



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 AM GMT

PDB ID : 2IX0
Title : RNASE II
Authors : Frazao, C.; Mcvey, C.E.; Amblar, M.; Barbas, A.; Vonnrhein, C.; Arraiano, C.M.; Carrondo, M.A.
Deposited on : 2006-07-05
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

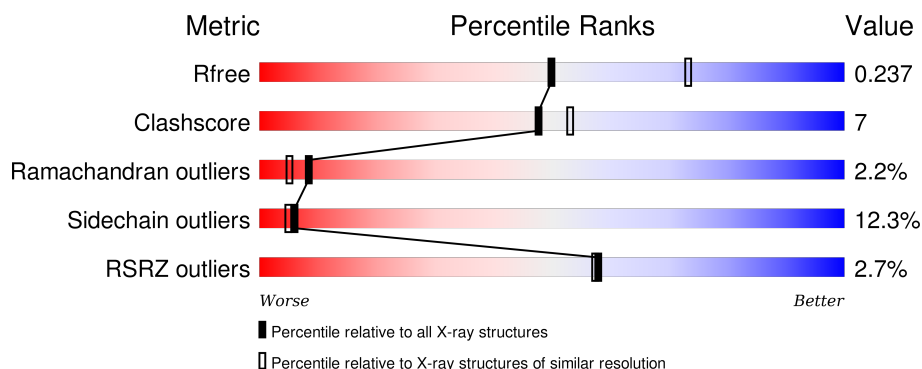
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	663	

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
2	C5P	A	1645	-	-	-	X

2 Entry composition [i](#)

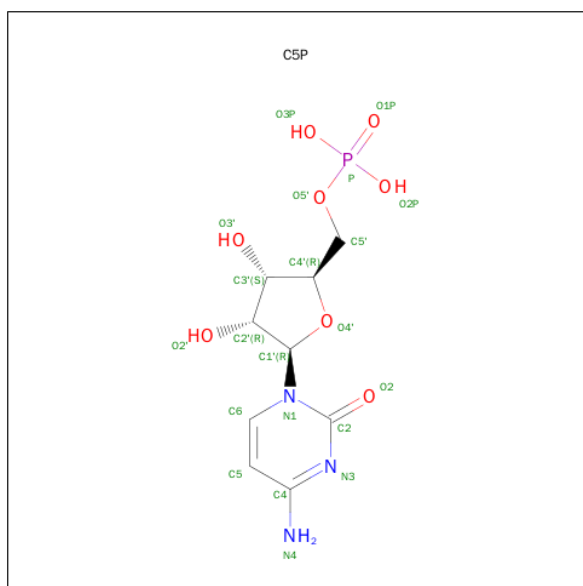
There are 5 unique types of molecules in this entry. The entry contains 5328 atoms, of which 1 is hydrogen and 0 are deuteriums.

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 EXORIBONUCLEASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	637	Total	C	H	N	O	S	0	18	0
			5160	3254	1	926	958	21			

- Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

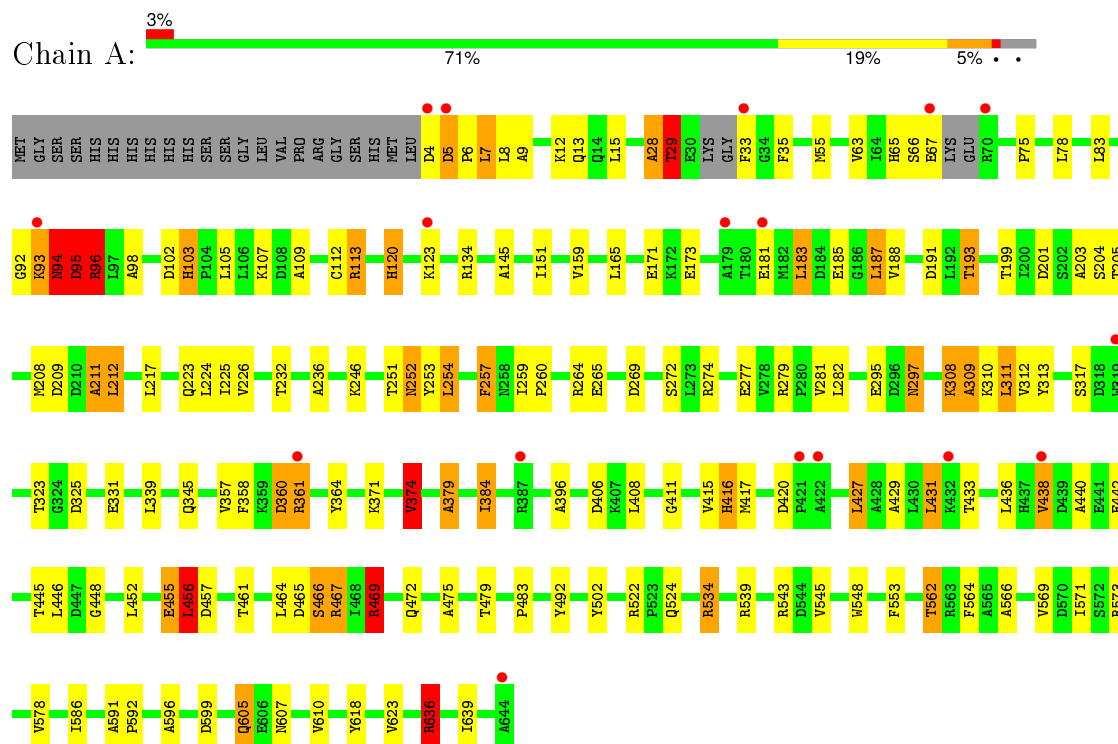
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	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: EXORIBONUCLEASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.84Å 125.72Å 66.24Å 90.00° 111.91° 90.00°	Depositor
Resolution (Å)	62.87 – 2.44 43.94 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.7 (62.87-2.44) 98.6 (43.94-2.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.236 0.198 , 0.237	Depositor DCC
R_{free} test set	1576 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31545 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5328	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, C5P

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	0.69	2/5326 (0.0%)	1.11	49/7204 (0.7%)

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	5	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	ASP	C-O	6.32	1.35	1.23
1	A	456	LEU	C-N	6.01	1.47	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	TYR	CD1-CE1-CZ	9.76	128.58	119.80
1	A	313	TYR	CG-CD2-CE2	9.53	128.92	121.30
1	A	253	TYR	CG-CD1-CE1	8.45	128.06	121.30
1	A	35	PHE	CG-CD2-CE2	8.30	129.93	120.80
1	A	257	PHE	CD1-CE1-CZ	8.24	129.99	120.10
1	A	225	ILE	CG1-CB-CG2	7.86	128.70	111.40
1	A	188	VAL	CA-CB-CG2	7.85	122.67	110.90
1	A	113	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	211	ALA	N-CA-CB	7.59	120.72	110.10
1	A	212	LEU	N-CA-C	7.20	130.44	111.00
1	A	252	ASN	CB-CA-C	7.12	124.63	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	VAL	CG1-CB-CG2	-7.03	99.65	110.90
1	A	374	VAL	CB-CA-C	6.89	124.49	111.40
1	A	120	HIS	N-CA-C	6.80	129.37	111.00
1	A	113	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	281	VAL	CG1-CB-CG2	6.56	121.40	110.90
1	A	309	ALA	N-CA-CB	6.51	119.21	110.10
1	A	416	HIS	CB-CA-C	6.49	123.39	110.40
1	A	357	VAL	CA-CB-CG2	6.48	120.62	110.90
1	A	457	ASP	CB-CA-C	-6.43	97.53	110.40
1	A	264	ARG	N-CA-C	6.37	128.19	111.00
1	A	427	LEU	CB-CA-C	6.20	121.98	110.20
1	A	534	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	596	ALA	N-CA-C	6.13	127.54	111.00
1	A	232	THR	CA-CB-CG2	6.06	120.88	112.40
1	A	636	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	203	ALA	N-CA-C	5.95	127.06	111.00
1	A	427	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	211	ALA	CB-CA-C	5.71	118.67	110.10
1	A	75	PRO	N-CA-C	5.70	126.91	112.10
1	A	534	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	457	ASP	CA-C-N	5.64	129.61	117.20
1	A	457	ASP	CA-C-O	-5.62	108.30	120.10
1	A	545	VAL	CG1-CB-CG2	5.57	119.81	110.90
1	A	188	VAL	CB-CA-C	5.54	121.93	111.40
1	A	440	ALA	N-CA-C	5.42	125.64	111.00
1	A	475	ALA	N-CA-C	5.42	125.64	111.00
1	A	469[A]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	469[B]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	29	THR	CA-CB-CG2	5.37	119.91	112.40
1	A	636	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	562	THR	CA-CB-CG2	5.30	119.82	112.40
1	A	212	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	522	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	564	PHE	CE1-CZ-CE2	5.17	129.31	120.00
1	A	562	THR	OG1-CB-CG2	5.16	121.87	110.00
1	A	618	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	A	415	VAL	CB-CA-C	5.08	121.06	111.40
1	A	639	ILE	CG1-CB-CG2	5.04	122.50	111.40

All (5) chirality outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
-----	-------	-----	------	------

Mol	Chain	Res	Type	Atom
1	A	208	MET	CA
1	A	211	ALA	CA
1	A	360	ASP	CA
1	A	374	VAL	CA
1	A	427	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ALA	Peptide
1	A	5[A]	ASP	Peptide
1	A	92	GLY	Peptide
1	A	93	LYS	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	5159	1	5124	77	0
2	A	21	0	12	2	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	145	0	0	1	0
All	All	5327	1	5136	77	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 7.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:GLU:O	1:A:445:THR:HG22	1.77	0.84
1:A:66:SER:O	1:A:67:GLU:HG3	1.86	0.76
1:A:171:GLU:OE2	1:A:534:ARG:NH2	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:OD1	1:A:193:THR:HB	1.91	0.71
1:A:183:LEU:HD21	1:A:236:ALA:HB2	1.73	0.70
1:A:5[A]:ASP:O	1:A:8:LEU:N	2.26	0.68
1:A:539[B]:ARG:HH11	1:A:539[B]:ARG:HG2	1.58	0.67
1:A:445:THR:HG23	1:A:448:GLY:H	1.58	0.67
1:A:374:VAL:HG22	1:A:553:PHE:CD1	2.30	0.67
1:A:55:MET:HE3	1:A:83:LEU:HD22	1.79	0.63
1:A:95:ASP:O	1:A:95:ASP:CG	2.37	0.62
1:A:566:ALA:HB1	1:A:578:VAL:HG13	1.81	0.62
1:A:93:LYS:O	1:A:95:ASP:N	2.33	0.62
1:A:199:THR:HG22	1:A:211:ALA:HB2	1.83	0.61
1:A:95:ASP:O	1:A:96[A]:ARG:HB2	1.99	0.61
1:A:317:SER:HA	1:A:384:ILE:CD1	2.32	0.60
1:A:431:LEU:HD23	1:A:438:VAL:HG21	1.86	0.58
1:A:185:GLU:HB2	1:A:187:LEU:HD22	1.86	0.57
1:A:66:SER:O	1:A:67:GLU:CG	2.52	0.57
1:A:431:LEU:HD23	1:A:438:VAL:CG2	2.35	0.56
1:A:571:ILE:HD13	1:A:610:VAL:HG23	1.88	0.55
1:A:259:ILE:N	1:A:259:ILE:HD12	2.21	0.55
1:A:274:ARG:HB2	1:A:277:GLU:HG3	1.89	0.54
1:A:5[A]:ASP:O	1:A:7:LEU:N	2.40	0.54
1:A:364:TYR:CD2	1:A:379:ALA:HB2	2.42	0.54
1:A:539[B]:ARG:CG	1:A:539[B]:ARG:HH11	2.20	0.53
1:A:411:GLY:O	1:A:479:THR:HA	2.09	0.53
1:A:95:ASP:O	1:A:96[B]:ARG:HB2	2.10	0.52
1:A:309:ALA:HB1	1:A:311:LEU:HD13	1.90	0.52
1:A:431:LEU:HD12	1:A:464:LEU:HD11	1.91	0.51
1:A:5[A]:ASP:H	1:A:9:ALA:HB2	1.75	0.51
1:A:55:MET:CE	1:A:83:LEU:HB2	2.42	0.49
1:A:4[A]:ASP:N	1:A:12:LYS:HZ1	2.11	0.48
1:A:358:PHE:CE2	1:A:361:ARG:HD3	2.49	0.48
1:A:226:VAL:HG21	1:A:396:ALA:HB2	1.95	0.48
1:A:5[A]:ASP:HB3	1:A:8:LEU:HB3	1.95	0.47
1:A:4[A]:ASP:HB3	1:A:9:ALA:HB2	1.96	0.47
1:A:5[A]:ASP:O	1:A:6:PRO:C	2.51	0.47
1:A:55:MET:HE1	1:A:83:LEU:HB2	1.96	0.47
1:A:103:HIS:CD2	1:A:105:LEU:H	2.32	0.46
1:A:429:ALA:O	1:A:433:THR:HG23	2.16	0.46
1:A:201:ASP:O	1:A:312:VAL:HA	2.16	0.46
1:A:265:GLU:O	1:A:269:ASP:HB3	2.15	0.46
1:A:309:ALA:HB1	1:A:311:LEU:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:HD2	1:A:105:LEU:H	1.64	0.46
1:A:246:LYS:HG3	1:A:502:TYR:CE2	2.51	0.46
1:A:358:PHE:CE2	1:A:361:ARG:CD	3.00	0.45
1:A:199:THR:O	1:A:311:LEU:HB2	2.17	0.45
1:A:252:ASN:ND2	5:A:2065:HOH:O	2.47	0.45
1:A:254:LEU:HB2	1:A:257:PHE:O	2.16	0.44
1:A:103:HIS:HB2	2:A:1645:C5P:H5'1	1.98	0.44
1:A:251:THR:HG23	1:A:260:PRO:HA	1.99	0.44
1:A:193:THR:O	1:A:308:LYS:NZ	2.47	0.43
1:A:469[A]:ARG:NH2	1:A:569:VAL:O	2.51	0.43
1:A:548[A]:TRP:CD2	1:A:636:ARG:HD3	2.53	0.43
1:A:591:ALA:HB3	1:A:592:PRO:HD3	1.99	0.43
1:A:28:ALA:O	1:A:29:THR:HG22	2.19	0.43
1:A:272:SER:O	1:A:279:ARG:HD2	2.18	0.43
1:A:4[A]:ASP:O	1:A:5[A]:ASP:HB2	2.19	0.42
1:A:102:ASP:HB3	2:A:1645:C5P:O3P	2.20	0.42
1:A:571:ILE:O	1:A:605:GLN:HA	2.20	0.42
1:A:98:ALA:HB1	1:A:109:ALA:HB1	2.01	0.42
1:A:436:LEU:HD11	1:A:455:GLU:CD	2.41	0.41
1:A:5[B]:ASP:HA	1:A:6:PRO:HD2	1.68	0.41
1:A:217:LEU:HD11	1:A:223:GLN:HB2	2.02	0.41
1:A:33:PHE:C	1:A:33:PHE:CD1	2.95	0.41
1:A:472:GLN:HA	1:A:472:GLN:NE2	2.35	0.41
1:A:452:LEU:O	1:A:456:LEU:HB2	2.21	0.40
1:A:112:CYS:HA	1:A:145:ALA:O	2.21	0.40
1:A:93:LYS:HD3	1:A:123[A]:LYS:HB3	2.04	0.40
1:A:466:SER:OG	1:A:467:ARG:NH2	2.47	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	648/663 (98%)	595 (92%)	38 (6%)	15 (2%)	8 4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	95	ASP
1	A	96[A]	ARG
1	A	96[B]	ARG
1	A	181	GLU
1	A	297	ASN
1	A	29	THR
1	A	120	HIS
1	A	379	ALA
1	A	151	ILE
1	A	159	VAL
1	A	492	TYR
1	A	360	ASP
1	A	465	ASP
1	A	103	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	548/553 (99%)	480 (88%)	68 (12%)	6 5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13[A]	GLN
1	A	13[B]	GLN
1	A	15	LEU
1	A	63	VAL
1	A	65	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	78	LEU
1	A	94	ASN
1	A	95	ASP
1	A	96[A]	ARG
1	A	96[B]	ARG
1	A	107	LYS
1	A	113	ARG
1	A	134	ARG
1	A	165	LEU
1	A	173	GLU
1	A	183	LEU
1	A	187	LEU
1	A	193	THR
1	A	204	SER
1	A	205	THR
1	A	208	MET
1	A	209	ASP
1	A	212	LEU
1	A	224	LEU
1	A	254	LEU
1	A	282	LEU
1	A	295	GLU
1	A	297	ASN
1	A	308	LYS
1	A	310	LYS
1	A	311	LEU
1	A	323	THR
1	A	325	ASP
1	A	331	GLU
1	A	339	LEU
1	A	345	GLN
1	A	360	ASP
1	A	361	ARG
1	A	371	LYS
1	A	374	VAL
1	A	384	ILE
1	A	406	ASP
1	A	408	LEU
1	A	416	HIS
1	A	417	MET
1	A	420	ASP
1	A	427	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	431	LEU
1	A	438	VAL
1	A	446	LEU
1	A	455	GLU
1	A	456	LEU
1	A	461	THR
1	A	466	SER
1	A	467	ARG
1	A	469[A]	ARG
1	A	469[B]	ARG
1	A	524	GLN
1	A	543	ARG
1	A	562	THR
1	A	573	ARG
1	A	586	ILE
1	A	599	ASP
1	A	605	GLN
1	A	607	ASN
1	A	623	VAL
1	A	636	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	169	ASN
1	A	252	ASN
1	A	414	ASN
1	A	437	HIS
1	A	472	GLN
1	A	524	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	C5P	A	1645	-	17,22,22	1.04	1 (5%)	22,33,33	2.83	8 (36%)

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
2	C5P	A	1645	-	-	0/6/26/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1645	C5P	C6-N1	2.83	1.39	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1645	C5P	C4'-O4'-C1'	-9.81	98.94	109.72
2	A	1645	C5P	O3P-P-O1P	-2.79	101.60	110.58
2	A	1645	C5P	C2'-C3'-C4'	-2.45	97.57	102.61
2	A	1645	C5P	C5-C4-N4	-2.19	117.94	121.31
2	A	1645	C5P	N4-C4-N3	2.89	121.77	116.50
2	A	1645	C5P	O2P-P-O1P	3.04	120.36	110.58
2	A	1645	C5P	O2P-P-O3P	3.30	119.95	107.38
2	A	1645	C5P	C2-N3-C4	3.62	120.72	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1645	C5P	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	637/663 (96%)	0.05	17 (2%) 58 57	19, 39, 68, 96	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ARG	4.9
1	A	422	ALA	4.5
1	A	67	GLU	4.1
1	A	179	ALA	3.5
1	A	4[A]	ASP	3.5
1	A	181	GLU	3.4
1	A	421	PRO	3.3
1	A	644	ALA	3.3
1	A	93	LYS	2.9
1	A	361	ARG	2.8
1	A	387	ARG	2.7
1	A	438	VAL	2.5
1	A	123[A]	LYS	2.5
1	A	319	TRP	2.4
1	A	33	PHE	2.3
1	A	432	LYS	2.2
1	A	5[A]	ASP	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	C5P	A	1645	21/21	0.94	0.30	13.66	34,66,90,91	0
4	CA	A	1647	1/1	0.98	0.10	-1.47	62,62,62,62	0
3	MG	A	1646	1/1	0.91	0.07	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.