



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 7SSJ / pdb_00007ssj
Title : Crystal structure of the DesK-DesR complex in the phosphatase state
Authors : Trajtenberg, F.; Buschiazzi, A.
Deposited on : 2021-11-11
Resolution : 2.52 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

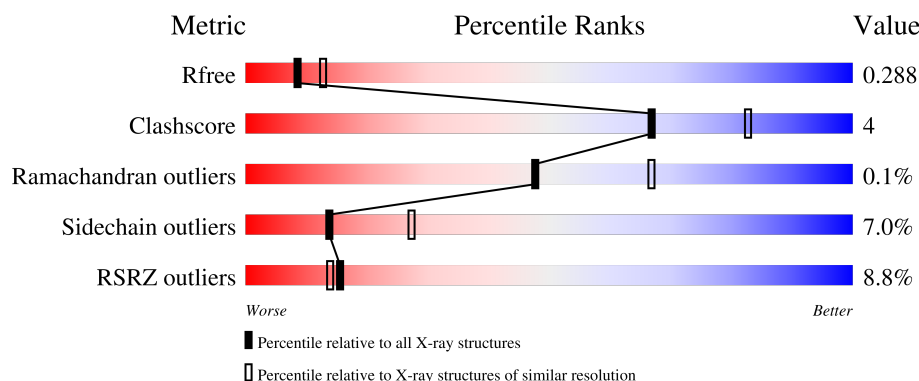
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	224	7% 83% 15% .
1	C	224	14% 86% 10% .
1	D	224	4% 84% 12% ..
2	B	139	% 74% 19% 6%
2	E	139	4% 83% 11% 6%

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Mol	Chain	Length	Quality of chain
2	F	139	21% 78% 14% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8101 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 Sensor histidine kinase DesK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1687	1050	304	328	5			
1	C	216	Total	C	N	O	S	0	1	0
			1675	1046	297	326	6			
1	D	218	Total	C	N	O	S	0	0	0
			1694	1057	304	327	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLY	-	expression tag	UNP O34757
A	148	SER	-	expression tag	UNP O34757
A	149	GLY	-	expression tag	UNP O34757
A	150	ILE	SER	engineered mutation	UNP O34757
A	153	LEU	SER	engineered mutation	UNP O34757
A	157	ILE	ARG	engineered mutation	UNP O34757
C	147	GLY	-	expression tag	UNP O34757
C	148	SER	-	expression tag	UNP O34757
C	149	GLY	-	expression tag	UNP O34757
C	150	ILE	SER	engineered mutation	UNP O34757
C	153	LEU	SER	engineered mutation	UNP O34757
C	157	ILE	ARG	engineered mutation	UNP O34757
D	147	GLY	-	expression tag	UNP O34757
D	148	SER	-	expression tag	UNP O34757
D	149	GLY	-	expression tag	UNP O34757
D	150	ILE	SER	engineered mutation	UNP O34757
D	153	LEU	SER	engineered mutation	UNP O34757
D	157	ILE	ARG	engineered mutation	UNP O34757

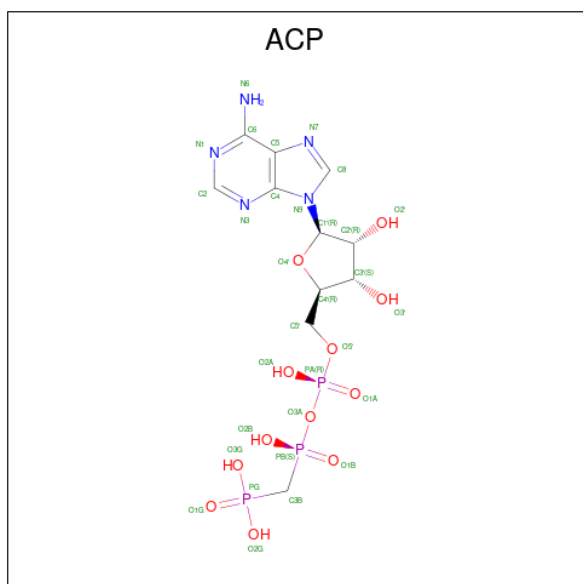
- Molecule 2 is a protein called Transcriptional regulatory protein DesR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			961	607	156	189	9			
2	E	131	Total	C	N	O	S	0	1	0
			991	626	163	193	9			
2	F	130	Total	C	N	O	S	0	0	0
			955	603	157	186	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP O34723
B	-2	SER	-	expression tag	UNP O34723
B	-1	GLY	-	expression tag	UNP O34723
B	0	SER	-	expression tag	UNP O34723
E	-3	GLY	-	expression tag	UNP O34723
E	-2	SER	-	expression tag	UNP O34723
E	-1	GLY	-	expression tag	UNP O34723
E	0	SER	-	expression tag	UNP O34723
F	-3	GLY	-	expression tag	UNP O34723
F	-2	SER	-	expression tag	UNP O34723
F	-1	GLY	-	expression tag	UNP O34723
F	0	SER	-	expression tag	UNP O34723

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

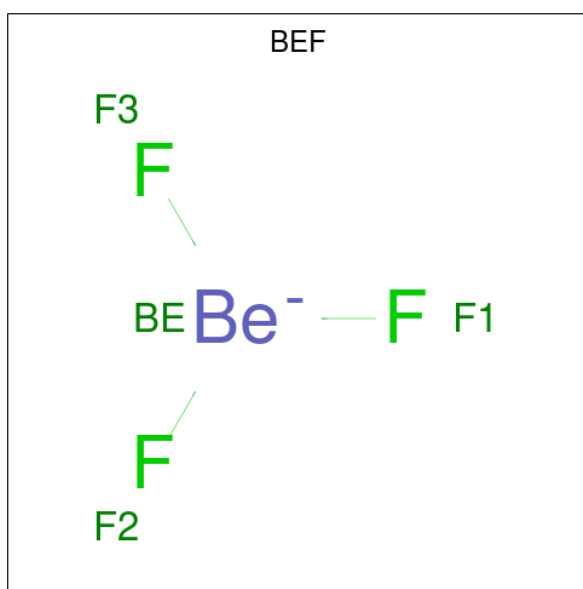


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Be	F	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	Be	F	0	0
			4	1	3		
5	F	1	Total	Be	F	0	0
			4	1	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

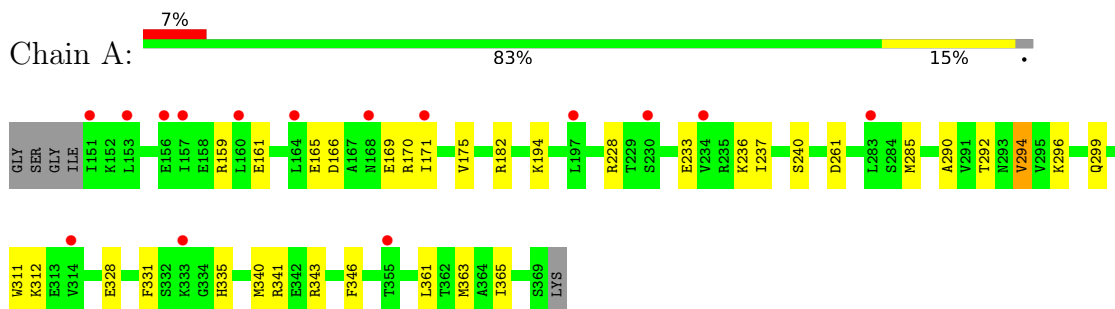
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	B	3	Total	O	0	0
			3	3		
7	C	2	Total	O	0	0
			2	2		
7	D	3	Total	O	0	0
			3	3		
7	E	5	Total	O	0	0
			5	5		
7	F	2	Total	O	0	0
			2	2		

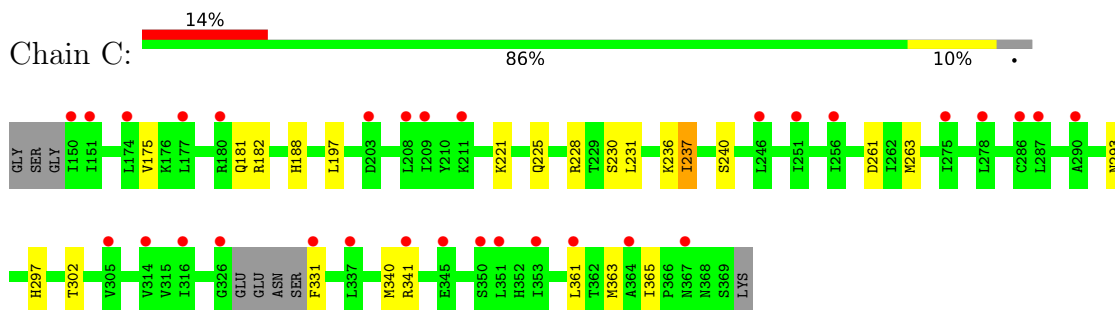
3 Residue-property plots [i](#)

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.

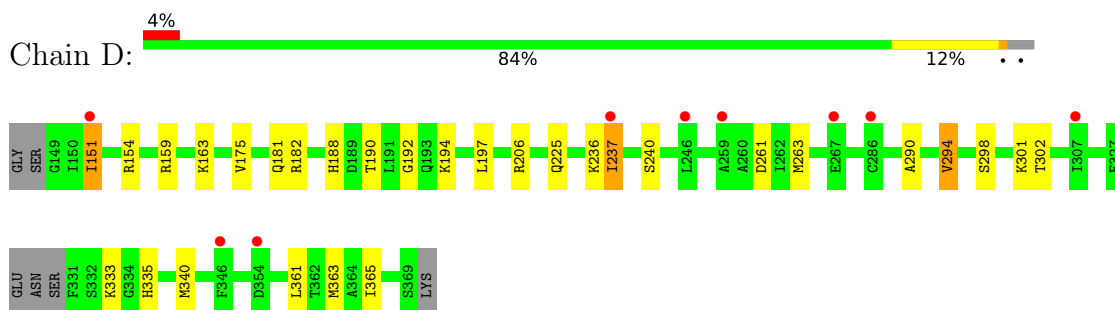
- Molecule 1: Sensor histidine kinase DesK



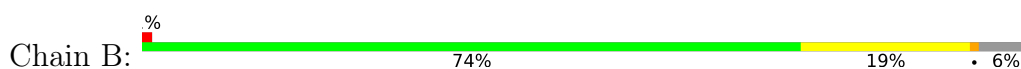
- Molecule 1: Sensor histidine kinase DesK

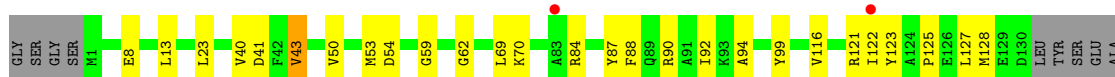


- Molecule 1: Sensor histidine kinase DesK

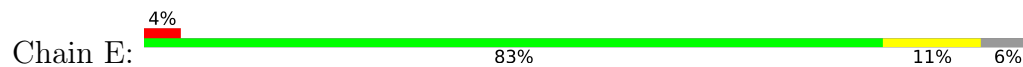


- Molecule 2: Transcriptional regulatory protein DesR

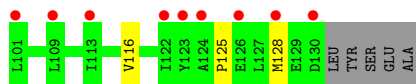
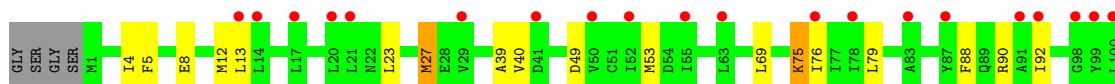
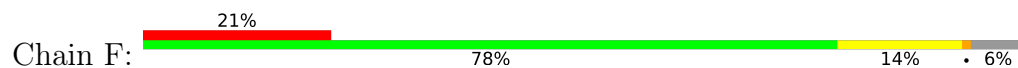




- Molecule 2: Transcriptional regulatory protein DesR



- Molecule 2: Transcriptional regulatory protein DesR



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.69Å 94.69Å 240.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.00 – 2.52 82.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	79.3 (82.00-2.52) 79.3 (82.00-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.253 , 0.289 0.249 , 0.288	Depositor DCC
R_{free} test set	1720 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	81.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8101	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, SO4, MG, ACP

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	0.81	0/1702	1.14	0/2295
1	C	0.69	0/1692	1.09	0/2279
1	D	0.73	0/1708	1.11	3/2297 (0.1%)
2	B	0.83	0/972	1.11	2/1311 (0.2%)
2	E	0.75	0/1005	1.08	1/1352 (0.1%)
2	F	0.72	0/966	1.10	2/1303 (0.2%)
All	All	0.75	0/8045	1.11	8/10837 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	SER	N-CA-C	5.93	117.41	111.07
2	B	53	MET	N-CA-C	5.57	117.51	108.26
2	F	76	ILE	N-CA-C	5.57	116.19	108.84
1	D	151	ILE	CA-C-N	5.48	127.90	120.44
1	D	151	ILE	C-N-CA	5.48	127.90	120.44
2	E	41	ASP	CA-CB-CG	5.34	117.94	112.60
2	F	53	MET	N-CA-C	5.31	117.07	108.26
2	B	41	ASP	CA-CB-CG	5.08	117.68	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1687	0	1680	17	0
1	C	1675	0	1674	13	0
1	D	1694	0	1711	14	0
2	B	961	0	954	12	0
2	E	991	0	1012	5	0
2	F	955	0	945	7	0
3	A	31	0	14	1	0
3	C	31	0	14	2	0
3	D	31	0	14	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	B	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
6	E	5	0	0	0	0
7	A	7	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
7	D	3	0	0	0	0
7	E	5	0	0	0	0
7	F	2	0	0	0	0
All	All	8101	0	8018	59	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 4.

All (59) 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:166:ASP:O	1:A:170:ARG:HB2	1.70	0.91
2:B:70:LYS:HE2	2:B:94:ALA:HA	1.61	0.82
1:D:361:LEU:HB3	1:D:363:MET:HE2	1.77	0.67
1:A:361:LEU:HB3	1:A:363:MET:HE2	1.77	0.66
1:A:311:TRP:HE1	1:A:312:LYS:NZ	1.93	0.66
1:C:361:LEU:HB3	1:C:363:MET:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:PRO:HA	2:B:128:MET:HE2	1.80	0.63
1:A:165:GLU:O	1:A:169:GLU:HB3	1.99	0.61
1:A:311:TRP:NE1	1:A:312:LYS:HZ3	1.98	0.61
1:A:311:TRP:NE1	1:A:312:LYS:NZ	2.49	0.61
1:A:331:PHE:CZ	1:A:341:ARG:NH1	2.69	0.61
1:C:331:PHE:CZ	1:C:341:ARG:NH1	2.69	0.60
1:C:197:LEU:HD21	2:E:12:MET:HE3	1.83	0.60
1:A:311:TRP:HE1	1:A:312:LYS:HZ1	1.50	0.59
2:F:49:ASP:O	2:F:75:LYS:HG2	2.06	0.55
1:C:221:LYS:NZ	1:D:206:ARG:HD2	2.23	0.54
1:D:340:MET:HE1	1:D:361:LEU:HD23	1.89	0.54
2:E:88:PHE:O	2:E:92:ILE:HG12	2.08	0.53
2:B:84:ARG:HB2	2:B:87:TYR:CE2	2.44	0.52
1:C:188:HIS:CE1	1:D:237:ILE:HD11	2.45	0.52
1:A:311:TRP:CD1	1:A:312:LYS:HG3	2.45	0.52
2:F:40:VAL:HA	2:F:69:LEU:HD21	1.91	0.51
2:E:99:TYR:CE2	2:E:127:LEU:HB3	2.46	0.50
1:C:263:MET:HB2	1:C:302:THR:HG22	1.94	0.50
2:F:125:PRO:HA	2:F:128:MET:HE2	1.94	0.50
1:C:340:MET:HE1	1:C:361:LEU:HD23	1.94	0.50
2:B:88:PHE:O	2:B:92:ILE:HG12	2.12	0.49
2:F:4:ILE:HD11	2:F:27:MET:HG2	1.94	0.49
1:C:237:ILE:HD11	1:D:188:HIS:CE1	2.48	0.48
2:B:43:VAL:HG21	2:B:69:LEU:HD13	1.95	0.48
1:C:221:LYS:HZ2	1:D:206:ARG:HD2	1.78	0.48
1:D:263:MET:HB2	1:D:302:THR:HG22	1.95	0.48
2:B:84:ARG:HB2	2:B:87:TYR:CD2	2.49	0.47
1:D:197:LEU:HD21	2:F:12:MET:HE3	1.97	0.46
1:A:233:GLU:HG3	1:A:346:PHE:CE2	2.52	0.45
1:A:166:ASP:O	1:A:170:ARG:CB	2.55	0.45
1:A:292:THR:O	1:A:296:LYS:HG3	2.17	0.45
2:B:121:ARG:HD3	2:B:123:TYR:OH	2.18	0.44
1:C:231:LEU:HD13	1:D:192:GLY:HA2	1.99	0.44
1:A:312:LYS:HZ2	2:B:59:GLY:HA3	1.83	0.44
1:C:297:HIS:CG	3:C:401:ACP:H2'	2.53	0.44
2:F:88:PHE:O	2:F:92:ILE:HG12	2.18	0.44
1:A:340:MET:HE1	1:A:361:LEU:HD23	2.00	0.43
2:E:54:ASP:O	2:E:57:MET:HE2	2.18	0.43
1:A:290:ALA:O	1:A:294:VAL:HG13	2.17	0.43
2:B:54:ASP:O	2:B:62:GLY:HA3	2.19	0.43
1:C:293:ASN:HB3	3:C:401:ACP:N7	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ARG:HE	1:D:163:LYS:HE2	1.84	0.43
2:B:40:VAL:HA	2:B:69:LEU:HD21	2.01	0.42
2:B:99:TYR:HE2	2:B:127:LEU:CB	2.31	0.42
1:A:335:HIS:HB3	3:A:401:ACP:O2A	2.19	0.42
2:F:5:PHE:CE2	2:F:39:ALA:HA	2.55	0.42
1:D:335:HIS:HB3	3:D:401:ACP:O2A	2.19	0.41
2:B:70:LYS:CE	2:B:94:ALA:HA	2.41	0.41
1:D:290:ALA:O	1:D:294:VAL:HG13	2.19	0.41
2:E:42:PHE:CE2	2:E:46:ARG:HG3	2.56	0.41
1:D:194:LYS:HA	1:D:194:LYS:HD3	1.95	0.41
1:C:181:GLN:OE1	1:D:181:GLN:OE1	2.39	0.41
1:A:285:MET:SD	1:A:343:ARG:NH1	2.94	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	217/224 (97%)	213 (98%)	3 (1%)	1 (0%)	24	41
1	C	213/224 (95%)	210 (99%)	3 (1%)	0	100	100
1	D	214/224 (96%)	213 (100%)	1 (0%)	0	100	100
2	B	128/139 (92%)	121 (94%)	7 (6%)	0	100	100
2	E	130/139 (94%)	121 (93%)	9 (7%)	0	100	100
2	F	128/139 (92%)	121 (94%)	7 (6%)	0	100	100
All	All	1030/1089 (95%)	999 (97%)	30 (3%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	GLU

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	178/199 (89%)	164 (92%)	14 (8%)	11	22
1	C	178/199 (89%)	168 (94%)	10 (6%)	19	37
1	D	181/199 (91%)	167 (92%)	14 (8%)	12	23
2	B	99/113 (88%)	91 (92%)	8 (8%)	11	22
2	E	106/113 (94%)	101 (95%)	5 (5%)	23	44
2	F	97/113 (86%)	89 (92%)	8 (8%)	10	21
All	All	839/936 (90%)	780 (93%)	59 (7%)	14	27

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

Mol	Chain	Res	Type
1	A	159	ARG
1	A	161	GLU
1	A	171	ILE
1	A	175	VAL
1	A	182	ARG
1	A	194	LYS
1	A	228	ARG
1	A	236	LYS
1	A	237	ILE
1	A	240	SER
1	A	261	ASP
1	A	294	VAL
1	A	299	GLN
1	A	365	ILE
2	B	8	GLU
2	B	13	LEU
2	B	23	LEU
2	B	43	VAL
2	B	50	VAL
2	B	90	ARG
2	B	116	VAL
2	B	122	ILE

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Mol	Chain	Res	Type
1	C	175	VAL
1	C	182	ARG
1	C	225	GLN
1	C	228	ARG
1	C	230	SER
1	C	236	LYS
1	C	237	ILE
1	C	240	SER
1	C	261	ASP
1	C	365	ILE
1	D	151	ILE
1	D	154	ARG
1	D	175	VAL
1	D	182	ARG
1	D	190	THR
1	D	225	GLN
1	D	236	LYS
1	D	237	ILE
1	D	240	SER
1	D	261	ASP
1	D	294	VAL
1	D	301	LYS
1	D	333	LYS
1	D	365	ILE
2	E	8	GLU
2	E	13	LEU
2	E	23	LEU
2	E	116	VAL
2	E	122	ILE
2	F	8	GLU
2	F	13	LEU
2	F	23	LEU
2	F	27	MET
2	F	75	LYS
2	F	79	LEU
2	F	90	ARG
2	F	116	VAL

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	255	GLN

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Mol	Chain	Res	Type
1	A	281	ASN
1	C	193	GLN
1	C	255	GLN
1	D	193	GLN
1	D	225	GLN
1	D	255	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](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\# Z > 2$
3	ACP	C	401	4	31,33,33	0.61	1 (3%)	47,52,52	0.60	1 (2%)
3	ACP	D	401	4	31,33,33	0.66	1 (3%)	47,52,52	0.68	1 (2%)
5	BEF	F	202	2	0,3,3	-	-	-	-	-
6	SO4	E	203	-	4,4,4	0.31	0	6,6,6	0.12	0
3	ACP	A	401	4	31,33,33	0.60	1 (3%)	47,52,52	0.56	1 (2%)
5	BEF	B	202	2	0,3,3	-	-	-	-	-
5	BEF	E	202	2	0,3,3	-	-	-	-	-

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	ACP	A	401	4	-	3/19/38/38	0/3/3/3
3	ACP	C	401	4	-	3/19/38/38	0/3/3/3
3	ACP	D	401	4	-	3/19/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ACP	PB-O3A	3.06	1.61	1.58
3	A	401	ACP	PB-O3A	2.93	1.61	1.58
3	D	401	ACP	PB-O3A	2.75	1.61	1.58

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ACP	O1B-PB-C3B	3.17	117.40	109.05
3	C	401	ACP	O1B-PB-C3B	2.94	116.79	109.05
3	A	401	ACP	O1B-PB-C3B	2.87	116.60	109.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

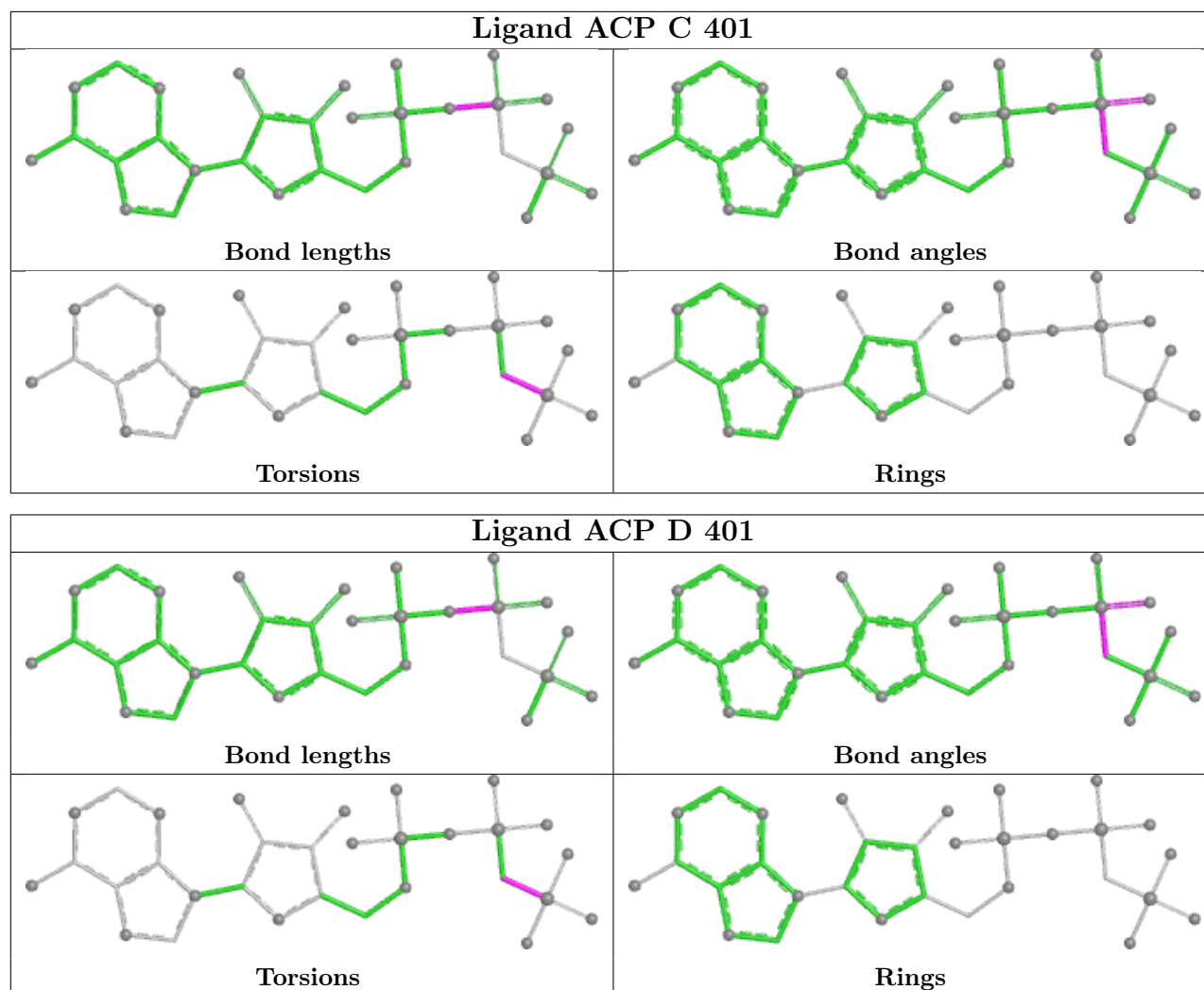
Mol	Chain	Res	Type	Atoms
3	A	401	ACP	PB-C3B-PG-O1G
3	A	401	ACP	PB-C3B-PG-O2G
3	C	401	ACP	PB-C3B-PG-O1G
3	C	401	ACP	PB-C3B-PG-O3G
3	D	401	ACP	PB-C3B-PG-O1G
3	D	401	ACP	PB-C3B-PG-O2G
3	D	401	ACP	PB-C3B-PG-O3G
3	A	401	ACP	PB-C3B-PG-O3G
3	C	401	ACP	PB-C3B-PG-O2G

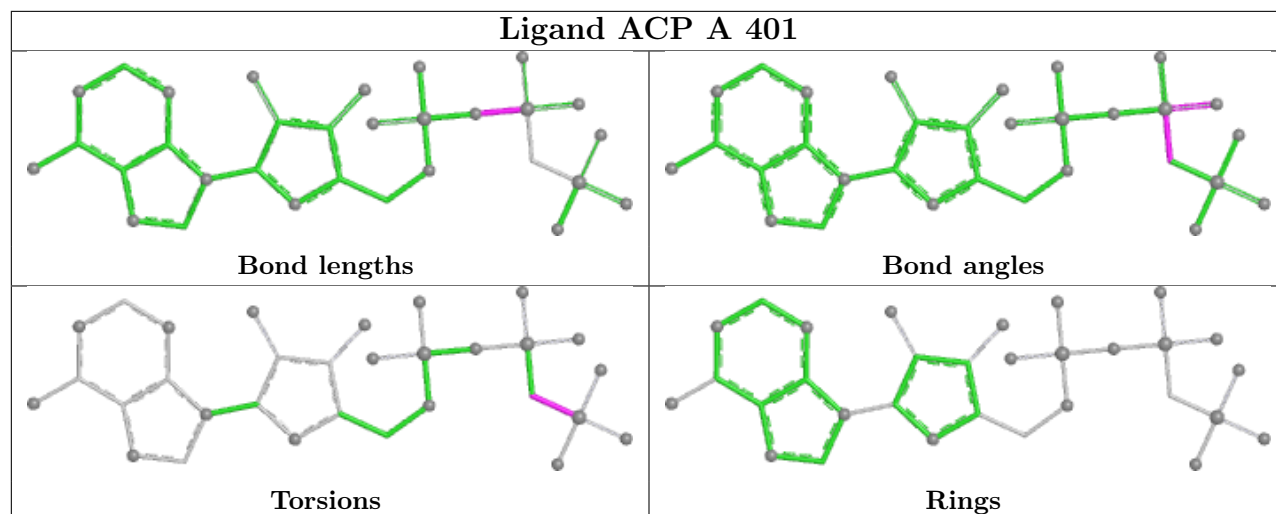
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	ACP	2	0
3	D	401	ACP	1	0
3	A	401	ACP	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	219/224 (97%)	0.66	15 (6%) 23 21	60, 85, 129, 139	11 (5%)
1	C	216/224 (96%)	1.03	31 (14%) 6 5	55, 132, 189, 212	1 (0%)
1	D	218/224 (97%)	0.60	9 (4%) 41 38	70, 108, 138, 159	0
2	B	130/139 (93%)	0.51	2 (1%) 72 69	60, 78, 109, 123	0
2	E	131/139 (94%)	0.54	6 (4%) 37 34	52, 81, 103, 115	1 (0%)
2	F	130/139 (93%)	1.36	29 (22%) 2 2	97, 119, 132, 136	0
All	All	1044/1089 (95%)	0.78	92 (8%) 15 14	52, 101, 150, 212	13 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	LYS	4.9
2	F	83	ALA	4.7
1	A	164	LEU	4.5
1	C	246	LEU	4.4
1	C	350	SER	4.2
1	C	150	ILE	4.2
1	A	156	GLU	4.1
1	A	151	ILE	4.0
1	C	337	LEU	4.0
2	F	109	LEU	3.8
2	E	21	LEU	3.7
2	F	78	ILE	3.7
2	F	20	LEU	3.5
1	C	331	PHE	3.5
1	C	174	LEU	3.5
1	C	177	LEU	3.4
1	D	151	ILE	3.4
1	A	153	LEU	3.4
1	C	353	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	101	LEU	3.3
1	A	333	LYS	3.2
1	C	290	ALA	3.2
1	A	160	LEU	3.2
2	F	99	TYR	3.2
2	F	100	LEU	3.1
2	F	17	LEU	3.0
2	F	55	ILE	2.9
1	C	341	ARG	2.9
1	C	351	LEU	2.8
1	C	203	ASP	2.8
1	C	180	ARG	2.8
2	F	87	TYR	2.8
2	F	98	GLY	2.8
1	A	171	ILE	2.8
2	F	52	ILE	2.8
1	D	246	LEU	2.8
2	F	123	TYR	2.7
1	A	355	THR	2.7
2	F	21	LEU	2.7
1	C	151	ILE	2.6
1	D	286	CYS	2.6
2	B	122	ILE	2.6
2	F	91	ALA	2.6
2	F	92	ILE	2.6
1	A	168	ASN	2.6
2	F	29	VAL	2.6
2	F	113	ILE	2.5
2	F	126	GLU	2.5
1	C	314	VAL	2.5
2	F	13	LEU	2.5
2	F	76	ILE	2.5
1	A	197	LEU	2.5
1	D	259	ALA	2.5
1	C	286	CYS	2.5
1	A	157	ILE	2.5
1	C	275	ILE	2.5
2	B	83	ALA	2.5
1	C	208	LEU	2.4
2	F	14	LEU	2.4
1	C	256	ILE	2.4
1	D	237	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	345	GLU	2.4
1	C	361	LEU	2.4
1	C	364	ALA	2.4
2	E	17	LEU	2.3
1	C	367	ASN	2.3
1	D	354	ASP	2.3
1	C	326	GLY	2.3
2	E	20	LEU	2.3
1	D	346	PHE	2.3
1	A	314	VAL	2.3
1	A	230	SER	2.3
2	E	127	LEU	2.3
1	C	287	LEU	2.2
1	C	278	LEU	2.2
2	F	130	ASP	2.2
1	C	209	ILE	2.2
1	C	251	ILE	2.2
2	F	124	ALA	2.2
2	E	71	ASP	2.2
1	C	316	ILE	2.1
2	F	122	ILE	2.1
2	E	130	ASP	2.1
1	C	305	VAL	2.1
1	A	283	LEU	2.1
1	A	234	VAL	2.1
2	F	50	VAL	2.1
1	D	267	GLU	2.1
2	F	128	MET	2.0
2	F	63	LEU	2.0
1	D	307	ILE	2.0
2	F	41	ASP	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

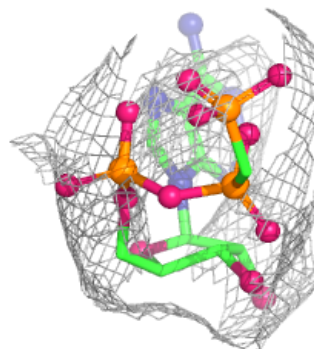
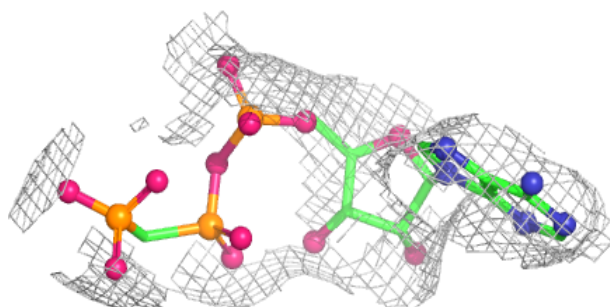
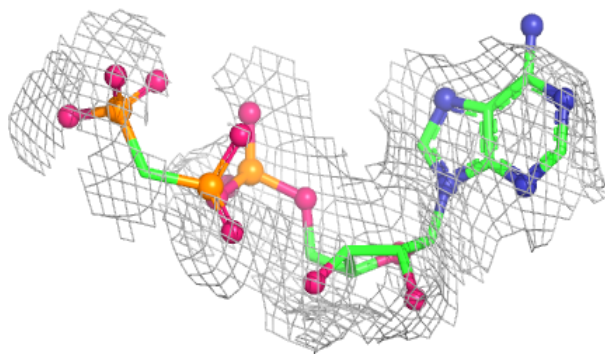
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	E	203	5/5	0.84	0.08	170,170,170,170	0
5	BEF	F	202	4/4	0.86	0.10	122,122,122,123	0
3	ACP	C	401	31/31	0.90	0.08	152,156,159,159	0
5	BEF	E	202	4/4	0.91	0.09	74,75,75,77	0
3	ACP	D	401	31/31	0.94	0.07	87,89,91,91	0
4	MG	F	201	1/1	0.94	0.08	133,133,133,133	0
5	BEF	B	202	4/4	0.94	0.08	72,72,73,73	0
3	ACP	A	401	31/31	0.95	0.06	90,92,97,97	0
4	MG	C	402	1/1	0.96	0.07	188,188,188,188	0
4	MG	E	201	1/1	0.99	0.05	77,77,77,77	0
4	MG	B	201	1/1	0.99	0.02	51,51,51,51	0
4	MG	D	402	1/1	0.99	0.05	89,89,89,89	0
4	MG	A	402	1/1	1.00	0.09	84,84,84,84	0

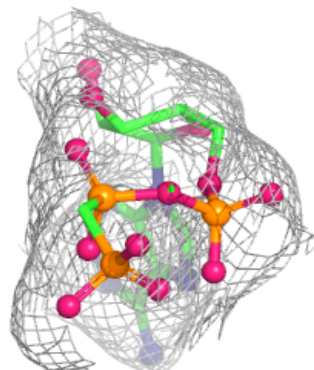
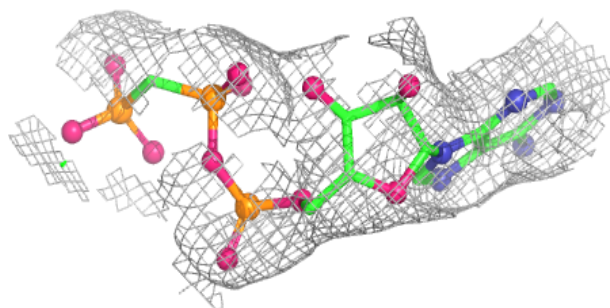
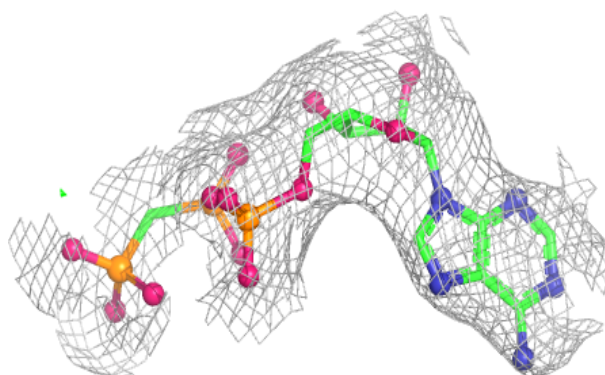
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

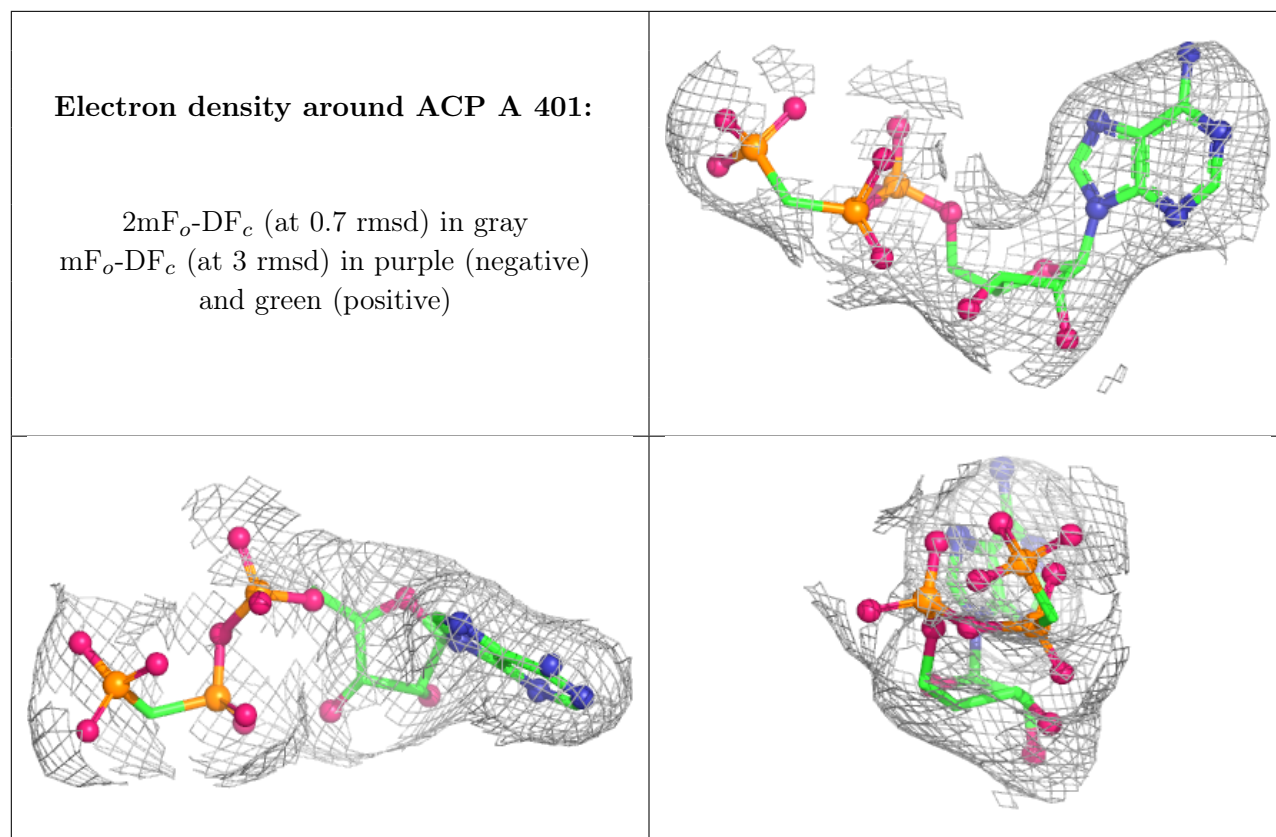
Electron density around ACP C 401:

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

**Electron density around ACP D 401:**

$2mF_o-DF_c$ (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.