:69:TYR:CG	1:B:463:MET:HG3	2.50	0.47
1:E:245:VAL:HG22	1:E:252:VAL:HG22	1.95	0.47
1:E:423:THR:C	6:E:820:HOH:O	2.53	0.47
1:C:94[B]:TYR:CE2	1:C:313:LYS:HE3	2.50	0.47
1:F:136:ASN:ND2	1:F:137:THR:HG23	2.29	0.47
1:A:60:VAL:HB	1:A:415:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:VAL:HG13	1:G:170:PRO:HD2	1.97	0.47
1:F:272:ASP:OD2	1:F:417:HIS:HE1	1.98	0.47
1:E:158:PHE:CD1	1:E:319:PRO:HG3	2.49	0.47
1:H:457:ASN:CG	3:H:521:GDU:HO3A	2.12	0.47
1:A:296:HIS:CE1	1:A:382:VAL:HG21	2.49	0.47
2:F:600:FAD:H9	2:F:600:FAD:H1'1	1.49	0.47
1:E:28:GLN:HE22	1:E:71:TYR:HE2	1.62	0.47
1:H:125:MET:HE1	1:H:188:LEU:HA	1.97	0.47
1:C:104:TYR:HH	1:C:204[B]:TRP:HZ3	1.60	0.46
1:D:338:ASN:C	1:D:339:GLN:HG3	2.36	0.46
1:H:348:THR:O	1:H:357:PRO:HG3	2.15	0.46
1:G:54:GLU:HG2	1:G:409:SER:OG	2.16	0.46
1:A:178[B]:TRP:HA	1:A:454:GLU:HG2	1.97	0.46
1:H:110:ILE:HD13	1:H:195:VAL:HG23	1.96	0.46
1:A:158:PHE:CD1	1:A:319:PRO:HG3	2.51	0.46
1:D:100:GLN:HG2	1:D:112:MET:HB3	1.98	0.46
1:A:69:TYR:CG	1:A:463:MET:HG3	2.50	0.46
1:D:245:VAL:HG22	1:D:252:VAL:HG22	1.97	0.46
1:D:434:LEU:HB2	1:D:435:PRO:HD3	1.96	0.46
1:B:182[B]:ARG:NH1	3:B:521:GDU:H4'	2.30	0.46
1:B:315[A]:TRP:HZ3	1:B:334:TYR:OH	1.97	0.46
1:A:419:TYR:HE1	2:A:600:FAD:HM73	1.81	0.46
1:A:306:ARG:CD	1:A:333:ASN:HD21	2.27	0.46
1:C:296:HIS:CE1	1:C:382:VAL:HG21	2.50	0.46
1:C:162:TYR:CZ	1:C:166:VAL:HG21	2.51	0.46
2:A:600:FAD:H1'1	2:A:600:FAD:H9	1.53	0.46
1:C:346:LEU:HD13	1:C:408:VAL:CG1	2.45	0.46
1:C:48:SER:O	1:C:60[A]:VAL:HG22	2.15	0.46
1:F:313[A]:LYS:HG3	1:F:333:ASN:HB3	1.97	0.46
1:E:110:ILE:HD13	1:E:195:VAL:HG23	1.97	0.46
1:H:93[A]:SER:HB3	1:H:104[A]:TYR:CB	2.46	0.46
1:E:65:ILE:HD13	3:E:521:GDU:C6'	2.45	0.46
1:A:65:ILE:HD13	1:A:315[B]:TRP:CZ2	2.51	0.46
1:C:303:ARG:NH2	6:C:634:HOH:O	2.41	0.46
1:D:348:THR:N	6:D:632:HOH:O	2.49	0.46
1:A:303:ARG:NH1	6:A:631:HOH:O	2.18	0.46
1:G:149:MET:SD	1:G:184:ALA:HA	2.55	0.46
1:E:372:LEU:HD23	1:E:395:LEU:HD21	1.98	0.46
1:B:326:TYR:CE1	1:B:327:ARG:HG2	2.51	0.46
1:E:302:VAL:HG12	1:E:407:ILE:HA	1.97	0.46
1:E:263:LYS:O	1:E:264:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:327:ARG:HH22	5:H:600:FDA:HN5	1.64	0.46
1:G:434:LEU:HB2	1:G:435:PRO:HD3	1.98	0.46
1:E:69:TYR:CG	1:E:463:MET:HG3	2.51	0.46
1:H:28:GLN:HE22	1:H:71:TYR:HE2	1.63	0.46
1:E:332:SER:HA	1:E:339:GLN:HE21	1.81	0.46
1:D:302:VAL:CG2	1:D:368:TRP:CE2	2.99	0.46
1:H:91[A]:ARG:NH2	1:H:204[A]:TRP:O	2.45	0.46
1:H:90[A]:GLN:HG3	1:H:91[A]:ARG:N	2.30	0.46
1:H:178[A]:TRP:HB2	1:H:454:GLU:HG3	1.96	0.46
1:D:91[B]:ARG:HD2	1:D:91[B]:ARG:C	2.35	0.46
1:A:345:LYS:HA	1:A:363:LYS:O	2.15	0.46
1:D:346:LEU:HD13	1:D:408:VAL:HG11	1.97	0.46
1:G:313:LYS:HB3	1:G:316:LEU:HD21	1.97	0.46
1:H:66[A]:PHE:HB2	1:H:207[A]:ASN:H	1.80	0.45
1:H:90[A]:GLN:HG3	1:H:91[A]:ARG:H	1.81	0.45
1:E:159:MET:HE3	1:E:183[B]:VAL:HG13	1.97	0.45
1:E:145:TRP:CH2	1:E:183[B]:VAL:HB	2.51	0.45
1:E:296:HIS:CE1	1:E:376:GLU:OE2	2.67	0.45
1:F:314[B]:CYS:O	1:F:329:THR:HA	2.16	0.45
1:G:284:VAL:O	1:G:287:THR:HG22	2.15	0.45
1:H:332:SER:HA	1:H:339:GLN:HE21	1.82	0.45
1:H:65[A]:ILE:HB	1:H:207[A]:ASN:ND2	2.31	0.45
1:C:64[A]:VAL:CG2	1:C:458:GLN:HB2	2.46	0.45
2:D:600:FAD:H1'1	2:D:600:FAD:H9	1.57	0.45
1:H:306:ARG:HD3	1:H:333:ASN:HD21	1.81	0.45
1:B:18:THR:OG1	1:B:461:SER:HB3	2.16	0.45
1:E:199:LYS:HD2	1:E:199:LYS:C	2.36	0.45
1:F:296:HIS:HE1	1:F:376:GLU:OE2	2.00	0.45
1:G:25:ARG:HH21	1:G:28:GLN:HE22	1.65	0.45
2:B:600:FAD:H1'1	2:B:600:FAD:H9	1.53	0.45
1:D:307:PRO:CB	1:D:309:ARG:HE	2.29	0.45
1:H:62[B]:GLY:HA2	1:H:331:PHE:HE1	1.81	0.45
1:C:178[A]:TRP:HB2	1:C:454:GLU:HG3	1.98	0.45
1:G:244:LYS:HB3	1:G:253:THR:HB	1.97	0.45
1:E:310:ILE:HG23	1:E:330:ILE:HG13	1.98	0.45
1:B:330:ILE:HB	1:B:333:ASN:HD22	1.82	0.45
1:F:306:ARG:HH12	1:F:312[A]:ASP:HB3	1.81	0.45
1:F:443:TRP:HE1	1:F:471:ASN:HD22	1.65	0.45
1:G:440:LYS:O	1:G:441:ASP:HB2	2.16	0.45
1:H:434:LEU:HB2	1:H:435:PRO:HD3	1.98	0.45
1:G:114:PRO:O	1:G:118:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:GLU:O	1:G:148:ARG:HG3	2.17	0.45
1:E:93:SER:OG	1:E:317:TYR:HE2	1.99	0.45
1:F:367:TYR:HE1	1:F:408:VAL:HG21	1.81	0.45
1:C:124:GLY:HA3	6:C:657:HOH:O	2.16	0.45
5:H:600:FDA:H1'1	5:H:600:FDA:H9	1.44	0.45
1:E:310:ILE:HG22	1:E:311:GLY:N	2.31	0.45
1:F:303:ARG:NH2	6:F:539:HOH:O	2.27	0.45
1:C:60[B]:VAL:HG13	1:C:415:PHE:CE2	2.52	0.45
1:E:157:LEU:HD23	1:E:157:LEU:HA	1.75	0.45
1:H:65[A]:ILE:HD13	1:H:315[A]:TRP:CZ2	2.52	0.45
1:B:418:GLY:O	2:B:600:FAD:HM83	2.17	0.45
1:C:13:ILE:HG21	1:C:269:MET:CE	2.46	0.45
1:C:175:GLN:HE21	1:C:178[A]:TRP:HD1	1.64	0.45
1:A:458:GLN:HG3	2:A:600:FAD:H2'	1.99	0.45
1:H:136:ASN:N	1:H:136:ASN:HD22	2.14	0.45
1:E:284:VAL:O	1:E:288:LYS:HG2	2.17	0.45
1:A:25:ARG:HH21	1:A:28:GLN:NE2	2.14	0.45
1:A:221:ILE:O	1:A:225:VAL:HG23	2.16	0.45
1:E:122:ILE:O	1:E:126:ILE:HG13	2.16	0.44
1:E:149:MET:HG3	1:E:186[B]:PRO:HD2	1.98	0.44
1:C:59[A]:ASP:C	1:C:61[A]:GLY:N	2.70	0.44
1:C:107:GLN:H	1:C:107:GLN:CD	2.20	0.44
1:G:175:GLN:NE2	1:G:177:ALA:HB3	2.33	0.44
1:F:263:LYS:NZ	6:F:529:HOH:O	2.49	0.44
1:B:14:GLY:O	1:B:19:GLY:HA3	2.17	0.44
1:A:180[A]:GLY:HA2	1:A:485:ASP:OD1	2.17	0.44
1:F:130:LEU:HD23	1:H:130:LEU:HD23	1.98	0.44
1:A:134:VAL:O	1:A:134:VAL:CG1	2.65	0.44
1:A:145:TRP:CE3	1:A:179[B]:LEU:HD22	2.52	0.44
1:D:296:HIS:CE1	1:D:382:VAL:HG21	2.52	0.44
1:H:197:LEU:HD23	1:H:199[A]:LYS:HD3	1.98	0.44
1:E:212:PHE:CD2	1:E:213:PRO:HD2	2.53	0.44
1:A:28:GLN:HE22	1:A:71:TYR:HE2	1.66	0.44
1:B:46:LEU:O	1:B:61:GLY:HA3	2.17	0.44
1:F:108:ASN:HD22	1:F:108:ASN:N	2.13	0.44
1:E:65:ILE:HD13	3:E:521:GDU:O6'	2.17	0.44
1:F:110:ILE:HD11	1:F:191:VAL:HG13	1.98	0.44
1:F:13:ILE:HG21	1:F:269:MET:CE	2.47	0.44
1:B:125:MET:HE2	1:B:188[B]:LEU:HA	1.99	0.44
1:A:310:ILE:O	1:A:313:LYS:HE2	2.17	0.44
1:H:91[A]:ARG:CD	1:H:207[A]:ASN:OD1	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:ILE:HD11	1:H:191:VAL:HG13	1.99	0.44
1:G:110:ILE:CG2	1:G:113:LEU:HD12	2.46	0.44
1:C:110:ILE:CD1	1:C:191:VAL:HG13	2.45	0.44
1:G:64:VAL:CG2	1:G:458:GLN:HB2	2.47	0.44
1:A:196:ILE:HD11	1:C:122:ILE:HG13	1.99	0.44
1:E:37:VAL:HG12	1:E:235:ARG:HB3	1.98	0.44
1:A:175:GLN:HE21	1:A:178[A]:TRP:HD1	1.65	0.44
2:A:600:FAD:O4	3:A:521:GDU:H2'	2.16	0.44
1:B:25:ARG:HG2	1:B:469:VAL:CG1	2.47	0.44
1:D:302:VAL:HG21	1:D:368:TRP:CE2	2.53	0.44
1:D:388:LEU:HB2	6:D:928:HOH:O	2.16	0.44
1:C:246:ASN:HD21	1:C:249:ASN:HD21	1.64	0.44
1:E:107:GLN:H	1:E:107:GLN:CD	2.20	0.44
1:A:91:ARG:HG3	1:A:208:ALA:C	2.38	0.44
1:C:207[B]:ASN:O	1:C:208[B]:ALA:C	2.56	0.44
1:H:284:VAL:O	1:H:287:THR:HG22	2.18	0.44
1:B:96:ARG:HB2	1:B:101:TRP:CZ3	2.53	0.44
1:H:455:VAL:HG13	1:H:484:PRO:HB3	2.00	0.44
1:H:315[B]:TRP:O	1:H:316:LEU:HD23	2.18	0.44
1:E:307:PRO:O	1:E:310:ILE:HB	2.17	0.44
1:H:295:THR:HG23	1:H:418:GLY:HA3	2.00	0.44
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.53	0.44
1:H:302:VAL:HG21	1:H:368:TRP:CE2	2.53	0.44
1:G:92:ILE:CG2	1:G:93:SER:N	2.80	0.44
1:A:110:ILE:HD11	1:A:191:VAL:HG13	2.00	0.43
1:F:136:ASN:N	1:F:136:ASN:HD22	2.06	0.43
2:F:600:FAD:O2'	2:F:600:FAD:O4'	2.32	0.43
1:G:315[A]:TRP:HA	1:G:315[A]:TRP:CE3	2.52	0.43
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.53	0.43
1:C:169:VAL:HG13	1:C:170:PRO:HD2	1.99	0.43
1:A:163:ASN:OD1	3:A:521:GDU:O3D	2.17	0.43
1:F:118:GLN:O	1:F:122:ILE:HG12	2.17	0.43
1:B:181[A]:GLU:HG2	1:B:485:ASP:OD2	2.18	0.43
1:C:14:GLY:O	1:C:19:GLY:HA3	2.18	0.43
1:C:425:GLU:OE2	1:C:425:GLU:N	2.52	0.43
1:E:383:ASN:O	1:E:387:ILE:HB	2.17	0.43
1:A:212:PHE:CG	1:A:213:PRO:HD2	2.54	0.43
1:D:14:GLY:O	1:D:19:GLY:HA3	2.18	0.43
1:B:64:VAL:CG2	1:B:458:GLN:HB2	2.48	0.43
1:E:32:PRO:HB3	1:F:504:PHE:CD2	2.54	0.43
1:B:149:MET:HB3	1:B:150:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ASP:OD1	1:H:272:ASP:N	2.52	0.43
1:B:51:VAL:HG22	1:B:57:LEU:HG	2.01	0.43
1:H:314:CYS:O	1:H:329:THR:HA	2.19	0.43
1:C:91[B]:ARG:NH1	1:C:207[B]:ASN:HB2	2.33	0.43
1:A:146:ILE:HD13	1:A:159:MET:HB3	2.01	0.43
1:A:65:ILE:CD1	3:A:521:GDU:H6'2	2.47	0.43
1:C:56:PHE:CD1	1:C:339:GLN:HB3	2.52	0.43
1:G:64:VAL:HG23	1:G:458:GLN:HB2	2.00	0.43
1:F:144:GLU:O	1:F:148:ARG:HG3	2.19	0.43
1:E:139:PRO:HG3	1:E:148:ARG:HD2	1.99	0.43
1:A:255:GLN:CA	1:A:255:GLN:HE21	2.31	0.43
1:E:334:TYR:CD1	1:E:334:TYR:N	2.86	0.43
1:A:455:VAL:HG11	1:A:480:THR:CG2	2.46	0.43
1:B:315[A]:TRP:CD2	1:B:315[A]:TRP:N	2.84	0.43
1:B:110:ILE:N	1:B:110:ILE:HD12	2.34	0.43
1:F:313[A]:LYS:O	1:F:314[A]:CYS:CB	2.66	0.43
1:G:56:PHE:CD1	1:G:339:GLN:HB3	2.53	0.43
1:E:25:ARG:HD3	1:E:470:ASP:OD1	2.17	0.43
1:C:93[A]:SER:HB3	1:C:104:TYR:CB	2.47	0.43
1:C:183[B]:VAL:HG13	3:C:521:GDU:O2	2.18	0.43
1:A:169:VAL:HG13	1:A:170:PRO:HD2	1.99	0.43
1:E:114:PRO:O	1:E:118:GLN:HG3	2.19	0.43
1:H:212:PHE:CG	1:H:213:PRO:HD2	2.52	0.43
1:F:345:LYS:HA	1:F:363:LYS:O	2.18	0.43
2:E:600:FAD:H5'1	2:E:600:FAD:PA	2.59	0.43
1:C:66[A]:PHE:HB2	1:C:91[A]:ARG:NH1	2.34	0.43
1:A:338:ASN:HB2	1:A:339:GLN:NE2	2.33	0.43
1:D:298:ILE:HB	1:D:372:LEU:HD11	2.01	0.43
1:C:325:PHE:CD2	1:C:372:LEU:HD23	2.53	0.43
1:H:61[B]:GLY:O	1:H:62[B]:GLY:C	2.57	0.43
1:C:59[A]:ASP:O	1:C:61[A]:GLY:N	2.49	0.43
1:G:280:ASP:O	1:G:284:VAL:HG23	2.19	0.43
1:C:372:LEU:HD11	1:C:395:LEU:HD21	2.00	0.43
1:F:69:TYR:CD1	1:F:463:MET:HG3	2.54	0.43
1:E:315[A]:TRP:O	1:E:316:LEU:HD23	2.19	0.43
1:D:306:ARG:CD	1:D:333:ASN:HD21	2.30	0.43
1:B:110:ILE:H	1:B:110:ILE:HD12	1.82	0.43
1:G:338:ASN:C	1:G:339:GLN:HG3	2.39	0.43
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.54	0.43
1:C:98:GLN:HE22	1:C:114:PRO:HG2	1.83	0.43
1:B:388:LEU:O	1:B:392:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ILE:O	1:F:225:VAL:HG23	2.19	0.43
1:H:183[B]:VAL:HG13	3:H:521:GDU:O2	2.19	0.42
1:A:145:TRP:CZ2	1:A:179[B]:LEU:HD13	2.53	0.42
1:H:346:LEU:HD13	1:H:408:VAL:CG1	2.48	0.42
1:F:150:MET:SD	1:F:186[B]:PRO:HG3	2.59	0.42
1:C:303:ARG:NH1	1:C:406:GLU:OE1	2.52	0.42
1:D:204:TRP:O	1:D:204:TRP:CE3	2.72	0.42
1:E:79:ALA:O	1:E:80:LEU:HD12	2.19	0.42
1:G:298:ILE:HB	1:G:372:LEU:CD1	2.49	0.42
1:A:299:GLY:HA3	1:A:411:TYR:HB3	2.02	0.42
1:G:82:LYS:O	1:G:85:ASP:HB2	2.19	0.42
1:E:14:GLY:O	1:E:19:GLY:HA3	2.19	0.42
1:E:306:ARG:CD	1:E:333:ASN:HD21	2.31	0.42
1:F:101:TRP:CH2	1:F:316[B]:LEU:HD13	2.54	0.42
1:E:158:PHE:HD1	1:E:319:PRO:HG3	1.83	0.42
1:A:14:GLY:O	1:A:19:GLY:HA3	2.19	0.42
1:E:429:ALA:O	1:E:433:ILE:HG13	2.20	0.42
1:B:79:ALA:O	1:B:80:LEU:HD12	2.18	0.42
1:H:65[A]:ILE:HG22	1:H:210:PHE:HB3	2.02	0.42
1:H:307:PRO:CG	1:H:310:ILE:HD13	2.48	0.42
1:A:338:ASN:HB2	1:A:339:GLN:HE21	1.84	0.42
1:D:315[B]:TRP:HZ3	1:D:334:TYR:HH	1.66	0.42
1:G:136:ASN:ND2	1:G:137:THR:HG23	2.33	0.42
1:C:298:ILE:HB	1:C:372:LEU:HB2	2.01	0.42
1:C:158:PHE:CD1	1:C:319:PRO:HG3	2.54	0.42
1:G:139:PRO:HB2	1:G:176:CYS:SG	2.59	0.42
1:B:37:VAL:HG12	1:B:235:ARG:HB3	2.01	0.42
1:E:175:GLN:NE2	1:E:177:ALA:HB3	2.34	0.42
1:C:61[B]:GLY:O	1:C:315[B]:TRP:HH2	2.02	0.42
1:C:165:LYS:O	1:C:375:SER:OG	2.31	0.42
1:G:197:LEU:HD12	1:G:197:LEU:HA	1.82	0.42
1:H:48:SER:O	1:H:60[A]:VAL:HG22	2.19	0.42
1:F:182:ARG:HB2	1:F:182:ARG:CZ	2.49	0.42
1:C:293:SER:OG	6:C:1244:HOH:O	2.21	0.42
1:E:278:MET:O	1:E:279:ASN:HB2	2.19	0.42
1:H:93[A]:SER:HB3	1:H:104[A]:TYR:HB2	2.01	0.42
1:E:162:TYR:HE2	3:E:521:GDU:H2D	1.84	0.42
1:D:346:LEU:HD13	1:D:408:VAL:CG1	2.50	0.42
1:D:166:VAL:HG22	1:D:326:TYR:CD1	2.54	0.42
1:E:125:MET:HE2	1:E:186[A]:PRO:HB2	2.02	0.42
1:A:92:ILE:C	1:A:314[B]:CYS:HG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HD12	6:B:538:HOH:O	2.19	0.42
1:E:346:LEU:HD12	1:E:367:TYR:CZ	2.55	0.42
1:B:56:PHE:CE1	1:B:339:GLN:HB3	2.55	0.42
1:C:67[B]:SER:HB2	1:C:72:PHE:CD2	2.54	0.42
1:C:306:ARG:HH11	1:C:333:ASN:HD21	1.66	0.42
1:A:116:GLU:OE1	1:A:116:GLU:N	2.43	0.42
1:H:91[A]:ARG:HD3	1:H:207[A]:ASN:CG	2.39	0.42
1:H:110:ILE:CD1	1:H:110:ILE:H	2.20	0.42
1:H:443:TRP:HE1	1:H:471:ASN:ND2	2.16	0.42
1:C:136:ASN:ND2	1:C:137:THR:HG23	2.35	0.42
1:D:102:VAL:HA	1:D:103:PRO:HD3	1.82	0.42
1:C:136:ASN:HD22	1:C:136:ASN:N	2.17	0.42
1:B:212:PHE:CD2	1:B:213:PRO:HD2	2.55	0.42
1:E:334:TYR:N	1:E:334:TYR:HD1	2.18	0.42
1:C:434:LEU:HB2	1:C:435:PRO:HD3	2.01	0.42
1:F:212:PHE:CD2	1:F:213:PRO:HD2	2.55	0.42
1:H:56:PHE:CD1	1:H:339:GLN:HB3	2.55	0.42
1:F:139:PRO:HG3	1:F:148:ARG:HD2	2.02	0.42
1:F:323:CYS:HA	1:F:324:PRO:HD3	1.90	0.42
1:B:499:ASP:OD1	6:B:1251:HOH:O	2.21	0.42
1:H:315[A]:TRP:CZ3	1:H:334:TYR:OH	2.66	0.41
1:H:91[A]:ARG:HE	1:H:91[A]:ARG:HB3	1.55	0.41
1:D:175:GLN:HE21	1:D:178:TRP:HD1	1.67	0.41
1:F:306:ARG:HG3	1:F:333:ASN:HD21	1.85	0.41
1:D:431:THR:O	1:D:435:PRO:HG2	2.20	0.41
1:C:46:LEU:O	1:C:60[A]:VAL:HG23	2.19	0.41
1:F:196:ILE:HD11	1:H:122:ILE:HG13	2.02	0.41
1:H:182[B]:ARG:HH12	3:H:521:GDU:H3'	1.85	0.41
1:C:64[B]:VAL:HG13	1:C:210[B]:PHE:CB	2.50	0.41
1:A:110:ILE:HD13	1:A:195:VAL:HG22	2.01	0.41
1:H:96:ARG:O	1:H:319:PRO:HD2	2.20	0.41
1:H:46:LEU:O	1:H:60[A]:VAL:HG23	2.20	0.41
1:G:241:LYS:HD3	1:G:255:GLN:HG3	2.02	0.41
1:H:20:LEU:O	1:H:24:LYS:HG2	2.20	0.41
1:F:157:LEU:HD23	1:F:157:LEU:HA	1.91	0.41
1:B:65:ILE:HG21	1:B:91[B]:ARG:HD3	2.01	0.41
1:C:175:GLN:HE22	1:C:178[A]:TRP:H	1.66	0.41
1:D:175:GLN:HE22	1:D:178:TRP:H	1.67	0.41
1:C:367:TYR:HE1	1:C:408:VAL:HG21	1.86	0.41
1:A:158:PHE:HD1	1:A:319:PRO:HG3	1.85	0.41
1:F:69:TYR:CG	1:F:463:MET:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ALA:C	1:D:80:LEU:HD12	2.40	0.41
1:E:197:LEU:HA	1:E:197:LEU:HD12	1.79	0.41
1:H:92[A]:ILE:HG13	1:H:93[A]:SER:H	1.83	0.41
1:B:110:ILE:HD13	1:B:195:VAL:HG23	2.02	0.41
1:H:160:ARG:N	1:H:161:PRO:HD2	2.36	0.41
1:E:122:ILE:HG13	1:G:196:ILE:HD11	2.02	0.41
1:G:419:TYR:HE1	2:G:600:FAD:HM73	1.85	0.41
1:F:175:GLN:HE21	1:F:178:TRP:HD1	1.68	0.41
1:D:307:PRO:HD2	1:D:310:ILE:HD12	2.02	0.41
1:B:157:LEU:HA	1:B:157:LEU:HD23	1.82	0.41
1:C:180[A]:GLY:HA2	1:C:485:ASP:OD1	2.21	0.41
1:F:296:HIS:CD2	1:F:412:HIS:CE1	2.92	0.41
1:C:64[B]:VAL:HG13	1:C:210[B]:PHE:CG	2.56	0.41
1:H:187[B]:ASN:HD22	1:H:190:ALA:H	1.68	0.41
1:F:28:GLN:HE22	1:F:71:TYR:HE2	1.67	0.41
1:H:87:TYR:CE2	1:H:336:PRO:HD2	2.55	0.41
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.93	0.41
1:H:107:GLN:HB2	1:H:107:GLN:HE21	1.71	0.41
1:H:315[A]:TRP:CE3	1:H:334:TYR:OH	2.74	0.41
1:D:204:TRP:O	1:D:204:TRP:CG	2.74	0.41
1:D:315[B]:TRP:HD1	1:D:317:TYR:HH	1.65	0.41
1:B:332:SER:HA	1:B:339:GLN:HE21	1.85	0.41
1:H:325:PHE:CD2	1:H:372:LEU:HD13	2.56	0.41
1:E:8:VAL:O	1:E:262:TYR:HA	2.20	0.41
1:H:457:ASN:CG	3:H:521:GDU:O3'	2.58	0.41
1:B:348:THR:OG1	6:B:828:HOH:O	2.22	0.41
1:G:327:ARG:NH1	3:G:521:GDU:O5'	2.53	0.41
1:C:105:PRO:HG2	1:C:201[B]:ALA:O	2.20	0.41
1:E:139:PRO:HB2	1:E:176:CYS:SG	2.61	0.41
1:C:87:TYR:CE2	1:C:336:PRO:HD2	2.56	0.41
1:A:245:VAL:HG22	1:A:278:MET:HG2	2.03	0.41
1:C:89:HIS:O	1:C:209[A]:THR:HA	2.21	0.41
1:B:63:HIS:CE1	1:B:315[A]:TRP:CZ3	3.09	0.41
1:A:175:GLN:HE22	1:A:178[A]:TRP:N	2.19	0.41
1:B:110:ILE:CD1	1:B:110:ILE:H	2.32	0.41
2:G:600:FAD:H1'1	2:G:600:FAD:H9	1.45	0.41
1:F:313[B]:LYS:HB3	1:F:316[B]:LEU:HD21	2.03	0.41
1:F:92:ILE:O	1:F:314[A]:CYS:HB2	2.21	0.41
1:A:149:MET:HG3	1:A:186[B]:PRO:HD2	2.01	0.41
1:E:110:ILE:HD11	1:E:191:VAL:HG13	2.01	0.41
1:B:272:ASP:OD2	1:B:417:HIS:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:PHE:CE1	1:G:339:GLN:HB3	2.56	0.41
1:C:162:TYR:CE2	1:C:166:VAL:HG21	2.56	0.41
1:C:246:ASN:ND2	1:C:249:ASN:HD21	2.18	0.41
1:E:375:SER:N	6:E:1170:HOH:O	2.53	0.41
1:A:86:TRP:CD2	1:A:211:ARG:HD2	2.56	0.41
1:A:316:LEU:O	1:A:327:ARG:HA	2.21	0.41
1:C:269:MET:HE1	5:C:600:FDA:N6A	2.35	0.41
1:D:204:TRP:NE1	1:D:207:ASN:HA	2.36	0.41
1:E:280:ASP:O	1:E:284:VAL:HG23	2.20	0.41
1:C:338:ASN:N	6:C:577:HOH:O	2.54	0.41
1:C:351:LEU:HB2	1:C:353:ASP:OD2	2.20	0.41
1:C:37:VAL:HG12	1:C:235:ARG:HB3	2.03	0.41
1:B:197:LEU:HD12	1:B:197:LEU:HA	1.80	0.41
1:B:380:LYS:HG2	1:B:380:LYS:O	2.20	0.41
1:H:65[A]:ILE:HG22	1:H:210:PHE:CB	2.51	0.40
1:B:145:TRP:CH2	1:B:183[B]:VAL:HB	2.56	0.40
1:E:145:TRP:O	1:E:149:MET:HB2	2.21	0.40
2:A:600:FAD:H2'	2:A:600:FAD:N1	2.36	0.40
1:D:125:MET:HE1	1:D:188:LEU:HA	2.03	0.40
1:H:149:MET:O	1:H:186[A]:PRO:HB3	2.21	0.40
1:H:126:ILE:HA	1:H:188:LEU:HD11	2.03	0.40
1:H:383:ASN:HB3	1:H:386:THR:OG1	2.21	0.40
1:H:206[A]:PRO:O	1:H:207[A]:ASN:C	2.59	0.40
1:E:65:ILE:HD13	3:E:521:GDU:H6'2	2.04	0.40
1:E:64:VAL:HG23	1:E:458:GLN:HB2	2.03	0.40
1:C:348:THR:N	6:C:634:HOH:O	2.54	0.40
1:B:125:MET:HE2	1:B:188[A]:LEU:HA	2.01	0.40
1:A:307:PRO:HB2	1:A:310:ILE:HG13	2.03	0.40
1:E:134:VAL:HG22	1:H:134:VAL:HG22	2.03	0.40
1:C:17:PRO:HG2	5:C:600:FDA:H4'	2.03	0.40
1:D:178:TRP:CA	1:D:454:GLU:HG2	2.51	0.40
1:E:332:SER:OG	1:E:369:SER:N	2.52	0.40
1:H:242:VAL:HG13	1:H:252:VAL:HG13	2.04	0.40
1:B:421:THR:HA	1:B:422:PRO:HD3	1.97	0.40
1:E:18:THR:OG1	1:E:461:SER:HB3	2.21	0.40
1:H:66[A]:PHE:HB2	1:H:207[A]:ASN:HA	2.03	0.40
1:B:182[A]:ARG:NH1	1:B:182[A]:ARG:CG	2.74	0.40
1:G:104:TYR:HD1	3:G:521:GDU:O4	2.04	0.40
1:F:306:ARG:NH1	1:F:311[A]:GLY:O	2.54	0.40
1:A:125:MET:HE2	1:A:188[A]:LEU:HA	2.03	0.40
1:G:25:ARG:HH21	1:G:28:GLN:NE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:VAL:O	1:G:185:ALA:N	2.54	0.40
1:G:46:LEU:O	1:G:61:GLY:HA3	2.21	0.40
1:E:348:THR:O	1:E:357:PRO:HG3	2.22	0.40
1:G:134:VAL:CG1	1:G:134:VAL:O	2.68	0.40
1:E:315[B]:TRP:N	1:E:315[B]:TRP:CE3	2.90	0.40
1:H:302:VAL:HG23	1:H:368:TRP:NE1	2.37	0.40
1:A:86:TRP:CE3	1:A:211:ARG:HD2	2.56	0.40
1:A:272:ASP:OD1	1:A:417:HIS:HE1	2.05	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	515/519 (99%)	501 (97%)	14 (3%)	0	100	100
1	B	523/519 (101%)	501 (96%)	22 (4%)	0	100	100
1	C	541/519 (104%)	509 (94%)	28 (5%)	4 (1%)	26	31
1	D	511/519 (98%)	494 (97%)	16 (3%)	1 (0%)	52	64
1	E	517/519 (100%)	487 (94%)	27 (5%)	3 (1%)	30	36
1	F	508/519 (98%)	490 (96%)	15 (3%)	3 (1%)	30	36
1	G	501/519 (96%)	481 (96%)	20 (4%)	0	100	100
1	H	545/519 (105%)	515 (94%)	26 (5%)	4 (1%)	26	31
All	All	4161/4152 (100%)	3978 (96%)	168 (4%)	15 (0%)	52	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	186[A]	PRO
1	E	186[B]	PRO

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Mol	Chain	Res	Type
1	E	187	ASN
1	C	208[B]	ALA
1	H	61[A]	GLY
1	H	61[B]	GLY
1	F	310	ILE
1	C	111	SER
1	F	187[A]	ASN
1	F	187[B]	ASN
1	D	207	ASN
1	C	61[A]	GLY
1	C	61[B]	GLY
1	H	62[A]	GLY
1	H	62[B]	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/441 (100%)	415 (94%)	25 (6%)	25	34
1	B	443/441 (100%)	413 (93%)	30 (7%)	20	25
1	C	459/441 (104%)	428 (93%)	31 (7%)	20	25
1	D	435/441 (99%)	406 (93%)	29 (7%)	20	26
1	E	438/441 (99%)	412 (94%)	26 (6%)	24	32
1	F	436/441 (99%)	413 (95%)	23 (5%)	28	37
1	G	430/441 (98%)	406 (94%)	24 (6%)	26	35
1	H	461/441 (104%)	427 (93%)	34 (7%)	17	21
All	All	3542/3528 (100%)	3320 (94%)	222 (6%)	24	29

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	54	GLU

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Mol	Chain	Res	Type
1	A	88	THR
1	A	90	GLN
1	A	92	ILE
1	A	100	GLN
1	A	107	GLN
1	A	110	ILE
1	A	136	ASN
1	A	175	GLN
1	A	197	LEU
1	A	245	VAL
1	A	254	LEU
1	A	255	GLN
1	A	287	THR
1	A	295	THR
1	A	302	VAL
1	A	309	ARG
1	A	339	GLN
1	A	382	VAL
1	A	388	LEU
1	A	454	GLU
1	A	470	ASP
1	A	510	GLN
1	A	511	LEU
1	B	25	ARG
1	B	54	GLU
1	B	88	THR
1	B	90	GLN
1	B	100	GLN
1	B	107	GLN
1	B	110	ILE
1	B	134	VAL
1	B	136	ASN
1	B	150	MET
1	B	175	GLN
1	B	182[A]	ARG
1	B	182[B]	ARG
1	B	183[A]	VAL
1	B	183[B]	VAL
1	B	188[A]	LEU
1	B	188[B]	LEU
1	B	197	LEU
1	B	204	TRP

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Mol	Chain	Res	Type
1	B	255	GLN
1	B	287	THR
1	B	295	THR
1	B	310	ILE
1	B	315[A]	TRP
1	B	315[B]	TRP
1	B	339	GLN
1	B	371	MET
1	B	382	VAL
1	B	387	ILE
1	B	470	ASP
1	C	25	ARG
1	C	54	GLU
1	C	63[A]	HIS
1	C	63[B]	HIS
1	C	80	LEU
1	C	88	THR
1	C	100	GLN
1	C	107	GLN
1	C	110	ILE
1	C	134	VAL
1	C	136	ASN
1	C	150	MET
1	C	157	LEU
1	C	175	GLN
1	C	182[A]	ARG
1	C	182[B]	ARG
1	C	197	LEU
1	C	254	LEU
1	C	255	GLN
1	C	287	THR
1	C	295	THR
1	C	302	VAL
1	C	309	ARG
1	C	312	ASP
1	C	339	GLN
1	C	356	ARG
1	C	361	GLU
1	C	387	ILE
1	C	388	LEU
1	C	470	ASP
1	C	511	LEU

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Mol	Chain	Res	Type
1	D	25	ARG
1	D	54	GLU
1	D	88	THR
1	D	100	GLN
1	D	107	GLN
1	D	110	ILE
1	D	134	VAL
1	D	136	ASN
1	D	175	GLN
1	D	181	GLU
1	D	188	LEU
1	D	197	LEU
1	D	199	LYS
1	D	200	THR
1	D	207	ASN
1	D	254	LEU
1	D	255	GLN
1	D	287	THR
1	D	295	THR
1	D	309	ARG
1	D	339	GLN
1	D	358	GLN
1	D	359	SER
1	D	382	VAL
1	D	387	ILE
1	D	388	LEU
1	D	454	GLU
1	D	470	ASP
1	D	511	LEU
1	E	25	ARG
1	E	54	GLU
1	E	65	ILE
1	E	88	THR
1	E	92	ILE
1	E	100	GLN
1	E	107	GLN
1	E	110	ILE
1	E	134	VAL
1	E	136	ASN
1	E	157	LEU
1	E	183[A]	VAL
1	E	183[B]	VAL

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Mol	Chain	Res	Type
1	E	197	LEU
1	E	199	LYS
1	E	204	TRP
1	E	254	LEU
1	E	255	GLN
1	E	287	THR
1	E	295	THR
1	E	339	GLN
1	E	371	MET
1	E	382	VAL
1	E	387	ILE
1	E	470	ASP
1	E	506	LYS
1	F	25	ARG
1	F	54	GLU
1	F	88	THR
1	F	92	ILE
1	F	100	GLN
1	F	107	GLN
1	F	108	ASN
1	F	110	ILE
1	F	136	ASN
1	F	175	GLN
1	F	197	LEU
1	F	255	GLN
1	F	287	THR
1	F	295	THR
1	F	302	VAL
1	F	309	ARG
1	F	339	GLN
1	F	387	ILE
1	F	388	LEU
1	F	470	ASP
1	F	507	SER
1	F	510	GLN
1	F	512	GLU
1	G	25	ARG
1	G	54	GLU
1	G	80	LEU
1	G	88	THR
1	G	100	GLN
1	G	107	GLN

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Mol	Chain	Res	Type
1	G	110	ILE
1	G	134	VAL
1	G	136	ASN
1	G	175	GLN
1	G	188	LEU
1	G	197	LEU
1	G	255	GLN
1	G	279	ASN
1	G	287	THR
1	G	295	THR
1	G	302	VAL
1	G	324	PRO
1	G	339	GLN
1	G	358	GLN
1	G	387	ILE
1	G	388	LEU
1	G	450	SER
1	G	470	ASP
1	H	25	ARG
1	H	54	GLU
1	H	63[A]	HIS
1	H	63[B]	HIS
1	H	65[A]	ILE
1	H	65[B]	ILE
1	H	88	THR
1	H	91[A]	ARG
1	H	91[B]	ARG
1	H	100	GLN
1	H	107	GLN
1	H	110	ILE
1	H	136	ASN
1	H	150	MET
1	H	175	GLN
1	H	181[A]	GLU
1	H	181[B]	GLU
1	H	182[A]	ARG
1	H	182[B]	ARG
1	H	188	LEU
1	H	197	LEU
1	H	209[A]	THR
1	H	209[B]	THR
1	H	254	LEU

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Mol	Chain	Res	Type
1	H	255	GLN
1	H	287	THR
1	H	295	THR
1	H	315[A]	TRP
1	H	315[B]	TRP
1	H	339	GLN
1	H	387	ILE
1	H	388	LEU
1	H	470	ASP
1	H	508	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	90	GLN
1	A	98	GLN
1	A	100	GLN
1	A	108	ASN
1	A	118	GLN
1	A	136	ASN
1	A	175	GLN
1	A	255	GLN
1	A	296	HIS
1	A	333	ASN
1	A	338	ASN
1	A	339	GLN
1	A	384	GLN
1	A	393	GLN
1	A	397	ASN
1	A	412	HIS
1	A	417	HIS
1	A	458	GLN
1	A	471	ASN
1	A	474	ASN
1	B	28	GLN
1	B	90	GLN
1	B	98	GLN
1	B	100	GLN
1	B	107	GLN
1	B	108	ASN
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	136	ASN
1	B	175	GLN
1	B	255	GLN
1	B	296	HIS
1	B	338	ASN
1	B	384	GLN
1	B	393	GLN
1	B	397	ASN
1	B	412	HIS
1	B	417	HIS
1	B	458	GLN
1	B	471	ASN
1	B	474	ASN
1	C	28	GLN
1	C	98	GLN
1	C	100	GLN
1	C	107	GLN
1	C	108	ASN
1	C	118	GLN
1	C	136	ASN
1	C	175	GLN
1	C	249	ASN
1	C	255	GLN
1	C	296	HIS
1	C	338	ASN
1	C	339	GLN
1	C	384	GLN
1	C	393	GLN
1	C	397	ASN
1	C	412	HIS
1	C	417	HIS
1	C	471	ASN
1	C	510	GLN
1	D	28	GLN
1	D	90	GLN
1	D	98	GLN
1	D	100	GLN
1	D	108	ASN
1	D	118	GLN
1	D	136	ASN
1	D	175	GLN
1	D	255	GLN

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Mol	Chain	Res	Type
1	D	296	HIS
1	D	333	ASN
1	D	338	ASN
1	D	339	GLN
1	D	384	GLN
1	D	393	GLN
1	D	397	ASN
1	D	412	HIS
1	D	417	HIS
1	D	458	GLN
1	D	471	ASN
1	E	28	GLN
1	E	98	GLN
1	E	100	GLN
1	E	107	GLN
1	E	108	ASN
1	E	118	GLN
1	E	136	ASN
1	E	175	GLN
1	E	255	GLN
1	E	296	HIS
1	E	333	ASN
1	E	338	ASN
1	E	339	GLN
1	E	384	GLN
1	E	393	GLN
1	E	397	ASN
1	E	412	HIS
1	E	417	HIS
1	E	458	GLN
1	E	471	ASN
1	F	28	GLN
1	F	90	GLN
1	F	98	GLN
1	F	100	GLN
1	F	107	GLN
1	F	108	ASN
1	F	118	GLN
1	F	136	ASN
1	F	175	GLN
1	F	255	GLN
1	F	296	HIS

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Mol	Chain	Res	Type
1	F	333	ASN
1	F	338	ASN
1	F	339	GLN
1	F	384	GLN
1	F	393	GLN
1	F	397	ASN
1	F	412	HIS
1	F	417	HIS
1	F	458	GLN
1	F	471	ASN
1	F	510	GLN
1	G	28	GLN
1	G	90	GLN
1	G	98	GLN
1	G	100	GLN
1	G	107	GLN
1	G	108	ASN
1	G	118	GLN
1	G	136	ASN
1	G	175	GLN
1	G	255	GLN
1	G	296	HIS
1	G	333	ASN
1	G	338	ASN
1	G	339	GLN
1	G	384	GLN
1	G	397	ASN
1	G	412	HIS
1	G	417	HIS
1	G	458	GLN
1	G	471	ASN
1	H	28	GLN
1	H	98	GLN
1	H	100	GLN
1	H	107	GLN
1	H	108	ASN
1	H	118	GLN
1	H	136	ASN
1	H	175	GLN
1	H	255	GLN
1	H	296	HIS
1	H	333	ASN

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Mol	Chain	Res	Type
1	H	338	ASN
1	H	339	GLN
1	H	358	GLN
1	H	384	GLN
1	H	393	GLN
1	H	397	ASN
1	H	412	HIS
1	H	417	HIS
1	H	471	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDU	A	521	-	29,38,38	1.79	7 (24%)	43,58,58	1.64	5 (11%)
2	FAD	A	600	-	48,58,58	2.21	12 (25%)	54,89,89	2.28	15 (27%)
3	GDU	B	521	-	29,38,38	1.81	8 (27%)	43,58,58	1.64	4 (9%)
2	FAD	B	600	-	48,58,58	2.29	15 (31%)	54,89,89	2.29	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDU	C	521	-	29,38,38	1.82	7 (24%)	43,58,58	1.62	5 (11%)
5	FDA	C	600	-	48,58,58	2.24	12 (25%)	54,89,89	2.26	15 (27%)
3	GDU	D	521	-	29,38,38	1.78	8 (27%)	43,58,58	1.71	5 (11%)
2	FAD	D	600	-	48,58,58	2.32	14 (29%)	54,89,89	2.24	16 (29%)
3	GDU	E	521	-	29,38,38	1.75	7 (24%)	43,58,58	2.00	8 (18%)
2	FAD	E	600	-	48,58,58	2.31	14 (29%)	54,89,89	2.27	17 (31%)
3	GDU	F	521	-	29,38,38	1.78	8 (27%)	43,58,58	1.72	5 (11%)
2	FAD	F	600	-	48,58,58	2.28	13 (27%)	54,89,89	2.42	17 (31%)
3	GDU	G	521	-	29,38,38	1.80	8 (27%)	43,58,58	1.70	5 (11%)
2	FAD	G	600	-	48,58,58	2.35	14 (29%)	54,89,89	2.36	21 (38%)
3	GDU	H	521	-	29,38,38	1.81	7 (24%)	43,58,58	1.69	6 (13%)
5	FDA	H	600	-	48,58,58	2.32	14 (29%)	54,89,89	2.39	14 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDU	A	521	-	-	0/19/59/59	0/3/3/3
2	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	GDU	B	521	-	-	0/19/59/59	0/3/3/3
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	GDU	C	521	-	-	0/19/59/59	0/3/3/3
5	FDA	C	600	-	-	0/30/50/50	0/6/6/6
3	GDU	D	521	-	-	0/19/59/59	0/3/3/3
2	FAD	D	600	-	-	0/30/50/50	0/6/6/6
3	GDU	E	521	-	-	0/19/59/59	0/3/3/3
2	FAD	E	600	-	-	0/30/50/50	0/6/6/6
3	GDU	F	521	-	-	0/19/59/59	0/3/3/3
2	FAD	F	600	-	-	0/30/50/50	0/6/6/6
3	GDU	G	521	-	-	0/19/59/59	0/3/3/3
2	FAD	G	600	-	-	0/30/50/50	0/6/6/6
3	GDU	H	521	-	-	0/19/59/59	0/3/3/3
5	FDA	H	600	-	-	0/30/50/50	0/6/6/6

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	600	FAD	C1'-N10	-8.39	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	600	FDA	C1'-N10	-8.31	1.39	1.48
2	D	600	FAD	C1'-N10	-8.24	1.39	1.48
2	E	600	FAD	C1'-N10	-8.23	1.39	1.48
2	B	600	FAD	C1'-N10	-7.98	1.40	1.48
2	F	600	FAD	C1'-N10	-7.86	1.40	1.48
5	C	600	FDA	C1'-N10	-7.85	1.40	1.48
2	A	600	FAD	C1'-N10	-7.00	1.41	1.48
5	H	600	FDA	C2B-C3B	-5.32	1.38	1.53
5	C	600	FDA	C2B-C3B	-5.17	1.39	1.53
2	E	600	FAD	C2B-C3B	-5.09	1.39	1.53
2	G	600	FAD	C2B-C3B	-5.05	1.39	1.53
2	D	600	FAD	C2B-C3B	-5.02	1.39	1.53
2	A	600	FAD	C2B-C3B	-5.01	1.39	1.53
2	B	600	FAD	C2B-C3B	-4.97	1.39	1.53
2	F	600	FAD	C2B-C3B	-4.95	1.39	1.53
3	C	521	GDU	PB-O3B	-4.01	1.49	1.60
5	H	600	FDA	C9A-C5X	-3.95	1.34	1.42
3	H	521	GDU	PB-O3B	-3.92	1.49	1.60
3	G	521	GDU	PB-O3B	-3.85	1.50	1.60
3	B	521	GDU	PB-O3B	-3.83	1.50	1.60
3	D	521	GDU	PB-O3B	-3.78	1.50	1.60
3	A	521	GDU	PB-O3B	-3.77	1.50	1.60
3	F	521	GDU	PB-O3B	-3.76	1.50	1.60
5	C	600	FDA	C9A-C5X	-3.72	1.35	1.42
3	E	521	GDU	PB-O3B	-3.63	1.50	1.60
2	F	600	FAD	C9A-C5X	-3.52	1.35	1.42
2	G	600	FAD	C9A-C5X	-3.49	1.35	1.42
3	G	521	GDU	C3D-C2D	-3.49	1.43	1.53
3	D	521	GDU	C3D-C2D	-3.45	1.44	1.53
2	D	600	FAD	C9A-C5X	-3.44	1.35	1.42
3	H	521	GDU	C3D-C2D	-3.43	1.44	1.53
2	D	600	FAD	C4'-C3'	-3.40	1.46	1.53
3	B	521	GDU	C3D-C2D	-3.38	1.44	1.53
2	B	600	FAD	C9A-C5X	-3.38	1.35	1.42
5	C	600	FDA	O3'-C3'	-3.36	1.34	1.43
5	H	600	FDA	O3'-C3'	-3.34	1.35	1.43
3	A	521	GDU	C3D-C2D	-3.32	1.44	1.53
3	A	521	GDU	C4'-C3'	-3.30	1.43	1.52
3	C	521	GDU	C3D-C2D	-3.30	1.44	1.53
2	A	600	FAD	C9A-C5X	-3.29	1.36	1.42
3	E	521	GDU	C3D-C2D	-3.27	1.44	1.53
3	F	521	GDU	C3D-C2D	-3.27	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	600	FDA	C9A-N10	-3.26	1.34	1.38
2	E	600	FAD	C9A-C5X	-3.20	1.36	1.42
3	H	521	GDU	C4'-C3'	-3.15	1.44	1.52
5	H	600	FDA	C4'-C3'	-3.13	1.47	1.53
2	B	600	FAD	O3'-C3'	-3.11	1.35	1.43
5	C	600	FDA	C4'-C3'	-3.10	1.47	1.53
2	A	600	FAD	O3'-C3'	-3.07	1.35	1.43
2	F	600	FAD	C4'-C3'	-3.06	1.47	1.53
2	D	600	FAD	O3'-C3'	-3.03	1.35	1.43
3	B	521	GDU	C4'-C3'	-3.01	1.44	1.52
2	F	600	FAD	O3'-C3'	-2.98	1.35	1.43
3	E	521	GDU	C4'-C3'	-2.98	1.44	1.52
3	C	521	GDU	C4'-C3'	-2.97	1.44	1.52
2	A	600	FAD	C4'-C3'	-2.97	1.47	1.53
2	G	600	FAD	O3'-C3'	-2.96	1.35	1.43
3	G	521	GDU	C4'-C3'	-2.95	1.44	1.52
2	G	600	FAD	C9A-N10	-2.95	1.34	1.38
2	E	600	FAD	O3'-C3'	-2.92	1.36	1.43
2	G	600	FAD	C4'-C3'	-2.91	1.47	1.53
3	F	521	GDU	C4'-C3'	-2.89	1.44	1.52
3	D	521	GDU	C4'-C3'	-2.88	1.44	1.52
3	H	521	GDU	O4D-C1D	-2.84	1.37	1.41
3	F	521	GDU	C3D-C4D	-2.81	1.45	1.53
3	B	521	GDU	O4D-C1D	-2.78	1.37	1.41
3	G	521	GDU	C3D-C4D	-2.77	1.45	1.53
3	B	521	GDU	C3D-C4D	-2.77	1.45	1.53
3	D	521	GDU	O4D-C1D	-2.75	1.37	1.41
3	C	521	GDU	C3D-C4D	-2.74	1.45	1.53
2	D	600	FAD	C9A-N10	-2.74	1.35	1.38
3	C	521	GDU	O4D-C1D	-2.74	1.37	1.41
3	A	521	GDU	C3D-C4D	-2.73	1.45	1.53
2	B	600	FAD	C4'-C3'	-2.72	1.47	1.53
2	E	600	FAD	C4'-C3'	-2.69	1.48	1.53
5	C	600	FDA	C9A-N10	-2.68	1.35	1.38
3	E	521	GDU	C3D-C4D	-2.68	1.45	1.53
2	E	600	FAD	C10-N10	-2.68	1.36	1.39
3	H	521	GDU	C3D-C4D	-2.67	1.45	1.53
3	D	521	GDU	C3D-C4D	-2.63	1.45	1.53
3	G	521	GDU	O4D-C1D	-2.60	1.37	1.41
3	E	521	GDU	O4D-C1D	-2.58	1.38	1.41
2	F	600	FAD	C9A-N10	-2.52	1.35	1.38
3	F	521	GDU	O4D-C1D	-2.51	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	600	FDA	O4B-C1B	-2.51	1.38	1.41
5	H	600	FDA	C10-N10	-2.47	1.36	1.39
3	A	521	GDU	O4D-C1D	-2.45	1.38	1.41
2	D	600	FAD	C10-N10	-2.40	1.36	1.39
2	B	600	FAD	O4B-C1B	-2.39	1.38	1.41
2	B	600	FAD	C9A-N10	-2.38	1.35	1.38
3	B	521	GDU	C3'-C2'	-2.38	1.46	1.52
3	C	521	GDU	C3'-C2'	-2.38	1.46	1.52
3	F	521	GDU	C3'-C2'	-2.31	1.46	1.52
3	G	521	GDU	C3'-C2'	-2.29	1.46	1.52
5	C	600	FDA	C10-N10	-2.28	1.36	1.39
2	A	600	FAD	C9A-N10	-2.26	1.35	1.38
3	D	521	GDU	C3'-C2'	-2.25	1.46	1.52
3	A	521	GDU	C3'-C2'	-2.24	1.46	1.52
2	E	600	FAD	O4B-C1B	-2.24	1.38	1.41
3	H	521	GDU	C3'-C2'	-2.22	1.46	1.52
2	D	600	FAD	O4B-C1B	-2.13	1.38	1.41
2	F	600	FAD	O4B-C1B	-2.12	1.38	1.41
2	B	600	FAD	C10-N10	-2.08	1.36	1.39
5	H	600	FDA	O3B-C3B	-2.06	1.38	1.43
2	E	600	FAD	C9A-N10	-2.04	1.36	1.38
2	G	600	FAD	O4B-C1B	-2.03	1.38	1.41
3	E	521	GDU	C3'-C2'	-2.01	1.47	1.52
2	G	600	FAD	C4X-N5	2.06	1.36	1.33
3	D	521	GDU	O5'-C5'	2.06	1.49	1.44
3	F	521	GDU	O5'-C5'	2.07	1.49	1.44
2	B	600	FAD	C4X-N5	2.10	1.36	1.33
3	B	521	GDU	O5'-C5'	2.11	1.49	1.44
2	D	600	FAD	P-O1P	2.12	1.58	1.51
3	G	521	GDU	O5'-C5'	2.14	1.49	1.44
2	F	600	FAD	P-O1P	2.21	1.59	1.51
2	A	600	FAD	P-O1P	2.28	1.59	1.51
2	B	600	FAD	P-O1P	2.30	1.59	1.51
2	G	600	FAD	P-O1P	2.34	1.59	1.51
5	H	600	FDA	O4'-C4'	2.48	1.48	1.43
2	E	600	FAD	P-O1P	2.50	1.60	1.51
5	C	600	FDA	O4'-C4'	2.55	1.49	1.43
2	F	600	FAD	O4'-C4'	2.63	1.49	1.43
2	B	600	FAD	O4'-C4'	2.68	1.49	1.43
2	E	600	FAD	O4'-C4'	2.70	1.49	1.43
5	H	600	FDA	C4-C4X	2.79	1.46	1.41
5	C	600	FDA	C4-C4X	2.85	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	O4'-C4'	2.85	1.49	1.43
2	G	600	FAD	O4'-C4'	2.87	1.49	1.43
2	A	600	FAD	O4'-C4'	2.87	1.49	1.43
2	D	600	FAD	C4-C4X	3.37	1.48	1.41
2	F	600	FAD	C4-C4X	3.37	1.48	1.41
2	E	600	FAD	C4-C4X	3.43	1.48	1.41
2	B	600	FAD	C4-C4X	3.48	1.48	1.41
2	G	600	FAD	C4-C4X	3.51	1.48	1.41
5	C	600	FDA	C7M-C7	3.54	1.58	1.51
2	A	600	FAD	C4-C4X	3.58	1.48	1.41
5	H	600	FDA	C7M-C7	3.64	1.58	1.51
3	H	521	GDU	O4-C4	3.72	1.33	1.24
3	F	521	GDU	O4-C4	3.72	1.33	1.24
3	C	521	GDU	O4-C4	3.72	1.33	1.24
3	G	521	GDU	O4-C4	3.74	1.33	1.24
3	D	521	GDU	O4-C4	3.75	1.33	1.24
3	B	521	GDU	O4-C4	3.77	1.33	1.24
3	A	521	GDU	O4-C4	3.80	1.33	1.24
3	E	521	GDU	O4-C4	3.81	1.33	1.24
2	B	600	FAD	C7M-C7	3.86	1.58	1.51
2	F	600	FAD	C7M-C7	3.93	1.59	1.51
2	G	600	FAD	C7M-C7	3.93	1.59	1.51
5	H	600	FDA	C4-N3	3.97	1.40	1.33
2	E	600	FAD	C7M-C7	4.00	1.59	1.51
2	A	600	FAD	C7M-C7	4.01	1.59	1.51
2	D	600	FAD	C7M-C7	4.02	1.59	1.51
5	C	600	FDA	C4-N3	4.06	1.40	1.33
5	H	600	FDA	C10-N1	4.51	1.43	1.35
2	D	600	FAD	C4-N3	4.63	1.41	1.33
2	A	600	FAD	C4-N3	4.65	1.41	1.33
2	F	600	FAD	C4-N3	4.65	1.41	1.33
5	C	600	FDA	C10-N1	4.73	1.43	1.35
2	E	600	FAD	C4-N3	4.75	1.41	1.33
2	B	600	FAD	C4-N3	4.76	1.41	1.33
2	G	600	FAD	C4-N3	4.79	1.42	1.33
2	D	600	FAD	C10-N1	4.85	1.43	1.35
2	E	600	FAD	C10-N1	4.90	1.43	1.35
2	A	600	FAD	C10-N1	4.96	1.43	1.35
2	B	600	FAD	C10-N1	4.98	1.43	1.35
2	F	600	FAD	C10-N1	5.24	1.44	1.35
2	G	600	FAD	C10-N1	5.25	1.44	1.35

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	600	FDA	N3A-C2A-N1A	-9.42	121.68	128.89
2	A	600	FAD	N3A-C2A-N1A	-9.34	121.75	128.89
2	F	600	FAD	N3A-C2A-N1A	-9.19	121.86	128.89
2	E	600	FAD	N3A-C2A-N1A	-9.13	121.90	128.89
2	B	600	FAD	N3A-C2A-N1A	-9.11	121.92	128.89
2	D	600	FAD	N3A-C2A-N1A	-9.01	121.99	128.89
2	G	600	FAD	N3A-C2A-N1A	-8.76	122.19	128.89
5	C	600	FDA	N3A-C2A-N1A	-8.44	122.43	128.89
2	F	600	FAD	O5B-PA-O1A	-5.77	87.22	109.62
2	F	600	FAD	C4B-O4B-C1B	-5.48	103.70	109.72
2	G	600	FAD	O5B-PA-O1A	-5.42	88.57	109.62
5	H	600	FDA	C4B-O4B-C1B	-5.09	104.13	109.72
2	E	600	FAD	O5B-PA-O1A	-4.94	90.42	109.62
3	E	521	GDU	C4D-O4D-C1D	-4.87	104.37	109.72
5	H	600	FDA	O5B-PA-O1A	-4.87	90.72	109.62
5	C	600	FDA	O5B-PA-O1A	-4.86	90.76	109.62
2	B	600	FAD	O5B-PA-O1A	-4.84	90.81	109.62
3	F	521	GDU	PB-O3A-PA	-4.83	119.15	132.73
3	C	521	GDU	PB-O3A-PA	-4.69	119.55	132.73
3	G	521	GDU	PB-O3A-PA	-4.67	119.62	132.73
2	D	600	FAD	O5B-PA-O1A	-4.55	91.97	109.62
3	D	521	GDU	PB-O3A-PA	-4.49	120.12	132.73
3	H	521	GDU	PB-O3A-PA	-4.45	120.25	132.73
2	B	600	FAD	O5'-P-O1P	-4.41	92.50	109.62
3	A	521	GDU	PB-O3A-PA	-4.40	120.37	132.73
5	C	600	FDA	O5'-P-O1P	-4.40	92.53	109.62
5	H	600	FDA	C4X-C10-N10	-4.37	117.94	120.52
5	H	600	FDA	O5'-P-O1P	-4.33	92.80	109.62
2	G	600	FAD	O5'-P-O1P	-4.27	93.04	109.62
3	B	521	GDU	PB-O3A-PA	-4.23	120.85	132.73
5	C	600	FDA	C4B-O4B-C1B	-4.19	105.12	109.72
3	E	521	GDU	PB-O3A-PA	-4.06	121.33	132.73
2	E	600	FAD	C4B-O4B-C1B	-4.03	105.29	109.72
2	A	600	FAD	O5'-P-O1P	-3.93	94.38	109.62
2	D	600	FAD	O5'-P-O1P	-3.92	94.40	109.62
2	A	600	FAD	O5B-PA-O1A	-3.91	94.46	109.62
2	E	600	FAD	O5'-P-O1P	-3.90	94.49	109.62
2	G	600	FAD	P-O3P-PA	-3.83	121.97	132.73
2	F	600	FAD	C4X-C10-N10	-3.83	118.27	120.52
5	C	600	FDA	C4X-C10-N10	-3.58	118.41	120.52
2	B	600	FAD	C4B-O4B-C1B	-3.53	105.84	109.72
2	D	600	FAD	P-O3P-PA	-3.47	122.97	132.73
2	G	600	FAD	C4X-C10-N10	-3.44	118.49	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	FAD	C4B-O4B-C1B	-3.40	105.98	109.72
2	G	600	FAD	C4B-O4B-C1B	-3.30	106.09	109.72
5	H	600	FDA	C4X-C4-N3	-3.29	119.09	123.59
2	A	600	FAD	C4B-O4B-C1B	-3.27	106.12	109.72
2	F	600	FAD	P-O3P-PA	-3.26	123.57	132.73
2	B	600	FAD	C4X-C10-N10	-3.22	118.62	120.52
5	C	600	FDA	C4X-C4-N3	-3.19	119.23	123.59
2	F	600	FAD	O5'-P-O1P	-3.15	97.41	109.62
2	A	600	FAD	P-O3P-PA	-2.90	124.59	132.73
2	D	600	FAD	C4X-C4-N3	-2.84	119.71	123.59
2	B	600	FAD	P-O3P-PA	-2.79	124.88	132.73
5	H	600	FDA	C1'-N10-C9A	-2.77	115.75	118.86
2	G	600	FAD	C1'-N10-C9A	-2.73	115.79	118.86
3	F	521	GDU	C4D-O4D-C1D	-2.69	106.77	109.72
2	D	600	FAD	C4X-C10-N10	-2.68	118.94	120.52
2	A	600	FAD	C4X-C4-N3	-2.64	119.98	123.59
3	C	521	GDU	C4D-O4D-C1D	-2.63	106.83	109.72
2	E	600	FAD	C4A-C5A-N7A	-2.63	107.06	109.48
2	B	600	FAD	C4X-C4-N3	-2.60	120.03	123.59
5	C	600	FDA	O2'-C2'-C1'	-2.58	103.60	109.94
2	E	600	FAD	C4X-C4-N3	-2.57	120.07	123.59
2	A	600	FAD	C4A-C5A-N7A	-2.56	107.13	109.48
2	G	600	FAD	O2'-C2'-C1'	-2.45	103.91	109.94
5	H	600	FDA	C4A-C5A-N7A	-2.44	107.23	109.48
2	F	600	FAD	C4X-C4-N3	-2.44	120.25	123.59
2	E	600	FAD	P-O3P-PA	-2.35	126.13	132.73
2	E	600	FAD	C4X-C10-N10	-2.32	119.15	120.52
5	H	600	FDA	O2'-C2'-C1'	-2.25	104.42	109.94
2	G	600	FAD	C4X-C4-N3	-2.23	120.55	123.59
5	C	600	FDA	C4A-C5A-N7A	-2.20	107.46	109.48
2	G	600	FAD	C4A-C5A-N7A	-2.18	107.47	109.48
2	F	600	FAD	C4A-C5A-N7A	-2.16	107.50	109.48
2	D	600	FAD	C4A-C5A-N7A	-2.13	107.52	109.48
2	F	600	FAD	O2'-C2'-C1'	-2.04	104.93	109.94
2	F	600	FAD	C1'-N10-C9A	-2.03	116.59	118.86
3	H	521	GDU	C4D-O4D-C1D	-2.00	107.52	109.72
2	G	600	FAD	O2P-P-O5'	2.02	118.64	108.46
2	G	600	FAD	O5B-C5B-C4B	2.05	116.67	109.12
2	G	600	FAD	O2'-C2'-C3'	2.05	114.17	109.02
2	E	600	FAD	O2P-P-O5'	2.07	118.90	108.46
5	H	600	FDA	O2P-P-O5'	2.07	118.91	108.46
3	E	521	GDU	C1'-C2'-C3'	2.07	114.06	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	FAD	C5X-C9A-N10	2.08	119.20	117.62
3	D	521	GDU	C2D-C3D-C4D	2.08	106.88	102.61
2	G	600	FAD	O3'-C3'-C2'	2.08	113.98	108.75
2	A	600	FAD	O3'-C3'-C2'	2.08	113.99	108.75
2	B	600	FAD	O2A-PA-O5B	2.11	119.09	108.46
2	F	600	FAD	O2P-P-O5'	2.12	119.16	108.46
5	C	600	FDA	O2A-PA-O5B	2.12	119.18	108.46
5	C	600	FDA	O2P-P-O5'	2.13	119.18	108.46
3	A	521	GDU	C2D-C3D-C4D	2.14	107.02	102.61
3	H	521	GDU	C4'-C3'-C2'	2.14	114.79	110.79
2	B	600	FAD	O5B-C5B-C4B	2.15	117.04	109.12
2	D	600	FAD	O5B-C5B-C4B	2.16	117.09	109.12
2	B	600	FAD	O2'-C2'-C3'	2.17	114.47	109.02
2	E	600	FAD	C4-C4X-N5	2.18	121.37	118.72
2	B	600	FAD	O2P-P-O5'	2.19	119.49	108.46
2	A	600	FAD	C4-C4X-N5	2.20	121.39	118.72
3	G	521	GDU	O5D-C5D-C4D	2.22	117.30	109.12
2	A	600	FAD	O2P-P-O5'	2.26	119.85	108.46
2	F	600	FAD	O2A-PA-O5B	2.26	119.87	108.46
2	D	600	FAD	O2A-PA-O5B	2.27	119.89	108.46
2	E	600	FAD	C4X-N5-C5X	2.35	119.47	116.76
5	C	600	FDA	C5X-C9A-N10	2.36	119.41	117.62
2	D	600	FAD	C4X-N5-C5X	2.37	119.48	116.76
2	E	600	FAD	O2'-C2'-C3'	2.38	115.01	109.02
2	E	600	FAD	O5B-C5B-C4B	2.39	117.92	109.12
2	G	600	FAD	O2A-PA-O5B	2.40	120.56	108.46
5	C	600	FDA	C4X-N5-C5X	2.41	119.53	116.76
2	G	600	FAD	C4-C4X-N5	2.45	121.70	118.72
2	E	600	FAD	O2A-PA-O5B	2.47	120.92	108.46
2	G	600	FAD	C5X-C9A-N10	2.52	119.54	117.62
2	A	600	FAD	C4X-N5-C5X	2.56	119.71	116.76
2	F	600	FAD	C4X-N5-C5X	2.65	119.81	116.76
3	A	521	GDU	O5'-C5'-C4'	2.66	114.67	109.68
2	B	600	FAD	C4X-N5-C5X	2.68	119.84	116.76
5	H	600	FDA	O2P-P-O3P	2.69	117.28	105.09
5	C	600	FDA	O2P-P-O3P	2.70	117.34	105.09
2	E	600	FAD	O2P-P-O3P	2.73	117.49	105.09
2	G	600	FAD	C4X-N5-C5X	2.79	119.97	116.76
2	D	600	FAD	O2P-P-O3P	2.80	117.81	105.09
3	C	521	GDU	O5'-C5'-C4'	2.83	114.99	109.68
2	B	600	FAD	C5X-C9A-N10	2.84	119.77	117.62
2	A	600	FAD	O2P-P-O3P	2.86	118.09	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	521	GDU	O5'-C5'-C4'	2.89	115.11	109.68
2	D	600	FAD	O3'-C3'-C2'	2.92	116.11	108.75
3	E	521	GDU	O4D-C1D-N1	3.01	114.43	108.08
2	F	600	FAD	C5X-C9A-N10	3.02	119.91	117.62
2	D	600	FAD	O2A-PA-O3P	3.04	118.87	105.09
2	A	600	FAD	C5X-C9A-N10	3.05	119.93	117.62
2	G	600	FAD	O2A-PA-O3P	3.05	118.91	105.09
2	B	600	FAD	O2P-P-O3P	3.09	119.12	105.09
2	G	600	FAD	O2P-P-O3P	3.17	119.45	105.09
2	B	600	FAD	O2A-PA-O3P	3.22	119.68	105.09
2	F	600	FAD	O2P-P-O3P	3.22	119.69	105.09
5	C	600	FDA	O2A-PA-O3P	3.23	119.73	105.09
3	F	521	GDU	O5'-C5'-C4'	3.27	115.83	109.68
5	H	600	FDA	C5X-C9A-N10	3.32	120.14	117.62
3	B	521	GDU	C3'-C4'-C5'	3.37	116.08	110.20
2	F	600	FAD	O2A-PA-O3P	3.38	120.45	105.09
3	A	521	GDU	C3'-C4'-C5'	3.40	116.12	110.20
3	E	521	GDU	O5'-C5'-C4'	3.40	116.06	109.68
2	E	600	FAD	O2A-PA-O3P	3.42	120.59	105.09
3	E	521	GDU	C4'-C3'-C2'	3.51	117.35	110.79
2	A	600	FAD	O2A-PA-O3P	3.54	121.13	105.09
3	C	521	GDU	C3'-C4'-C5'	3.55	116.38	110.20
3	B	521	GDU	O5'-C5'-C4'	3.62	116.47	109.68
3	G	521	GDU	O5'-C5'-C4'	3.65	116.53	109.68
3	D	521	GDU	O5'-C5'-C4'	3.68	116.59	109.68
3	H	521	GDU	C3'-C4'-C5'	3.73	116.70	110.20
5	H	600	FDA	O2A-PA-O3P	3.79	122.28	105.09
3	G	521	GDU	C3'-C4'-C5'	3.81	116.84	110.20
3	D	521	GDU	C3'-C4'-C5'	4.01	117.19	110.20
3	F	521	GDU	C3'-C4'-C5'	4.20	117.52	110.20
3	E	521	GDU	C3'-C4'-C5'	4.60	118.22	110.20
3	C	521	GDU	C4-N3-C2	5.41	119.50	114.14
2	G	600	FAD	C4-N3-C2	5.46	119.97	115.25
5	H	600	FDA	C4-N3-C2	5.51	120.01	115.25
2	E	600	FAD	C4-N3-C2	5.52	120.02	115.25
3	F	521	GDU	C4-N3-C2	5.56	119.65	114.14
3	E	521	GDU	C4-N3-C2	5.61	119.70	114.14
3	H	521	GDU	C4-N3-C2	5.62	119.71	114.14
2	B	600	FAD	C4-N3-C2	5.67	120.14	115.25
2	D	600	FAD	C4-N3-C2	5.69	120.16	115.25
3	B	521	GDU	C4-N3-C2	5.73	119.81	114.14
2	F	600	FAD	C4-N3-C2	5.81	120.27	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	521	GDU	C4-N3-C2	5.82	119.90	114.14
3	A	521	GDU	C4-N3-C2	5.82	119.90	114.14
3	G	521	GDU	C4-N3-C2	5.88	119.97	114.14
2	A	600	FAD	C4-N3-C2	5.96	120.40	115.25
5	C	600	FDA	C4-N3-C2	6.09	120.51	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	521	GDU	10	0
2	A	600	FAD	6	0
3	B	521	GDU	10	0
2	B	600	FAD	4	0
3	C	521	GDU	7	0
5	C	600	FDA	6	0
3	D	521	GDU	4	0
2	D	600	FAD	2	0
3	E	521	GDU	12	0
2	E	600	FAD	2	0
3	F	521	GDU	3	0
2	F	600	FAD	6	0
3	G	521	GDU	8	0
2	G	600	FAD	4	0
3	H	521	GDU	11	0
5	H	600	FDA	6	0

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	504/519 (97%)	0.58	46 (9%) 11 17	27, 50, 80, 137	0
1	B	510/519 (98%)	0.85	75 (14%) 3 5	28, 53, 88, 163	0
1	C	511/519 (98%)	0.89	69 (13%) 4 6	28, 54, 84, 138	10 (1%)
1	D	510/519 (98%)	0.63	61 (11%) 6 9	30, 52, 87, 150	0
1	E	510/519 (98%)	1.06	94 (18%) 2 2	30, 56, 89, 147	2 (0%)
1	F	504/519 (97%)	0.50	38 (7%) 17 24	31, 53, 85, 137	0
1	G	504/519 (97%)	0.66	54 (10%) 8 12	28, 53, 85, 140	0
1	H	511/519 (98%)	0.93	77 (15%) 3 5	27, 54, 82, 137	6 (1%)
All	All	4064/4152 (97%)	0.76	514 (12%) 5 8	27, 53, 85, 163	18 (0%)

All (514) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	GLY	16.7
1	C	204[B]	TRP	15.3
1	E	202	GLY	13.6
1	H	204[A]	TRP	12.8
1	E	201	ALA	12.6
1	E	204	TRP	12.4
1	H	205[A]	GLY	12.1
1	H	184[A]	ALA	11.3
1	B	203	ASN	10.8
1	D	206	PRO	10.7
1	H	511	LEU	10.2
1	D	202	GLY	9.9
1	H	2	THR	9.5
1	H	202[A]	GLY	9.4
1	C	206[B]	PRO	9.3
1	D	204	TRP	9.1

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Mol	Chain	Res	Type	RSRZ
1	C	511	LEU	9.0
1	C	205[B]	GLY	8.9
1	E	184[A]	ALA	8.6
1	C	202[B]	GLY	8.5
1	G	308	GLU	8.5
1	A	315[A]	TRP	8.5
1	B	185[A]	ALA	8.4
1	H	183[A]	VAL	8.3
1	F	310	ILE	8.3
1	D	207	ASN	7.9
1	G	511	LEU	7.9
1	A	183[A]	VAL	7.8
1	G	310	ILE	7.8
1	D	200	THR	7.6
1	D	203	ASN	7.6
1	E	183[A]	VAL	7.6
1	D	201	ALA	7.6
1	E	315[A]	TRP	7.5
1	B	183[A]	VAL	7.4
1	D	205	GLY	7.4
1	B	184[A]	ALA	7.3
1	C	203[B]	ASN	7.3
1	H	185[A]	ALA	7.3
1	F	315[A]	TRP	7.2
1	H	182[A]	ARG	7.2
1	A	184[A]	ALA	7.2
1	B	511	LEU	7.2
1	C	183[A]	VAL	7.2
1	E	2	THR	7.1
1	B	181[A]	GLU	7.1
1	F	309	ARG	7.0
1	D	308	GLU	6.9
1	B	204	TRP	6.9
1	C	315[A]	TRP	6.9
1	H	315[A]	TRP	6.9
1	E	511	LEU	6.9
1	F	511	LEU	6.9
1	B	356	ARG	6.8
1	C	201[B]	ALA	6.7
1	F	2	THR	6.7
1	B	315[A]	TRP	6.7
1	E	307	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	310	ILE	6.4
1	G	183	VAL	6.4
1	G	307	PRO	6.4
1	E	352	ALA	6.4
1	H	207[A]	ASN	6.3
1	E	185[A]	ALA	6.2
1	B	2	THR	6.2
1	A	182[A]	ARG	6.1
1	E	401	LEU	6.1
1	C	358	GLN	6.1
1	C	61[A]	GLY	6.0
1	A	309	ARG	6.0
1	D	310	ILE	6.0
1	H	358	GLN	6.0
1	C	182[A]	ARG	6.0
1	F	184	ALA	5.9
1	E	182[A]	ARG	5.9
1	A	185[A]	ALA	5.9
1	E	310	ILE	5.9
1	D	511	LEU	5.9
1	F	206	PRO	5.8
1	B	307	PRO	5.7
1	E	360	THR	5.7
1	E	3	HIS	5.5
1	H	206[A]	PRO	5.5
1	C	185[A]	ALA	5.5
1	E	351	LEU	5.5
1	E	362	ALA	5.4
1	B	182[A]	ARG	5.4
1	F	183	VAL	5.4
1	D	315[A]	TRP	5.3
1	B	359	SER	5.3
1	H	61[A]	GLY	5.3
1	F	512	GLU	5.2
1	B	358	GLN	5.2
1	E	392	ILE	5.2
1	E	309	ARG	5.2
1	G	184	ALA	5.2
1	G	309	ARG	5.2
1	G	200	THR	5.1
1	C	207[B]	ASN	5.1
1	A	186[A]	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	3	HIS	5.0
1	D	309	ARG	5.0
1	E	357	PRO	5.0
1	C	2	THR	5.0
1	E	358	GLN	4.9
1	H	65[A]	ILE	4.9
1	F	207	ASN	4.9
1	C	360	THR	4.9
1	E	407	ILE	4.8
1	H	186[A]	PRO	4.8
1	D	2	THR	4.8
1	E	200	THR	4.8
1	C	62[A]	GLY	4.8
1	B	305	SER	4.7
1	E	312	ASP	4.7
1	F	186[A]	PRO	4.7
1	C	186[A]	PRO	4.7
1	C	512	GLU	4.7
1	D	307	PRO	4.7
1	C	212[A]	PHE	4.6
1	H	512	GLU	4.6
1	H	200[A]	THR	4.6
1	B	201	ALA	4.5
1	H	91[A]	ARG	4.5
1	G	315[A]	TRP	4.5
1	E	393	GLN	4.5
1	B	91[A]	ARG	4.4
1	B	205	GLY	4.4
1	H	62[A]	GLY	4.4
1	E	281	GLN	4.4
1	C	184[A]	ALA	4.3
1	F	509	ALA	4.3
1	G	512	GLU	4.3
1	D	18	THR	4.3
1	B	206	PRO	4.3
1	E	356	ARG	4.2
1	E	385	GLU	4.2
1	F	313[A]	LYS	4.2
1	B	353	ASP	4.2
1	D	266	VAL	4.2
1	E	353	ASP	4.1
1	E	205	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	310	ILE	4.1
1	C	346	LEU	4.1
1	G	266	VAL	4.1
1	C	359	SER	4.0
1	E	359	SER	4.0
1	E	313	LYS	4.0
1	A	2	THR	4.0
1	H	92[A]	ILE	4.0
1	D	238	GLU	4.0
1	E	303	ARG	4.0
1	C	92[A]	ILE	4.0
1	E	355	SER	4.0
1	F	307	PRO	4.0
1	G	138	LYS	3.9
1	B	360	THR	3.9
1	A	181[A]	GLU	3.9
1	A	314[A]	CYS	3.9
1	G	22	ALA	3.9
1	G	199	LYS	3.9
1	G	510	GLN	3.9
1	C	199	LYS	3.8
1	E	181[A]	GLU	3.8
1	E	199	LYS	3.8
1	B	367	TYR	3.8
1	D	6	ILE	3.8
1	H	66[A]	PHE	3.8
1	E	405	ASP	3.8
1	H	510	GLN	3.8
1	C	347	PRO	3.8
1	C	356	ARG	3.7
1	E	396	VAL	3.7
1	H	201[A]	ALA	3.7
1	E	391	CYS	3.7
1	H	181[A]	GLU	3.7
1	E	347	PRO	3.7
1	E	368	TRP	3.7
1	B	3	HIS	3.7
1	G	21	GLY	3.7
1	E	198	GLY	3.7
1	D	22	ALA	3.7
1	E	399	GLU	3.7
1	G	83	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	110	ILE	3.6
1	E	378	SER	3.6
1	H	345	LYS	3.6
1	A	511	LEU	3.6
1	D	469	VAL	3.6
1	G	466	VAL	3.6
1	B	385	GLU	3.6
1	C	181[A]	GLU	3.6
1	E	208	ALA	3.6
1	H	208[A]	ALA	3.6
1	C	3	HIS	3.6
1	E	341	GLU	3.6
1	B	509	ALA	3.6
1	G	311	GLY	3.6
1	C	104	TYR	3.6
1	A	200	THR	3.5
1	D	3	HIS	3.5
1	G	509	ALA	3.5
1	H	356	ARG	3.5
1	D	19	GLY	3.5
1	D	208	ALA	3.5
1	E	406	GLU	3.5
1	E	404	THR	3.5
1	H	104[A]	TYR	3.5
1	C	65[A]	ILE	3.5
1	C	396	VAL	3.4
1	B	365	GLY	3.4
1	C	208[B]	ALA	3.4
1	H	359	SER	3.4
1	G	469	VAL	3.4
1	B	137	THR	3.4
1	D	268	THR	3.4
1	B	186[A]	PRO	3.4
1	H	329	THR	3.3
1	E	389	ALA	3.3
1	G	267	SER	3.3
1	C	200	THR	3.3
1	H	509	ALA	3.3
1	D	17	PRO	3.3
1	C	329	THR	3.3
1	F	181	GLU	3.3
1	C	386	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	203	ASN	3.2
1	A	311	GLY	3.2
1	E	350	GLN	3.2
1	H	63[A]	HIS	3.2
1	A	46	LEU	3.2
1	G	2	THR	3.2
1	E	383	ASN	3.2
1	B	389	ALA	3.2
1	E	186[A]	PRO	3.2
1	E	346	LEU	3.2
1	D	314[A]	CYS	3.2
1	G	462	PHE	3.2
1	D	510	GLN	3.2
1	B	306	ARG	3.2
1	G	345	LYS	3.2
1	H	365	GLY	3.1
1	A	341	GLU	3.1
1	G	3	HIS	3.1
1	F	84	ASP	3.1
1	C	345	LYS	3.1
1	E	408	VAL	3.1
1	B	309	ARG	3.1
1	E	56	PHE	3.1
1	D	267	SER	3.1
1	E	400	MET	3.1
1	B	469	VAL	3.1
1	B	352	ALA	3.0
1	E	345	LYS	3.0
1	F	510	GLN	3.0
1	D	21	GLY	3.0
1	A	270	ALA	3.0
1	G	18	THR	3.0
1	A	466	VAL	3.0
1	H	355	SER	3.0
1	D	313	LYS	3.0
1	E	206	PRO	3.0
1	D	13	ILE	3.0
1	E	402	LYS	3.0
1	A	509	ALA	3.0
1	E	305	SER	3.0
1	G	268	THR	3.0
1	E	469	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	64[A]	VAL	2.9
1	C	404	THR	2.9
1	D	209	THR	2.9
1	H	347	PRO	2.9
1	C	354	GLY	2.9
1	E	381	PRO	2.9
1	E	403	PRO	2.9
1	H	308	GLU	2.9
1	C	93[A]	SER	2.9
1	E	349	MET	2.9
1	D	12	VAL	2.9
1	G	12	VAL	2.9
1	E	308	GLU	2.9
1	G	20	LEU	2.9
1	A	512	GLU	2.8
1	E	384	GLN	2.8
1	C	99	GLY	2.8
1	E	365	GLY	2.8
1	F	466	VAL	2.8
1	D	91[A]	ARG	2.8
1	A	268	THR	2.8
1	C	469	VAL	2.8
1	B	355	SER	2.8
1	G	305	SER	2.8
1	F	62	GLY	2.8
1	E	179[A]	LEU	2.8
1	B	303	ARG	2.8
1	E	367	TYR	2.8
1	C	63[A]	HIS	2.7
1	D	20	LEU	2.7
1	G	196	ILE	2.7
1	B	357	PRO	2.7
1	G	385	GLU	2.7
1	F	449	GLY	2.7
1	B	361	GLU	2.7
1	H	112	MET	2.7
1	H	361	GLU	2.7
1	H	346	LEU	2.7
1	D	468	ALA	2.7
1	E	464	LEU	2.7
1	B	468	ALA	2.7
1	D	258	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	306	ARG	2.7
1	F	308	GLU	2.7
1	H	60[A]	VAL	2.7
1	B	342	ALA	2.7
1	D	199	LYS	2.7
1	E	115	LYS	2.7
1	A	449	GLY	2.7
1	C	406	GLU	2.7
1	G	265	LEU	2.6
1	H	461	SER	2.6
1	E	116	GLU	2.6
1	E	311	GLY	2.6
1	A	308	GLU	2.6
1	E	361	GLU	2.6
1	A	62	GLY	2.6
1	G	23	ALA	2.6
1	H	268	THR	2.6
1	H	383	ASN	2.6
1	C	314	CYS	2.6
1	D	23	ALA	2.6
1	A	199	LYS	2.6
1	E	306	ARG	2.6
1	E	344	LYS	2.6
1	G	140	LYS	2.6
1	A	180[A]	GLY	2.6
1	E	190	ALA	2.6
1	C	362	ALA	2.5
1	B	266	VAL	2.5
1	B	464	LEU	2.5
1	D	466	VAL	2.5
1	A	3	HIS	2.5
1	H	140	LYS	2.5
1	C	351	LEU	2.5
1	E	348	THR	2.5
1	H	179[A]	LEU	2.5
1	B	199	LYS	2.5
1	E	363	LYS	2.5
1	G	468	ALA	2.5
1	C	510	GLN	2.5
1	A	266	VAL	2.5
1	A	469	VAL	2.5
1	B	180[A]	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	268	THR	2.5
1	B	473	VAL	2.5
1	A	13	ILE	2.5
1	G	313	LYS	2.5
1	B	393	GLN	2.5
1	D	509	ALA	2.5
1	D	259	THR	2.5
1	A	17	PRO	2.5
1	H	203[A]	ASN	2.5
1	D	446	GLY	2.4
1	G	185	ALA	2.4
1	B	200	THR	2.4
1	B	207	ASN	2.4
1	H	371	MET	2.4
1	C	509	ALA	2.4
1	E	267	SER	2.4
1	B	347	PRO	2.4
1	G	181	GLU	2.4
1	G	446	GLY	2.4
1	A	447	ARG	2.4
1	H	507	SER	2.4
1	H	419	TYR	2.4
1	E	124	GLY	2.4
1	D	461	SER	2.4
1	H	83	GLU	2.4
1	B	466	VAL	2.4
1	D	345	LYS	2.4
1	F	115	LYS	2.4
1	H	12	VAL	2.4
1	B	273	PHE	2.4
1	H	3	HIS	2.4
1	B	312	ASP	2.4
1	D	465	GLY	2.4
1	E	302	VAL	2.4
1	G	119	VAL	2.4
1	A	138	LYS	2.4
1	B	405	ASP	2.3
1	D	311	GLY	2.3
1	A	305	SER	2.3
1	A	271	VAL	2.3
1	D	472	ILE	2.3
1	H	453	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	405	ASP	2.3
1	E	207	ASN	2.3
1	E	507	SER	2.3
1	G	306	ARG	2.3
1	H	466	VAL	2.3
1	A	18	THR	2.3
1	H	362	ALA	2.3
1	H	462	PHE	2.3
1	E	180[A]	GLY	2.3
1	H	363	LYS	2.3
1	C	464	LEU	2.3
1	B	510	GLN	2.3
1	B	472	ILE	2.3
1	D	256	ASP	2.3
1	E	342	ALA	2.3
1	D	16	GLY	2.3
1	G	19	GLY	2.3
1	C	308	GLU	2.3
1	C	357	PRO	2.3
1	H	469	VAL	2.3
1	G	238	GLU	2.3
1	C	209[A]	THR	2.3
1	E	510	GLN	2.3
1	H	342	ALA	2.3
1	H	384	GLN	2.3
1	B	179[A]	LEU	2.3
1	C	393	GLN	2.2
1	B	362	ALA	2.2
1	H	209[A]	THR	2.2
1	H	396	VAL	2.2
1	C	317	TYR	2.2
1	E	143	ASP	2.2
1	F	337	TYR	2.2
1	A	462	PHE	2.2
1	H	197	LEU	2.2
1	B	138	LYS	2.2
1	E	436	LYS	2.2
1	H	22	ALA	2.2
1	B	10	VAL	2.2
1	F	461	SER	2.2
1	G	473	VAL	2.2
1	H	314	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	464	LEU	2.2
1	C	21	GLY	2.2
1	F	311[A]	GLY	2.2
1	H	357	PRO	2.2
1	G	364	GLU	2.2
1	G	342	ALA	2.2
1	B	196	ILE	2.2
1	F	110	ILE	2.2
1	F	314[A]	CYS	2.2
1	F	446	GLY	2.2
1	H	364	GLU	2.2
1	B	265	LEU	2.2
1	F	403	PRO	2.2
1	A	342	ALA	2.2
1	G	382	VAL	2.2
1	C	94[A]	TYR	2.2
1	C	367	TYR	2.2
1	B	406	GLU	2.2
1	H	385	GLU	2.2
1	G	13	ILE	2.2
1	A	382	VAL	2.2
1	D	443	TRP	2.2
1	B	314	CYS	2.2
1	G	182	ARG	2.1
1	C	456	GLY	2.1
1	A	273	PHE	2.1
1	E	114	PRO	2.1
1	F	238	GLU	2.1
1	H	381	PRO	2.1
1	F	259	THR	2.1
1	H	330	ILE	2.1
1	G	269	MET	2.1
1	B	341	GLU	2.1
1	B	474	ASN	2.1
1	C	64[A]	VAL	2.1
1	C	455	VAL	2.1
1	F	266	VAL	2.1
1	H	93[A]	SER	2.1
1	C	312	ASP	2.1
1	A	269	MET	2.1
1	B	304	GLY	2.1
1	C	60[A]	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	255	GLN	2.1
1	E	98	GLN	2.1
1	A	66	PHE	2.1
1	A	329	THR	2.1
1	A	337	TYR	2.1
1	D	184	ALA	2.1
1	H	449	GLY	2.1
1	C	355	SER	2.1
1	G	17	PRO	2.1
1	G	366	PRO	2.1
1	E	432	GLN	2.1
1	B	12	VAL	2.1
1	B	26	LEU	2.1
1	B	386	THR	2.1
1	C	66[A]	PHE	2.1
1	D	464	LEU	2.1
1	D	5	ASP	2.1
1	A	450	SER	2.1
1	C	385	GLU	2.0
1	F	456	GLY	2.0
1	H	311	GLY	2.0
1	B	391	CYS	2.0
1	F	185	ALA	2.0
1	C	178[A]	TRP	2.0
1	B	465	GLY	2.0
1	H	447	ARG	2.0
1	D	281	GLN	2.0
1	B	11	LEU	2.0
1	C	377	SER	2.0
1	F	428	GLY	2.0
1	D	473	VAL	2.0
1	B	308	GLU	2.0
1	D	305	SER	2.0
1	B	53	PRO	2.0
1	D	445	ARG	2.0
1	F	17	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GDU	F	521	36/36	0.55	0.71	7.05	41,69,87,93	36
3	GDU	D	521	36/36	0.67	0.54	5.07	49,70,84,88	36
3	GDU	G	521	36/36	0.73	0.41	4.17	56,75,90,90	36
3	GDU	A	521	36/36	0.67	0.67	2.89	48,67,79,83	36
3	GDU	B	521	36/36	0.64	0.58	2.78	43,62,81,86	36
3	GDU	E	521	36/36	0.62	0.58	2.41	48,69,78,84	36
3	GDU	H	521	36/36	0.82	0.57	1.83	45,67,85,85	36
3	GDU	C	521	36/36	0.85	0.47	1.73	31,57,76,85	36
2	FAD	F	600	53/53	0.93	0.19	-0.11	34,50,63,69	0
2	FAD	E	600	53/53	0.95	0.16	-0.12	36,55,64,69	0
2	FAD	B	600	53/53	0.94	0.17	-0.21	36,48,62,70	0
2	FAD	G	600	53/53	0.95	0.17	-0.31	34,48,60,63	0
2	FAD	D	600	53/53	0.94	0.19	-0.32	30,47,56,60	0
2	FAD	A	600	53/53	0.95	0.19	-0.37	30,42,57,66	0
5	FDA	C	600	53/53	0.93	0.17	-0.57	33,51,64,82	0
5	FDA	H	600	53/53	0.94	0.19	-0.62	28,53,65,76	0
4	CL	A	522	1/1	0.53	0.18	-	103,103,103,103	0
4	CL	B	1	1/1	0.60	0.15	-	99,99,99,99	0

6.5 Other polymers ⓘ

There are no such residues in this entry.