



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 06:29 PM EDT

PDB ID : 1P4E
Title : Flpe W330F mutant-DNA Holliday Junction Complex
Authors : Rice, P.A.; Chen, Y.
Deposited on : 2003-04-23
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

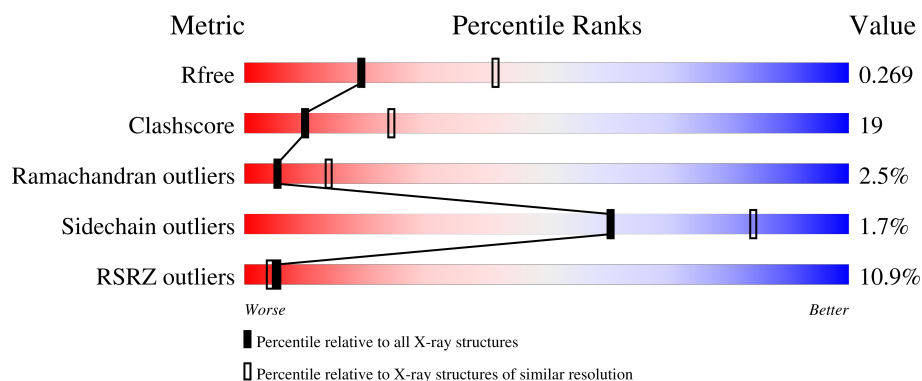
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	E	13	<div> <div>15%</div> <div>85%</div> </div>
1	F	13	<div> <div>38%</div> <div>54%</div> <div>8%</div> </div>
2	I	20	<div> <div>10%</div> <div>35%</div> <div>65%</div> </div>
2	J	20	<div> <div>45%</div> <div>55%</div> </div>
3	G	33	<div> <div>30%</div> <div>70%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	33	
4	A	429	
4	B	429	
5	C	429	
5	D	429	

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
5	PTR	D	343	-	-	X	-
6	2PO	H	513	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16070 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 DNA chain called 5'-D(*TP*AP*AP*GP*TP*TP*CP*CP*TP*AP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			259	127	41	79	12			
1	F	13	Total	C	N	O	P	0	0	0
			259	127	41	79	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	P	0	0	0
			395	189	75	112	19			
2	J	20	Total	C	N	O	P	0	0	0
			395	189	75	112	19			

- Molecule 3 is a DNA chain called 33-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	33	Total	C	N	O	P	0	0	0
			657	316	116	193	32			
3	H	33	Total	C	N	O	P	0	0	0
			654	316	116	191	31			

- Molecule 4 is a protein called Recombinase FLP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	400	Total	C	N	O	S	0	0	0
			3242	2086	546	599	11			
4	B	413	Total	C	N	O	S	0	0	0
			3357	2157	573	616	11			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	PRO	SEE REMARK 999	UNP P03870
A	5	ASP	GLY	variant	UNP P03870
A	33	SER	LEU	SEE REMARK 999	UNP P03870
A	108	ASN	TYR	SEE REMARK 999	UNP P03870
A	294	PRO	SER	SEE REMARK 999	UNP P03870
A	330	PHE	TRP	engineered mutation	UNP P03870
A	424	GLY	-	expression tag	UNP P03870
A	425	HIS	-	expression tag	UNP P03870
A	426	HIS	-	expression tag	UNP P03870
A	427	HIS	-	expression tag	UNP P03870
A	428	HIS	-	expression tag	UNP P03870
A	429	HIS	-	expression tag	UNP P03870
A	430	HIS	-	expression tag	UNP P03870
B	2	SER	PRO	SEE REMARK 999	UNP P03870
B	5	ASP	GLY	variant	UNP P03870
B	33	SER	LEU	SEE REMARK 999	UNP P03870
B	108	ASN	TYR	SEE REMARK 999	UNP P03870
B	294	PRO	SER	SEE REMARK 999	UNP P03870
B	330	PHE	TRP	engineered mutation	UNP P03870
B	424	GLY	-	expression tag	UNP P03870
B	425	HIS	-	expression tag	UNP P03870
B	426	HIS	-	expression tag	UNP P03870
B	427	HIS	-	expression tag	UNP P03870
B	428	HIS	-	expression tag	UNP P03870
B	429	HIS	-	expression tag	UNP P03870
B	430	HIS	-	expression tag	UNP P03870

- Molecule 5 is a protein called Recombinase FLP protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	C	400	Total	C	N	O	P	S	0	0	0
			3263	2100	551	600	1	11			
5	D	409	Total	C	N	O	P	S	0	0	0
			3319	2132	562	613	1	11			

There are 26 discrepancies between the modelled and reference sequences:

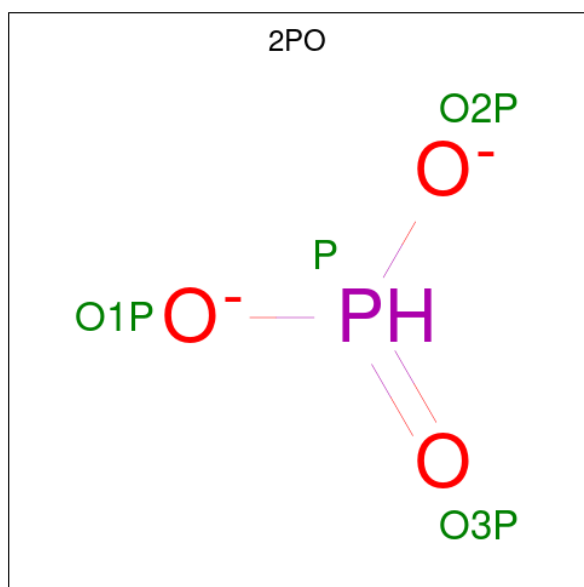
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	PRO	SEE REMARK 999	UNP P03870
C	5	ASP	GLY	variant	UNP P03870
C	33	SER	LEU	SEE REMARK 999	UNP P03870
C	108	ASN	TYR	SEE REMARK 999	UNP P03870
C	294	PRO	SER	SEE REMARK 999	UNP P03870

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Chain	Residue	Modelled	Actual	Comment	Reference
C	330	PHE	TRP	engineered mutation	UNP P03870
C	424	GLY	-	expression tag	UNP P03870
C	425	HIS	-	expression tag	UNP P03870
C	426	HIS	-	expression tag	UNP P03870
C	427	HIS	-	expression tag	UNP P03870
C	428	HIS	-	expression tag	UNP P03870
C	429	HIS	-	expression tag	UNP P03870
C	430	HIS	-	expression tag	UNP P03870
D	2	SER	PRO	SEE REMARK 999	UNP P03870
D	5	ASP	GLY	variant	UNP P03870
D	33	SER	LEU	SEE REMARK 999	UNP P03870
D	108	ASN	TYR	SEE REMARK 999	UNP P03870
D	294	PRO	SER	SEE REMARK 999	UNP P03870
D	330	PHE	TRP	engineered mutation	UNP P03870
D	424	GLY	-	expression tag	UNP P03870
D	425	HIS	-	expression tag	UNP P03870
D	426	HIS	-	expression tag	UNP P03870
D	427	HIS	-	expression tag	UNP P03870
D	428	HIS	-	expression tag	UNP P03870
D	429	HIS	-	expression tag	UNP P03870
D	430	HIS	-	expression tag	UNP P03870

- Molecule 6 is PHOSPHONATE (three-letter code: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	P	0	0
			4	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	9	Total O 9 9	0	0
7	F	13	Total O 13 13	0	0
7	J	19	Total O 19 19	0	0
7	G	19	Total O 19 19	0	0
7	H	14	Total O 14 14	0	0
7	A	2	Total O 2 2	0	0
7	B	98	Total O 98 98	0	0
7	C	24	Total O 24 24	0	0
7	D	68	Total O 68 68	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: 5'-D(*TP*AP*AP*GP*TP*TP*CP*CP*TP*AP*TP*TP*C)-3'

Chain E: 



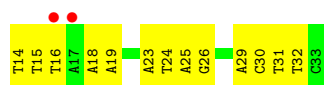
- Molecule 1: 5'-D(*TP*AP*AP*GP*TP*TP*CP*CP*TP*AP*TP*TP*C)-3'

Chain F: 



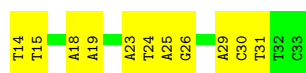
- Molecule 2: 5'-D(*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*TP*AP*GP*GP*AP*AP*CP*TP*TP*C)-3'

Chain I: 



- Molecule 2: 5'-D(*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*TP*AP*GP*GP*AP*AP*CP*TP*TP*C)-3'

Chain J: 



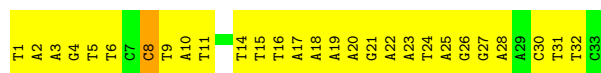
- Molecule 3: 33-MER

Chain G: 



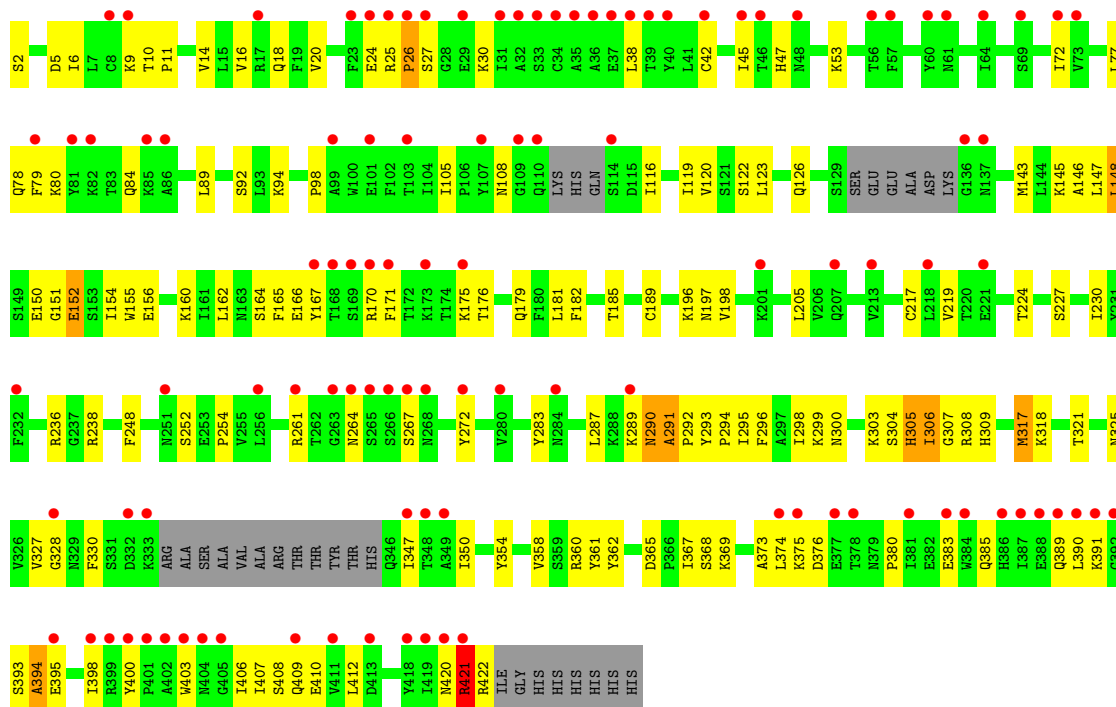
- Molecule 3: 33-MER

Chain H: 15% 82% .



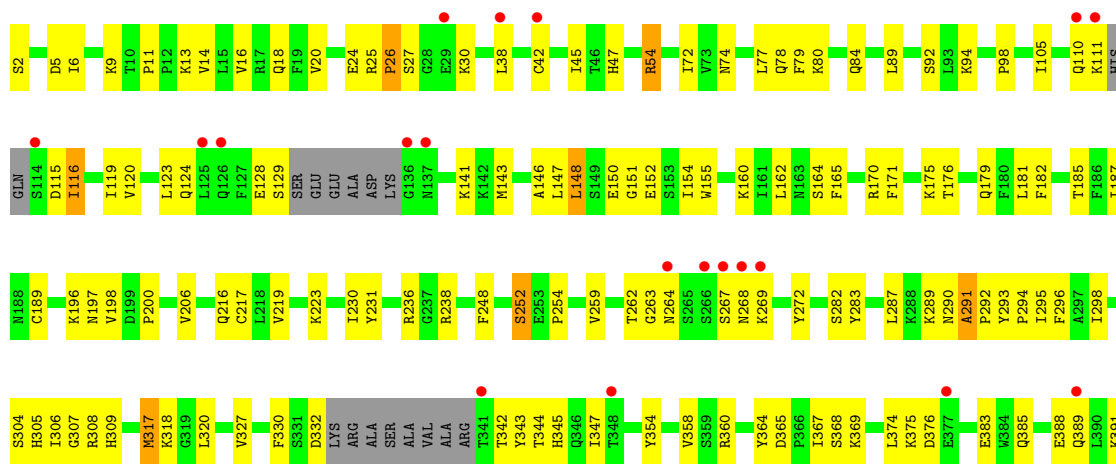
• Molecule 4: Recombinase FLP protein

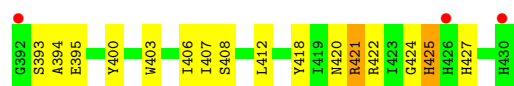
Chain A: 25% 59% 31% . 7%



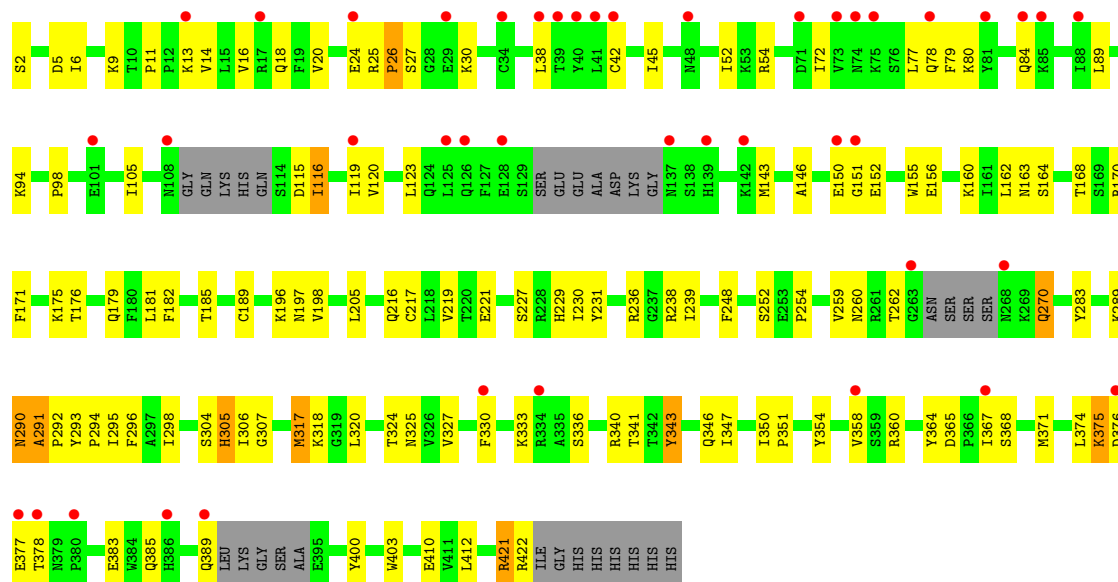
• Molecule 4: Recombinase FLP protein

Chain B: 5% 61% 33% . .

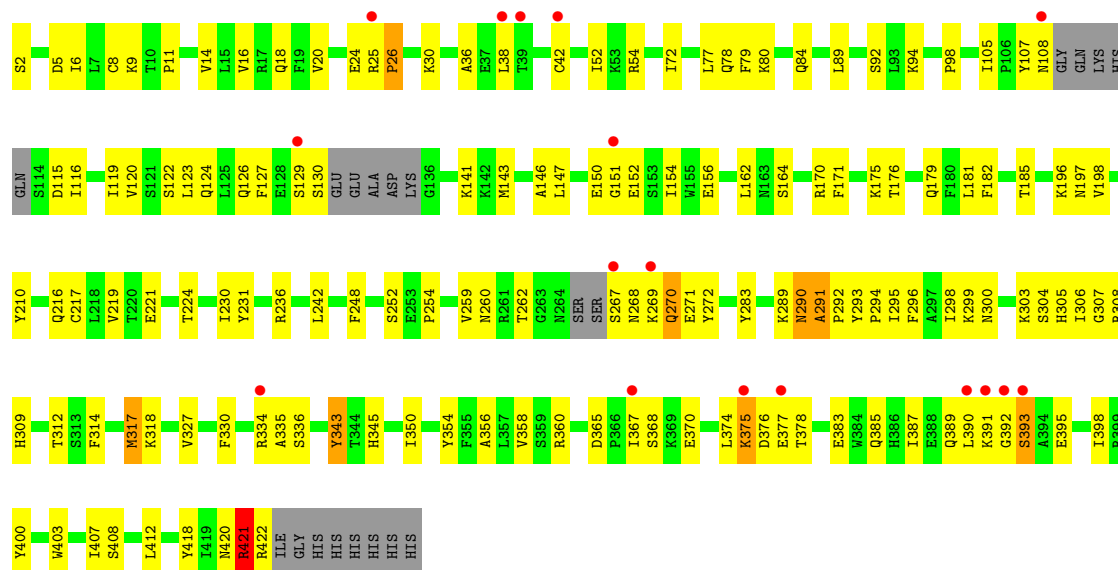




• Molecule 5: Recombinase FLP protein



• Molecule 5: Recombinase FLP protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.76Å 116.72Å 142.05Å 90.00° 97.64° 90.00°	Depositor
Resolution (Å)	21.98 – 2.70 21.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.8 (21.98-2.70) 90.9 (21.98-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.275 0.230 , 0.269	Depositor DCC
R_{free} test set	6513 reflections (9.42%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16070	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: PTR, 2PO

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	E	0.44	0/288	0.84	0/442
1	F	0.62	0/288	0.94	0/442
2	I	0.44	0/444	0.85	0/685
2	J	0.55	0/444	0.89	0/685
3	G	0.52	0/736	0.89	0/1135
3	H	0.50	0/732	0.88	0/1127
4	A	0.32	0/3311	0.55	0/4468
4	B	0.44	0/3434	0.62	0/4637
5	C	0.36	0/3316	0.59	1/4475 (0.0%)
5	D	0.41	0/3373	0.61	1/4552 (0.0%)
All	All	0.41	0/16366	0.66	2/22648 (0.0%)

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	F	0	1
3	H	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	270	GLN	N-CA-C	-5.44	96.32	111.00
5	D	270	GLN	N-CA-C	-5.38	96.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	8	DC	Sidechain
3	H	8	DC	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	E	259	0	150	22	0
1	F	259	0	150	9	0
2	I	395	0	216	22	0
2	J	395	0	216	20	0
3	G	657	0	365	27	0
3	H	654	0	366	56	0
4	A	3242	0	3278	122	0
4	B	3357	0	3371	130	0
5	C	3263	0	3295	101	0
5	D	3319	0	3352	123	0
6	H	4	0	0	2	0
7	A	2	0	0	0	0
7	B	98	0	0	10	0
7	C	24	0	0	3	0
7	D	68	0	0	6	0
7	F	13	0	0	0	0
7	G	19	0	0	0	0
7	H	14	0	0	2	0
7	I	9	0	0	1	0
7	J	19	0	0	0	0
All	All	16070	0	14759	580	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 19.

All (580) 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)
3:H:15:DT:H2''	3:H:16:DT:H5''	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:25:DA:H2''	2:I:26:DG:H5'	1.45	0.97
1:E:4:DG:H2''	1:E:5:DT:H5''	1.47	0.96
2:J:25:DA:H2''	2:J:26:DG:H5'	1.46	0.95
3:H:1:DT:H5'	3:H:1:DT:H6	1.32	0.95
3:H:16:DT:H6	3:H:16:DT:H5'	1.31	0.93
3:H:15:DT:H2''	3:H:16:DT:C5'	2.03	0.87
1:F:8:DC:H2'	1:F:9:DT:H72	1.59	0.85
1:E:2:DA:H2''	1:E:3:DA:N7	1.92	0.83
1:E:8:DC:H2'	1:E:9:DT:H72	1.58	0.83
3:G:8:DC:H2'	3:G:9:DT:H72	1.61	0.82
3:H:8:DC:H2'	3:H:9:DT:H72	1.61	0.82
3:H:15:DT:C2'	3:H:16:DT:H5''	2.13	0.79
3:H:23:DA:H2'	3:H:24:DT:H72	1.64	0.79
1:E:4:DG:H2''	1:E:5:DT:C5'	2.13	0.78
4:B:141:LYS:HE2	7:C:431:HOH:O	1.84	0.78
1:E:2:DA:H2''	1:E:3:DA:C8	2.18	0.77
3:H:16:DT:H5'	3:H:16:DT:C6	2.19	0.77
4:B:342:THR:HG22	5:D:312:THR:HG22	1.67	0.77
2:J:30:DC:H2''	2:J:31:DT:C5'	2.15	0.77
1:E:5:DT:H2'	1:E:6:DT:H71	1.66	0.77
5:D:421:ARG:O	5:D:421:ARG:HD3	1.85	0.76
4:B:110:GLN:O	4:B:111:LYS:HG2	1.86	0.76
3:G:15:DT:H1'	3:G:16:DT:H5''	1.68	0.75
1:E:4:DG:C2'	1:E:5:DT:H5''	2.15	0.74
2:I:30:DC:H2''	2:I:31:DT:C5'	2.17	0.74
2:I:30:DC:H2''	2:I:31:DT:H5'	1.70	0.74
2:J:23:DA:H2'	2:J:24:DT:H71	1.68	0.74
5:C:336:SER:O	5:C:340:ARG:HG3	1.87	0.74
2:J:30:DC:H2''	2:J:31:DT:H5'	1.70	0.74
4:A:421:ARG:HD3	4:A:421:ARG:O	1.88	0.74
5:C:325:ASN:HA	5:C:330:PHE:HD1	1.51	0.73
5:C:421:ARG:O	5:C:421:ARG:HD3	1.88	0.73
3:H:1:DT:H5'	3:H:1:DT:C6	2.20	0.73
4:A:84:GLN:HA	4:A:84:GLN:NE2	2.03	0.73
1:E:13:DC:H3'	5:D:343:PTR:HE1	1.70	0.73
5:C:385:GLN:O	5:C:389:GLN:HG2	1.89	0.72
4:B:309:HIS:HD2	5:C:343:PTR:HA	1.55	0.72
5:D:152:GLU:HA	5:D:156:GLU:OE1	1.88	0.72
5:D:294:PRO:HG2	7:D:461:HOH:O	1.89	0.72
4:A:385:GLN:O	4:A:389:GLN:HG2	1.89	0.72
4:B:421:ARG:HH11	4:B:421:ARG:HG2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:84:GLN:HA	5:C:84:GLN:NE2	2.05	0.71
4:B:84:GLN:HA	4:B:84:GLN:NE2	2.04	0.71
1:E:3:DA:H1'	1:E:4:DG:H5''	1.71	0.71
4:B:385:GLN:O	4:B:389:GLN:HG2	1.91	0.71
5:D:38:LEU:HD21	5:D:79:PHE:CE2	2.26	0.71
3:H:2:DA:H2''	3:H:3:DA:N7	2.06	0.70
1:E:8:DC:OP2	4:A:2:SER:HB2	1.91	0.70
4:A:116:ILE:HD11	5:D:92:SER:HB3	1.72	0.70
5:C:38:LEU:HD21	5:C:79:PHE:CE2	2.26	0.70
4:A:38:LEU:HD21	4:A:79:PHE:CE2	2.26	0.70
5:C:25:ARG:HB2	5:C:30:LYS:NZ	2.07	0.70
4:B:38:LEU:HD21	4:B:79:PHE:CE2	2.27	0.70
5:D:385:GLN:O	5:D:389:GLN:HG2	1.92	0.70
5:D:84:GLN:HA	5:D:84:GLN:NE2	2.06	0.70
3:H:8:DC:H2'	3:H:9:DT:C7	2.22	0.69
2:I:18:DA:H1'	2:I:19:DA:H5''	1.75	0.69
2:I:23:DA:H2'	2:I:24:DT:H72	1.75	0.69
5:D:25:ARG:HB3	5:D:30:LYS:HZ3	1.58	0.69
2:J:18:DA:H1'	2:J:19:DA:H5''	1.73	0.69
4:A:238:ARG:HG3	4:A:238:ARG:HH11	1.58	0.68
4:A:395:GLU:HA	4:A:398:ILE:HD12	1.76	0.68
5:D:52:ILE:HG22	5:D:262:THR:CG2	2.24	0.68
4:B:25:ARG:HB3	4:B:30:LYS:NZ	2.08	0.68
5:D:143:MET:HE2	7:D:498:HOH:O	1.94	0.67
3:G:20:DA:H2''	3:G:21:DG:H5'	1.76	0.67
3:H:20:DA:H2''	3:H:21:DG:C5'	2.24	0.67
2:I:29:DA:H2''	2:I:30:DC:H5''	1.76	0.67
4:A:53:LYS:HE2	4:A:261:ARG:NH2	2.10	0.67
2:I:18:DA:H2''	2:I:19:DA:H5'	1.76	0.67
2:J:18:DA:H2''	2:J:19:DA:H5'	1.77	0.67
4:A:236:ARG:HH11	4:A:374:LEU:HD12	1.60	0.66
5:C:365:ASP:OD2	5:C:367:ILE:HG22	1.94	0.66
4:B:421:ARG:O	4:B:421:ARG:HD3	1.94	0.66
5:C:54:ARG:NH1	5:C:259:VAL:O	2.28	0.66
3:G:8:DC:H2'	3:G:9:DT:C7	2.25	0.66
5:D:196:LYS:HE3	5:D:197:ASN:ND2	2.11	0.66
3:H:14:DT:H2''	3:H:15:DT:C6	2.30	0.66
5:D:421:ARG:HH11	5:D:421:ARG:HG2	1.61	0.66
4:A:84:GLN:HA	4:A:84:GLN:HE21	1.61	0.66
4:A:143:MET:CG	4:A:298:ILE:HD11	2.26	0.66
5:C:421:ARG:HG2	5:C:421:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:377:GLU:HG3	5:D:378:THR:H	1.60	0.65
1:F:8:DC:H2'	1:F:9:DT:C7	2.26	0.65
3:H:10:DA:H1'	3:H:11:DT:H5''	1.78	0.65
5:D:143:MET:HG3	5:D:298:ILE:HD11	1.78	0.65
5:D:365:ASP:OD2	5:D:367:ILE:HG22	1.97	0.65
4:A:325:ASN:ND2	5:D:334:ARG:O	2.30	0.65
5:D:54:ARG:NH1	5:D:259:VAL:O	2.29	0.65
3:G:10:DA:H1'	3:G:11:DT:H5''	1.79	0.64
2:J:29:DA:H2''	2:J:30:DC:H5''	1.78	0.64
4:B:124:GLN:OE1	5:C:13:LYS:HG2	1.98	0.64
4:B:84:GLN:HA	4:B:84:GLN:HE21	1.63	0.64
5:C:377:GLU:HG3	5:C:378:THR:H	1.62	0.64
1:E:8:DC:H2'	1:E:9:DT:C7	2.26	0.64
4:A:421:ARG:HG2	4:A:421:ARG:HH11	1.62	0.63
1:F:4:DG:H1'	1:F:5:DT:H5''	1.81	0.63
4:A:5:ASP:O	4:A:9:LYS:HG2	1.99	0.63
5:C:84:GLN:HA	5:C:84:GLN:HE21	1.64	0.63
4:A:196:LYS:HE3	4:A:197:ASN:ND2	2.13	0.62
3:H:14:DT:H5''	6:H:513:2PO:P	2.39	0.62
4:A:176:THR:CG2	4:A:248:PHE:HA	2.30	0.62
4:A:272:TYR:HE1	4:A:406:ILE:HD12	1.65	0.62
4:A:254:PRO:HG3	4:A:403:TRP:CZ3	2.34	0.62
4:A:283:TYR:HE2	4:A:304:SER:HA	1.65	0.62
4:A:25:ARG:HB2	4:A:30:LYS:NZ	2.13	0.62
4:B:254:PRO:HG3	4:B:403:TRP:CE3	2.35	0.62
4:B:120:VAL:HG11	5:C:16:VAL:HG21	1.82	0.62
4:B:383:GLU:CG	4:B:421:ARG:HE	2.12	0.62
4:A:365:ASP:OD2	4:A:367:ILE:HG22	2.00	0.61
4:B:343:TYR:HB2	5:D:309:HIS:CD2	2.35	0.61
4:B:388:GLU:O	4:B:391:LYS:HE3	1.99	0.61
5:D:267:SER:OG	5:D:269:LYS:HE2	2.01	0.61
3:G:29:DA:H1'	3:G:30:DC:H5''	1.81	0.61
4:A:389:GLN:O	4:A:391:LYS:HD2	2.00	0.61
4:A:393:SER:C	4:A:395:GLU:H	2.03	0.61
5:D:5:ASP:O	5:D:9:LYS:HG2	2.00	0.61
5:D:150:GLU:O	5:D:152:GLU:N	2.33	0.61
4:B:267:SER:O	4:B:268:ASN:ND2	2.34	0.61
5:C:5:ASP:O	5:C:9:LYS:HG2	2.00	0.61
5:C:196:LYS:HE3	5:C:197:ASN:ND2	2.14	0.61
3:H:23:DA:H2'	3:H:24:DT:C7	2.30	0.61
5:D:271:GLU:HG3	5:D:272:TYR:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:23:DA:H2''	3:H:24:DT:C6	2.37	0.60
4:A:116:ILE:O	4:A:120:VAL:HG23	2.00	0.60
4:B:294:PRO:HG2	7:B:461:HOH:O	2.01	0.60
4:A:321:THR:HB	5:D:335:ALA:HB2	1.84	0.60
4:A:143:MET:HG3	4:A:298:ILE:HD11	1.83	0.60
1:E:5:DT:C2'	1:E:6:DT:H71	2.32	0.60
3:H:14:DT:H5''	6:H:513:2PO:O1P	2.02	0.60
4:A:361:TYR:CD2	4:A:380:PRO:HD3	2.37	0.60
5:D:24:GLU:O	5:D:26:PRO:HD3	2.01	0.59
5:C:176:THR:CG2	5:C:248:PHE:HA	2.33	0.59
3:H:22:DA:H1'	3:H:23:DA:H5''	1.85	0.59
4:B:176:THR:CG2	4:B:248:PHE:HA	2.33	0.59
4:B:365:ASP:OD2	4:B:367:ILE:HG22	2.02	0.59
5:C:116:ILE:O	5:C:120:VAL:HG23	2.03	0.59
3:H:30:DC:H2''	3:H:31:DT:H5''	1.85	0.59
5:D:176:THR:CG2	5:D:248:PHE:HA	2.32	0.59
5:D:308:ARG:HH12	5:D:330:PHE:HE2	1.50	0.59
4:A:27:SER:HB3	4:A:30:LYS:HE2	1.84	0.59
4:B:5:ASP:O	4:B:9:LYS:HG2	2.03	0.59
5:C:27:SER:HB3	5:C:30:LYS:HE2	1.85	0.59
5:C:377:GLU:HG3	5:C:378:THR:N	2.17	0.59
3:H:20:DA:H2''	3:H:21:DG:H5'	1.85	0.59
5:D:116:ILE:O	5:D:120:VAL:HG23	2.02	0.59
5:D:383:GLU:CG	5:D:421:ARG:HE	2.16	0.59
4:A:227:SER:HB2	4:A:347:ILE:HG21	1.84	0.58
3:H:5:DT:H2''	3:H:6:DT:H5'	1.84	0.58
2:I:31:DT:H2''	2:I:32:DT:C6	2.39	0.58
2:J:14:DT:H2'	2:J:15:DT:C6	2.38	0.58
3:G:5:DT:H2''	3:G:6:DT:H5'	1.86	0.58
3:H:30:DC:H2''	3:H:31:DT:C5'	2.34	0.58
4:B:148:LEU:CD1	4:B:154:ILE:HD11	2.34	0.58
4:A:26:PRO:HB3	4:A:72:ILE:HG23	1.86	0.58
5:D:84:GLN:HA	5:D:84:GLN:HE21	1.67	0.58
4:A:383:GLU:CG	4:A:421:ARG:HE	2.16	0.57
3:G:23:DA:H2'	3:G:24:DT:H72	1.85	0.57
5:C:383:GLU:CG	5:C:421:ARG:HE	2.16	0.57
4:B:54:ARG:NH1	4:B:259:VAL:O	2.36	0.57
4:B:98:PRO:HD2	7:B:460:HOH:O	2.03	0.57
5:D:94:LYS:HE3	5:D:98:PRO:O	2.04	0.57
4:B:309:HIS:HE1	7:B:505:HOH:O	1.87	0.57
5:D:317:MET:HE3	7:D:481:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:DC:H2''	1:E:9:DT:C6	2.40	0.57
4:B:94:LYS:HE3	4:B:98:PRO:O	2.04	0.57
4:B:189:CYS:HB3	4:B:327:VAL:HG12	1.87	0.57
5:C:254:PRO:HG3	5:C:403:TRP:CE3	2.40	0.57
2:J:25:DA:C2'	2:J:26:DG:H5'	2.29	0.56
4:B:24:GLU:O	4:B:26:PRO:HD3	2.04	0.56
5:C:94:LYS:HE3	5:C:98:PRO:O	2.05	0.56
5:D:377:GLU:HG3	5:D:378:THR:N	2.19	0.56
2:I:25:DA:C2'	2:I:26:DG:H5'	2.29	0.56
4:A:94:LYS:HE3	4:A:98:PRO:O	2.05	0.56
3:H:22:DA:H2''	3:H:23:DA:OP2	2.05	0.56
5:D:146:ALA:O	5:D:150:GLU:HG3	2.06	0.56
1:F:8:DC:H2''	1:F:9:DT:C6	2.40	0.56
4:B:13:LYS:HG2	5:D:124:GLN:OE1	2.06	0.56
4:B:196:LYS:HE3	4:B:197:ASN:ND2	2.21	0.56
5:C:25:ARG:HB2	5:C:30:LYS:HZ3	1.70	0.56
5:C:14:VAL:O	5:C:18:GLN:HG3	2.06	0.56
2:I:23:DA:H2'	2:I:24:DT:C7	2.36	0.56
3:H:20:DA:H2''	3:H:21:DG:H5''	1.87	0.56
2:J:30:DC:H2''	2:J:31:DT:H5''	1.86	0.56
2:J:23:DA:H2'	2:J:24:DT:C7	2.35	0.56
1:E:2:DA:N3	4:A:170:ARG:NH1	2.42	0.55
3:H:15:DT:H3'	7:H:516:HOH:O	2.04	0.55
4:A:14:VAL:O	4:A:18:GLN:HG3	2.06	0.55
4:A:309:HIS:HD2	5:D:343:PTR:HA	1.72	0.55
4:A:198:VAL:HG22	4:A:219:VAL:HG22	1.88	0.55
4:B:393:SER:C	4:B:395:GLU:H	2.09	0.55
5:C:146:ALA:O	5:C:150:GLU:HG3	2.07	0.55
4:B:84:GLN:HE21	4:B:84:GLN:CA	2.19	0.55
4:B:272:TYR:CE1	4:B:406:ILE:HD12	2.41	0.55
5:C:181:LEU:O	5:C:185:THR:HG23	2.06	0.55
5:D:24:GLU:C	5:D:26:PRO:HD3	2.27	0.55
4:A:84:GLN:HE21	4:A:84:GLN:CA	2.19	0.55
3:H:19:DA:H3'	4:A:108:ASN:ND2	2.21	0.54
4:A:24:GLU:O	4:A:26:PRO:HD3	2.07	0.54
4:B:424:GLY:O	4:B:425:HIS:CG	2.60	0.54
4:B:111:LYS:HG3	4:B:111:LYS:O	2.06	0.54
5:C:24:GLU:C	5:C:26:PRO:HD3	2.28	0.54
5:D:14:VAL:O	5:D:18:GLN:HG3	2.08	0.54
5:D:367:ILE:HG23	5:D:368:SER:H	1.72	0.54
4:A:24:GLU:C	4:A:26:PRO:HD3	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:24:GLU:O	5:C:26:PRO:HD3	2.08	0.54
5:D:164:SER:CB	5:D:292:PRO:HG3	2.38	0.54
4:B:14:VAL:O	4:B:18:GLN:HG3	2.08	0.54
5:C:227:SER:CB	5:C:347:ILE:HD11	2.38	0.54
3:G:30:DC:H1'	3:G:31:DT:H5''	1.89	0.54
3:H:2:DA:H2''	3:H:3:DA:C8	2.43	0.54
4:B:25:ARG:HB3	4:B:30:LYS:HZ3	1.71	0.54
4:B:116:ILE:O	4:B:120:VAL:HG23	2.07	0.54
5:D:26:PRO:HB3	5:D:72:ILE:HG23	1.90	0.54
4:A:176:THR:HG23	4:A:248:PHE:HA	1.90	0.53
4:A:317:MET:HE1	4:A:318:LYS:HA	1.90	0.53
4:B:24:GLU:C	4:B:26:PRO:HD3	2.27	0.53
5:D:25:ARG:HB3	5:D:30:LYS:NZ	2.22	0.53
4:A:143:MET:HG2	4:A:298:ILE:HD11	1.89	0.53
4:B:176:THR:HG23	4:B:248:PHE:HA	1.90	0.53
4:B:383:GLU:HG3	4:B:421:ARG:HE	1.73	0.53
3:H:31:DT:H2''	3:H:32:DT:C6	2.44	0.53
5:C:143:MET:HG3	5:C:298:ILE:HD11	1.90	0.53
3:G:16:DT:H5'	3:G:16:DT:C6	2.43	0.53
4:A:164:SER:CB	4:A:292:PRO:HG3	2.39	0.53
4:B:368:SER:O	4:B:369:LYS:HB2	2.08	0.53
5:C:367:ILE:HG23	5:C:368:SER:N	2.24	0.53
5:D:107:TYR:O	5:D:108:ASN:C	2.47	0.53
3:H:17:DA:O5'	3:H:17:DA:H8	1.92	0.53
4:A:152:GLU:HA	4:A:156:GLU:OE1	2.09	0.53
5:C:26:PRO:HB3	5:C:72:ILE:HG23	1.89	0.53
5:D:327:VAL:HA	5:D:350:ILE:CD1	2.39	0.53
3:G:2:DA:H1'	3:G:3:DA:C8	2.44	0.53
3:G:1:DT:H2'	3:G:2:DA:C8	2.43	0.53
4:A:254:PRO:HG3	4:A:403:TRP:CE3	2.44	0.53
5:D:42:CYS:HA	5:D:89:LEU:HD11	1.91	0.53
5:D:52:ILE:HG22	5:D:262:THR:HG23	1.90	0.53
4:A:368:SER:O	4:A:369:LYS:HB2	2.08	0.53
4:B:27:SER:HB3	4:B:30:LYS:HE2	1.91	0.53
5:D:52:ILE:HG22	5:D:262:THR:HG21	1.91	0.53
5:C:198:VAL:HG22	5:C:219:VAL:HG22	1.91	0.52
2:J:25:DA:H3'	5:D:303:LYS:HG3	1.90	0.52
3:H:8:DC:H2''	3:H:9:DT:C6	2.45	0.52
5:C:283:TYR:HE2	5:C:304:SER:HA	1.73	0.52
1:E:3:DA:H2''	1:E:4:DG:H5'	1.92	0.52
4:A:181:LEU:O	4:A:185:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:26:PRO:HB3	4:B:72:ILE:HG23	1.89	0.52
5:D:198:VAL:HG22	5:D:219:VAL:HG22	1.91	0.52
4:A:42:CYS:HA	4:A:89:LEU:HD11	1.91	0.52
4:B:198:VAL:HG22	4:B:219:VAL:HG22	1.92	0.52
5:C:176:THR:HG23	5:C:248:PHE:HA	1.92	0.52
4:B:2:SER:O	4:B:6:ILE:HG13	2.09	0.52
4:B:148:LEU:HD13	4:B:154:ILE:HD11	1.92	0.52
5:C:84:GLN:HE21	5:C:84:GLN:CA	2.22	0.52
5:C:367:ILE:HG23	5:C:368:SER:H	1.74	0.52
2:J:18:DA:H2''	2:J:19:DA:C5'	2.40	0.52
5:C:42:CYS:HA	5:C:89:LEU:HD11	1.91	0.52
5:D:147:LEU:HD13	5:D:293:TYR:CD2	2.45	0.52
1:F:3:DA:H2''	1:F:4:DG:H5'	1.92	0.52
4:A:374:LEU:C	4:A:376:ASP:H	2.13	0.52
4:B:374:LEU:C	4:B:376:ASP:H	2.13	0.52
5:D:254:PRO:HG3	5:D:403:TRP:CE3	2.45	0.52
4:A:374:LEU:O	4:A:376:ASP:N	2.43	0.51
5:C:236:ARG:CZ	5:C:376:ASP:HB2	2.40	0.51
3:H:20:DA:C2'	3:H:21:DG:H5''	2.40	0.51
4:A:383:GLU:HG3	4:A:421:ARG:HE	1.75	0.51
4:B:120:VAL:CG1	5:C:16:VAL:HG21	2.41	0.51
4:A:145:LYS:HD3	5:D:345:HIS:O	2.11	0.51
5:C:227:SER:HB3	5:C:347:ILE:HD11	1.93	0.51
5:D:367:ILE:HG23	5:D:368:SER:N	2.24	0.51
2:I:18:DA:H2''	2:I:19:DA:C5'	2.39	0.51
5:C:164:SER:CB	5:C:292:PRO:HG3	2.39	0.51
4:A:120:VAL:HG11	5:D:16:VAL:HG21	1.93	0.51
2:I:29:DA:C2'	2:I:30:DC:H5''	2.39	0.51
3:G:10:DA:H1'	3:G:11:DT:C5'	2.41	0.51
3:H:1:DT:H2'	3:H:2:DA:C8	2.45	0.51
4:A:272:TYR:CE1	4:A:406:ILE:HD12	2.46	0.51
4:A:308:ARG:NH1	5:D:343:PTR:O2P	2.44	0.51
4:B:252:SER:HB3	7:B:502:HOH:O	2.11	0.51
5:D:176:THR:HG23	5:D:248:PHE:HA	1.92	0.51
5:D:289:LYS:C	5:D:291:ALA:H	2.13	0.51
1:E:13:DC:H4'	5:D:343:PTR:O1P	2.11	0.50
3:G:21:DG:OP1	4:B:47:HIS:NE2	2.44	0.50
2:I:15:DT:H2''	2:I:16:DT:O4'	2.11	0.50
5:D:216:GLN:HG3	5:D:231:TYR:CE2	2.46	0.50
1:E:10:DA:H1'	1:E:11:DT:H5''	1.93	0.50
4:B:374:LEU:O	4:B:376:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:30:DC:H2''	2:I:31:DT:H5''	1.90	0.50
4:B:400:TYR:CD1	4:B:412:LEU:HD22	2.46	0.50
4:A:305:HIS:O	4:A:308:ARG:N	2.43	0.50
5:C:374:LEU:O	5:C:376:ASP:N	2.44	0.50
5:D:170:ARG:HG2	5:D:171:PHE:CE1	2.46	0.50
5:C:238:ARG:O	5:C:239:ILE:HD13	2.11	0.50
5:D:181:LEU:O	5:D:185:THR:HG23	2.12	0.50
4:B:309:HIS:CE1	7:B:505:HOH:O	2.63	0.50
3:H:10:DA:H1'	3:H:11:DT:C5'	2.42	0.50
4:A:80:LYS:HA	4:A:105:ILE:O	2.11	0.50
4:B:283:TYR:HE2	4:B:304:SER:HA	1.77	0.49
5:C:289:LYS:C	5:C:291:ALA:H	2.15	0.49
4:B:143:MET:CG	4:B:298:ILE:HD11	2.42	0.49
5:C:221:GLU:OE2	5:C:260:ASN:ND2	2.44	0.49
2:J:29:DA:C2'	2:J:30:DC:H5''	2.41	0.49
5:C:383:GLU:HG3	5:C:421:ARG:HE	1.76	0.49
5:D:217:CYS:SG	5:D:230:ILE:HB	2.52	0.49
5:D:267:SER:O	5:D:269:LYS:HG2	2.13	0.49
4:A:148:LEU:CD1	4:A:154:ILE:HD11	2.42	0.49
4:A:166:GLU:HG3	4:A:167:TYR:CE1	2.47	0.49
4:B:92:SER:HB3	5:D:116:ILE:HD11	1.94	0.49
4:B:217:CYS:SG	4:B:230:ILE:HB	2.52	0.49
4:B:289:LYS:C	4:B:291:ALA:H	2.15	0.49
5:D:8:CYS:HA	7:D:466:HOH:O	2.11	0.49
5:D:306:ILE:HG23	5:D:307:GLY:N	2.26	0.49
4:A:308:ARG:NH2	4:A:328:GLY:O	2.46	0.49
4:B:238:ARG:HG3	4:B:238:ARG:HH11	1.77	0.49
5:C:52:ILE:HG22	5:C:262:THR:CG2	2.41	0.49
5:D:420:ASN:C	5:D:422:ARG:H	2.16	0.49
3:H:10:DA:H2''	3:H:11:DT:OP2	2.13	0.49
4:A:205:LEU:HD12	4:A:410:GLU:HG2	1.94	0.49
4:B:120:VAL:HG21	5:C:16:VAL:HG21	1.95	0.49
4:B:164:SER:CB	4:B:292:PRO:HG3	2.42	0.49
3:H:23:DA:H5'	3:H:23:DA:H8	1.78	0.49
4:B:181:LEU:O	4:B:185:THR:HG23	2.12	0.49
5:D:80:LYS:HA	5:D:105:ILE:O	2.11	0.49
3:G:8:DC:H2''	3:G:9:DT:C6	2.48	0.49
4:B:254:PRO:HG3	4:B:403:TRP:CZ3	2.47	0.49
4:B:391:LYS:C	4:B:393:SER:H	2.16	0.49
5:C:2:SER:O	5:C:6:ILE:HG13	2.12	0.49
3:G:23:DA:H2'	3:G:24:DT:C7	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:DG:H2''	3:H:28:DA:H5'	1.95	0.49
4:A:420:ASN:C	4:A:422:ARG:H	2.15	0.49
2:J:25:DA:H5'	5:D:303:LYS:HB2	1.94	0.49
4:B:42:CYS:HA	4:B:89:LEU:HD11	1.94	0.49
5:C:150:GLU:O	5:C:152:GLU:N	2.46	0.49
4:B:80:LYS:HA	4:B:105:ILE:O	2.12	0.48
4:B:418:TYR:O	4:B:422:ARG:HB2	2.13	0.48
5:C:163:ASN:N	5:C:163:ASN:HD22	2.11	0.48
1:E:2:DA:C2	4:A:170:ARG:NH1	2.81	0.48
4:A:25:ARG:HB2	4:A:30:LYS:HZ1	1.77	0.48
4:A:289:LYS:C	4:A:291:ALA:H	2.16	0.48
4:B:170:ARG:HG2	4:B:171:PHE:CE1	2.48	0.48
5:D:25:ARG:O	5:D:25:ARG:HG2	2.13	0.48
3:H:17:DA:H2''	3:H:18:DA:O5'	2.13	0.48
5:D:77:LEU:HD23	5:D:77:LEU:C	2.33	0.48
4:B:295:ILE:HG23	4:B:296:PHE:N	2.28	0.48
5:C:25:ARG:HB2	5:C:30:LYS:HZ1	1.76	0.48
5:C:80:LYS:HA	5:C:105:ILE:O	2.13	0.48
4:A:367:ILE:HD13	5:D:370:GLU:HA	1.96	0.48
3:G:4:DG:H1'	3:G:5:DT:H5''	1.95	0.48
4:B:143:MET:HG3	4:B:298:ILE:HD11	1.96	0.48
4:A:77:LEU:C	4:A:77:LEU:HD23	2.34	0.48
4:A:328:GLY:HA3	4:A:330:PHE:CE1	2.47	0.48
5:C:254:PRO:HG3	5:C:403:TRP:CZ3	2.49	0.48
3:H:16:DT:C5'	3:H:16:DT:C6	2.95	0.48
4:B:25:ARG:HB3	4:B:30:LYS:HZ1	1.77	0.48
5:C:317:MET:HE1	5:C:318:LYS:HA	1.96	0.48
5:D:236:ARG:CZ	5:D:376:ASP:HB2	2.44	0.48
4:A:170:ARG:HG2	4:A:171:PHE:CE1	2.49	0.47
4:B:236:ARG:HH11	4:B:374:LEU:HD12	1.79	0.47
3:H:4:DG:H1'	3:H:5:DT:H5''	1.95	0.47
4:A:306:ILE:HG23	4:A:307:GLY:N	2.29	0.47
4:A:325:ASN:HD21	5:D:335:ALA:HA	1.80	0.47
4:A:2:SER:O	4:A:6:ILE:HG13	2.14	0.47
3:G:27:DG:H2''	3:G:28:DA:H5'	1.96	0.47
4:B:268:ASN:ND2	7:B:450:HOH:O	2.48	0.47
5:D:395:GLU:O	5:D:395:GLU:HG2	2.14	0.47
4:A:217:CYS:SG	4:A:230:ILE:HB	2.54	0.47
5:C:170:ARG:HG2	5:C:171:PHE:CE1	2.49	0.47
5:D:84:GLN:HE21	5:D:84:GLN:CA	2.25	0.47
5:C:340:ARG:HB3	5:C:340:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:383:GLU:HG3	5:D:421:ARG:HE	1.77	0.47
4:B:317:MET:HG3	5:C:346:GLN:CD	2.35	0.47
4:B:320:LEU:HD21	4:B:364:TYR:CZ	2.50	0.47
3:H:21:DG:OP1	4:A:47:HIS:NE2	2.46	0.47
3:H:23:DA:H2''	3:H:24:DT:H6	1.77	0.47
4:B:354:TYR:CZ	4:B:358:VAL:HG21	2.50	0.47
5:C:168:THR:HG23	7:C:433:HOH:O	2.14	0.47
3:H:26:DG:O3'	4:A:299:LYS:HE3	2.14	0.47
3:G:10:DA:H2''	3:G:11:DT:OP2	2.15	0.46
4:B:306:ILE:HG23	4:B:307:GLY:N	2.30	0.46
4:B:342:THR:HG22	5:D:312:THR:CG2	2.41	0.46
4:B:77:LEU:HD23	4:B:77:LEU:C	2.35	0.46
5:C:175:LYS:O	5:C:179:GLN:HG3	2.15	0.46
5:D:162:LEU:HD13	5:D:182:PHE:HD2	1.79	0.46
4:A:236:ARG:NH1	4:A:374:LEU:HD12	2.30	0.46
4:B:116:ILE:HD11	5:C:45:ILE:HD11	1.97	0.46
5:D:2:SER:O	5:D:6:ILE:HG13	2.16	0.46
2:J:14:DT:H2'	2:J:15:DT:C5	2.50	0.46
4:B:175:LYS:O	4:B:179:GLN:HG3	2.15	0.46
4:B:216:GLN:HG3	4:B:231:TYR:CE2	2.51	0.46
4:B:427:HIS:O	4:B:427:HIS:ND1	2.44	0.46
5:D:36:ALA:HB3	7:D:443:HOH:O	2.15	0.46
3:H:5:DT:H2''	3:H:6:DT:C5'	2.46	0.46
4:B:393:SER:O	4:B:395:GLU:N	2.38	0.46
4:B:268:ASN:O	4:B:269:LYS:HB3	2.15	0.46
5:C:324:THR:HG22	5:C:330:PHE:CE1	2.51	0.46
4:B:293:TYR:HB3	4:B:294:PRO:HD2	1.97	0.46
5:C:293:TYR:HB3	5:C:294:PRO:HD2	1.97	0.46
1:F:2:DA:H2''	1:F:3:DA:N7	2.31	0.46
5:C:375:LYS:O	5:C:376:ASP:C	2.54	0.46
5:C:11:PRO:HB2	5:C:14:VAL:HG23	1.98	0.45
5:C:77:LEU:C	5:C:77:LEU:HD23	2.35	0.45
5:C:155:TRP:CE2	5:C:360:ARG:HD2	2.51	0.45
1:F:10:DA:H1'	1:F:11:DT:H5''	1.97	0.45
3:H:26:DG:OP1	4:A:303:LYS:NZ	2.49	0.45
4:A:16:VAL:O	4:A:20:VAL:HG23	2.16	0.45
4:B:367:ILE:CD1	5:C:371:MET:HG2	2.46	0.45
5:C:16:VAL:O	5:C:20:VAL:HG23	2.17	0.45
3:G:15:DT:C1'	3:G:16:DT:H5''	2.43	0.45
3:H:14:DT:H2'	3:H:15:DT:H72	1.97	0.45
3:H:20:DA:H1'	3:H:21:DG:H5''	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:26:DG:P	4:A:303:LYS:NZ	2.89	0.45
4:B:344:THR:C	5:D:141:LYS:HD3	2.37	0.45
5:C:320:LEU:HD21	5:C:364:TYR:CE2	2.51	0.45
5:D:418:TYR:O	5:D:422:ARG:HG3	2.16	0.45
3:H:20:DA:P	4:A:108:ASN:HD21	2.39	0.45
4:A:293:TYR:HB3	4:A:294:PRO:HD2	1.98	0.45
4:A:362:TYR:CE2	4:A:373:ALA:HB2	2.51	0.45
5:D:143:MET:CE	5:D:294:PRO:HB2	2.45	0.45
5:C:217:CYS:SG	5:C:230:ILE:HB	2.57	0.45
5:C:400:TYR:CD1	5:C:412:LEU:HD22	2.50	0.45
5:D:360:ARG:O	5:D:374:LEU:HD12	2.16	0.45
3:G:17:DA:H2''	3:G:18:DA:C8	2.52	0.45
4:B:420:ASN:C	4:B:422:ARG:H	2.20	0.45
4:B:421:ARG:NH1	4:B:421:ARG:CG	2.80	0.45
5:D:78:GLN:NE2	5:D:105:ILE:HD11	2.32	0.45
4:A:236:ARG:NH1	4:A:374:LEU:CD1	2.80	0.45
5:C:324:THR:HG22	5:C:330:PHE:HE1	1.81	0.45
5:D:317:MET:HE1	5:D:318:LYS:HA	1.99	0.45
4:A:116:ILE:CD1	5:D:92:SER:HB3	2.44	0.45
4:A:354:TYR:CZ	4:A:358:VAL:HG21	2.52	0.45
3:G:30:DC:H2''	3:G:31:DT:C5'	2.47	0.45
4:A:11:PRO:HB2	4:A:14:VAL:HG23	1.97	0.45
4:A:175:LYS:O	4:A:179:GLN:HG3	2.17	0.45
3:G:30:DC:H2''	3:G:31:DT:H5'	1.98	0.45
4:A:148:LEU:N	4:A:148:LEU:CD2	2.80	0.45
4:B:110:GLN:O	4:B:111:LYS:CG	2.63	0.45
5:D:119:ILE:O	5:D:123:LEU:HG	2.17	0.45
3:H:22:DA:C2	3:H:23:DA:C4	3.05	0.44
4:A:295:ILE:HG23	4:A:296:PHE:N	2.32	0.44
4:B:148:LEU:N	4:B:148:LEU:CD2	2.80	0.44
4:B:345:HIS:CD2	4:B:347:ILE:HD11	2.52	0.44
3:G:20:DA:H1'	3:G:21:DG:H5''	1.99	0.44
3:H:26:DG:P	4:A:303:LYS:HZ3	2.39	0.44
4:A:400:TYR:CD1	4:A:412:LEU:HD22	2.52	0.44
5:C:162:LEU:HD13	5:C:182:PHE:HD2	1.82	0.44
5:C:216:GLN:HG3	5:C:231:TYR:CE2	2.52	0.44
5:D:421:ARG:HH11	5:D:421:ARG:CG	2.29	0.44
4:B:162:LEU:HD13	4:B:182:PHE:HD2	1.82	0.44
5:D:175:LYS:O	5:D:179:GLN:HG3	2.17	0.44
3:H:17:DA:O5'	3:H:17:DA:C8	2.69	0.44
5:C:360:ARG:O	5:C:374:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:164:SER:HB3	5:D:292:PRO:HG3	2.00	0.44
1:F:2:DA:H2''	1:F:3:DA:C8	2.53	0.44
4:A:78:GLN:NE2	4:A:105:ILE:HD11	2.33	0.44
4:B:306:ILE:CG2	4:B:307:GLY:N	2.81	0.44
5:D:224:THR:HB	7:D:482:HOH:O	2.17	0.44
4:B:289:LYS:HG3	7:B:491:HOH:O	2.18	0.44
4:B:308:ARG:NH1	4:B:330:PHE:CZ	2.86	0.44
4:B:393:SER:C	4:B:395:GLU:N	2.71	0.44
4:A:160:LYS:HE3	4:A:160:LYS:HB2	1.91	0.44
4:B:128:GLU:O	4:B:129:SER:C	2.56	0.44
2:I:24:DT:H4'	5:C:305:HIS:CE1	2.53	0.43
4:A:119:ILE:O	4:A:123:LEU:HG	2.18	0.43
2:I:15:DT:H5'	4:A:224:THR:CG2	2.48	0.43
4:A:155:TRP:CE2	4:A:360:ARG:HD2	2.53	0.43
4:B:155:TRP:HD1	7:B:497:HOH:O	2.01	0.43
4:B:200:PRO:HG3	4:B:272:TYR:HB3	1.99	0.43
5:C:306:ILE:HG23	5:C:307:GLY:N	2.33	0.43
5:D:154:ILE:HG21	5:D:314:PHE:HB2	2.00	0.43
5:D:221:GLU:OE2	5:D:260:ASN:ND2	2.46	0.43
5:D:295:ILE:HG23	5:D:296:PHE:N	2.33	0.43
1:F:4:DG:H1'	1:F:5:DT:C5'	2.48	0.43
4:A:165:PHE:HZ	4:A:287:LEU:HD13	1.83	0.43
4:B:365:ASP:OD2	4:B:365:ASP:C	2.55	0.43
5:C:152:GLU:HA	5:C:156:GLU:OE1	2.18	0.43
5:D:387:ILE:O	5:D:390:LEU:HB3	2.19	0.43
2:I:14:DT:H5''	5:D:343:PTR:P	2.59	0.43
5:C:78:GLN:NE2	5:C:105:ILE:HD11	2.33	0.43
5:D:293:TYR:HB3	5:D:294:PRO:HD2	1.99	0.43
5:D:395:GLU:HA	5:D:398:ILE:HD12	2.01	0.43
3:G:5:DT:H2''	3:G:6:DT:C5'	2.47	0.43
5:D:129:SER:O	5:D:130:SER:O	2.36	0.43
5:C:295:ILE:HG23	5:C:296:PHE:N	2.33	0.43
5:C:354:TYR:CZ	5:C:358:VAL:HG21	2.54	0.43
5:D:16:VAL:O	5:D:20:VAL:HG23	2.17	0.43
4:A:162:LEU:HD13	4:A:182:PHE:HD2	1.82	0.43
5:C:229:HIS:HE1	7:C:442:HOH:O	2.01	0.43
4:A:146:ALA:O	4:A:147:LEU:C	2.57	0.43
4:A:164:SER:HB3	4:A:292:PRO:HG3	2.00	0.43
4:B:11:PRO:HB2	4:B:14:VAL:HG23	2.01	0.43
4:B:16:VAL:O	4:B:20:VAL:HG23	2.19	0.43
2:I:15:DT:H2'	2:I:16:DT:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:11:PRO:HG3	5:D:127:PHE:CE2	2.52	0.43
4:B:119:ILE:O	4:B:123:LEU:HG	2.18	0.43
5:D:306:ILE:CG2	5:D:307:GLY:N	2.81	0.43
5:D:375:LYS:O	5:D:375:LYS:HG3	2.18	0.43
4:A:182:PHE:HB2	4:A:283:TYR:OH	2.19	0.43
4:A:306:ILE:CG2	4:A:307:GLY:N	2.82	0.42
5:D:400:TYR:CD1	5:D:412:LEU:HD22	2.53	0.42
4:A:238:ARG:HG3	4:A:238:ARG:NH1	2.28	0.42
4:B:116:ILE:CD1	5:C:45:ILE:HD11	2.49	0.42
2:I:25:DA:H2''	2:I:26:DG:C5'	2.33	0.42
4:B:78:GLN:NE2	4:B:105:ILE:HD11	2.35	0.42
4:B:320:LEU:HD21	4:B:364:TYR:CE2	2.55	0.42
5:C:119:ILE:O	5:C:123:LEU:HG	2.19	0.42
2:I:14:DT:O3'	4:A:224:THR:HG21	2.18	0.42
2:I:29:DA:H5''	7:I:248:HOH:O	2.19	0.42
4:B:187:ILE:HD13	4:B:187:ILE:HA	1.79	0.42
5:D:391:LYS:O	5:D:393:SER:N	2.46	0.42
4:B:146:ALA:O	4:B:147:LEU:C	2.57	0.42
4:B:155:TRP:CE2	4:B:360:ARG:HD2	2.55	0.42
5:C:333:LYS:HA	5:C:333:LYS:HD3	1.89	0.42
4:B:317:MET:HE1	4:B:318:LYS:HA	2.01	0.42
5:D:354:TYR:CZ	5:D:358:VAL:HG21	2.55	0.42
1:E:13:DC:H3'	5:D:343:PTR:CE1	2.45	0.42
4:A:10:THR:HA	4:A:11:PRO:HD3	1.92	0.42
4:A:394:ALA:HB1	4:A:409:GLN:NE2	2.35	0.42
1:E:2:DA:OP1	1:E:2:DA:H4'	2.20	0.42
3:G:23:DA:H2''	3:G:24:DT:C6	2.54	0.42
4:A:25:ARG:HB2	4:A:30:LYS:HZ3	1.83	0.42
5:D:210:TYR:CG	5:D:356:ALA:HB2	2.55	0.42
1:E:1:DT:O5'	1:E:1:DT:H6	2.03	0.41
5:D:374:LEU:O	5:D:376:ASP:N	2.53	0.41
3:H:24:DT:H4'	4:A:305:HIS:CE1	2.55	0.41
1:E:10:DA:C2	3:H:25:DA:C2	3.09	0.41
2:J:14:DT:H5''	4:B:223:LYS:NZ	2.34	0.41
4:A:407:ILE:O	4:A:408:SER:C	2.59	0.41
4:B:115:ASP:O	4:B:119:ILE:HG13	2.20	0.41
4:B:206:VAL:CG1	7:B:483:HOH:O	2.68	0.41
5:C:182:PHE:HB2	5:C:283:TYR:OH	2.21	0.41
5:D:375:LYS:O	5:D:376:ASP:C	2.56	0.41
4:A:299:LYS:O	4:A:300:ASN:HB2	2.20	0.41
4:B:262:THR:O	4:B:263:GLY:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:189:CYS:HB3	4:A:327:VAL:HG12	2.03	0.41
4:A:327:VAL:HG22	4:A:350:ILE:HD13	2.03	0.41
4:A:328:GLY:HA3	4:A:330:PHE:HE1	1.84	0.41
5:C:115:ASP:O	5:C:119:ILE:HG13	2.20	0.41
5:C:160:LYS:HE3	5:C:160:LYS:HB2	1.91	0.41
5:D:283:TYR:HE2	5:D:304:SER:HA	1.85	0.41
2:J:18:DA:H1'	2:J:19:DA:C5'	2.47	0.41
5:D:407:ILE:O	5:D:408:SER:C	2.59	0.41
2:I:23:DA:H5''	2:I:23:DA:H8	1.86	0.41
4:B:160:LYS:HE3	4:B:160:LYS:HB2	1.92	0.41
4:B:407:ILE:O	4:B:408:SER:C	2.59	0.41
5:D:290:ASN:O	5:D:292:PRO:N	2.53	0.41
2:J:30:DC:C2'	2:J:31:DT:H5''	2.51	0.41
4:A:393:SER:C	4:A:395:GLU:N	2.71	0.41
4:B:120:VAL:CG2	5:C:16:VAL:HG21	2.50	0.41
2:J:25:DA:H2''	2:J:26:DG:C5'	2.35	0.41
4:A:122:SER:O	4:A:126:GLN:HG3	2.21	0.41
4:B:74:ASN:HB3	7:B:478:HOH:O	2.20	0.41
4:B:189:CYS:SG	4:B:189:CYS:O	2.79	0.41
4:B:306:ILE:HD12	4:B:306:ILE:HA	1.84	0.41
5:C:205:LEU:HD12	5:C:410:GLU:HG2	2.02	0.41
4:B:236:ARG:NH1	4:B:374:LEU:HD12	2.36	0.41
5:C:374:LEU:C	5:C:376:ASP:H	2.23	0.41
4:A:116:ILE:HD12	5:D:92:SER:O	2.21	0.40
4:A:238:ARG:HH11	4:A:238:ARG:CG	2.29	0.40
4:B:45:ILE:HD13	4:B:92:SER:HB2	2.02	0.40
4:B:238:ARG:HG3	4:B:238:ARG:NH1	2.35	0.40
5:C:290:ASN:O	5:C:292:PRO:N	2.53	0.40
4:A:290:ASN:O	4:A:292:PRO:N	2.54	0.40
4:B:16:VAL:HG21	5:D:120:VAL:HG11	2.03	0.40
4:B:165:PHE:HZ	4:B:287:LEU:HD13	1.86	0.40
5:C:350:ILE:HA	5:C:351:PRO:HD3	1.94	0.40
5:C:421:ARG:NH1	5:C:421:ARG:CG	2.84	0.40
5:D:11:PRO:HB2	5:D:14:VAL:HG23	2.03	0.40
3:G:6:DT:H5'	3:G:6:DT:C6	2.56	0.40
5:C:375:LYS:O	5:C:375:LYS:HG3	2.22	0.40
5:D:242:LEU:HD23	5:D:242:LEU:HA	1.87	0.40
5:D:299:LYS:O	5:D:300:ASN:HB2	2.21	0.40
3:H:1:DT:H2''	3:H:2:DA:O5'	2.21	0.40
4:A:45:ILE:HD13	4:A:92:SER:HB2	2.04	0.40
5:C:189:CYS:HB3	5:C:327:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:122:SER:O	5:D:126:GLN:HG3	2.21	0.40
3:H:21:DG:N2	7:H:525:HOH:O	2.44	0.40
4:A:236:ARG:HH11	4:A:374:LEU:CD1	2.29	0.40
5:C:290:ASN:O	5:C:291:ALA:C	2.59	0.40
5:D:115:ASP:O	5:D:119:ILE:HG13	2.21	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	
4	A	392/429 (91%)	345 (88%)	36 (9%)	11 (3%)	5	11
4	B	405/429 (94%)	363 (90%)	32 (8%)	10 (2%)	5	14
5	C	389/429 (91%)	356 (92%)	25 (6%)	8 (2%)	7	18
5	D	400/429 (93%)	361 (90%)	28 (7%)	11 (3%)	5	11
All	All	1586/1716 (92%)	1425 (90%)	121 (8%)	40 (2%)	5	14

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	152	GLU
4	A	267	SER
4	A	375	LYS
4	B	152	GLU
4	B	375	LYS
5	C	151	GLY
5	C	375	LYS
5	D	151	GLY
5	D	375	LYS
4	A	150	GLU

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Mol	Chain	Res	Type
4	A	306	ILE
4	B	150	GLU
5	C	26	PRO
5	C	270	GLN
5	C	341	THR
4	A	26	PRO
4	A	151	GLY
4	A	394	ALA
4	A	421	ARG
4	B	26	PRO
4	B	394	ALA
5	D	26	PRO
5	D	268	ASN
5	D	393	SER
5	D	421	ARG
4	A	291	ALA
4	B	291	ALA
4	B	425	HIS
5	C	291	ALA
5	D	270	GLN
5	D	290	ASN
5	D	291	ALA
4	A	290	ASN
5	C	290	ASN
5	D	336	SER
4	B	290	ASN
4	B	116	ILE
4	B	151	GLY
5	D	392	GLY
5	C	116	ILE

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
4	A	364/388 (94%)	357 (98%)	7 (2%)	57 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	376/388 (97%)	367 (98%)	9 (2%)	49	77
5	C	364/387 (94%)	359 (99%)	5 (1%)	67	86
5	D	370/387 (96%)	366 (99%)	4 (1%)	73	90
All	All	1474/1550 (95%)	1449 (98%)	25 (2%)	60	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	148	LEU
4	A	252	SER
4	A	264	ASN
4	A	305	HIS
4	A	317	MET
4	A	390	LEU
4	A	421	ARG
4	B	54	ARG
4	B	148	LEU
4	B	252	SER
4	B	264	ASN
4	B	282	SER
4	B	305	HIS
4	B	317	MET
4	B	332	ASP
4	B	421	ARG
5	C	252	SER
5	C	305	HIS
5	C	317	MET
5	C	421	ARG
5	C	422	ARG
5	D	252	SER
5	D	305	HIS
5	D	317	MET
5	D	421	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	61	ASN
4	A	74	ASN
4	A	78	GLN

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Mol	Chain	Res	Type
4	A	84	GLN
4	A	108	ASN
4	A	163	ASN
4	A	197	ASN
4	A	268	ASN
4	A	309	HIS
4	A	409	GLN
4	B	74	ASN
4	B	78	GLN
4	B	84	GLN
4	B	163	ASN
4	B	197	ASN
4	B	309	HIS
4	B	345	HIS
4	B	409	GLN
4	B	428	HIS
4	B	430	HIS
5	C	61	ASN
5	C	74	ASN
5	C	78	GLN
5	C	84	GLN
5	C	139	HIS
5	C	163	ASN
5	C	197	ASN
5	C	346	GLN
5	D	61	ASN
5	D	74	ASN
5	D	78	GLN
5	D	84	GLN
5	D	163	ASN
5	D	197	ASN
5	D	309	HIS
5	D	345	HIS
5	D	346	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	PTR	C	343	5,1	11,15,17	1.95	3 (27%)	12,19,24	0.86	0
5	PTR	D	343	5,1	11,15,17	1.85	3 (27%)	12,19,24	1.02	1 (8%)

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	PTR	C	343	5,1	-	0/7/10/13	0/1/1/1
5	PTR	D	343	5,1	-	0/7/10/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	343	PTR	OH-CZ	4.03	1.46	1.40
5	C	343	PTR	OH-CZ	4.03	1.46	1.40
5	C	343	PTR	CE1-CD1	2.76	1.43	1.38
5	C	343	PTR	CE2-CD2	2.24	1.42	1.38
5	D	343	PTR	CE2-CD2	2.19	1.42	1.38
5	D	343	PTR	CE1-CZ	2.10	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	343	PTR	CD2-CE2-CZ	-2.12	117.14	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	343	PTR	1	0
5	D	343	PTR	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	2PO	H	513	3	0,3,3	-	-	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	513	2PO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	E	13/13 (100%)	0.67	0 100 100	71, 106, 117, 124	0
1	F	13/13 (100%)	-0.99	0 100 100	34, 36, 46, 57	0
2	I	20/20 (100%)	0.65	2 (10%) 7 5	65, 109, 135, 137	0
2	J	20/20 (100%)	-0.42	0 100 100	27, 56, 86, 99	0
3	G	33/33 (100%)	-0.26	0 100 100	25, 79, 101, 102	0
3	H	33/33 (100%)	-0.19	0 100 100	33, 75, 127, 136	0
4	A	400/429 (93%)	1.51	107 (26%) 0 0	66, 125, 165, 177	0
4	B	413/429 (96%)	-0.04	22 (5%) 26 25	21, 48, 107, 133	0
5	C	399/429 (93%)	0.52	43 (10%) 5 4	46, 85, 141, 157	0
5	D	408/429 (95%)	-0.03	17 (4%) 36 35	25, 55, 94, 122	0
All	All	1752/1848 (94%)	0.44	191 (10%) 5 4	21, 74, 149, 177	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	32	ALA	7.8
4	A	268	ASN	7.2
4	A	25	ARG	7.2
4	A	42	CYS	6.6
4	A	405	GLY	6.6
4	A	169	SER	6.5
4	A	392	GLY	6.3
4	A	261	ARG	6.2
5	D	267	SER	5.9
5	C	386	HIS	5.9
5	D	391	LYS	5.8
5	C	268	ASN	5.7
4	A	377	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
4	A	403	TRP	5.6
4	A	375	LYS	5.5
4	B	430	HIS	5.4
4	A	333	LYS	5.3
4	A	267	SER	5.2
4	A	26	PRO	5.2
4	A	39	THR	5.1
5	C	378	THR	5.1
4	A	265	SER	5.1
4	A	256	LEU	4.9
4	A	389	GLN	4.9
4	A	374	LEU	4.9
4	B	267	SER	4.8
4	A	40	TYR	4.8
5	C	377	GLU	4.7
4	A	81	TYR	4.6
5	C	125	LEU	4.5
4	B	392	GLY	4.3
4	A	27	SER	4.3
4	A	347	ILE	4.3
4	A	34	CYS	4.2
5	C	29	GLU	4.1
4	A	421	ARG	4.0
4	A	168	THR	4.0
5	C	119	ILE	4.0
4	A	69	SER	4.0
5	C	389	GLN	4.0
5	C	376	ASP	4.0
4	A	266	SER	3.9
4	A	332	ASP	3.9
4	B	136	GLY	3.9
5	C	126	GLN	3.9
4	A	23	PHE	3.8
4	B	137	ASN	3.8
5	C	39	THR	3.8
2	I	16	DT	3.8
4	A	420	ASN	3.8
4	B	266	SER	3.6
5	C	73	VAL	3.6
4	A	390	LEU	3.6
4	A	110	GLN	3.5
5	C	88	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
5	C	334	ARG	3.5
4	A	48	ASN	3.5
4	A	103	THR	3.5
4	A	418	TYR	3.5
4	A	29	GLU	3.5
4	A	79	PHE	3.5
4	A	328	GLY	3.5
4	A	400	TYR	3.5
4	A	38	LEU	3.4
4	A	136	GLY	3.4
4	A	386	HIS	3.4
4	A	175	LYS	3.4
4	A	31	ILE	3.4
5	C	84	GLN	3.4
4	A	107	TYR	3.4
4	A	348	THR	3.4
5	D	334	ARG	3.4
4	A	384	TRP	3.3
4	A	101	GLU	3.3
4	B	264	ASN	3.3
5	D	108	ASN	3.3
4	A	289	LYS	3.3
4	A	391	LYS	3.3
5	D	269	LYS	3.3
4	A	167	TYR	3.3
4	A	399	ARG	3.3
4	A	201	LYS	3.3
4	A	56	THR	3.3
5	C	330	PHE	3.2
4	A	37	GLU	3.2
4	B	377	GLU	3.2
4	A	207	GLN	3.2
4	A	388	GLU	3.2
5	C	151	GLY	3.2
5	C	48	ASN	3.2
5	C	42	CYS	3.1
5	C	108	ASN	3.1
5	C	74	ASN	3.1
4	A	413	ASP	3.1
4	B	268	ASN	3.1
4	A	36	ALA	3.0
4	A	45	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
4	A	401	PRO	3.0
4	A	137	ASN	3.0
4	A	114	SER	3.0
4	A	72	ILE	3.0
4	A	221	GLU	3.0
4	A	35	ALA	3.0
4	B	111	LYS	3.0
5	D	392	GLY	2.9
5	C	41	LEU	2.9
5	C	75	LYS	2.9
4	A	378	THR	2.9
4	A	24	GLU	2.9
4	B	341	THR	2.9
5	C	150	GLU	2.8
5	C	17	ARG	2.8
4	A	86	ALA	2.8
5	D	393	SER	2.8
4	A	251	ASN	2.7
4	B	348	THR	2.7
4	A	411	VAL	2.7
4	A	60	TYR	2.7
5	C	139	HIS	2.7
5	C	24	GLU	2.7
5	D	367	ILE	2.7
5	D	25	ARG	2.7
4	A	398	ILE	2.7
4	A	82	LYS	2.6
5	C	367	ILE	2.6
5	C	85	LYS	2.6
5	C	38	LEU	2.6
4	A	381	ILE	2.6
4	A	409	GLN	2.6
4	A	213	VAL	2.5
5	C	142	LYS	2.5
5	C	40	TYR	2.5
4	A	109	GLY	2.4
4	B	126	GLN	2.4
4	A	64	ILE	2.4
5	C	71	ASP	2.4
5	D	39	THR	2.4
4	A	387	ILE	2.4
5	C	128	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	218	LEU	2.4
4	B	110	GLN	2.4
4	A	402	ALA	2.4
2	I	17	DA	2.4
4	A	170	ARG	2.4
4	B	426	HIS	2.4
4	A	263	GLY	2.3
4	B	125	LEU	2.3
5	D	38	LEU	2.3
4	A	404	ASN	2.3
4	A	171	PHE	2.3
4	A	173	LYS	2.3
4	A	85	LYS	2.3
4	A	349	ALA	2.3
4	A	8	CYS	2.3
4	A	61	ASN	2.3
5	C	34	CYS	2.3
4	B	269	LYS	2.3
4	A	383	GLU	2.2
5	C	78	GLN	2.2
4	A	33	SER	2.2
4	A	99	ALA	2.2
4	A	232	PHE	2.2
4	A	57	PHE	2.2
4	A	264	ASN	2.2
4	A	46	THR	2.2
4	A	9	LYS	2.2
4	A	272	TYR	2.2
5	C	81	TYR	2.2
5	D	129	SER	2.2
5	D	42	CYS	2.2
5	C	101	GLU	2.2
5	C	263	GLY	2.2
5	C	380	PRO	2.2
4	B	38	LEU	2.1
4	A	17	ARG	2.1
4	B	114	SER	2.1
5	C	137	ASN	2.1
4	A	395	GLU	2.1
4	B	42	CYS	2.1
5	C	13	LYS	2.1
4	A	280	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	D	390	LEU	2.1
5	C	358	VAL	2.1
5	D	375	LYS	2.0
4	A	73	VAL	2.0
5	D	377	GLU	2.0
5	D	151	GLY	2.0
4	B	389	GLN	2.0
4	A	419	ILE	2.0
4	A	284	ASN	2.0
4	B	29	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PTR	D	343	15/17	0.89	0.20	71,78,80,80	0
5	PTR	C	343	15/17	0.98	0.13	38,41,45,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
6	2PO	H	513	4/4	0.93	0.20	85,85,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.