



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:12 AM UTC

PDB ID : 4IAO / pdb_00004iao
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

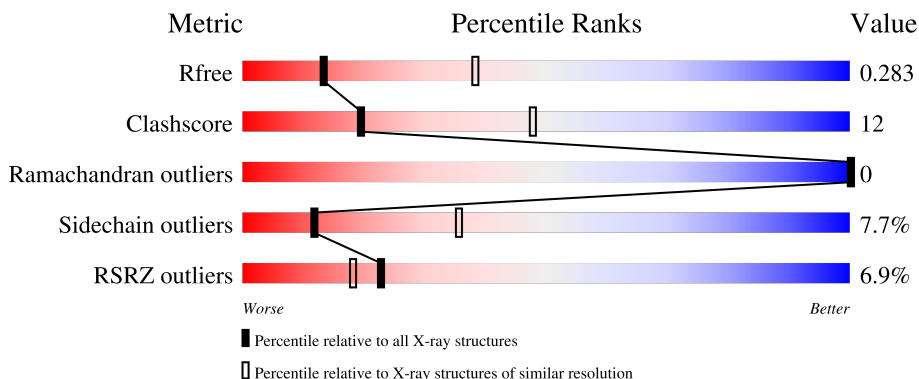
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	492	7% 61% 23% • 14%
1	B	492	7% 62% 21% • 13%
2	C	159	3% 41% 19% • 39%
2	D	159	% 40% 21% • 38%

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			

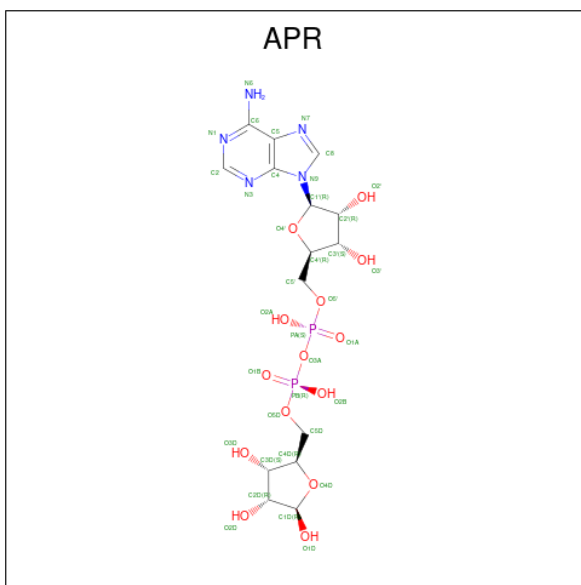
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).



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

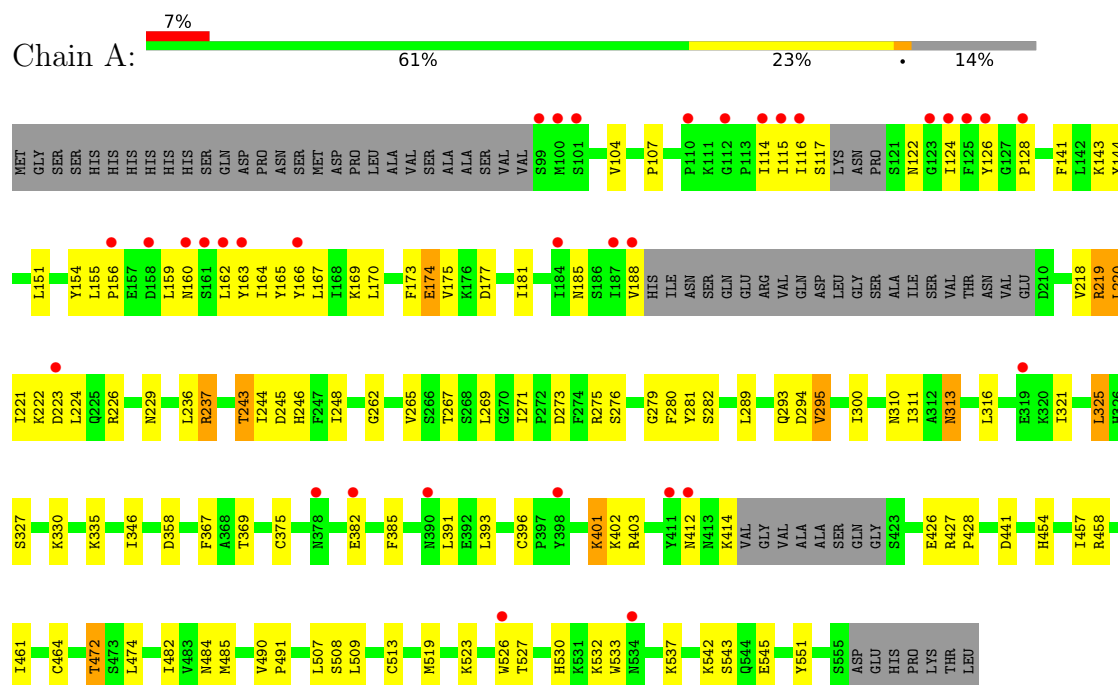
- Molecule 5 is water.

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

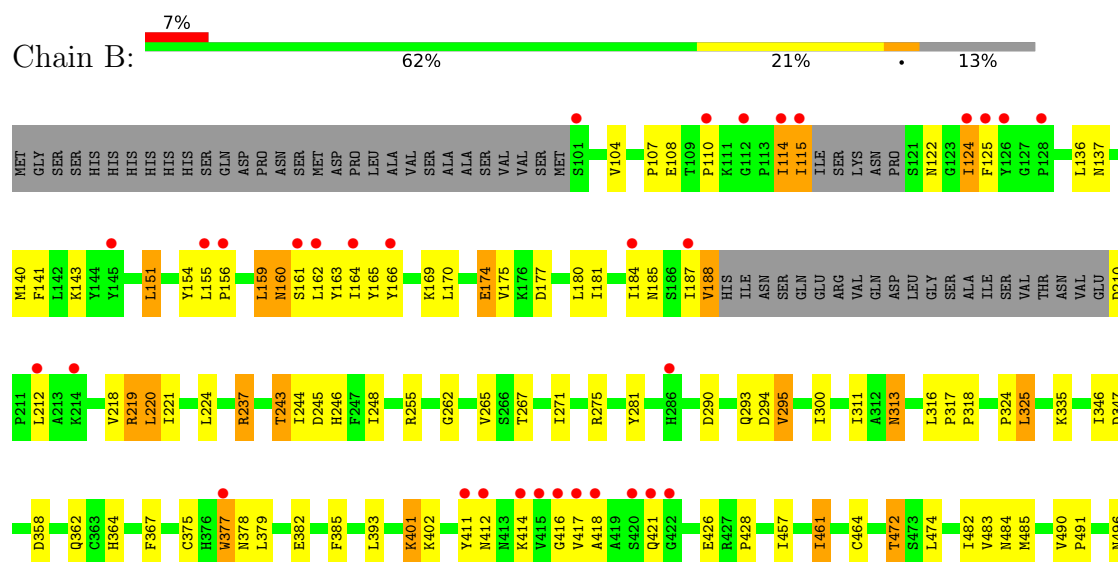
3 Residue-property plots

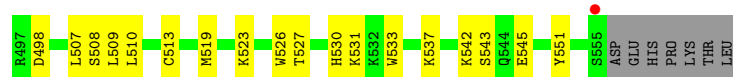
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NAD-dependent histone deacetylase SIR2

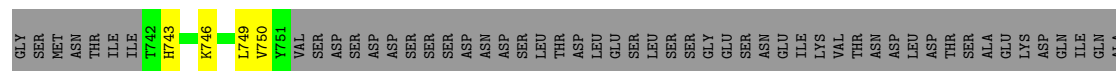


• Molecule 1: NAD-dependent histone deacetylase SIR2

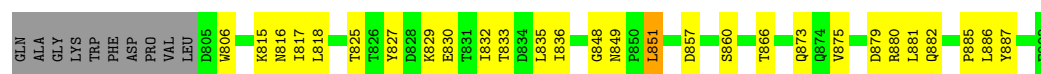
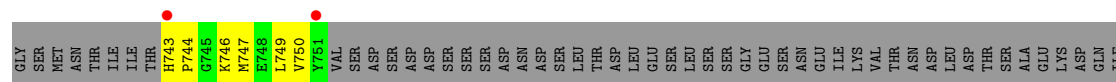
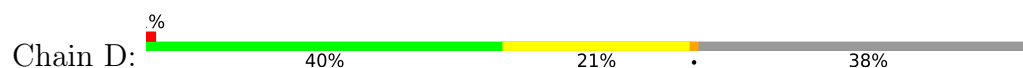




• Molecule 2: Regulatory protein SIR4



• 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, α , β , γ	166.41Å 178.75Å 121.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.43 – 2.90 36.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.7 (36.43-2.90) 89.1 (36.43-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.227 , 0.269 (Not available) , 0.283	Depositor DCC
R_{free} test set	1815 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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

5.1 Standard geometry

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	0.39	0/3501	0.83	8/4734 (0.2%)
1	B	0.40	0/3521	0.84	2/4764 (0.0%)
2	C	0.35	0/816	0.86	4/1103 (0.4%)
2	D	0.36	0/833	0.85	2/1127 (0.2%)
All	All	0.39	0/8671	0.84	16/11728 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	821	ILE	N-CA-C	8.06	118.64	110.82
1	A	159	LEU	N-CA-C	6.87	117.10	108.45
1	B	124	ILE	N-CA-C	6.76	117.45	110.36
2	D	849	ASN	CA-C-N	5.80	125.42	119.56
2	D	849	ASN	C-N-CA	5.80	125.42	119.56
1	A	124	ILE	N-CA-C	5.40	116.13	110.62
1	A	279	GLY	N-CA-C	5.40	121.55	112.85
2	C	849	ASN	CA-C-N	5.39	125.01	119.56
2	C	849	ASN	C-N-CA	5.39	125.01	119.56
1	A	275	ARG	N-CA-C	5.23	119.76	113.17
1	A	396	CYS	CA-C-N	5.20	124.82	119.05
1	A	396	CYS	C-N-CA	5.20	124.82	119.05
2	C	858	ILE	N-CA-C	-5.14	104.55	111.44
1	B	461	ILE	N-CA-C	5.05	115.67	110.36
1	A	427	ARG	CA-C-N	5.03	125.56	120.38
1	A	427	ARG	C-N-CA	5.03	125.56	120.38

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	3419	0	3462	84	0
1	B	3438	0	3480	88	0
2	C	799	0	783	28	0
2	D	814	0	790	28	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
5	B	44	0	0	1	0
5	C	7	0	0	1	0
5	D	12	0	0	2	0
All	All	8654	0	8557	199	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 12.

All (199) 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:HD3	2:C:877:LYS:H	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:HD2	2:C:880:ARG:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:HG2	1:B:416:GLY:H	1.63	0.63
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
2:D:746:LYS:NZ	5:D:903:HOH:O	2.36	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
1:A:294:ASP:HB3	1:A:300:ILE:HD12	1.88	0.56
1:A:313:ASN:HD22	1:A:313:ASN:H	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
2:C:746:LYS:NZ	5:C:903:HOH:O	2.29	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:A:519:MET:HE3	1:A:523:LYS:HE3	1.92	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:B:377:TRP:CD1	1:B:377:TRP:C	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:ILE:HD13	1:B:519:MET:HE1	1.92	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:164:ILE:HD11	2:C:832:ILE:HD13	1.92	0.50
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
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
1:B:174:GLU:HG3	2:D:882:GLN:HB2	1.93	0.50
2:C:743:HIS:HB2	2:C:746:LYS:HG3	1.94	0.50
2:D:832:ILE:O	2:D:836:ILE:HG12	2.12	0.49
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:161:SER:OG	1:B:212:LEU:HB2	2.13	0.48
1:B:187:ILE:HG23	1:B:188:VAL:N	2.28	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:482:ILE:HA	1:B:485:MET:HE3	1.95	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:B:519:MET:HE3	1:B:523:LYS:HE3	1.96	0.47
1:A:273:ASP:OD2	1:A:276:SER:OG	2.24	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HH11	2:C:880:ARG:HE	1.64	0.46
1:A:244:ILE:HD13	1:A:519:MET:HE1	1.98	0.46
1:A:310:ASN:OD1	1:A:414:LYS:HB3	2.16	0.46
1:A:482:ILE:HA	1:A:485:MET:HE3	1.97	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:293:GLN:OE1	2:D:749:LEU:HD22	2.17	0.45
1:B:382:GLU:HA	1:B:385:PHE:CD2	2.52	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
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:HD23	1:A:393:LEU:HA	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:144:TYR:O	2:C:845:TYR:HB2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:D:830:GLU:HG3	1.63	0.42
1:B:364:HIS:CE1	2:D:747:MET:HE3	2.54	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:HE2	1:B:531:LYS:HB3	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:A:219:ARG:HH12	2:C:880:ARG:HB3	1.85	0.42
1:B:496:ASN:HD22	1:B:498:ASP:H	1.65	0.42
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.88	0.42
1:A:165:TYR:HE1	1:A:175:VAL:HB	1.85	0.42
1:A:166:TYR:HD1	1:A:169:LYS:HG3	1.85	0.42
1:B:311:ILE:C	1:B:311:ILE:HD12	2.45	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
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:HB3	1:B:143:LYS:HE3	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:HD23	1:B:316:LEU:HA	1.91	0.41
1:B:533:TRP:CE2	1:B:537:LYS:HB3	2.55	0.41
1:B:159:LEU:H	1:B:159:LEU:HG	1.75	0.41
1:B:255:ARG:HD3	1:B:255:ARG:HA	1.90	0.41
1:B:114:ILE:HG13	1:B:114:ILE:H	1.66	0.41
2:D:835:LEU:HD12	2:D:835:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:GLU:HA	1:A:385:PHE:CD2	2.56	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: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:173:PHE:CE1	2:C:883:TYR:HD1	2.39	0.40
1:A:224:LEU:HD23	2:C:836:ILE:HD12	2.04	0.40
1:A:369:THR:OG1	1:A:441:ASP:OD2	2.24	0.40
1:A:393:LEU:HB2	1:A:412:ASN:HB2	2.02	0.40
2:C:835:LEU:HD12	2:C:835:LEU:HA	1.86	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

5.3.1 Protein backbone

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 ⓘ

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	344/443 (78%)	320 (93%)	24 (7%)	14	40
1	B	386/443 (87%)	357 (92%)	29 (8%)	12	37
2	C	91/148 (62%)	82 (90%)	9 (10%)	7	24
2	D	92/148 (62%)	84 (91%)	8 (9%)	9	30
All	All	913/1182 (77%)	843 (92%)	70 (8%)	12	35

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	126	TYR
1	A	151	LEU
1	A	160	ASN
1	A	174	GLU
1	A	218	VAL
1	A	219	ARG
1	A	220	LEU
1	A	237	ARG
1	A	243	THR
1	A	265	VAL
1	A	282	SER
1	A	289	LEU
1	A	295	VAL
1	A	313	ASN
1	A	325	LEU
1	A	358	ASP
1	A	375	CYS
1	A	401	LYS
1	A	457	ILE
1	A	464	CYS
1	A	472	THR

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Mol	Chain	Res	Type
1	A	474	LEU
1	A	508	SER
1	B	104	VAL
1	B	114	ILE
1	B	115	ILE
1	B	151	LEU
1	B	159	LEU
1	B	160	ASN
1	B	174	GLU
1	B	188	VAL
1	B	218	VAL
1	B	219	ARG
1	B	220	LEU
1	B	237	ARG
1	B	243	THR
1	B	265	VAL
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	401	LYS
1	B	457	ILE
1	B	464	CYS
1	B	472	THR
1	B	474	LEU
1	B	483	VAL
1	B	508	SER
2	C	750	VAL
2	C	816	ASN
2	C	818	LEU
2	C	825	THR
2	C	851	LEU
2	C	866	THR
2	C	875	VAL
2	C	877	LYS
2	C	880	ARG
2	D	750	VAL
2	D	806	TRP

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Mol	Chain	Res	Type
2	D	816	ASN
2	D	818	LEU
2	D	851	LEU
2	D	866	THR
2	D	875	VAL
2	D	881	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	229	ASN
1	A	303	HIS
1	A	313	ASN
1	A	364	HIS
1	A	376	HIS
1	A	378	ASN
1	A	390	ASN
1	A	412	ASN
1	A	433	ASN
1	A	489	HIS
1	A	496	ASN
1	B	185	ASN
1	B	229	ASN
1	B	313	ASN
1	B	341	ASN
1	B	376	HIS
1	B	390	ASN
1	B	412	ASN
1	B	433	ASN
1	B	489	HIS
1	B	496	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	39,39,39	2.19	13 (33%)	56,60,60	1.88	14 (25%)
4	APR	B	602	-	39,39,39	2.15	12 (30%)	56,60,60	1.90	13 (23%)

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	-	-	7/22/54/54	0/4/4/4
4	APR	B	602	-	-	8/22/54/54	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	APR	C1D-C2D	-6.83	1.44	1.52
4	A	602	APR	C1D-C2D	-6.79	1.44	1.52
4	A	602	APR	PA-O3A	-5.10	1.54	1.59
4	B	602	APR	PA-O3A	-4.49	1.54	1.59
4	A	602	APR	C3'-C2'	-4.36	1.41	1.53
4	B	602	APR	C3'-C2'	-4.26	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	APR	C3D-C2D	-3.66	1.43	1.53
4	A	602	APR	C3D-C2D	-3.65	1.43	1.53
4	B	602	APR	C6-N6	3.29	1.42	1.34
4	A	602	APR	C6-N6	3.26	1.42	1.34
4	B	602	APR	O4D-C1D	-3.23	1.39	1.43
4	B	602	APR	O4'-C4'	-3.15	1.38	1.45
4	A	602	APR	O4'-C4'	-3.08	1.38	1.45
4	A	602	APR	C3D-C4D	-3.06	1.45	1.53
4	A	602	APR	O4D-C4D	-2.95	1.38	1.45
4	A	602	APR	O4D-C1D	-2.90	1.39	1.43
4	B	602	APR	C3D-C4D	-2.82	1.45	1.53
4	B	602	APR	C3'-C4'	-2.68	1.46	1.53
4	B	602	APR	O4D-C4D	-2.61	1.39	1.45
4	A	602	APR	C3'-C4'	-2.46	1.46	1.53
4	B	602	APR	C2'-C1'	-2.27	1.46	1.53
4	A	602	APR	C2'-C1'	-2.23	1.46	1.53
4	A	602	APR	C8-N9	-2.08	1.34	1.37
4	A	602	APR	C5-N7	-2.04	1.35	1.39
4	B	602	APR	C8-N9	-2.03	1.34	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	APR	N3-C2-N1	-5.53	120.21	128.58
4	B	602	APR	C5-C4-N3	-5.41	119.26	126.72
4	B	602	APR	N3-C2-N1	-5.40	120.41	128.58
4	A	602	APR	C5-C4-N3	-5.39	119.29	126.72
4	A	602	APR	C2-N3-C4	3.97	121.52	111.83
4	B	602	APR	C2-N3-C4	3.93	121.44	111.83
4	A	602	APR	C4-C5-N7	-3.90	106.12	110.58
4	B	602	APR	C4-C5-N7	-3.82	106.22	110.58
4	B	602	APR	N3-C4-N9	3.68	133.43	127.17
4	B	602	APR	N9-C8-N7	-3.67	108.72	113.94
4	A	602	APR	N9-C8-N7	-3.63	108.78	113.94
4	A	602	APR	C5-N7-C8	3.46	108.89	103.45
4	B	602	APR	C5-N7-C8	3.46	108.89	103.45
4	A	602	APR	N3-C4-N9	3.43	133.01	127.17
4	A	602	APR	O5'-C5'-C4'	3.27	120.13	108.99
4	B	602	APR	O5'-C5'-C4'	3.03	119.32	108.99
4	B	602	APR	C4-N9-C8	2.96	108.84	105.74
4	B	602	APR	C2'-C1'-N9	2.72	120.07	113.30
4	A	602	APR	C4-N9-C8	2.62	108.49	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	APR	C1D-C2D-C3D	2.60	105.48	102.29
4	A	602	APR	C1D-C2D-C3D	2.50	105.37	102.29
4	B	602	APR	O5D-C5D-C4D	2.48	117.45	108.99
4	A	602	APR	C2'-C3'-C4'	2.15	106.75	102.61
4	A	602	APR	O5D-C5D-C4D	2.11	116.19	108.99
4	B	602	APR	C4-N9-C1'	-2.10	121.73	126.63
4	A	602	APR	C4-N9-C1'	-2.07	121.79	126.63
4	A	602	APR	C2'-C1'-N9	2.02	118.32	113.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

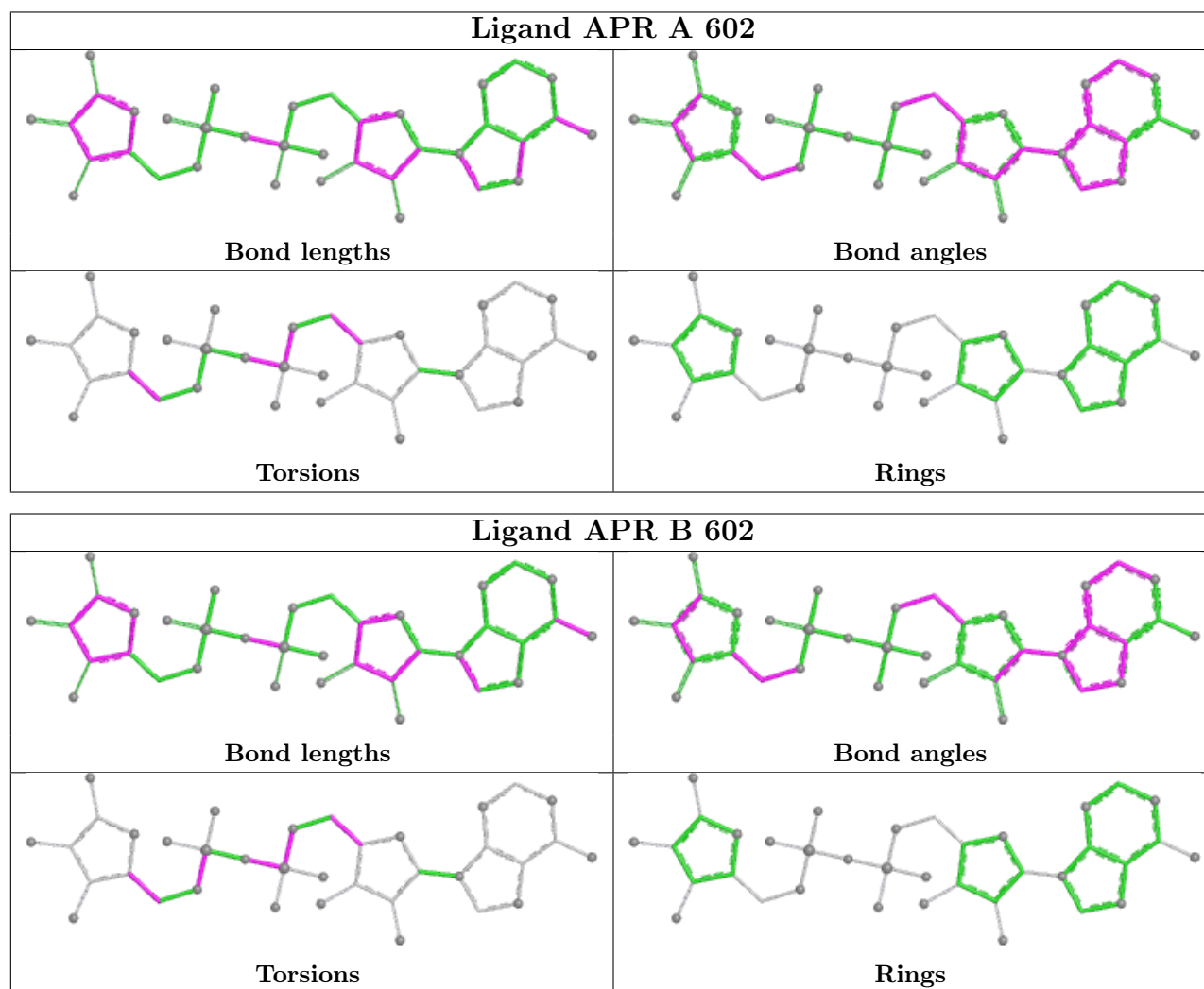
There are no ring outliers.

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, 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	425/492 (86%)	0.49	33 (7%) 19 16	38, 70, 127, 161	0
1	B	429/492 (87%)	0.45	33 (7%) 19 16	40, 69, 127, 157	0
2	C	97/159 (61%)	0.44	4 (4%) 41 33	52, 87, 136, 155	0
2	D	98/159 (61%)	0.62	2 (2%) 65 56	50, 89, 142, 160	0
All	All	1049/1302 (80%)	0.48	72 (6%) 23 18	38, 73, 130, 161	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	VAL	5.9
1	B	161	SER	5.3
1	B	162	LEU	4.9
1	A	115	ILE	4.4
1	B	411	TYR	4.3
1	B	115	ILE	4.0
1	A	166	TYR	4.0
1	A	187	ILE	3.9
1	B	422	GLY	3.5
1	B	125	PHE	3.5
1	B	420	SER	3.5
1	A	128	PRO	3.5
1	B	421	GLN	3.5
1	A	184	ILE	3.4
1	B	155	LEU	3.4
1	A	116	ILE	3.3
1	A	188	VAL	3.2
2	C	825	THR	3.2
1	B	145	TYR	3.1
1	B	128	PRO	3.0
1	B	124	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	GLY	3.0
1	B	416	GLY	3.0
1	A	161	SER	2.9
1	B	187	ILE	2.9
1	A	114	ILE	2.8
1	B	112	GLY	2.8
2	D	743	HIS	2.8
1	A	124	ILE	2.7
1	A	112	GLY	2.7
1	B	184	ILE	2.6
1	A	160	ASN	2.6
1	B	415	VAL	2.6
1	A	382	GLU	2.6
1	B	377	TRP	2.5
1	A	162	LEU	2.5
1	A	412	ASN	2.5
1	A	534	ASN	2.5
1	B	212	LEU	2.5
1	A	158	ASP	2.4
1	A	223	ASP	2.4
1	A	126	TYR	2.4
1	B	412	ASN	2.4
1	A	110	PRO	2.4
1	B	214	LYS	2.4
1	B	164	ILE	2.4
1	A	319	GLU	2.3
1	B	156	PRO	2.3
1	A	378	ASN	2.3
1	A	390	ASN	2.3
2	C	878	LYS	2.3
1	A	411	TYR	2.3
1	A	526	TRP	2.3
1	A	398	TYR	2.3
1	B	414	LYS	2.2
1	B	110	PRO	2.2
1	A	156	PRO	2.2
1	A	101	SER	2.2
1	B	101	SER	2.2
1	B	166	TYR	2.2
1	B	555	SER	2.2
2	C	826	THR	2.1
1	A	99	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	114	ILE	2.1
1	B	418	ALA	2.1
2	D	751	TYR	2.1
2	C	817	ILE	2.0
1	B	286	HIS	2.0
1	A	125	PHE	2.0
1	A	100	MET	2.0
1	A	163	TYR	2.0
1	B	126	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

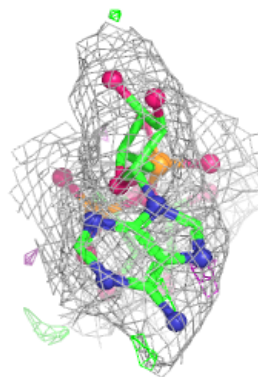
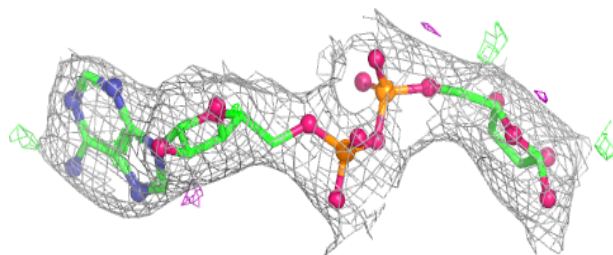
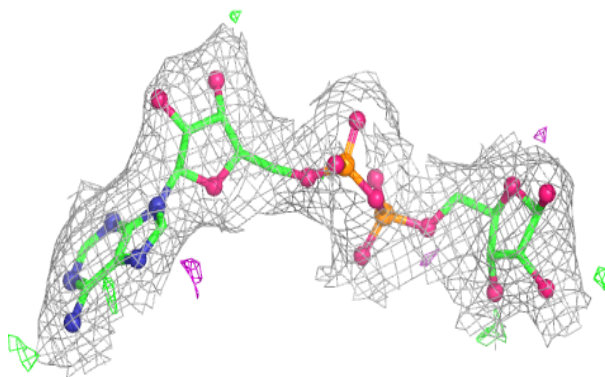
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	APR	A	602	36/36	0.95	0.09	43,62,70,75	0
4	APR	B	602	36/36	0.95	0.08	50,60,72,78	0
3	ZN	A	601	1/1	0.99	0.08	57,57,57,57	0
3	ZN	B	601	1/1	0.99	0.09	52,52,52,52	0

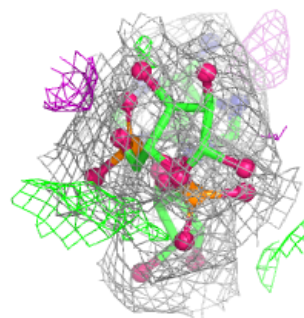
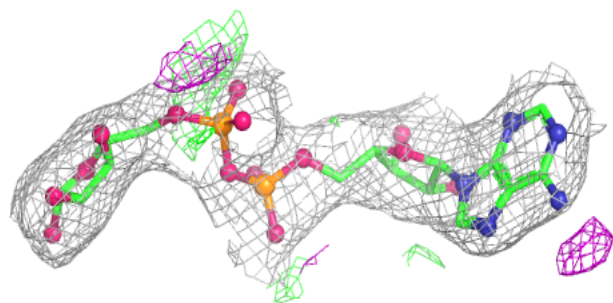
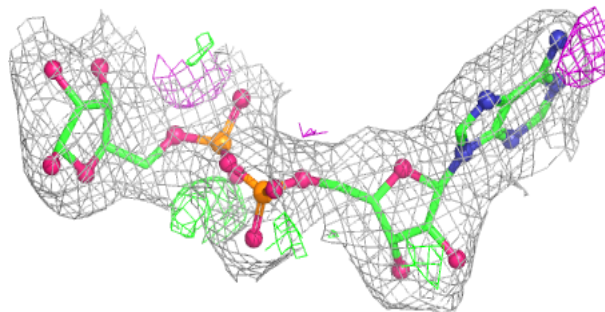
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APR A 602:

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

**Electron density around APR B 602:**

$2mF_o-DF_c$ (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.