Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 02:37 PM EST

PDB ID	:	5T16
Title	:	Crystal structure of yeast RNase III (Rnt1p) complexed with a non-hydrolyzable RNA substrate analog
Authors	:	Song, H.; Ji, X.
Deposited on	:	2016-08-18
Resolution	:	2.78 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

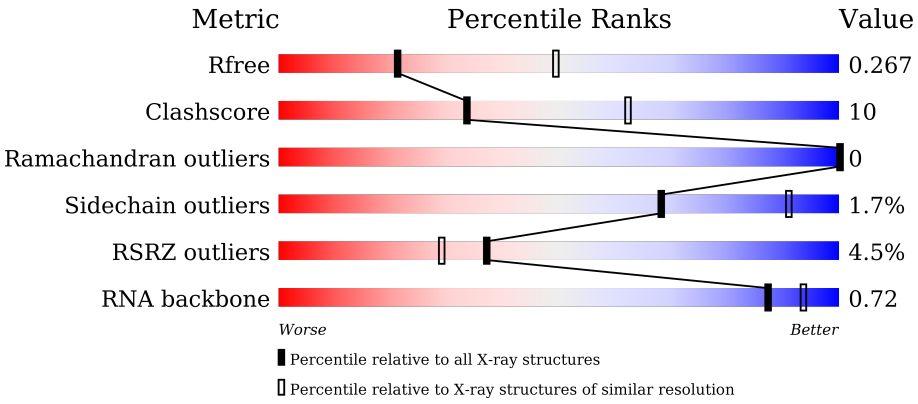
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)
RNA backbone	2183	1015 (3.16-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	276	4% 86% 13%
1	B	276	5% 81% 17%
1	I	276	5% 81% 19%
1	J	276	5% 74% 22%

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Mol	Chain	Length	Quality of chain
2	C	119	64% 29% 5%
2	D	119	3% 74% 21%
2	E	119	5% 67% 29%
2	F	119	11% 65% 31%
2	K	119	4% 77% 18%
2	L	119	4% 71% 25%
2	M	119	3% 66% 26% 6%
2	N	119	6% 69% 28%
3	G	34	53% 41% 6%
3	H	34	50% 47%
3	O	34	47% 44% 6%
3	P	34	41% 53%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	F	201	-	-	-	X
4	EDO	H	101	-	-	-	X
4	EDO	I	501	-	-	-	X
4	EDO	I	502	-	-	-	X
4	EDO	I	504	-	-	-	X
4	EDO	I	505	-	-	-	X
4	EDO	J	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19568 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 Ribonuclease 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2212	1406	389	409	8			
1	B	269	Total	C	N	O	S	0	0	0
			2161	1374	381	398	8			
1	I	276	Total	C	N	O	S	0	0	0
			2212	1406	389	409	8			
1	J	267	Total	C	N	O	S	0	0	0
			2141	1361	379	393	8			

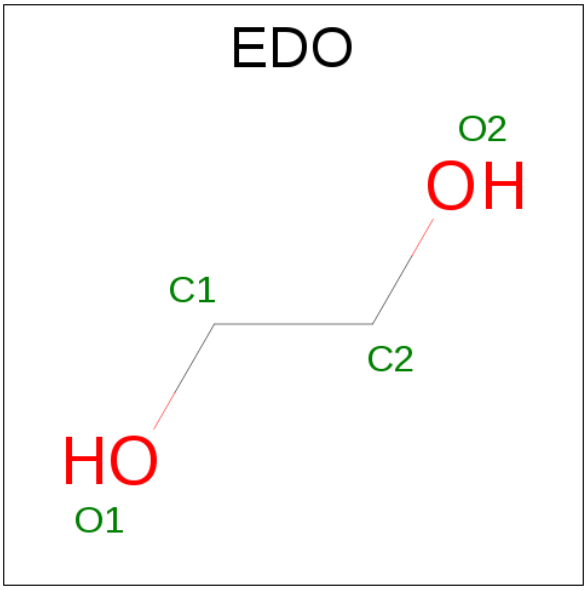
- Molecule 2 is a protein called Ribonuclease 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	113	Total	C	N	O	S	0	0	0
			925	589	150	185	1			
2	D	116	Total	C	N	O	S	0	0	0
			959	609	160	189	1			
2	E	115	Total	C	N	O	S	0	0	0
			948	603	156	188	1			
2	F	115	Total	C	N	O	S	0	0	0
			948	603	156	188	1			
2	K	114	Total	C	N	O	S	0	0	0
			936	595	154	186	1			
2	L	116	Total	C	N	O	S	0	0	0
			959	609	160	189	1			
2	M	112	Total	C	N	O	S	0	0	0
			917	584	148	184	1			
2	N	117	Total	C	N	O	S	0	0	0
			968	614	161	192	1			

- Molecule 3 is a RNA chain called RNA substrate analog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	34	Total	C	N	O	P	S	0	0	0
			721	323	127	236	33	2			
3	H	34	Total	C	N	O	P	S	0	0	0
			721	323	127	236	33	2			
3	O	34	Total	C	N	O	P	S	0	0	0
			721	323	127	236	33	2			
3	P	34	Total	C	N	O	P	S	0	0	0
			721	323	127	236	33	2			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

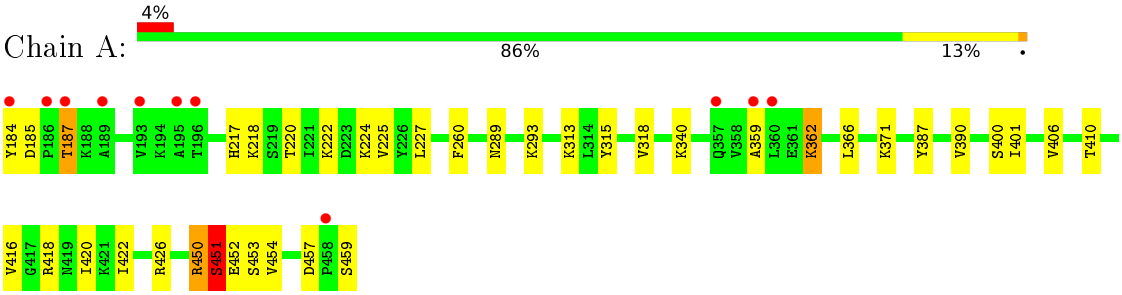
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	43	Total O 43 43	0	0
5	B	44	Total O 44 44	0	0
5	C	15	Total O 15 15	0	0
5	D	12	Total O 12 12	0	0
5	E	7	Total O 7 7	0	0
5	F	9	Total O 9 9	0	0
5	G	20	Total O 20 20	0	0
5	H	25	Total O 25 25	0	0
5	I	51	Total O 51 51	0	0
5	J	46	Total O 46 46	0	0
5	K	12	Total O 12 12	0	0
5	L	13	Total O 13 13	0	0
5	M	6	Total O 6 6	0	0
5	N	14	Total O 14 14	0	0
5	O	27	Total O 27 27	0	0
5	P	14	Total O 14 14	0	0

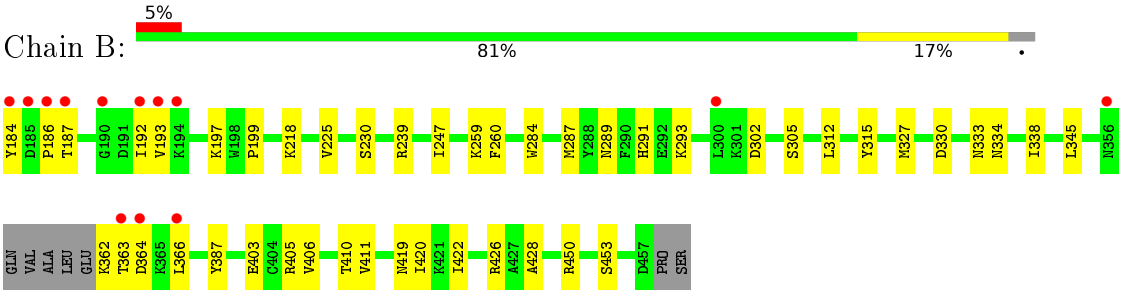
3 Residue-property plots (i)

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

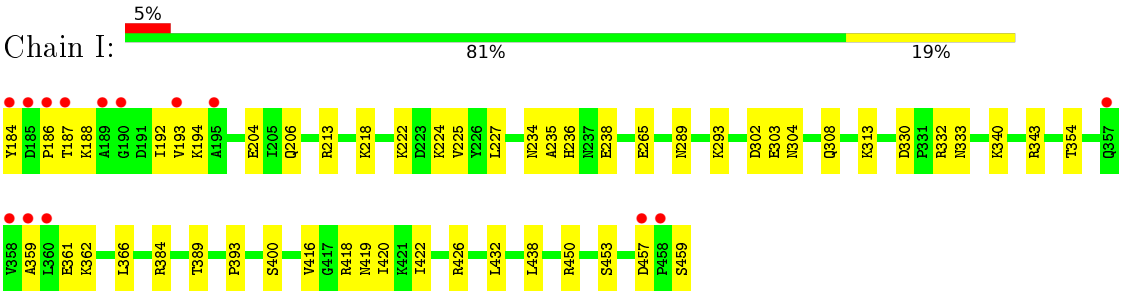
- Molecule 1: Ribonuclease 3



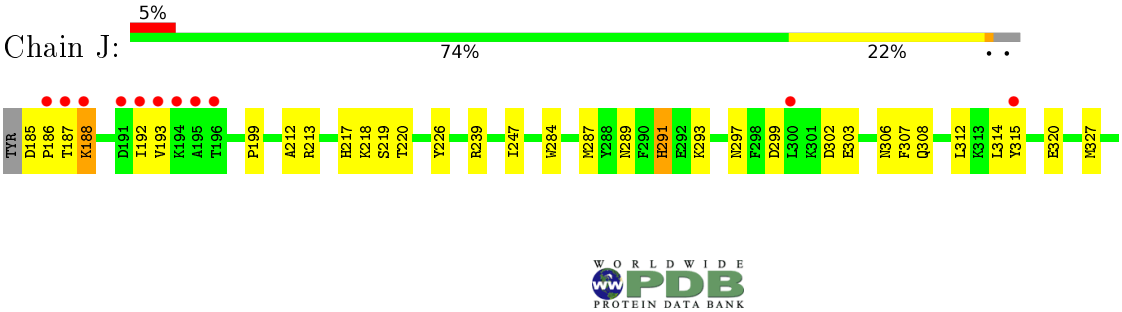
- Molecule 1: Ribonuclease 3



- Molecule 1: Ribonuclease 3

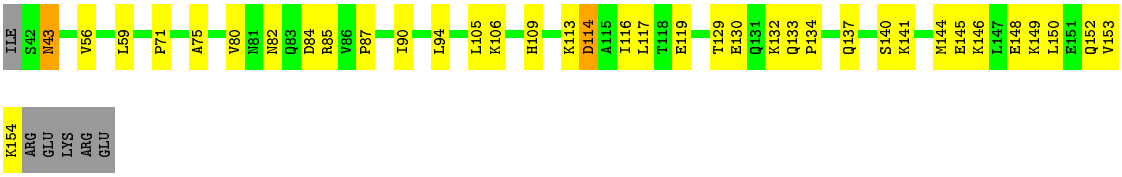


- Molecule 1: Ribonuclease 3



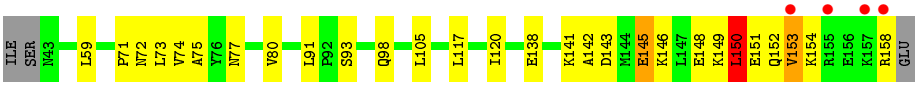
• Molecule 2: Ribonuclease 3

Chain C:



• Molecule 2: Ribonuclease 3

Chain D:

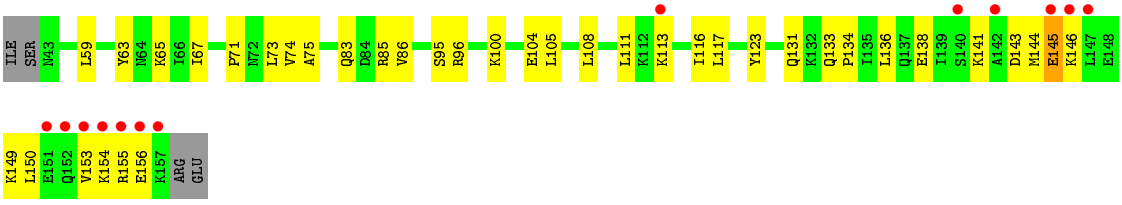


• Molecule 2: Ribonuclease 3

Chain E:

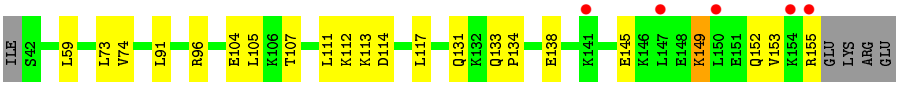
• Molecule 2: Ribonuclease 3

Chain F:



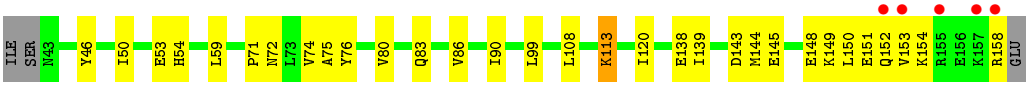
• Molecule 2: Ribonuclease 3

Chain K:

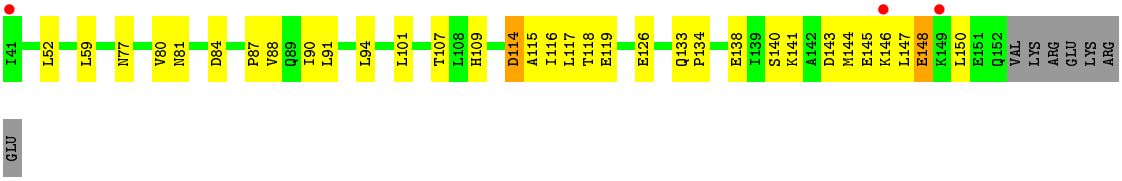


• Molecule 2: Ribonuclease 3

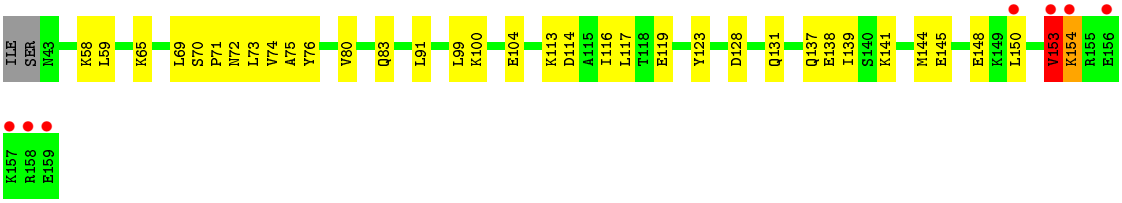
Chain L:



• Molecule 2: Ribonuclease 3



• Molecule 2: Ribonuclease 3



• Molecule 3: RNA substrate analog

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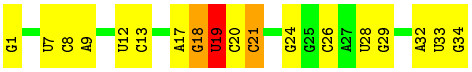

• Molecule 3: RNA substrate analog

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.04Å 164.06Å 176.85Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	38.98 – 2.78 39.94 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.98-2.78) 98.2 (39.94-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.77Å)	Xtriage
Refinement program	PHENIX (dev_2376: ???)	Depositor
R, R_{free}	0.226 , 0.265 0.222 , 0.267	Depositor DCC
R_{free} test set	990 reflections (1.15%)	DCC
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19568	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.09 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2043e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 73W

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	0.53	0/2252	0.67	0/3036
1	B	0.54	0/2199	0.68	0/2961
1	I	0.53	0/2252	0.72	1/3036 (0.0%)
1	J	0.56	1/2178 (0.0%)	0.68	0/2933
2	C	0.53	0/937	0.71	0/1267
2	D	0.57	0/971	0.76	1/1310 (0.1%)
2	E	0.63	0/960	0.77	0/1296
2	F	0.63	0/960	0.99	3/1296 (0.2%)
2	K	0.62	0/948	0.83	2/1281 (0.2%)
2	L	0.54	0/971	0.69	0/1310
2	M	0.61	0/929	0.72	0/1257
2	N	0.70	1/980 (0.1%)	0.87	1/1322 (0.1%)
3	G	0.70	0/782	1.10	1/1215 (0.1%)
3	H	0.69	0/782	1.23	3/1215 (0.2%)
3	O	0.70	0/782	1.17	2/1215 (0.2%)
3	P	0.66	0/782	1.24	6/1215 (0.5%)
All	All	0.59	2/19665 (0.0%)	0.84	20/27165 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	C	0	1
2	K	0	1
2	M	0	1
2	N	0	2
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	153	VAL	CA-CB	5.17	1.65	1.54
1	J	404	CYS	CB-SG	-5.07	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	144	MET	CB-CA-C	-15.60	79.20	110.40
2	F	145	GLU	N-CA-CB	-12.78	87.60	110.60
3	P	19	U	C5-C4-O4	9.09	131.35	125.90
3	H	19	U	C5-C4-O4	8.22	130.83	125.90
3	P	19	U	N3-C4-O4	-7.64	114.05	119.40
3	H	19	U	N3-C4-O4	-7.10	114.43	119.40
3	P	19	U	N3-C2-O2	-6.94	117.34	122.20
3	H	19	U	N3-C2-O2	-6.92	117.36	122.20
2	N	154	LYS	CB-CG-CD	6.25	127.84	111.60
2	D	150	LEU	CA-CB-CG	5.83	128.71	115.30
1	I	194	LYS	N-CA-C	-5.43	96.34	111.00
3	P	21	C	N1-C2-O2	5.42	122.15	118.90
2	K	111	LEU	N-CA-C	-5.41	96.40	111.00
3	O	19	U	N3-C2-O2	-5.37	118.44	122.20
2	K	153	VAL	CG1-CB-CG2	5.32	119.41	110.90
3	P	25	G	C4-N9-C1'	5.32	133.41	126.50
3	G	19	U	O4'-C1'-N1	5.29	112.43	108.20
2	F	145	GLU	N-CA-C	5.14	124.89	111.00
3	P	19	U	N1-C2-N3	5.10	117.96	114.90
3	O	21	C	N3-C4-N4	-5.06	114.46	118.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	ARG	Peptide
1	A	451	SER	Peptide
2	C	114	ASP	Peptide
2	K	114	ASP	Peptide
2	M	114	ASP	Peptide
2	N	114	ASP	Peptide
2	N	153	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2212	0	2270	31	0
1	B	2161	0	2218	30	0
1	I	2212	0	2270	43	0
1	J	2141	0	2202	46	0
2	C	925	0	945	34	0
2	D	959	0	985	30	0
2	E	948	0	972	32	0
2	F	948	0	972	37	0
2	K	936	0	958	19	0
2	L	959	0	985	20	0
2	M	917	0	934	26	0
2	N	968	0	991	34	0
3	G	721	0	356	12	0
3	H	721	0	356	14	0
3	O	721	0	356	13	0
3	P	721	0	356	16	0
4	A	4	0	6	0	0
4	E	4	0	6	0	0
4	F	4	0	6	1	0
4	H	4	0	6	0	0
4	I	20	0	30	2	0
4	J	4	0	6	2	0
5	A	43	0	0	4	0
5	B	44	0	0	2	0
5	C	15	0	0	6	0
5	D	12	0	0	1	0
5	E	7	0	0	1	0
5	F	9	0	0	0	0
5	G	20	0	0	3	0
5	H	25	0	0	2	0
5	I	51	0	0	4	0
5	J	46	0	0	6	0
5	K	12	0	0	1	0
5	L	13	0	0	0	0
5	M	6	0	0	1	0
5	N	14	0	0	0	0
5	O	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	14	0	0	2	0
All	All	19568	0	18186	382	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 10.

All (382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:GLU:HA	2:D:148:GLU:HG2	1.55	0.89
2:K:107:THR:HG21	2:L:139:ILE:HD12	1.55	0.88
3:P:3:73W:SP2	5:P:111:HOH:O	2.33	0.84
2:F:145:GLU:HA	2:F:149:LYS:HE2	1.60	0.83
1:I:450:ARG:HA	1:I:453:SER:HB3	1.60	0.83
1:J:394:THR:HB	4:J:501:EDO:H11	1.57	0.83
1:I:225:VAL:HG11	3:P:15:U:H4'	1.61	0.82
1:B:450:ARG:HA	1:B:453:SER:HB3	1.59	0.82
2:E:154:LYS:HA	2:E:157:LYS:HG2	1.62	0.81
2:C:82:ASN:HB3	2:C:85:ARG:HH11	1.43	0.80
3:P:3:73W:N4	5:P:101:HOH:O	2.13	0.80
2:L:150:LEU:O	2:L:154:LYS:HG3	1.81	0.79
1:J:218:LYS:HE3	3:O:26:C:H5"	1.65	0.78
1:A:218:LYS:HE3	3:H:26:C:H5"	1.64	0.77
2:M:87:PRO:HG2	2:M:90:ILE:HG13	1.64	0.77
2:E:152:GLN:O	2:E:156:GLU:HG3	1.85	0.76
2:M:107:THR:HG21	2:N:139:ILE:HD12	1.66	0.76
2:M:148:GLU:H	2:M:148:GLU:CD	1.90	0.75
2:C:149:LYS:HA	2:C:152:GLN:HB3	1.70	0.73
1:I:393:PRO:HD3	1:I:400:SER:HB2	1.72	0.71
1:B:366:LEU:HD21	1:B:422:ILE:HG23	1.73	0.71
2:F:145:GLU:O	2:F:149:LYS:HG2	1.92	0.70
2:E:78:GLU:O	2:E:82:ASN:ND2	2.25	0.69
1:J:185:ASP:HB3	1:J:186:PRO:CD	2.22	0.69
2:D:145:GLU:CA	2:D:148:GLU:HG2	2.19	0.69
3:G:2:C:OP2	5:G:101:HOH:O	2.09	0.69
2:C:145:GLU:OE1	2:C:145:GLU:N	2.24	0.69
1:J:291:HIS:CD2	1:J:291:HIS:H	2.11	0.68
2:E:146:LYS:O	2:E:150:LEU:HD13	1.94	0.68
2:N:139:ILE:HD11	2:N:144:MET:SD	2.35	0.67
2:N:150:LEU:HA	2:N:153:VAL:HG12	1.73	0.67
2:M:140:SER:HB3	2:M:143:ASP:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ASP:O	1:A:459:SER:N	2.24	0.67
2:D:145:GLU:CD	2:D:145:GLU:H	1.98	0.67
1:I:457:ASP:O	1:I:459:SER:N	2.27	0.67
2:F:108:LEU:HA	2:F:113:LYS:NZ	2.10	0.66
2:M:146:LYS:O	2:M:150:LEU:HG	1.94	0.66
1:I:366:LEU:HD21	1:I:422:ILE:HG23	1.78	0.66
2:C:137:GLN:HB2	5:C:201:HOH:O	1.95	0.65
2:E:119:GLU:N	2:E:119:GLU:OE1	2.26	0.65
1:I:213:ARG:HH11	4:I:501:EDO:H21	1.62	0.65
2:M:133:GLN:HG3	2:M:134:PRO:HD2	1.77	0.65
1:A:184:TYR:HA	1:A:185:ASP:O	1.97	0.65
3:G:8:C:H2'	3:G:9:A:H8	1.61	0.65
2:C:85:ARG:HH12	1:I:332:ARG:NH2	1.95	0.65
2:N:119:GLU:HG2	2:N:137:GLN:HE22	1.60	0.65
2:F:105:LEU:HA	2:F:108:LEU:HD12	1.80	0.64
2:N:116:ILE:HD12	2:N:116:ILE:H	1.62	0.64
1:I:384:ARG:NH1	5:I:602:HOH:O	2.30	0.64
1:B:289:ASN:HA	1:B:291:HIS:CE1	2.32	0.63
2:L:71:PRO:HB2	2:L:75:ALA:HB3	1.79	0.63
1:J:348:PRO:HA	1:J:351:GLU:HG2	1.78	0.63
1:A:313:LYS:NZ	5:A:604:HOH:O	2.31	0.63
2:E:119:GLU:O	2:E:123:TYR:N	2.31	0.62
2:F:116:ILE:HD12	2:F:116:ILE:H	1.62	0.62
3:G:18:G:OP2	5:G:102:HOH:O	2.15	0.62
2:F:108:LEU:HD23	2:F:113:LYS:HG3	1.80	0.62
1:J:450:ARG:HA	1:J:453:SER:HB3	1.81	0.62
2:K:152:GLN:O	2:K:155:ARG:HG3	2.00	0.62
2:C:141:LYS:NZ	5:C:202:HOH:O	2.33	0.62
1:I:218:LYS:HE3	3:P:26:C:H5"	1.81	0.62
3:O:8:C:H2'	3:O:9:A:H8	1.65	0.61
1:J:420:ILE:HG13	3:P:7:U:OP1	2.00	0.61
1:B:192:ILE:HG22	1:B:193:VAL:HG13	1.83	0.61
2:E:149:LYS:O	2:E:153:VAL:HG23	2.00	0.61
1:A:366:LEU:HD21	1:A:422:ILE:HG23	1.82	0.61
2:M:116:ILE:HD12	2:N:116:ILE:HD13	1.82	0.61
1:A:222:LYS:NZ	3:H:26:C:OP1	2.33	0.61
2:L:138:GLU:OE1	2:L:138:GLU:N	2.34	0.61
2:N:153:VAL:O	2:N:154:LYS:HG2	2.01	0.60
2:N:137:GLN:H	2:N:137:GLN:CD	2.04	0.60
2:E:63:TYR:CD1	2:E:117:LEU:HD21	2.37	0.60
1:I:313:LYS:HE3	3:P:3:73W:SP1	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:ASN:OD1	2:C:43:ASN:N	2.33	0.60
2:D:149:LYS:HA	2:D:152:GLN:HB3	1.83	0.60
1:I:330:ASP:OD2	1:I:333:ASN:HB2	2.01	0.60
2:D:93:SER:OG	5:D:201:HOH:O	2.17	0.59
1:B:199:PRO:HG3	1:B:287:MET:HG2	1.85	0.59
1:J:421:LYS:O	1:J:425:ILE:HD13	2.03	0.59
2:M:145:GLU:HA	2:M:148:GLU:CD	2.23	0.59
2:E:157:LYS:HD3	2:E:157:LYS:N	2.17	0.59
3:H:32:A:H2'	3:H:33:U:C6	2.38	0.59
1:A:313:LYS:HE3	3:H:3:73W:SP1	2.43	0.59
2:F:111:LEU:HD12	2:F:113:LYS:NZ	2.19	0.58
2:C:130:GLU:HA	2:C:132:LYS:NZ	2.18	0.58
1:J:186:PRO:HB3	1:J:188:LYS:HD3	1.84	0.58
1:A:225:VAL:HG21	3:H:15:U:H4'	1.85	0.58
1:A:450:ARG:HA	1:A:453:SER:HB3	1.84	0.58
1:I:416:VAL:O	1:I:426:ARG:NH1	2.38	0.57
2:L:46:TYR:CZ	2:L:50:ILE:HD11	2.40	0.57
2:D:154:LYS:O	2:D:154:LYS:HD2	2.05	0.57
1:B:420:ILE:HG13	3:H:7:U:OP1	2.05	0.57
2:D:154:LYS:HD2	2:D:154:LYS:C	2.25	0.57
1:B:259:LYS:HG2	1:B:260:PHE:CE1	2.39	0.57
2:L:149:LYS:O	2:L:153:VAL:HG23	2.05	0.57
1:A:359:ALA:HA	1:A:418:ARG:HD3	1.87	0.57
1:J:291:HIS:HD2	1:J:291:HIS:H	1.52	0.57
1:A:184:TYR:HA	1:A:185:ASP:C	2.25	0.56
2:F:133:GLN:HG3	2:F:134:PRO:HD2	1.87	0.56
2:E:143:ASP:HB3	2:F:111:LEU:HD13	1.88	0.56
2:D:149:LYS:O	2:D:152:GLN:HB3	2.06	0.56
2:K:131:GLN:OE1	2:K:133:GLN:N	2.34	0.56
2:D:151:GLU:HA	2:D:154:LYS:HB3	1.88	0.56
2:K:149:LYS:HA	2:K:152:GLN:HB3	1.86	0.56
2:E:138:GLU:N	2:E:138:GLU:OE1	2.38	0.56
2:C:150:LEU:O	2:C:153:VAL:HG12	2.06	0.55
2:N:72:ASN:OD1	2:N:74:VAL:HG12	2.06	0.55
2:C:85:ARG:HH12	1:I:332:ARG:HH21	1.55	0.55
2:K:73:LEU:HD11	2:K:104:GLU:HG2	1.89	0.55
2:L:72:ASN:OD1	2:L:74:VAL:HG22	2.05	0.55
2:E:101:LEU:HB2	2:F:123:TYR:CE1	2.42	0.55
2:F:138:GLU:OE1	2:F:138:GLU:N	2.39	0.55
1:J:289:ASN:O	1:J:293:LYS:HG3	2.07	0.55
2:C:119:GLU:OE2	5:C:201:HOH:O	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:PRO:HB2	2:D:75:ALA:HB3	1.88	0.55
1:J:239:ARG:HB2	5:J:607:HOH:O	2.07	0.55
1:J:185:ASP:HB3	1:J:186:PRO:HD2	1.88	0.55
1:J:291:HIS:N	1:J:291:HIS:CD2	2.76	0.54
2:M:115:ALA:O	2:M:119:GLU:HG3	2.07	0.54
2:E:150:LEU:O	2:E:153:VAL:HB	2.08	0.54
1:A:416:VAL:O	1:A:426:ARG:NH1	2.40	0.54
2:D:154:LYS:HZ1	2:D:158:ARG:NH1	2.06	0.54
2:L:139:ILE:HD11	2:L:144:MET:SD	2.47	0.54
2:M:148:GLU:OE2	2:M:148:GLU:N	2.41	0.54
3:P:32:A:H2'	3:P:33:U:C6	2.42	0.54
1:B:187:THR:O	1:B:187:THR:HG22	2.08	0.54
1:J:419:ASN:OD1	1:J:422:ILE:HG12	2.08	0.54
2:K:113:LYS:NZ	2:L:143:ASP:OD2	2.39	0.54
1:A:289:ASN:O	1:A:293:LYS:HG3	2.08	0.53
2:M:77:ASN:HA	2:M:80:VAL:HG12	1.89	0.53
1:J:403:GLU:OE1	1:J:405:ARG:NH2	2.40	0.53
2:M:117:LEU:HD21	2:N:117:LEU:HD21	1.90	0.53
2:E:119:GLU:HA	2:E:122:ASP:HB2	1.91	0.53
2:N:83:GLN:HB3	2:N:91:LEU:HD21	1.91	0.53
1:I:186:PRO:HB2	1:I:188:LYS:H	1.74	0.53
1:J:213:ARG:NH1	5:J:607:HOH:O	2.41	0.53
2:E:133:GLN:NE2	2:E:134:PRO:HD2	2.24	0.53
1:I:359:ALA:HA	1:I:418:ARG:CD	2.39	0.53
2:M:138:GLU:OE1	2:M:138:GLU:N	2.42	0.53
2:C:140:SER:HB3	5:C:203:HOH:O	2.09	0.52
1:I:236:HIS:CE1	1:I:238:GLU:HG2	2.45	0.52
1:B:366:LEU:HD11	1:B:426:ARG:NH2	2.25	0.52
1:J:395:ALA:HB3	4:J:501:EDO:H22	1.90	0.52
1:B:218:LYS:HE3	3:G:26:C:H5"	1.90	0.52
3:G:1:G:H5'	3:H:34:G:H3'	1.93	0.51
3:H:12:U:H2'	3:H:13:C:C6	2.45	0.51
2:F:63:TYR:CE1	2:F:117:LEU:HD13	2.45	0.51
2:N:141:LYS:N	2:N:141:LYS:HD3	2.26	0.51
2:M:91:LEU:HD23	2:M:94:LEU:HD12	1.93	0.51
3:G:14:A:OP2	5:G:103:HOH:O	2.19	0.51
2:C:82:ASN:HB3	2:C:85:ARG:NH1	2.21	0.51
2:C:113:LYS:NZ	2:D:143:ASP:OD2	2.24	0.51
2:E:73:LEU:HD12	2:E:104:GLU:HG2	1.93	0.51
1:I:340:LYS:HD2	1:I:343:ARG:HH21	1.76	0.51
2:N:58:LYS:NZ	3:P:16:G:OP1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:LYS:O	2:C:150:LEU:HD13	2.11	0.50
3:H:9:A:H2'	3:H:10:U:C6	2.46	0.50
1:J:185:ASP:O	1:J:186:PRO:C	2.47	0.50
2:C:117:LEU:HD21	2:D:117:LEU:HD21	1.92	0.50
2:F:108:LEU:HA	2:F:113:LYS:HZ3	1.75	0.50
1:I:265:GLU:HG2	5:O:113:HOH:O	2.10	0.50
2:K:149:LYS:HB2	2:K:152:GLN:HB3	1.93	0.50
2:N:73:LEU:HD11	2:N:104:GLU:HG2	1.93	0.50
1:J:330:ASP:OD2	1:J:333:ASN:HB2	2.12	0.50
2:L:145:GLU:HA	2:L:148:GLU:HB3	1.93	0.50
2:N:150:LEU:HA	2:N:153:VAL:CG1	2.41	0.50
1:B:387:TYR:HE2	5:B:510:HOH:O	1.94	0.50
2:F:155:ARG:HG2	2:F:156:GLU:HG2	1.94	0.50
2:L:86:VAL:HB	2:L:90:ILE:HD11	1.93	0.50
1:A:359:ALA:HA	1:A:418:ARG:CD	2.42	0.50
2:D:72:ASN:OD1	2:D:74:VAL:HG22	2.12	0.50
1:I:359:ALA:HA	1:I:418:ARG:HD3	1.93	0.50
2:M:107:THR:HG21	2:N:139:ILE:CD1	2.40	0.50
1:B:330:ASP:OD2	1:B:333:ASN:HB2	2.12	0.49
3:O:32:A:H2'	3:O:33:U:C6	2.47	0.49
2:F:145:GLU:HG2	2:F:146:LYS:N	2.27	0.49
2:M:77:ASN:O	2:M:81:ASN:ND2	2.45	0.49
2:K:59:LEU:HD12	2:L:59:LEU:HD12	1.93	0.49
2:L:76:TYR:O	2:L:80:VAL:HG13	2.11	0.49
2:C:59:LEU:HD12	2:D:59:LEU:HD12	1.95	0.49
1:J:351:GLU:HG3	1:J:352:GLU:N	2.28	0.49
2:C:129:THR:O	2:C:132:LYS:NZ	2.39	0.49
3:O:8:C:H2'	3:O:9:A:C8	2.45	0.49
2:F:116:ILE:HD11	4:F:201:EDO:O1	2.13	0.49
1:I:420:ILE:HG13	3:O:7:U:OP1	2.13	0.48
2:F:150:LEU:O	2:F:153:VAL:HB	2.13	0.48
1:I:289:ASN:O	1:I:293:LYS:HG3	2.14	0.48
1:J:212:ALA:HB2	2:K:91:LEU:HD12	1.94	0.48
2:C:109:HIS:ND1	2:C:114:ASP:OD2	2.45	0.48
2:E:104:GLU:OE1	2:F:136:LEU:HG	2.13	0.48
2:E:152:GLN:HB3	2:E:155:ARG:HH21	1.78	0.48
1:J:303:GLU:HA	1:J:308:GLN:HG3	1.96	0.48
1:I:222:LYS:NZ	3:P:26:C:OP1	2.37	0.48
2:C:144:MET:O	2:C:148:GLU:HG3	2.13	0.48
2:N:144:MET:O	2:N:148:GLU:HG3	2.13	0.48
2:D:77:ASN:HA	2:D:80:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:320:GLU:OE1	5:J:601:HOH:O	2.20	0.48
2:E:53:GLU:OE2	2:F:96:ARG:NH1	2.38	0.48
5:A:642:HOH:O	1:B:230:SER:HB2	2.13	0.48
2:F:73:LEU:HD11	2:F:104:GLU:HG2	1.96	0.48
3:H:31:C:OP2	5:H:201:HOH:O	2.20	0.48
1:A:225:VAL:HG23	5:A:630:HOH:O	2.13	0.48
2:F:150:LEU:O	2:F:154:LYS:HG3	2.14	0.48
1:J:289:ASN:HA	1:J:291:HIS:CD2	2.49	0.48
1:J:312:LEU:HD23	1:J:315:TYR:CE2	2.48	0.48
3:P:19:U:H5'	3:P:21:C:H1'	1.96	0.47
2:N:100:LYS:O	2:N:104:GLU:HG3	2.14	0.47
2:N:71:PRO:HB2	2:N:75:ALA:HB3	1.96	0.47
1:A:451:SER:HA	1:A:453:SER:N	2.29	0.47
2:D:145:GLU:O	2:D:149:LYS:HG3	2.13	0.47
1:J:192:ILE:HG22	1:J:193:VAL:HG13	1.96	0.47
1:B:428:ALA:N	5:B:510:HOH:O	2.47	0.47
2:D:142:ALA:HA	2:D:145:GLU:OE2	2.14	0.47
1:I:187:THR:HG23	1:I:192:ILE:HA	1.96	0.47
1:J:284:TRP:CD1	1:J:345:LEU:HD22	2.49	0.47
1:B:289:ASN:O	1:B:293:LYS:HG3	2.14	0.47
2:D:154:LYS:NZ	2:D:158:ARG:NH1	2.63	0.47
1:A:420:ILE:HG13	3:G:7:U:OP1	2.14	0.47
1:I:354:THR:O	1:I:361:GLU:HG3	2.15	0.47
5:E:305:HOH:O	2:F:65:LYS:HE2	2.14	0.47
2:L:83:GLN:O	2:L:86:VAL:HG22	2.15	0.47
2:N:145:GLU:H	2:N:145:GLU:CD	2.18	0.47
2:D:149:LYS:HA	2:D:152:GLN:CB	2.45	0.47
1:I:192:ILE:O	1:I:193:VAL:HG22	2.15	0.47
2:K:117:LEU:HD12	2:K:117:LEU:HA	1.72	0.47
2:K:138:GLU:N	2:K:138:GLU:OE1	2.48	0.47
2:F:111:LEU:HD12	2:F:113:LYS:HZ1	1.79	0.47
1:A:451:SER:HB2	1:A:454:VAL:HG12	1.96	0.47
2:C:133:GLN:HB3	2:C:134:PRO:HD2	1.97	0.47
1:I:192:ILE:HG22	1:I:193:VAL:H	1.79	0.47
1:A:390:VAL:HG23	1:A:401:ILE:HB	1.95	0.46
1:J:369:ASN:OD1	1:J:372:ARG:HD2	2.15	0.46
1:J:443:LYS:NZ	5:J:610:HOH:O	2.48	0.46
1:A:260:PHE:O	1:B:239:ARG:NH2	2.48	0.46
1:A:451:SER:HA	1:A:452:GLU:C	2.36	0.46
2:C:106:LYS:HE2	5:C:204:HOH:O	2.15	0.46
2:M:126:GLU:HG3	2:M:126:GLU:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:HIS:HA	2:C:114:ASP:OD2	2.16	0.46
3:O:34:G:C2	3:P:1:G:H1'	2.50	0.46
1:I:400:SER:O	1:I:416:VAL:HA	2.15	0.46
2:N:65:LYS:HD2	2:N:65:LYS:HA	1.77	0.46
2:D:145:GLU:HA	2:D:148:GLU:CG	2.38	0.46
2:F:141:LYS:HD2	2:F:141:LYS:O	2.16	0.46
1:I:453:SER:OG	5:I:601:HOH:O	2.21	0.46
2:K:149:LYS:O	2:K:149:LYS:HG3	2.16	0.46
2:C:105:LEU:HD21	2:D:120:ILE:HD11	1.98	0.46
1:J:226:TYR:CE2	2:L:53:GLU:HB3	2.51	0.46
2:C:87:PRO:HG2	2:C:90:ILE:HG13	1.97	0.45
2:E:101:LEU:HD13	2:F:123:TYR:CD2	2.51	0.45
1:J:199:PRO:HG3	1:J:287:MET:HG2	1.97	0.45
1:A:224:LYS:HB2	1:A:227:LEU:HD12	1.97	0.45
2:C:130:GLU:HA	2:C:132:LYS:HZ1	1.81	0.45
2:E:84:ASP:N	2:E:84:ASP:OD1	2.45	0.45
2:N:137:GLN:N	2:N:137:GLN:CD	2.69	0.45
2:D:149:LYS:O	2:D:153:VAL:HG13	2.17	0.45
2:C:85:ARG:NH1	1:I:332:ARG:NH2	2.64	0.45
2:L:46:TYR:CE1	2:L:50:ILE:HD11	2.51	0.45
2:M:148:GLU:CD	2:M:148:GLU:N	2.61	0.45
2:M:59:LEU:HD12	2:N:59:LEU:HD12	1.97	0.45
2:D:141:LYS:HB2	2:D:141:LYS:HE3	1.69	0.45
3:H:32:A:H2'	3:H:33:U:H6	1.78	0.45
1:A:340:LYS:NZ	5:A:606:HOH:O	2.48	0.45
2:C:109:HIS:HA	2:C:114:ASP:CG	2.37	0.45
2:C:84:ASP:OD1	2:C:84:ASP:N	2.47	0.45
1:B:405:ARG:HG2	1:B:411:VAL:HG22	1.99	0.45
2:M:101:LEU:HB2	2:N:123:TYR:CE1	2.51	0.45
1:J:219:SER:HB2	1:J:297:ASN:HB3	1.98	0.45
2:K:149:LYS:HD2	2:K:152:GLN:HG2	1.98	0.45
1:B:247:ILE:HG13	1:B:327:MET:HG3	1.98	0.44
1:B:362:LYS:HB3	1:B:363:THR:H	1.34	0.44
1:J:247:ILE:HG13	1:J:327:MET:HG3	1.99	0.44
1:J:335:LEU:HB3	1:J:336:PRO:HD3	1.98	0.44
1:A:217:HIS:O	1:A:220:THR:HB	2.17	0.44
1:I:224:LYS:HB2	1:I:227:LEU:HD12	1.99	0.44
1:B:184:TYR:O	1:B:186:PRO:HD2	2.18	0.44
1:B:419:ASN:OD1	1:B:422:ILE:HG12	2.17	0.44
3:G:1:G:H8	3:G:1:G:HO5'	1.64	0.44
2:N:76:TYR:O	2:N:80:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:453:SER:CB	3:O:18:G:H21	2.30	0.44
3:P:32:A:H2'	3:P:33:U:H6	1.82	0.44
1:B:259:LYS:HG3	1:B:259:LYS:O	2.18	0.44
1:B:284:TRP:CD1	1:B:345:LEU:HD22	2.53	0.44
1:J:406:VAL:HG13	1:J:412:LEU:HD11	2.00	0.44
2:M:109:HIS:HE1	5:M:205:HOH:O	1.98	0.44
2:F:63:TYR:CE1	2:F:67:ILE:HD11	2.53	0.44
2:N:141:LYS:O	2:N:144:MET:HB2	2.17	0.44
2:M:52:LEU:HD21	2:N:70:SER:HB2	1.99	0.44
2:N:99:LEU:HD23	2:N:99:LEU:HA	1.75	0.44
1:J:299:ASP:OD2	1:J:302:ASP:HB2	2.18	0.44
2:E:77:ASN:O	2:E:81:ASN:ND2	2.51	0.43
1:I:234:ASN:HA	4:I:501:EDO:H12	1.99	0.43
1:J:457:ASP:HB2	5:J:630:HOH:O	2.18	0.43
2:M:144:MET:O	2:M:147:LEU:N	2.40	0.43
3:H:31:C:H2'	3:H:32:A:H8	1.82	0.43
1:I:419:ASN:OD1	1:I:422:ILE:HG12	2.18	0.43
3:P:9:A:H2'	3:P:10:U:C6	2.53	0.43
1:A:362:LYS:HA	1:A:362:LYS:HD2	1.37	0.43
1:A:371:LYS:HD3	1:A:387:TYR:CE1	2.53	0.43
2:D:150:LEU:O	2:D:154:LYS:HB3	2.18	0.43
2:F:150:LEU:HA	2:F:150:LEU:HD12	1.85	0.43
1:I:303:GLU:HA	1:I:308:GLN:HG3	1.99	0.43
2:M:101:LEU:HD13	2:N:123:TYR:CD2	2.54	0.43
3:P:12:U:H2'	3:P:13:C:C6	2.53	0.43
2:K:74:VAL:HG11	2:L:151:GLU:HG3	1.99	0.43
2:K:145:GLU:OE1	2:K:145:GLU:N	2.43	0.43
2:L:99:LEU:HD23	2:L:99:LEU:HA	1.86	0.43
2:E:152:GLN:HA	2:E:155:ARG:HE	1.83	0.43
1:A:315:TYR:O	1:A:318:VAL:HG12	2.18	0.43
2:E:82:ASN:O	2:E:83:GLN:HB2	2.18	0.43
2:E:59:LEU:HD12	2:F:59:LEU:HD12	2.01	0.43
3:P:33:U:H2'	3:P:34:G:O4'	2.19	0.43
1:B:312:LEU:HD23	1:B:315:TYR:CE2	2.54	0.43
2:E:58:LYS:NZ	2:E:61:GLU:OE1	2.50	0.43
1:J:307:PHE:HE1	1:J:314:LEU:HD13	1.83	0.43
2:N:138:GLU:N	2:N:138:GLU:OE1	2.52	0.43
1:B:334:ASN:O	1:B:338:ILE:HG13	2.19	0.42
1:B:363:THR:OG1	1:B:364:ASP:N	2.51	0.42
2:D:138:GLU:OE1	2:D:138:GLU:N	2.52	0.42
3:G:8:C:H2'	3:G:9:A:C8	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:O	1:A:416:VAL:HA	2.19	0.42
2:F:149:LYS:O	2:F:153:VAL:HG23	2.18	0.42
1:I:213:ARG:HG3	1:I:235:ALA:O	2.19	0.42
1:J:424:GLY:HA3	5:J:608:HOH:O	2.19	0.42
2:K:105:LEU:HD21	2:L:120:ILE:HD11	2.01	0.42
2:K:96:ARG:NH2	5:K:204:HOH:O	2.51	0.42
1:A:406:VAL:HG22	1:A:410:THR:HB	2.01	0.42
2:C:85:ARG:HH22	1:I:332:ARG:CZ	2.32	0.42
2:F:100:LYS:O	2:F:104:GLU:HG3	2.19	0.42
1:I:184:TYR:N	5:I:609:HOH:O	2.52	0.42
2:C:56:VAL:HG11	2:D:98:GLN:HA	2.01	0.42
1:J:217:HIS:O	1:J:220:THR:HB	2.19	0.42
1:B:302:ASP:HB3	1:B:305:SER:HB2	2.02	0.42
2:C:80:VAL:HG12	2:C:94:LEU:HD22	2.01	0.42
2:E:154:LYS:HD3	2:E:154:LYS:N	2.35	0.42
3:O:20:C:O2'	5:O:101:HOH:O	2.21	0.42
2:E:77:ASN:HA	2:E:80:VAL:HG12	2.02	0.42
2:N:141:LYS:O	2:N:144:MET:N	2.51	0.42
3:O:19:U:H5'	3:O:21:C:H1'	2.01	0.42
2:C:116:ILE:HD12	5:C:208:HOH:O	2.20	0.41
2:C:71:PRO:HB2	2:C:75:ALA:HB3	2.02	0.41
2:D:91:LEU:HA	2:D:91:LEU:HD23	1.92	0.41
1:I:192:ILE:C	1:I:193:VAL:HG22	2.40	0.41
3:H:33:U:H2'	3:H:34:G:O4'	2.20	0.41
2:K:133:GLN:HB3	2:K:134:PRO:HD2	2.01	0.41
2:L:108:LEU:HD22	2:L:113:LYS:HB2	2.02	0.41
2:E:113:LYS:NZ	2:F:143:ASP:OD2	2.52	0.41
1:B:406:VAL:HG22	1:B:410:THR:HB	2.03	0.41
2:F:108:LEU:HA	2:F:113:LYS:HZ2	1.86	0.41
3:G:9:A:H2'	3:G:10:U:C6	2.55	0.41
1:A:184:TYR:N	1:A:185:ASP:HB3	2.35	0.41
1:B:225:VAL:HG21	3:G:15:U:H4'	2.03	0.41
2:E:123:TYR:OH	2:F:104:GLU:OE2	2.36	0.41
1:I:204:GLU:OE1	1:I:206:GLN:NE2	2.45	0.41
1:J:347:LYS:HB3	1:J:348:PRO:HD3	2.03	0.41
1:A:184:TYR:CZ	1:A:187:THR:HG23	2.56	0.41
2:F:85:ARG:NH1	2:F:85:ARG:HG3	2.35	0.41
1:I:450:ARG:NH1	5:I:608:HOH:O	2.50	0.41
2:N:69:LEU:HA	2:N:69:LEU:HD23	1.84	0.41
1:J:448:ILE:HA	1:J:449:PRO:HD3	2.00	0.41
2:M:109:HIS:HA	2:M:114:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:143:ASP:OD1	2:N:113:LYS:NZ	2.48	0.41
2:E:58:LYS:HA	2:E:61:GLU:HB3	2.02	0.41
1:J:188:LYS:HE2	1:J:188:LYS:HB2	1.89	0.41
3:O:32:A:H2'	3:O:33:U:H6	1.86	0.41
1:B:403:GLU:OE1	1:B:405:ARG:NH2	2.48	0.40
2:D:73:LEU:HD12	2:D:73:LEU:HA	1.89	0.40
2:K:104:GLU:O	2:K:107:THR:HB	2.21	0.40
2:E:100:LYS:O	2:E:104:GLU:HG3	2.21	0.40
3:G:12:U:H2'	3:G:13:C:C6	2.56	0.40
2:D:105:LEU:HD23	2:D:105:LEU:HA	1.88	0.40
2:F:83:GLN:O	2:F:86:VAL:HG22	2.21	0.40
1:I:192:ILE:O	1:I:193:VAL:CG2	2.69	0.40
1:I:302:ASP:OD1	1:I:304:ASN:N	2.54	0.40
3:H:3:73W:SP1	5:H:218:HOH:O	2.63	0.40
1:J:192:ILE:HG22	1:J:193:VAL:H	1.86	0.40
2:F:131:GLN:HA	2:F:131:GLN:OE1	2.20	0.40
2:F:71:PRO:HB2	2:F:75:ALA:HB3	2.04	0.40
1:I:432:LEU:HA	1:I:438:LEU:HD11	2.04	0.40
2:N:128:ASP:HB3	2:N:131:GLN:HB3	2.04	0.40
3:O:12:U:H2'	3:O:13:C:C6	2.56	0.40
1:J:306:ASN:O	3:O:28:U:H4'	2.21	0.40
3:O:1:G:H5'	3:P:34:G:H3'	2.02	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	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	B	265/276 (96%)	260 (98%)	5 (2%)	0	100	100
1	I	274/276 (99%)	268 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	263/276 (95%)	257 (98%)	6 (2%)	0	100	100
2	C	111/119 (93%)	108 (97%)	3 (3%)	0	100	100
2	D	114/119 (96%)	113 (99%)	1 (1%)	0	100	100
2	E	113/119 (95%)	108 (96%)	5 (4%)	0	100	100
2	F	113/119 (95%)	110 (97%)	3 (3%)	0	100	100
2	K	112/119 (94%)	108 (96%)	4 (4%)	0	100	100
2	L	114/119 (96%)	113 (99%)	1 (1%)	0	100	100
2	M	110/119 (92%)	106 (96%)	4 (4%)	0	100	100
2	N	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
All	All	1978/2056 (96%)	1930 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/242 (100%)	239 (99%)	3 (1%)	78	94
1	B	236/242 (98%)	235 (100%)	1 (0%)	93	98
1	I	242/242 (100%)	240 (99%)	2 (1%)	86	96
1	J	234/242 (97%)	231 (99%)	3 (1%)	76	93
2	C	106/112 (95%)	104 (98%)	2 (2%)	65	90
2	D	109/112 (97%)	105 (96%)	4 (4%)	41	75
2	E	108/112 (96%)	106 (98%)	2 (2%)	65	90
2	F	108/112 (96%)	106 (98%)	2 (2%)	65	90
2	K	107/112 (96%)	105 (98%)	2 (2%)	65	90
2	L	109/112 (97%)	105 (96%)	4 (4%)	41	75
2	M	105/112 (94%)	100 (95%)	5 (5%)	31	64
2	N	110/112 (98%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1816/1864 (97%)	1786 (98%)	30 (2%)	68 91

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	THR
1	A	362	LYS
1	A	451	SER
1	B	197	LYS
2	C	43	ASN
2	C	154	LYS
2	D	145	GLU
2	D	146	LYS
2	D	150	LEU
2	D	153	VAL
2	E	84	ASP
2	E	137	GLN
2	F	74	VAL
2	F	95	SER
1	I	362	LYS
1	I	389	THR
1	J	187	THR
1	J	188	LYS
1	J	291	HIS
2	K	112	LYS
2	K	149	LYS
2	L	54	HIS
2	L	113	LYS
2	L	152	GLN
2	L	158	ARG
2	M	84	ASP
2	M	88	VAL
2	M	118	THR
2	M	141	LYS
2	M	148	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	133	GLN
1	J	291	HIS

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Mol	Chain	Res	Type
2	L	152	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	32/34 (94%)	5 (15%)	0
3	H	32/34 (94%)	5 (15%)	0
3	O	32/34 (94%)	5 (15%)	0
3	P	32/34 (94%)	5 (15%)	0
All	All	128/136 (94%)	20 (15%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	17	A
3	G	18	G
3	G	19	U
3	G	24	G
3	G	29	G
3	H	17	A
3	H	18	G
3	H	19	U
3	H	24	G
3	H	29	G
3	O	17	A
3	O	18	G
3	O	19	U
3	O	24	G
3	O	29	G
3	P	17	A
3	P	18	G
3	P	19	U
3	P	24	G
3	P	29	G

There are no RNA pucker outliers to report.

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

4 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	$\#\|Z\| > 2$
3	73W	G	3	3	14,21,22	1.18	1 (7%)	18,30,33	1.54	4 (22%)
3	73W	H	3	3	14,21,22	1.04	1 (7%)	18,30,33	1.62	4 (22%)
3	73W	O	3	3	14,21,22	1.02	0	18,30,33	1.48	4 (22%)
3	73W	P	3	3	14,21,22	1.17	1 (7%)	18,30,33	1.49	4 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	73W	G	3	3	-	0/3/25/26	0/2/2/2
3	73W	H	3	3	-	0/3/25/26	0/2/2/2
3	73W	O	3	3	-	0/3/25/26	0/2/2/2
3	73W	P	3	3	-	0/3/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	3	73W	O3'-C3'	-2.30	1.37	1.43
3	H	3	73W	O3'-C3'	-2.11	1.38	1.43
3	G	3	73W	C2'-C1'	2.85	1.58	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	3	73W	C2'-C3'-C4'	-3.42	95.64	102.64
3	O	3	73W	O2'-C2'-C1'	-2.87	102.63	111.61
3	G	3	73W	C2'-C3'-C4'	-2.85	96.81	102.64
3	O	3	73W	C2'-C3'-C4'	-2.73	97.04	102.64
3	H	3	73W	C5-C4-N4	-2.69	116.89	121.19
3	H	3	73W	O2'-C2'-C1'	-2.48	103.86	111.61
3	P	3	73W	C5-C4-N4	-2.25	117.59	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3	73W	O2'-C2'-C1'	-2.18	104.80	111.61
3	P	3	73W	O2'-C2'-C1'	-2.07	105.14	111.61
3	H	3	73W	C5-C4-N3	2.18	124.56	121.79
3	O	3	73W	C6-C5-C4	2.22	118.30	117.44
3	G	3	73W	C6-C5-C4	2.33	118.35	117.44
3	P	3	73W	C5-C4-N3	2.38	124.82	121.79
3	O	3	73W	O4'-C1'-N1	2.61	113.06	108.10
3	G	3	73W	O4'-C1'-N1	3.11	114.02	108.10
3	P	3	73W	O4'-C1'-N1	3.85	115.42	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3	73W	2	0
3	P	3	73W	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands 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	$\#\|Z\| > 2$
4	EDO	A	501	-	3,3,3	0.44	0	2,2,2	0.46	0
4	EDO	E	201	-	3,3,3	0.50	0	2,2,2	0.26	0
4	EDO	F	201	-	3,3,3	0.57	0	2,2,2	0.26	0
4	EDO	H	101	-	3,3,3	0.44	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	I	501	-	3,3,3	0.56	0	2,2,2	0.33	0
4	EDO	I	502	-	3,3,3	0.52	0	2,2,2	0.30	0
4	EDO	I	503	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	I	504	-	3,3,3	0.47	0	2,2,2	0.53	0
4	EDO	I	505	-	3,3,3	0.64	0	2,2,2	0.10	0
4	EDO	J	501	-	3,3,3	0.60	0	2,2,2	0.11	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
4	EDO	A	501	-	-	0/1/1/1	0/0/0/0
4	EDO	E	201	-	-	0/1/1/1	0/0/0/0
4	EDO	F	201	-	-	0/1/1/1	0/0/0/0
4	EDO	H	101	-	-	0/1/1/1	0/0/0/0
4	EDO	I	501	-	-	0/1/1/1	0/0/0/0
4	EDO	I	502	-	-	0/1/1/1	0/0/0/0
4	EDO	I	503	-	-	0/1/1/1	0/0/0/0
4	EDO	I	504	-	-	0/1/1/1	0/0/0/0
4	EDO	I	505	-	-	0/1/1/1	0/0/0/0
4	EDO	J	501	-	-	0/1/1/1	0/0/0/0

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	201	EDO	1	0
4	I	501	EDO	2	0
4	J	501	EDO	2	0

5.7 Other polymers

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, 95^{th} 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	276/276 (100%)	0.05	11 (3%) 42 34	34, 50, 77, 86	0
1	B	269/276 (97%)	0.03	13 (4%) 34 26	34, 51, 78, 89	0
1	I	276/276 (100%)	0.06	14 (5%) 32 23	34, 49, 79, 100	0
1	J	267/276 (96%)	0.05	15 (5%) 28 20	32, 49, 77, 87	0
2	C	113/119 (94%)	-0.02	0 100 100	42, 61, 83, 98	0
2	D	116/119 (97%)	0.01	4 (3%) 49 41	37, 60, 85, 93	0
2	E	115/119 (96%)	0.31	6 (5%) 31 23	41, 68, 91, 97	0
2	F	115/119 (96%)	0.35	13 (11%) 7 4	46, 68, 91, 95	0
2	K	114/119 (95%)	0.11	5 (4%) 38 30	40, 63, 87, 92	0
2	L	116/119 (97%)	0.05	5 (4%) 39 31	41, 64, 87, 92	0
2	M	112/119 (94%)	0.17	3 (2%) 58 50	41, 64, 85, 96	0
2	N	117/119 (98%)	0.23	7 (5%) 25 18	40, 65, 88, 95	0
3	G	33/34 (97%)	-0.58	0 100 100	35, 54, 79, 83	0
3	H	33/34 (97%)	-0.82	0 100 100	38, 54, 68, 73	0
3	O	33/34 (97%)	-0.66	0 100 100	35, 54, 75, 78	0
3	P	33/34 (97%)	-0.80	0 100 100	36, 54, 68, 74	0
All	All	2138/2192 (97%)	0.05	96 (4%) 37 29	32, 56, 84, 100	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	358	VAL	7.5
2	F	142	ALA	5.6
1	B	363	THR	5.1
1	A	359	ALA	4.5
1	B	186	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
2	L	157	LYS	4.2
1	B	364	ASP	4.2
1	J	357	GLN	4.1
1	I	360	LEU	4.1
1	J	192	ILE	4.0
1	I	359	ALA	4.0
1	I	186	PRO	4.0
2	L	158	ARG	3.9
2	E	139	ILE	3.8
1	I	185	ASP	3.7
1	I	187	THR	3.7
2	N	159	GLU	3.7
2	F	155	ARG	3.6
2	D	158	ARG	3.5
1	A	360	LEU	3.5
1	I	184	TYR	3.5
2	L	155	ARG	3.5
1	J	300	LEU	3.4
1	B	184	TYR	3.3
2	E	156	GLU	3.3
1	J	186	PRO	3.3
2	F	113	LYS	3.3
2	N	154	LYS	3.3
2	N	158	ARG	3.2
1	J	193	VAL	3.2
2	M	41	ILE	3.2
2	F	157	LYS	3.2
2	K	155	ARG	3.2
1	J	194	LYS	3.1
1	I	358	VAL	3.1
2	D	155	ARG	3.0
2	K	147	LEU	3.0
2	F	147	LEU	3.0
1	A	195	ALA	3.0
1	A	357	GLN	3.0
1	I	193	VAL	2.9
1	J	191	ASP	2.9
2	D	153	VAL	2.9
2	E	153	VAL	2.9
1	B	193	VAL	2.8
1	J	195	ALA	2.8
1	B	192	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	195	ALA	2.8
2	N	156	GLU	2.8
2	F	140	SER	2.8
2	L	153	VAL	2.7
2	F	146	LYS	2.7
1	I	189	ALA	2.7
2	D	157	LYS	2.7
1	B	356	ASN	2.7
2	E	157	LYS	2.7
1	J	315	TYR	2.6
1	B	194	LYS	2.6
2	F	145	GLU	2.6
1	I	357	GLN	2.6
1	A	184	TYR	2.6
2	K	154	LYS	2.6
1	J	196	THR	2.6
1	B	300	LEU	2.6
1	A	193	VAL	2.6
2	F	156	GLU	2.6
2	F	153	VAL	2.5
2	N	157	LYS	2.5
1	J	188	LYS	2.5
2	F	152	GLN	2.5
1	I	457	ASP	2.5
2	F	151	GLU	2.5
2	N	153	VAL	2.5
1	I	190	GLY	2.4
1	A	187	THR	2.4
2	E	152	GLN	2.4
2	N	150	LEU	2.3
2	L	152	GLN	2.2
1	B	190	GLY	2.2
2	E	147	LEU	2.2
2	M	146	LYS	2.2
1	A	196	THR	2.2
2	M	149	LYS	2.1
1	B	366	LEU	2.1
1	B	187	THR	2.1
1	B	185	ASP	2.1
1	A	186	PRO	2.1
1	J	418	ARG	2.1
1	J	187	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	458	PRO	2.1
2	F	154	LYS	2.1
1	A	189	ALA	2.1
1	J	356	ASN	2.0
2	K	150	LEU	2.0
1	A	458	PRO	2.0
2	K	141	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	73W	G	3	20/21	0.95	0.14	-	49,58,77,79	0
3	73W	O	3	20/21	0.96	0.14	-	48,58,83,87	0
3	73W	H	3	20/21	0.96	0.13	-	42,55,81,85	0
3	73W	P	3	20/21	0.95	0.14	-	44,56,93,95	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	J	501	4/4	0.81	0.61	14.02	68,75,76,82	0
4	EDO	F	201	4/4	0.61	0.76	10.92	83,84,86,87	0
4	EDO	I	505	4/4	0.82	0.47	6.74	56,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	I	501	4/4	0.77	0.39	6.23	58,58,70,80	0
4	EDO	H	101	4/4	0.94	0.47	5.40	58,58,64,65	0
4	EDO	I	502	4/4	0.88	0.29	5.24	69,72,75,75	0
4	EDO	I	504	4/4	0.86	0.26	3.37	54,54,54,55	0
4	EDO	A	501	4/4	0.94	0.17	-0.18	56,57,57,60	0
4	EDO	E	201	4/4	0.92	0.10	-	70,77,77,80	0
4	EDO	I	503	4/4	0.84	0.42	-	58,64,66,70	0

6.5 Other polymers

There are no such residues in this entry.