



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:44 pm BST

PDB ID : 5IUN
Title : Crystal structure of the DesK-DesR complex in the phosphatase state
Authors : Trajtenberg, F.; Imelio, J.A.; Larrieux, N.; Buschiazzi, A.
Deposited on : 2016-03-18
Resolution : 2.79 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

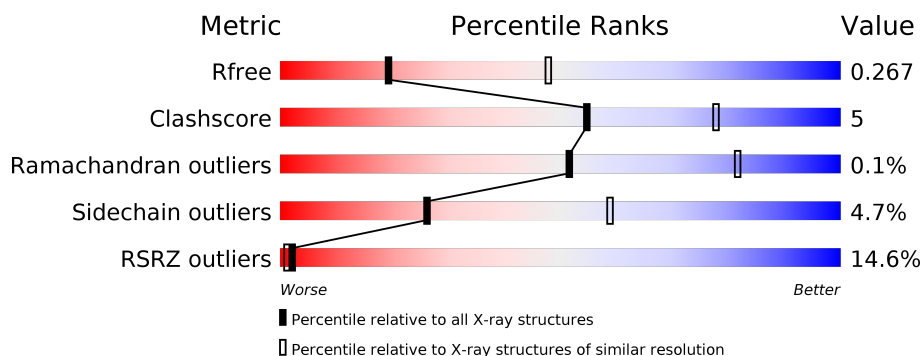
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	<div> <div>26%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	224	<div> <div>12%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div> </div>
1	E	224	<div> <div>11%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
2	C	139	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>.</div> <div>6%</div> </div> </div>
2	D	139	<div> <div>24%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>.</div> <div>6%</div> </div> </div>
2	F	139	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>..</div> <div>7%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8112 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	216	Total	C	N	O	S	0	0	0
			1689	1055	305	323	6			
1	B	216	Total	C	N	O	S	0	0	0
			1697	1061	301	329	6			
1	E	220	Total	C	N	O	S	0	0	0
			1707	1066	303	332	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
B	147	GLY	-	expression tag	UNP O34757
B	148	SER	-	expression tag	UNP O34757
B	149	GLY	-	expression tag	UNP O34757
B	150	ILE	SER	engineered mutation	UNP O34757
B	153	LEU	SER	engineered mutation	UNP O34757
B	157	ILE	ARG	engineered mutation	UNP O34757
E	147	GLY	-	expression tag	UNP O34757
E	148	SER	-	expression tag	UNP O34757
E	149	GLY	-	expression tag	UNP O34757
E	150	ILE	SER	engineered mutation	UNP O34757
E	153	LEU	SER	engineered mutation	UNP O34757
E	157	ILE	ARG	engineered mutation	UNP O34757

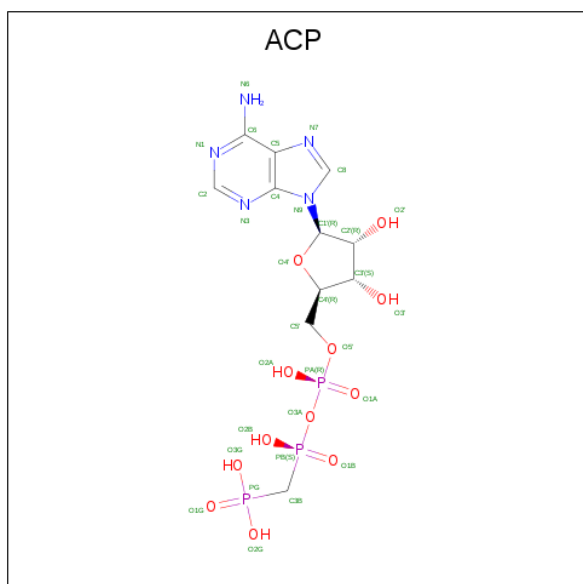
- Molecule 2 is a protein called Transcriptional regulatory protein DesR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	0	0
			979	618	162	190	9			
2	D	130	Total	C	N	O	S	0	0	0
			946	600	154	184	8			
2	F	129	Total	C	N	O	S	0	0	0
			954	604	156	185	9			

There are 12 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
D	-3	GLY	-	expression tag	UNP O34723
D	-2	SER	-	expression tag	UNP O34723
D	-1	GLY	-	expression tag	UNP O34723
D	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 (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

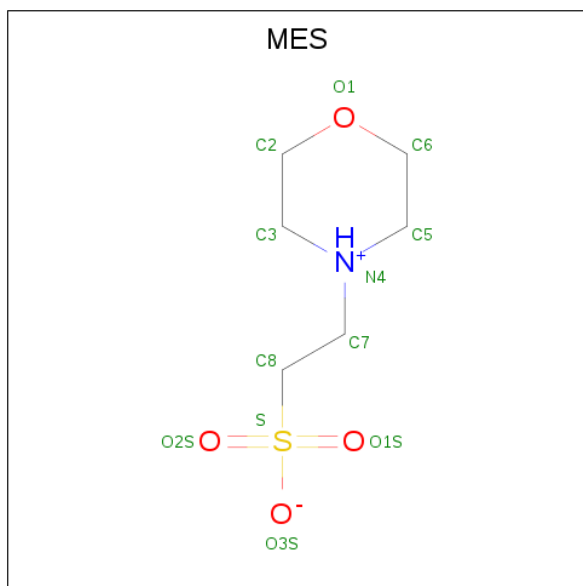


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

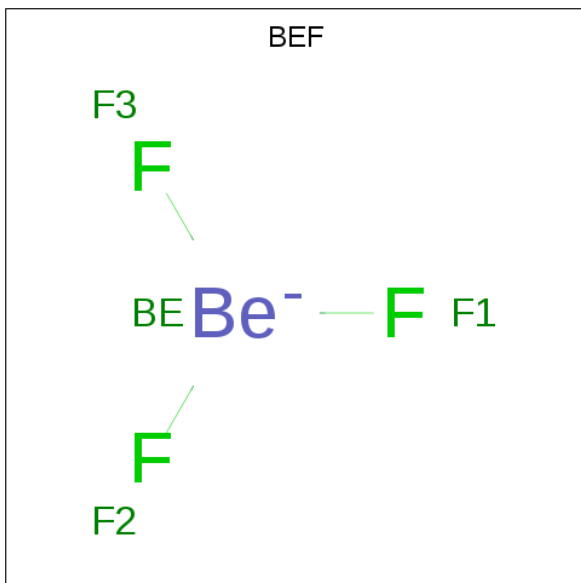
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	Be	F	0	0
			4	1	3		
6	D	1	Total	Be	F	0	0
			4	1	3		
6	F	1	Total	Be	F	0	0
			4	1	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

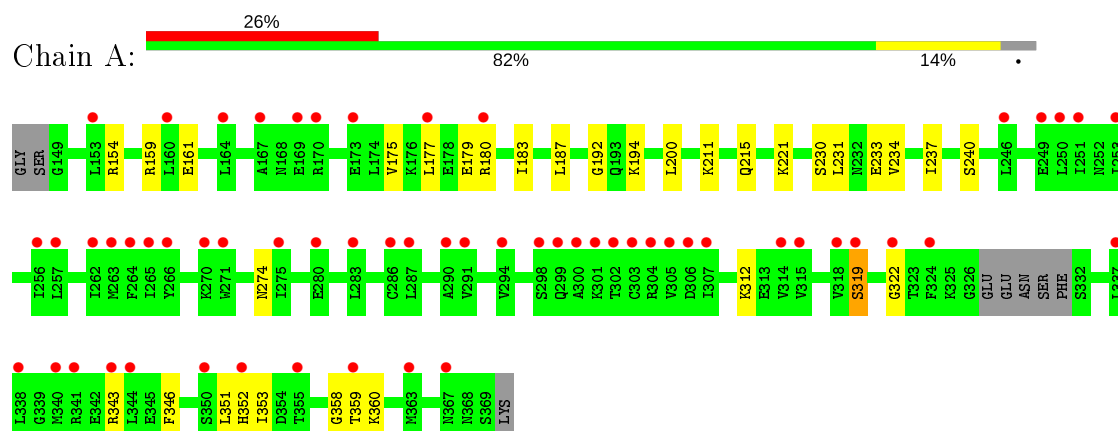
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	O	0	0
			2	2		
8	B	1	Total	O	0	0
			1	1		
8	C	3	Total	O	0	0
			3	3		
8	D	2	Total	O	0	0
			2	2		
8	E	2	Total	O	0	0
			2	2		
8	F	2	Total	O	0	0
			2	2		

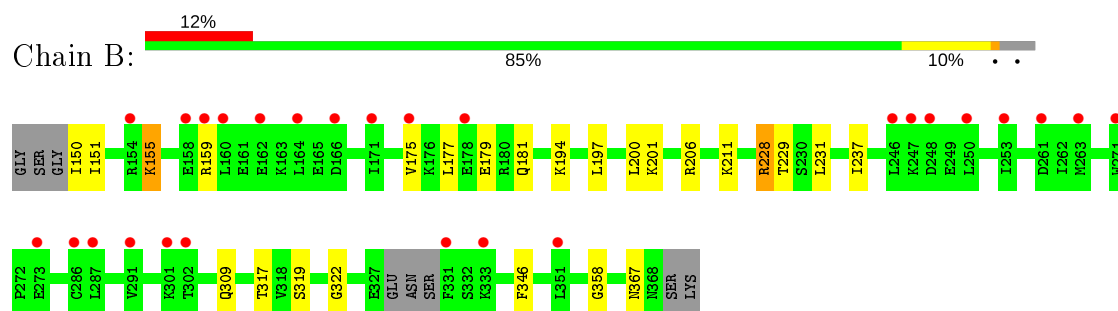
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

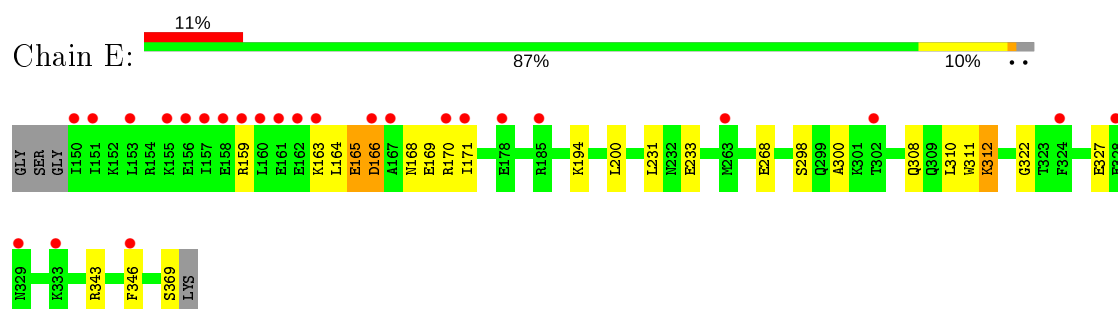
- Molecule 1: Sensor histidine kinase DesK



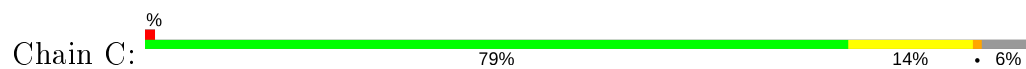
- Molecule 1: Sensor histidine kinase DesK



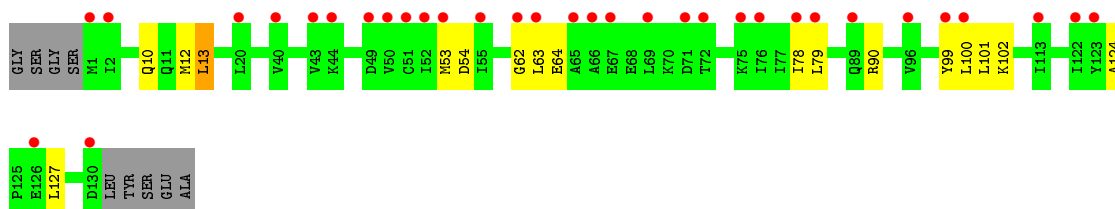
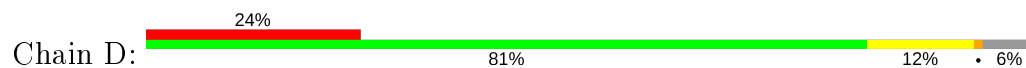
- Molecule 1: Sensor histidine kinase DesK



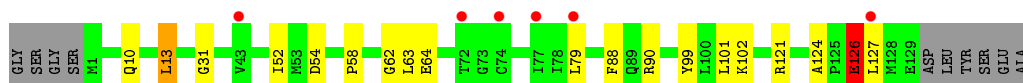
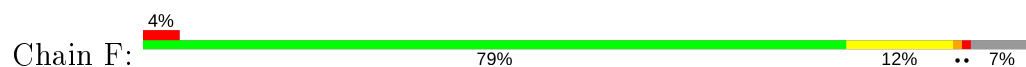
- Molecule 2: Transcriptional regulatory protein DesR



- 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	94.33Å 94.33Å 239.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.35 – 2.79 48.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.35-2.79) 99.5 (48.35-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.213 , 0.248 0.230 , 0.267	Depositor DCC
R_{free} test set	1568 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: MG, ACP, BEF, SO4, MES

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	0.46	0/1703	0.71	0/2289
1	B	0.49	0/1710	0.71	0/2296
1	E	0.58	0/1723	0.76	0/2320
2	C	0.49	0/990	0.71	0/1333
2	D	0.45	0/957	0.66	0/1294
2	F	0.51	0/965	0.73	1/1302 (0.1%)
All	All	0.50	0/8048	0.72	1/10834 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	126	GLU	CA-CB-CG	5.25	124.94	113.40

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	1689	0	1730	17	0
1	B	1697	0	1737	17	0
1	E	1707	0	1716	12	0
2	C	979	0	990	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	946	0	937	20	0
2	F	954	0	957	14	0
3	A	31	0	14	0	0
3	B	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
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	13	2	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
6	F	4	0	0	0	0
7	C	5	0	0	0	0
8	A	2	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
All	All	8112	0	8122	84	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 (84) 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:D:124:ALA:HB3	2:D:127:LEU:HD23	1.59	0.84
1:E:166:ASP:O	1:E:170:ARG:HB2	1.81	0.80
1:B:197:LEU:HD21	2:D:12:MET:HG2	1.69	0.74
2:C:124:ALA:HB3	2:C:127:LEU:HD12	1.69	0.74
1:A:353:ILE:HD11	1:A:359:THR:HG23	1.68	0.73
1:A:319:SER:HB3	1:A:360:LYS:HG2	1.71	0.73
2:D:99:TYR:CE1	2:D:127:LEU:HG	2.25	0.71
2:F:88:PHE:HD1	2:F:99:TYR:HD2	1.40	0.70
2:C:99:TYR:HE1	2:C:127:LEU:HD22	1.55	0.69
1:A:177:LEU:HD12	1:B:181:GLN:HG3	1.74	0.68
2:C:99:TYR:CD1	2:C:127:LEU:HD13	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:GLU:HG3	2:C:90:ARG:HH22	1.59	0.66
2:C:82:PHE:HB2	2:C:84:ARG:HD2	1.78	0.65
2:D:64:GLU:HG3	2:D:90:ARG:HH22	1.62	0.64
2:F:64:GLU:HG3	2:F:90:ARG:HH12	1.64	0.62
2:F:88:PHE:HD1	2:F:99:TYR:CD2	2.18	0.62
1:A:180:ARG:HA	1:A:183:ILE:HD12	1.81	0.61
1:A:187:LEU:HD22	1:A:237:ILE:HG13	1.83	0.61
1:E:165:GLU:O	1:E:169:GLU:HB2	1.99	0.61
2:C:99:TYR:HD1	2:C:127:LEU:HD13	1.66	0.60
1:E:200:LEU:HD12	2:F:13:LEU:HD23	1.83	0.60
2:F:101:LEU:HD11	2:F:126:GLU:HG2	1.84	0.59
2:C:52:ILE:CG2	2:C:79:LEU:HD22	2.32	0.59
1:B:201:LYS:NZ	2:D:12:MET:CG	2.65	0.59
1:B:201:LYS:NZ	2:D:12:MET:HG3	2.17	0.59
2:D:99:TYR:HE1	2:D:127:LEU:HG	1.69	0.58
1:A:353:ILE:HD11	1:A:359:THR:CG2	2.35	0.55
2:D:124:ALA:HB3	2:D:127:LEU:CD2	2.33	0.55
2:D:79:LEU:HG	2:D:102:LYS:HG2	1.88	0.54
1:E:194:LYS:HE3	1:E:346:PHE:O	2.08	0.54
2:F:124:ALA:HB3	2:F:127:LEU:HD12	1.89	0.54
2:F:101:LEU:CD1	2:F:126:GLU:HG2	2.38	0.54
2:D:101:LEU:HG	2:D:127:LEU:HD21	1.90	0.53
1:E:233:GLU:HG3	1:E:346:PHE:CE2	2.41	0.53
2:F:52:ILE:CG2	2:F:79:LEU:HD22	2.39	0.52
1:A:215:GLN:HE22	5:A:403:MES:H82	1.73	0.52
1:B:155:LYS:HD3	1:B:159:ARG:HE	1.75	0.52
2:D:99:TYR:CD1	2:D:127:LEU:HG	2.44	0.52
1:E:312:LYS:HB3	2:F:58:PRO:HB2	1.92	0.52
1:B:228:ARG:NH1	1:B:229:THR:HG22	2.25	0.52
2:C:64:GLU:HG3	2:C:90:ARG:NH2	2.24	0.51
1:B:200:LEU:HD12	2:D:13:LEU:HD23	1.93	0.50
1:A:192:GLY:HA2	1:B:231:LEU:HD13	1.93	0.49
2:F:88:PHE:CD1	2:F:99:TYR:HD2	2.26	0.49
2:D:64:GLU:HG3	2:D:90:ARG:NH2	2.25	0.49
1:B:201:LYS:HZ2	2:D:12:MET:HG3	1.77	0.48
1:B:175:VAL:O	1:B:179:GLU:HG2	2.13	0.48
5:A:403:MES:H52	2:F:31:GLY:HA2	1.96	0.48
1:E:164:LEU:HG	1:E:168:ASN:ND2	2.29	0.48
2:F:64:GLU:HG3	2:F:90:ARG:NH1	2.29	0.47
1:A:233:GLU:O	1:A:237:ILE:HG12	2.15	0.47
1:E:311:TRP:CE3	1:E:312:LYS:HG2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLN:HE22	1:B:367:ASN:HD21	1.63	0.46
1:E:298:SER:OG	1:E:300:ALA:HB2	2.15	0.46
1:B:201:LYS:HZ2	2:D:12:MET:CG	2.28	0.46
2:D:79:LEU:HG	2:D:102:LYS:HA	1.98	0.45
2:D:79:LEU:HD12	2:D:100:LEU:HB2	1.97	0.45
1:A:230:SER:O	1:A:234:VAL:HG23	2.16	0.45
1:B:194:LYS:HE3	1:B:346:PHE:O	2.16	0.45
2:C:99:TYR:CE1	2:C:127:LEU:HD13	2.52	0.45
2:C:99:TYR:CE1	2:C:127:LEU:HD22	2.44	0.45
1:B:228:ARG:HH12	1:B:229:THR:HG22	1.82	0.44
2:C:1:MET:HG3	1:E:310:LEU:HD22	1.99	0.44
1:B:177:LEU:O	1:B:181:GLN:HG2	2.17	0.44
2:F:63:LEU:HD13	2:F:90:ARG:HD3	1.99	0.44
2:C:82:PHE:CB	2:C:84:ARG:HD2	2.47	0.44
2:F:54:ASP:O	2:F:62:GLY:HA3	2.19	0.43
1:E:298:SER:OG	1:E:322:GLY:HA3	2.19	0.43
1:A:233:GLU:HG3	1:A:346:PHE:CE1	2.54	0.43
1:E:159:ARG:O	1:E:163:LYS:HD3	2.20	0.42
1:A:200:LEU:HD12	2:C:13:LEU:HD23	2.01	0.42
2:C:54:ASP:O	2:C:62:GLY:HA3	2.19	0.42
1:A:312:LYS:CB	2:C:58:PRO:HB2	2.49	0.41
2:D:53:MET:HB3	2:D:78:ILE:HD13	2.03	0.41
1:A:221:LYS:HG3	1:B:206:ARG:HD3	2.01	0.41
2:C:63:LEU:HD13	2:C:90:ARG:HD3	2.02	0.41
2:D:54:ASP:O	2:D:62:GLY:HA3	2.21	0.41
2:D:63:LEU:HD13	2:D:90:ARG:HD3	2.02	0.41
1:A:351:LEU:HD23	1:A:351:LEU:C	2.41	0.41
1:B:322:GLY:O	1:B:358:GLY:HA2	2.21	0.41
2:C:40:VAL:HA	2:C:69:LEU:HD21	2.03	0.40
2:C:53:MET:HB3	2:C:78:ILE:HD13	2.03	0.40
1:A:194:LYS:HE3	1:A:346:PHE:O	2.21	0.40
1:A:322:GLY:O	1:A:358:GLY:HA2	2.21	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	212/224 (95%)	209 (99%)	3 (1%)	0	100	100
1	B	212/224 (95%)	210 (99%)	2 (1%)	0	100	100
1	E	218/224 (97%)	213 (98%)	5 (2%)	0	100	100
2	C	129/139 (93%)	126 (98%)	2 (2%)	1 (1%)	19	49
2	D	128/139 (92%)	126 (98%)	2 (2%)	0	100	100
2	F	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
All	All	1026/1089 (94%)	1009 (98%)	16 (2%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	129	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	183/199 (92%)	171 (93%)	12 (7%)	16	44
1	B	185/199 (93%)	177 (96%)	8 (4%)	29	62
1	E	183/199 (92%)	173 (94%)	10 (6%)	21	52
2	C	103/113 (91%)	100 (97%)	3 (3%)	42	76
2	D	96/113 (85%)	94 (98%)	2 (2%)	53	84
2	F	99/113 (88%)	94 (95%)	5 (5%)	24	55
All	All	849/936 (91%)	809 (95%)	40 (5%)	26	59

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ARG
1	A	159	ARG
1	A	161	GLU
1	A	175	VAL
1	A	179	GLU
1	A	211	LYS
1	A	231	LEU
1	A	240	SER
1	A	274	ASN
1	A	319	SER
1	A	343	ARG
1	A	352	HIS
1	B	150	ILE
1	B	151	ILE
1	B	155	LYS
1	B	211	LYS
1	B	228	ARG
1	B	237	ILE
1	B	317	THR
1	B	319	SER
2	C	13	LEU
2	C	84	ARG
2	C	85	PRO
2	D	10	GLN
2	D	13	LEU
1	E	165	GLU
1	E	166	ASP
1	E	171	ILE
1	E	231	LEU
1	E	268	GLU
1	E	308	GLN
1	E	312	LYS
1	E	327	GLU
1	E	343	ARG
1	E	369	SER
2	F	10	GLN
2	F	13	LEU
2	F	102	LYS
2	F	121	ARG
2	F	126	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	279	ASN
1	A	352	HIS
1	B	255	GLN
1	B	279	ASN
1	B	309	GLN
1	B	367	ASN
1	B	368	ASN
2	C	10	GLN
2	C	11	GLN
2	D	10	GLN
2	D	11	GLN
1	E	224	GLN
1	E	255	GLN
1	E	279	ASN
2	F	10	GLN
2	F	11	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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
6	BEF	F	202	2	0,3,3	0.00	-	-		
3	ACP	E	401	4	27,33,33	0.95	1 (3%)	32,52,52	0.89	2 (6%)
7	SO4	C	203	-	4,4,4	0.23	0	6,6,6	0.12	0
3	ACP	A	401	4	27,33,33	0.92	2 (7%)	32,52,52	1.04	2 (6%)
6	BEF	C	202	2	0,3,3	0.00	-	-		
3	ACP	B	401	4	27,33,33	0.91	1 (3%)	32,52,52	0.88	2 (6%)
6	BEF	D	202	2	0,3,3	0.00	-	-		
5	MES	A	403	-	12,12,12	0.71	0	14,16,16	0.39	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	ACP	E	401	4	-	3/15/38/38	0/3/3/3
3	ACP	B	401	4	-	3/15/38/38	0/3/3/3
3	ACP	A	401	4	-	3/15/38/38	0/3/3/3
5	MES	A	403	-	-	4/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ACP	PB-O2B	-3.10	1.49	1.56
3	B	401	ACP	PB-O2B	-3.02	1.49	1.56
3	A	401	ACP	PG-O1G	2.23	1.54	1.50
3	A	401	ACP	PG-O2G	-2.12	1.50	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ACP	O1G-PG-C3B	-3.83	102.98	111.24
3	E	401	ACP	C5-C6-N6	2.51	124.17	120.35
3	B	401	ACP	C5-C6-N6	2.39	123.99	120.35
3	A	401	ACP	C5-C6-N6	2.28	123.82	120.35
3	E	401	ACP	O1G-PG-C3B	-2.12	106.67	111.24
3	B	401	ACP	O1G-PG-C3B	-2.09	106.74	111.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

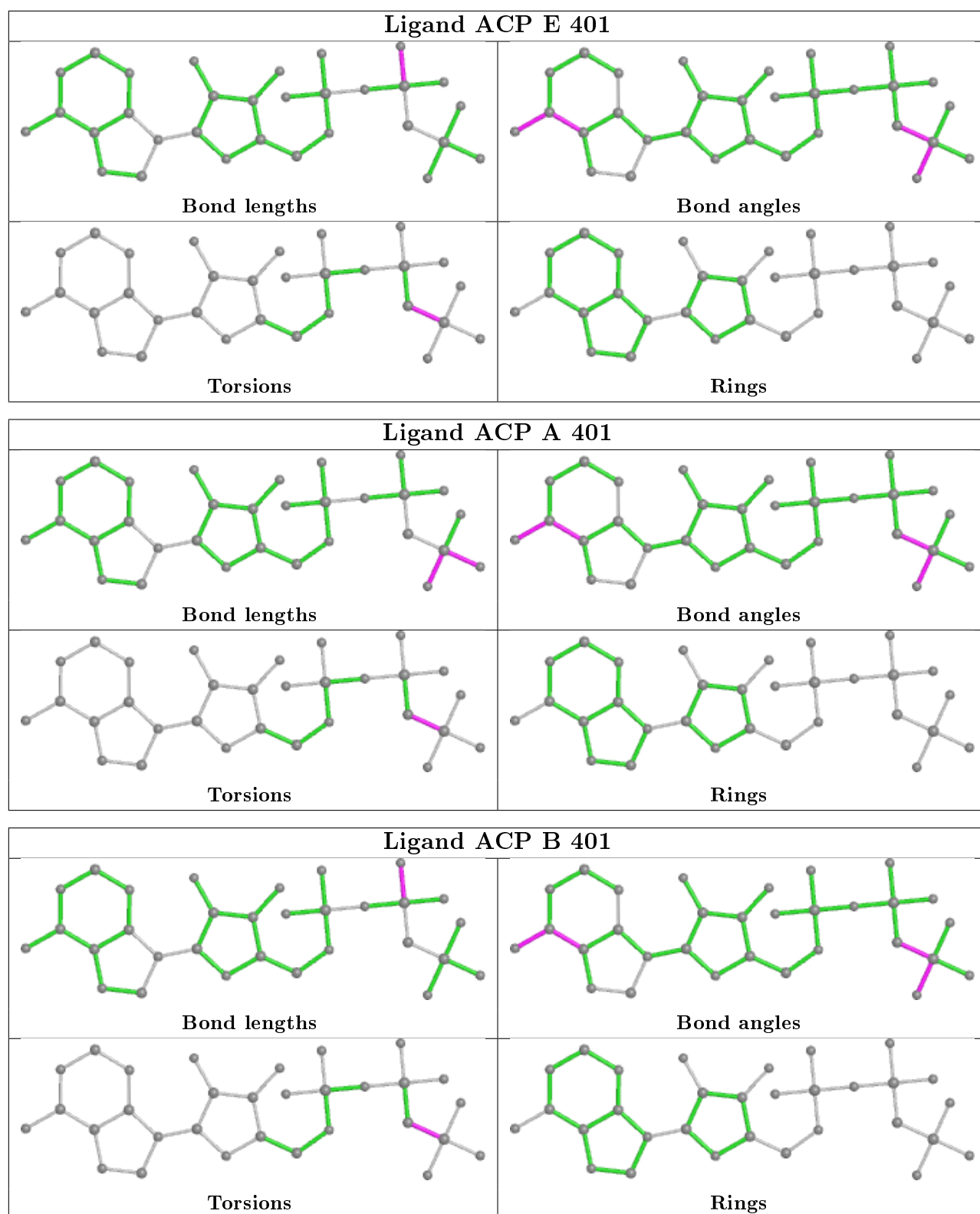
Mol	Chain	Res	Type	Atoms
3	E	401	ACP	PB-C3B-PG-O1G
3	E	401	ACP	PB-C3B-PG-O2G
3	E	401	ACP	PB-C3B-PG-O3G
3	A	401	ACP	PB-C3B-PG-O1G
3	A	401	ACP	PB-C3B-PG-O2G
3	A	401	ACP	PB-C3B-PG-O3G
3	B	401	ACP	PB-C3B-PG-O1G
3	B	401	ACP	PB-C3B-PG-O2G
3	B	401	ACP	PB-C3B-PG-O3G
5	A	403	MES	C7-C8-S-O3S
5	A	403	MES	C7-C8-S-O1S
5	A	403	MES	C7-C8-S-O2S
5	A	403	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	MES	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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	216/224 (96%)	1.32	59 (27%) 0 0	72, 142, 193, 210	0
1	B	216/224 (96%)	0.84	27 (12%) 3 2	72, 114, 154, 175	0
1	E	220/224 (98%)	0.79	25 (11%) 5 3	58, 93, 156, 172	0
2	C	131/139 (94%)	0.38	2 (1%) 73 68	71, 93, 128, 145	0
2	D	130/139 (93%)	1.18	33 (25%) 0 0	114, 150, 177, 190	0
2	F	129/139 (92%)	0.57	6 (4%) 31 22	69, 95, 142, 173	0
All	All	1042/1089 (95%)	0.88	152 (14%) 2 1	58, 113, 175, 210	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	ILE	9.3
1	B	171	ILE	8.7
2	D	63	LEU	8.4
1	B	246	LEU	8.2
1	B	331	PHE	6.5
1	A	305	VAL	6.2
1	A	355	THR	6.1
1	B	160	LEU	6.0
1	A	275	ILE	5.9
2	D	71	ASP	5.7
2	D	53	MET	5.6
1	A	299	GLN	5.4
1	B	178	GLU	5.4
1	E	328	GLU	5.4
1	B	247	LYS	5.3
2	F	72	THR	5.3
1	E	162	GLU	5.2
1	A	253	ILE	5.0
1	B	250	LEU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	266	TYR	4.7
1	A	246	LEU	4.7
1	E	153	LEU	4.7
1	A	287	LEU	4.6
2	D	40	VAL	4.6
1	B	162	GLU	4.6
1	B	154	ARG	4.5
1	A	291	VAL	4.5
1	A	306	ASP	4.5
1	E	167	ALA	4.5
1	A	263	MET	4.4
2	D	113	ILE	4.4
1	E	163	LYS	4.4
1	A	294	VAL	4.3
1	B	302	THR	4.3
2	D	50	VAL	4.3
1	A	300	ALA	4.0
1	E	150	ILE	3.9
1	E	166	ASP	3.9
1	E	156	GLU	3.9
1	A	324	PHE	3.8
2	D	69	LEU	3.8
1	A	264	PHE	3.8
1	A	170	ARG	3.7
1	B	158	GLU	3.7
1	E	160	LEU	3.7
2	D	76	ILE	3.7
1	A	341	ARG	3.7
1	B	159	ARG	3.7
1	B	253	ILE	3.6
1	A	270	LYS	3.6
2	D	52	ILE	3.6
1	A	337	LEU	3.6
1	A	319	SER	3.6
1	A	303	CYS	3.5
1	E	263	MET	3.5
2	F	74	CYS	3.5
1	A	164	LEU	3.5
1	E	158	GLU	3.5
2	D	65	ALA	3.5
1	E	329	ASN	3.5
1	E	159	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	171	ILE	3.4
1	A	286	CYS	3.4
1	A	251	ILE	3.4
2	C	44	LYS	3.4
1	B	273	GLU	3.4
1	A	304	ARG	3.4
1	A	169	GLU	3.3
1	A	280	GLU	3.3
2	D	44	LYS	3.3
1	B	287	LEU	3.3
1	A	283	LEU	3.3
1	A	271	TRP	3.2
2	D	122	ILE	3.2
1	A	167	ALA	3.2
1	A	307	ILE	3.2
2	D	79	LEU	3.1
1	A	257	LEU	3.1
2	D	66	ALA	3.1
1	A	250	LEU	3.1
2	D	67	GLU	3.0
1	A	177	LEU	2.9
1	A	314	VAL	2.9
2	F	127	LEU	2.9
1	A	315	VAL	2.9
2	D	43	VAL	2.9
1	A	262	ILE	2.9
1	A	352	HIS	2.9
2	D	75	LYS	2.9
2	D	99	TYR	2.9
1	A	249	GLU	2.9
1	A	344	LEU	2.9
1	A	173	GLU	2.8
1	A	160	LEU	2.8
1	A	363	MET	2.8
2	D	89	GLN	2.8
2	D	100	LEU	2.8
2	D	62	GLY	2.7
1	A	359	THR	2.7
1	B	261	ASP	2.7
1	A	153	LEU	2.7
2	D	55	ILE	2.7
2	D	96	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	318	VAL	2.7
1	A	340	MET	2.7
1	A	298	SER	2.6
2	D	78	ILE	2.6
1	E	155	LYS	2.6
1	A	302	THR	2.6
1	A	290	ALA	2.6
2	D	123	TYR	2.6
1	E	302	THR	2.5
2	D	49	ASP	2.5
1	B	333	LYS	2.5
1	A	367	ASN	2.5
1	B	166	ASP	2.5
1	E	333	LYS	2.5
1	A	343	ARG	2.5
2	D	1	MET	2.5
1	E	151	ILE	2.4
1	B	263	MET	2.4
2	F	77	ILE	2.4
1	A	265	ILE	2.4
2	F	43	VAL	2.4
2	C	88	PHE	2.4
1	E	324	PHE	2.4
1	B	286	CYS	2.3
2	F	79	LEU	2.3
1	A	338	LEU	2.3
1	B	164	LEU	2.3
1	E	170	ARG	2.3
1	E	346	PHE	2.3
2	D	130	ASP	2.3
1	B	248	ASP	2.3
1	A	322	GLY	2.3
1	B	271	TRP	2.3
2	D	51	CYS	2.3
1	A	256	ILE	2.2
1	A	301	LYS	2.2
2	D	72	THR	2.2
1	B	291	VAL	2.1
1	A	350	SER	2.1
2	D	20	LEU	2.1
1	B	175	VAL	2.1
1	E	178	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	301	LYS	2.1
1	B	351	LEU	2.1
2	D	2	ILE	2.1
1	E	185	ARG	2.1
1	A	180	ARG	2.0
2	D	126	GLU	2.0
1	E	161	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

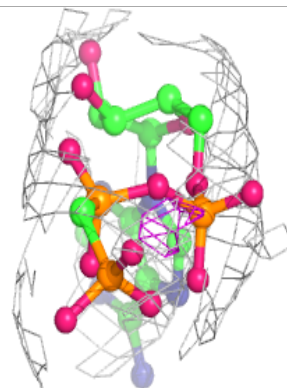
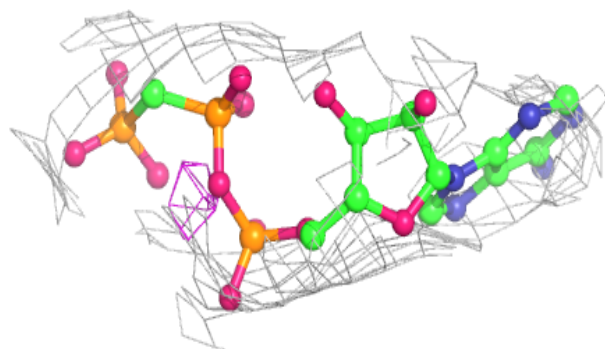
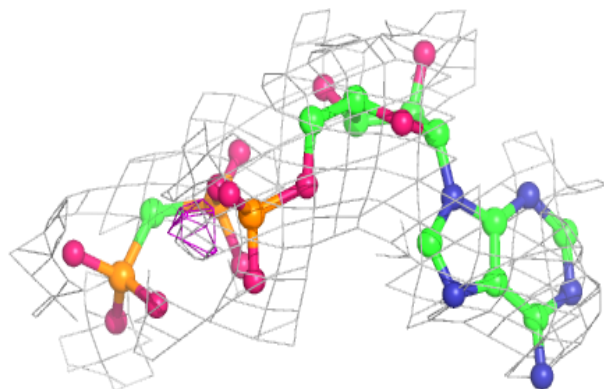
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	C	203	5/5	0.80	0.20	173,173,174,174	0
5	MES	A	403	12/12	0.81	0.27	146,149,156,156	0
3	ACP	A	401	31/31	0.86	0.17	153,161,177,180	0
4	MG	A	402	1/1	0.88	0.05	186,186,186,186	0
4	MG	B	402	1/1	0.90	0.09	117,117,117,117	0
3	ACP	E	401	31/31	0.94	0.17	89,100,114,117	0
4	MG	D	201	1/1	0.95	0.16	142,142,142,142	0
4	MG	E	402	1/1	0.95	0.16	99,99,99,99	0
3	ACP	B	401	31/31	0.95	0.18	93,99,107,110	0
6	BEF	C	202	4/4	0.96	0.20	78,82,82,88	0
4	MG	F	201	1/1	0.97	0.22	79,79,79,79	0
6	BEF	D	202	4/4	0.98	0.14	117,120,121,122	0
6	BEF	F	202	4/4	0.98	0.19	79,81,82,89	0
4	MG	C	201	1/1	0.99	0.20	101,101,101,101	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.

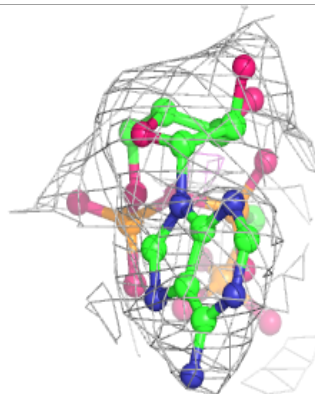
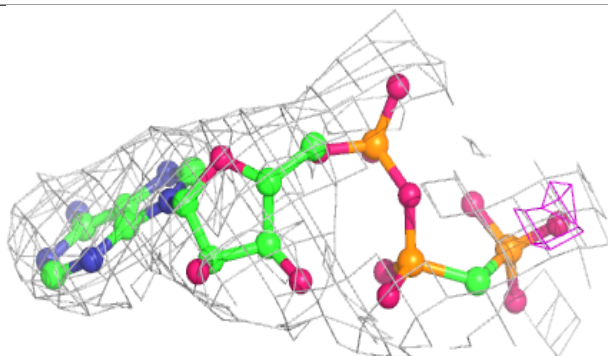
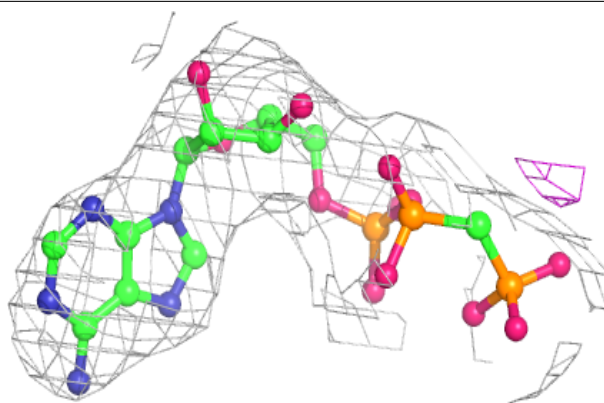
Electron density around ACP A 401:

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

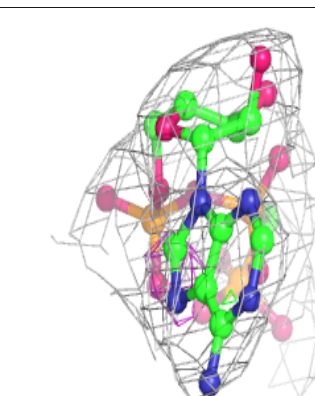
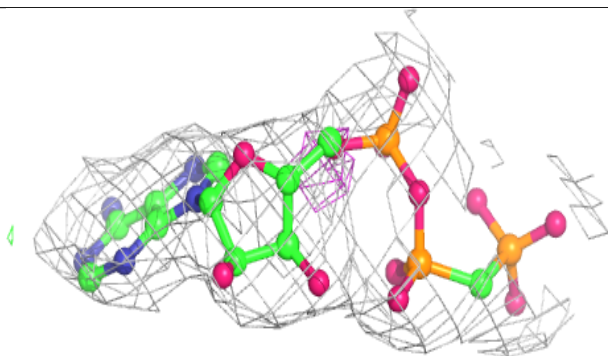
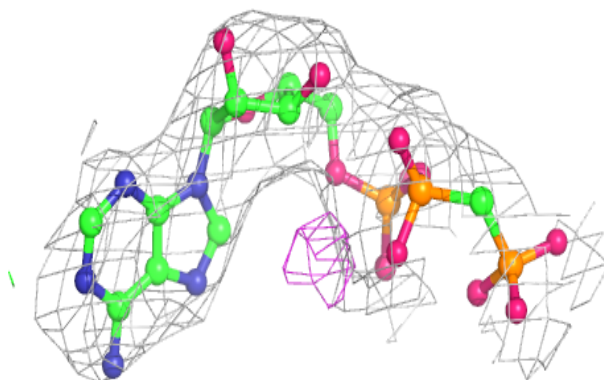


Electron density around ACP E 401:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.