



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 AM UTC

PDB ID : 5IUL / pdb_00005iul
Title : Crystal structure of the DesK-DesR complex in the phosphotransfer state with high Mg²⁺ (150 mM) and BeF₃
Authors : Trajtenberg, F.; Imelio, J.A.; Larrieux, N.; Buschiazzi, A.
Deposited on : 2016-03-18
Resolution : 3.15 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

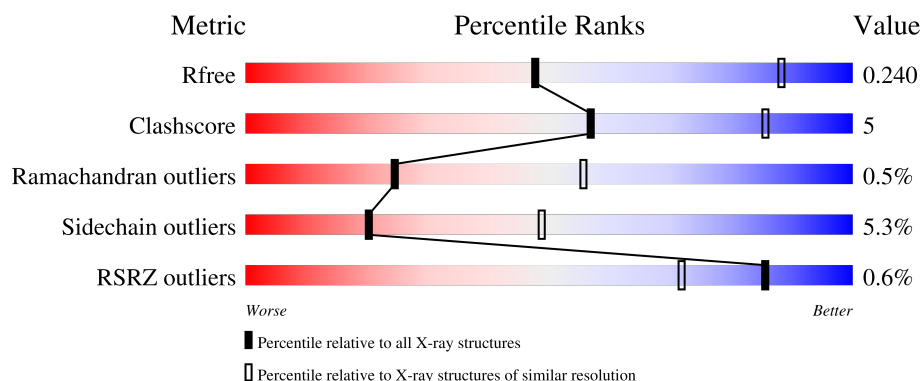
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

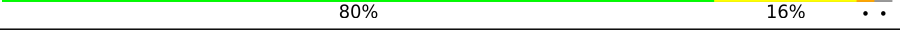
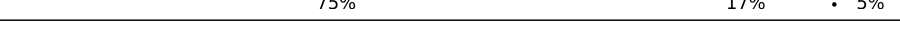
The reported resolution of this entry is 3.15 Å.

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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	218	 83% 13% .
1	B	218	 75% 16% . 5%
1	D	218	 80% 16% . .
1	E	218	 75% 17% . 5%
2	C	139	 82% 12% . 5%

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Mol	Chain	Length	Quality of chain
2	F	139	% 81% 13% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8859 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	211	Total	C	N	O	S	0	0	0
			1696	1056	301	332	7			
1	B	207	Total	C	N	O	S	0	0	0
			1644	1020	295	323	6			
1	D	213	Total	C	N	O	S	0	0	0
			1708	1062	303	336	7			
1	E	207	Total	C	N	O	S	0	0	0
			1643	1019	296	322	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP O34757
A	188	GLU	HIS	engineered mutation	UNP O34757
B	153	GLY	-	expression tag	UNP O34757
B	188	GLU	HIS	engineered mutation	UNP O34757
D	153	GLY	-	expression tag	UNP O34757
D	188	GLU	HIS	engineered mutation	UNP O34757
E	153	GLY	-	expression tag	UNP O34757
E	188	GLU	HIS	engineered mutation	UNP O34757

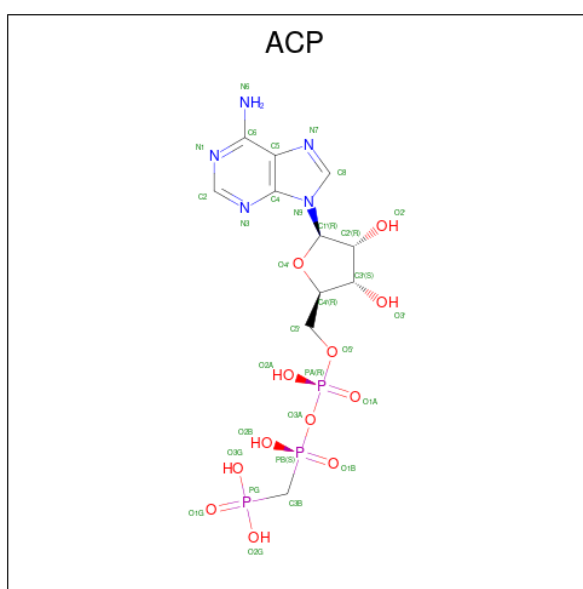
- Molecule 2 is a protein called Transcriptional regulatory protein DesR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	132	Total	C	N	O	S	0	0	0
			1006	635	165	197	9			
2	F	132	Total	C	N	O	S	0	0	0
			1012	641	165	197	9			

There are 8 discrepancies between the modelled and reference sequences:

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

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total 2	K 2	0	0

- Molecule 6 is water.

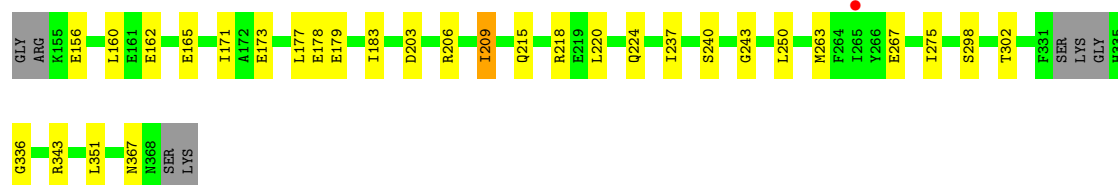
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	1	Total 1	O 1	0	0
6	C	6	Total 6	O 6	0	0
6	D	3	Total 3	O 3	0	0
6	E	1	Total 1	O 1	0	0
6	F	4	Total 4	O 4	0	0

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.

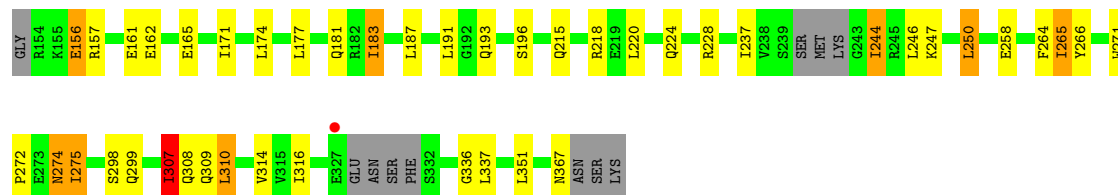
- Molecule 1: Sensor histidine kinase DesK

Chain A: 



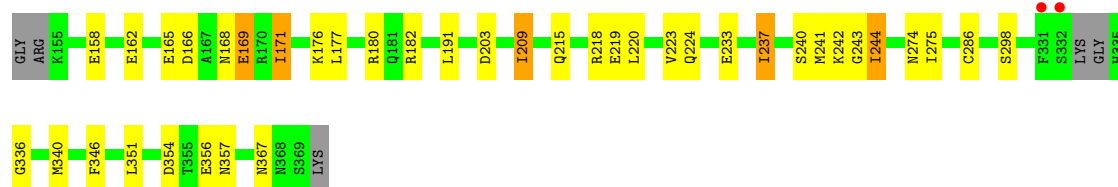
- Molecule 1: Sensor histidine kinase DesK

Chain B: 



- Molecule 1: Sensor histidine kinase DesK

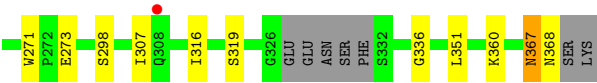
Chain D: 



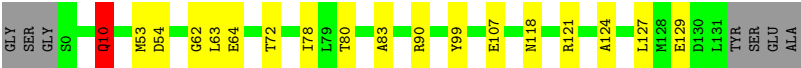
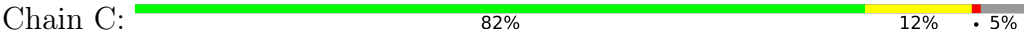
- Molecule 1: Sensor histidine kinase DesK

Chain E: 

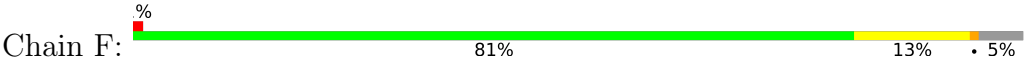




● Molecule 2: Transcriptional regulatory protein DesR



● Molecule 2: Transcriptional regulatory protein DesR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.19Å 116.68Å 91.88Å 90.00° 117.10° 90.00°	Depositor
Resolution (Å)	38.59 – 3.15 38.59 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.59-3.15) 97.7 (38.59-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.18Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.190 , 0.231 0.199 , 0.240	Depositor DCC
R_{free} test set	1361 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8859	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: ACP, K, MG

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	0/1710	1.38	8/2292 (0.3%)
1	B	0.82	0/1654	1.49	18/2216 (0.8%)
1	D	0.80	1/1722 (0.1%)	1.38	15/2308 (0.6%)
1	E	0.84	2/1653 (0.1%)	1.41	21/2215 (0.9%)
2	C	0.90	0/1017	1.38	5/1366 (0.4%)
2	F	0.87	0/1024	1.33	3/1376 (0.2%)
All	All	0.84	3/8780 (0.0%)	1.40	70/11773 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	243	GLY	C-N	6.23	1.40	1.33
1	E	237	ILE	CA-C	5.40	1.59	1.52
1	E	238	VAL	CA-C	5.37	1.59	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ILE	N-CA-C	-9.27	102.57	113.42
1	B	265	ILE	CB-CG1-CD1	7.95	130.49	113.80
1	D	244	ILE	N-CA-CB	7.54	119.19	110.82
1	E	180	ARG	CA-C-N	7.04	130.05	120.54
1	E	180	ARG	C-N-CA	7.04	130.05	120.54
1	B	336	GLY	N-CA-C	6.85	120.44	112.50
1	B	244	ILE	CA-C-N	6.69	135.88	121.64
1	B	244	ILE	C-N-CA	6.69	135.88	121.64
1	D	237	ILE	CA-C-N	6.54	129.75	120.53
1	D	237	ILE	C-N-CA	6.54	129.75	120.53
2	C	72	THR	N-CA-C	-6.38	101.33	110.59
1	B	274	ASN	CA-C-N	6.33	130.44	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ASN	C-N-CA	6.33	130.44	121.96
1	E	336	GLY	N-CA-C	6.31	119.82	112.50
1	E	155	LYS	N-CA-C	-6.25	105.69	113.38
1	E	298	SER	N-CA-C	6.17	118.08	111.36
1	E	157	ARG	N-CA-C	-6.15	104.48	111.07
1	E	237	ILE	CB-CA-C	6.05	116.58	110.65
1	D	336	GLY	N-CA-C	6.01	119.94	112.73
1	E	367	ASN	CA-C-N	5.96	132.42	121.70
1	E	367	ASN	C-N-CA	5.96	132.42	121.70
1	A	336	GLY	N-CA-C	5.90	119.81	112.73
1	D	171	ILE	CA-C-N	5.88	128.08	120.44
1	D	171	ILE	C-N-CA	5.88	128.08	120.44
1	B	157	ARG	N-CA-C	-5.79	104.66	110.97
1	A	298	SER	N-CA-C	5.72	117.60	111.36
1	B	298	SER	N-CA-C	5.72	117.60	111.36
1	B	162	GLU	CA-C-N	5.72	128.22	120.38
1	B	162	GLU	C-N-CA	5.72	128.22	120.38
1	D	298	SER	N-CA-C	5.71	117.58	111.36
1	B	307	ILE	CB-CA-C	5.67	116.87	110.41
2	C	129	GLU	CA-C-N	5.65	132.33	121.54
2	C	129	GLU	C-N-CA	5.65	132.33	121.54
2	F	125	PRO	CA-C-N	5.55	127.72	120.28
2	F	125	PRO	C-N-CA	5.55	127.72	120.28
1	A	243	GLY	CA-C-N	5.52	129.53	121.80
1	A	243	GLY	C-N-CA	5.52	129.53	121.80
1	B	157	ARG	CA-C-N	5.33	127.43	120.28
1	B	157	ARG	C-N-CA	5.33	127.43	120.28
1	E	157	ARG	CA-C-N	5.33	127.37	120.44
1	E	157	ARG	C-N-CA	5.33	127.37	120.44
1	E	244	ILE	CA-C-N	5.32	127.84	120.29
1	E	244	ILE	C-N-CA	5.32	127.84	120.29
1	D	176	LYS	CA-C-N	5.25	127.32	120.28
1	D	176	LYS	C-N-CA	5.25	127.32	120.28
1	D	191	LEU	CA-C-N	5.21	125.88	119.99
1	D	191	LEU	C-N-CA	5.21	125.88	119.99
1	E	162	GLU	CA-C-N	5.20	127.97	120.38
1	E	162	GLU	C-N-CA	5.20	127.97	120.38
1	E	168	ASN	CA-C-N	5.19	127.18	120.44
1	E	168	ASN	C-N-CA	5.19	127.18	120.44
1	D	346	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	156	GLU	CA-C-N	5.16	127.46	120.65
1	B	156	GLU	C-N-CA	5.16	127.46	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLU	CA-C-N	5.15	127.18	120.28
1	A	162	GLU	C-N-CA	5.15	127.18	120.28
1	B	307	ILE	N-CA-CB	-5.12	105.68	112.34
2	F	131	LEU	N-CA-C	-5.11	103.72	111.34
1	D	169	GLU	CA-C-N	5.08	127.51	120.29
1	D	169	GLU	C-N-CA	5.08	127.51	120.29
2	C	10	GLN	CA-C-N	5.08	127.34	120.38
2	C	10	GLN	C-N-CA	5.08	127.34	120.38
1	B	310	LEU	CD1-CG-CD2	5.07	121.96	110.80
1	A	178	GLU	N-CA-C	-5.07	105.44	110.97
1	E	368	ASN	CA-CB-CG	5.07	117.67	112.60
1	E	168	ASN	CA-CB-CG	5.04	117.64	112.60
1	E	177	LEU	CA-C-N	5.04	127.29	120.38
1	E	177	LEU	C-N-CA	5.04	127.29	120.38
1	D	203	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	203	ASP	CA-CB-CG	5.01	117.61	112.60

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	1696	0	1742	13	0
1	B	1644	0	1686	25	0
1	D	1708	0	1752	17	0
1	E	1643	0	1686	22	0
2	C	1006	0	1033	10	0
2	F	1012	0	1037	9	0
3	A	31	0	14	0	0
3	B	31	0	14	1	0
3	D	31	0	14	0	0
3	E	31	0	14	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	C	2	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	6	0	0	0	0
6	D	3	0	0	0	0
6	E	1	0	0	0	0
6	F	4	0	0	0	0
All	All	8859	0	8992	82	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 5.

All (82) 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:220:LEU:HD21	1:B:220:LEU:HD21	1.50	0.92
1:B:187:LEU:HD22	1:B:191:LEU:HD12	1.65	0.79
1:B:308:GLN:HB2	1:B:310:LEU:HD21	1.65	0.78
1:E:244:ILE:HG22	1:E:247:LYS:H	1.54	0.73
1:D:242:LYS:HA	1:E:181:GLN:HE22	1.55	0.71
1:E:319:SER:HB2	1:E:360:LYS:HG2	1.71	0.71
1:B:307:ILE:HG13	1:B:316:ILE:HG12	1.75	0.69
1:E:319:SER:CB	1:E:360:LYS:HG2	2.22	0.69
1:B:244:ILE:HG22	1:B:247:LYS:H	1.59	0.68
1:B:275:ILE:HG12	1:B:314:VAL:HG21	1.75	0.66
2:C:64:GLU:HG3	2:C:90:ARG:HH22	1.62	0.65
2:F:99:TYR:CE2	2:F:127:LEU:HB3	2.31	0.65
2:F:64:GLU:HG3	2:F:90:ARG:HH22	1.63	0.64
1:A:343:ARG:HG3	1:B:174:LEU:HD11	1.81	0.63
1:B:308:GLN:HB2	1:B:310:LEU:CD2	2.30	0.62
1:D:286:CYS:HB3	1:D:340:MET:HE3	1.81	0.61
1:D:354:ASP:OD1	1:D:356:GLU:HG2	2.01	0.61
1:B:250:LEU:HB2	1:B:271:TRP:CH2	2.37	0.60
2:F:99:TYR:HE2	2:F:127:LEU:HB3	1.67	0.59
2:F:10:GLN:HB2	2:F:13:LEU:HD12	1.83	0.59
1:B:264:PHE:CE2	1:B:266:TYR:CD1	2.93	0.56
1:D:224:GLN:HE22	1:E:206:ARG:HD3	1.70	0.56
1:A:156:GLU:H	1:A:156:GLU:CD	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:GLU:HA	1:E:271:TRP:CD1	2.42	0.55
1:B:337:LEU:HD13	3:B:401:ACP:O5'	2.06	0.55
1:E:307:ILE:HG13	1:E:316:ILE:HG12	1.90	0.53
1:A:263:MET:HE2	1:A:302:THR:HG22	1.90	0.52
2:C:64:GLU:HG3	2:C:90:ARG:NH2	2.25	0.52
1:D:356:GLU:HG3	1:D:357:ASN:H	1.75	0.51
1:B:215:GLN:HA	1:B:218:ARG:HD2	1.93	0.50
1:E:215:GLN:HA	1:E:218:ARG:HD2	1.92	0.50
2:F:64:GLU:HG3	2:F:90:ARG:NH2	2.26	0.49
1:E:246:LEU:HD21	1:E:307:ILE:HD11	1.94	0.49
1:B:274:ASN:C	1:B:275:ILE:HG13	2.37	0.49
1:E:206:ARG:HA	1:E:209:ILE:HD12	1.94	0.49
1:A:215:GLN:HA	1:A:218:ARG:HD2	1.94	0.48
1:E:177:LEU:O	1:E:181:GLN:HB2	2.14	0.47
1:B:308:GLN:CB	1:B:310:LEU:HD21	2.42	0.47
2:C:124:ALA:HB3	2:C:127:LEU:HD12	1.97	0.47
1:D:215:GLN:HA	1:D:218:ARG:HD2	1.95	0.47
1:B:271:TRP:HA	1:B:307:ILE:CG2	2.45	0.47
1:E:187:LEU:HD22	1:E:191:LEU:HD12	1.96	0.47
1:B:351:LEU:C	1:B:351:LEU:HD23	2.40	0.46
2:C:53:MET:HB3	2:C:78:ILE:HD13	1.97	0.46
1:D:275:ILE:HA	1:D:367:ASN:OD1	2.15	0.46
2:C:83:ALA:HB2	2:C:127:LEU:HD23	1.96	0.46
1:D:241:MET:HE1	1:E:183:ILE:HG22	1.98	0.46
1:D:209:ILE:HD11	1:E:220:LEU:HD12	1.97	0.46
1:D:220:LEU:HD21	1:E:220:LEU:HD21	1.98	0.46
1:B:272:PRO:HD3	1:B:307:ILE:HG23	1.97	0.46
1:E:264:PHE:CE2	1:E:266:TYR:CD1	3.04	0.45
1:A:275:ILE:HA	1:A:367:ASN:OD1	2.16	0.45
1:E:351:LEU:C	1:E:351:LEU:HD23	2.41	0.45
2:F:53:MET:HB3	2:F:78:ILE:HD13	1.97	0.45
1:D:351:LEU:C	1:D:351:LEU:HD23	2.42	0.45
2:F:63:LEU:HD13	2:F:90:ARG:HD3	1.99	0.45
1:A:183:ILE:HG21	1:B:183:ILE:HG21	1.98	0.45
1:A:351:LEU:C	1:A:351:LEU:HD23	2.42	0.45
1:A:183:ILE:HD13	1:B:183:ILE:HG21	1.98	0.45
1:D:220:LEU:HD21	1:E:220:LEU:CD2	2.47	0.44
1:D:224:GLN:HE22	1:E:206:ARG:HH11	1.65	0.44
2:C:63:LEU:HD13	2:C:90:ARG:HD3	2.00	0.44
1:D:158:GLU:O	1:D:162:GLU:HG2	2.18	0.43
1:B:250:LEU:C	1:B:250:LEU:HD23	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLN:O	1:B:228:ARG:HG2	2.18	0.43
2:C:54:ASP:O	2:C:62:GLY:HA3	2.19	0.43
1:B:193:GLN:HG3	2:C:10:GLN:OE1	2.19	0.43
1:D:219:GLU:O	1:D:223:VAL:HG23	2.20	0.42
1:B:246:LEU:HG	1:B:271:TRP:CZ3	2.54	0.42
1:D:180:ARG:HB3	1:E:237:ILE:HG23	2.02	0.42
1:D:244:ILE:HD12	1:D:244:ILE:H	1.85	0.42
1:E:238:VAL:HB	1:E:243:GLY:N	2.34	0.42
1:E:264:PHE:CE2	1:E:266:TYR:CG	3.09	0.41
2:F:128:MET:C	2:F:130:ASP:H	2.28	0.41
2:F:54:ASP:O	2:F:62:GLY:HA3	2.20	0.41
1:A:209:ILE:HD11	1:B:220:LEU:HD12	2.03	0.41
1:B:177:LEU:O	1:B:181:GLN:HG2	2.20	0.41
2:C:99:TYR:CZ	2:C:127:LEU:HD22	2.56	0.41
1:A:179:GLU:OE1	1:A:179:GLU:HA	2.21	0.40
2:C:80:THR:CG2	2:C:99:TYR:HE1	2.34	0.40
1:A:206:ARG:HA	1:A:209:ILE:HD12	2.03	0.40
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.90	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	207/218 (95%)	201 (97%)	5 (2%)	1 (0%)	24	55
1	B	201/218 (92%)	195 (97%)	6 (3%)	0	100	100
1	D	209/218 (96%)	199 (95%)	9 (4%)	1 (0%)	24	55
1	E	201/218 (92%)	192 (96%)	7 (4%)	2 (1%)	12	41
2	C	130/139 (94%)	127 (98%)	3 (2%)	0	100	100
2	F	130/139 (94%)	126 (97%)	3 (2%)	1 (1%)	16	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1078/1150 (94%)	1040 (96%)	33 (3%)	5 (0%)	24	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ILE
1	E	367	ASN
1	E	236	LYS
2	F	129	GLU
1	D	209	ILE

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	189/194 (97%)	180 (95%)	9 (5%)	23	52
1	B	181/194 (93%)	167 (92%)	14 (8%)	12	37
1	D	191/194 (98%)	180 (94%)	11 (6%)	18	46
1	E	181/194 (93%)	172 (95%)	9 (5%)	22	50
2	C	109/113 (96%)	105 (96%)	4 (4%)	30	58
2	F	109/113 (96%)	105 (96%)	4 (4%)	30	58
All	All	960/1002 (96%)	909 (95%)	51 (5%)	20	49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LEU
1	A	165	GLU
1	A	171	ILE
1	A	173	GLU
1	A	177	LEU
1	A	224	GLN
1	A	237	ILE

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Mol	Chain	Res	Type
1	A	240	SER
1	A	267	GLU
1	B	156	GLU
1	B	161	GLU
1	B	165	GLU
1	B	171	ILE
1	B	183	ILE
1	B	196	SER
1	B	250	LEU
1	B	258	GLU
1	B	265	ILE
1	B	275	ILE
1	B	299	GLN
1	B	307	ILE
1	B	309	GLN
1	B	367	ASN
2	C	10	GLN
2	C	107	GLU
2	C	118	ASN
2	C	121	ARG
1	D	165	GLU
1	D	166	ASP
1	D	168	ASN
1	D	169	GLU
1	D	171	ILE
1	D	177	LEU
1	D	182	ARG
1	D	233	GLU
1	D	237	ILE
1	D	240	SER
1	D	274	ASN
1	E	156	GLU
1	E	173	GLU
1	E	181	GLN
1	E	188	GLU
1	E	196	SER
1	E	203	ASP
1	E	229	THR
1	E	250	LEU
1	E	273	GLU
2	F	107	GLU
2	F	118	ASN

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Mol	Chain	Res	Type
2	F	131	LEU
2	F	132	TYR

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	225	GLN
1	A	281	ASN
1	B	274	ASN
2	C	89	GLN
1	D	274	ASN
1	D	281	ASN
1	E	181	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 12 ligands modelled in this entry, 8 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
3	ACP	B	401	4	31,33,33	0.98	4 (12%)	47,52,52	0.68	1 (2%)
3	ACP	D	401	4	31,33,33	0.78	2 (6%)	47,52,52	0.62	1 (2%)
3	ACP	A	401	4	31,33,33	0.46	0	47,52,52	0.59	1 (2%)
3	ACP	E	401	4	31,33,33	0.95	3 (9%)	47,52,52	0.61	1 (2%)

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	B	401	4	-	3/19/38/38	0/3/3/3
3	ACP	D	401	4	-	3/19/38/38	0/3/3/3
3	ACP	A	401	4	-	3/19/38/38	0/3/3/3
3	ACP	E	401	4	-	3/19/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ACP	PB-O2B	-3.34	1.48	1.56
3	B	401	ACP	PB-O2B	-3.32	1.48	1.56
3	D	401	ACP	PG-O1G	2.49	1.55	1.50
3	B	401	ACP	PG-O1G	2.38	1.55	1.50
3	D	401	ACP	PG-O3G	-2.26	1.49	1.55
3	E	401	ACP	PG-O1G	2.25	1.54	1.50
3	E	401	ACP	PG-O3G	-2.24	1.49	1.55
3	B	401	ACP	PG-O3G	-2.23	1.50	1.55
3	B	401	ACP	PB-O1B	2.02	1.56	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ACP	O3G-PG-O2G	2.80	115.93	107.96
3	E	401	ACP	O3G-PG-O2G	2.45	114.94	107.96
3	B	401	ACP	O3G-PG-O2G	2.44	114.93	107.96
3	A	401	ACP	O1G-PG-C3B	-2.31	106.33	111.37

There are no chirality outliers.

All (12) 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	A	401	ACP	PB-C3B-PG-O3G
3	B	401	ACP	PB-C3B-PG-O1G
3	B	401	ACP	PB-C3B-PG-O2G
3	B	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	E	401	ACP	PB-C3B-PG-O1G
3	E	401	ACP	PB-C3B-PG-O2G
3	E	401	ACP	PB-C3B-PG-O3G

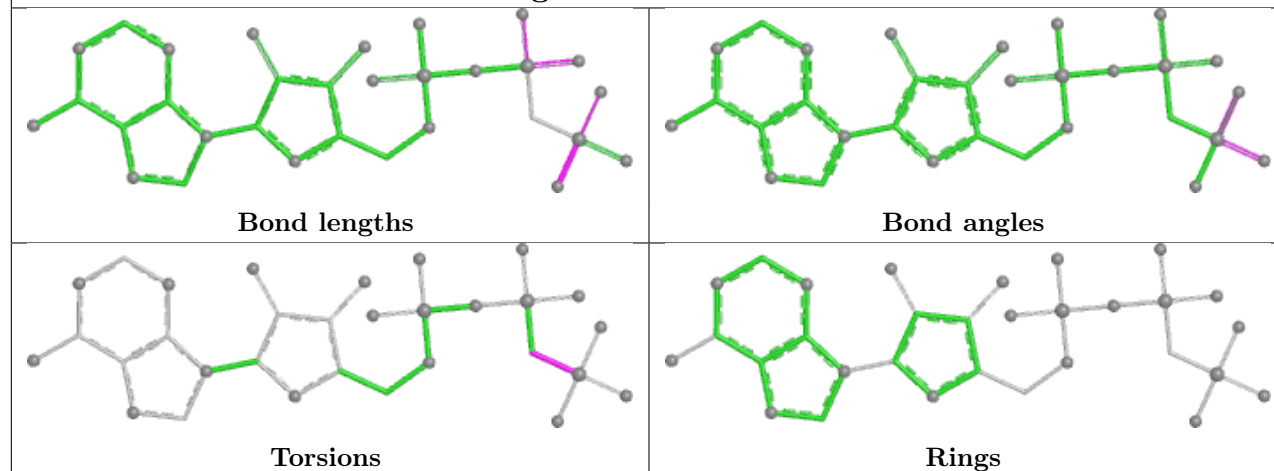
There are no ring outliers.

1 monomer is involved in 1 short contact:

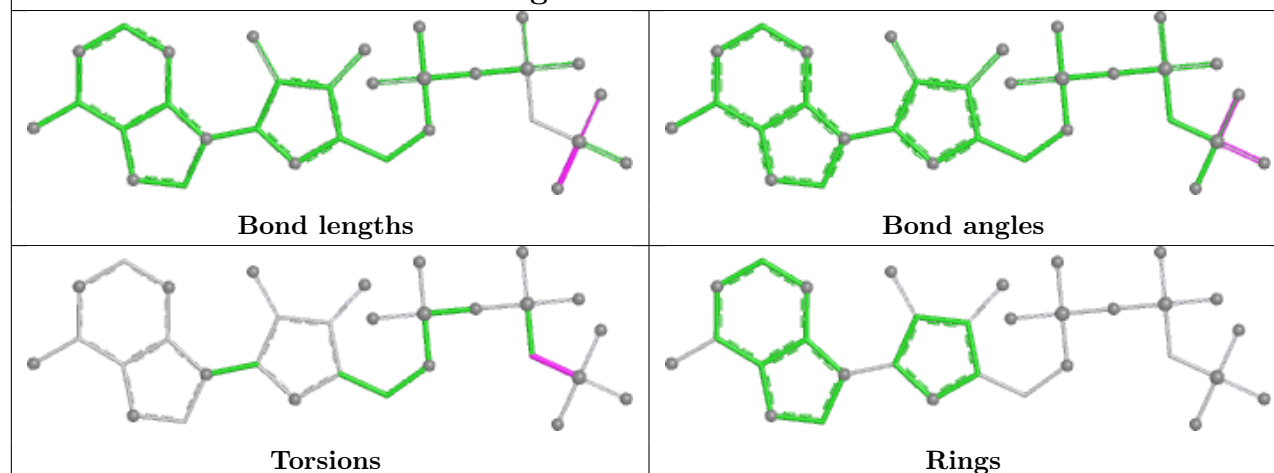
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ACP	1	0

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.

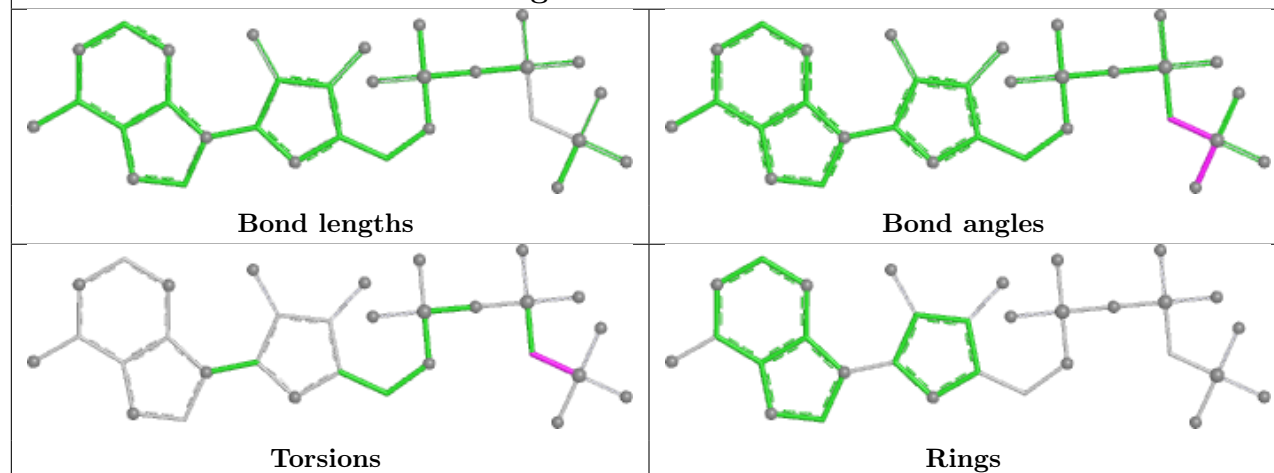
Ligand ACP B 401

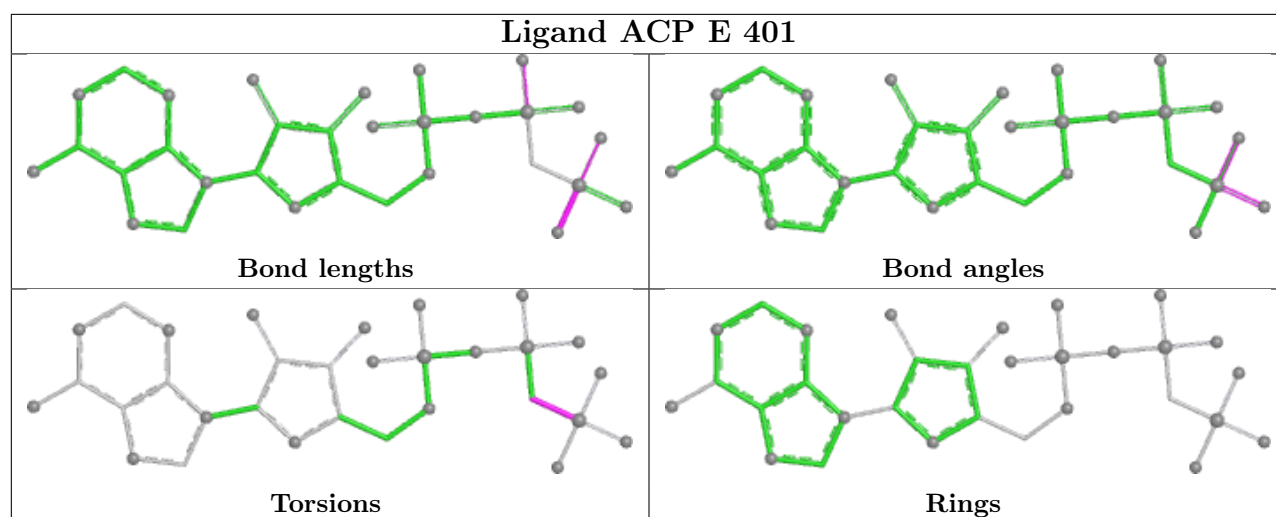


Ligand ACP D 401



Ligand ACP A 401





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	211/218 (96%)	0.08	1 (0%) 87 75	47, 86, 148, 173	0
1	B	207/218 (94%)	0.05	1 (0%) 87 75	49, 89, 126, 171	0
1	D	213/218 (97%)	-0.02	2 (0%) 81 64	43, 81, 139, 174	0
1	E	207/218 (94%)	0.07	1 (0%) 87 75	49, 87, 124, 156	0
2	C	132/139 (94%)	-0.15	0 100 100	49, 73, 104, 126	0
2	F	132/139 (94%)	-0.07	2 (1%) 72 52	51, 77, 115, 141	0
All	All	1102/1150 (95%)	0.01	7 (0%) 85 72	43, 84, 135, 174	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	332	SER	3.3
2	F	131	LEU	2.5
1	E	308	GLN	2.5
2	F	132	TYR	2.4
1	B	327	GLU	2.1
1	A	265	ILE	2.1
1	D	331	PHE	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

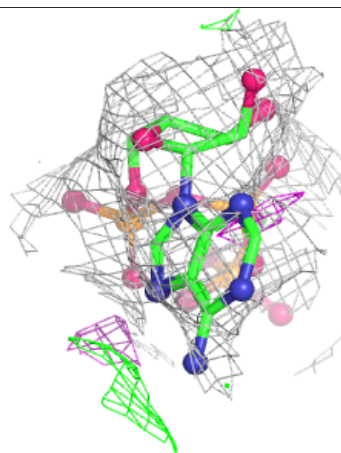
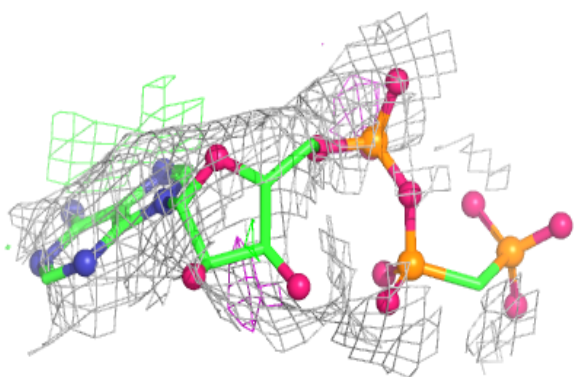
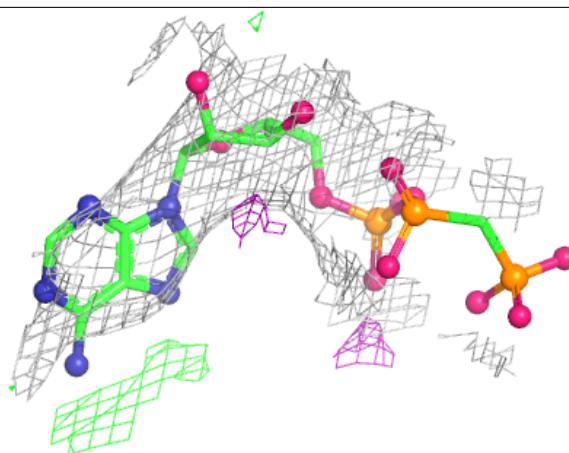
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	402	1/1	0.77	0.14	291,291,291,291	0
3	ACP	A	401	31/31	0.84	0.11	127,137,143,145	0
3	ACP	D	401	31/31	0.86	0.11	135,142,152,156	0
4	MG	A	402	1/1	0.91	0.09	196,196,196,196	0
5	K	C	203	1/1	0.91	0.07	123,123,123,123	0
3	ACP	B	401	31/31	0.93	0.08	85,98,111,116	0
3	ACP	E	401	31/31	0.95	0.07	81,100,114,121	0
5	K	C	202	1/1	0.96	0.06	80,80,80,80	0
4	MG	B	402	1/1	0.98	0.05	85,85,85,85	0
4	MG	F	201	1/1	0.99	0.05	57,57,57,57	0
4	MG	C	201	1/1	0.99	0.04	82,82,82,82	0
4	MG	E	402	1/1	0.99	0.05	72,72,72,72	0

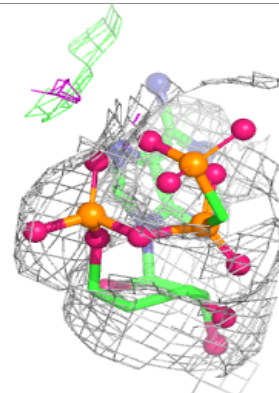
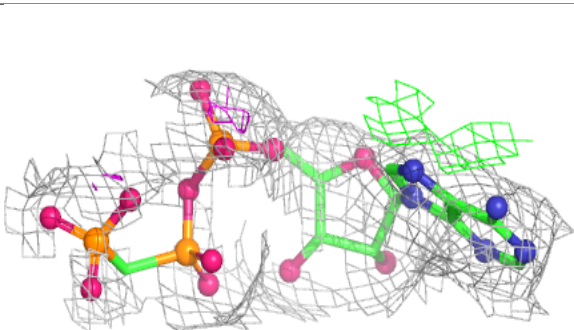
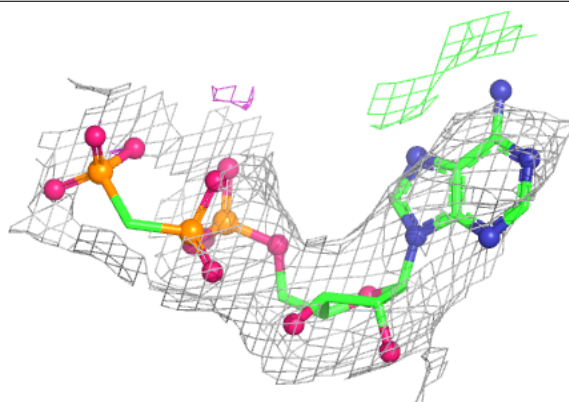
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP A 401:

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

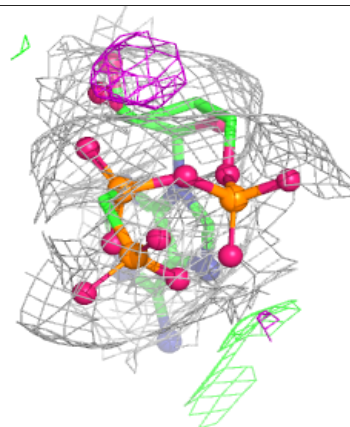
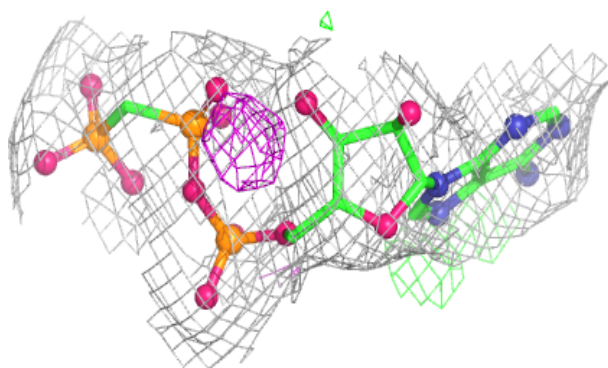
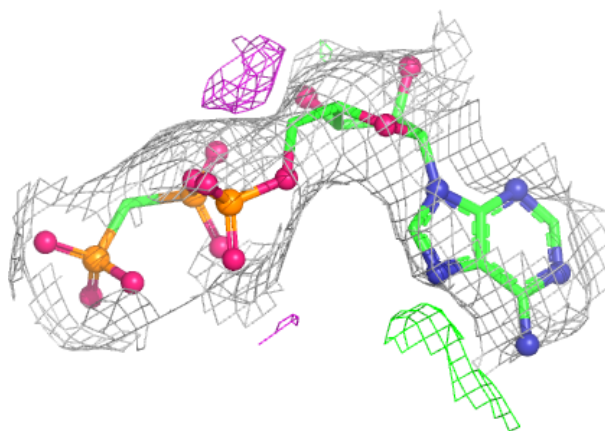
**Electron density around ACP D 401:**

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

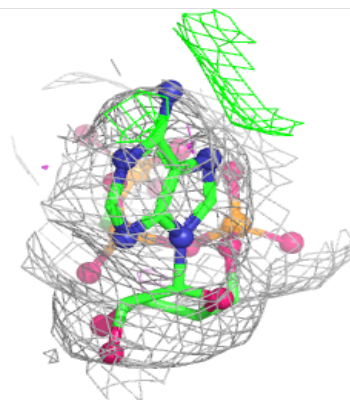
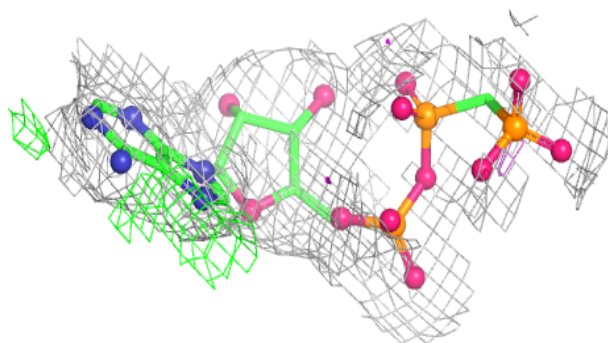
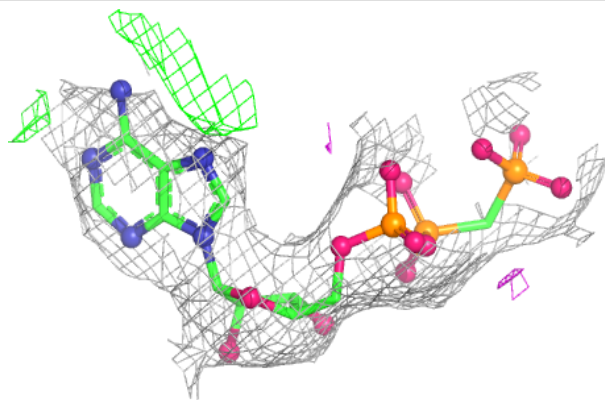


Electron density around ACP B 401:

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

**Electron density around ACP E 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.