



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 08:08 PM JST

PDB ID : 7XOZ
Title : Crystal structure of RPPT-TIR
Authors : Song, W.; Jia, A.; Huang, S.; Chai, J.
Deposited on : 2022-05-02
Resolution : 2.52 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 : 2.36
buster-report : 1.1.7 (2018)
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) : 2.36

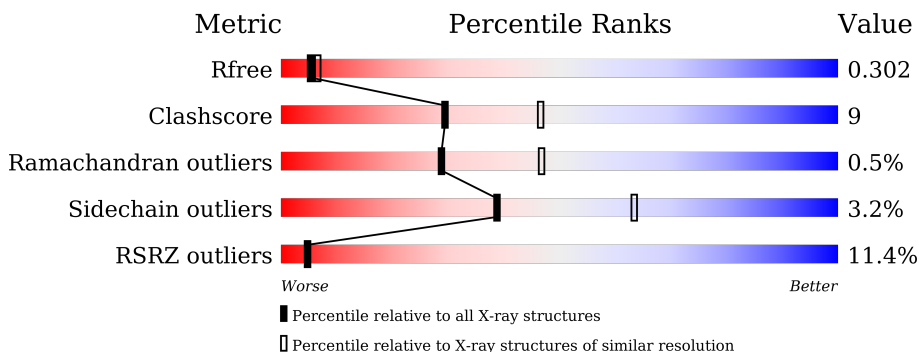
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	165	
1	F	165	
2	B	165	
2	E	165	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10514 atoms, of which 5248 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.

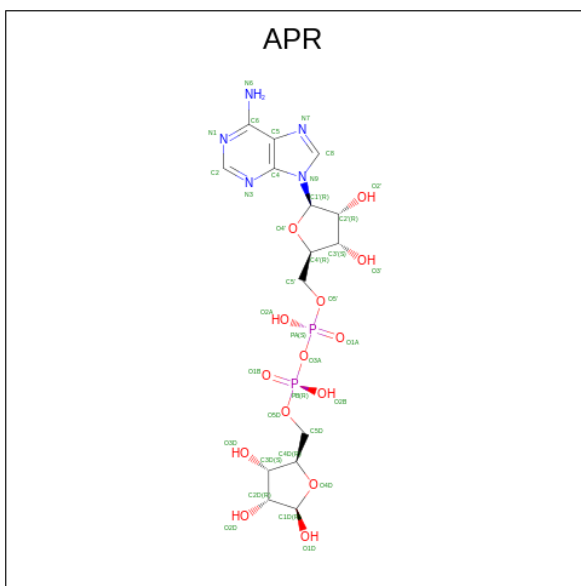
- Molecule 1 is a protein called ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	165	Total	C	H	N	O	S	0	0	0
			2675	844	1347	232	245	7			
1	F	156	Total	C	H	N	O	S	0	0	0
			2513	799	1263	214	230	7			

- Molecule 2 is a protein called ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	165	Total	C	H	N	O	S	0	0	0
			2643	839	1324	229	244	7			
2	E	157	Total	C	H	N	O	S	0	0	0
			2527	803	1272	217	228	7			

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	P	0	0
			57	15	21	5	14	2		
3	B	1	Total	C	H	N	O	P	0	0
			57	15	21	5	14	2		

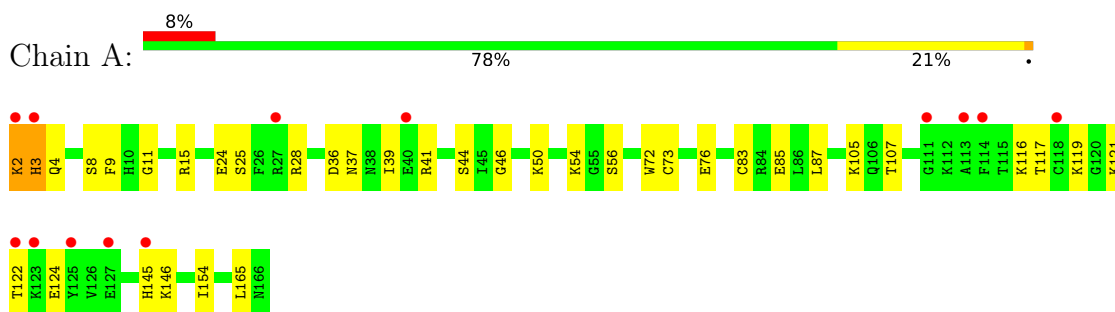
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	5	Total	O	0	0
			5	5		
4	E	11	Total	O	0	0
			11	11		
4	F	14	Total	O	0	0
			14	14		

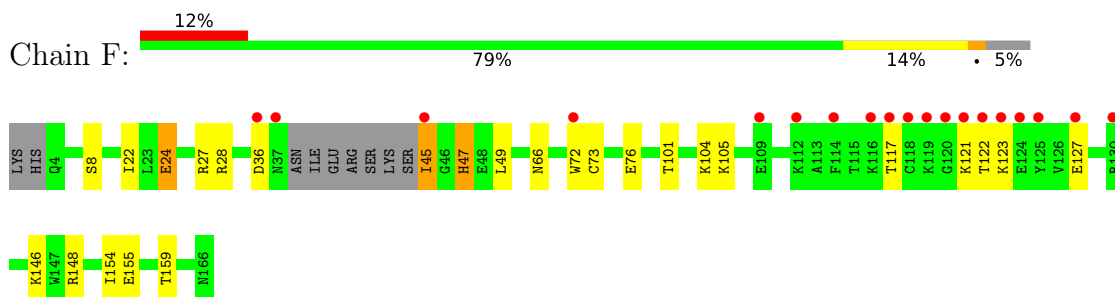
3 Residue-property plots [i](#)

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.

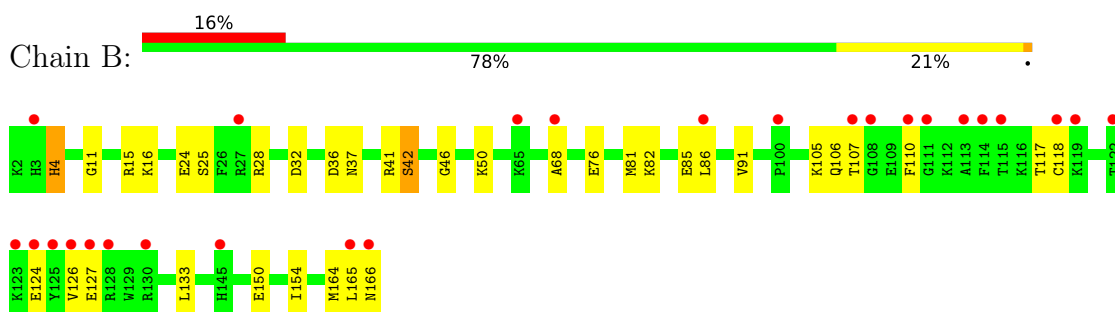
- Molecule 1: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase



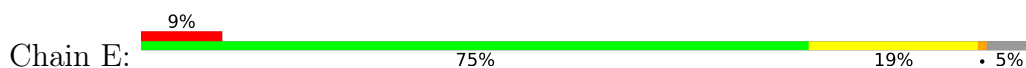
- Molecule 1: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase

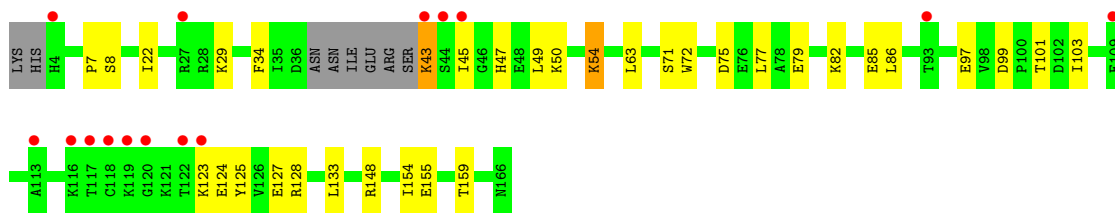


- Molecule 2: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase



- Molecule 2: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.80Å 81.13Å 70.71Å 90.00° 112.33° 90.00°	Depositor
Resolution (Å)	39.12 – 2.52 39.12 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.12-2.52) 78.9 (39.12-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.29 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20_4478	Depositor
R, R_{free}	0.258 , 0.297 0.259 , 0.302	Depositor DCC
R_{free} test set	1234 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.547	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10514	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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 56.14 % 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 2.8592e-05. 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: APR

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	0.48	0/1353	0.61	0/1815
1	F	0.48	1/1273 (0.1%)	0.59	0/1708
2	B	0.43	0/1345	0.56	0/1807
2	E	0.48	1/1279 (0.1%)	0.60	0/1716
All	All	0.47	2/5250 (0.0%)	0.59	0/7046

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	54	LYS	CD-CE	5.32	1.64	1.51
1	F	73	CYS	CB-SG	-5.10	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1328	1347	1347	28	0
1	F	1250	1263	1265	19	0
2	B	1319	1324	1324	31	0
2	E	1255	1272	1271	31	0
3	A	36	21	21	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	36	21	21	2	0
4	A	12	0	0	12	0
4	B	5	0	0	1	0
4	E	11	0	0	4	0
4	F	14	0	0	4	0
All	All	5266	5248	5249	99	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 9.

All (99) 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:83:CYS:SG	4:A:310:HOH:O	2.07	1.11
1:A:76:GLU:OE1	3:A:201:APR:O2D	1.86	0.93
1:A:72:TRP:O	4:A:301:HOH:O	1.91	0.87
1:A:117:THR:O	4:A:302:HOH:O	1.93	0.85
2:E:155:GLU:O	2:E:159:THR:HG23	1.79	0.83
2:E:63:LEU:HD13	2:E:103:ILE:HD13	1.59	0.83
1:F:27:ARG:NH2	4:F:201:HOH:O	2.10	0.83
2:B:85:GLU:OE2	4:B:301:HOH:O	2.03	0.75
1:A:73:CYS:C	4:A:301:HOH:O	2.25	0.75
1:A:105:LYS:O	1:A:107:THR:HG23	1.86	0.74
2:E:75:ASP:OD2	4:E:201:HOH:O	2.06	0.73
2:B:86:LEU:HD11	2:E:82:LYS:HG2	1.71	0.73
1:A:85:GLU:OE2	4:A:303:HOH:O	2.07	0.71
1:A:2:LYS:N	4:A:304:HOH:O	2.26	0.69
1:A:76:GLU:N	4:A:301:HOH:O	1.92	0.68
2:E:123:LYS:NZ	2:E:127:GLU:OE2	2.23	0.67
2:E:97:GLU:OE2	4:E:202:HOH:O	2.14	0.65
1:A:73:CYS:O	4:A:301:HOH:O	2.15	0.65
2:B:86:LEU:HD12	2:E:86:LEU:HD12	1.79	0.64
1:A:2:LYS:HB2	1:A:165:LEU:HD13	1.78	0.64
1:F:104:LYS:HE3	1:F:105:LYS:HE2	1.80	0.62
2:B:82:LYS:HG2	2:E:86:LEU:HD11	1.83	0.60
2:B:46:GLY:O	2:B:50:LYS:HG2	2.01	0.60
1:A:46:GLY:O	1:A:50:LYS:HG2	2.03	0.59
2:E:50:LYS:NZ	2:E:79:GLU:HB2	2.17	0.59
2:E:45:ILE:HG23	2:E:49:LEU:HD23	1.84	0.59
2:B:127:GLU:HB2	2:E:124:GLU:HG2	1.84	0.59
1:F:8:SER:HB2	1:F:76:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:CYS:SG	2:B:126:VAL:HG13	2.45	0.57
1:F:66:ASN:ND2	4:F:203:HOH:O	2.31	0.57
2:B:82:LYS:NZ	2:E:85:GLU:OE2	2.36	0.56
1:A:54:LYS:HA	4:A:310:HOH:O	2.06	0.55
1:F:123:LYS:NZ	1:F:127:GLU:OE2	2.33	0.55
2:B:41:ARG:O	2:B:42:SER:CB	2.55	0.55
2:B:86:LEU:O	2:E:54:LYS:NZ	2.38	0.55
2:B:127:GLU:HG3	2:E:124:GLU:HG2	1.88	0.54
2:B:24:GLU:OE2	2:B:28:ARG:HG3	2.07	0.54
2:E:49:LEU:HD22	2:E:72:TRP:CZ2	2.42	0.54
1:F:45:ILE:C	1:F:45:ILE:HD13	2.27	0.54
2:E:99:ASP:OD2	2:E:101:THR:HG22	2.08	0.54
2:B:41:ARG:O	2:B:42:SER:HB3	2.08	0.53
1:F:117:THR:O	1:F:121:LYS:HG3	2.09	0.53
1:A:76:GLU:HB2	4:A:301:HOH:O	2.09	0.52
1:A:116:LYS:HA	1:A:119:LYS:HE2	1.91	0.52
1:A:145:HIS:CE1	1:A:146:LYS:HG3	2.44	0.52
2:B:105:LYS:O	2:B:107:THR:HG23	2.09	0.51
2:B:36:ASP:OD1	2:B:37:ASN:N	2.43	0.51
1:A:87:LEU:HD12	4:A:310:HOH:O	2.12	0.51
2:B:106:GLN:HE21	2:B:133:LEU:HB2	1.75	0.51
2:B:164:MET:O	2:B:166:ASN:N	2.44	0.50
1:F:155:GLU:O	1:F:159:THR:HG23	2.10	0.50
2:B:4:HIS:CE1	2:B:165:LEU:HD13	2.47	0.50
1:F:45:ILE:HD12	1:F:72:TRP:NE1	2.26	0.50
1:A:36:ASP:OD1	1:A:37:ASN:N	2.45	0.49
1:F:45:ILE:HD12	1:F:72:TRP:CD1	2.47	0.49
2:B:127:GLU:CB	2:E:124:GLU:HG2	2.42	0.48
1:A:122:THR:HB	1:A:124:GLU:OE1	2.14	0.48
1:F:28:ARG:NH2	4:F:204:HOH:O	2.39	0.48
2:E:50:LYS:HZ3	2:E:79:GLU:HB2	1.77	0.48
2:E:29:LYS:HE3	2:E:159:THR:HG22	1.96	0.47
1:F:45:ILE:O	1:F:45:ILE:HG23	2.15	0.47
2:B:76:GLU:OE2	3:B:201:APR:HR'1	2.15	0.47
1:A:76:GLU:CD	3:A:201:APR:O2D	2.52	0.47
1:A:4:GLN:HB3	1:A:56:SER:HA	1.97	0.47
2:B:127:GLU:CG	2:E:124:GLU:HG2	2.44	0.46
2:E:45:ILE:HG13	2:E:75:ASP:HB3	1.98	0.46
2:E:43:LYS:N	2:E:71:SER:OG	2.49	0.45
2:B:68:ALA:HB2	2:B:110:PHE:CZ	2.52	0.45
1:A:39:ILE:O	1:A:41:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:GLY:HA3	3:B:201:APR:O2A	2.15	0.45
2:E:22:ILE:CG1	2:E:154:ILE:HD12	2.47	0.45
1:A:9:PHE:O	3:A:201:APR:HR'3	2.17	0.45
1:F:45:ILE:HD12	1:F:72:TRP:HE1	1.82	0.44
1:A:24:GLU:HG3	1:A:28:ARG:NH1	2.32	0.44
2:B:117:THR:O	2:B:117:THR:HG22	2.17	0.44
1:A:25:SER:OG	1:A:154:ILE:HG22	2.18	0.44
2:B:4:HIS:HB2	2:B:32:ASP:HB3	2.00	0.44
2:B:106:GLN:NE2	2:B:133:LEU:HB2	2.32	0.44
1:F:24:GLU:OE1	1:F:27:ARG:NH2	2.51	0.43
2:B:150:GLU:O	2:B:154:ILE:HG12	2.18	0.43
2:E:7:PRO:HD2	2:E:34:PHE:O	2.17	0.43
1:F:36:ASP:OD1	1:F:49:LEU:HD13	2.18	0.43
1:F:117:THR:O	1:F:117:THR:HG22	2.19	0.43
1:F:28:ARG:NE	4:F:204:HOH:O	2.32	0.43
2:E:125:TYR:HE2	4:E:201:HOH:O	2.01	0.43
1:A:11:GLY:HA2	1:A:15:ARG:HB2	1.99	0.43
1:F:45:ILE:HG21	1:F:72:TRP:CD1	2.55	0.42
2:E:43:LYS:CB	4:E:201:HOH:O	2.69	0.41
2:B:81:MET:HE1	2:B:91:VAL:HG21	2.02	0.41
1:A:121:LYS:N	4:A:305:HOH:O	2.52	0.41
2:B:24:GLU:HG3	2:B:28:ARG:NH2	2.35	0.41
2:B:124:GLU:HG2	2:E:127:GLU:HB2	2.02	0.41
2:E:22:ILE:HG12	2:E:154:ILE:HD12	2.02	0.41
2:B:11:GLY:CA	2:B:15:ARG:HB2	2.51	0.41
2:E:50:LYS:HZ2	2:E:79:GLU:HB2	1.85	0.41
1:F:22:ILE:CG1	1:F:154:ILE:HD12	2.50	0.41
1:A:11:GLY:CA	1:A:15:ARG:HB2	2.52	0.40
2:E:77:LEU:CD2	2:E:133:LEU:HD23	2.51	0.40
2:E:125:TYR:CE2	2:E:128:ARG:NH2	2.90	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	163/165 (99%)	156 (96%)	6 (4%)	1 (1%)	25	41
1	F	152/165 (92%)	147 (97%)	4 (3%)	1 (1%)	22	37
2	B	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	25	41
2	E	153/165 (93%)	149 (97%)	4 (3%)	0	100	100
All	All	631/660 (96%)	610 (97%)	18 (3%)	3 (0%)	29	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	F	47	HIS
2	B	42	SER

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	145/145 (100%)	141 (97%)	4 (3%)	43	68
1	F	135/145 (93%)	128 (95%)	7 (5%)	23	41
2	B	143/145 (99%)	140 (98%)	3 (2%)	53	76
2	E	135/145 (93%)	131 (97%)	4 (3%)	41	66
All	All	558/580 (96%)	540 (97%)	18 (3%)	39	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	HIS
1	A	8	SER
1	A	44	SER
2	B	4	HIS

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Mol	Chain	Res	Type
2	B	16	LYS
2	B	25	SER
2	E	8	SER
2	E	43	LYS
2	E	47	HIS
2	E	148	ARG
1	F	24	GLU
1	F	45	ILE
1	F	47	HIS
1	F	101	THR
1	F	122	THR
1	F	146	LYS
1	F	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
3	APR	A	201	-	34,39,39	0.57	0	40,60,60	1.03	3 (7%)
3	APR	B	201	-	34,39,39	0.66	0	40,60,60	0.97	3 (7%)

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	APR	A	201	-	-	4/18/54/54	0/4/4/4
3	APR	B	201	-	-	4/18/54/54	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	APR	C3'-C2'-C1'	2.98	105.46	100.98
3	A	201	APR	C5-C6-N6	2.50	124.16	120.35
3	A	201	APR	O2'-C2'-C1'	-2.22	102.64	110.85
3	B	201	APR	C5-C6-N6	2.16	123.64	120.35
3	B	201	APR	O4'-C4'-C3'	-2.14	100.87	105.11
3	B	201	APR	C1D-C2D-C3D	2.09	104.91	102.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

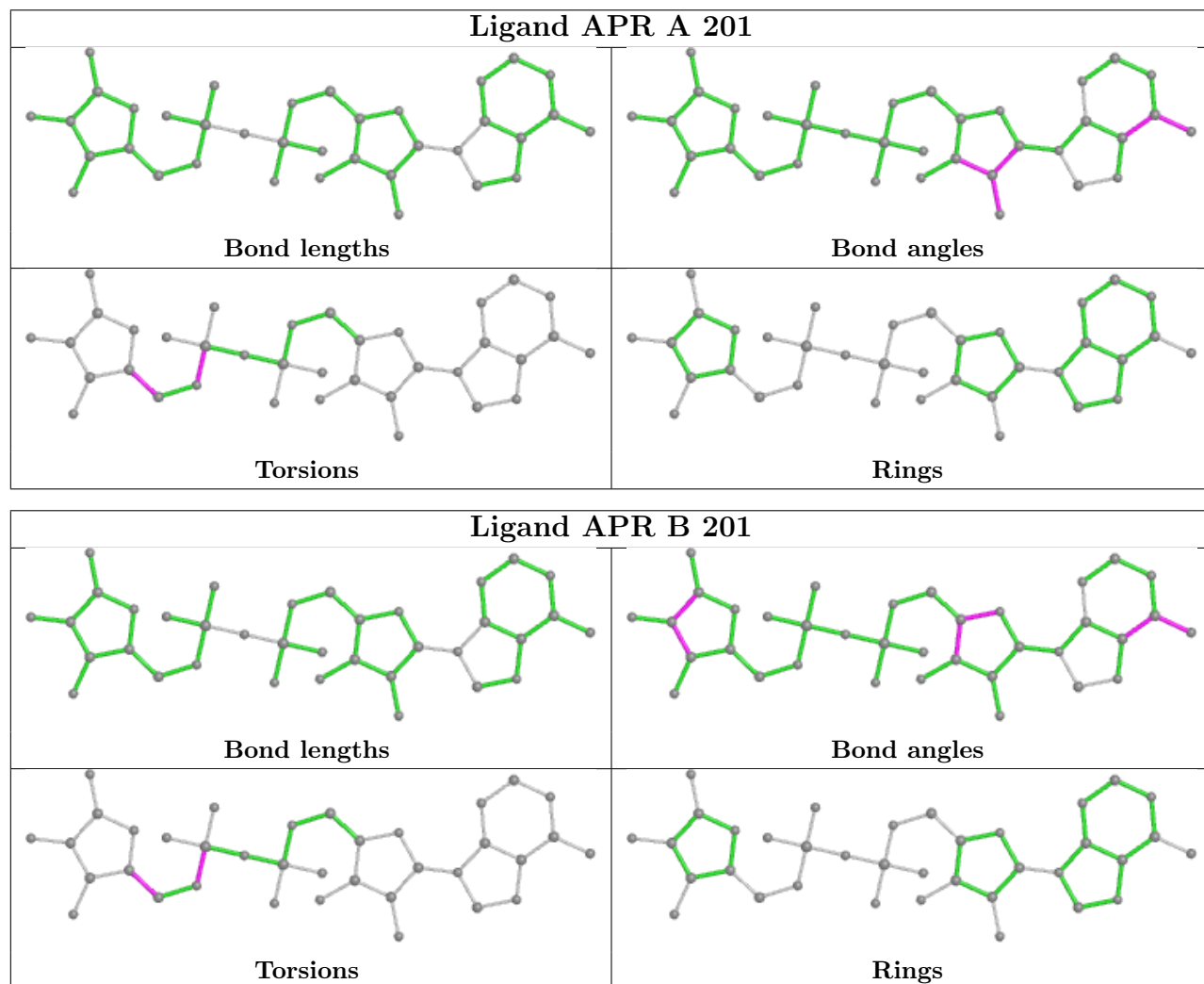
Mol	Chain	Res	Type	Atoms
3	A	201	APR	C5D-O5D-PB-O1B
3	A	201	APR	C5D-O5D-PB-O2B
3	B	201	APR	C5D-O5D-PB-O3A
3	A	201	APR	C3D-C4D-C5D-O5D
3	B	201	APR	C5D-O5D-PB-O1B
3	B	201	APR	C5D-O5D-PB-O2B
3	A	201	APR	C5D-O5D-PB-O3A
3	B	201	APR	O4D-C4D-C5D-O5D

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	APR	3	0
3	B	201	APR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	165/165 (100%)	0.71	13 (7%) 12 13	38, 52, 88, 105	0
1	F	156/165 (94%)	0.83	19 (12%) 4 4	42, 58, 98, 119	0
2	B	165/165 (100%)	1.02	26 (15%) 2 1	48, 63, 110, 124	0
2	E	157/165 (95%)	0.65	15 (9%) 8 8	37, 49, 79, 92	0
All	All	643/660 (97%)	0.80	73 (11%) 5 5	37, 56, 97, 124	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	5.7
1	A	2	LYS	5.7
2	B	108	GLY	5.1
1	F	122	THR	4.6
1	F	118	CYS	4.5
1	A	125	TYR	4.5
2	B	111	GLY	4.5
2	B	123	LYS	4.2
2	B	118	CYS	4.2
1	F	119	LYS	4.2
1	F	109	GLU	4.0
1	F	120	GLY	4.0
1	F	121	LYS	3.9
2	B	124	GLU	3.8
2	B	125	TYR	3.8
2	E	43	LYS	3.7
2	E	122	THR	3.7
1	F	125	TYR	3.6
2	B	165	LEU	3.6
1	A	122	THR	3.6
2	B	127	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	45	ILE	3.3
1	A	111	GLY	3.3
1	F	37	ASN	3.2
1	A	118	CYS	3.2
1	F	36	ASP	3.2
2	B	114	PHE	3.2
1	F	112	LYS	3.1
1	F	127	GLU	2.9
2	B	68	ALA	2.9
2	B	166	ASN	2.8
2	B	107	THR	2.7
2	B	130	ARG	2.7
1	A	113	ALA	2.7
1	F	117	THR	2.7
2	B	122	THR	2.7
1	A	27	ARG	2.6
2	E	117	THR	2.6
1	F	130	ARG	2.6
1	F	124	GLU	2.5
2	E	44	SER	2.5
1	F	123	LYS	2.5
2	E	123	LYS	2.5
2	B	86	LEU	2.5
2	B	115	THR	2.5
2	E	120	GLY	2.5
2	E	118	CYS	2.4
1	F	72	TRP	2.4
1	A	114	PHE	2.4
2	E	116	LYS	2.4
2	E	4	HIS	2.4
1	A	145	HIS	2.3
2	B	119	LYS	2.3
2	B	126	VAL	2.3
2	B	113	ALA	2.3
2	E	109	GLU	2.3
2	B	100	PRO	2.3
2	B	145	HIS	2.2
2	B	128	ARG	2.2
1	A	40	GLU	2.2
2	E	93	THR	2.2
1	A	123	LYS	2.2
2	E	27	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	3	HIS	2.2
2	B	65	LYS	2.2
2	E	45	ILE	2.1
2	E	119	LYS	2.1
2	E	113	ALA	2.1
1	A	127	GLU	2.0
2	B	110	PHE	2.0
1	F	116	LYS	2.0
2	B	27	ARG	2.0
1	F	114	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

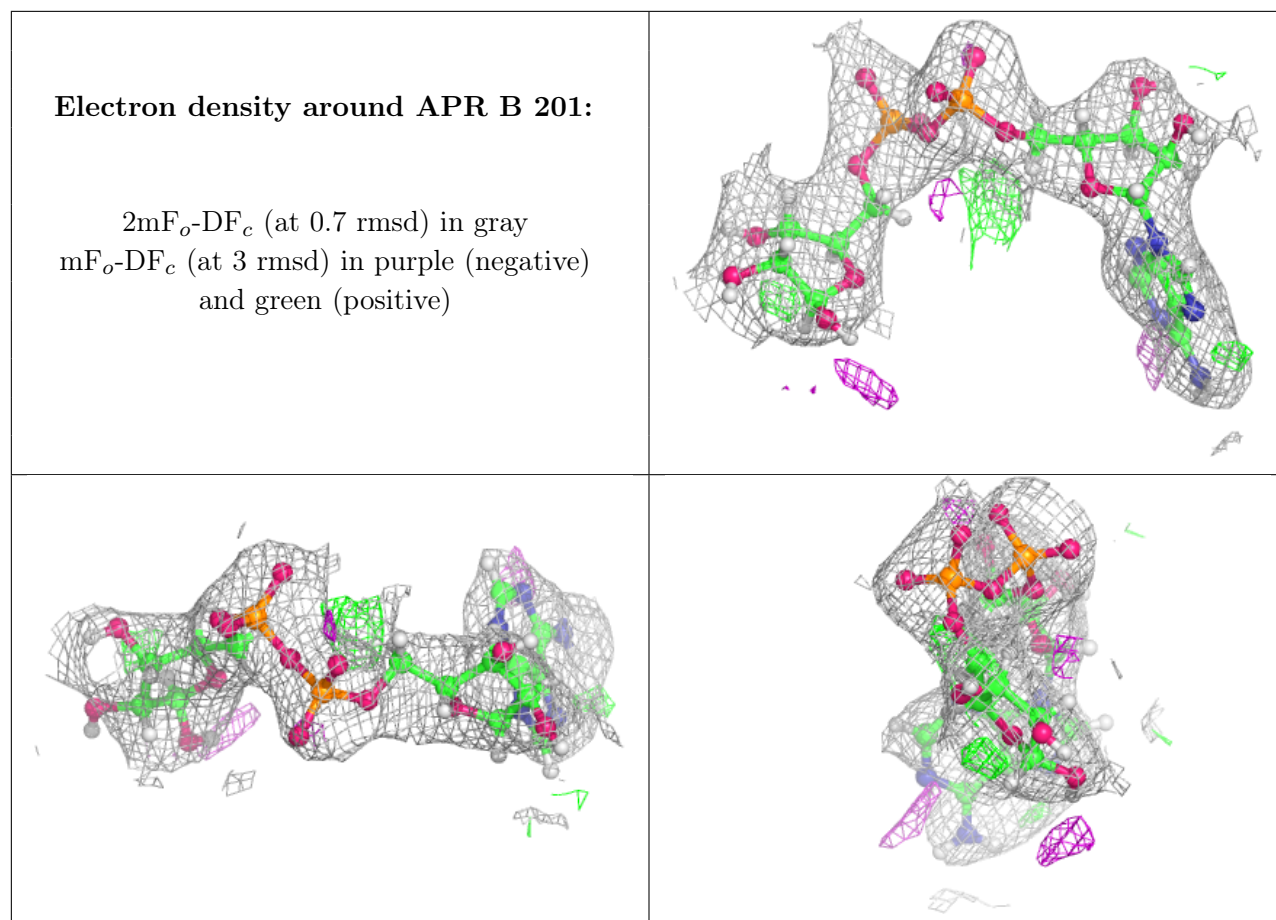
There are no monosaccharides in this entry.

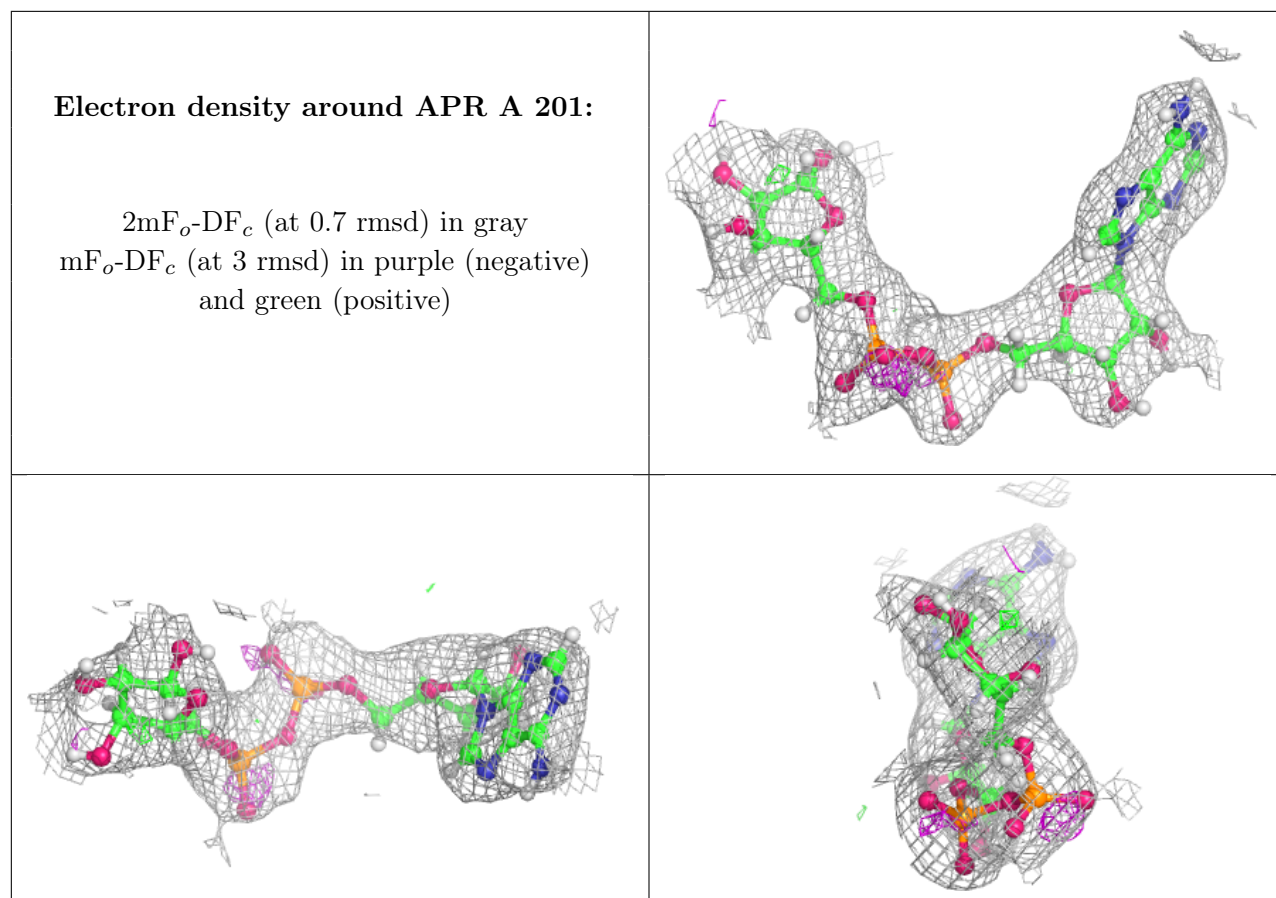
6.4 Ligands [i](#)

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
3	APR	B	201	36/36	0.92	0.20	47,58,73,78	0
3	APR	A	201	36/36	0.94	0.17	39,49,60,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.