



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:36 PM UTC

PDB ID : 3CF6 / pdb_00003cf6
Title : Structure of Epac2 in complex with cyclic-AMP and Rap
Authors : Rehmann, H.; Arias-Palomo, E.; Hadders, M.A.; Schwede, F.; Llorca, O.; Bos, J.L.
Deposited on : 2008-03-02
Resolution : 2.20 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

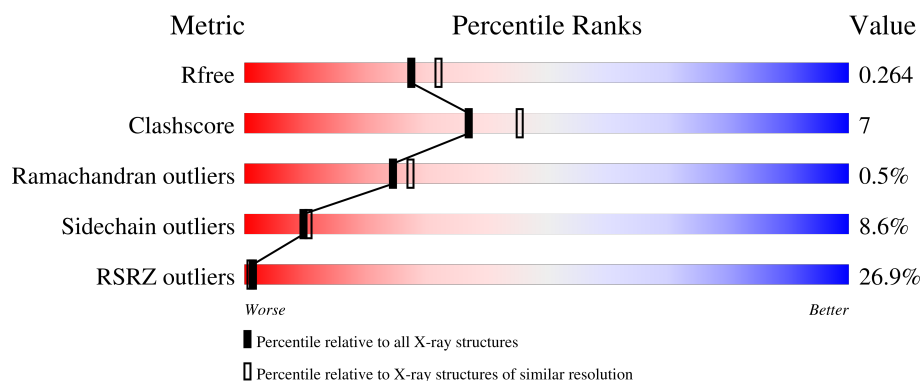
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	E	694	17% 74% 14% • 10%
2	R	167	56% 57% 26% 5% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6561 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 Rap guanine nucleotide exchange factor (GEF) 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	627	Total	C	N	O	S	0	0	0
			5052	3222	871	928	31			

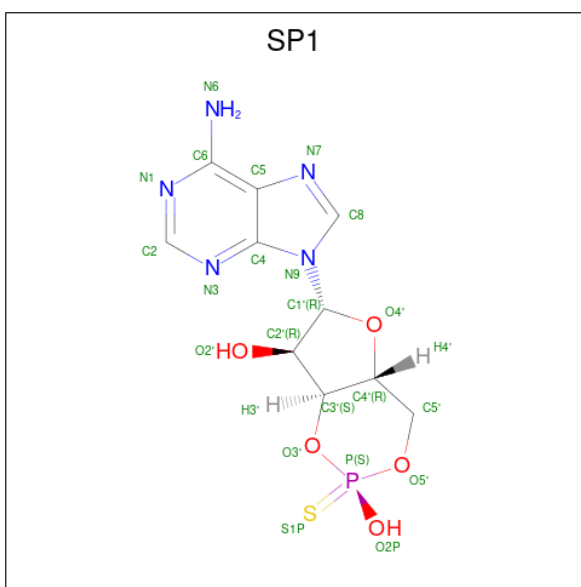
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	300	GLY	-	expression tag	UNP A2ASW3
E	301	SER	-	expression tag	UNP A2ASW3
E	302	PRO	-	expression tag	UNP A2ASW3
E	303	GLU	-	expression tag	UNP A2ASW3
E	304	SER	-	expression tag	UNP A2ASW3
E	305	PHE	-	expression tag	UNP A2ASW3

- Molecule 2 is a protein called Ras-related protein Rap-1b.

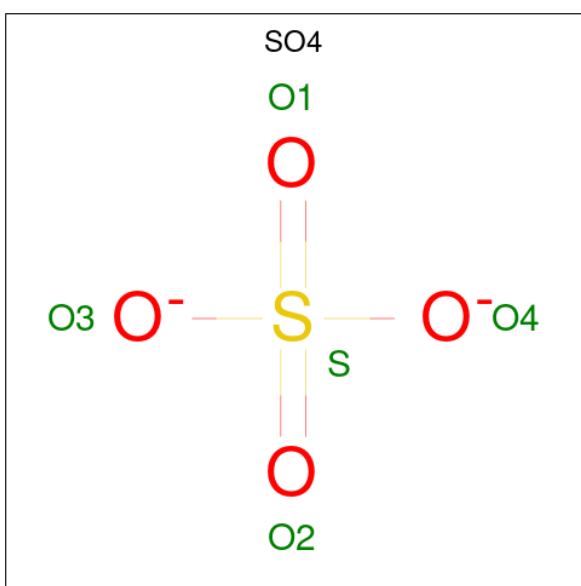
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	150	Total	C	N	O	S	0	0	0
			1186	748	196	236	6			

- Molecule 3 is 6-(6-AMINO-PURIN-9-YL)-2-THIOXO-TETRAHYDRO-2-FURO[3,2-D][1,3,2]DIOXAPHOSPHININE-2,7-DIOL (CCD ID: SP1) (formula: C₁₀H₁₂N₅O₅PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	S	0	0
			22	10	5	5	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			22	10	5	5	1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	1	Total	O S	0	0
			5	4 1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	251	Total 251	O 251	0	0
5	R	23	Total 23	O 23	0	0

L144	S146	A148	K149	S150	K151	I152	M153	V154	M155	E156	I157	F158	Y159	D160	L161	V162	K163	Q164	I165	ASN	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.37Å 149.03Å 225.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.20 48.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.56-2.20) 99.0 (48.56-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.265 0.242 , 0.264	Depositor DCC
R_{free} test set	5214 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6561	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: SP1, SO4

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	E	0.73	1/5152 (0.0%)	0.98	11/6963 (0.2%)
2	R	0.77	1/1198 (0.1%)	0.99	4/1610 (0.2%)
All	All	0.74	2/6350 (0.0%)	0.99	15/8573 (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
2	R	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	102	ARG	C-N	9.36	1.46	1.33
1	E	792	THR	CA-CB	5.01	1.59	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	899	GLU	CA-C-N	9.86	130.53	120.38
1	E	899	GLU	C-N-CA	9.86	130.53	120.38
1	E	456	VAL	CB-CA-C	8.36	118.49	110.63
1	E	456	VAL	N-CA-C	-7.27	106.81	113.71
1	E	900	PRO	N-CA-C	6.92	119.14	110.70
2	R	95	ASP	N-CA-C	6.43	118.28	111.28
1	E	453	ASP	N-CA-C	6.16	120.03	111.90
1	E	900	PRO	CA-C-N	-6.09	112.22	119.84
1	E	900	PRO	C-N-CA	-6.09	112.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	28	PHE	N-CA-C	5.82	123.20	110.80
1	E	432	LYS	N-CA-C	5.60	117.06	111.07
2	R	102	ARG	O-C-N	5.35	129.71	122.59
1	E	409	VAL	N-CA-C	5.34	116.12	110.72
1	E	879	GLU	N-CA-C	5.27	117.02	111.28
2	R	29	VAL	N-CA-C	-5.13	105.12	112.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	R	86	ALA	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	E	5052	0	5081	58	0
2	R	1186	0	1180	37	0
3	E	44	0	22	0	0
4	R	5	0	0	1	0
5	E	251	0	0	3	0
5	R	23	0	0	1	0
All	All	6561	0	6283	89	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 7.

All (89) 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)
2:R:14:VAL:CG2	2:R:89:THR:HG21	1.92	0.99
1:E:766:ASP:OD1	1:E:801:ARG:HD3	1.71	0.90
1:E:774:HIS:HD2	1:E:776:LEU:H	1.18	0.90
1:E:905:PHE:HZ	2:R:67:MET:HE1	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:VAL:HG13	1:E:489:LYS:HG2	1.57	0.86
2:R:87:GLN:HG3	2:R:88:SER:H	1.40	0.84
2:R:87:GLN:CG	2:R:88:SER:H	1.91	0.82
2:R:101:LEU:O	2:R:102:ARG:HB2	1.82	0.79
1:E:380:LEU:HD11	1:E:428:LEU:HD13	1.66	0.77
1:E:850:MET:SD	1:E:882:MET:HE1	2.26	0.75
1:E:905:PHE:CZ	2:R:67:MET:HE1	2.21	0.75
1:E:887:ASN:CG	1:E:892:ARG:HH12	1.96	0.74
1:E:369:GLN:HE22	1:E:389:TYR:H	1.36	0.73
2:R:63:GLN:HG2	5:R:176:HOH:O	1.89	0.71
1:E:887:ASN:CG	1:E:892:ARG:NH1	2.49	0.70
1:E:344:THR:O	1:E:348:ARG:HG2	1.92	0.69
2:R:14:VAL:HG21	2:R:89:THR:HG21	1.71	0.67
1:E:747:VAL:O	1:E:751:GLU:HB2	1.94	0.67
1:E:815:LEU:HD23	1:E:984:MET:CE	2.25	0.66
1:E:782:THR:OG1	1:E:913:MET:HG2	1.96	0.66
5:E:1128:HOH:O	2:R:65:THR:HG22	1.98	0.63
1:E:818:GLN:H	1:E:818:GLN:CD	2.07	0.63
1:E:846:PHE:CD2	1:E:882:MET:HE3	2.35	0.61
1:E:313:ILE:HG22	1:E:329:ILE:HD11	1.82	0.61
2:R:87:GLN:CG	2:R:88:SER:N	2.62	0.61
2:R:84:ILE:HG22	2:R:126:VAL:O	2.01	0.60
1:E:900:PRO:O	1:E:902:LEU:N	2.34	0.60
2:R:14:VAL:HG23	2:R:89:THR:HG21	1.79	0.60
1:E:815:LEU:HD23	1:E:984:MET:HE3	1.83	0.59
2:R:87:GLN:HG3	2:R:88:SER:N	2.15	0.59
1:E:762:MET:HE1	1:E:832:ILE:HG21	1.86	0.58
1:E:815:LEU:CD2	1:E:984:MET:HE1	2.34	0.58
1:E:774:HIS:CD2	1:E:776:LEU:H	2.10	0.57
1:E:405:LYS:HE2	1:E:480:TYR:OH	2.04	0.56
2:R:41:ARG:HG2	2:R:54:GLU:HG2	1.86	0.56
2:R:70:LEU:O	2:R:74:ASN:ND2	2.37	0.56
2:R:124:ARG:HH22	2:R:145:GLU:CD	2.14	0.55
1:E:333:LEU:HA	1:E:336:ILE:HD12	1.88	0.55
2:R:124:ARG:NH2	2:R:145:GLU:OE1	2.39	0.55
1:E:456:VAL:HG13	1:E:489:LYS:CG	2.34	0.54
1:E:785:ARG:HG2	1:E:790:LYS:O	2.08	0.53
1:E:886:ARG:N	2:R:54:GLU:OE2	2.30	0.53
1:E:766:ASP:OD2	1:E:844:SER:OG	2.23	0.53
2:R:76:GLN:O	2:R:110:PRO:HG2	2.10	0.52
1:E:887:ASN:OD1	1:E:892:ARG:NH1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:LEU:HB3	1:E:356:PHE:HB2	1.92	0.51
1:E:716:LEU:HD11	1:E:722:LEU:HD13	1.92	0.51
2:R:110:PRO:HB3	2:R:164:GLN:HB3	1.93	0.50
2:R:84:ILE:HD11	2:R:115:GLY:O	2.11	0.50
2:R:65:THR:HG23	2:R:68:ARG:NH2	2.27	0.50
1:E:815:LEU:CD2	1:E:984:MET:CE	2.89	0.50
1:E:918:GLU:HG2	2:R:17:SER:OG	2.12	0.49
2:R:44:VAL:HG13	2:R:159:TYR:HE2	1.77	0.49
1:E:519:HIS:HD2	1:E:523:MET:O	1.95	0.49
1:E:405:LYS:NZ	1:E:445:ASN:O	2.45	0.49
2:R:14:VAL:HG21	2:R:89:THR:CG2	2.39	0.48
1:E:769:LEU:HD23	1:E:801:ARG:HD2	1.96	0.48
2:R:82:TYR:HB3	2:R:93:LEU:HD11	1.97	0.47
2:R:14:VAL:CG2	2:R:89:THR:CG2	2.80	0.47
1:E:901:PRO:HD3	1:E:949:GLN:HB2	1.97	0.47
2:R:28:PHE:O	2:R:28:PHE:CG	2.66	0.46
1:E:341:HIS:CE1	1:E:443:GLU:OE2	2.69	0.45
1:E:831:LYS:O	1:E:835:HIS:HD2	2.00	0.45
2:R:80:LEU:HB3	2:R:93:LEU:HD22	1.99	0.45
1:E:899:GLU:HB3	1:E:900:PRO:HD2	1.99	0.45
1:E:934:ARG:NH1	5:E:996:HOH:O	2.41	0.45
1:E:864:TRP:O	1:E:872:LYS:HE2	2.17	0.44
2:R:23:PHE:CD2	2:R:55:ILE:HD11	2.52	0.44
1:E:900:PRO:HD3	1:E:945:TYR:OH	2.18	0.44
1:E:930:PHE:O	1:E:934:ARG:HG3	2.18	0.44
2:R:158:PHE:O	2:R:162:VAL:HG23	2.17	0.44
1:E:935:MET:HE1	2:R:32:TYR:O	2.17	0.44
1:E:819:LEU:O	1:E:823:VAL:HG23	2.17	0.44
1:E:869:SER:HA	1:E:872:LYS:HB2	2.00	0.43
1:E:882:MET:HB3	1:E:882:MET:HE2	1.81	0.43
1:E:380:LEU:HD11	1:E:428:LEU:CD1	2.44	0.43
1:E:489:LYS:NZ	5:E:1156:HOH:O	2.52	0.43
1:E:367:PHE:CZ	1:E:418:ILE:HG13	2.55	0.42
1:E:900:PRO:HD3	1:E:945:TYR:CZ	2.55	0.42
2:R:16:LYS:HG3	4:R:168:SO4:O3	2.19	0.41
2:R:41:ARG:HA	2:R:53:LEU:O	2.20	0.41
1:E:889:ARG:NH1	2:R:37:GLU:OE1	2.53	0.41
2:R:121:GLU:HA	2:R:124:ARG:HB2	2.03	0.41
1:E:917:HIS:HD2	1:E:932:LYS:NZ	2.18	0.41
1:E:394:VAL:HG13	1:E:451:GLU:HG2	2.03	0.41
1:E:507:ALA:O	1:E:511:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:746:THR:HG22	1:E:749:THR:HB	2.02	0.41
1:E:982:SER:O	1:E:986:HIS:HD2	2.04	0.40
2:R:43:GLN:HB2	2:R:52:MET:HE1	2.02	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	E	619/694 (89%)	607 (98%)	11 (2%)	1 (0%)	43	51
2	R	144/167 (86%)	132 (92%)	9 (6%)	3 (2%)	5	3
All	All	763/861 (89%)	739 (97%)	20 (3%)	4 (0%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	900	PRO
2	R	102	ARG
2	R	87	GLN
2	R	157	ILE

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	E	562/615 (91%)	519 (92%)	43 (8%)	12	13
2	R	132/147 (90%)	115 (87%)	17 (13%)	4	4
All	All	694/762 (91%)	634 (91%)	60 (9%)	10	10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	312	MET
1	E	326	LEU
1	E	334	LEU
1	E	344	THR
1	E	348	ARG
1	E	353	VAL
1	E	366	LEU
1	E	391	LYS
1	E	394	VAL
1	E	428	LEU
1	E	442	VAL
1	E	443	GLU
1	E	456	VAL
1	E	508	THR
1	E	546	GLN
1	E	573	LEU
1	E	574	LEU
1	E	584	LEU
1	E	596	ARG
1	E	643	ARG
1	E	652	VAL
1	E	679	SER
1	E	691	LEU
1	E	694	VAL
1	E	696	MET
1	E	707	SER
1	E	710	VAL
1	E	722	LEU
1	E	728	GLU
1	E	738	GLU
1	E	755	SER
1	E	769	LEU
1	E	785	ARG
1	E	801	ARG
1	E	806	GLN

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Mol	Chain	Res	Type
1	E	818	GLN
1	E	852	LEU
1	E	881	LEU
1	E	892	ARG
1	E	918	GLU
1	E	944	ARG
1	E	969	VAL
1	E	974	VAL
2	R	14	VAL
2	R	29	VAL
2	R	44	VAL
2	R	51	CYS
2	R	53	LEU
2	R	68	ARG
2	R	80	LEU
2	R	84	ILE
2	R	94	GLN
2	R	104	LYS
2	R	106	THR
2	R	107	ASP
2	R	109	VAL
2	R	112	ILE
2	R	120	LEU
2	R	134	LEU
2	R	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	369	GLN
1	E	424	ASN
1	E	445	ASN
1	E	478	GLN
1	E	519	HIS
1	E	535	HIS
1	E	542	GLN
1	E	546	GLN
1	E	761	GLN
1	E	774	HIS
1	E	806	GLN
1	E	835	HIS
1	E	917	HIS

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Mol	Chain	Res	Type
1	E	983	GLN
1	E	986	HIS
2	R	43	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SP1	E	3	-	25,25,25	2.23	5 (20%)	38,39,39	2.38	11 (28%)
3	SP1	E	2	-	25,25,25	2.22	9 (36%)	38,39,39	2.09	11 (28%)
4	SO4	R	168	-	4,4,4	0.29	0	6,6,6	1.01	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SP1	E	3	-	-	1/4/31/31	0/4/4/4
3	SP1	E	2	-	-	0/4/31/31	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	SP1	P-O2P	6.67	1.76	1.54
3	E	3	SP1	P-O2P	5.92	1.73	1.54
3	E	3	SP1	C5-C4	5.01	1.48	1.39
3	E	2	SP1	C5-C4	4.75	1.47	1.39
3	E	3	SP1	P-S1P	4.30	2.00	1.90
3	E	3	SP1	P-O3'	4.00	1.62	1.57
3	E	2	SP1	P-O5'	3.43	1.62	1.57
3	E	3	SP1	C5-C6	3.04	1.49	1.41
3	E	2	SP1	C8-N7	2.55	1.36	1.31
3	E	2	SP1	P-O3'	2.29	1.60	1.57
3	E	2	SP1	C5-C6	2.25	1.47	1.41
3	E	2	SP1	P-S1P	2.20	1.95	1.90
3	E	2	SP1	O3'-C3'	-2.11	1.41	1.44
3	E	2	SP1	C5-N7	-2.02	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	SP1	C5-C4-N3	-6.05	118.38	126.72
3	E	3	SP1	O3'-P-S1P	-5.66	107.30	115.04
3	E	3	SP1	N3-C4-N9	5.34	136.24	127.17
3	E	2	SP1	C5-C4-N3	-5.29	119.43	126.72
3	E	2	SP1	N3-C4-N9	4.93	135.55	127.17
3	E	3	SP1	C2-N3-C4	3.99	121.56	111.83
3	E	2	SP1	N3-C2-N1	-3.87	122.73	128.58
3	E	2	SP1	O3'-P-S1P	-3.69	110.00	115.04
3	E	2	SP1	O5'-P-S1P	-3.58	108.98	114.06
3	E	2	SP1	C2-N3-C4	3.54	120.47	111.83
3	E	3	SP1	O3'-C3'-C2'	3.30	118.84	115.61
3	E	3	SP1	N3-C2-N1	-3.26	123.64	128.58
3	E	3	SP1	O5'-P-S1P	-3.19	109.53	114.06
3	E	3	SP1	C4-C5-N7	-3.19	106.94	110.58
3	E	2	SP1	C4-N9-C8	2.90	108.78	105.74
3	E	3	SP1	O2P-P-O5'	2.86	114.14	107.16
3	E	3	SP1	C5-N7-C8	2.78	107.82	103.45
3	E	3	SP1	C4-N9-C8	2.77	108.65	105.74
3	E	2	SP1	O2P-P-O5'	2.59	113.47	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	SP1	C2-N1-C6	2.12	122.21	118.73
3	E	2	SP1	N6-C6-N1	2.09	123.03	118.38
3	E	2	SP1	C5'-C4'-C3'	-2.04	108.72	112.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

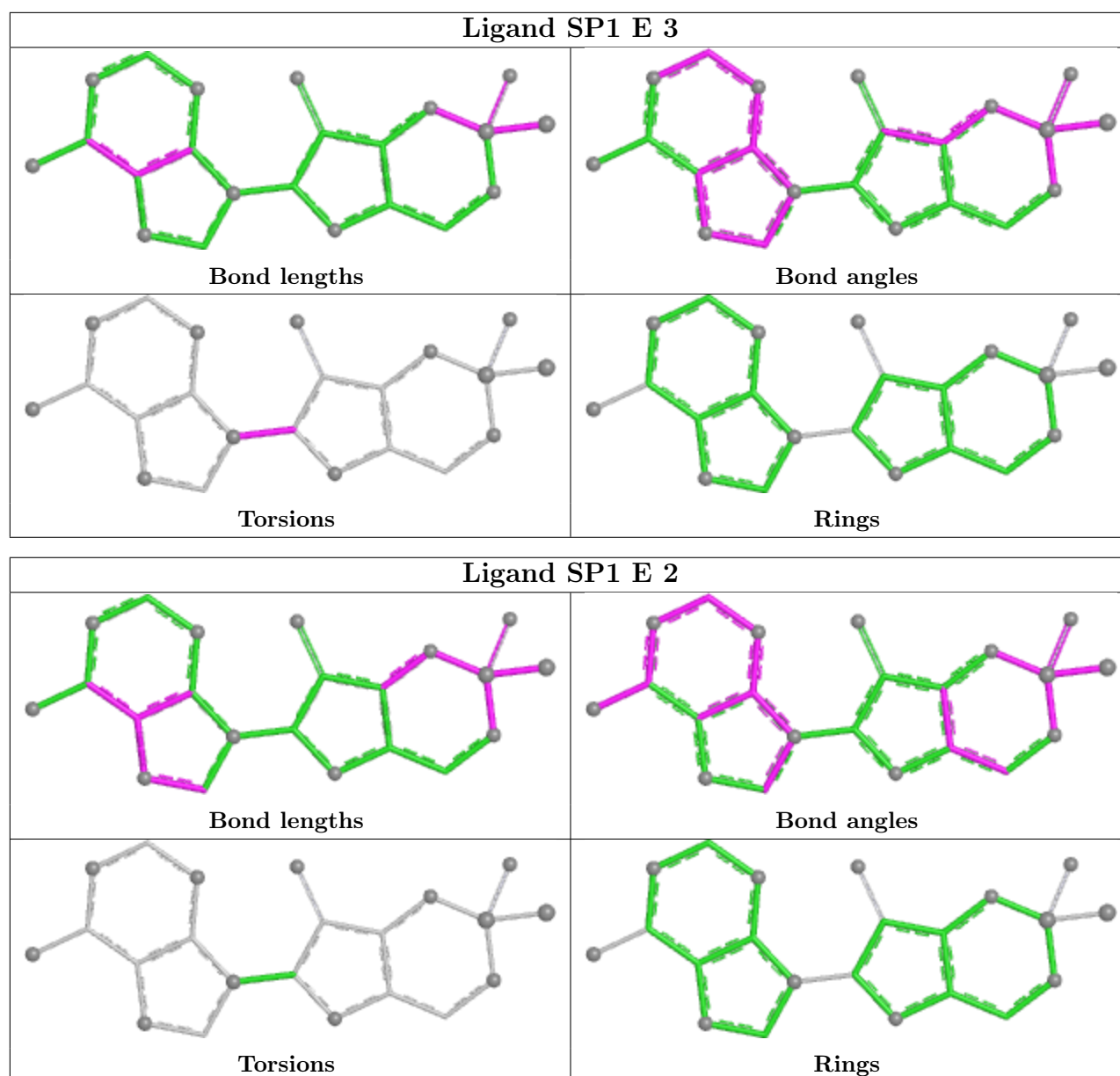
Mol	Chain	Res	Type	Atoms
3	E	3	SP1	O4'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	168	SO4	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	E	627/694 (90%)	0.93	116 (18%) 3 2	28, 43, 67, 85	0
2	R	150/167 (89%)	2.76	93 (62%) 0 0	35, 60, 86, 91	0
All	All	777/861 (90%)	1.28	209 (26%) 1 1	28, 45, 76, 91	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	900	PRO	9.2
2	R	134	LEU	9.0
2	R	142	ALA	8.0
2	R	106	THR	7.4
1	E	612	VAL	6.1
2	R	131	GLY	6.0
2	R	108	ASP	6.0
2	R	90	PHE	6.0
1	E	312	MET	6.0
2	R	127	GLY	5.8
2	R	105	ASP	5.8
2	R	93	LEU	5.7
2	R	125	VAL	5.6
2	R	118	CYS	5.6
1	E	686	GLY	5.5
2	R	115	GLY	5.5
2	R	50	GLN	5.5
2	R	52	MET	5.4
1	E	452	HIS	5.4
2	R	113	LEU	5.3
2	R	133	ASN	5.2
2	R	132	GLN	5.2
2	R	51	CYS	5.2
1	E	478	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
2	R	104	LYS	5.1
2	R	4	TYR	5.0
2	R	120	LEU	5.0
1	E	901	PRO	4.9
2	R	126	VAL	4.9
2	R	89	THR	4.9
2	R	162	VAL	4.8
2	R	107	ASP	4.7
2	R	130	GLN	4.6
1	E	952	ASN	4.5
2	R	146	SER	4.5
1	E	310	MET	4.5
2	R	128	LYS	4.5
2	R	159	TYR	4.4
1	E	685	LEU	4.4
2	R	3	GLU	4.4
2	R	144	LEU	4.4
1	E	869	SER	4.3
1	E	572	ASP	4.3
2	R	114	VAL	4.3
1	E	441	ASP	4.3
1	E	874	PHE	4.2
1	E	311	ARG	4.2
2	R	129	GLU	4.2
1	E	658	CYS	4.1
2	R	112	ILE	4.1
2	R	101	LEU	4.1
2	R	86	ALA	4.0
2	R	87	GLN	4.0
2	R	84	ILE	4.0
1	E	987	ARG	3.9
2	R	164	GLN	3.9
1	E	318	PRO	3.9
2	R	100	ILE	3.9
2	R	110	PRO	3.9
2	R	121	GLU	3.9
2	R	143	PHE	3.9
1	E	688	GLY	3.8
2	R	94	GLN	3.7
1	E	501	GLU	3.7
1	E	861	ALA	3.7
1	E	337	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	R	149	LYS	3.7
2	R	161	LEU	3.6
1	E	324	ASP	3.6
2	R	158	PHE	3.5
2	R	53	LEU	3.5
1	E	611	ILE	3.5
2	R	109	VAL	3.5
2	R	157	ILE	3.5
1	E	314	LEU	3.5
2	R	95	ASP	3.5
1	E	507	ALA	3.4
2	R	153	ASN	3.4
1	E	462	VAL	3.4
2	R	103	VAL	3.4
1	E	603	GLU	3.4
1	E	824	GLN	3.4
2	R	98	GLU	3.3
2	R	97	ARG	3.3
2	R	5	LYS	3.3
2	R	75	GLY	3.2
1	E	331	ASP	3.2
2	R	44	VAL	3.2
2	R	81	VAL	3.2
2	R	111	MET	3.2
1	E	865	GLU	3.1
1	E	876	ALA	3.1
2	R	122	ASP	3.1
1	E	442	VAL	3.1
1	E	356	PHE	3.1
1	E	875	TYR	3.1
2	R	82	TYR	3.1
1	E	708	ASN	3.1
1	E	687	SER	3.0
2	R	163	ARG	3.0
2	R	55	ILE	3.0
1	E	873	LYS	3.0
2	R	57	ASP	3.0
1	E	962	HIS	3.0
1	E	866	LYS	3.0
2	R	36	ILE	3.0
1	E	448	ARG	3.0
2	R	80	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	437	ARG	2.9
2	R	152	ILE	2.9
1	E	581	MET	2.9
1	E	689	GLU	2.9
1	E	964	ASP	2.9
2	R	160	ASP	2.9
1	E	315	ARG	2.9
1	E	454	GLN	2.9
2	R	116	ASN	2.9
1	E	868	PRO	2.9
2	R	96	LEU	2.9
2	R	99	GLN	2.9
1	E	867	LEU	2.8
1	E	701	GLU	2.8
2	R	119	ASP	2.8
1	E	455	ASP	2.8
2	R	154	VAL	2.8
1	E	313	ILE	2.8
1	E	880	SER	2.8
1	E	372	GLU	2.8
1	E	819	LEU	2.8
2	R	102	ARG	2.8
1	E	925	ASP	2.7
1	E	506	GLU	2.7
1	E	818	GLN	2.7
1	E	433	GLU	2.7
1	E	838	GLU	2.7
2	R	147	SER	2.7
1	E	644	GLN	2.6
1	E	820	SER	2.6
1	E	609	GLU	2.6
1	E	445	ASN	2.6
1	E	453	ASP	2.6
2	R	91	ASN	2.6
2	R	85	THR	2.6
1	E	756	LYS	2.6
1	E	864	TRP	2.6
2	R	156	GLU	2.6
1	E	355	ILE	2.6
1	E	877	GLU	2.6
1	E	317	PRO	2.5
1	E	502	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	990	PRO	2.5
1	E	885	SER	2.5
1	E	354	LEU	2.5
1	E	679	SER	2.5
1	E	440	ARG	2.5
1	E	335	HIS	2.5
1	E	871	PHE	2.5
1	E	353	VAL	2.5
1	E	505	ASN	2.5
1	E	332	GLU	2.4
2	R	37	GLU	2.4
1	E	504	LEU	2.4
2	R	148	ALA	2.4
1	E	881	LEU	2.4
1	E	341	HIS	2.4
1	E	683	ASP	2.3
1	E	969	VAL	2.3
2	R	41	ARG	2.3
1	E	926	ASN	2.3
1	E	897	LYS	2.3
1	E	973	ASN	2.3
2	R	117	LYS	2.3
2	R	124	ARG	2.3
1	E	399	GLU	2.3
2	R	76	GLN	2.3
1	E	870	LYS	2.3
1	E	965	VAL	2.3
1	E	610	LYS	2.2
1	E	859	ARG	2.2
1	E	682	ALA	2.2
1	E	760	TYR	2.2
2	R	13	GLY	2.2
1	E	492	GLU	2.2
1	E	604	GLN	2.2
1	E	326	LEU	2.2
1	E	862	LEU	2.2
1	E	509	ASP	2.2
1	E	831	LYS	2.2
2	R	79	ALA	2.2
2	R	88	SER	2.2
1	E	608	LEU	2.1
2	R	7	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	74	ASN	2.1
1	E	835	HIS	2.1
1	E	748	GLY	2.1
1	E	863	THR	2.1
1	E	886	ARG	2.1
1	E	411	ASP	2.1
2	R	123	GLU	2.1
1	E	602	LYS	2.1
1	E	757	ASP	2.1
1	E	667	ARG	2.1
1	E	575	GLN	2.1
2	R	6	LEU	2.1
1	E	499	ARG	2.1
1	E	508	THR	2.0
1	E	334	LEU	2.0
1	E	643	ARG	2.0
2	R	151	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no 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.

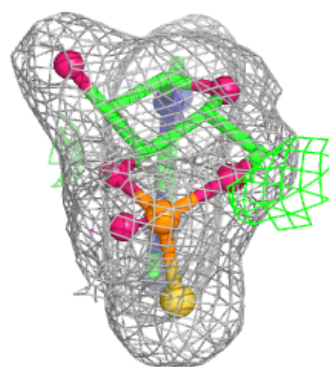
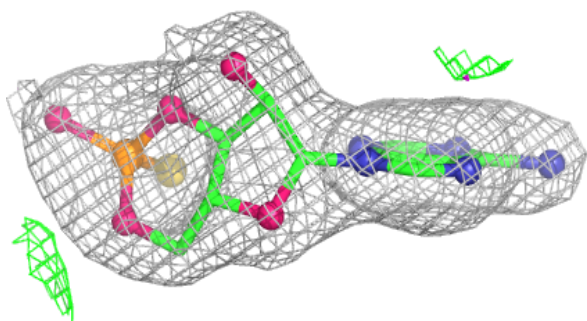
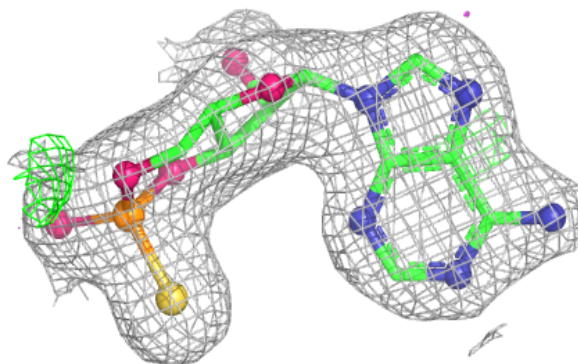
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SP1	E	3	22/22	0.98	0.06	32,36,39,40	0
4	SO4	R	168	5/5	0.98	0.06	34,35,37,39	0
3	SP1	E	2	22/22	0.99	0.05	27,30,34,36	0

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.

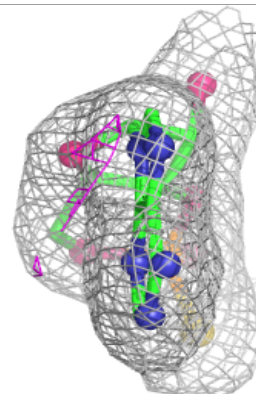
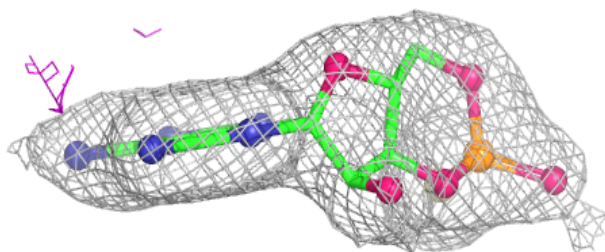
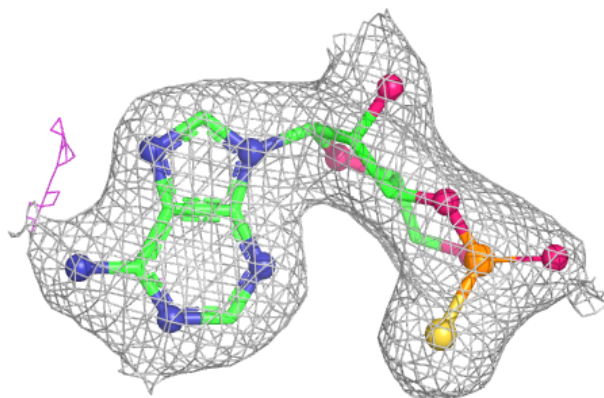
Electron density around SP1 E 3:

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



Electron density around SP1 E 2:

$2mF_o-DF_c$ (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.