



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 08:55 PM EDT

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

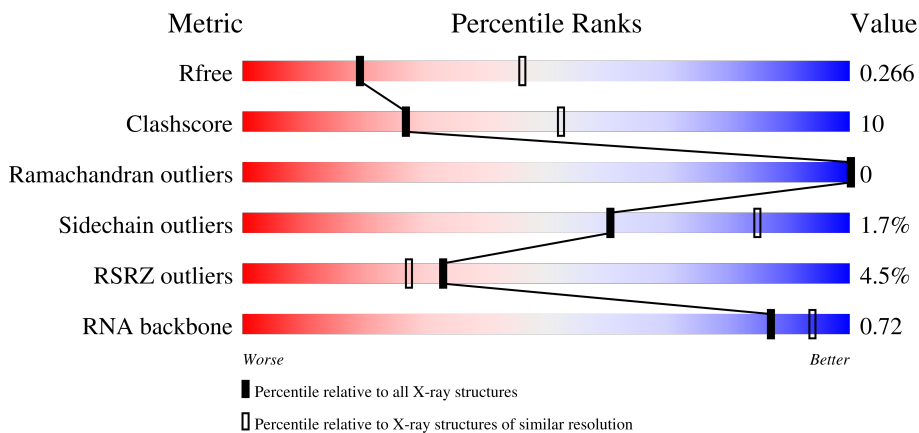
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




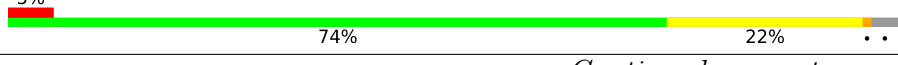
The reported resolution of this entry is 2.78 Å.

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.






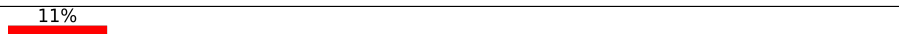
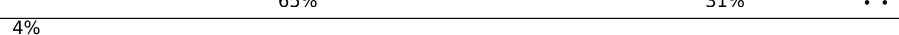




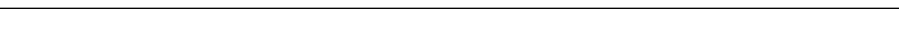
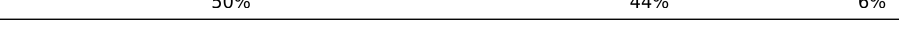

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)
RNA backbone	3102	1092 (3.06-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	276	 4% 86% 13%
1	B	276	 5% 81% 17%
1	I	276	 5% 81% 19%
1	J	276	 5% 74% 22%

Continued on next page...

Continued from previous page...

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

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

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	276	Total 2212	C 1406	N 389	O 409	S 8	0	0	0
1	B	269	Total 2161	C 1374	N 381	O 398	S 8	0	0	0
1	I	276	Total 2212	C 1406	N 389	O 409	S 8	0	0	0
1	J	267	Total 2141	C 1361	N 379	O 393	S 8	0	0	0

- Molecule 2 is a protein called Ribonuclease 3.

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

- 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: C₂H₆O₂).



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		

Continued on next page...

Continued from previous page...

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

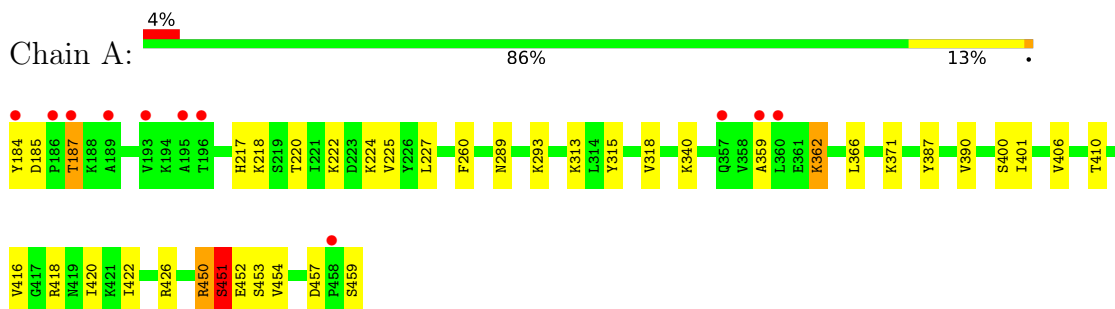
- Molecule 5 is water.

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

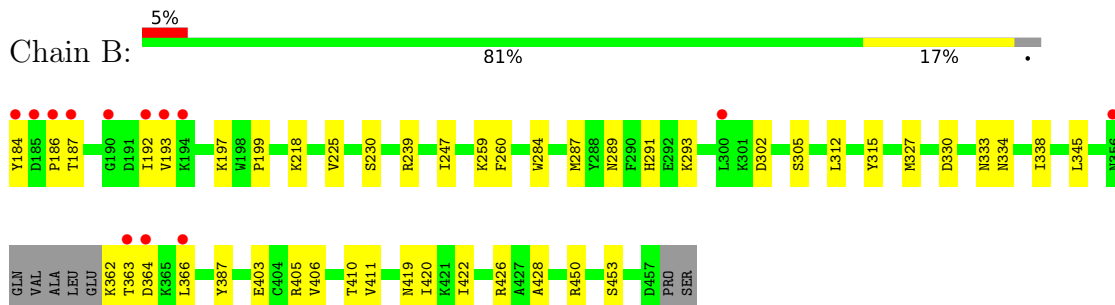
3 Residue-property plots [i](#)

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.

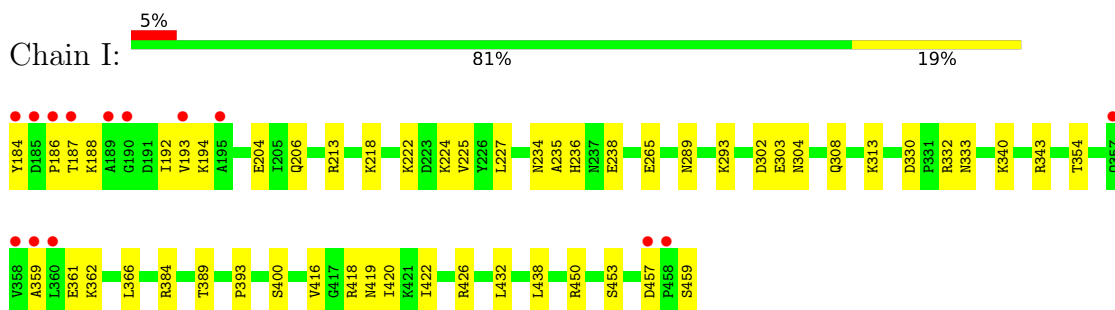
- Molecule 1: Ribonuclease 3



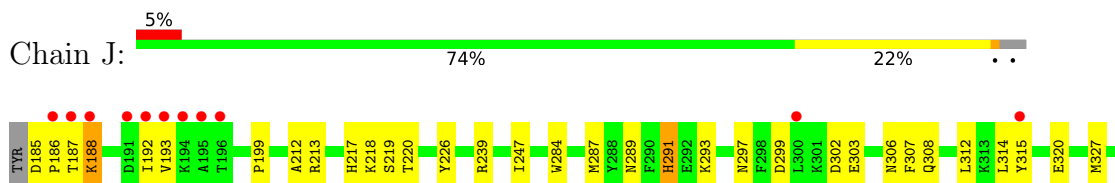
- Molecule 1: Ribonuclease 3

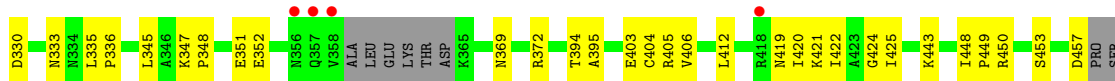


- Molecule 1: Ribonuclease 3

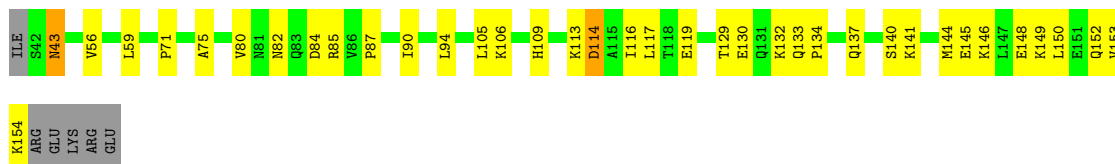


- Molecule 1: Ribonuclease 3

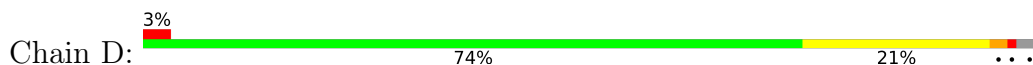




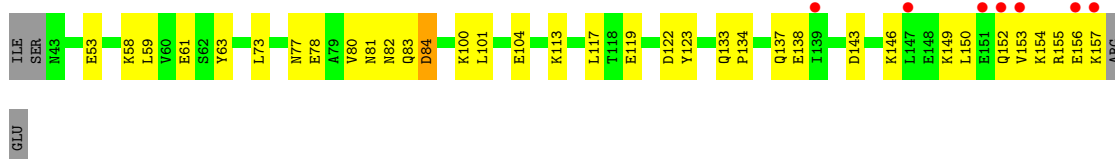
- Molecule 2: Ribonuclease 3



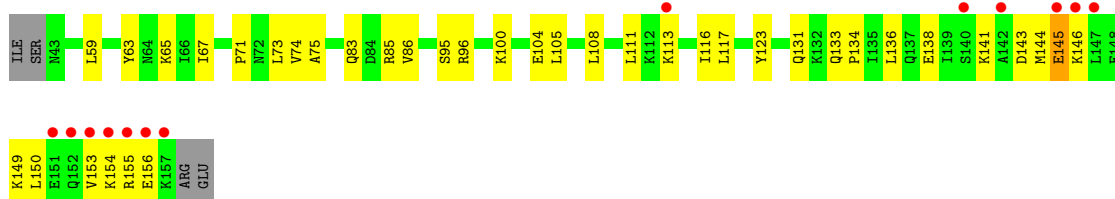
- Molecule 2: Ribonuclease 3



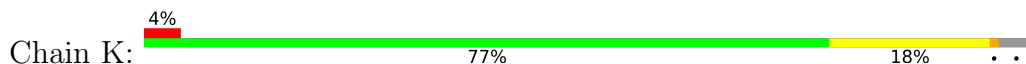
- Molecule 2: Ribonuclease 3



- Molecule 2: Ribonuclease 3



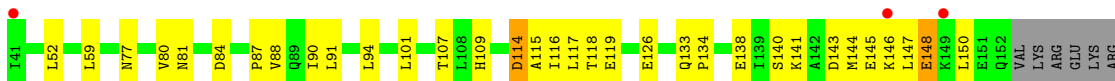
- Molecule 2: Ribonuclease 3



- Molecule 2: Ribonuclease 3



- Molecule 2: Ribonuclease 3



GLU

- Molecule 2: Ribonuclease 3



K157
R158
E159

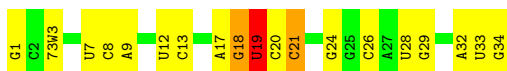
- Molecule 3: RNA substrate analog



- Molecule 3: RNA substrate analog

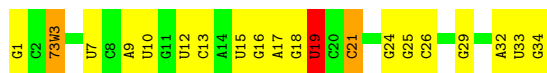


- Molecule 3: RNA substrate analog



- Molecule 3: RNA substrate analog





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (dev_2376: ???)	Depositor
R, R_{free}	0.226 , 0.265 0.226 , 0.266	Depositor DCC
R_{free} test set	998 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtrriage
Anisotropy	0.382	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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(°)	Ideal(°)
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

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

Continued on next page...

Continued from previous page...

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:CD	2:M:148:GLU:H	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:N	2:C:145:GLU:OE1	2.24	0.69
1:J:291:HIS:H	1:J:291:HIS:CD2	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

Continued on next page...

Continued from previous page...

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:OE1	2:E:119:GLU:N	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:H	2:F:116:ILE:HD12	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:N	2:L:138:GLU:OE1	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

Continued on next page...

Continued from previous page...

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:HD2	2:D:154:LYS:O	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:H	1:J:291:HIS:HD2	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:OE1	2:E:138:GLU:N	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:N	2:F:138:GLU:OE1	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

Continued on next page...

Continued from previous page...

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:CD2	1:J:291:HIS:N	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:HD3	2:N:141:LYS:N	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

Continued on next page...

Continued from previous page...

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:I:222:LYS:NZ	3:P:26:C:OP1	2.37	0.48
1:J:303:GLU:HA	1:J:308:GLN:HG3	1.96	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

Continued on next page...

Continued from previous page...

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:71:PRO:HB2	2:N:75:ALA:HB3	1.96	0.47
2:N:100:LYS:O	2:N:104:GLU:HG3	2.14	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:A:420:ILE:HG13	3:G:7:U:OP1	2.14	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
5:E:305:HOH:O	2:F:65:LYS:HE2	2.14	0.47
1:I:354:THR:O	1:I:361:GLU:HG3	2.15	0.47
2:L:83:GLN:O	2:L:86:VAL:HG22	2.15	0.47
2:N:145:GLU:CD	2:N:145:GLU:H	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:O	2:M:126:GLU:HG3	2.14	0.46

Continued on next page...

Continued from previous page...

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:OD1	2:E:84:ASP:N	2.45	0.45
2:N:137:GLN:CD	2:N:137:GLN:N	2.69	0.45
2:C:85:ARG:NH1	1:I:332:ARG:NH2	2.64	0.45
2:D:149:LYS:O	2:D:153:VAL:HG13	2.17	0.45
2:L:46:TYR:CE1	2:L:50:ILE:HD11	2.51	0.45
2:M:59:LEU:HD12	2:N:59:LEU:HD12	1.97	0.45
2:M:148:GLU:CD	2:M:148:GLU:N	2.61	0.45
2:D:141:LYS:HE3	2:D:141:LYS:HB2	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:N	2:C:84:ASP:OD1	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

Continued on next page...

Continued from previous page...

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:O	1:B:259:LYS:HG3	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:HA	2:N:99:LEU:HD23	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:HD12	2:F:150:LEU:HA	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:59:LEU:HD12	2:F:59:LEU:HD12	2.01	0.43
2:E:82:ASN:O	2:E:83:GLN:HB2	2.18	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:N	2:D:138:GLU:OE1	2.52	0.42
3:G:8:C:H2'	3:G:9:A:C8	2.46	0.42

Continued on next page...

Continued from previous page...

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:96:ARG:NH2	5:K:204:HOH:O	2.51	0.42
2:K:105:LEU:HD21	2:L:120:ILE:HD11	2.01	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:71:PRO:HB2	2:C:75:ALA:HB3	2.02	0.41
2:C:116:ILE:HD12	5:C:208:HOH:O	2.20	0.41
2:D:91:LEU:HD23	2:D:91:LEU:HA	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:HD23	2:N:69:LEU:HA	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

Continued on next page...

Continued from previous page...

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:HB2	1:J:188:LYS:HE2	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:HA	2:D:105:LEU:HD23	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:71:PRO:HB2	2:F:75:ALA:HB3	2.04	0.40
2:F:131:GLN:OE1	2:F:131:GLN:HA	2.20	0.40
1:I:432:LEU:HA	1:I:438:LEU:HD11	2.04	0.40
1:J:306:ASN:O	3:O:28:U:H4'	2.21	0.40
2:N:128:ASP:HB3	2:N:131:GLN:HB3	2.04	0.40
3:O:1:G:H5'	3:P:34:G:H3'	2.02	0.40
3:O:12:U:H2'	3:O:13:C:C6	2.56	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

Continued on next page...

Continued from previous page...

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%)	71	90
1	B	236/242 (98%)	235 (100%)	1 (0%)	91	96
1	I	242/242 (100%)	240 (99%)	2 (1%)	81	93
1	J	234/242 (97%)	231 (99%)	3 (1%)	69	89
2	C	106/112 (95%)	104 (98%)	2 (2%)	57	83
2	D	109/112 (97%)	105 (96%)	4 (4%)	34	65
2	E	108/112 (96%)	106 (98%)	2 (2%)	57	83
2	F	108/112 (96%)	106 (98%)	2 (2%)	57	83
2	K	107/112 (96%)	105 (98%)	2 (2%)	57	83
2	L	109/112 (97%)	105 (96%)	4 (4%)	34	65
2	M	105/112 (94%)	100 (95%)	5 (5%)	25	55
2	N	110/112 (98%)	110 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1816/1864 (97%)	1786 (98%)	30 (2%)	60 85

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

Sometimes 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	152	GLN

5.3.3 RNA [i](#)

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 [i](#)

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	H	3	3	18,21,22	1.33	2 (11%)	26,30,33	1.24	2 (7%)
3	73W	P	3	3	18,21,22	1.63	3 (16%)	26,30,33	1.20	2 (7%)
3	73W	G	3	3	18,21,22	1.38	2 (11%)	26,30,33	1.12	2 (7%)
3	73W	O	3	3	18,21,22	1.30	2 (11%)	26,30,33	1.08	3 (11%)

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	H	3	3	-	0/7/25/26	0/2/2/2
3	73W	P	3	3	-	2/7/25/26	0/2/2/2
3	73W	G	3	3	-	2/7/25/26	0/2/2/2
3	73W	O	3	3	-	2/7/25/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	3	73W	O5'-C5'	-4.35	1.34	1.44
3	H	3	73W	C2-N1	3.71	1.48	1.40
3	G	3	73W	C2-N1	3.39	1.47	1.40
3	O	3	73W	C2-N1	3.39	1.47	1.40
3	P	3	73W	C2-N1	3.21	1.46	1.40
3	P	3	73W	O3'-C3'	-2.31	1.37	1.43
3	G	3	73W	C2-N3	2.18	1.40	1.36
3	H	3	73W	O3'-C3'	-2.12	1.38	1.43
3	O	3	73W	C2-N3	2.03	1.40	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	73W	C2'-C3'-C4'	-3.60	95.64	102.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	73W	O4'-C1'-N1	3.09	115.42	108.36
3	G	3	73W	C2'-C3'-C4'	-3.00	96.81	102.64
3	O	3	73W	C2'-C3'-C4'	-2.88	97.04	102.64
3	G	3	73W	O4'-C1'-N1	2.47	114.02	108.36
3	H	3	73W	C5-C4-N4	-2.34	116.89	120.57
3	O	3	73W	O2'-C2'-C1'	-2.21	102.63	110.02
3	O	3	73W	O4'-C1'-N1	2.05	113.06	108.36
3	P	3	73W	C5-C4-N3	2.05	124.82	121.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	3	73W	O4'-C4'-C5'-O5'
3	O	3	73W	O4'-C4'-C5'-O5'
3	P	3	73W	C3'-C4'-C5'-O5'
3	G	3	73W	O4'-C4'-C5'-O5'
3	O	3	73W	C3'-C4'-C5'-O5'
3	G	3	73W	C3'-C4'-C5'-O5'

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 monosaccharides 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	0.45	0	2,2,2	0.39	0
4	EDO	F	201	-	3,3,3	0.59	0	2,2,2	0.21	0
4	EDO	I	504	-	3,3,3	0.49	0	2,2,2	0.46	0
4	EDO	I	501	-	3,3,3	0.58	0	2,2,2	0.28	0
4	EDO	H	101	-	3,3,3	0.46	0	2,2,2	0.47	0
4	EDO	I	502	-	3,3,3	0.54	0	2,2,2	0.24	0
4	EDO	I	505	-	3,3,3	0.66	0	2,2,2	0.11	0
4	EDO	J	501	-	3,3,3	0.62	0	2,2,2	0.07	0
4	EDO	I	503	-	3,3,3	0.52	0	2,2,2	0.31	0
4	EDO	E	201	-	3,3,3	0.51	0	2,2,2	0.20	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	-	-	1/1/1/1	-
4	EDO	F	201	-	-	0/1/1/1	-
4	EDO	I	504	-	-	1/1/1/1	-
4	EDO	I	501	-	-	1/1/1/1	-
4	EDO	H	101	-	-	1/1/1/1	-
4	EDO	I	502	-	-	1/1/1/1	-
4	EDO	I	505	-	-	1/1/1/1	-
4	EDO	J	501	-	-	0/1/1/1	-
4	EDO	I	503	-	-	1/1/1/1	-
4	EDO	E	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	EDO	O1-C1-C2-O2
4	I	503	EDO	O1-C1-C2-O2
4	I	505	EDO	O1-C1-C2-O2
4	I	501	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	504	EDO	O1-C1-C2-O2
4	I	502	EDO	O1-C1-C2-O2
4	H	101	EDO	O1-C1-C2-O2

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.05	11 (3%) 38 33	34, 50, 77, 86	0
1	B	269/276 (97%)	0.03	13 (4%) 30 24	34, 51, 78, 89	0
1	I	276/276 (100%)	0.06	14 (5%) 28 22	34, 49, 79, 100	0
1	J	267/276 (96%)	0.05	15 (5%) 24 19	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%) 45 39	37, 60, 85, 93	0
2	E	115/119 (96%)	0.32	7 (6%) 21 16	41, 68, 91, 97	0
2	F	115/119 (96%)	0.35	13 (11%) 5 3	46, 68, 91, 95	0
2	K	114/119 (95%)	0.12	5 (4%) 34 28	40, 63, 87, 92	0
2	L	116/119 (97%)	0.05	5 (4%) 35 30	41, 64, 87, 92	0
2	M	112/119 (94%)	0.17	3 (2%) 54 49	41, 64, 85, 96	0
2	N	117/119 (98%)	0.23	7 (5%) 21 16	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%)	-0.81	0 100 100	36, 54, 68, 74	0
All	All	2138/2192 (97%)	0.05	97 (4%) 33 27	32, 56, 84, 100	0

All (97) 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
2	L	157	LYS	4.3

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	154	LYS	2.1
1	I	458	PRO	2.1
2	K	150	LEU	2.0
1	A	458	PRO	2.0
1	A	189	ALA	2.0
1	J	356	ASN	2.0
2	K	141	LYS	2.0
2	E	151	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
3	73W	G	3	20/21	0.95	0.14	49,58,77,79	0
3	73W	P	3	20/21	0.95	0.14	44,56,93,95	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

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
4	EDO	F	201	4/4	0.61	0.76	83,84,86,87	0
4	EDO	I	501	4/4	0.76	0.40	58,58,70,80	0
4	EDO	J	501	4/4	0.81	0.60	68,75,76,82	0
4	EDO	I	505	4/4	0.82	0.48	56,60,62,62	0
4	EDO	I	503	4/4	0.84	0.43	58,64,66,70	0
4	EDO	I	504	4/4	0.86	0.26	54,54,54,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	I	502	4/4	0.88	0.29	69,72,75,75	0
4	EDO	E	201	4/4	0.92	0.11	70,77,77,80	0
4	EDO	A	501	4/4	0.94	0.17	56,57,57,60	0
4	EDO	H	101	4/4	0.94	0.47	58,58,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.