



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:27 am BST

PDB ID : 4IAO  
Title : Crystal structure of Sir2 C543S mutant in complex with SID domain of Sir4  
Authors : Hsu, H.C.; Wang, C.L.; Wang, M.; Yang, N.; Chen, Z.; Sternglanz, R.; Xu, R.M.  
Deposited on : 2012-12-07  
Resolution : 2.90 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

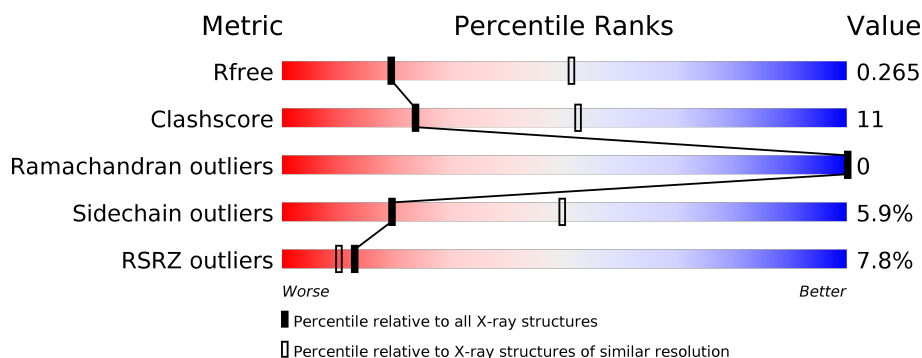
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	492	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>21%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	492	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>21%</div> <div>•</div> <div>13%</div> </div> </div>
2	C	159	<div> <div>6%</div> <div> <div></div> <div>45%</div> <div>14%</div> <div>•</div> <div>39%</div> </div> </div>
2	D	159	<div> <div>7%</div> <div> <div></div> <div>44%</div> <div>16%</div> <div>•</div> <div>38%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8654 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 NAD-dependent histone deacetylase SIR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3419	2212	574	614	19			
1	B	429	Total	C	N	O	S	0	0	0
			3438	2223	579	618	18			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	MET	-	EXPRESSION TAG	UNP P06700
A	72	GLY	-	EXPRESSION TAG	UNP P06700
A	73	SER	-	EXPRESSION TAG	UNP P06700
A	74	SER	-	EXPRESSION TAG	UNP P06700
A	75	HIS	-	EXPRESSION TAG	UNP P06700
A	76	HIS	-	EXPRESSION TAG	UNP P06700
A	77	HIS	-	EXPRESSION TAG	UNP P06700
A	78	HIS	-	EXPRESSION TAG	UNP P06700
A	79	HIS	-	EXPRESSION TAG	UNP P06700
A	80	HIS	-	EXPRESSION TAG	UNP P06700
A	81	SER	-	EXPRESSION TAG	UNP P06700
A	82	GLN	-	EXPRESSION TAG	UNP P06700
A	83	ASP	-	EXPRESSION TAG	UNP P06700
A	84	PRO	-	EXPRESSION TAG	UNP P06700
A	85	ASN	-	EXPRESSION TAG	UNP P06700
A	86	SER	-	EXPRESSION TAG	UNP P06700
A	543	SER	CYS	ENGINEERED MUTATION	UNP P06700
B	71	MET	-	EXPRESSION TAG	UNP P06700
B	72	GLY	-	EXPRESSION TAG	UNP P06700
B	73	SER	-	EXPRESSION TAG	UNP P06700
B	74	SER	-	EXPRESSION TAG	UNP P06700
B	75	HIS	-	EXPRESSION TAG	UNP P06700
B	76	HIS	-	EXPRESSION TAG	UNP P06700
B	77	HIS	-	EXPRESSION TAG	UNP P06700
B	78	HIS	-	EXPRESSION TAG	UNP P06700

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Chain	Residue	Modelled	Actual	Comment	Reference
B	79	HIS	-	EXPRESSION TAG	UNP P06700
B	80	HIS	-	EXPRESSION TAG	UNP P06700
B	81	SER	-	EXPRESSION TAG	UNP P06700
B	82	GLN	-	EXPRESSION TAG	UNP P06700
B	83	ASP	-	EXPRESSION TAG	UNP P06700
B	84	PRO	-	EXPRESSION TAG	UNP P06700
B	85	ASN	-	EXPRESSION TAG	UNP P06700
B	86	SER	-	EXPRESSION TAG	UNP P06700
B	543	SER	CYS	ENGINEERED MUTATION	UNP P06700

- Molecule 2 is a protein called Regulatory protein SIR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	97	Total	C	N	O	S	0	0	0
			799	508	132	157	2			
2	D	98	Total	C	N	O	S	0	0	0
			814	519	134	159	2			

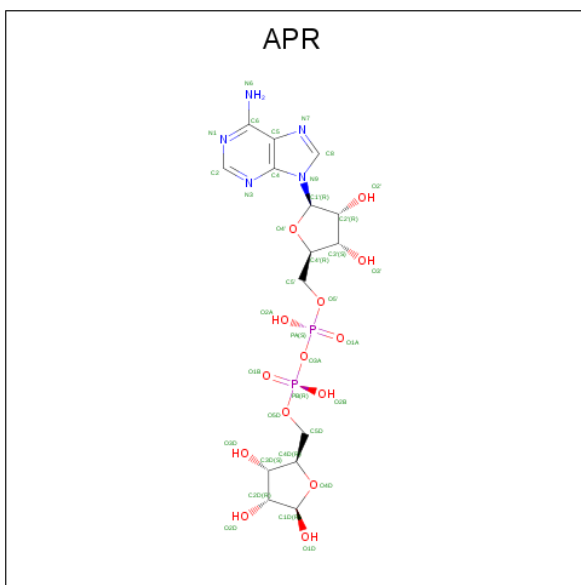
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	735	GLY	-	EXPRESSION TAG	UNP P11978
C	736	SER	-	EXPRESSION TAG	UNP P11978
D	735	GLY	-	EXPRESSION TAG	UNP P11978
D	736	SER	-	EXPRESSION TAG	UNP P11978

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

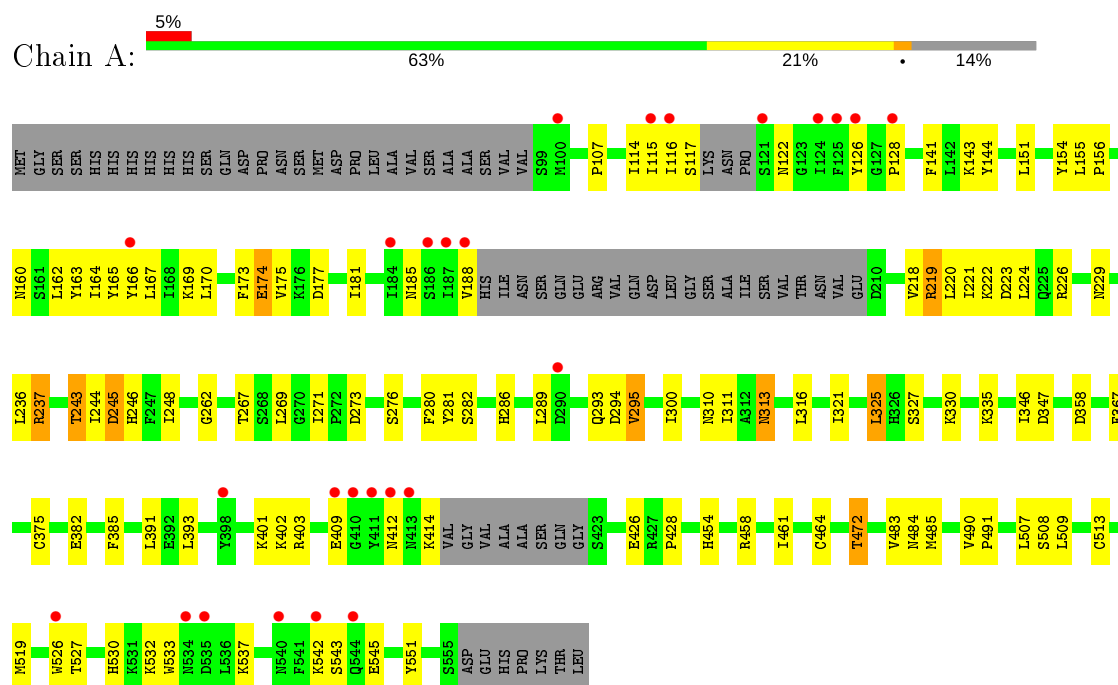
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	47	Total O 47 47	0	0
5	B	44	Total O 44 44	0	0
5	C	7	Total O 7 7	0	0
5	D	12	Total O 12 12	0	0

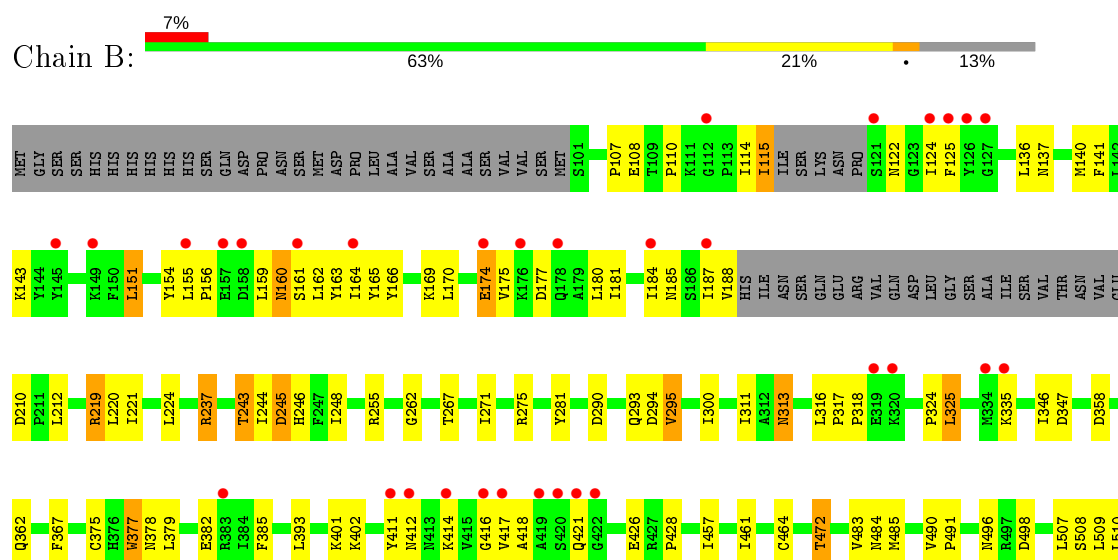
### 3 Residue-property plots

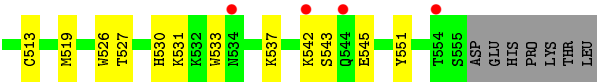
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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: NAD-dependent histone deacetylase SIR2

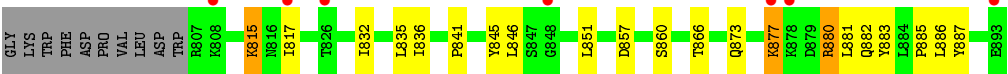
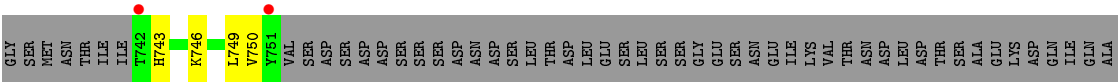


- Molecule 1: NAD-dependent histone deacetylase SIR2

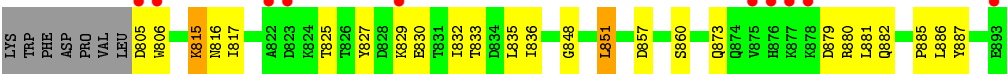




• Molecule 2: Regulatory protein SIR4



• Molecule 2: Regulatory protein SIR4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.41Å 178.75Å 121.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.43 – 2.90 48.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.7 (36.43-2.90) 89.9 (48.57-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.227 , 0.269 0.223 , 0.265	Depositor DCC
$R_{free}$ test set	1813 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.4	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.15 % 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 5.0646e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.31	0/3501	0.50	0/4734
1	B	0.31	0/3521	0.52	0/4764
2	C	0.28	0/816	0.48	0/1103
2	D	0.29	0/833	0.49	0/1127
All	All	0.31	0/8671	0.50	0/11728

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 [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	3419	0	3462	81	0
1	B	3438	0	3480	84	0
2	C	799	0	783	28	0
2	D	814	0	790	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	21	1	0
4	B	36	0	21	1	0
5	A	47	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	44	0	0	1	0
5	C	7	0	0	1	0
5	D	12	0	0	1	0
All	All	8654	0	8557	191	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 11.

All (191) 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:116:ILE:HB	1:A:128:PRO:HG2	1.59	0.83
1:B:221:ILE:HG23	2:D:836:ILE:HD13	1.64	0.77
1:A:221:ILE:HG23	2:C:836:ILE:HD13	1.69	0.75
1:B:412:ASN:HD21	1:B:418:ALA:HB1	1.51	0.74
2:D:817:ILE:HG23	2:D:835:LEU:HD21	1.71	0.73
1:B:124:ILE:HA	1:B:188:VAL:HG21	1.72	0.72
2:C:877:LYS:H	2:C:877:LYS:HD3	1.55	0.72
1:B:160:ASN:HD21	1:B:162:LEU:HB2	1.55	0.71
2:C:817:ILE:HG23	2:C:835:LEU:HD21	1.74	0.69
1:B:237:ARG:HB2	2:D:887:TYR:CE1	2.30	0.66
1:B:107:PRO:HG3	1:B:141:PHE:HA	1.78	0.66
1:B:401:LYS:HG3	1:B:402:LYS:H	1.61	0.65
1:B:156:PRO:HG3	1:B:163:TYR:CZ	2.33	0.64
1:A:401:LYS:HG3	1:A:402:LYS:H	1.62	0.63
2:C:880:ARG:H	2:C:880:ARG:HD2	1.63	0.63
1:B:414:LYS:HG2	1:B:416:GLY:H	1.63	0.63
2:C:746:LYS:NZ	5:C:903:HOH:O	2.29	0.62
1:A:237:ARG:HB2	2:C:887:TYR:CE1	2.34	0.62
1:A:244:ILE:O	1:A:248:ILE:HG12	2.00	0.61
1:A:122:ASN:H	1:A:188:VAL:HG13	1.66	0.60
1:B:164:ILE:HD11	2:D:832:ILE:HD13	1.83	0.59
1:A:155:LEU:HD21	1:A:167:LEU:HD11	1.84	0.59
1:A:325:LEU:HD13	1:A:513:CYS:HB2	1.84	0.59
1:B:294:ASP:HB3	1:B:300:ILE:HD12	1.84	0.58
1:A:114:ILE:HG23	1:A:154:TYR:O	2.02	0.58
1:A:243:THR:HG22	1:A:246:HIS:CG	2.38	0.58
1:A:107:PRO:HG3	1:A:141:PHE:HA	1.87	0.57
1:A:114:ILE:HD11	1:A:163:TYR:HD1	1.69	0.57
1:B:187:ILE:HG23	1:B:188:VAL:H	1.69	0.56
1:B:461:ILE:HG21	1:B:485:MET:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:HB3	1:A:300:ILE:HD12	1.88	0.56
1:A:313:ASN:H	1:A:313:ASN:HD22	1.53	0.55
1:A:164:ILE:HB	1:A:220:LEU:HD23	1.89	0.55
1:B:401:LYS:HE2	1:B:402:LYS:HG3	1.89	0.55
1:A:115:ILE:HB	1:A:128:PRO:HB3	1.89	0.54
1:B:484:ASN:HD21	2:D:873:GLN:HE22	1.55	0.54
1:A:426:GLU:O	1:A:428:PRO:HD3	2.08	0.54
1:B:124:ILE:HG13	1:B:125:PHE:N	2.23	0.53
1:B:219:ARG:HH22	2:D:880:ARG:HD2	1.73	0.53
1:B:110:PRO:HG3	1:B:154:TYR:CZ	2.43	0.53
2:D:829:LYS:HG3	2:D:830:GLU:H	1.71	0.53
1:B:244:ILE:O	1:B:248:ILE:HG12	2.07	0.53
1:B:154:TYR:CD1	1:B:170:LEU:HD21	2.44	0.53
1:B:243:THR:HG22	1:B:246:HIS:CG	2.44	0.53
1:A:116:ILE:HB	1:A:128:PRO:CG	2.36	0.52
1:A:117:SER:HA	1:A:163:TYR:OH	2.09	0.52
1:B:281:TYR:OH	4:B:602:APR:O1D	2.26	0.52
1:B:156:PRO:HG2	1:B:159:LEU:HB3	1.91	0.52
1:A:267:THR:HA	1:A:271:ILE:O	2.10	0.51
1:A:177:ASP:O	1:A:181:ILE:HG13	2.10	0.51
1:B:325:LEU:HD13	1:B:513:CYS:HB2	1.92	0.51
1:A:223:ASP:OD1	2:C:880:ARG:HG3	2.10	0.51
1:B:210:ASP:HB2	2:D:825:THR:O	2.11	0.51
1:A:116:ILE:HG23	1:A:163:TYR:CE1	2.45	0.51
1:A:154:TYR:CD1	1:A:170:LEU:HD21	2.44	0.51
1:B:417:VAL:HA	1:B:421:GLN:O	2.11	0.51
1:B:114:ILE:HG13	1:B:154:TYR:O	2.10	0.51
2:C:832:ILE:O	2:C:836:ILE:HG12	2.11	0.51
1:A:401:LYS:HE2	1:A:402:LYS:HG3	1.92	0.51
1:B:426:GLU:O	1:B:428:PRO:HD3	2.11	0.51
1:A:219:ARG:NH1	2:C:880:ARG:HE	2.09	0.50
1:B:177:ASP:O	1:B:181:ILE:HG13	2.11	0.50
1:A:164:ILE:HD11	2:C:832:ILE:HD13	1.92	0.50
2:D:879:ASP:OD1	2:D:880:ARG:N	2.44	0.50
2:C:857:ASP:HA	2:C:860:SER:HB3	1.93	0.50
1:A:281:TYR:CZ	1:A:293:GLN:HG2	2.47	0.50
1:A:293:GLN:OE1	2:C:749:LEU:HD22	2.12	0.50
1:B:164:ILE:HB	1:B:220:LEU:HD23	1.93	0.50
2:C:743:HIS:HB2	2:C:746:LYS:HG3	1.94	0.50
1:B:174:GLU:HG3	2:D:882:GLN:HB2	1.93	0.50
2:D:832:ILE:O	2:D:836:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:857:ASP:HA	2:D:860:SER:HB3	1.94	0.49
1:A:484:ASN:HD21	2:C:873:GLN:HE22	1.61	0.49
1:B:313:ASN:HD22	1:B:313:ASN:H	1.61	0.49
1:A:181:ILE:HG22	1:A:185:ASN:HD21	1.78	0.48
1:B:187:ILE:HG23	1:B:188:VAL:N	2.28	0.48
1:B:161:SER:OG	1:B:212:LEU:HB2	2.13	0.48
1:B:165:TYR:CE2	1:B:169:LYS:HD2	2.47	0.48
1:B:267:THR:HA	1:B:271:ILE:O	2.13	0.48
1:B:166:TYR:HD1	1:B:169:LYS:HG3	1.78	0.48
1:A:174:GLU:HG3	2:C:882:GLN:HB2	1.96	0.48
1:B:181:ILE:HG22	1:B:185:ASN:HD21	1.79	0.47
1:A:273:ASP:OD2	1:A:276:SER:OG	2.24	0.47
1:B:244:ILE:HD13	1:B:519:MET:HE1	1.97	0.47
1:B:271:ILE:HD11	1:B:318:PRO:HG3	1.96	0.47
1:B:393:LEU:HD11	1:B:411:TYR:HE2	1.78	0.47
1:B:377:TRP:C	1:B:377:TRP:CD1	2.88	0.47
1:B:275:ARG:HH12	2:D:749:LEU:HD13	1.80	0.47
1:B:262:GLY:HA3	1:B:472:THR:HB	1.97	0.46
1:B:219:ARG:HH12	2:D:880:ARG:HD2	1.81	0.46
1:A:244:ILE:HD13	1:A:519:MET:HE1	1.98	0.46
1:A:243:THR:HG22	1:A:246:HIS:ND1	2.31	0.46
2:D:885:PRO:O	2:D:886:LEU:HD23	2.16	0.46
1:A:165:TYR:CE2	1:A:169:LYS:HD2	2.51	0.46
1:A:219:ARG:HH11	2:C:880:ARG:HE	1.64	0.46
1:A:310:ASN:OD1	1:A:414:LYS:HB3	2.16	0.46
2:C:880:ARG:HG2	2:C:881:LEU:H	1.80	0.45
1:A:155:LEU:HD11	1:A:167:LEU:HD11	1.99	0.45
1:B:382:GLU:HA	1:B:385:PHE:CD2	2.52	0.45
1:B:293:GLN:OE1	2:D:749:LEU:HD22	2.17	0.45
1:A:262:GLY:HA3	1:A:472:THR:HB	1.98	0.45
1:B:108:GLU:HG2	1:B:137:ASN:OD1	2.16	0.45
1:A:545:GLU:HB2	1:A:551:TYR:CE2	2.52	0.44
1:A:221:ILE:HG23	2:C:836:ILE:CD1	2.44	0.44
2:D:815:LYS:HE3	2:D:815:LYS:HB3	1.83	0.44
2:D:829:LYS:O	2:D:833:THR:HG23	2.17	0.44
1:B:324:PRO:HG3	1:B:530:HIS:HD2	1.82	0.44
1:B:243:THR:HG23	1:B:245:ASP:H	1.82	0.44
1:B:295:VAL:HG21	1:B:311:ILE:HG12	2.00	0.44
1:B:151:LEU:O	1:B:155:LEU:HG	2.18	0.44
1:B:346:ILE:HD12	1:B:367:PHE:CE1	2.53	0.44
1:B:156:PRO:HG3	1:B:163:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD23	2:D:836:ILE:HD12	2.00	0.44
1:A:222:LYS:HB3	1:A:226:ARG:HH12	1.82	0.44
1:A:530:HIS:NE2	1:A:532:LYS:HG3	2.33	0.44
1:B:542:LYS:HD3	1:B:543:SER:N	2.31	0.44
2:D:829:LYS:HG3	2:D:830:GLU:HG3	1.99	0.44
1:A:281:TYR:OH	4:A:602:APR:O1D	2.31	0.44
2:C:815:LYS:HE3	2:C:815:LYS:HB3	1.86	0.44
1:B:243:THR:HG22	1:B:246:HIS:ND1	2.33	0.43
1:B:507:LEU:HD21	1:B:509:LEU:HD21	1.98	0.43
1:A:116:ILE:HG12	1:A:117:SER:N	2.33	0.43
1:A:393:LEU:HA	1:A:393:LEU:HD23	1.90	0.43
1:A:229:ASN:ND2	2:C:841:PRO:HD2	2.33	0.43
1:A:403:ARG:HH12	1:A:412:ASN:HB3	1.84	0.43
1:B:545:GLU:HB2	1:B:551:TYR:CE2	2.53	0.43
2:C:885:PRO:O	2:C:886:LEU:HD23	2.19	0.43
1:A:461:ILE:HG21	1:A:485:MET:HG3	1.99	0.43
1:A:542:LYS:HD3	1:A:543:SER:N	2.33	0.43
1:A:144:TYR:O	2:C:845:TYR:HB2	2.19	0.43
2:D:851:LEU:HA	2:D:851:LEU:HD12	1.77	0.43
1:A:143:LYS:HD3	1:A:236:LEU:CD1	2.48	0.43
1:A:313:ASN:H	1:A:313:ASN:ND2	2.17	0.43
1:A:507:LEU:HD21	1:A:509:LEU:HD21	2.01	0.43
1:B:136:LEU:O	1:B:140:MET:HG3	2.19	0.43
2:D:848:GLY:O	5:D:908:HOH:O	2.22	0.42
2:D:830:GLU:HG3	2:D:830:GLU:H	1.63	0.42
2:D:743:HIS:HA	2:D:744:PRO:HD3	1.91	0.42
1:A:401:LYS:HG3	1:A:402:LYS:N	2.33	0.42
1:A:412:ASN:O	1:A:412:ASN:ND2	2.52	0.42
1:B:531:LYS:HB3	1:B:531:LYS:HE2	1.87	0.42
1:A:223:ASP:HB3	2:C:881:LEU:HD21	2.01	0.42
1:A:527:THR:HG23	1:A:533:TRP:NE1	2.34	0.42
1:B:115:ILE:HD12	1:B:122:ASN:ND2	2.35	0.42
1:B:527:THR:HG23	1:B:533:TRP:NE1	2.34	0.42
1:B:496:ASN:HD22	1:B:498:ASP:H	1.65	0.42
1:A:219:ARG:HH12	2:C:880:ARG:HB3	1.85	0.42
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.88	0.42
1:A:166:TYR:HD1	1:A:169:LYS:HG3	1.85	0.42
1:A:165:TYR:HE1	1:A:175:VAL:HB	1.85	0.42
1:B:401:LYS:HG3	1:B:402:LYS:N	2.33	0.42
1:B:496:ASN:ND2	1:B:498:ASP:H	2.17	0.42
1:A:280:PHE:HZ	1:A:311:ILE:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:O	1:A:414:LYS:HG2	2.19	0.42
1:B:151:LEU:HD12	1:B:151:LEU:HA	1.81	0.42
1:A:116:ILE:HG13	1:A:122:ASN:HD22	1.85	0.42
1:A:490:VAL:HA	1:A:491:PRO:HD3	1.92	0.42
1:B:377:TRP:HD1	1:B:378:ASN:N	2.18	0.42
2:C:846:LEU:HD23	2:C:846:LEU:HA	1.91	0.41
1:B:143:LYS:HE3	1:B:143:LYS:HB3	1.94	0.41
1:B:335:LYS:HE3	1:B:526:TRP:CE2	2.55	0.41
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.92	0.41
1:A:327:SER:HA	1:A:330:LYS:HB3	2.02	0.41
1:B:243:THR:HG23	1:B:245:ASP:N	2.35	0.41
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.91	0.41
1:B:533:TRP:CE2	1:B:537:LYS:HB3	2.55	0.41
1:B:159:LEU:HG	1:B:159:LEU:H	1.75	0.41
1:B:255:ARG:HA	1:B:255:ARG:HD3	1.90	0.41
1:B:114:ILE:H	1:B:114:ILE:HG13	1.66	0.41
2:D:835:LEU:HA	2:D:835:LEU:HD12	1.88	0.41
1:A:335:LYS:HE3	1:A:526:TRP:CE2	2.56	0.41
1:B:161:SER:HB3	2:D:827:TYR:HE2	1.86	0.41
1:B:180:LEU:O	1:B:184:ILE:HG13	2.21	0.41
1:B:346:ILE:HD12	1:B:367:PHE:HE1	1.85	0.41
1:A:156:PRO:HG2	1:A:163:TYR:CE1	2.55	0.41
1:A:243:THR:HG23	1:A:245:ASP:H	1.86	0.41
1:A:454:HIS:HB3	1:A:458:ARG:NH1	2.35	0.41
1:A:533:TRP:CE2	1:A:537:LYS:HB3	2.56	0.41
1:B:317:PRO:HB3	1:B:347:ASP:HA	2.03	0.41
1:B:362:GLN:HB3	5:B:724:HOH:O	2.21	0.41
1:B:496:ASN:O	1:B:510:LEU:HA	2.20	0.41
1:A:382:GLU:HA	1:A:385:PHE:CD2	2.56	0.41
1:A:295:VAL:HG21	1:A:311:ILE:HG12	2.03	0.41
1:A:346:ILE:HD12	1:A:367:PHE:CE1	2.56	0.40
1:A:269:LEU:HD13	1:A:321:ILE:HD12	2.02	0.40
1:B:490:VAL:HA	1:B:491:PRO:HD3	1.94	0.40
1:A:224:LEU:HD23	2:C:836:ILE:HD12	2.04	0.40
1:A:393:LEU:HB2	1:A:412:ASN:HB2	2.02	0.40
2:C:835:LEU:HA	2:C:835:LEU:HD12	1.86	0.40
1:A:173:PHE:CE1	2:C:883:TYR:HD1	2.39	0.40
1:B:165:TYR:HE1	1:B:175:VAL:HB	1.86	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	417/492 (85%)	402 (96%)	15 (4%)	0	100	100
1	B	423/492 (86%)	412 (97%)	11 (3%)	0	100	100
2	C	93/159 (58%)	89 (96%)	4 (4%)	0	100	100
2	D	94/159 (59%)	91 (97%)	3 (3%)	0	100	100
All	All	1027/1302 (79%)	994 (97%)	33 (3%)	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	386/443 (87%)	363 (94%)	23 (6%)	19	49
1	B	386/443 (87%)	365 (95%)	21 (5%)	22	54
2	C	91/148 (62%)	85 (93%)	6 (7%)	16	44
2	D	92/148 (62%)	86 (94%)	6 (6%)	17	45
All	All	955/1182 (81%)	899 (94%)	56 (6%)	19	49

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

Mol	Chain	Res	Type
1	A	126	TYR
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	160	ASN
1	A	174	GLU
1	A	218	VAL
1	A	219	ARG
1	A	237	ARG
1	A	243	THR
1	A	245	ASP
1	A	282	SER
1	A	286	HIS
1	A	289	LEU
1	A	295	VAL
1	A	313	ASN
1	A	325	LEU
1	A	347	ASP
1	A	358	ASP
1	A	375	CYS
1	A	409	GLU
1	A	464	CYS
1	A	472	THR
1	A	483	VAL
1	A	508	SER
1	B	115	ILE
1	B	151	LEU
1	B	160	ASN
1	B	174	GLU
1	B	219	ARG
1	B	237	ARG
1	B	243	THR
1	B	245	ASP
1	B	290	ASP
1	B	295	VAL
1	B	313	ASN
1	B	325	LEU
1	B	358	ASP
1	B	375	CYS
1	B	377	TRP
1	B	379	LEU
1	B	457	ILE
1	B	464	CYS
1	B	472	THR
1	B	483	VAL
1	B	508	SER

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Mol	Chain	Res	Type
2	C	750	VAL
2	C	815	LYS
2	C	851	LEU
2	C	866	THR
2	C	877	LYS
2	C	880	ARG
2	D	805	ASP
2	D	806	TRP
2	D	815	LYS
2	D	816	ASN
2	D	851	LEU
2	D	881	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	185	ASN
1	A	229	ASN
1	A	303	HIS
1	A	313	ASN
1	A	378	ASN
1	A	390	ASN
1	A	412	ASN
1	B	185	ASN
1	B	229	ASN
1	B	313	ASN
1	B	378	ASN
1	B	390	ASN
1	B	412	ASN
2	C	743	HIS
2	C	873	GLN
2	C	882	GLN
2	D	873	GLN
2	D	882	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	602	-	34,39,39	2.18	10 (29%)	40,60,60	1.60	9 (22%)
4	APR	B	602	-	34,39,39	2.19	10 (29%)	40,60,60	1.57	8 (20%)

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	602	-	-	7/18/54/54	0/4/4/4
4	APR	B	602	-	-	8/18/54/54	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	APR	C1D-C2D	-6.72	1.44	1.52
4	A	602	APR	C1D-C2D	-6.67	1.44	1.52
4	B	602	APR	C2'-C1'	-4.89	1.46	1.53
4	A	602	APR	C2'-C1'	-4.80	1.46	1.53
4	A	602	APR	C3'-C2'	-4.31	1.41	1.53
4	B	602	APR	C3'-C2'	-4.21	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	APR	C3D-C2D	-3.62	1.43	1.53
4	A	602	APR	C3D-C2D	-3.60	1.43	1.53
4	B	602	APR	O4D-C1D	-3.37	1.39	1.43
4	B	602	APR	O4'-C4'	-3.14	1.38	1.45
4	A	602	APR	O4'-C4'	-3.06	1.38	1.45
4	A	602	APR	C3D-C4D	-3.04	1.45	1.53
4	A	602	APR	O4D-C1D	-3.03	1.39	1.43
4	A	602	APR	O4D-C4D	-2.94	1.38	1.45
4	B	602	APR	C3D-C4D	-2.80	1.45	1.53
4	B	602	APR	C3'-C4'	-2.66	1.46	1.53
4	B	602	APR	O4D-C4D	-2.60	1.39	1.45
4	A	602	APR	C3'-C4'	-2.45	1.46	1.53
4	B	602	APR	C6-N6	2.35	1.42	1.34
4	A	602	APR	C6-N6	2.33	1.42	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	APR	N3-C2-N1	-5.42	120.21	128.68
4	B	602	APR	N3-C2-N1	-5.29	120.41	128.68
4	A	602	APR	O5'-C5'-C4'	3.24	120.13	108.99
4	A	602	APR	PB-O3A-PA	-3.21	121.79	132.83
4	A	602	APR	C4-C5-N7	-3.15	106.12	109.40
4	B	602	APR	C4-C5-N7	-3.05	106.22	109.40
4	B	602	APR	O5'-C5'-C4'	3.00	119.32	108.99
4	B	602	APR	C1'-N9-C4	-2.80	121.73	126.64
4	A	602	APR	C1'-N9-C4	-2.76	121.79	126.64
4	B	602	APR	PB-O3A-PA	-2.67	123.67	132.83
4	B	602	APR	C1D-C2D-C3D	2.54	105.48	102.30
4	B	602	APR	O5D-C5D-C4D	2.46	117.45	108.99
4	A	602	APR	C1D-C2D-C3D	2.45	105.37	102.30
4	A	602	APR	C2'-C3'-C4'	2.12	106.75	102.64
4	A	602	APR	O5D-C5D-C4D	2.09	116.19	108.99
4	B	602	APR	O4'-C1'-C2'	-2.07	103.91	106.93
4	A	602	APR	C3'-C2'-C1'	2.04	104.06	100.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	APR	C3'-C4'-C5'-O5'
4	A	602	APR	C5'-O5'-PA-O3A

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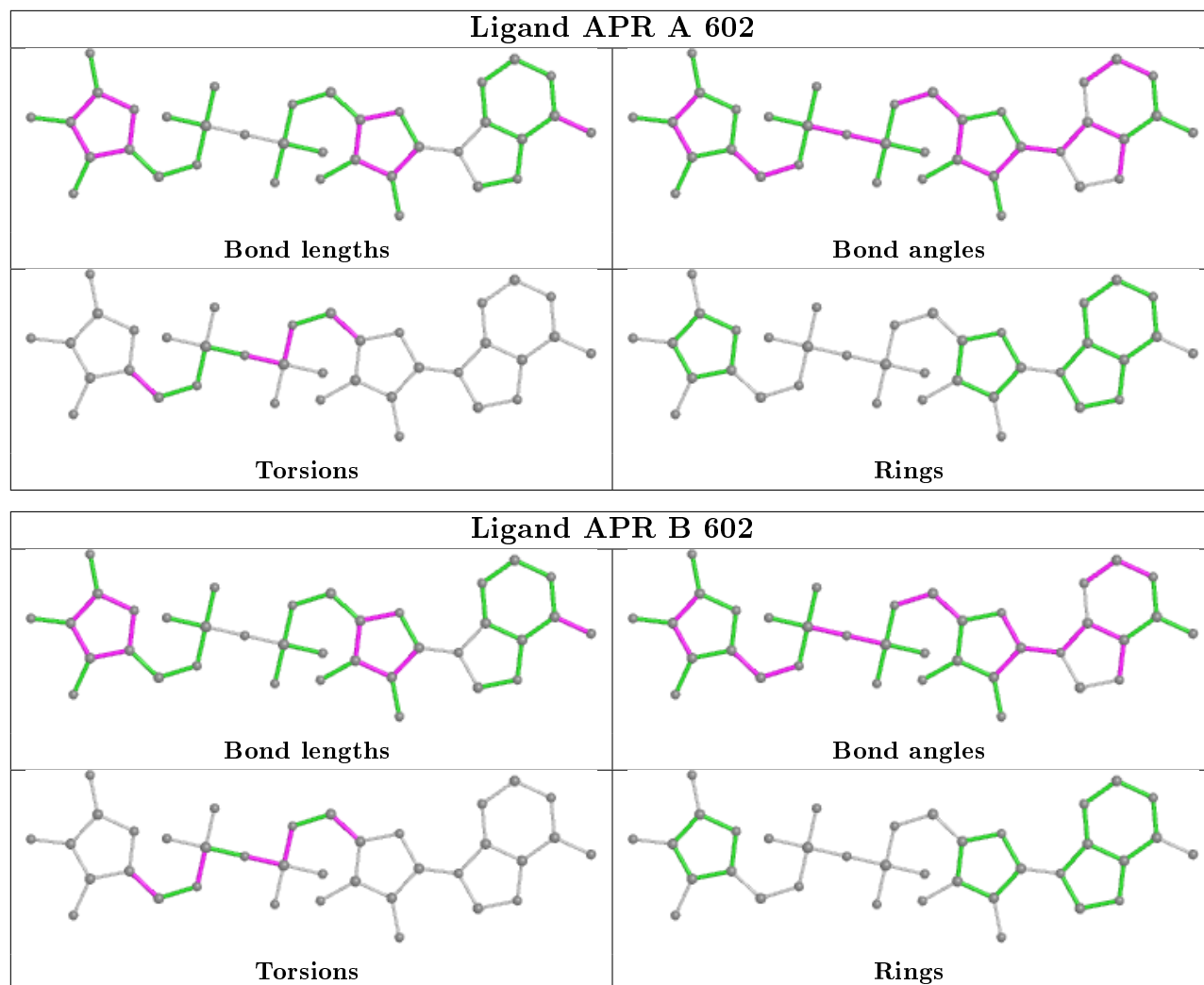
Mol	Chain	Res	Type	Atoms
4	A	602	APR	PB-O3A-PA-O5'
4	B	602	APR	C3'-C4'-C5'-O5'
4	B	602	APR	C5'-O5'-PA-O3A
4	B	602	APR	C5D-O5D-PB-O1B
4	A	602	APR	O4D-C4D-C5D-O5D
4	B	602	APR	O4D-C4D-C5D-O5D
4	A	602	APR	O4'-C4'-C5'-O5'
4	B	602	APR	O4'-C4'-C5'-O5'
4	B	602	APR	PB-O3A-PA-O5'
4	A	602	APR	C3D-C4D-C5D-O5D
4	B	602	APR	C5D-O5D-PB-O3A
4	A	602	APR	C5'-O5'-PA-O2A
4	B	602	APR	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	APR	1	0
4	B	602	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 [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, 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	425/492 (86%)	0.18	26 (6%) 21 17	38, 70, 127, 161	0
1	B	429/492 (87%)	0.26	36 (8%) 11 8	40, 69, 127, 157	0
2	C	97/159 (61%)	0.43	9 (9%) 8 6	52, 87, 136, 155	0
2	D	98/159 (61%)	0.51	11 (11%) 5 4	50, 89, 142, 160	0
All	All	1049/1302 (80%)	0.27	82 (7%) 13 10	38, 73, 130, 161	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	GLN	7.7
1	B	422	GLY	6.1
2	C	878	LYS	5.6
1	B	416	GLY	5.5
1	B	124	ILE	5.3
1	B	125	PHE	5.2
1	B	161	SER	5.0
1	A	125	PHE	4.7
2	D	806	TRP	4.4
1	A	124	ILE	4.4
1	A	412	ASN	4.3
1	A	413	ASN	4.0
1	B	411	TYR	4.0
1	B	419	ALA	3.8
2	C	808	LYS	3.6
1	B	112	GLY	3.5
1	B	420	SER	3.5
2	C	893	GLU	3.5
1	B	126	TYR	3.5
2	D	877	LYS	3.4
1	A	126	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	187	ILE	3.2
1	A	187	ILE	3.1
1	B	542	LYS	3.1
1	B	417	VAL	3.1
1	A	115	ILE	3.0
1	B	157	GLU	3.0
1	A	186	SER	2.9
1	B	158	ASP	2.9
2	C	826	THR	2.9
1	A	121	SER	2.8
2	C	751	TYR	2.7
1	B	414	LYS	2.7
1	A	128	PRO	2.7
1	B	145	TYR	2.7
1	B	184	ILE	2.7
1	B	155	LEU	2.7
1	B	178	GLN	2.6
1	A	411	TYR	2.6
1	A	290	ASP	2.6
2	D	875	VAL	2.6
1	B	534	ASN	2.6
1	B	544	GLN	2.6
2	D	822	ALA	2.6
1	B	121	SER	2.5
2	D	743	HIS	2.5
1	A	540	ASN	2.4
1	B	412	ASN	2.4
2	D	876	HIS	2.3
1	A	184	ILE	2.3
1	A	534	ASN	2.3
2	C	877	LYS	2.3
1	B	149	LYS	2.3
1	A	166	TYR	2.3
1	B	554	THR	2.3
2	D	893	GLU	2.3
2	D	829	LYS	2.2
1	B	174	GLU	2.2
1	B	319	GLU	2.2
1	A	398	TYR	2.2
2	C	742	THR	2.2
1	B	127	GLY	2.2
2	D	823	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLN	2.2
1	A	535	ASP	2.2
1	A	526	TRP	2.2
1	A	116	ILE	2.2
1	A	410	GLY	2.2
1	B	320	LYS	2.2
1	B	334	MET	2.1
1	B	383	ARG	2.1
2	D	805	ASP	2.1
1	B	164	ILE	2.1
1	A	100	MET	2.1
2	C	817	ILE	2.1
1	A	542	LYS	2.1
2	C	848	GLY	2.1
1	B	335	LYS	2.0
1	A	188	VAL	2.0
1	A	409	GLU	2.0
1	B	176	LYS	2.0
2	D	878	LYS	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 carbohydrates in this entry.

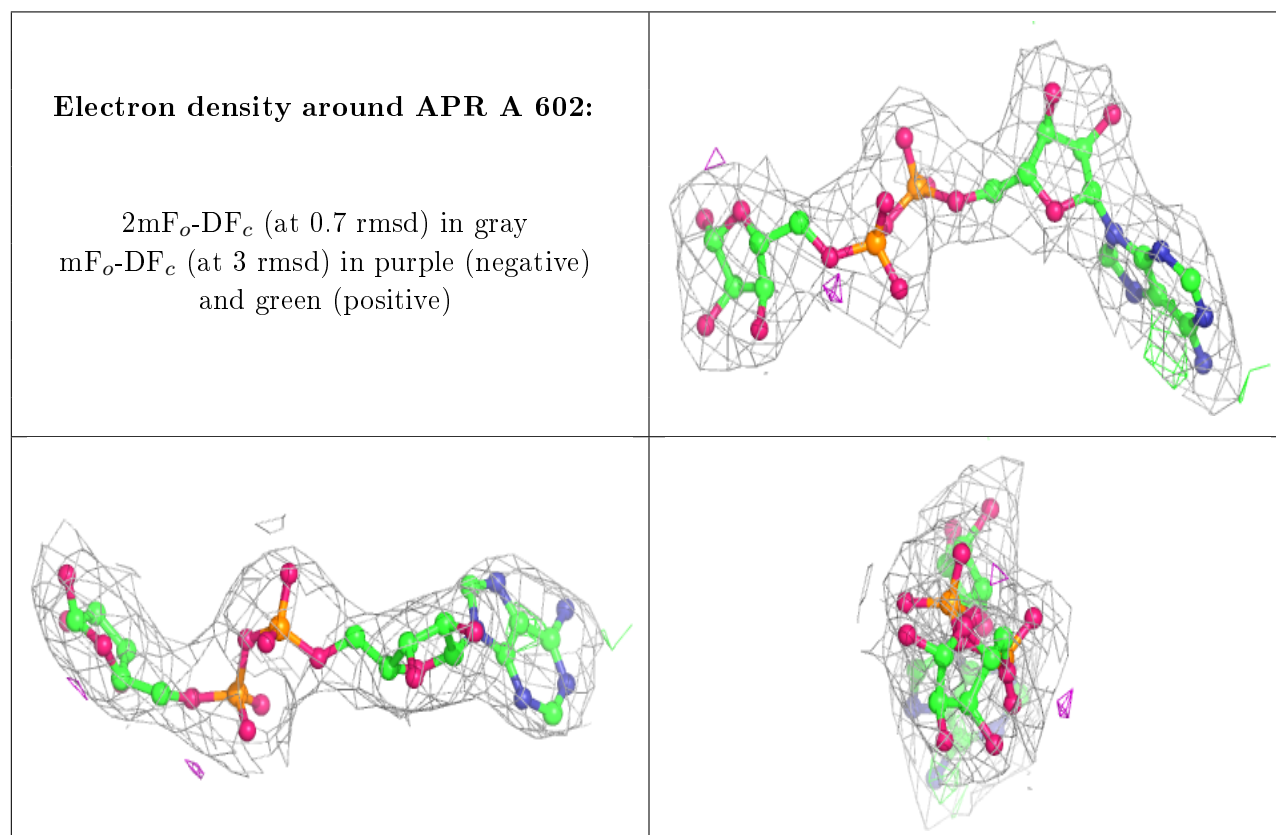
## 6.4 Ligands [i](#)

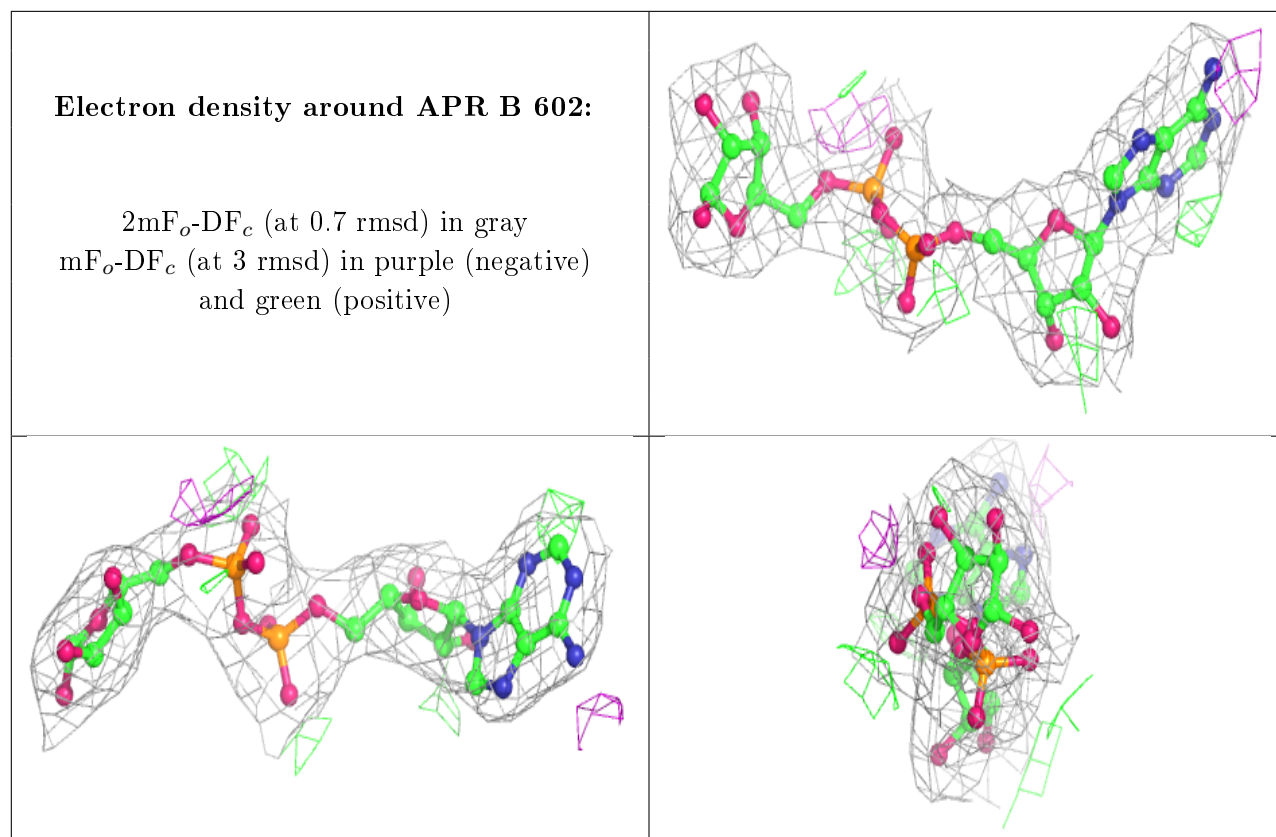
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	APR	A	602	36/36	0.97	0.18	43,62,70,75	0
4	APR	B	602	36/36	0.97	0.17	50,60,72,78	0
3	ZN	A	601	1/1	0.99	0.15	57,57,57,57	0
3	ZN	B	601	1/1	1.00	0.15	52,52,52,52	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.