



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:49 pm BST

PDB ID : 1Q17  
Title : Structure of the yeast Hst2 protein deacetylase in ternary complex with 2'-O-acetyl ADP ribose and histone peptide  
Authors : Zhao, K.; Chai, X.; Marmorstein, R.  
Deposited on : 2003-07-18  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

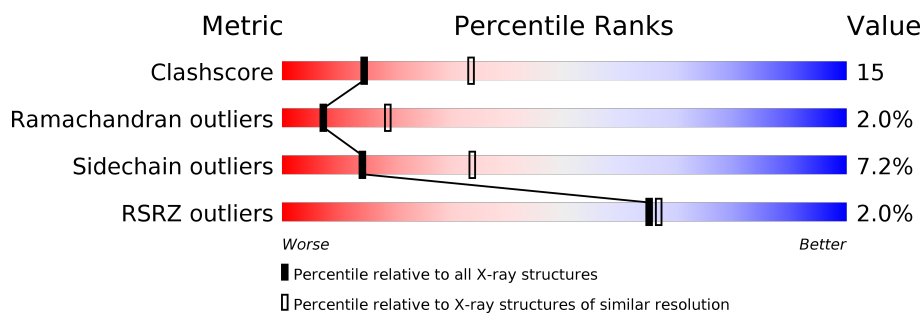
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	300	<div> <div>2%</div> <div>69%</div> <div>24%</div> <div>• •</div> </div>
1	B	300	<div> <div>%</div> <div>64%</div> <div>29%</div> <div>• • •</div> </div>
1	C	300	<div> <div>3%</div> <div>64%</div> <div>31%</div> <div>• •</div> </div>

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
3	CL	A	703	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7261 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 HST2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2301	1486	379	424	12			
1	B	294	Total	C	N	O	S	0	0	0
			2337	1508	388	429	12			
1	C	295	Total	C	N	O	S	0	0	0
			2346	1514	390	430	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P53686
A	-4	HIS	-	EXPRESSION TAG	UNP P53686
A	-3	GLY	-	EXPRESSION TAG	UNP P53686
A	-2	MET	-	EXPRESSION TAG	UNP P53686
A	-1	ALA	-	EXPRESSION TAG	UNP P53686
A	0	SER	-	EXPRESSION TAG	UNP P53686
B	-5	HIS	-	EXPRESSION TAG	UNP P53686
B	-4	HIS	-	EXPRESSION TAG	UNP P53686
B	-3	GLY	-	EXPRESSION TAG	UNP P53686
B	-2	MET	-	EXPRESSION TAG	UNP P53686
B	-1	ALA	-	EXPRESSION TAG	UNP P53686
B	0	SER	-	EXPRESSION TAG	UNP P53686
C	-5	HIS	-	EXPRESSION TAG	UNP P53686
C	-4	HIS	-	EXPRESSION TAG	UNP P53686
C	-3	GLY	-	EXPRESSION TAG	UNP P53686
C	-2	MET	-	EXPRESSION TAG	UNP P53686
C	-1	ALA	-	EXPRESSION TAG	UNP P53686
C	0	SER	-	EXPRESSION TAG	UNP P53686

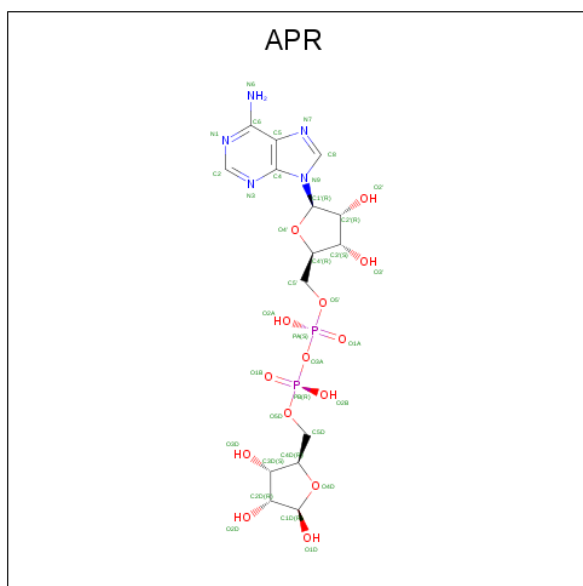
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).

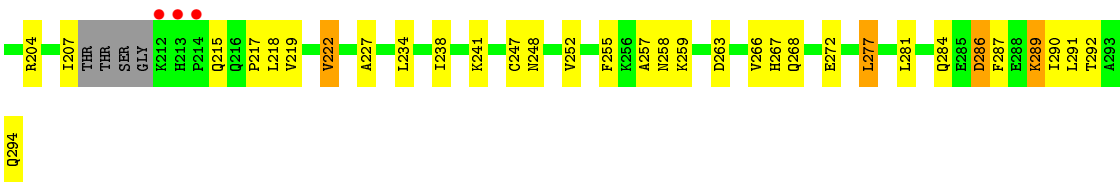


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
4	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
4	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total 56	O 56	0	0
5	B	51	Total 51	O 51	0	0
5	C	55	Total 55	O 55	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.16 Å   109.68 Å   85.83 Å 90.00°   104.90°   90.00°	Depositor
Resolution (Å)	28.88 – 2.70 28.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.88-2.70) 97.0 (28.88-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 2.68 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.186 ,      0.247 0.189 ,      (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APR, ZN, CL

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	0.36	0/2360	0.61	0/3198
1	B	0.36	0/2399	0.60	0/3251
1	C	0.36	0/2408	0.60	0/3263
All	All	0.36	0/7167	0.60	0/9712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2301	0	2284	61	0
1	B	2337	0	2314	84	0
1	C	2346	0	2326	79	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	2	0
3	B	2	0	0	1	0
3	C	1	0	0	0	0
4	A	36	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	36	0	17	0	0
4	C	36	0	19	1	0
5	A	56	0	0	3	0
5	B	51	0	0	2	0
5	C	55	0	0	1	0
All	All	7261	0	6978	217	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 15.

All (217) 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:B:162:HIS:HB2	1:B:163:PRO:HD3	1.34	1.02
1:C:104:GLN:HE22	1:C:127:LYS:H	1.06	1.01
1:C:162:HIS:HB2	1:C:163:PRO:HD3	1.45	0.99
1:A:104:GLN:HE22	1:A:127:LYS:H	1.01	0.99
1:B:104:GLN:HE21	1:B:130:LEU:HD12	1.34	0.92
1:B:104:GLN:HE22	1:B:127:LYS:H	1.15	0.90
1:B:215:GLN:HA	1:B:215:GLN:HE21	1.40	0.84
1:A:162:HIS:HB2	1:A:163:PRO:HD3	1.59	0.83
1:B:57:ARG:HG3	1:B:58:LEU:HD22	1.63	0.80
1:A:165:LYS:HD2	1:A:165:LYS:H	1.46	0.80
1:B:162:HIS:HB2	1:B:163:PRO:CD	2.12	0.80
1:C:104:GLN:HE21	1:C:130:LEU:HD12	1.49	0.78
1:A:10:MET:SD	1:C:64:GLU:HG3	2.24	0.77
1:C:162:HIS:CB	1:C:163:PRO:HD3	2.15	0.76
1:C:165:LYS:HD3	1:C:165:LYS:H	1.47	0.76
1:A:258:ASN:HD22	1:A:258:ASN:N	1.84	0.74
1:B:64:GLU:HG3	1:C:10:MET:SD	2.27	0.74
1:B:184:PHE:CE1	1:C:3:VAL:HG22	2.23	0.74
1:C:170:CYS:SG	1:C:172:VAL:HG12	2.30	0.71
1:C:121:GLU:HG2	5:C:1004:HOH:O	1.89	0.71
1:B:170:CYS:SG	1:B:172:VAL:HG12	2.32	0.70
1:C:25:ALA:HB2	1:C:215:GLN:HB3	1.74	0.69
1:B:84:LYS:HA	1:B:84:LYS:HE2	1.75	0.69
1:B:182:VAL:HG11	1:B:188:LEU:HD23	1.74	0.68
1:A:104:GLN:HE21	1:A:130:LEU:HD12	1.60	0.67
1:B:215:GLN:HA	1:B:215:GLN:NE2	2.09	0.67
1:B:60:LEU:HD11	1:B:66:VAL:HG22	1.77	0.66
1:C:151:PRO:CB	1:C:153:GLN:HE21	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:HE3	1:C:263:ASP:HB2	1.77	0.65
1:C:197:LEU:O	1:C:201:GLU:HG2	1.96	0.65
1:C:241:LYS:N	1:C:241:LYS:HD2	2.10	0.65
1:A:78:PRO:HG2	5:A:1037:HOH:O	1.95	0.65
1:B:265:ILE:HD12	1:B:265:ILE:N	2.12	0.65
1:B:243:LYS:HE3	1:B:264:LEU:HD13	1.78	0.65
1:B:284:GLN:O	1:B:288:GLU:HG2	1.97	0.65
1:B:23:PRO:O	1:B:24:ASN:HB2	1.96	0.64
1:A:153:GLN:H	1:A:153:GLN:CD	2.01	0.64
1:B:55:LEU:HD13	1:B:66:VAL:HG21	1.78	0.64
1:A:104:GLN:HE22	1:A:127:LYS:N	1.85	0.64
1:A:162:HIS:CB	1:A:163:PRO:HD3	2.27	0.64
1:C:182:VAL:HG11	1:C:188:LEU:HD23	1.79	0.63
1:A:145:GLY:HA3	1:A:175:GLU:HG3	1.82	0.62
1:C:152:PRO:HD2	1:C:153:GLN:NE2	2.15	0.62
1:A:104:GLN:NE2	1:A:127:LYS:H	1.85	0.62
1:A:222:VAL:HB	1:A:247:CYS:HB3	1.80	0.61
1:C:151:PRO:HB3	1:C:153:GLN:HE21	1.65	0.61
1:B:60:LEU:CD1	1:B:66:VAL:HG22	2.30	0.61
1:C:31:VAL:HG12	1:C:222:VAL:HG13	1.83	0.61
1:B:198:ASN:O	1:B:201:GLU:HG2	2.01	0.60
1:C:143:CYS:SG	1:C:170:CYS:HB2	2.42	0.60
1:B:39:CYS:SG	1:B:94:SER:HB3	2.41	0.59
1:B:264:LEU:HG	5:B:1032:HOH:O	2.02	0.59
1:B:12:VAL:HG13	1:B:277:LEU:HA	1.83	0.59
1:A:104:GLN:NE2	1:A:127:LYS:HG3	2.18	0.58
1:A:154:VAL:HG23	5:A:1032:HOH:O	2.02	0.58
1:C:222:VAL:HB	1:C:247:CYS:HB3	1.84	0.58
1:A:204:ARG:NH2	3:A:703:CL:CL	2.72	0.58
1:A:152:PRO:HD2	1:A:153:GLN:OE1	2.04	0.57
1:C:158:LYS:HE2	1:C:166:ASP:O	2.04	0.57
1:C:104:GLN:NE2	1:C:127:LYS:H	1.89	0.57
1:C:23:PRO:O	1:C:24:ASN:HB2	2.04	0.57
1:A:285:GLU:H	1:A:285:GLU:CD	2.07	0.57
1:C:167:PHE:O	1:C:169:LYS:HG3	2.04	0.57
1:B:26:LYS:HB3	1:B:110:LYS:HB2	1.85	0.57
1:C:151:PRO:HB3	1:C:153:GLN:NE2	2.20	0.57
1:B:248:ASN:O	1:B:267:HIS:HA	2.05	0.56
1:B:12:VAL:CG1	1:B:277:LEU:HA	2.35	0.56
1:A:19:MET:HE3	1:A:108:VAL:HG11	1.88	0.56
1:C:204:ARG:HH11	1:C:204:ARG:HG3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:O	1:A:205:GLU:HG3	2.05	0.56
1:C:266:VAL:HG11	1:C:268:GLN:HE21	1.70	0.56
1:C:104:GLN:NE2	1:C:127:LYS:HG3	2.21	0.56
1:C:162:HIS:HB2	1:C:163:PRO:CD	2.29	0.56
1:C:286:ASP:O	1:C:289:LYS:HD3	2.06	0.56
1:C:196:TRP:CE2	1:C:234:LEU:HD22	2.42	0.55
1:C:165:LYS:HD3	1:C:165:LYS:N	2.16	0.55
1:C:286:ASP:O	1:C:290:ILE:HG13	2.06	0.54
1:A:161:GLU:OE2	1:A:165:LYS:HD3	2.07	0.54
1:B:201:GLU:O	1:B:205:GLU:HG3	2.07	0.54
1:B:12:VAL:HG11	1:B:276:GLN:O	2.08	0.54
1:B:76:PRO:HG2	1:B:167:PHE:CE1	2.43	0.54
1:C:126:VAL:HB	1:C:131:ILE:HD11	1.89	0.54
1:C:152:PRO:HD2	1:C:153:GLN:HE22	1.71	0.54
1:C:96:PHE:O	1:C:99:LEU:HB3	2.06	0.54
1:A:143:CYS:SG	1:A:175:GLU:HB2	2.48	0.53
1:A:3:VAL:HG21	1:A:6:ALA:HB2	1.91	0.53
1:C:289:LYS:HD3	1:C:290:ILE:N	2.24	0.53
1:B:154:VAL:O	1:B:157:SER:HB3	2.08	0.53
1:B:158:LYS:HG3	1:B:168:VAL:HG23	1.90	0.53
1:A:165:LYS:H	1:A:165:LYS:CD	2.18	0.53
1:C:16:ALA:O	1:C:20:LYS:HG3	2.09	0.53
1:A:234:LEU:HB2	1:A:235:PRO:HD3	1.91	0.53
1:B:73:GLN:HA	1:B:176:LEU:CD1	2.39	0.53
1:B:287:PHE:O	1:B:291:LEU:HG	2.09	0.52
1:C:132:ILE:HD11	1:C:195:THR:HG21	1.92	0.52
1:A:126:VAL:HB	1:A:131:ILE:HD11	1.91	0.52
1:A:240:ARG:NH1	3:A:703:CL:CL	2.80	0.52
1:C:20:LYS:O	1:C:23:PRO:HD3	2.08	0.52
1:C:286:ASP:HA	1:C:289:LYS:HD2	1.92	0.51
1:A:110:LYS:HG3	1:A:202:TRP:CH2	2.46	0.51
1:B:71:PHE:HE2	1:B:78:PRO:HG3	1.74	0.51
1:B:84:LYS:HE2	1:B:84:LYS:CA	2.40	0.51
1:C:248:ASN:O	1:C:267:HIS:HA	2.10	0.51
1:C:5:THR:HG22	1:C:5:THR:O	2.10	0.51
1:A:64:GLU:HG3	1:B:10:MET:SD	2.50	0.51
1:B:12:VAL:HG13	1:B:277:LEU:HD23	1.92	0.51
1:A:162:HIS:HB2	1:A:163:PRO:CD	2.35	0.51
1:B:102:LEU:HD12	1:B:287:PHE:CD1	2.46	0.50
1:C:140:HIS:CD2	1:C:149:VAL:HG13	2.46	0.50
1:C:139:ALA:O	1:C:152:PRO:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:VAL:HG11	1:C:238:ILE:HD11	1.92	0.50
1:B:77:LEU:N	1:B:78:PRO:HD2	2.26	0.50
1:C:84:LYS:HB2	1:C:84:LYS:NZ	2.26	0.50
1:A:5:THR:HB	1:C:227:ALA:HB1	1.94	0.49
1:A:140:HIS:CD2	1:A:149:VAL:HG13	2.48	0.49
1:B:84:LYS:HA	1:B:84:LYS:CE	2.41	0.49
1:B:23:PRO:O	1:B:24:ASN:CB	2.61	0.49
1:C:286:ASP:O	1:C:289:LYS:CD	2.61	0.49
1:B:73:GLN:HA	1:B:176:LEU:HD12	1.94	0.49
1:C:27:VAL:HG22	1:C:218:LEU:HB3	1.95	0.49
1:C:289:LYS:HD3	1:C:290:ILE:HG13	1.94	0.49
1:A:110:LYS:O	1:A:110:LYS:HD3	2.13	0.49
1:A:39:CYS:SG	1:A:94:SER:HB3	2.53	0.48
1:B:98:TYR:O	1:B:101:LYS:HB3	2.13	0.48
1:A:122:ARG:HH11	1:A:122:ARG:HG3	1.78	0.48
1:A:122:ARG:NH1	1:A:128:ASP:OD2	2.46	0.48
1:A:57:ARG:HG3	1:A:58:LEU:HD12	1.93	0.48
1:B:75:ASP:OD1	1:B:78:PRO:HD2	2.13	0.48
1:A:229:TYR:HB3	1:A:230:PRO:HA	1.94	0.48
1:B:62:TYR:HD1	1:B:64:GLU:HG2	1.79	0.48
1:C:266:VAL:CG1	1:C:268:GLN:HE21	2.26	0.48
1:C:44:PHE:CE1	4:C:1003:APR:HR'3	2.49	0.48
1:B:87:TYR:CE2	1:B:156:LYS:HD3	2.49	0.48
1:A:257:ALA:C	1:A:258:ASN:HD22	2.17	0.48
1:C:113:TYR:OH	1:C:196:TRP:HA	2.14	0.47
1:A:71:PHE:HE2	1:A:78:PRO:HG3	1.80	0.47
1:A:162:HIS:O	1:A:164:ILE:HD12	2.13	0.47
1:A:21:SER:C	1:A:23:PRO:HD3	2.35	0.47
1:B:61:PRO:HB2	1:B:62:TYR:CD2	2.50	0.47
1:C:162:HIS:CB	1:C:163:PRO:CD	2.88	0.47
1:A:239:PRO:HB2	1:A:242:VAL:HG23	1.96	0.47
1:C:204:ARG:HH11	1:C:204:ARG:CG	2.28	0.47
1:A:10:MET:O	1:A:13:ARG:HB3	2.15	0.47
1:C:108:VAL:O	1:C:108:VAL:HG13	2.15	0.47
1:A:95:LYS:HG3	5:A:1004:HOH:O	2.14	0.46
1:C:39:CYS:SG	1:C:94:SER:HB3	2.55	0.46
1:B:140:HIS:HB2	1:B:150:TYR:O	2.15	0.46
1:C:61:PRO:HB2	1:C:62:TYR:HD2	1.80	0.46
1:C:277:LEU:HD22	1:C:281:LEU:CD1	2.46	0.46
1:A:31:VAL:HG12	1:A:222:VAL:HG13	1.98	0.46
1:B:162:HIS:O	1:B:164:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ARG:O	1:C:207:ILE:HG12	2.16	0.46
1:A:92:ARG:HH11	1:A:92:ARG:HG3	1.81	0.45
1:B:142:HIS:HE1	1:B:178:LYS:NZ	2.13	0.45
1:C:69:VAL:HG11	1:C:186:GLU:CG	2.47	0.45
1:B:265:ILE:CD1	1:B:265:ILE:N	2.77	0.45
1:A:153:GLN:N	1:A:153:GLN:OE1	2.37	0.45
1:A:165:LYS:N	1:A:165:LYS:HD2	2.23	0.45
1:A:162:HIS:CB	1:A:163:PRO:CD	2.95	0.45
1:C:290:ILE:O	1:C:294:GLN:HG2	2.16	0.45
1:B:153:GLN:H	1:B:153:GLN:CD	2.19	0.45
1:B:139:ALA:O	1:B:152:PRO:HG3	2.16	0.45
1:B:31:VAL:HG12	1:B:222:VAL:HG13	1.98	0.45
1:B:102:LEU:O	1:B:102:LEU:HD23	2.17	0.45
1:B:173:CYS:SG	1:B:175:GLU:HB2	2.56	0.45
1:B:181:ILE:O	1:B:181:ILE:HG13	2.17	0.45
1:A:258:ASN:ND2	1:A:258:ASN:N	2.56	0.44
1:B:111:ARG:HG3	1:B:112:VAL:H	1.82	0.44
1:B:165:LYS:HB3	1:B:166:ASP:H	1.60	0.44
1:B:110:LYS:HG3	1:B:202:TRP:CZ2	2.51	0.44
1:B:110:LYS:HG3	1:B:202:TRP:CH2	2.52	0.44
1:B:111:ARG:HG3	1:B:112:VAL:N	2.33	0.43
1:C:101:LYS:O	1:C:104:GLN:HB3	2.18	0.43
1:B:188:LEU:HB3	1:B:189:PRO:HD2	2.00	0.43
1:B:110:LYS:HD3	1:B:110:LYS:O	2.19	0.43
1:C:9:GLU:O	1:C:13:ARG:HB2	2.18	0.43
1:A:97:HIS:O	1:A:100:LEU:HB2	2.18	0.43
1:C:25:ALA:O	1:C:108:VAL:HG22	2.18	0.43
1:B:61:PRO:HB2	1:B:62:TYR:HD2	1.83	0.43
1:A:8:THR:O	1:A:12:VAL:HG23	2.19	0.43
1:B:238:ILE:HD12	1:B:244:ARG:HD2	2.01	0.43
1:A:216:GLN:HA	1:A:217:PRO:HD3	1.78	0.43
1:C:287:PHE:CE2	1:C:291:LEU:HD11	2.55	0.42
1:A:61:PRO:HB2	1:A:62:TYR:CD2	2.55	0.42
1:C:292:THR:C	1:C:294:GLN:H	2.23	0.42
1:B:26:LYS:HB2	1:B:202:TRP:CH2	2.54	0.42
1:B:141:CYS:HA	1:B:179:PRO:HA	2.00	0.42
1:A:108:VAL:O	1:A:108:VAL:HG12	2.20	0.42
1:B:196:TRP:CE2	1:B:234:LEU:HD22	2.54	0.42
1:B:215:GLN:NE2	1:B:215:GLN:CA	2.77	0.42
1:B:204:ARG:NH2	3:B:704:CL:CL	2.90	0.42
1:B:251:THR:OG1	1:B:267:HIS:HE1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:HA	1:B:88:PRO:HD3	1.91	0.42
1:C:151:PRO:HB2	1:C:153:GLN:HE21	1.83	0.42
1:B:229:TYR:HB3	1:B:230:PRO:HA	2.02	0.41
1:B:171:ASP:O	1:B:171:ASP:OD2	2.38	0.41
1:C:158:LYS:HE3	1:C:165:LYS:O	2.20	0.41
1:A:0:SER:HB2	1:C:186:GLU:O	2.20	0.41
1:B:261:PRO:HD2	5:B:1044:HOH:O	2.20	0.41
1:C:77:LEU:HB3	1:C:78:PRO:HD3	2.01	0.41
1:A:204:ARG:NH1	1:A:239:PRO:HG3	2.36	0.41
1:B:151:PRO:HB3	1:B:153:GLN:OE1	2.21	0.41
1:B:51:LEU:O	1:B:55:LEU:HG	2.20	0.41
1:C:146:CYS:SG	1:C:148:LYS:HB2	2.61	0.41
1:C:143:CYS:SG	1:C:175:GLU:HB2	2.60	0.41
1:C:219:VAL:HG11	1:C:238:ILE:CD1	2.51	0.41
1:B:234:LEU:HB2	1:B:235:PRO:CD	2.50	0.40
1:B:62:TYR:HB3	1:C:9:GLU:CB	2.51	0.40
1:C:73:GLN:OE1	1:C:74:SER:HB3	2.22	0.40
1:B:69:VAL:HG22	1:B:184:PHE:O	2.22	0.40
1:A:151:PRO:HA	1:A:152:PRO:HD3	1.94	0.40
1:A:202:TRP:CZ3	1:A:203:LEU:HD23	2.57	0.40
1:A:207:ILE:HG22	1:A:216:GLN:OE1	2.21	0.40
1:B:158:LYS:HG3	1:B:168:VAL:CG2	2.51	0.40
1:B:287:PHE:CE2	1:B:291:LEU:HD11	2.56	0.40
1:B:71:PHE:CE2	1:B:78:PRO:HG3	2.54	0.40
1:C:252:VAL:O	1:C:255:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	286/300 (95%)	263 (92%)	18 (6%)	5 (2%)	<b>9</b> <b>23</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	290/300 (97%)	255 (88%)	28 (10%)	7 (2%)	6	15
1	C	291/300 (97%)	260 (89%)	26 (9%)	5 (2%)	9	23
All	All	867/900 (96%)	778 (90%)	72 (8%)	17 (2%)	7	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	LYS
1	B	165	LYS
1	B	172	VAL
1	C	257	ALA
1	A	164	ILE
1	C	180	ALA
1	C	217	PRO
1	B	153	GLN
1	B	84	LYS
1	B	162	HIS
1	B	163	PRO
1	C	83	ALA
1	A	162	HIS
1	A	180	ALA
1	C	162	HIS
1	B	164	ILE
1	A	217	PRO

### 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	255/264 (97%)	236 (92%)	19 (8%)	13	31
1	B	259/264 (98%)	243 (94%)	16 (6%)	18	40
1	C	260/264 (98%)	239 (92%)	21 (8%)	11	27
All	All	774/792 (98%)	718 (93%)	56 (7%)	14	34



All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	57	ARG
1	A	64	GLU
1	A	66	VAL
1	A	77	LEU
1	A	85	GLU
1	A	87	TYR
1	A	102	LEU
1	A	107	ASP
1	A	109	LEU
1	A	153	GLN
1	A	172	VAL
1	A	218	LEU
1	A	222	VAL
1	A	246	LEU
1	A	258	ASN
1	A	277	LEU
1	A	285	GLU
1	A	286	ASP
1	B	69	VAL
1	B	70	ASP
1	B	77	LEU
1	B	84	LYS
1	B	102	LEU
1	B	109	LEU
1	B	122	ARG
1	B	153	GLN
1	B	197	LEU
1	B	204	ARG
1	B	222	VAL
1	B	246	LEU
1	B	264	LEU
1	B	272	GLU
1	B	277	LEU
1	B	294	GLN
1	C	3	VAL
1	C	37	THR
1	C	66	VAL
1	C	73	GLN
1	C	77	LEU
1	C	82	LEU
1	C	108	VAL

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Mol	Chain	Res	Type
1	C	109	LEU
1	C	128	ASP
1	C	142	HIS
1	C	153	GLN
1	C	158	LYS
1	C	165	LYS
1	C	173	CYS
1	C	222	VAL
1	C	258	ASN
1	C	272	GLU
1	C	277	LEU
1	C	284	GLN
1	C	286	ASP
1	C	289	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	104	GLN
1	A	140	HIS
1	A	142	HIS
1	A	248	ASN
1	A	258	ASN
1	A	294	GLN
1	B	24	ASN
1	B	90	ASN
1	B	104	GLN
1	B	123	GLN
1	B	140	HIS
1	B	142	HIS
1	B	215	GLN
1	B	248	ASN
1	B	267	HIS
1	B	294	GLN
1	C	24	ASN
1	C	90	ASN
1	C	104	GLN
1	C	140	HIS
1	C	153	GLN
1	C	248	ASN
1	C	267	HIS

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Mol	Chain	Res	Type
1	C	268	GLN
1	C	284	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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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$
4	APR	A	1001	-	34,39,39	3.77	13 (38%)	40,60,60	2.48	17 (42%)
4	APR	C	1003	-	34,39,39	3.72	12 (35%)	40,60,60	2.51	15 (37%)
4	APR	B	1002	-	34,39,39	3.76	10 (29%)	40,60,60	2.61	15 (37%)

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	APR	A	1001	-	-	4/18/54/54	0/4/4/4
4	APR	C	1003	-	-	3/18/54/54	0/4/4/4
4	APR	B	1002	-	-	3/18/54/54	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	APR	C1D-C2D	-13.16	1.37	1.52
4	C	1003	APR	O2D-C2D	-12.86	1.12	1.43
4	B	1002	APR	C1D-C2D	-12.79	1.37	1.52
4	B	1002	APR	O2D-C2D	-11.71	1.15	1.43
4	C	1003	APR	C1D-C2D	-11.08	1.39	1.52
4	A	1001	APR	O2D-C2D	-10.71	1.17	1.43
4	B	1002	APR	O4D-C1D	6.99	1.51	1.43
4	A	1001	APR	O4D-C1D	6.65	1.51	1.43
4	C	1003	APR	O4D-C1D	6.14	1.50	1.43
4	B	1002	APR	O1D-C1D	-5.62	1.21	1.39
4	A	1001	APR	O1D-C1D	-5.25	1.22	1.39
4	C	1003	APR	O1D-C1D	-5.20	1.23	1.39
4	C	1003	APR	C3D-C4D	-4.60	1.41	1.53
4	B	1002	APR	PB-O2B	-4.35	1.34	1.55
4	C	1003	APR	PB-O2B	-4.33	1.35	1.55
4	A	1001	APR	PB-O2B	-4.26	1.35	1.55
4	B	1002	APR	C4-N3	4.07	1.41	1.35
4	A	1001	APR	C3D-C4D	-4.07	1.42	1.53
4	B	1002	APR	C2-N1	4.06	1.41	1.33
4	C	1003	APR	C2-N1	3.88	1.41	1.33
4	A	1001	APR	C4-N3	3.82	1.40	1.35
4	A	1001	APR	C2-N1	3.76	1.40	1.33
4	C	1003	APR	C4-N3	3.62	1.40	1.35
4	A	1001	APR	O5D-C5D	3.59	1.58	1.44
4	B	1002	APR	O5D-C5D	3.54	1.58	1.44
4	A	1001	APR	O4D-C4D	3.54	1.52	1.45
4	C	1003	APR	O4D-C4D	3.31	1.52	1.45
4	C	1003	APR	O5D-C5D	2.89	1.55	1.44
4	A	1001	APR	C3D-C2D	2.89	1.61	1.53
4	B	1002	APR	C3D-C4D	-2.63	1.46	1.53
4	C	1003	APR	C5D-C4D	-2.23	1.44	1.51
4	B	1002	APR	PA-O2A	-2.19	1.45	1.55
4	C	1003	APR	C3D-C2D	2.15	1.59	1.53
4	A	1001	APR	PA-O2A	-2.05	1.45	1.55
4	A	1001	APR	PB-O1B	-2.03	1.43	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	APR	C1D-C2D-C3D	8.33	112.72	102.30
4	C	1003	APR	C1D-C2D-C3D	7.72	111.96	102.30
4	A	1001	APR	C1D-C2D-C3D	7.53	111.73	102.30
4	B	1002	APR	O1D-C1D-O4D	-6.52	102.78	111.13
4	C	1003	APR	O3D-C3D-C2D	5.39	129.26	111.82
4	C	1003	APR	O5D-PB-O1B	-5.33	88.25	109.07
4	A	1001	APR	O5D-PB-O1B	-4.90	89.93	109.07
4	C	1003	APR	O1D-C1D-O4D	-4.89	104.87	111.13
4	A	1001	APR	O3D-C3D-C2D	4.84	127.49	111.82
4	A	1001	APR	O1D-C1D-O4D	-4.72	105.08	111.13
4	B	1002	APR	O5D-PB-O1B	-4.72	90.63	109.07
4	B	1002	APR	O3D-C3D-C2D	4.34	125.86	111.82
4	B	1002	APR	O5'-PA-O1A	4.04	124.86	109.07
4	A	1001	APR	O5'-PA-O1A	4.04	124.85	109.07
4	C	1003	APR	O5'-PA-O1A	3.95	124.49	109.07
4	C	1003	APR	O2A-PA-O1A	-3.46	95.12	112.24
4	C	1003	APR	O2D-C2D-C1D	-3.19	103.03	111.82
4	A	1001	APR	O2A-PA-O1A	-3.16	96.61	112.24
4	B	1002	APR	O2A-PA-O1A	-3.15	96.68	112.24
4	B	1002	APR	C1'-N9-C4	-3.10	121.20	126.64
4	B	1002	APR	PB-O3A-PA	3.09	143.42	132.83
4	A	1001	APR	O1D-C1D-C2D	3.08	125.10	110.39
4	A	1001	APR	O2D-C2D-C1D	-3.04	103.44	111.82
4	A	1001	APR	O4D-C4D-C3D	3.03	111.12	105.11
4	C	1003	APR	C1'-N9-C4	-3.02	121.33	126.64
4	C	1003	APR	O1D-C1D-C2D	2.93	124.40	110.39
4	B	1002	APR	O1D-C1D-C2D	2.93	124.38	110.39
4	B	1002	APR	O4D-C4D-C3D	2.84	110.73	105.11
4	C	1003	APR	PB-O3A-PA	2.84	142.56	132.83
4	A	1001	APR	O4D-C1D-C2D	2.81	107.92	104.46
4	B	1002	APR	C5D-C4D-C3D	2.80	125.67	115.18
4	A	1001	APR	PB-O3A-PA	2.72	142.15	132.83
4	A	1001	APR	C1'-N9-C4	-2.66	121.96	126.64
4	B	1002	APR	C5-C6-N6	2.42	124.03	120.35
4	C	1003	APR	N3-C2-N1	-2.36	124.99	128.68
4	B	1002	APR	O2D-C2D-C1D	-2.35	105.33	111.82
4	A	1001	APR	C5-C6-N6	2.35	123.93	120.35
4	C	1003	APR	O4D-C4D-C3D	2.34	109.74	105.11
4	A	1001	APR	C3'-C2'-C1'	2.31	104.46	100.98
4	C	1003	APR	O4'-C1'-C2'	-2.30	103.56	106.93
4	B	1002	APR	C3'-C2'-C1'	2.26	104.38	100.98
4	A	1001	APR	N3-C2-N1	-2.24	125.17	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	APR	C5-C6-N6	2.24	123.76	120.35
4	B	1002	APR	N3-C2-N1	-2.13	125.35	128.68
4	A	1001	APR	O3'-C3'-C2'	2.10	118.61	111.82
4	A	1001	APR	O2B-PB-O5D	2.00	117.05	107.75
4	C	1003	APR	O2B-PB-O5D	2.00	117.04	107.75

There are no chirality outliers.

All (10) torsion outliers are listed below:

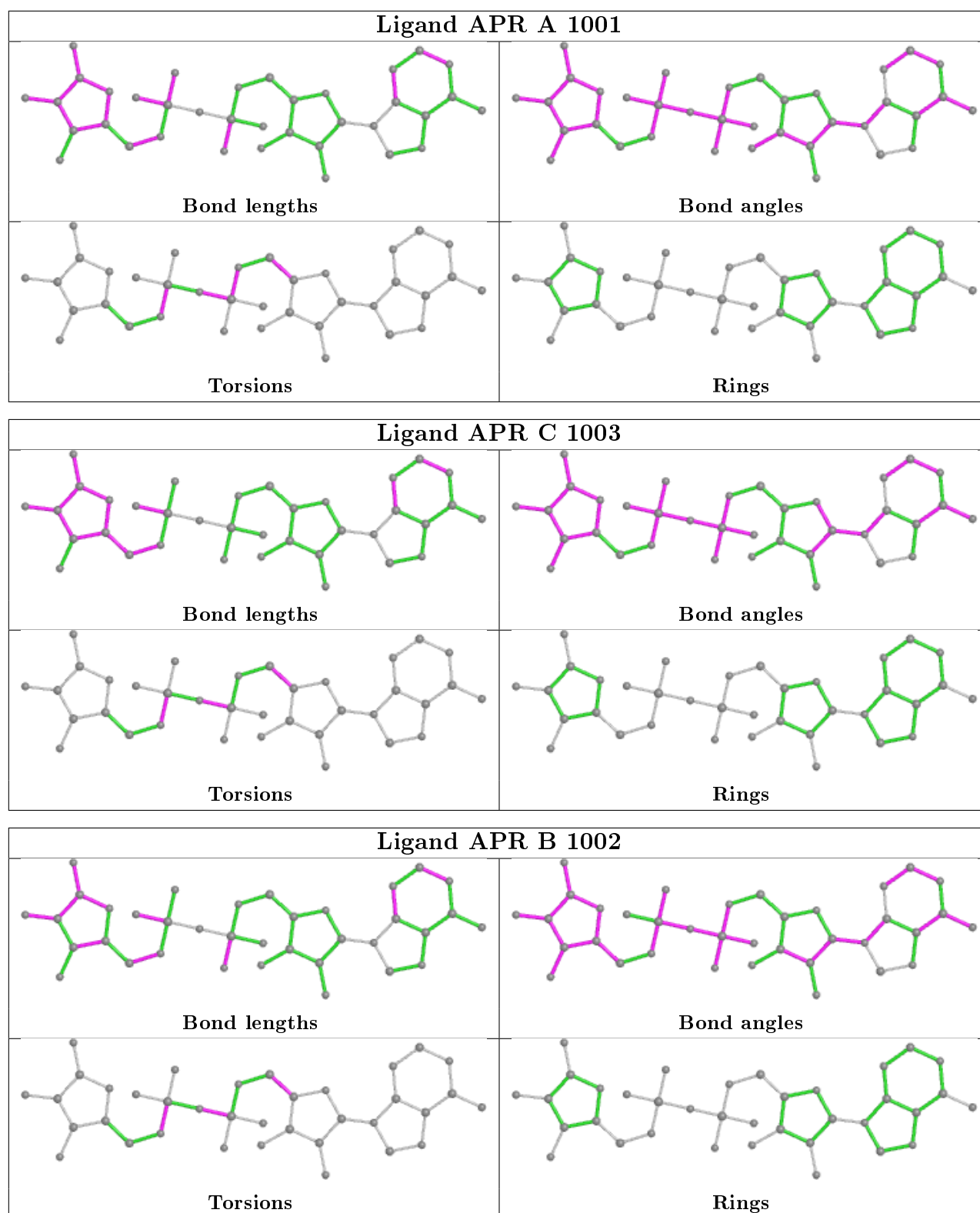
Mol	Chain	Res	Type	Atoms
4	A	1001	APR	C5'-O5'-PA-O1A
4	A	1001	APR	PB-O3A-PA-O1A
4	C	1003	APR	PB-O3A-PA-O1A
4	B	1002	APR	PB-O3A-PA-O1A
4	B	1002	APR	O4'-C4'-C5'-O5'
4	A	1001	APR	O4'-C4'-C5'-O5'
4	C	1003	APR	O4'-C4'-C5'-O5'
4	A	1001	APR	C5D-O5D-PB-O1B
4	C	1003	APR	C5D-O5D-PB-O1B
4	B	1002	APR	C5D-O5D-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1003	APR	1	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	290/300 (96%)	-0.38	6 (2%) 63 65	23, 44, 75, 120	0
1	B	294/300 (98%)	-0.21	4 (1%) 75 77	26, 47, 84, 145	0
1	C	295/300 (98%)	-0.31	8 (2%) 54 55	26, 47, 88, 127	0
All	All	879/900 (97%)	-0.30	18 (2%) 65 67	23, 46, 85, 145	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	HIS	4.8
1	A	162	HIS	3.8
1	A	165	LYS	3.7
1	B	165	LYS	3.6
1	A	294	GLN	3.2
1	C	165	LYS	3.2
1	C	166	ASP	3.0
1	B	-5	HIS	2.9
1	A	293	ALA	2.8
1	C	213	HIS	2.4
1	C	212	LYS	2.3
1	C	162	HIS	2.3
1	A	220	ILE	2.3
1	C	-4	HIS	2.3
1	B	163	PRO	2.2
1	A	-2	MET	2.2
1	C	214	PRO	2.2
1	C	154	VAL	2.0

### 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 ⓘ

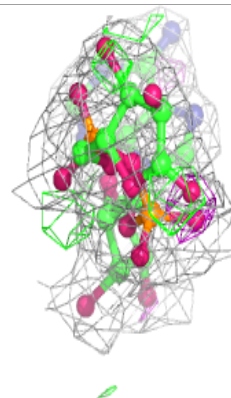
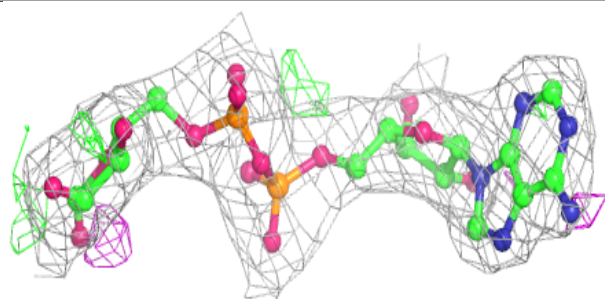
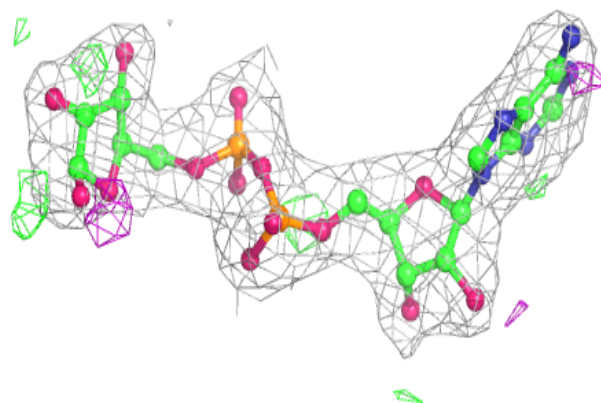
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	C	701	1/1	0.96	0.13	56,56,56,56	0
4	APR	C	1003	36/36	0.97	0.14	25,36,45,49	0
3	CL	B	704	1/1	0.97	0.17	43,43,43,43	0
4	APR	B	1002	36/36	0.97	0.15	22,36,48,50	0
4	APR	A	1001	36/36	0.97	0.14	24,35,48,57	0
3	CL	A	703	1/1	0.98	0.12	46,46,46,46	0
3	CL	B	702	1/1	0.98	0.17	48,48,48,48	0
2	ZN	A	401	1/1	0.99	0.08	53,53,53,53	0
2	ZN	B	401	1/1	0.99	0.05	61,61,61,61	0
2	ZN	C	401	1/1	1.00	0.10	63,63,63,63	0

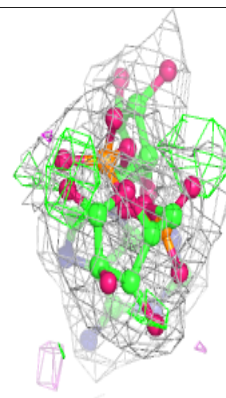
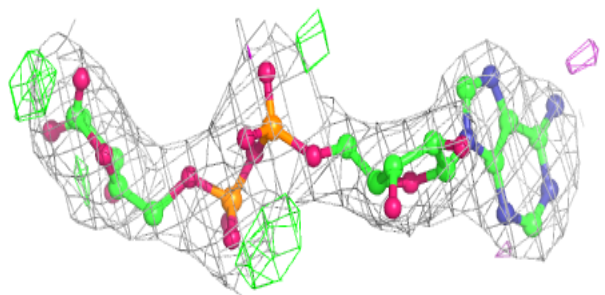
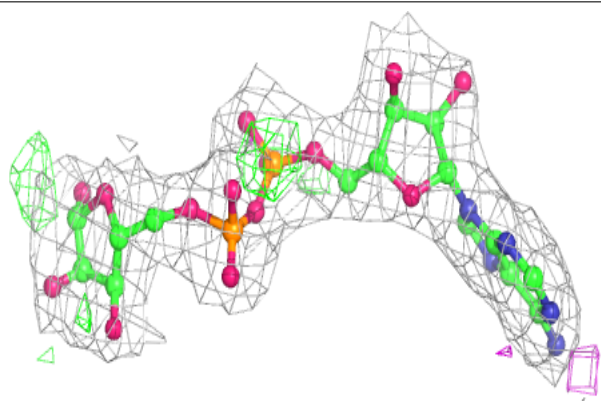
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

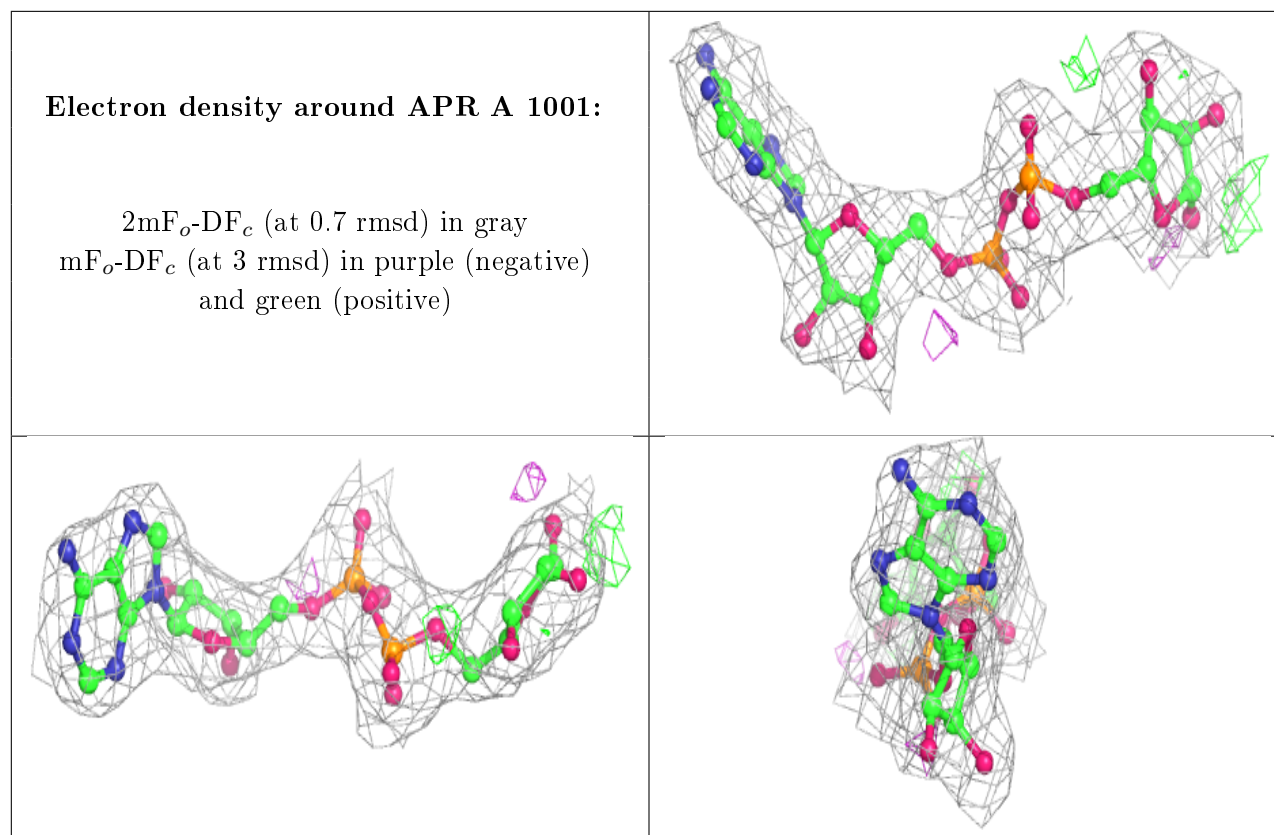
**Electron density around APR C 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around APR B 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.