



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:09 PM UTC

PDB ID : 4BV2 / pdb_00004bv2
Title : CRYSTAL STRUCTURE OF SIR2 IN COMPLEX WITH THE INHIBITOR
EX-527, 2'-O-ACETYL-ADP-RIBOSE AND DEACETYLATED P53-
PEPTIDE
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Deposited on : 2013-06-24
Resolution : 3.30 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

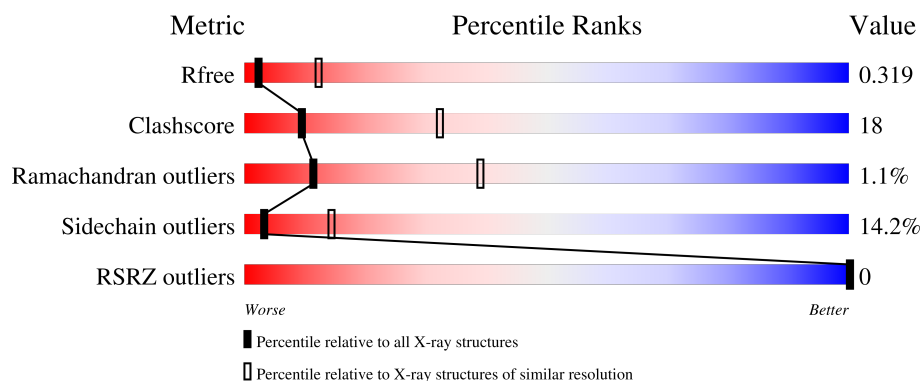
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	246	
1	B	246	
2	E	13	
2	H	13	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3853 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 PROTEIN DEACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1846	1184	305	348	9			
1	B	230	Total	C	N	O	S	0	0	0
			1805	1159	299	338	9			

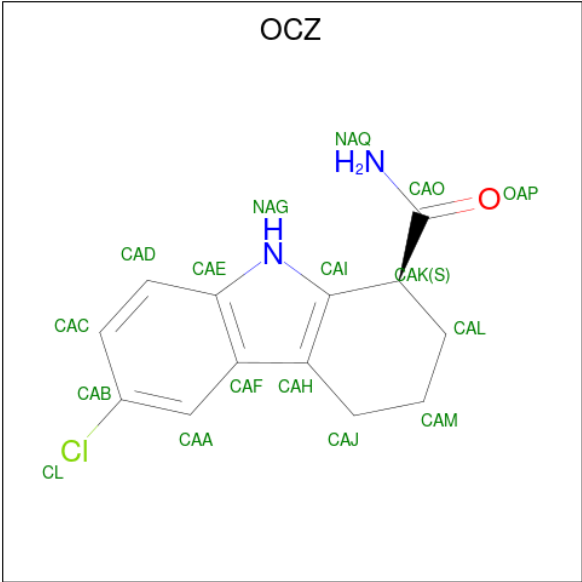
- Molecule 2 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	S	0	0	0
			44	29	9	5	1			
2	H	5	Total	C	N	O	S	0	0	0
			44	29	9	5	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

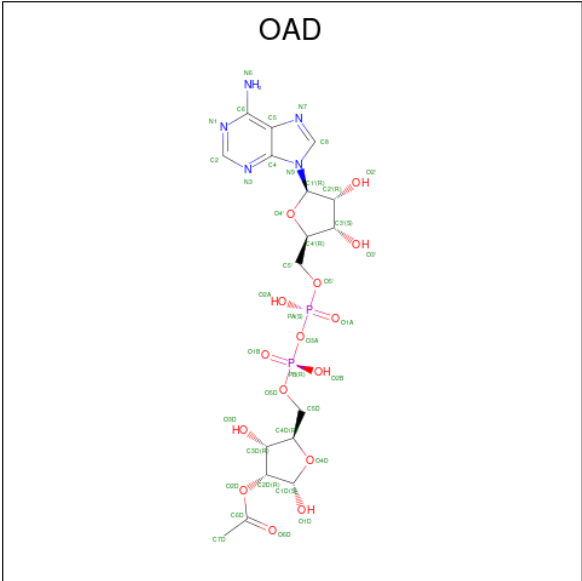
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (1S)-6-chloro-2,3,4,9-tetrahydro-1H-carbazole-1- carboxamide (CCD ID: OCZ) (formula: C₁₃H₁₃ClN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
4	B	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		

- Molecule 5 is 2'-O-ACETYL ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: OAD) (formula: C₁₇H₂₅N₅O₁₅P₂).



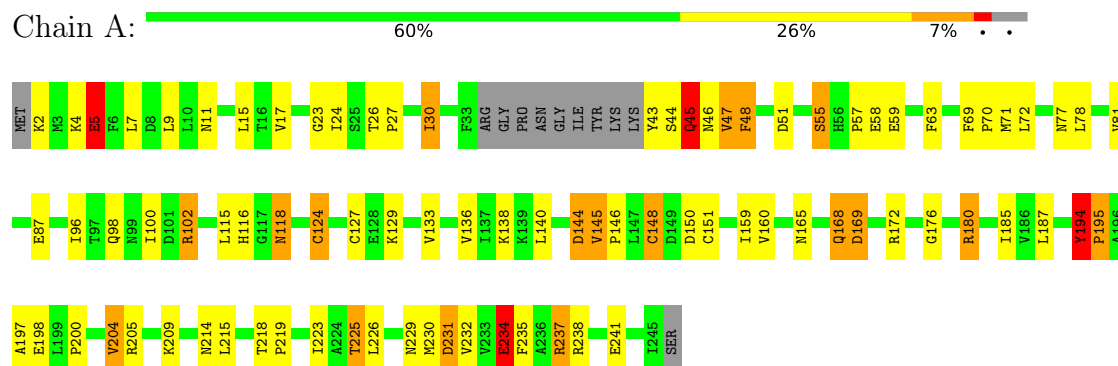
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			39	17	5	15	2		

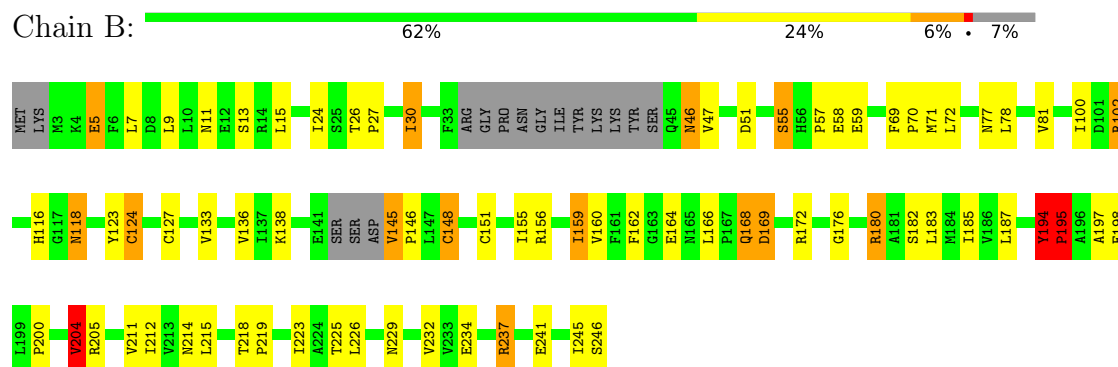
3 Residue-property plots

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 PROTEIN DEACETYLASE



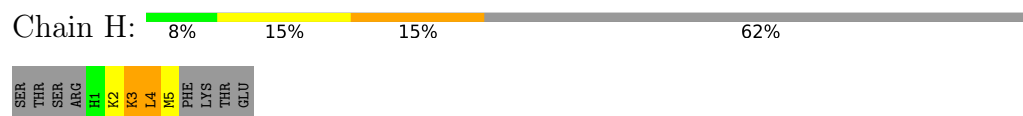
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE



• Molecule 2: CELLULAR TUMOR ANTIGEN P53



• Molecule 2: CELLULAR TUMOR ANTIGEN P53



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	45.95Å 45.95Å 241.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.47 – 3.30 60.47 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.47-3.30) 99.7 (60.47-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.245 , 0.318 0.244 , 0.319	Depositor DCC
R_{free} test set	374 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	99.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 123.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.297 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3853	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: OCZ, OAD, 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	0.72	1/1879 (0.1%)	1.15	6/2540 (0.2%)
1	B	0.69	0/1836	1.63	6/2481 (0.2%)
2	E	0.80	0/44	1.12	0/55
2	H	0.68	0/44	0.83	0/55
All	All	0.71	1/3803 (0.0%)	1.40	12/5131 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ASP	C-O	-5.22	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	TYR	CA-C-N	46.37	177.80	119.84
1	B	194	TYR	C-N-CA	46.37	177.80	119.84
1	A	194	TYR	CA-C-N	20.75	145.77	119.84
1	A	194	TYR	C-N-CA	20.75	145.77	119.84
1	B	194	TYR	C-N-CD	-12.04	75.62	125.00
1	A	194	TYR	C-N-CD	-9.42	86.36	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	GLN	N-CA-C	9.16	130.30	110.80
1	B	195	PRO	N-CA-C	-6.22	99.66	112.47
1	A	234	GLU	CA-CB-CG	5.62	125.35	114.10
1	A	5	GLU	CA-CB-CG	5.59	125.27	114.10
1	B	195	PRO	CA-N-CD	-5.26	104.64	112.00
1	B	204	VAL	CB-CA-C	5.08	119.00	112.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Peptide
1	B	194	TYR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1846	0	1862	76	2
1	B	1805	0	1825	57	0
2	E	44	0	55	5	0
2	H	44	0	55	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	17	0	13	1	0
4	B	17	0	13	2	0
5	A	39	0	23	11	0
5	B	39	0	23	5	0
All	All	3853	0	3869	138	2

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 18.

All (138) 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:168:GLN:NE2	1:A:168:GLN:H	1.49	1.09
1:A:180:ARG:HG3	1:A:180:ARG:HH11	1.14	1.07
1:B:168:GLN:H	1:B:168:GLN:NE2	1.51	1.07
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.23	1.03
1:B:102:ARG:HH11	1:B:102:ARG:HG3	1.30	0.95
1:B:214:ASN:HD22	1:B:215:LEU:N	1.63	0.95
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.30	0.95
1:A:194:TYR:HB2	2:E:4:LEU:HD12	1.46	0.93
1:A:168:GLN:H	1:A:168:GLN:HE21	1.03	0.93
1:B:168:GLN:HE21	1:B:168:GLN:N	1.67	0.91
1:A:214:ASN:HD22	1:A:215:LEU:N	1.69	0.90
1:B:168:GLN:H	1:B:168:GLN:HE21	0.91	0.86
1:A:2:LYS:N	1:A:238:ARG:HH21	1.77	0.83
5:A:1248:OAD:O4D	5:A:1248:OAD:O1B	1.98	0.82
1:A:168:GLN:HE21	1:A:168:GLN:N	1.78	0.81
1:B:194:TYR:CD1	1:B:197:ALA:HB3	2.16	0.80
1:A:180:ARG:HG3	1:A:180:ARG:NH1	1.92	0.80
1:B:148:CYS:SG	1:B:151:CYS:N	2.56	0.79
1:A:214:ASN:HD21	5:A:1248:OAD:H'1	1.49	0.78
1:A:98:GLN:HB3	5:A:1248:OAD:HR'4	1.66	0.78
1:A:165:ASN:OD1	2:E:2:LYS:HB3	1.85	0.76
1:A:2:LYS:N	1:A:238:ARG:NH2	2.33	0.76
1:A:214:ASN:ND2	5:A:1248:OAD:H'1	2.00	0.76
1:A:148:CYS:SG	1:A:151:CYS:N	2.59	0.76
1:A:194:TYR:CD1	1:A:197:ALA:HB3	2.21	0.75
1:A:24:ILE:HA	1:A:232:VAL:HG11	1.70	0.73
1:A:230:MET:HE3	1:A:234:GLU:HG3	1.69	0.73
1:B:102:ARG:HH11	1:B:102:ARG:CG	2.01	0.73
1:A:194:TYR:CE1	1:A:197:ALA:HB3	2.24	0.72
1:B:214:ASN:ND2	5:B:1248:OAD:O2'	2.20	0.72
1:B:237:ARG:O	1:B:241:GLU:HG2	1.90	0.71
1:A:237:ARG:O	1:A:241:GLU:HG2	1.89	0.71
1:B:5:GLU:HB2	1:B:226:LEU:HD11	1.71	0.71
1:B:194:TYR:CE1	1:B:197:ALA:HB3	2.24	0.71
1:B:180:ARG:HG3	1:B:180:ARG:NH1	2.01	0.69
1:B:51:ASP:O	1:B:55:SER:OG	2.12	0.68
1:B:24:ILE:HA	1:B:232:VAL:HG11	1.76	0.67
1:B:102:ARG:HG3	1:B:102:ARG:NH1	2.05	0.66
1:A:2:LYS:HD3	1:A:4:LYS:HD2	1.79	0.65
1:A:116:HIS:ND1	5:A:1248:OAD:O3D	2.30	0.64
1:A:194:TYR:CB	2:E:4:LEU:HD12	2.26	0.64
1:A:23:GLY:HA2	5:A:1248:OAD:C8	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:C	1:B:118:ASN:HD22	2.05	0.63
1:B:69:PHE:N	1:B:70:PRO:HD2	2.15	0.62
1:A:102:ARG:HH11	1:A:102:ARG:CG	2.08	0.62
1:A:231:ASP:HA	5:A:1248:OAD:N1	2.16	0.60
1:B:214:ASN:HD22	1:B:214:ASN:C	2.08	0.60
1:A:44:SER:HB2	1:A:47:VAL:HG21	1.84	0.60
1:A:57:PRO:HB2	1:A:145:VAL:HG11	1.82	0.60
1:B:185:ILE:HG22	1:B:187:LEU:CD1	2.32	0.59
4:B:1247:OCZ:CAC	5:B:1248:OAD:O6D	2.51	0.59
1:A:136:VAL:HG13	1:A:146:PRO:HG3	1.85	0.59
1:B:136:VAL:HG13	1:B:146:PRO:HG3	1.83	0.58
1:A:51:ASP:O	1:A:55:SER:OG	2.22	0.58
1:B:159:ILE:HG21	4:B:1247:OCZ:CL	2.41	0.57
5:B:1248:OAD:C6D	2:H:3:LYS:NZ	2.68	0.57
1:A:200:PRO:O	1:A:204:VAL:HG23	2.05	0.57
1:B:200:PRO:O	1:B:204:VAL:HG23	2.05	0.57
1:A:214:ASN:HD22	1:A:214:ASN:C	2.12	0.56
1:B:214:ASN:HD22	1:B:215:LEU:H	1.51	0.56
1:A:69:PHE:N	1:A:70:PRO:HD2	2.20	0.56
1:A:5:GLU:HG2	1:A:226:LEU:HD21	1.88	0.55
1:A:214:ASN:HD21	5:A:1248:OAD:C1'	2.19	0.55
1:A:58:GLU:HG2	1:A:59:GLU:N	2.21	0.54
1:A:118:ASN:C	1:A:118:ASN:HD22	2.16	0.54
1:B:100:ILE:HG21	1:B:159:ILE:HG12	1.88	0.54
1:B:164:GLU:O	2:H:2:LYS:HB2	2.08	0.54
2:H:3:LYS:O	2:H:4:LEU:HB3	2.07	0.54
1:A:129:LYS:HD2	1:A:150:ASP:HB2	1.90	0.53
1:A:102:ARG:HG3	1:A:102:ARG:NH1	2.09	0.53
1:A:159:ILE:HG21	4:A:1247:OCZ:CL	2.46	0.52
1:A:124:CYS:HB2	1:A:148:CYS:CB	2.39	0.52
1:B:124:CYS:HB2	1:B:148:CYS:CB	2.40	0.52
1:A:194:TYR:HB2	2:E:4:LEU:CD1	2.32	0.51
1:A:116:HIS:HA	1:A:160:VAL:HB	1.92	0.50
1:B:26:THR:OG1	1:B:27:PRO:HD3	2.12	0.50
1:B:162:PHE:HA	2:H:3:LYS:HB3	1.94	0.50
1:A:7:LEU:O	1:A:11:ASN:ND2	2.43	0.50
1:A:124:CYS:HB2	1:A:148:CYS:HB3	1.94	0.50
1:B:218:THR:HB	1:B:219:PRO:CD	2.42	0.50
1:B:185:ILE:HG22	1:B:187:LEU:HD11	1.94	0.49
1:B:146:PRO:HB2	1:B:155:ILE:HD12	1.95	0.49
1:A:168:GLN:NE2	1:A:168:GLN:N	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ALA:O	1:A:200:PRO:HD2	2.13	0.49
1:B:166:LEU:HD13	1:B:195:PRO:HG2	1.94	0.49
1:A:5:GLU:N	1:A:5:GLU:OE1	2.44	0.48
1:B:123:TYR:CZ	1:B:156:ARG:HD3	2.47	0.48
1:B:46:ASN:N	1:B:46:ASN:OD1	2.45	0.48
1:A:57:PRO:HB2	1:A:145:VAL:CG1	2.43	0.48
1:B:176:GLY:O	1:B:180:ARG:NH1	2.46	0.48
1:B:116:HIS:HA	1:B:160:VAL:HB	1.95	0.48
1:B:185:ILE:HG22	1:B:187:LEU:HD12	1.96	0.48
1:A:176:GLY:O	1:A:180:ARG:NH1	2.47	0.47
1:B:57:PRO:HB2	1:B:145:VAL:HG11	1.96	0.47
1:B:13:SER:OG	1:B:182:SER:OG	2.28	0.47
1:B:245:ILE:O	1:B:246:SER:C	2.57	0.47
1:A:26:THR:OG1	5:A:1248:OAD:N7	2.43	0.47
1:B:194:TYR:HD1	1:B:197:ALA:HB3	1.72	0.47
1:A:214:ASN:HD22	1:A:215:LEU:H	1.54	0.47
1:A:96:ILE:CG2	1:A:115:LEU:HD11	2.45	0.46
1:A:230:MET:CE	1:A:234:GLU:HG3	2.42	0.46
1:A:100:ILE:HG21	1:A:159:ILE:HG12	1.97	0.46
1:B:124:CYS:HB2	1:B:148:CYS:HB3	1.97	0.46
1:B:169:ASP:O	1:B:172:ARG:HG2	2.16	0.46
1:A:30:ILE:HG23	1:A:71:MET:HG2	1.98	0.46
1:A:72:LEU:HD21	1:A:133:VAL:HG11	1.99	0.45
1:B:7:LEU:O	1:B:11:ASN:ND2	2.47	0.45
1:A:44:SER:CB	1:A:47:VAL:HG21	2.46	0.45
1:A:218:THR:HB	1:A:219:PRO:HD2	1.99	0.45
1:A:9:LEU:HD12	1:A:226:LEU:HD12	1.97	0.45
1:B:102:ARG:CG	1:B:102:ARG:NH1	2.71	0.44
1:B:58:GLU:HG2	1:B:59:GLU:N	2.31	0.44
1:A:230:MET:O	5:A:1248:OAD:H2	2.17	0.44
1:A:140:LEU:HD21	1:A:146:PRO:HD3	2.00	0.44
1:A:26:THR:OG1	1:A:27:PRO:HD3	2.18	0.44
1:A:194:TYR:HD1	1:A:194:TYR:HA	1.72	0.44
1:B:77:ASN:O	1:B:81:VAL:HG23	2.18	0.43
1:B:214:ASN:ND2	1:B:214:ASN:C	2.76	0.43
5:B:1248:OAD:C6D	2:H:3:LYS:HZ1	2.31	0.43
1:B:218:THR:HB	1:B:219:PRO:HD2	1.99	0.43
1:B:9:LEU:HD12	1:B:226:LEU:HD12	1.99	0.43
1:A:48:PHE:HE1	1:A:63:PHE:CZ	2.37	0.43
1:A:144:ASP:OD1	1:A:144:ASP:N	2.52	0.43
1:A:43:TYR:O	1:A:44:SER:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:HIS:CE1	5:A:1248:OAD:O3D	2.72	0.42
1:A:77:ASN:OD1	1:A:77:ASN:C	2.62	0.42
1:B:72:LEU:HD21	1:B:133:VAL:HG11	2.01	0.42
1:A:209:LYS:HD3	1:A:225:THR:HG21	2.01	0.42
1:A:44:SER:HB2	1:A:47:VAL:CG2	2.49	0.41
1:A:194:TYR:CB	2:E:4:LEU:CD1	2.95	0.41
1:B:30:ILE:HG23	1:B:71:MET:HG2	2.03	0.41
1:A:169:ASP:O	1:A:172:ARG:HG2	2.20	0.41
1:A:185:ILE:HG22	1:A:187:LEU:CD1	2.51	0.41
1:B:185:ILE:CG2	1:B:187:LEU:HD11	2.51	0.41
1:B:232:VAL:N	5:B:1248:OAD:N1	2.68	0.41
1:A:230:MET:HE2	1:A:235:PHE:HA	2.03	0.40
1:A:77:ASN:O	1:A:81:VAL:HG23	2.21	0.40
1:B:183:LEU:HD11	1:B:211:VAL:HG23	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:OE2	1:A:87:GLU:O[1_565]	1.88	0.32
1:A:11:ASN:OD1	1:A:45:GLN:NE2[1_545]	2.10	0.10

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	231/246 (94%)	226 (98%)	3 (1%)	2 (1%)	14	43
1	B	224/246 (91%)	221 (99%)	2 (1%)	1 (0%)	30	60
2	E	3/13 (23%)	2 (67%)	1 (33%)	0	100	100
2	H	3/13 (23%)	1 (33%)	0	2 (67%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	461/518 (89%)	450 (98%)	6 (1%)	5 (1%)	11	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	PRO
1	B	195	PRO
2	H	4	LEU
1	A	45	GLN
2	H	3	LYS

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	205/215 (95%)	176 (86%)	29 (14%)	3	14
1	B	200/215 (93%)	172 (86%)	28 (14%)	3	15
2	E	5/13 (38%)	4 (80%)	1 (20%)	1	6
2	H	5/13 (38%)	4 (80%)	1 (20%)	1	6
All	All	415/456 (91%)	356 (86%)	59 (14%)	3	14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	15	LEU
1	A	17	VAL
1	A	30	ILE
1	A	46	ASN
1	A	47	VAL
1	A	48	PHE
1	A	55	SER
1	A	78	LEU
1	A	102	ARG

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Mol	Chain	Res	Type
1	A	118	ASN
1	A	124	CYS
1	A	127	CYS
1	A	138	LYS
1	A	144	ASP
1	A	145	VAL
1	A	148	CYS
1	A	168	GLN
1	A	169	ASP
1	A	180	ARG
1	A	195	PRO
1	A	198	GLU
1	A	204	VAL
1	A	205	ARG
1	A	223	ILE
1	A	225	THR
1	A	229	ASN
1	A	234	GLU
1	A	237	ARG
1	B	5	GLU
1	B	15	LEU
1	B	30	ILE
1	B	46	ASN
1	B	47	VAL
1	B	55	SER
1	B	78	LEU
1	B	102	ARG
1	B	118	ASN
1	B	124	CYS
1	B	127	CYS
1	B	138	LYS
1	B	145	VAL
1	B	148	CYS
1	B	159	ILE
1	B	168	GLN
1	B	169	ASP
1	B	180	ARG
1	B	195	PRO
1	B	198	GLU
1	B	204	VAL
1	B	205	ARG
1	B	212	ILE

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Mol	Chain	Res	Type
1	B	223	ILE
1	B	225	THR
1	B	229	ASN
1	B	234	GLU
1	B	237	ARG
2	E	3	LYS
2	H	5	MET

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

Mol	Chain	Res	Type
1	A	118	ASN
1	A	168	GLN
1	A	214	ASN
1	B	56	HIS
1	B	118	ASN
1	B	168	GLN
1	B	214	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	OCZ	A	1247	-	19,19,19	3.52	10 (52%)	23,28,28	1.99	6 (26%)
5	OAD	A	1248	-	42,42,42	1.82	10 (23%)	58,64,64	2.20	23 (39%)
5	OAD	B	1248	-	42,42,42	1.72	11 (26%)	58,64,64	2.36	20 (34%)
4	OCZ	B	1247	-	19,19,19	3.52	9 (47%)	23,28,28	1.52	4 (17%)

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	OCZ	A	1247	-	-	0/4/14/14	0/3/3/3
5	OAD	A	1248	-	-	10/26/58/58	0/4/4/4
5	OAD	B	1248	-	-	11/26/58/58	0/4/4/4
4	OCZ	B	1247	-	-	0/4/14/14	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	OCZ	CAJ-CAH	-8.86	1.39	1.50
4	B	1247	OCZ	CAJ-CAH	-7.40	1.40	1.50
4	B	1247	OCZ	CAK-CAI	-6.71	1.43	1.50
4	A	1247	OCZ	CAK-CAI	-6.42	1.44	1.50
4	B	1247	OCZ	CAF-CAE	-5.93	1.34	1.41
4	A	1247	OCZ	CAF-CAE	-5.26	1.34	1.41
4	A	1247	OCZ	CAK-CAO	-5.25	1.42	1.52
4	B	1247	OCZ	CAF-CAH	-5.23	1.34	1.44
4	B	1247	OCZ	CAK-CAO	-4.69	1.43	1.52
5	A	1248	OAD	C2-N3	4.59	1.42	1.33
4	A	1247	OCZ	CAF-CAH	-4.37	1.36	1.44
4	B	1247	OCZ	CAI-NAG	-4.31	1.33	1.38
5	A	1248	OAD	C5-N7	-4.13	1.31	1.39
4	A	1247	OCZ	CAI-NAG	-3.98	1.33	1.38
5	B	1248	OAD	C2-N3	3.90	1.40	1.33
5	B	1248	OAD	PB-O1B	3.73	1.63	1.50
4	B	1247	OCZ	CAD-CAE	-3.64	1.33	1.39
5	A	1248	OAD	C5-C6	-3.63	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1248	OAD	PA-O1A	3.61	1.63	1.50
5	B	1248	OAD	C5-C4	-3.59	1.32	1.39
5	A	1248	OAD	C1D-C2D	-3.55	1.49	1.52
5	A	1248	OAD	C2-N1	3.53	1.40	1.33
5	B	1248	OAD	C8-N9	-3.09	1.32	1.37
5	A	1248	OAD	PB-O1B	3.01	1.61	1.50
4	B	1247	OCZ	CAE-NAG	-2.98	1.33	1.38
5	B	1248	OAD	C5-N7	-2.84	1.33	1.39
5	B	1248	OAD	PA-O3A	2.71	1.62	1.59
5	B	1248	OAD	C1D-C2D	2.70	1.55	1.52
5	A	1248	OAD	C5-C4	-2.68	1.34	1.39
4	B	1247	OCZ	CAA-CAF	-2.66	1.35	1.39
4	A	1247	OCZ	CAD-CAE	-2.64	1.35	1.39
5	B	1248	OAD	C2-N1	2.60	1.38	1.33
5	A	1248	OAD	C8-N9	-2.35	1.33	1.37
4	A	1247	OCZ	CAL-CAK	-2.30	1.50	1.55
5	A	1248	OAD	C4-N9	-2.25	1.33	1.37
5	B	1248	OAD	C5-C6	-2.24	1.34	1.41
5	B	1248	OAD	O1D-C1D	2.20	1.46	1.39
4	A	1247	OCZ	CAA-CAB	2.17	1.41	1.38
4	A	1247	OCZ	CAE-NAG	-2.12	1.34	1.38
5	A	1248	OAD	PA-O1A	2.02	1.57	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1248	OAD	N3-C2-N1	-8.19	116.19	128.58
5	A	1248	OAD	C2D-O2D-C6D	-7.30	106.38	117.72
5	B	1248	OAD	N9-C8-N7	-5.84	105.65	113.94
5	B	1248	OAD	C5-C4-N3	-4.90	119.97	126.72
5	A	1248	OAD	C5-C4-N3	-4.85	120.04	126.72
5	A	1248	OAD	N3-C2-N1	-4.65	121.54	128.58
4	A	1247	OCZ	CAH-CAI-NAG	-4.63	106.07	110.22
5	B	1248	OAD	C5-N7-C8	4.28	110.17	103.45
5	B	1248	OAD	C2-N3-C4	4.10	121.84	111.83
5	A	1248	OAD	C6-C5-C4	4.08	122.75	117.18
5	B	1248	OAD	C4-N9-C8	4.02	109.96	105.74
4	B	1247	OCZ	CAH-CAI-NAG	-3.94	106.69	110.22
5	B	1248	OAD	C4'-O4'-C1'	-3.87	100.93	109.47
5	A	1248	OAD	N9-C8-N7	-3.86	108.46	113.94
5	A	1248	OAD	C5-C6-N6	-3.74	114.02	123.29
4	A	1247	OCZ	CAM-CAL-CAK	-3.72	106.85	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	OCZ	CAA-CAB-CL	3.55	123.62	119.17
4	A	1247	OCZ	CAF-CAH-CAI	3.45	109.24	106.90
5	B	1248	OAD	C4-C5-N7	-3.27	106.84	110.58
5	B	1248	OAD	N3-C4-N9	3.22	132.65	127.17
5	A	1248	OAD	O4'-C1'-N9	3.05	113.94	108.09
5	A	1248	OAD	O2D-C6D-C7D	2.99	116.42	111.09
4	B	1247	OCZ	CAA-CAB-CL	2.95	122.87	119.17
5	B	1248	OAD	O1D-C1D-O4D	-2.94	107.37	111.12
5	A	1248	OAD	O3A-PA-O1A	-2.90	101.98	110.70
5	B	1248	OAD	O4D-C4D-C3D	-2.89	99.43	105.15
5	B	1248	OAD	C5-C6-N6	-2.84	116.25	123.29
5	B	1248	OAD	O2D-C6D-C7D	2.82	116.11	111.09
5	A	1248	OAD	O2B-PB-O3A	2.80	114.83	107.27
5	A	1248	OAD	N3-C4-N9	2.77	131.88	127.17
4	B	1247	OCZ	CAC-CAB-CAA	-2.72	117.98	121.53
5	A	1248	OAD	C5-N7-C8	2.64	107.60	103.45
5	B	1248	OAD	C2D-C3D-C4D	-2.55	96.51	101.99
4	A	1247	OCZ	CAK-CAO-NAQ	-2.54	114.32	116.93
5	B	1248	OAD	C3'-C2'-C1'	-2.45	96.82	101.46
4	A	1247	OCZ	CAD-CAC-CAB	-2.42	116.81	119.24
5	A	1248	OAD	C4'-O4'-C1'	-2.28	104.44	109.47
5	A	1248	OAD	O1D-C1D-O4D	2.25	113.98	111.12
4	B	1247	OCZ	CAF-CAH-CAI	2.23	108.42	106.90
5	A	1248	OAD	C5-C6-N1	2.20	123.09	117.51
5	B	1248	OAD	C5'-C4'-C3'	-2.19	107.33	115.21
5	B	1248	OAD	C2D-O2D-C6D	-2.18	114.34	117.72
5	A	1248	OAD	O4'-C1'-C2'	-2.16	101.98	106.62
5	B	1248	OAD	C5-C6-N1	2.14	122.96	117.51
5	A	1248	OAD	O4'-C4'-C5'	-2.13	102.52	109.33
5	A	1248	OAD	C5'-C4'-C3'	-2.12	107.60	115.21
5	A	1248	OAD	C5-C4-N9	2.09	108.08	105.81
5	B	1248	OAD	O2B-PB-O3A	2.04	112.80	107.27
5	B	1248	OAD	C4-N9-C1'	-2.04	121.86	126.63
5	A	1248	OAD	N6-C6-N1	2.03	122.89	118.38
5	A	1248	OAD	C2-N3-C4	2.02	116.75	111.83
5	A	1248	OAD	O4D-C4D-C3D	-2.01	101.15	105.15
5	A	1248	OAD	O4D-C4D-C5D	2.01	115.77	109.33

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1248	OAD	C5'-O5'-PA-O1A
5	A	1248	OAD	C7D-C6D-O2D-C2D
5	A	1248	OAD	C4D-C5D-O5D-PB
5	B	1248	OAD	C5D-O5D-PB-O3A
5	B	1248	OAD	C5D-O5D-PB-O2B
5	B	1248	OAD	C7D-C6D-O2D-C2D
5	B	1248	OAD	O4D-C4D-C5D-O5D
5	B	1248	OAD	O6D-C6D-O2D-C2D
5	A	1248	OAD	O6D-C6D-O2D-C2D
5	B	1248	OAD	C3'-C4'-C5'-O5'
5	B	1248	OAD	C3D-C4D-C5D-O5D
5	A	1248	OAD	C3'-C4'-C5'-O5'
5	A	1248	OAD	O4'-C4'-C5'-O5'
5	B	1248	OAD	O4'-C4'-C5'-O5'
5	B	1248	OAD	C4'-C5'-O5'-PA
5	A	1248	OAD	PB-O3A-PA-O5'
5	A	1248	OAD	C1D-C2D-O2D-C6D
5	B	1248	OAD	C5D-O5D-PB-O1B
5	A	1248	OAD	PA-O3A-PB-O2B
5	B	1248	OAD	C4D-C5D-O5D-PB
5	A	1248	OAD	PA-O3A-PB-O1B

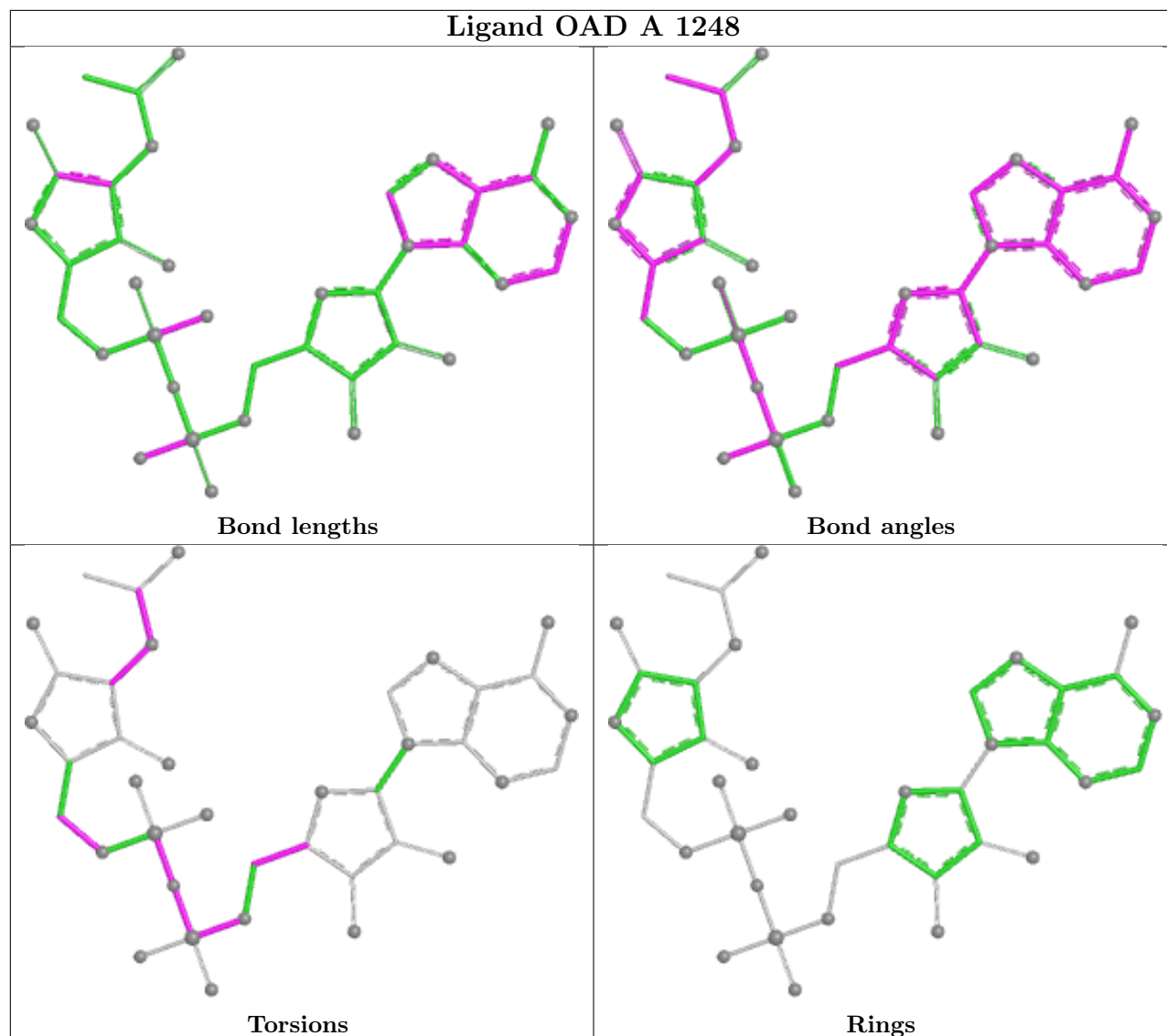
There are no ring outliers.

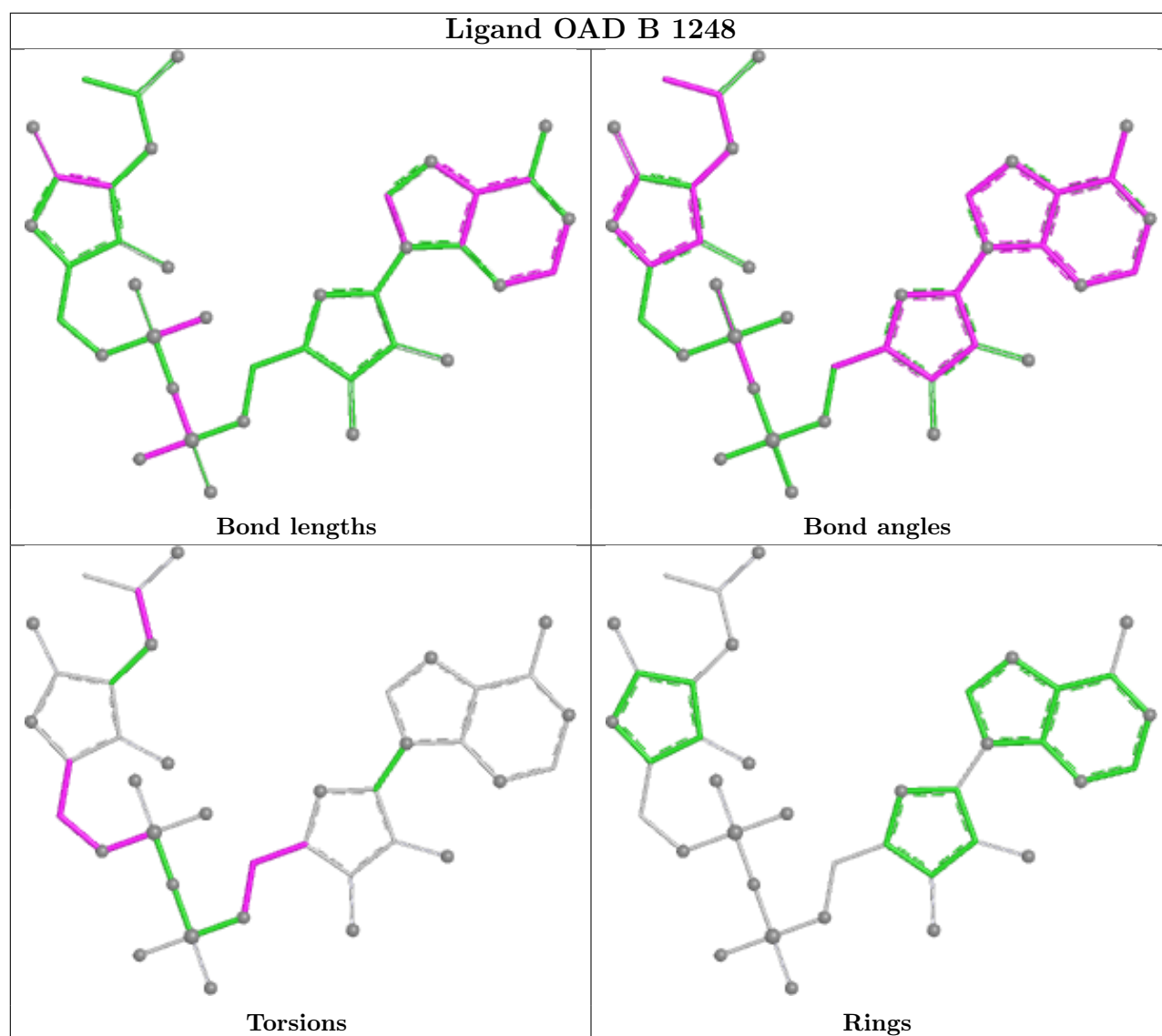
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1247	OCZ	1	0
5	A	1248	OAD	11	0
5	B	1248	OAD	5	0
4	B	1247	OCZ	2	0

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

Ligand OAD A 1248





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	235/246 (95%)	-0.87	0 100 100	72, 111, 151, 173	0
1	B	230/246 (93%)	-0.88	0 100 100	75, 114, 158, 181	0
2	E	5/13 (38%)	-1.01	0 100 100	84, 89, 94, 109	0
2	H	5/13 (38%)	-1.00	0 100 100	92, 100, 114, 129	0
All	All	475/518 (91%)	-0.88	0 100 100	72, 112, 155, 181	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OAD	A	1248	39/39	0.98	0.07	90,105,156,159	0
4	OCZ	A	1247	17/17	0.99	0.08	81,97,126,160	0
4	OCZ	B	1247	17/17	0.99	0.08	89,102,124,132	0
3	ZN	A	1246	1/1	0.99	0.02	122,122,122,122	0

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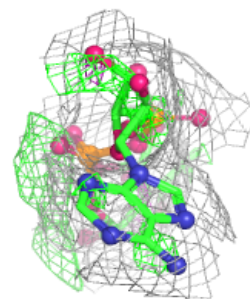
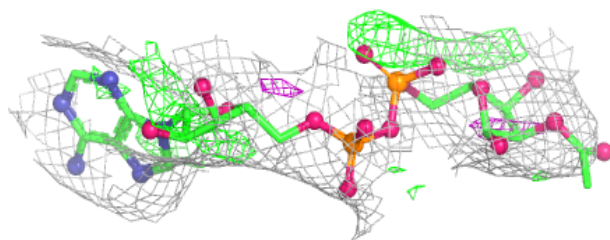
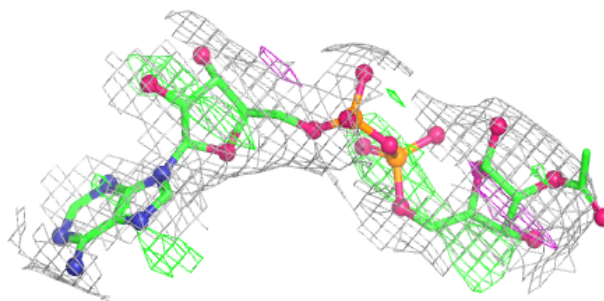
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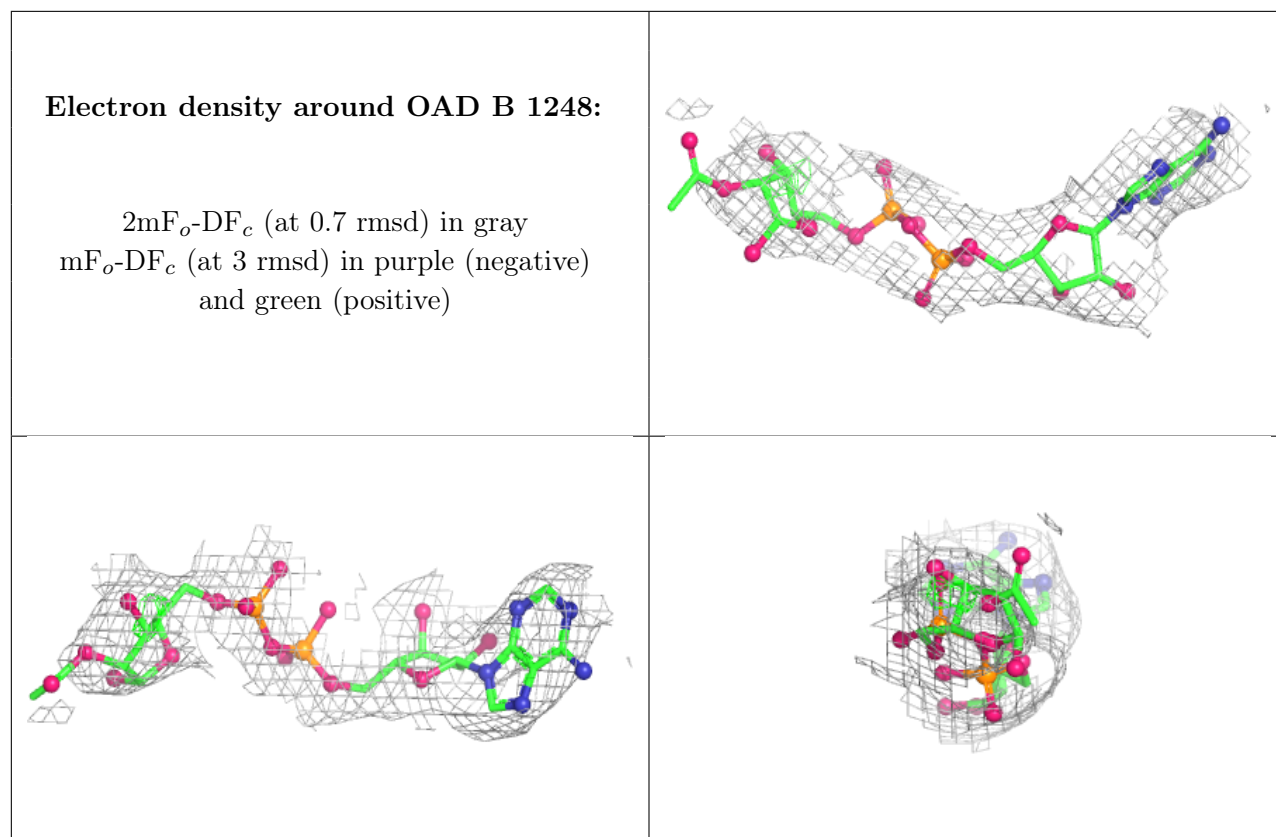
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OAD	B	1248	39/39	0.99	0.06	109,116,142,148	0
3	ZN	B	1249	1/1	1.00	0.01	131,131,131,131	0

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 OAD A 1248:

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.