



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:08 AM UTC

PDB ID : 7XD8 / pdb_00007xd8
Title : Crystal Structure of Dengue Virus Serotype 2 (DENV2) Polymerase Elongation Complex (Native Form)
Authors : Wu, J.; Wang, X.; Gong, P.
Deposited on : 2022-03-26
Resolution : 2.85 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

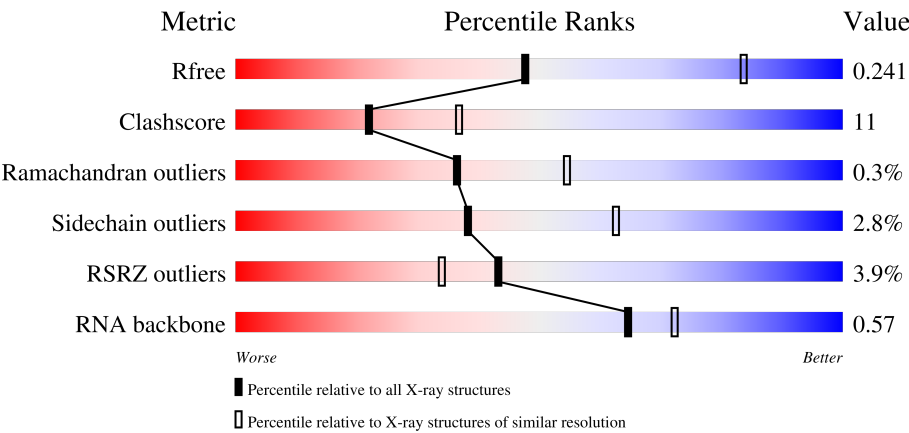
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.85 Å.

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



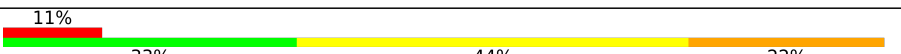
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	647	% 72% 23% ..
1	D	647	% 74% 22% .
1	G	647	% 73% 23% ..
1	J	647	% 73% 22% ..

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Mol	Chain	Length	Quality of chain
1	M	647	
1	P	647	
2	B	30	
2	E	30	
2	H	30	
2	K	30	
2	N	30	
2	Q	30	
3	C	9	
3	F	9	
3	I	9	
3	L	9	
3	O	9	
3	R	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31489 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 NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4900	3082	871	914	33			
1	D	621	Total	C	N	O	S	0	0	0
			4917	3095	873	915	34			
1	G	623	Total	C	N	O	S	0	0	0
			4874	3067	867	906	34			
1	J	623	Total	C	N	O	S	0	0	0
			4901	3086	871	910	34			
1	M	624	Total	C	N	O	S	0	0	0
			4909	3086	873	916	34			
1	P	611	Total	C	N	O	S	0	0	0
			4160	2587	753	790	30			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	901	GLY	-	expression tag	UNP Q91H74
A	902	SER	-	expression tag	UNP Q91H74
A	903	SER	-	expression tag	UNP Q91H74
A	904	SER	-	expression tag	UNP Q91H74
A	905	HIS	-	expression tag	UNP Q91H74
A	906	HIS	-	expression tag	UNP Q91H74
A	907	HIS	-	expression tag	UNP Q91H74
A	908	HIS	-	expression tag	UNP Q91H74
A	909	HIS	-	expression tag	UNP Q91H74
A	910	HIS	-	expression tag	UNP Q91H74
D	901	GLY	-	expression tag	UNP Q91H74
D	902	SER	-	expression tag	UNP Q91H74
D	903	SER	-	expression tag	UNP Q91H74
D	904	SER	-	expression tag	UNP Q91H74
D	905	HIS	-	expression tag	UNP Q91H74
D	906	HIS	-	expression tag	UNP Q91H74
D	907	HIS	-	expression tag	UNP Q91H74

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Chain	Residue	Modelled	Actual	Comment	Reference
D	908	HIS	-	expression tag	UNP Q91H74
D	909	HIS	-	expression tag	UNP Q91H74
D	910	HIS	-	expression tag	UNP Q91H74
G	901	GLY	-	expression tag	UNP Q91H74
G	902	SER	-	expression tag	UNP Q91H74
G	903	SER	-	expression tag	UNP Q91H74
G	904	SER	-	expression tag	UNP Q91H74
G	905	HIS	-	expression tag	UNP Q91H74
G	906	HIS	-	expression tag	UNP Q91H74
G	907	HIS	-	expression tag	UNP Q91H74
G	908	HIS	-	expression tag	UNP Q91H74
G	909	HIS	-	expression tag	UNP Q91H74
G	910	HIS	-	expression tag	UNP Q91H74
J	901	GLY	-	expression tag	UNP Q91H74
J	902	SER	-	expression tag	UNP Q91H74
J	903	SER	-	expression tag	UNP Q91H74
J	904	SER	-	expression tag	UNP Q91H74
J	905	HIS	-	expression tag	UNP Q91H74
J	906	HIS	-	expression tag	UNP Q91H74
J	907	HIS	-	expression tag	UNP Q91H74
J	908	HIS	-	expression tag	UNP Q91H74
J	909	HIS	-	expression tag	UNP Q91H74
J	910	HIS	-	expression tag	UNP Q91H74
M	901	GLY	-	expression tag	UNP Q91H74
M	902	SER	-	expression tag	UNP Q91H74
M	903	SER	-	expression tag	UNP Q91H74
M	904	SER	-	expression tag	UNP Q91H74
M	905	HIS	-	expression tag	UNP Q91H74
M	906	HIS	-	expression tag	UNP Q91H74
M	907	HIS	-	expression tag	UNP Q91H74
M	908	HIS	-	expression tag	UNP Q91H74
M	909	HIS	-	expression tag	UNP Q91H74
M	910	HIS	-	expression tag	UNP Q91H74
P	901	GLY	-	expression tag	UNP Q91H74
P	902	SER	-	expression tag	UNP Q91H74
P	903	SER	-	expression tag	UNP Q91H74
P	904	SER	-	expression tag	UNP Q91H74
P	905	HIS	-	expression tag	UNP Q91H74
P	906	HIS	-	expression tag	UNP Q91H74
P	907	HIS	-	expression tag	UNP Q91H74
P	908	HIS	-	expression tag	UNP Q91H74
P	909	HIS	-	expression tag	UNP Q91H74

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Chain	Residue	Modelled	Actual	Comment	Reference
P	910	HIS	-	expression tag	UNP Q91H74

- Molecule 2 is a RNA chain called RNA (30-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			251	113	42	84	12			
2	E	11	Total	C	N	O	P	0	0	0
			229	103	37	78	11			
2	H	11	Total	C	N	O	P	0	0	0
			229	103	37	78	11			
2	K	12	Total	C	N	O	P	0	0	0
			251	113	42	84	12			
2	N	12	Total	C	N	O	P	0	0	0
			251	113	42	84	12			
2	Q	11	Total	C	N	O	P	0	0	0
			229	103	37	78	11			

- Molecule 3 is a RNA chain called RNA (9-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			195	87	36	63	9			
3	F	9	Total	C	N	O	P	0	0	0
			195	87	36	63	9			
3	I	9	Total	C	N	O	P	0	0	0
			195	87	36	63	9			
3	L	9	Total	C	N	O	P	0	0	0
			194	87	36	62	9			
3	O	9	Total	C	N	O	P	0	0	0
			195	87	36	63	9			
3	R	9	Total	C	N	O	P	0	0	0
			195	87	36	63	9			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

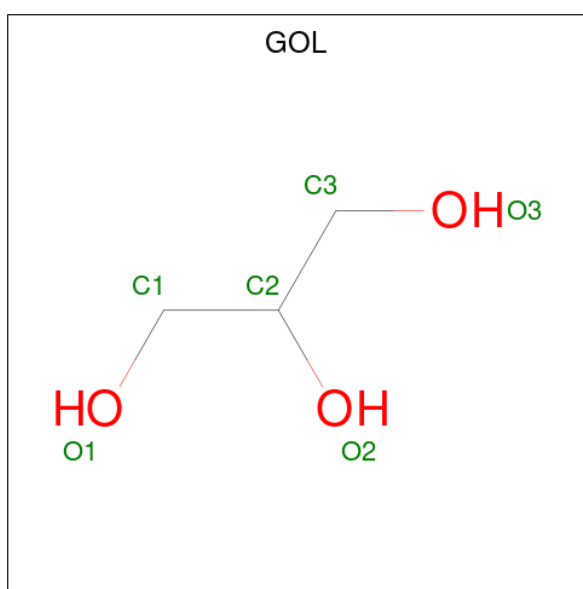
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	Zn 2	0	0
4	J	2	Total 2	Zn 2	0	0
4	M	2	Total 2	Zn 2	0	0
4	P	2	Total 2	Zn 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0
5	M	1	Total 6	C 3	O 3	0	0
5	P	1	Total 6	C 3	O 3	0	0

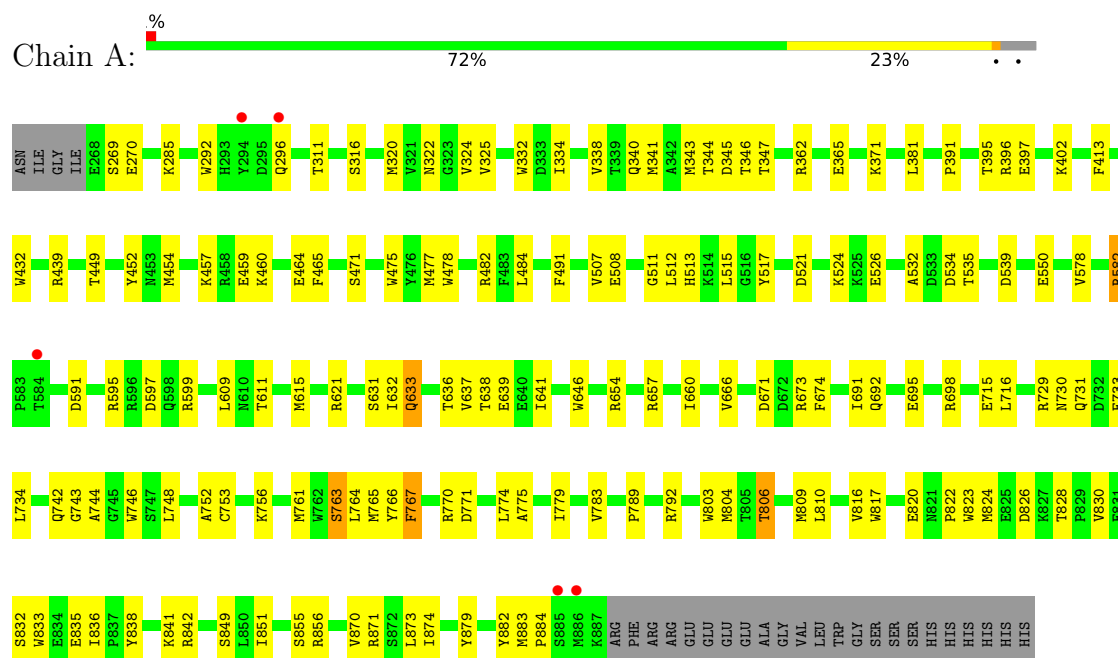
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total 29	O 29	0	0
6	B	8	Total 8	O 8	0	0
6	C	2	Total 2	O 2	0	0
6	D	26	Total 26	O 26	0	0
6	E	6	Total 6	O 6	0	0
6	F	6	Total 6	O 6	0	0
6	G	33	Total 33	O 33	0	0
6	H	2	Total 2	O 2	0	0
6	I	2	Total 2	O 2	0	0
6	J	29	Total 29	O 29	0	0
6	K	5	Total 5	O 5	0	0
6	L	1	Total 1	O 1	0	0
6	M	23	Total 23	O 23	0	0
6	N	3	Total 3	O 3	0	0
6	P	1	Total 1	O 1	0	0
6	R	1	Total 1	O 1	0	0

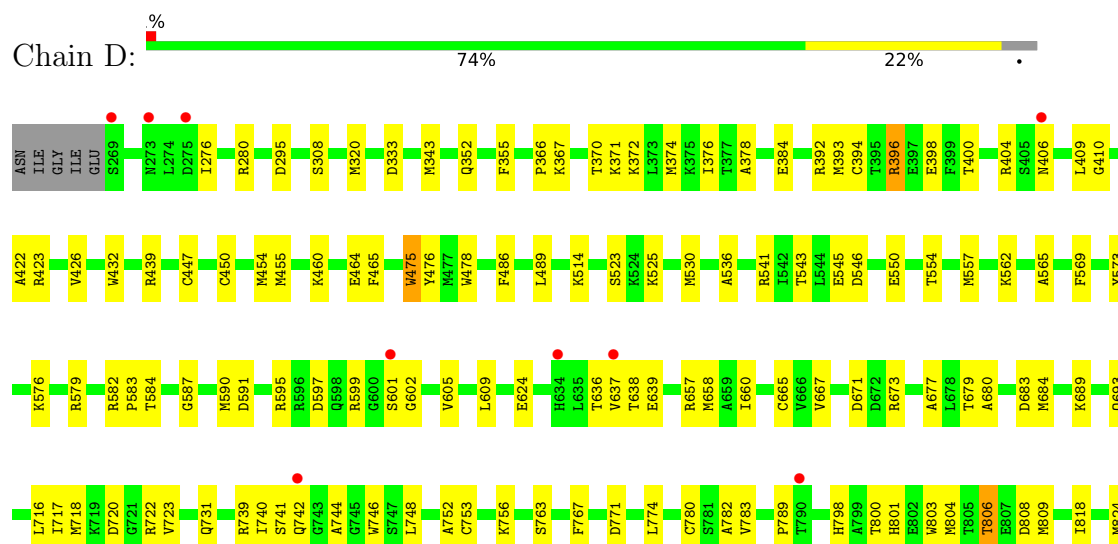
3 Residue-property plots [i](#)

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

• Molecule 1: NS5

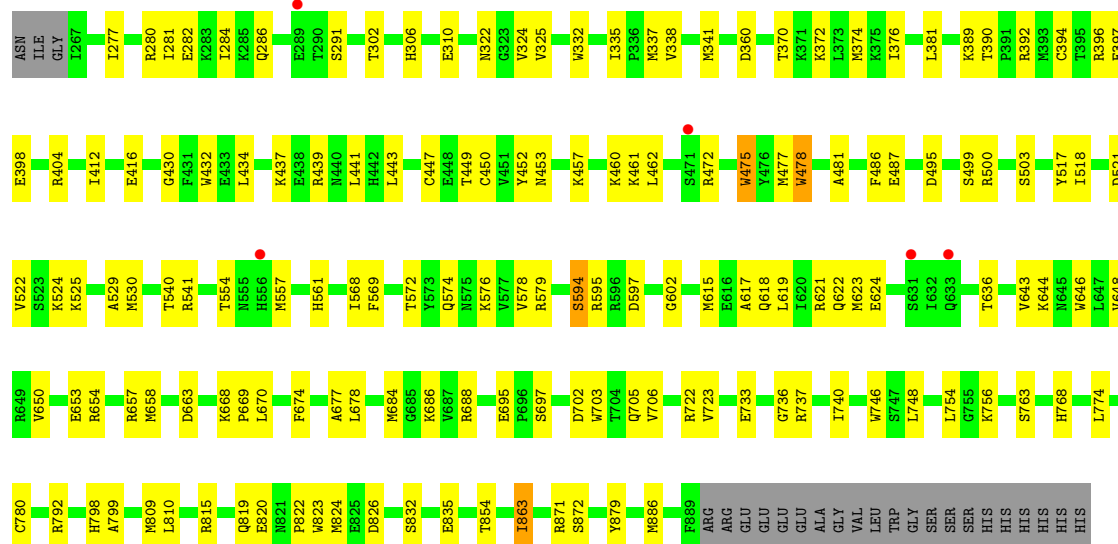
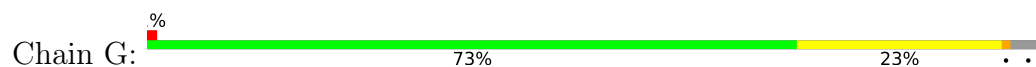


• Molecule 1: NS5

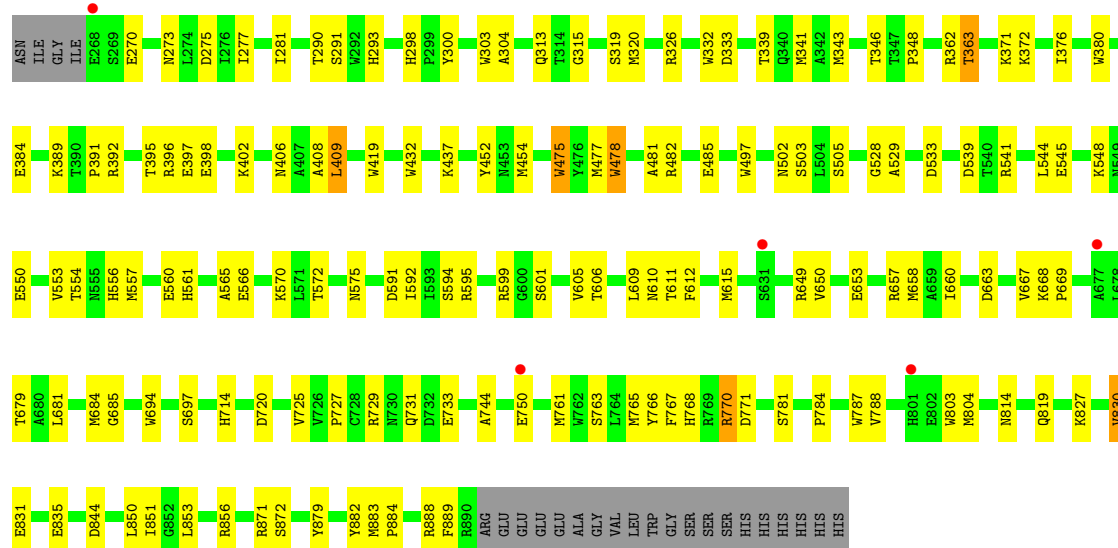




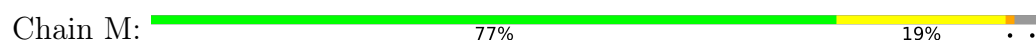
• Molecule 1: NS5

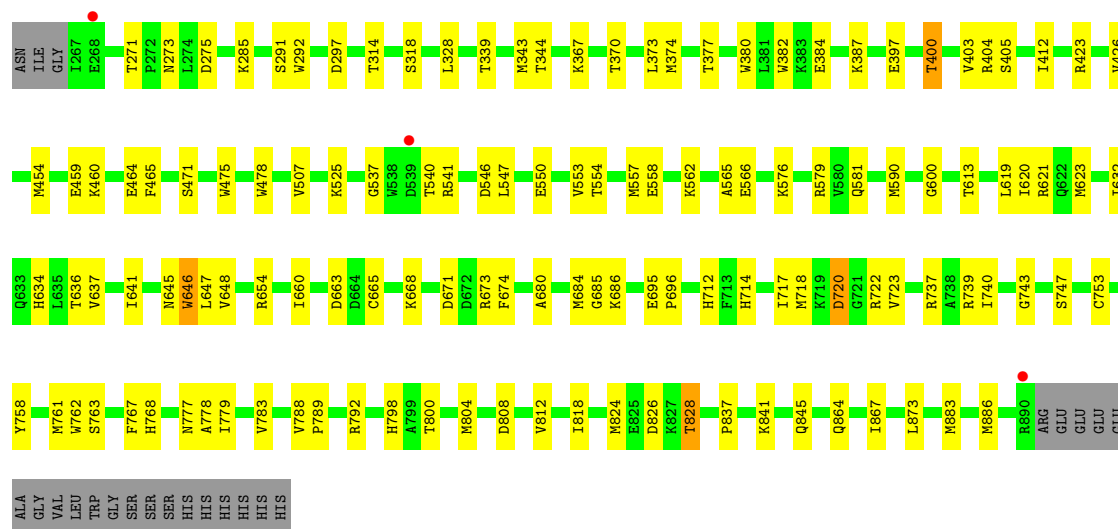


• Molecule 1: NS5

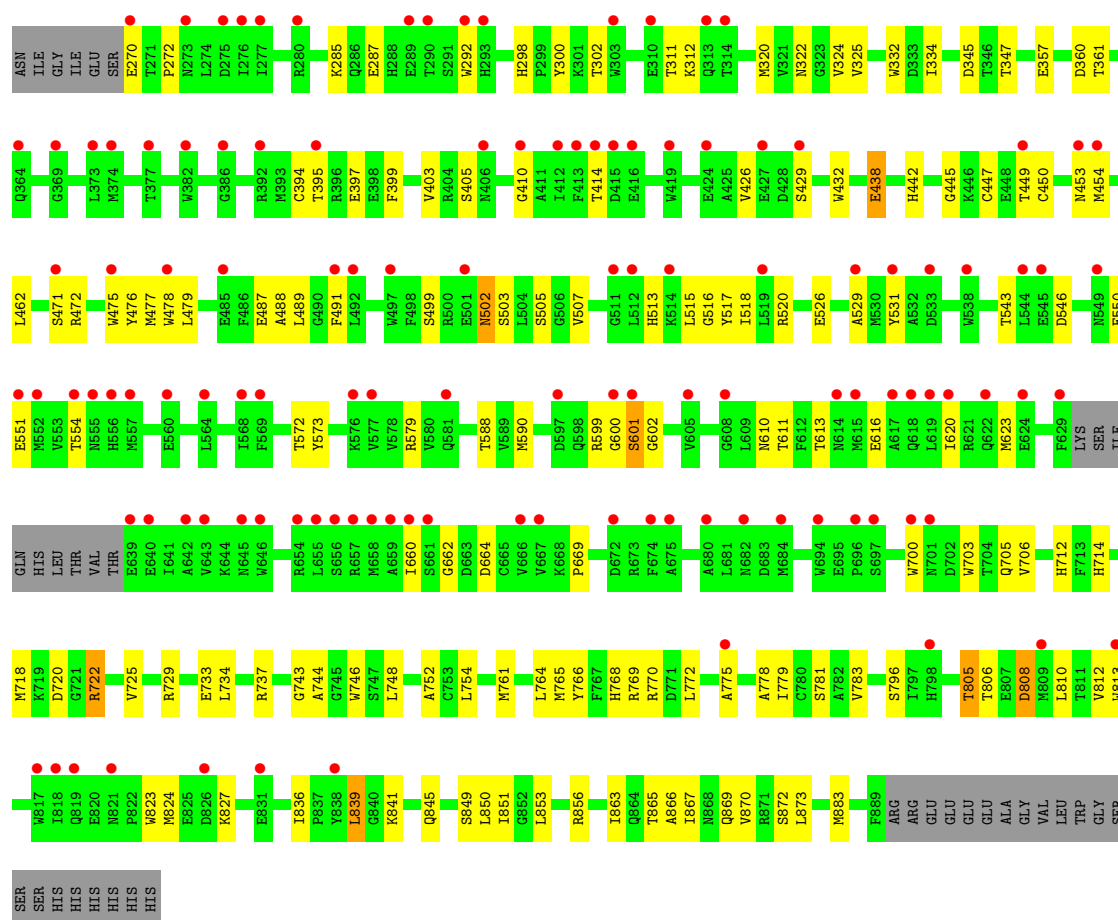


• Molecule 1: NS5





• Molecule 1: NS5



• Molecule 2: RNA (30-mer)





● Molecule 2: RNA (30-mer)



● Molecule 2: RNA (30-mer)



● Molecule 2: RNA (30-mer)



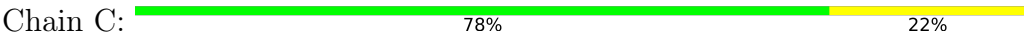
● Molecule 2: RNA (30-mer)



● Molecule 2: RNA (30-mer)



● Molecule 3: RNA (9-mer)



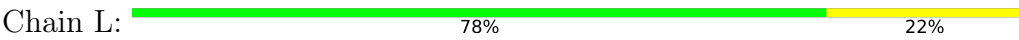
● Molecule 3: RNA (9-mer)



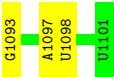
● Molecule 3: RNA (9-mer)



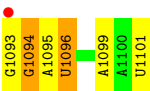
● Molecule 3: RNA (9-mer)



● Molecule 3: RNA (9-mer)



● Molecule 3: RNA (9-mer)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	141.73Å 156.32Å 174.42Å 90.00° 94.22° 90.00°	Depositor
Resolution (Å)	49.92 – 2.85 49.92 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.92-2.85) 87.5 (49.92-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.199 , 0.243 0.199 , 0.241	Depositor DCC
R_{free} test set	7872 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31489	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/5018	0.63	0/6812
1	D	0.40	0/5036	0.61	0/6833
1	G	0.37	0/4994	0.58	0/6789
1	J	0.38	0/5021	0.60	0/6819
1	M	0.40	0/5027	0.61	0/6826
1	P	0.34	0/4259	0.54	0/5848
2	B	0.48	0/279	0.69	0/431
2	E	0.39	0/254	0.57	0/392
2	H	0.38	0/254	0.61	0/392
2	K	0.37	0/279	0.63	0/431
2	N	0.35	0/279	0.56	0/431
2	Q	0.34	0/254	0.60	0/392
3	C	0.60	1/218 (0.5%)	0.62	0/336
3	F	0.60	1/218 (0.5%)	0.62	0/336
3	I	0.62	1/218 (0.5%)	0.69	0/336
3	L	0.60	1/217 (0.5%)	0.57	0/334
3	O	0.54	1/218 (0.5%)	0.64	0/336
3	R	0.55	1/218 (0.5%)	0.79	0/336
All	All	0.40	6/32261 (0.0%)	0.60	0/44410

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	J	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1093	G	OP3-P	6.55	1.61	1.48
3	L	1093	G	OP3-P	6.37	1.61	1.48
3	F	1093	G	OP3-P	6.35	1.61	1.48
3	C	1093	G	OP3-P	6.32	1.61	1.48
3	O	1093	G	OP3-P	5.99	1.60	1.48
3	R	1093	G	OP3-P	5.93	1.60	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	770	ARG	Sidechain

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	4900	0	4643	101	0
1	D	4917	0	4668	103	0
1	G	4874	0	4560	101	0
1	J	4901	0	4624	104	0
1	M	4909	0	4631	94	0
1	P	4160	0	3302	110	0
2	B	251	0	129	13	0
2	E	229	0	118	2	0
2	H	229	0	118	3	0
2	K	251	0	129	6	0
2	N	251	0	129	4	0
2	Q	229	0	118	5	0
3	C	195	0	97	2	0
3	F	195	0	97	1	0
3	I	195	0	97	1	0
3	L	194	0	97	2	0
3	O	195	0	97	2	0
3	R	195	0	97	5	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	M	2	0	0	0	0
4	P	2	0	0	0	0
5	C	6	0	8	3	0
5	D	6	0	8	2	0
5	E	6	0	8	0	0
5	M	6	0	8	3	0
5	P	6	0	8	0	0
6	A	29	0	0	3	0
6	B	8	0	0	1	0
6	C	2	0	0	0	0
6	D	26	0	0	3	0
6	E	6	0	0	1	0
6	F	6	0	0	0	0
6	G	33	0	0	4	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	29	0	0	0	0
6	K	5	0	0	0	0
6	L	1	0	0	0	0
6	M	23	0	0	1	0
6	N	3	0	0	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0
All	All	31489	0	27791	632	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 11.

All (632) 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:P:447:CYS:SG	1:P:450:CYS:HB2	1.93	1.06
1:P:475:TRP:CE3	1:P:600:GLY:HA2	2.04	0.93
1:M:778:ALA:HA	1:M:883:MET:HE1	1.56	0.86
1:M:475:TRP:HZ3	1:M:576:LYS:HD2	1.39	0.86
1:A:753:CYS:HB3	1:A:789:PRO:HG3	1.60	0.84
1:J:781:SER:HB3	1:J:882:TYR:H	1.42	0.83
1:J:395:THR:HG22	1:J:397:GLU:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:753:CYS:HB3	1:M:789:PRO:HG3	1.60	0.83
1:J:658:MET:HG2	1:J:667:VAL:HG22	1.60	0.82
1:J:731:GLN:HE22	1:J:771:ASP:HB2	1.42	0.82
1:A:457:LYS:NZ	2:B:1000:G:O6	2.12	0.82
1:D:579:ARG:HB2	1:D:590:MET:HE3	1.62	0.81
1:J:804:MET:HE3	2:K:1007:U:H5'	1.63	0.81
1:D:873:LEU:HD22	1:M:873:LEU:HD22	1.65	0.79
1:D:856:ARG:HH12	1:D:888:ARG:HH22	1.31	0.79
1:D:731:GLN:HE22	1:D:771:ASP:HB2	1.47	0.78
1:D:595:ARG:HD2	1:D:597:ASP:HB2	1.66	0.78
1:J:599:ARG:NH1	1:J:610:ASN:OD1	2.17	0.78
1:P:410:GLY:HA3	1:P:478:TRP:HA	1.65	0.78
1:G:774:LEU:HG	1:G:886:MET:HE1	1.66	0.77
1:M:343:MET:HE2	1:M:740:ILE:HD12	1.68	0.76
1:D:343:MET:HE2	1:D:740:ILE:HD12	1.68	0.76
1:M:717:ILE:HD13	1:M:723:VAL:HG12	1.67	0.76
1:P:477:MET:HE1	1:P:572:THR:HG23	1.68	0.75
1:P:611:THR:HG23	1:P:660:ILE:HG22	1.71	0.73
1:A:761:MET:HE3	1:A:766:TYR:HE2	1.55	0.72
1:D:752:ALA:HB1	1:D:783:VAL:HG22	1.71	0.71
1:A:775:ALA:O	1:A:779:ILE:HG13	1.90	0.71
1:D:753:CYS:HB3	1:D:789:PRO:HG3	1.72	0.71
1:G:277:ILE:HD12	1:G:281:ILE:HD11	1.73	0.71
1:M:400:THR:HG22	1:M:426:VAL:HB	1.72	0.71
1:G:460:LYS:HE2	1:G:740:ILE:HG13	1.72	0.70
1:G:302:THR:HG22	1:G:360:ASP:OD1	1.90	0.70
1:P:475:TRP:CZ3	1:P:600:GLY:HA2	2.27	0.70
1:J:731:GLN:NE2	1:J:771:ASP:HB2	2.05	0.70
1:P:438:GLU:OE1	1:P:449:THR:HB	1.90	0.70
1:D:557:MET:HE1	1:D:565:ALA:HB3	1.74	0.70
1:A:636:THR:HG22	1:A:638:THR:H	1.55	0.69
1:A:316:SER:H	1:A:346:THR:HG23	1.58	0.69
1:D:396:ARG:HG2	1:D:432:TRP:CZ3	2.28	0.69
1:D:804:MET:HE2	1:D:808:ASP:HB3	1.74	0.69
1:P:599:ARG:HH11	1:P:599:ARG:HG3	1.57	0.69
1:P:507:VAL:HG23	1:P:518:ILE:HD12	1.72	0.69
1:A:482:ARG:NH2	2:B:1001:A:OP1	2.26	0.69
1:D:716:LEU:HD12	1:D:839:LEU:HD23	1.75	0.69
1:P:805:THR:HG23	1:P:808:ASP:H	1.56	0.69
1:M:557:MET:HE2	1:M:562:LYS:HA	1.74	0.69
1:P:770:ARG:HB2	1:P:851:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:851:ILE:HA	1:P:856:ARG:HD2	1.75	0.68
1:J:727:PRO:HG2	1:J:765:MET:HG3	1.76	0.68
1:D:410:GLY:HA3	1:D:478:TRP:HA	1.75	0.68
1:D:856:ARG:NH1	1:D:888:ARG:HH22	1.92	0.68
2:B:1000:G:H2'	2:B:1001:A:C8	2.29	0.67
1:J:452:TYR:CZ	1:J:477:MET:HE2	2.28	0.67
1:G:595:ARG:HE	1:G:597:ASP:HB2	1.59	0.67
1:D:595:ARG:HH11	1:D:597:ASP:HB2	1.59	0.66
1:G:439:ARG:O	1:G:443:LEU:HD12	1.96	0.66
1:M:864:GLN:HA	1:M:867:ILE:HD12	1.78	0.66
1:J:557:MET:HE3	1:J:561:HIS:CE1	2.31	0.66
1:G:499:SER:O	1:G:503:SER:OG	2.10	0.66
1:G:824:MET:HE3	1:G:824:MET:HA	1.78	0.66
1:M:557:MET:HE1	1:M:565:ALA:HB3	1.77	0.65
1:A:764:LEU:HG	1:A:765:MET:HE2	1.78	0.65
1:A:270:GLU:HB2	1:A:362:ARG:HH12	1.61	0.65
1:A:365:GLU:OE2	1:A:371:LYS:NZ	2.30	0.65
1:A:695:GLU:HG3	1:D:541:ARG:HH22	1.61	0.65
1:G:557:MET:HE3	1:G:561:HIS:CD2	2.32	0.65
1:G:618:GLN:HB3	1:G:658:MET:HE2	1.79	0.65
1:P:394:CYS:HB2	1:P:487:GLU:HA	1.77	0.65
1:D:595:ARG:HH11	1:D:597:ASP:CB	2.09	0.65
1:D:856:ARG:HH12	1:D:888:ARG:NH2	1.94	0.64
1:G:525:LYS:HD2	1:G:657:ARG:HG2	1.80	0.64
1:P:502:ASN:O	1:P:502:ASN:ND2	2.30	0.64
1:J:298:HIS:HD2	1:J:300:TYR:H	1.43	0.64
1:A:526:GLU:O	1:A:657:ARG:NH2	2.30	0.64
1:P:775:ALA:O	1:P:779:ILE:HG13	1.97	0.64
1:M:620:ILE:HA	1:M:623:MET:HE2	1.78	0.64
1:J:566:GLU:O	1:J:570:LYS:HG3	1.98	0.64
1:G:282:GLU:O	1:G:286:GLN:HG2	1.98	0.63
1:J:320:MET:HE3	1:J:744:ALA:H	1.63	0.63
1:P:450:CYS:HB3	1:P:477:MET:HE2	1.80	0.63
1:P:805:THR:OG1	1:P:806:THR:N	2.30	0.62
1:P:429:SER:HA	1:P:432:TRP:HD1	1.63	0.62
1:A:508:GLU:HG2	6:A:2125:HOH:O	1.98	0.62
1:D:780:CYS:SG	1:D:809:MET:HE1	2.39	0.62
1:M:680:ALA:O	1:M:684:MET:HG3	1.98	0.62
1:G:478:TRP:CD1	1:G:481:ALA:H	2.16	0.62
1:P:733:GLU:HB3	1:P:737:ARG:NH1	2.14	0.62
1:G:530:MET:HE1	1:G:703:TRP:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:TRP:HA	1:G:335:ILE:HD13	1.81	0.61
1:M:344:THR:HG21	1:M:471:SER:HB2	1.81	0.61
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.36	0.61
1:A:763:SER:O	1:A:767:PHE:HB3	2.00	0.61
1:J:850:LEU:HD23	1:J:853:LEU:HD12	1.83	0.61
1:A:761:MET:HE3	1:A:766:TYR:CE2	2.36	0.61
1:M:525:LYS:O	1:M:668:LYS:NZ	2.34	0.61
1:J:570:LYS:O	1:J:575:ASN:ND2	2.34	0.60
1:J:304:ALA:HB3	1:J:594:SER:HB2	1.83	0.60
1:G:623:MET:HE1	1:G:643:VAL:HG13	1.83	0.60
1:M:722:ARG:HB3	1:M:824:MET:HE1	1.84	0.60
1:D:573:TYR:O	1:D:576:LYS:NZ	2.20	0.60
1:P:808:ASP:O	1:P:812:VAL:HG23	2.02	0.60
1:A:395:THR:HG22	1:A:397:GLU:H	1.67	0.60
1:D:756:LYS:NZ	6:D:2101:HOH:O	2.33	0.59
1:G:500:ARG:NH2	1:G:658:MET:O	2.35	0.59
1:J:396:ARG:HH21	1:J:432:TRP:HB3	1.66	0.59
1:J:814:ASN:HD21	1:J:830:VAL:H	1.49	0.59
1:M:370:THR:CG2	1:M:632:ILE:HB	2.32	0.59
1:P:579:ARG:CB	1:P:590:MET:HE1	2.32	0.59
1:P:770:ARG:HD2	1:P:851:ILE:HD13	1.84	0.59
1:P:733:GLU:HB3	1:P:737:ARG:HH12	1.68	0.59
1:P:572:THR:HG22	1:P:573:TYR:HD1	1.67	0.59
1:G:280:ARG:O	1:G:284:ILE:HG13	2.03	0.58
1:G:306:HIS:HE1	1:G:594:SER:HB3	1.68	0.58
1:J:533:ASP:OD2	1:J:697:SER:OG	2.13	0.58
1:M:343:MET:HE1	1:M:460:LYS:HG2	1.85	0.58
1:J:539:ASP:OD2	1:J:601:SER:OG	2.17	0.58
1:J:763:SER:O	1:J:767:PHE:HB3	2.02	0.58
1:P:778:ALA:HA	1:P:883:MET:HE1	1.84	0.58
1:D:554:THR:HG22	1:D:557:MET:HE2	1.85	0.58
1:A:621:ARG:HD3	1:A:674:PHE:CZ	2.38	0.58
1:A:636:THR:HG22	1:A:638:THR:N	2.18	0.58
1:P:429:SER:HA	1:P:432:TRP:CD1	2.39	0.58
1:J:477:MET:HE1	1:J:572:THR:HB	1.86	0.58
1:G:372:LYS:O	1:G:376:ILE:HG12	2.04	0.58
1:J:605:VAL:HB	1:J:609:LEU:HD12	1.84	0.57
1:P:761:MET:HE1	3:R:1099:A:H5'	1.85	0.57
1:D:557:MET:HE1	1:D:565:ALA:CB	2.33	0.57
1:A:873:LEU:HD12	1:P:873:LEU:HD22	1.85	0.57
1:M:779:ILE:O	1:M:783:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:HG3	1:A:465:PHE:CD2	2.40	0.57
1:G:530:MET:HE3	1:G:706:VAL:HG21	1.87	0.57
1:A:731:GLN:HE22	1:A:771:ASP:HB2	1.68	0.57
1:J:372:LYS:O	1:J:376:ILE:HG13	2.04	0.57
1:J:888:ARG:HD3	1:J:889:PHE:CE1	2.39	0.57
1:D:392:ARG:HH12	1:D:398:GLU:CD	2.13	0.57
1:M:339:THR:HB	5:M:2003:GOL:H32	1.87	0.57
1:J:770:ARG:HG3	1:J:844:ASP:OD2	2.05	0.57
1:J:761:MET:HE2	3:L:1099:A:H5'	1.87	0.57
1:P:302:THR:HG21	1:P:361:THR:C	2.30	0.57
1:A:457:LYS:HG3	1:A:459:GLU:HG2	1.85	0.57
1:M:550:GLU:OE2	1:M:613:THR:OG1	2.22	0.57
3:R:1094:G:C8	3:R:1094:G:H5''	2.40	0.57
1:D:774:LEU:HG	1:D:886:MET:HE1	1.87	0.56
1:J:409:LEU:HD21	1:J:419:TRP:HB2	1.86	0.56
1:A:770:ARG:NH2	1:A:841:LYS:HA	2.20	0.56
1:D:367:LYS:HE3	1:D:683:ASP:OD1	2.06	0.56
1:G:306:HIS:CE1	1:G:594:SER:HB3	2.40	0.56
1:M:663:ASP:N	1:M:663:ASP:OD1	2.36	0.56
1:M:343:MET:HE2	1:M:740:ILE:CD1	2.36	0.56
1:G:394:CYS:HB3	1:G:486:PHE:CE1	2.41	0.56
1:G:617:ALA:HA	1:G:684:MET:HE1	1.88	0.56
1:D:731:GLN:NE2	1:D:771:ASP:HB2	2.18	0.56
1:A:646:TRP:CH2	1:A:654:ARG:HG3	2.42	0.55
2:B:1007:U:H2'	2:B:1008:C:C6	2.42	0.55
1:J:819:GLN:O	1:J:827:LYS:NZ	2.39	0.55
1:D:280:ARG:NH1	1:D:447:CYS:SG	2.80	0.55
1:P:841:LYS:O	1:P:845:GLN:HG3	2.06	0.55
1:J:871:ARG:HD3	1:J:879:TYR:CG	2.42	0.55
1:G:832:SER:HB3	1:G:835:GLU:HG3	1.89	0.55
1:J:389:LYS:HD3	1:J:502:ASN:ND2	2.21	0.55
1:M:646:TRP:CZ2	1:M:654:ARG:HG3	2.41	0.55
1:D:756:LYS:HD3	1:D:803:TRP:CZ3	2.42	0.55
3:R:1094:G:H5''	3:R:1094:G:H8	1.72	0.55
1:D:717:ILE:HD13	1:D:723:VAL:HG22	1.88	0.55
1:G:337:MET:HG2	6:G:2125:HOH:O	2.06	0.55
1:M:454:MET:HE2	1:M:475:TRP:NE1	2.22	0.55
1:P:513:HIS:CD2	1:P:513:HIS:H	2.24	0.55
1:P:703:TRP:O	1:P:706:VAL:HG12	2.07	0.55
1:P:311:THR:OG1	1:P:312:LYS:N	2.40	0.55
1:A:320:MET:HG3	1:A:744:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:746:TRP:CH2	1:P:748:LEU:HB2	2.42	0.54
1:A:824:MET:HE3	1:A:824:MET:HA	1.88	0.54
1:D:746:TRP:CH2	1:D:748:LEU:HB2	2.41	0.54
1:P:489:LEU:HA	1:P:491:PHE:CE1	2.43	0.54
1:G:370:THR:O	1:G:374:MET:HG3	2.07	0.54
1:M:557:MET:HE1	1:M:565:ALA:CB	2.38	0.54
1:A:691:ILE:HD12	1:A:698:ARG:CZ	2.38	0.54
1:M:412:ILE:HA	1:M:579:ARG:NH1	2.22	0.54
1:A:804:MET:HE3	1:A:809:MET:HG3	1.90	0.54
1:J:332:TRP:NE1	1:J:850:LEU:HD11	2.22	0.54
1:A:731:GLN:NE2	1:A:771:ASP:HB2	2.23	0.54
1:A:806:THR:HG22	1:A:882:TYR:CD2	2.43	0.54
1:D:543:THR:OG1	1:D:546:ASP:OD1	2.13	0.54
1:J:482:ARG:HA	1:J:485:GLU:HG2	1.88	0.54
2:K:998:A:H5''	2:K:998:A:H8	1.72	0.54
1:M:403:VAL:HG22	1:M:404:ARG:O	2.08	0.54
1:M:405:SER:HB3	1:M:423:ARG:HB2	1.89	0.54
1:P:332:TRP:CE2	1:P:850:LEU:HD22	2.43	0.54
1:D:333:ASP:OD1	1:D:739:ARG:NH2	2.31	0.53
1:J:554:THR:HA	1:J:557:MET:SD	2.49	0.53
1:J:888:ARG:O	1:J:888:ARG:HG2	2.08	0.53
1:A:637:VAL:O	1:A:641:ILE:HG12	2.08	0.53
1:G:277:ILE:O	1:G:281:ILE:HD12	2.07	0.53
1:G:500:ARG:NH1	6:G:2103:HOH:O	2.40	0.53
1:M:475:TRP:CZ3	1:M:576:LYS:HD2	2.32	0.53
1:A:830:VAL:HG13	1:A:835:GLU:HB2	1.91	0.53
1:M:777:ASN:HD22	1:M:886:MET:HE2	1.72	0.53
1:D:392:ARG:NH1	1:D:398:GLU:OE2	2.33	0.53
1:D:782:ALA:HB2	1:D:867:ILE:HG23	1.90	0.53
1:P:475:TRP:HE3	1:P:600:GLY:HA2	1.65	0.53
1:P:765:MET:O	1:P:768:HIS:HE1	1.91	0.53
2:B:1000:G:H2'	2:B:1001:A:H8	1.72	0.53
1:G:452:TYR:CZ	1:G:477:MET:HE2	2.44	0.53
1:G:518:ILE:O	1:G:522:VAL:HG23	2.09	0.53
1:G:521:ASP:O	1:G:524:LYS:HB2	2.09	0.53
1:M:841:LYS:O	1:M:845:GLN:HG3	2.09	0.53
1:M:475:TRP:HZ3	1:M:576:LYS:CD	2.18	0.53
1:A:320:MET:HE3	1:A:743:GLY:HA3	1.91	0.52
1:A:521:ASP:HA	1:A:524:LYS:HE2	1.91	0.52
1:D:557:MET:HE3	1:D:562:LYS:HA	1.90	0.52
1:D:806:THR:HG21	1:D:885:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:554:THR:HA	1:G:557:MET:SD	2.49	0.52
1:M:370:THR:HG22	1:M:632:ILE:HB	1.91	0.52
1:A:792:ARG:NH1	3:C:1098:U:OP2	2.42	0.52
1:M:763:SER:O	1:M:767:PHE:HB3	2.10	0.52
1:P:572:THR:HG22	1:P:573:TYR:CD1	2.45	0.52
1:A:550:GLU:OE2	1:A:599:ARG:NH2	2.23	0.52
1:D:718:MET:HA	1:D:837:PRO:HG3	1.92	0.52
1:M:459:GLU:OE2	1:M:471:SER:OG	2.25	0.52
1:A:611:THR:HG23	1:A:660:ILE:HG22	1.92	0.52
1:J:599:ARG:HD3	1:J:606:THR:HA	1.92	0.52
1:M:761:MET:HE3	1:M:762:TRP:CD1	2.45	0.52
1:D:742:GLN:OE1	1:D:742:GLN:N	2.42	0.52
1:P:543:THR:OG1	1:P:546:ASP:OD2	2.27	0.52
1:D:536:ALA:HB2	1:D:689:LYS:HB2	1.90	0.52
1:P:551:GLU:O	1:P:554:THR:HG22	2.10	0.52
1:G:780:CYS:SG	1:G:809:MET:HE1	2.50	0.51
1:D:392:ARG:HH11	1:D:394:CYS:HA	1.75	0.51
1:G:619:LEU:O	1:G:623:MET:HG3	2.10	0.51
2:H:1000:G:H2'	2:H:1001:A:C8	2.46	0.51
1:G:568:ILE:O	1:G:572:THR:OG1	2.26	0.51
1:J:541:ARG:HG3	1:J:541:ARG:HH11	1.76	0.51
1:P:320:MET:HE2	1:P:744:ALA:O	2.10	0.51
1:P:752:ALA:HB1	1:P:783:VAL:HG13	1.92	0.51
1:G:389:LYS:NZ	1:G:495:ASP:O	2.27	0.51
1:A:883:MET:N	1:A:884:PRO:HD2	2.26	0.51
1:D:475:TRP:N	1:D:475:TRP:CD1	2.79	0.51
1:G:646:TRP:CZ2	1:G:654:ARG:HG3	2.46	0.51
1:A:345:ASP:OD1	1:A:347:THR:OG1	2.26	0.51
1:D:804:MET:CE	1:D:808:ASP:HB3	2.39	0.51
1:P:849:SER:OG	1:P:851:ILE:HG13	2.10	0.51
1:P:426:VAL:HA	1:P:432:TRP:CZ2	2.46	0.51
1:P:475:TRP:O	1:P:602:GLY:HA3	2.10	0.51
1:J:550:GLU:CD	1:J:599:ARG:HH22	2.19	0.50
1:J:653:GLU:O	1:J:657:ARG:HG3	2.12	0.50
1:M:808:ASP:O	1:M:812:VAL:HG23	2.10	0.50
1:P:287:GLU:OE1	1:P:414:THR:N	2.29	0.50
1:P:324:VAL:HG13	1:P:870:VAL:HG11	1.93	0.50
1:P:395:THR:HG23	1:P:397:GLU:H	1.74	0.50
1:M:712:HIS:CD2	1:M:714:HIS:CE1	3.00	0.50
1:D:352:GLN:HG3	1:D:583:PRO:HD2	1.94	0.50
1:G:475:TRP:CD1	1:G:475:TRP:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:605:VAL:CB	1:J:609:LEU:HD12	2.42	0.50
1:P:322:ASN:OD1	1:P:325:VAL:HG23	2.12	0.50
1:P:866:ALA:O	1:P:870:VAL:HG23	2.12	0.50
1:A:343:MET:HE2	1:A:742:GLN:HG3	1.93	0.50
1:D:371:LYS:HG2	1:D:545:GLU:CD	2.36	0.50
1:P:520:ARG:HD3	1:P:703:TRP:CH2	2.46	0.50
1:G:530:MET:HG2	1:G:668:LYS:HB2	1.94	0.50
1:P:270:GLU:O	1:P:272:PRO:HD3	2.11	0.50
1:P:865:THR:O	1:P:869:GLN:HG3	2.12	0.50
3:F:1097:A:H2'	3:F:1098:U:C6	2.47	0.50
1:G:416:GLU:HB3	1:G:478:TRP:CZ3	2.47	0.50
1:J:503:SER:C	1:J:505:SER:H	2.19	0.50
1:A:692:GLN:HB2	1:A:695:GLU:HB2	1.94	0.50
1:G:452:TYR:HB2	1:G:578:VAL:HG22	1.93	0.50
1:J:270:GLU:HB2	1:J:362:ARG:HH21	1.77	0.50
1:J:544:LEU:O	1:J:548:LYS:HG3	2.11	0.50
1:M:412:ILE:HA	1:M:579:ARG:HH12	1.77	0.50
2:B:1007:U:H1'	5:C:1201:GOL:O3	2.11	0.49
1:M:454:MET:HB2	1:M:579:ARG:O	2.12	0.49
1:D:804:MET:HE2	1:D:808:ASP:CB	2.39	0.49
1:M:798:HIS:HE1	1:M:800:THR:OG1	1.95	0.49
1:P:531:TYR:CE2	1:P:669:PRO:HG3	2.47	0.49
1:A:871:ARG:HE	1:A:879:TYR:HB3	1.77	0.49
1:D:372:LYS:O	1:D:376:ILE:HD12	2.13	0.49
1:P:770:ARG:HD2	1:P:851:ILE:CD1	2.42	0.49
1:D:460:LYS:NZ	1:D:740:ILE:O	2.44	0.49
1:J:883:MET:N	1:J:884:PRO:HD2	2.27	0.49
1:M:318:SER:HB2	1:M:743:GLY:O	2.12	0.49
1:M:581:GLN:HG2	1:M:590:MET:HE2	1.94	0.49
1:D:426:VAL:HG13	1:D:432:TRP:HZ2	1.77	0.49
1:D:378:ALA:HB2	5:D:2003:GOL:H32	1.95	0.49
1:M:739:ARG:HH21	5:M:2003:GOL:H12	1.77	0.49
1:M:343:MET:CE	1:M:460:LYS:HG2	2.43	0.49
1:J:391:PRO:HG2	1:J:556:HIS:O	2.13	0.49
1:M:546:ASP:OD2	1:M:686:LYS:NZ	2.44	0.49
1:P:602:GLY:HA2	2:Q:1000:G:N3	2.27	0.49
1:P:761:MET:O	1:P:761:MET:HG2	2.05	0.49
1:P:285:LYS:HA	1:P:292:TRP:CZ3	2.47	0.49
1:A:789:PRO:HB2	5:C:1201:GOL:H2	1.94	0.49
1:D:308:SER:HA	1:D:590:MET:O	2.13	0.49
1:D:809:MET:HE2	6:D:2108:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:302:THR:HG22	1:P:360:ASP:OD1	2.12	0.49
1:P:345:ASP:OD1	1:P:347:THR:OG1	2.28	0.49
1:D:554:THR:HA	1:D:557:MET:HG3	1.94	0.48
1:J:406:ASN:HD22	1:J:406:ASN:H	1.59	0.48
1:M:460:LYS:HD3	1:M:737:ARG:HG2	1.94	0.48
2:N:1000:G:H2'	2:N:1001:A:C8	2.47	0.48
1:A:322:ASN:OD1	1:A:325:VAL:HG23	2.13	0.48
1:A:402:LYS:NZ	2:B:1003:U:OP2	2.40	0.48
1:J:396:ARG:HG2	1:J:432:TRP:CZ3	2.48	0.48
1:P:600:GLY:O	1:P:601:SER:C	2.56	0.48
1:A:770:ARG:NH1	1:A:838:TYR:HB3	2.28	0.48
1:J:804:MET:CE	2:K:1007:U:H5'	2.39	0.48
1:M:373:LEU:O	1:M:377:THR:HG23	2.13	0.48
1:A:532:ALA:HB2	1:A:666:VAL:HG22	1.95	0.48
1:G:475:TRP:CZ3	1:G:576:LYS:HD2	2.49	0.48
1:A:511:GLY:O	1:A:515:LEU:HD13	2.14	0.48
1:D:447:CYS:SG	1:D:450:CYS:HB2	2.54	0.48
1:G:871:ARG:HG2	1:G:879:TYR:CZ	2.48	0.48
1:P:320:MET:HE3	1:P:743:GLY:HA3	1.95	0.48
1:D:756:LYS:NZ	6:D:2102:HOH:O	2.46	0.48
1:G:457:LYS:NZ	2:H:1000:G:O6	2.31	0.48
1:G:621:ARG:HD3	1:G:674:PHE:CZ	2.49	0.48
1:J:363:THR:HG21	1:J:541:ARG:HD3	1.94	0.48
1:M:792:ARG:NH1	3:O:1098:U:P	2.86	0.48
1:D:582:ARG:NH1	1:D:591:ASP:OD1	2.47	0.48
1:G:530:MET:HE1	1:G:703:TRP:CA	2.44	0.48
1:J:454:MET:HE3	1:J:454:MET:HB2	1.73	0.48
1:P:769:ARG:HB2	1:P:772:LEU:HB2	1.94	0.48
1:P:599:ARG:HG3	1:P:599:ARG:NH1	2.27	0.47
1:A:517:TYR:HB3	1:A:823:TRP:CE2	2.50	0.47
1:A:671:ASP:CG	1:A:673:ARG:HE	2.21	0.47
1:G:768:HIS:CD2	1:G:768:HIS:H	2.31	0.47
1:M:739:ARG:HE	5:M:2003:GOL:C1	2.27	0.47
1:G:396:ARG:HG2	1:G:432:TRP:CZ3	2.49	0.47
1:J:402:LYS:NZ	2:K:1003:U:OP2	2.43	0.47
1:M:637:VAL:O	1:M:641:ILE:HG12	2.14	0.47
1:P:471:SER:OG	1:P:472:ARG:N	2.48	0.47
1:A:396:ARG:HD3	1:A:432:TRP:CE3	2.49	0.47
1:G:557:MET:HE3	1:G:561:HIS:NE2	2.29	0.47
1:M:285:LYS:HG3	1:M:292:TRP:CE2	2.49	0.47
1:P:746:TRP:CZ3	1:P:748:LEU:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:579:ARG:CB	1:D:590:MET:HE3	2.40	0.47
1:J:814:ASN:ND2	1:J:830:VAL:H	2.13	0.47
1:M:541:ARG:HD2	1:M:685:GLY:O	2.15	0.47
1:P:620:ILE:HA	1:P:623:MET:HE2	1.97	0.47
1:P:662:GLY:HA3	3:R:1101:U:O2'	2.15	0.47
1:G:540:THR:OG1	1:G:541:ARG:HD2	2.15	0.47
1:A:730:ASN:HB3	1:A:733:GLU:HG3	1.95	0.47
1:D:409:LEU:HD11	1:D:422:ALA:HA	1.97	0.47
1:J:319:SER:HB3	1:J:343:MET:HG2	1.97	0.47
1:A:344:THR:HG21	1:A:471:SER:HB2	1.97	0.47
1:D:624:GLU:HG2	1:D:677:ALA:HB1	1.97	0.47
1:D:818:ILE:HA	1:D:824:MET:HG2	1.97	0.47
1:G:798:HIS:CD2	1:G:799:ALA:H	2.33	0.47
1:J:396:ARG:NH2	1:J:432:TRP:HB3	2.30	0.47
1:P:766:TYR:HA	1:P:768:HIS:CE1	2.50	0.47
1:D:660:ILE:HG12	1:D:665:CYS:HB2	1.97	0.46
1:J:395:THR:HB	1:J:398:GLU:HG3	1.98	0.46
1:J:557:MET:HE1	1:J:565:ALA:CB	2.45	0.46
1:M:273:ASN:OD1	1:M:275:ASP:HB3	2.16	0.46
1:P:703:TRP:H	1:P:703:TRP:CD1	2.32	0.46
1:A:871:ARG:HD3	1:A:879:TYR:CD1	2.49	0.46
1:M:460:LYS:HE3	1:M:758:TYR:OH	2.15	0.46
1:P:324:VAL:HG21	1:P:752:ALA:HA	1.98	0.46
1:P:450:CYS:HB3	1:P:477:MET:CE	2.45	0.46
1:A:870:VAL:O	1:A:874:ILE:HG13	2.15	0.46
1:G:754:LEU:HD22	1:G:792:ARG:HG3	1.98	0.46
1:A:826:ASP:OD1	1:A:828:THR:OG1	2.26	0.46
1:D:404:ARG:NH1	1:D:406:ASN:OD1	2.49	0.46
1:J:761:MET:CE	3:L:1099:A:H5'	2.46	0.46
1:M:768:HIS:CD2	1:M:768:HIS:H	2.33	0.46
1:P:449:THR:O	1:P:449:THR:HG22	2.15	0.46
1:A:729:ARG:HD3	1:A:734:LEU:HD21	1.96	0.46
1:A:439:ARG:HG3	1:A:484:LEU:HD21	1.97	0.46
1:D:426:VAL:HG13	1:D:432:TRP:CZ2	2.50	0.46
1:D:489:LEU:HD21	1:D:569:PHE:CE2	2.51	0.46
1:J:557:MET:HE1	1:J:565:ALA:HB2	1.96	0.46
1:M:718:MET:HA	1:M:837:PRO:HG3	1.97	0.46
1:A:332:TRP:HB3	1:A:338:VAL:HG21	1.96	0.46
1:A:851:ILE:HA	1:A:856:ARG:HD2	1.97	0.46
1:G:798:HIS:HD2	1:G:799:ALA:H	1.63	0.46
1:D:355:PHE:CE2	1:D:454:MET:HE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:392:ARG:NH2	1:G:398:GLU:OE2	2.49	0.46
1:J:541:ARG:HD2	1:J:685:GLY:O	2.15	0.46
2:B:1007:U:O2	5:C:1201:GOL:H11	2.16	0.46
1:G:324:VAL:HG23	6:G:2108:HOH:O	2.15	0.46
1:G:404:ARG:NH1	2:H:1001:A:OP2	2.48	0.46
1:G:624:GLU:HB3	1:G:677:ALA:HB1	1.98	0.46
1:A:513:HIS:HB2	1:A:817:TRP:CH2	2.51	0.45
1:G:623:MET:HE1	1:G:643:VAL:HG22	1.98	0.45
1:P:531:TYR:HE2	1:P:669:PRO:HG3	1.80	0.45
3:R:1096:U:H5''	3:R:1096:U:H6	1.80	0.45
1:D:658:MET:HG2	1:D:667:VAL:HG22	1.98	0.45
1:P:720:ASP:OD2	1:P:722:ARG:NH2	2.49	0.45
1:A:341:MET:HE2	1:A:341:MET:HB2	1.84	0.45
1:G:756:LYS:HE3	6:G:2106:HOH:O	2.16	0.45
1:M:464:GLU:HG2	1:M:465:PHE:CE2	2.51	0.45
1:M:720:ASP:OD1	1:M:722:ARG:NH2	2.49	0.45
1:G:517:TYR:HB3	1:G:823:TRP:CE2	2.52	0.45
1:G:525:LYS:O	1:G:668:LYS:HE2	2.16	0.45
1:P:863:ILE:O	1:P:867:ILE:HG12	2.16	0.45
1:A:632:ILE:O	1:A:633:GLN:HB2	2.16	0.45
1:G:722:ARG:HD3	1:G:826:ASP:HB3	1.98	0.45
1:M:367:LYS:HD2	1:M:367:LYS:HA	1.65	0.45
1:P:729:ARG:HD3	1:P:734:LEU:HD21	1.98	0.45
2:Q:1000:G:H2'	2:Q:1001:A:C8	2.52	0.45
1:A:774:LEU:HD12	1:A:774:LEU:HA	1.70	0.45
1:J:729:ARG:NH2	1:J:733:GLU:OE1	2.42	0.45
1:J:831:GLU:HB2	1:J:835:GLU:OE2	2.17	0.45
1:G:447:CYS:SG	1:G:450:CYS:HB2	2.57	0.45
1:J:341:MET:HE2	1:J:341:MET:HB2	1.75	0.45
1:J:784:PRO:HB2	1:J:787:TRP:CG	2.52	0.45
1:G:733:GLU:HB3	1:G:737:ARG:NH1	2.31	0.45
1:M:660:ILE:HG12	1:M:665:CYS:HB2	1.99	0.45
1:A:316:SER:N	1:A:346:THR:HG23	2.29	0.44
1:D:680:ALA:O	1:D:684:MET:HG3	2.17	0.44
1:M:718:MET:HE1	1:M:818:ILE:HD11	1.97	0.44
1:A:746:TRP:CH2	1:A:748:LEU:HB2	2.52	0.44
1:G:462:LEU:HA	1:G:462:LEU:HD23	1.62	0.44
1:J:591:ASP:C	1:J:592:ILE:HD13	2.43	0.44
1:M:826:ASP:OD1	1:M:828:THR:OG1	2.35	0.44
2:Q:1001:A:H2'	2:Q:1002:U:H6	1.82	0.44
1:A:391:PRO:HB3	1:A:491:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:NH1	2:B:1000:G:O3'	2.43	0.44
1:D:804:MET:HE3	6:E:1204:HOH:O	2.17	0.44
1:D:475:TRP:O	1:D:602:GLY:HA3	2.17	0.44
1:J:303:TRP:CD2	1:J:595:ARG:HB2	2.53	0.44
1:M:547:LEU:HD23	1:M:547:LEU:HA	1.61	0.44
1:A:482:ARG:HH22	2:B:1001:A:P	2.39	0.44
1:D:394:CYS:HB3	1:D:486:PHE:CE1	2.52	0.44
1:D:609:LEU:HD23	1:D:609:LEU:HA	1.82	0.44
1:D:624:GLU:OE2	1:D:679:THR:OG1	2.35	0.44
1:J:478:TRP:CD1	1:J:481:ALA:H	2.35	0.44
1:M:824:MET:HE3	1:M:824:MET:HA	2.00	0.44
1:P:507:VAL:HG21	1:P:515:LEU:HG	1.99	0.44
2:Q:1003:U:H2'	2:Q:1004:A:C8	2.52	0.44
1:D:295:ASP:CG	1:D:582:ARG:HH22	2.25	0.44
1:G:291:SER:HB3	1:G:310:GLU:HG3	1.99	0.44
1:D:550:GLU:CD	1:D:599:ARG:HH12	2.25	0.44
1:G:569:PHE:O	1:G:574:GLN:HG2	2.18	0.44
1:J:333:ASP:O	1:J:339:THR:HG21	2.18	0.44
1:J:391:PRO:HD3	1:J:497:TRP:CZ2	2.53	0.44
1:J:475:TRP:CD1	1:J:475:TRP:N	2.86	0.44
1:M:423:ARG:HA	1:M:423:ARG:HD3	1.82	0.44
1:A:343:MET:SD	1:A:460:LYS:HG2	2.58	0.43
1:A:452:TYR:CZ	1:A:477:MET:HE2	2.53	0.43
1:D:884:PRO:HA	1:D:889:PHE:C	2.43	0.43
1:G:622:GLN:HE21	1:G:658:MET:CE	2.31	0.43
1:G:746:TRP:CH2	1:G:748:LEU:HB2	2.53	0.43
1:J:788:VAL:HG22	1:J:803:TRP:CD1	2.53	0.43
1:M:671:ASP:OD2	1:M:673:ARG:NH2	2.47	0.43
1:A:770:ARG:HH21	1:A:841:LYS:HA	1.82	0.43
1:A:820:GLU:O	1:A:822:PRO:HD3	2.18	0.43
1:D:343:MET:HE3	1:D:741:SER:C	2.43	0.43
1:G:646:TRP:O	1:G:650:VAL:HG22	2.19	0.43
1:P:529:ALA:HB1	1:P:700:TRP:C	2.43	0.43
1:A:752:ALA:HB1	1:A:783:VAL:HG22	1.99	0.43
1:M:384:GLU:HA	1:M:387:LYS:HD3	1.99	0.43
1:A:413:PHE:HE2	1:A:449:THR:HA	1.83	0.43
1:A:849:SER:OG	1:A:851:ILE:HG12	2.18	0.43
1:D:355:PHE:CD2	1:D:454:MET:HE1	2.54	0.43
1:G:774:LEU:HA	1:G:886:MET:HE1	2.00	0.43
1:M:777:ASN:ND2	1:M:886:MET:HE2	2.33	0.43
2:Q:1001:A:H2'	2:Q:1002:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ARG:NH2	1:A:591:ASP:OD1	2.50	0.43
1:D:378:ALA:HB2	5:D:2003:GOL:C3	2.49	0.43
1:A:285:LYS:HG3	1:A:292:TRP:CE2	2.54	0.43
1:D:343:MET:HE1	1:D:460:LYS:HE2	2.01	0.43
1:D:804:MET:HE2	1:D:804:MET:HA	2.00	0.43
1:P:517:TYR:CE1	1:P:725:VAL:HB	2.53	0.43
1:P:520:ARG:HD3	1:P:703:TRP:CZ2	2.54	0.43
1:P:703:TRP:HA	1:P:706:VAL:HG12	2.01	0.43
1:A:324:VAL:HG23	6:A:2110:HOH:O	2.17	0.43
1:A:454:MET:HE3	1:A:578:VAL:HG11	2.01	0.43
1:A:631:SER:HB2	1:D:465:PHE:CZ	2.54	0.43
1:G:322:ASN:OD1	1:G:325:VAL:HG23	2.18	0.43
1:M:621:ARG:HG2	1:M:674:PHE:CE1	2.54	0.43
1:D:671:ASP:OD2	1:D:673:ARG:NH2	2.38	0.43
1:D:849:SER:OG	1:D:851:ILE:HG12	2.18	0.43
3:I:1097:A:H2'	3:I:1098:U:C6	2.54	0.43
1:D:824:MET:HE3	1:D:825:GLU:N	2.33	0.43
1:J:319:SER:HB3	1:J:343:MET:HB2	2.00	0.43
1:J:529:ALA:O	1:J:669:PRO:HD2	2.19	0.43
1:J:681:LEU:HA	1:J:684:MET:HE3	2.00	0.43
1:M:400:THR:CG2	1:M:426:VAL:HB	2.45	0.43
1:M:886:MET:HE3	1:M:886:MET:HB2	1.86	0.43
1:A:770:ARG:NH2	1:A:841:LYS:CA	2.82	0.43
1:G:653:GLU:OE1	1:G:654:ARG:NH1	2.49	0.43
1:P:298:HIS:HD2	1:P:300:TYR:H	1.67	0.43
1:P:599:ARG:NE	1:P:610:ASN:OD1	2.49	0.43
1:A:513:HIS:HD2	6:B:1104:HOH:O	2.02	0.42
1:A:539:ASP:OD1	1:A:599:ARG:HG2	2.19	0.42
1:A:636:THR:HB	1:A:639:GLU:HB2	2.01	0.42
1:A:716:LEU:HD12	1:A:716:LEU:HA	1.77	0.42
6:A:2125:HOH:O	2:B:1003:U:H4'	2.18	0.42
2:E:1004:A:H2'	2:E:1005:U:C6	2.53	0.42
1:G:374:MET:SD	1:G:684:MET:HG2	2.59	0.42
1:J:609:LEU:HD23	1:J:609:LEU:HA	1.85	0.42
1:J:612:PHE:HA	1:J:615:MET:HE3	2.01	0.42
1:M:720:ASP:OD2	1:M:720:ASP:N	2.52	0.42
1:P:453:ASN:N	1:P:476:TYR:O	2.34	0.42
1:A:534:ASP:OD1	1:A:534:ASP:N	2.52	0.42
1:G:338:VAL:HG13	1:G:736:GLY:HA2	2.01	0.42
1:G:819:GLN:HG2	1:G:820:GLU:HG2	2.01	0.42
1:J:750:GLU:OE2	1:J:750:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:475:TRP:CE3	1:M:600:GLY:HA2	2.53	0.42
1:P:712:HIS:CD2	1:P:714:HIS:CD2	3.08	0.42
1:P:768:HIS:HB2	1:P:839:LEU:CD1	2.48	0.42
1:P:850:LEU:O	1:P:853:LEU:HB2	2.18	0.42
1:A:270:GLU:HA	1:A:362:ARG:HH22	1.85	0.42
1:A:792:ARG:HH11	3:C:1098:U:P	2.42	0.42
1:D:525:LYS:HD2	1:D:657:ARG:HG2	2.01	0.42
1:D:746:TRP:CZ3	1:M:873:LEU:HD11	2.54	0.42
1:G:644:LYS:O	1:G:648:VAL:HG13	2.19	0.42
1:D:637:VAL:HG21	1:P:357:GLU:HG3	2.01	0.42
1:A:512:LEU:O	1:A:512:LEU:HG	2.15	0.42
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.66	0.42
1:J:291:SER:O	1:J:293:HIS:HD2	2.03	0.42
1:J:871:ARG:HD3	1:J:879:TYR:CD2	2.54	0.42
1:M:382:TRP:CZ2	1:M:553:VAL:HB	2.55	0.42
1:G:688:ARG:NH2	1:G:695:GLU:O	2.52	0.42
1:P:516:GLY:C	1:P:725:VAL:HG11	2.44	0.42
1:A:833:TRP:CE3	1:A:836:ILE:HD12	2.54	0.42
1:D:366:PRO:O	1:D:371:LYS:HE3	2.20	0.42
1:D:455:MET:SD	1:D:476:TYR:HE2	2.42	0.42
1:G:341:MET:HE3	1:G:461:LYS:N	2.34	0.42
1:G:457:LYS:HD3	1:G:472:ARG:CZ	2.49	0.42
1:J:277:ILE:HG13	1:J:281:ILE:HD12	2.01	0.42
1:J:883:MET:N	1:J:884:PRO:CD	2.83	0.42
1:M:412:ILE:HG23	1:M:579:ARG:HH11	1.84	0.42
1:M:562:LYS:NZ	1:M:566:GLU:OE2	2.52	0.42
2:N:1007:U:H2'	2:N:1008:C:C6	2.55	0.42
1:G:437:LYS:O	1:G:441:LEU:HD13	2.20	0.42
1:J:768:HIS:CD2	1:J:768:HIS:H	2.38	0.42
1:P:722:ARG:HD2	1:P:824:MET:SD	2.60	0.42
2:B:1004:A:H2'	2:B:1005:U:C6	2.55	0.42
1:D:720:ASP:OD2	1:D:722:ARG:NH2	2.52	0.42
1:G:678:LEU:HD22	1:G:688:ARG:NH1	2.35	0.42
1:G:863:ILE:HD12	1:G:863:ILE:HA	1.85	0.42
1:J:315:GLY:HA3	1:J:346:THR:O	2.20	0.42
1:J:319:SER:CB	1:J:343:MET:HG2	2.50	0.42
1:J:437:LYS:HE2	1:J:437:LYS:HB3	1.75	0.42
1:J:851:ILE:HA	1:J:856:ARG:HD2	2.01	0.42
1:M:380:TRP:CD1	1:M:647:LEU:HB3	2.55	0.42
2:N:999:C:H6	2:N:999:C:O5'	2.03	0.42
1:A:810:LEU:HB2	1:A:833:TRP:NE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:392:ARG:NH1	1:J:398:GLU:OE2	2.52	0.42
1:P:462:LEU:HD23	1:P:462:LEU:HA	1.75	0.42
1:D:320:MET:HG3	1:D:744:ALA:C	2.45	0.41
1:G:374:MET:HG2	1:G:684:MET:HE3	2.01	0.41
1:G:530:MET:HE1	1:G:703:TRP:CB	2.50	0.41
1:P:454:MET:CG	1:P:475:TRP:HD1	2.33	0.41
1:J:550:GLU:HG2	1:J:609:LEU:HD22	2.01	0.41
1:M:297:ASP:N	1:M:297:ASP:OD1	2.52	0.41
1:M:634:HIS:HE1	1:M:636:THR:HA	1.85	0.41
1:P:507:VAL:HG23	1:P:518:ILE:CD1	2.47	0.41
1:P:761:MET:SD	1:P:766:TYR:HE2	2.43	0.41
1:D:400:THR:O	1:D:423:ARG:NH2	2.37	0.41
1:D:763:SER:O	1:D:767:PHE:HB3	2.21	0.41
1:G:663:ASP:OD1	1:G:663:ASP:N	2.49	0.41
1:J:714:HIS:O	1:J:725:VAL:HA	2.21	0.41
1:M:374:MET:HE1	6:M:2108:HOH:O	2.19	0.41
1:M:720:ASP:HB2	1:M:722:ARG:HG3	2.01	0.41
1:D:523:SER:CB	1:D:530:MET:HE1	2.51	0.41
1:G:475:TRP:O	1:G:602:GLY:HA3	2.21	0.41
1:G:702:ASP:OD1	1:G:705:GLN:NE2	2.53	0.41
1:G:810:LEU:HD12	1:G:810:LEU:HA	1.80	0.41
1:D:370:THR:O	1:D:374:MET:HG3	2.20	0.41
1:D:584:THR:OG1	1:D:587:GLY:O	2.31	0.41
1:D:636:THR:HG23	1:D:639:GLU:OE1	2.21	0.41
1:G:529:ALA:O	1:G:669:PRO:HD2	2.21	0.41
1:J:273:ASN:OD1	1:J:275:ASP:HB3	2.20	0.41
1:J:784:PRO:HB2	1:J:787:TRP:CD1	2.56	0.41
1:P:298:HIS:HD2	1:P:300:TYR:N	2.18	0.41
1:P:442:HIS:CD2	1:P:447:CYS:HA	2.55	0.41
1:P:764:LEU:HG	1:P:765:MET:SD	2.60	0.41
1:G:619:LEU:HD23	1:G:619:LEU:HA	1.83	0.41
1:J:371:LYS:HG2	1:J:545:GLU:HG3	2.03	0.41
1:J:408:ALA:HB2	2:K:999:C:H5'	2.01	0.41
1:J:612:PHE:O	1:J:615:MET:HB2	2.20	0.41
1:J:765:MET:HE2	1:J:765:MET:HB2	1.89	0.41
1:J:784:PRO:HG2	1:J:787:TRP:CE2	2.56	0.41
1:M:454:MET:HE2	1:M:475:TRP:CE2	2.55	0.41
1:M:645:ASN:O	1:M:648:VAL:N	2.53	0.41
1:P:810:LEU:HD12	1:P:810:LEU:HA	1.87	0.41
1:P:813:TRP:CE2	1:P:836:ILE:HD13	2.55	0.41
1:D:393:MET:HE1	1:D:439:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:381:LEU:HD21	1:G:615:MET:HE2	2.02	0.41
1:G:439:ARG:NH1	1:G:487:GLU:OE2	2.54	0.41
2:K:1007:U:H2'	2:K:1008:C:C6	2.55	0.41
1:M:557:MET:CE	1:M:562:LYS:HA	2.47	0.41
1:P:700:TRP:CD1	1:P:705:GLN:HB3	2.56	0.41
2:B:1006:A:H2'	2:B:1007:U:O4'	2.20	0.41
1:D:595:ARG:HH11	1:D:597:ASP:HB3	1.84	0.41
1:D:798:HIS:CE1	1:D:801:HIS:H	2.39	0.41
1:G:557:MET:HE3	1:G:561:HIS:CE1	2.55	0.41
1:G:820:GLU:O	1:G:822:PRO:HD3	2.21	0.41
1:J:649:ARG:HG2	1:J:650:VAL:HG13	2.01	0.41
1:M:619:LEU:HD23	1:M:619:LEU:HA	1.72	0.41
1:P:503:SER:C	1:P:505:SER:H	2.28	0.41
1:A:595:ARG:NE	1:A:597:ASP:OD1	2.31	0.41
1:A:611:THR:O	1:A:615:MET:HG3	2.20	0.41
1:A:695:GLU:HG2	1:D:693:GLN:NE2	2.36	0.41
1:A:770:ARG:HH11	1:A:770:ARG:CG	2.34	0.41
1:J:611:THR:HG23	1:J:660:ILE:HG22	2.03	0.41
1:J:679:THR:HG22	1:J:694:TRP:HE1	1.85	0.41
1:M:554:THR:HA	1:M:557:MET:SD	2.60	0.41
1:M:788:VAL:HA	1:M:789:PRO:HD3	1.96	0.41
2:N:1000:G:H2'	2:N:1001:A:H8	1.85	0.41
2:E:1000:G:H2'	2:E:1001:A:C8	2.56	0.40
1:J:605:VAL:CG2	1:J:609:LEU:HD12	2.52	0.40
1:M:537:GLY:O	1:M:540:THR:OG1	2.39	0.40
1:P:399:PHE:O	1:P:403:VAL:HG13	2.21	0.40
1:D:863:ILE:HD12	1:D:863:ILE:HA	1.94	0.40
1:J:313:GLN:HG3	1:J:348:PRO:HG2	2.03	0.40
1:P:399:PHE:HE2	1:P:479:LEU:HD11	1.86	0.40
1:A:756:LYS:HE2	1:A:803:TRP:CE3	2.56	0.40
1:A:826:ASP:CG	1:A:828:THR:HG1	2.22	0.40
1:G:412:ILE:HG23	1:G:579:ARG:NH1	2.36	0.40
1:G:430:GLY:O	1:G:434:LEU:HD13	2.21	0.40
1:G:541:ARG:O	1:G:686:LYS:NZ	2.54	0.40
1:J:550:GLU:OE1	1:J:599:ARG:NH2	2.54	0.40
1:M:397:GLU:HA	1:M:400:THR:OG1	2.21	0.40
1:P:718:MET:HB2	1:P:718:MET:HE3	1.63	0.40
1:P:768:HIS:HB2	1:P:839:LEU:HD13	2.04	0.40
1:D:605:VAL:HG21	1:D:609:LEU:HD12	2.03	0.40
1:J:761:MET:SD	1:J:766:TYR:HE2	2.44	0.40
1:M:645:ASN:O	1:M:646:TRP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:695:GLU:CD	1:M:696:PRO:HD2	2.46	0.40
1:P:781:SER:HB2	1:P:867:ILE:HD12	2.03	0.40
1:A:340:GLN:HA	1:P:334:ILE:HG22	2.04	0.40
1:G:530:MET:HE3	1:G:530:MET:HB2	1.71	0.40
1:G:815:ARG:HA	1:G:819:GLN:HB3	2.03	0.40
1:J:380:TRP:O	1:J:384:GLU:HG2	2.22	0.40
1:J:528:GLY:O	1:J:668:LYS:HE3	2.21	0.40
1:M:328:LEU:HD22	1:M:779:ILE:HD13	2.04	0.40
3:O:1097:A:H2'	3:O:1098:U:C6	2.56	0.40
1:P:517:TYR:HB3	1:P:823:TRP:CE2	2.57	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	618/647 (96%)	586 (95%)	30 (5%)	2 (0%)	36	54
1	D	619/647 (96%)	592 (96%)	26 (4%)	1 (0%)	43	62
1	G	621/647 (96%)	605 (97%)	16 (3%)	0	100	100
1	J	621/647 (96%)	595 (96%)	26 (4%)	0	100	100
1	M	622/647 (96%)	593 (95%)	27 (4%)	2 (0%)	36	54
1	P	607/647 (94%)	559 (92%)	42 (7%)	6 (1%)	12	25
All	All	3708/3882 (96%)	3530 (95%)	167 (4%)	11 (0%)	36	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	601	SER
1	M	646	TRP

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Mol	Chain	Res	Type
1	A	767	PHE
1	D	601	SER
1	P	488	ALA
1	P	499	SER
1	A	507	VAL
1	M	804	MET
1	P	839	LEU
1	P	827	LYS
1	P	445	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	505/564 (90%)	488 (97%)	17 (3%)	32	58
1	D	508/564 (90%)	498 (98%)	10 (2%)	48	71
1	G	494/564 (88%)	479 (97%)	15 (3%)	36	61
1	J	502/564 (89%)	490 (98%)	12 (2%)	43	67
1	M	504/564 (89%)	494 (98%)	10 (2%)	48	71
1	P	318/564 (56%)	303 (95%)	15 (5%)	23	47
All	All	2831/3384 (84%)	2752 (97%)	79 (3%)	38	62

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	SER
1	A	296	GLN
1	A	311	THR
1	A	334	ILE
1	A	381	LEU
1	A	475	TRP
1	A	478	TRP
1	A	535	THR
1	A	582	ARG

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Mol	Chain	Res	Type
1	A	633	GLN
1	A	715	GLU
1	A	763	SER
1	A	806	THR
1	A	816	VAL
1	A	832	SER
1	A	842	ARG
1	A	855	SER
1	D	276	ILE
1	D	384	GLU
1	D	396	ARG
1	D	464	GLU
1	D	475	TRP
1	D	514	LYS
1	D	638	THR
1	D	800	THR
1	D	806	THR
1	D	855	SER
1	G	390	THR
1	G	397	GLU
1	G	449	THR
1	G	453	ASN
1	G	475	TRP
1	G	478	TRP
1	G	594	SER
1	G	636	THR
1	G	670	LEU
1	G	697	SER
1	G	723	VAL
1	G	763	SER
1	G	854	THR
1	G	863	ILE
1	G	872	SER
1	J	290	THR
1	J	326	ARG
1	J	363	THR
1	J	409	LEU
1	J	475	TRP
1	J	478	TRP
1	J	553	VAL
1	J	560	GLU
1	J	663	ASP

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Mol	Chain	Res	Type
1	J	720	ASP
1	J	830	VAL
1	J	872	SER
1	M	271	THR
1	M	291	SER
1	M	314	THR
1	M	400	THR
1	M	478	TRP
1	M	507	VAL
1	M	558	GLU
1	M	720	ASP
1	M	747	SER
1	M	828	THR
1	P	405	SER
1	P	438	GLU
1	P	502	ASN
1	P	526	GLU
1	P	550	GLU
1	P	588	THR
1	P	613	THR
1	P	616	GLU
1	P	664	ASP
1	P	722	ARG
1	P	754	LEU
1	P	796	SER
1	P	805	THR
1	P	808	ASP
1	P	872	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	288	HIS
1	A	296	GLN
1	A	298	HIS
1	A	417	ASN
1	A	453	ASN
1	A	502	ASN
1	A	555	ASN
1	A	575	ASN
1	A	618	GLN

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Mol	Chain	Res	Type
1	A	692	GLN
1	A	730	ASN
1	A	731	GLN
1	A	819	GLN
1	D	288	HIS
1	D	298	HIS
1	D	618	GLN
1	D	622	GLN
1	D	705	GLN
1	D	731	GLN
1	D	777	ASN
1	D	864	GLN
1	G	306	HIS
1	G	340	GLN
1	G	513	HIS
1	G	618	GLN
1	G	622	GLN
1	G	731	GLN
1	G	786	HIS
1	G	798	HIS
1	G	819	GLN
1	J	293	HIS
1	J	298	HIS
1	J	351	GLN
1	J	406	ASN
1	J	417	ASN
1	J	731	GLN
1	J	801	HIS
1	J	814	ASN
1	M	313	GLN
1	M	406	ASN
1	M	440	ASN
1	M	513	HIS
1	M	618	GLN
1	M	682	ASN
1	M	701	ASN
1	M	731	GLN
1	M	768	HIS
1	M	777	ASN
1	M	798	HIS
1	P	298	HIS
1	P	513	HIS

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Mol	Chain	Res	Type
1	P	603	GLN
1	P	614	ASN
1	P	730	ASN
1	P	768	HIS
1	P	821	ASN
1	P	845	GLN
1	P	862	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	11/30 (36%)	0	0
2	E	10/30 (33%)	0	0
2	H	10/30 (33%)	0	0
2	K	11/30 (36%)	1 (9%)	0
2	N	11/30 (36%)	0	0
2	Q	10/30 (33%)	1 (10%)	0
3	C	8/9 (88%)	0	0
3	F	8/9 (88%)	1 (12%)	0
3	I	8/9 (88%)	1 (12%)	0
3	L	8/9 (88%)	0	0
3	O	8/9 (88%)	0	0
3	R	8/9 (88%)	3 (37%)	0
All	All	111/234 (47%)	7 (6%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	F	1094	G
3	I	1094	G
2	K	1007	U
2	Q	1000	G
3	R	1094	G
3	R	1095	A
3	R	1096	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	D	2003	-	5,5,5	1.34	0	5,5,5	1.46	1 (20%)
5	GOL	C	1201	-	5,5,5	1.17	0	5,5,5	0.79	0
5	GOL	P	2003	-	5,5,5	1.40	1 (20%)	5,5,5	0.81	0
5	GOL	M	2003	-	5,5,5	1.52	2 (40%)	5,5,5	0.82	0
5	GOL	E	1101	-	5,5,5	1.58	2 (40%)	5,5,5	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	2003	-	-	2/4/4/4	-
5	GOL	C	1201	-	-	4/4/4/4	-
5	GOL	P	2003	-	-	2/4/4/4	-
5	GOL	M	2003	-	-	0/4/4/4	-
5	GOL	E	1101	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1101	GOL	C3-C2	2.53	1.61	1.51
5	M	2003	GOL	C1-C2	2.47	1.61	1.51
5	P	2003	GOL	C1-C2	2.42	1.61	1.51
5	E	1101	GOL	C1-C2	2.38	1.60	1.51
5	M	2003	GOL	C3-C2	2.28	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2003	GOL	C3-C2-C1	-2.47	102.74	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1201	GOL	O1-C1-C2-C3
5	C	1201	GOL	C1-C2-C3-O3
5	C	1201	GOL	O2-C2-C3-O3
5	D	2003	GOL	O1-C1-C2-C3
5	P	2003	GOL	O2-C2-C3-O3
5	P	2003	GOL	C1-C2-C3-O3
5	C	1201	GOL	O1-C1-C2-O2
5	D	2003	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2003	GOL	2	0
5	C	1201	GOL	3	0
5	M	2003	GOL	3	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	620/647 (95%)	-0.20	5 (0%) 82 78	42, 61, 81, 119	0
1	D	621/647 (95%)	-0.15	9 (1%) 73 67	44, 65, 91, 110	0
1	G	623/647 (96%)	-0.10	5 (0%) 82 78	48, 70, 97, 133	0
1	J	623/647 (96%)	-0.10	5 (0%) 82 78	50, 68, 90, 135	0
1	M	624/647 (96%)	-0.22	3 (0%) 87 85	46, 63, 84, 115	0
1	P	611/647 (94%)	1.15	121 (19%) 3 3	54, 116, 154, 177	0
2	B	12/30 (40%)	-0.45	0 100 100	46, 51, 85, 113	2 (16%)
2	E	11/30 (36%)	-0.48	0 100 100	55, 59, 72, 95	0
2	H	11/30 (36%)	-0.23	1 (9%) 15 11	56, 65, 76, 80	1 (9%)
2	K	12/30 (40%)	0.01	1 (8%) 17 13	55, 65, 86, 107	2 (16%)
2	N	12/30 (40%)	-0.22	0 100 100	53, 58, 75, 92	2 (16%)
2	Q	11/30 (36%)	0.44	0 100 100	85, 96, 108, 112	0
3	C	9/9 (100%)	-1.07	0 100 100	47, 53, 54, 57	0
3	F	9/9 (100%)	-0.60	0 100 100	52, 56, 70, 79	0
3	I	9/9 (100%)	-0.46	0 100 100	58, 63, 68, 79	0
3	L	9/9 (100%)	-0.40	0 100 100	60, 64, 77, 79	0
3	O	9/9 (100%)	-0.06	0 100 100	56, 59, 83, 88	0
3	R	9/9 (100%)	0.83	1 (11%) 10 8	85, 92, 108, 109	0
All	All	3845/4116 (93%)	0.05	151 (3%) 43 34	42, 67, 129, 177	7 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	569	PHE	5.5
1	P	416	GLU	4.6
1	P	656	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	P	412	ILE	4.3
1	P	597	ASP	4.3
1	P	675	ALA	4.3
1	M	268	GLU	4.2
1	P	497	TRP	4.1
1	P	639	GLU	4.1
1	P	608	GLY	4.0
1	P	512	LEU	3.9
1	P	303	TRP	3.9
1	P	485	GLU	3.8
1	P	544	LEU	3.8
1	P	551	GLU	3.8
1	P	478	TRP	3.8
1	P	545	GLU	3.7
1	P	581	GLN	3.7
1	P	564	LEU	3.7
1	D	634	HIS	3.7
1	P	674	PHE	3.6
1	P	817	TRP	3.6
1	P	619	LEU	3.6
1	G	633	GLN	3.6
1	P	531	TYR	3.6
1	A	885	SER	3.5
1	P	276	ILE	3.5
1	P	643	VAL	3.4
1	P	684	MET	3.4
1	P	514	LYS	3.4
1	P	819	GLN	3.4
1	P	373	LEU	3.3
1	P	395	THR	3.3
1	P	314	THR	3.3
1	P	414	THR	3.3
1	P	666	VAL	3.2
1	P	369	GLY	3.2
1	P	549	ASN	3.1
1	P	277	ILE	3.1
1	P	672	ASP	3.1
1	P	615	MET	3.1
1	P	270	GLU	3.0
1	P	560	GLU	2.9
1	P	682	ASN	2.9
1	P	392	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	P	382	TRP	2.9
1	P	696	PRO	2.9
1	J	268	GLU	2.9
1	P	374	MET	2.8
1	P	629	PHE	2.8
1	P	471	SER	2.8
1	P	620	ILE	2.8
1	P	415	ASP	2.8
1	P	798	HIS	2.8
1	P	273	ASN	2.8
1	P	576	LYS	2.8
1	P	453	ASN	2.7
1	P	655	LEU	2.7
1	D	275	ASP	2.7
1	D	269	SER	2.7
1	P	660	ILE	2.6
1	D	637	VAL	2.6
1	P	624	GLU	2.6
1	P	501	GLU	2.6
1	P	475	TRP	2.5
1	P	554	THR	2.5
1	P	280	ARG	2.5
1	P	601	SER	2.5
1	P	511	GLY	2.5
1	A	294	TYR	2.5
1	G	631	SER	2.5
1	P	552	MET	2.5
1	P	680	ALA	2.5
1	P	406	ASN	2.5
1	P	413	PHE	2.4
1	P	617	ALA	2.4
1	J	631	SER	2.4
1	J	750	GLU	2.4
1	P	289	GLU	2.4
1	P	529	ALA	2.4
1	P	694	TRP	2.4
1	D	273	ASN	2.4
1	P	701	ASN	2.4
1	P	568	ILE	2.4
1	G	556	HIS	2.4
1	P	826	ASP	2.4
1	P	310	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	364	GLN	2.4
1	P	821	ASN	2.3
1	A	886	MET	2.3
1	P	697	SER	2.3
1	J	801	HIS	2.3
1	P	449	THR	2.3
1	P	492	LEU	2.3
1	P	818	ILE	2.3
1	P	640	GLU	2.3
1	P	642	ALA	2.3
1	P	659	ALA	2.3
1	P	618	GLN	2.3
1	P	293	HIS	2.3
1	P	667	VAL	2.3
1	P	491	PHE	2.3
1	M	539	ASP	2.3
1	D	742	GLN	2.3
1	P	556	HIS	2.3
3	R	1093	G	2.3
1	D	790	THR	2.3
1	A	296	GLN	2.2
1	P	622	GLN	2.2
1	P	813	TRP	2.2
1	P	661	SER	2.2
1	P	831	GLU	2.2
1	P	809	MET	2.2
1	J	677	ALA	2.2
1	P	614	ASN	2.2
1	M	890	ARG	2.2
1	P	377	THR	2.2
1	P	419	TRP	2.2
1	P	410	GLY	2.2
1	P	657	ARG	2.2
2	K	998	A	2.2
1	G	471	SER	2.2
1	P	519	LEU	2.2
1	P	313	GLN	2.1
1	P	533	ASP	2.1
1	P	427	GLU	2.1
1	P	275	ASP	2.1
1	A	584	THR	2.1
2	H	999	C	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	454	MET	2.1
1	P	600	GLY	2.1
1	P	654	ARG	2.1
1	P	429	SER	2.1
1	P	645	ASN	2.1
1	P	292	TRP	2.1
1	P	646	TRP	2.1
1	P	700	TRP	2.1
1	P	838	TYR	2.1
1	P	658	MET	2.0
1	P	424	GLU	2.0
1	P	557	MET	2.0
1	D	601	SER	2.0
1	P	577	VAL	2.0
1	D	406	ASN	2.0
1	P	555	ASN	2.0
1	P	386	GLY	2.0
1	P	290	THR	2.0
1	P	775	ALA	2.0
1	G	289	GLU	2.0
1	P	538	TRP	2.0
1	P	605	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	P	2003	6/6	0.73	0.23	59,61,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	P	2002	1/1	0.91	0.07	142,142,142,142	1
5	GOL	D	2003	6/6	0.92	0.18	66,67,68,72	0
5	GOL	M	2003	6/6	0.94	0.12	53,56,60,63	0
5	GOL	C	1201	6/6	0.94	0.17	46,53,59,63	6
5	GOL	E	1101	6/6	0.95	0.16	57,61,64,66	0
4	ZN	P	2001	1/1	0.98	0.04	90,90,90,90	0
4	ZN	M	2002	1/1	0.99	0.03	52,52,52,52	1
4	ZN	A	2001	1/1	0.99	0.03	51,51,51,51	1
4	ZN	A	2002	1/1	0.99	0.03	51,51,51,51	1
4	ZN	G	2001	1/1	0.99	0.03	51,51,51,51	1
4	ZN	G	2002	1/1	0.99	0.03	68,68,68,68	1
4	ZN	J	2001	1/1	0.99	0.03	55,55,55,55	1
4	ZN	J	2002	1/1	0.99	0.02	65,65,65,65	0
4	ZN	M	2001	1/1	0.99	0.03	68,68,68,68	0
4	ZN	D	2002	1/1	1.00	0.02	74,74,74,74	0
4	ZN	D	2001	1/1	1.00	0.04	47,47,47,47	1

6.5 Other polymers [i](#)

There are no such residues in this entry.