



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 01:56 PM EDT

PDB ID : 7SSJ
Title : Crystal structure of the DesK-DesR complex in the phosphatase state
Authors : Trajtenberg, F.; Buschiazzo, 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

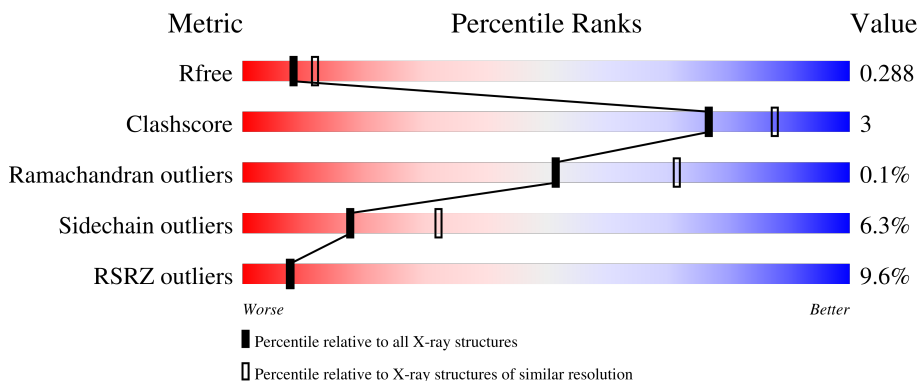
1 Overall quality at a glance i

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.



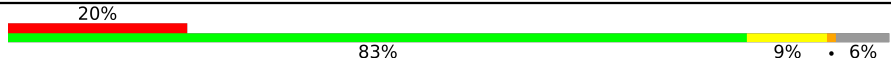
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">84% 12% ..</p>
1	C	224	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">88% 8% ..</p>
1	D	224	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">87% 10% ..</p>
2	B	139	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">76% 17% 6%</p>
2	E	139	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">88% 6% 6%</p>

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Mol	Chain	Length	Quality of chain
2	F	139	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into four segments: a red segment labeled '20%', a large green segment labeled '83%', a yellow segment labeled '9%', and a small grey segment labeled '6%'.</p>

2 Entry composition i

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
			Total	C	N	O	S			
1	A	219	Total 1687	C 1050	N 304	O 328	S 5	0	0	0
1	C	216	Total 1675	C 1046	N 297	O 326	S 6	0	1	0
1	D	218	Total 1694	C 1057	N 304	O 327	S 6	0	0	0

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

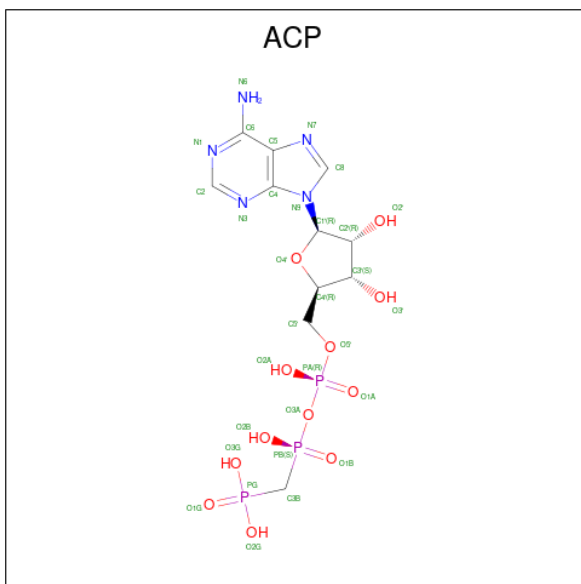
- Molecule 2 is a protein called Transcriptional regulatory protein DesR.

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

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 (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

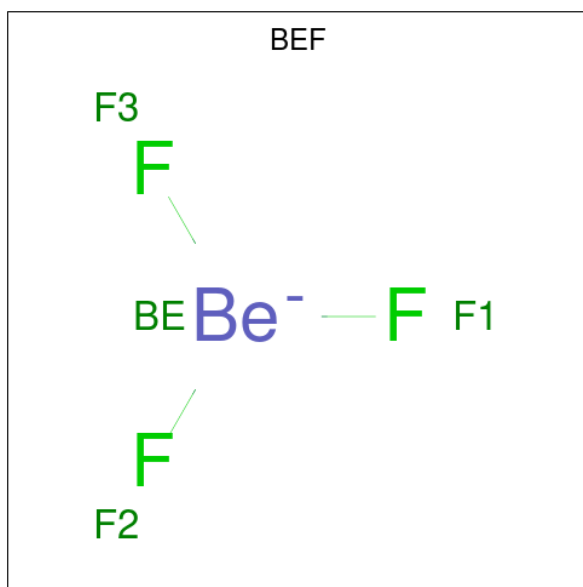


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	C	1	Total 31	C 11	N 5	O 12	P 3	0	0
3	D	1	Total 31	C 11	N 5	O 12	P 3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	Total 1	Mg 1	0	0
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 BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



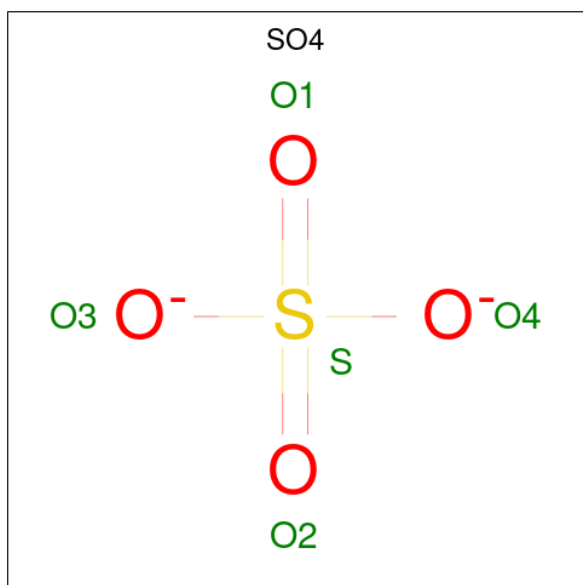
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
5	B	1	Total 4	Be 1	F 3	0	0

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

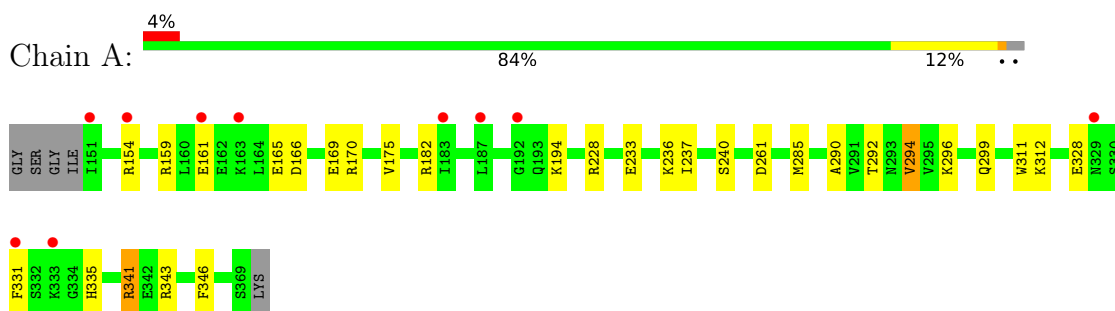
- Molecule 7 is water.

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

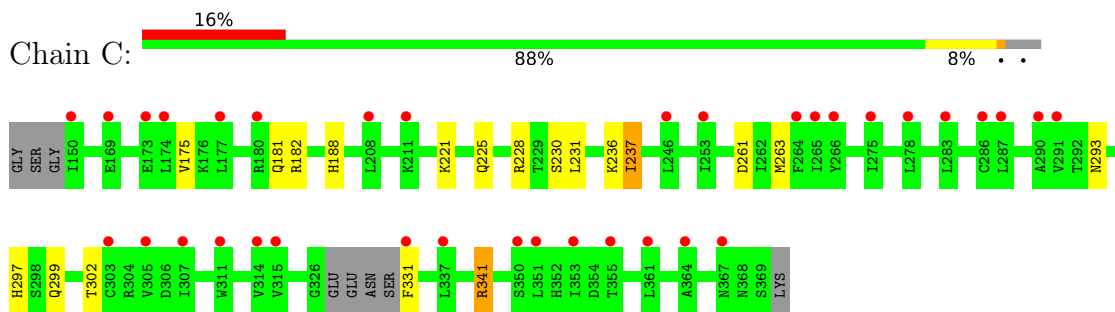
3 Residue-property plots [i](#)

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.

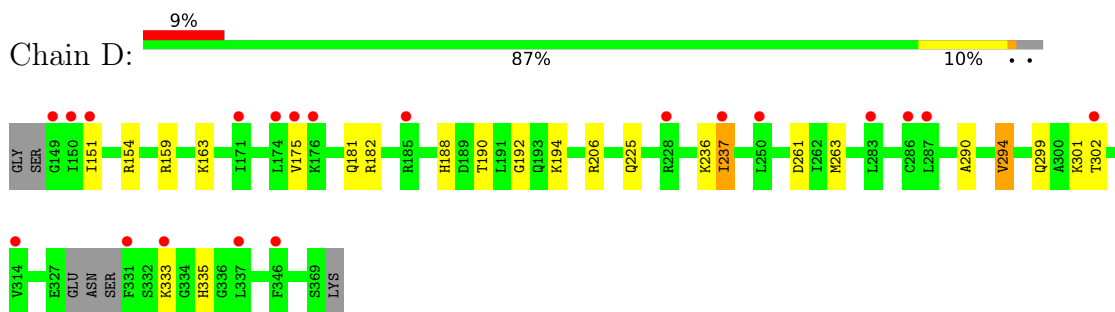
- Molecule 1: Sensor histidine kinase DesK



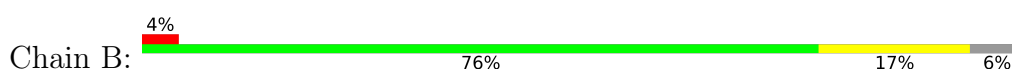
- Molecule 1: Sensor histidine kinase DesK

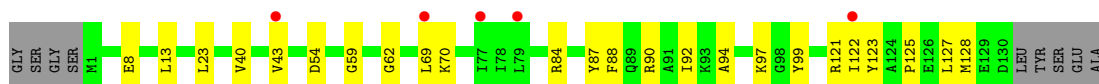


- Molecule 1: Sensor histidine kinase DesK

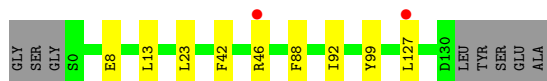
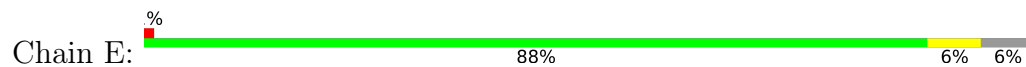


- Molecule 2: Transcriptional regulatory protein DesR

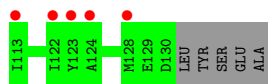
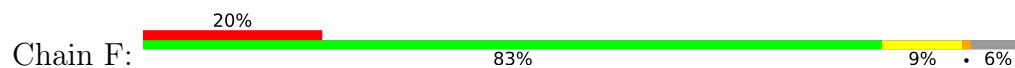




- Molecule 2: Transcriptional regulatory protein DesR



- Molecule 2: Transcriptional regulatory protein DesR



4 Data and refinement statistics i

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) 79.2 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
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

Xtrriage'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: MG, ACP, SO4, BEF

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	0.47	0/1702	0.60	0/2295
1	C	0.37	0/1692	0.53	0/2279
1	D	0.41	0/1708	0.57	0/2297
2	B	0.48	0/972	0.60	0/1311
2	E	0.43	0/1005	0.59	0/1352
2	F	0.37	0/966	0.56	0/1303
All	All	0.42	0/8045	0.57	0/10837

There are no bond length outliers.

There are no bond angle outliers.

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	13	0
1	C	1675	0	1674	10	0
1	D	1694	0	1711	11	0
2	B	961	0	954	13	0
2	E	991	0	1012	3	0
2	F	955	0	945	5	0
3	A	31	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	48	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 3.

All (48) 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:A:311:TRP:HE1	1:A:312:LYS:NZ	1.93	0.66
1:A:165:GLU:O	1:A:169:GLU:HB3	1.99	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:A:312:LYS:HZ2	2:B:59:GLY:HA3	1.69	0.57
1:A:311:TRP:NE1	1:A:312:LYS:NZ	2.49	0.57
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
2:E:88:PHE:O	2:E:92:ILE:HG12	2.08	0.53
2:B:125:PRO:HA	2:B:128:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:221:LYS:HZ3	1:D:206:ARG:HD2	1.78	0.48
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: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: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: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: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
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
2:B:125:PRO:HA	2:B:128:MET:CE	2.50	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/224 (97%)	213 (98%)	3 (1%)	1 (0%)	29	47
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%)	51	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/199 (89%)	164 (92%)	14 (8%)	12	22
1	C	178/199 (89%)	168 (94%)	10 (6%)	21	38
1	D	181/199 (91%)	168 (93%)	13 (7%)	14	26
2	B	99/113 (88%)	93 (94%)	6 (6%)	18	34
2	E	106/113 (94%)	103 (97%)	3 (3%)	43	68
2	F	97/113 (86%)	90 (93%)	7 (7%)	14	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	839/936 (90%)	786 (94%)	53 (6%)	18	32

All (53) 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	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	341	ARG
2	B	8	GLU
2	B	13	LEU
2	B	23	LEU
2	B	90	ARG
2	B	97	LYS
2	B	122	ILE
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	261	ASP
1	C	299	GLN
1	C	341	ARG
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

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Mol	Chain	Res	Type
1	D	237	ILE
1	D	261	ASP
1	D	294	VAL
1	D	299	GLN
1	D	301	LYS
1	D	333	LYS
2	E	8	GLU
2	E	13	LEU
2	E	23	LEU
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	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	281	ASN
1	C	193	GLN
1	C	255	GLN
1	D	193	GLN
1	D	225	GLN
1	D	255	GLN
2	F	89	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 monosaccharides in this entry.

5.6 Ligand geometry

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	27,33,33	0.80	1 (3%)	32,52,52	0.87	2 (6%)
3	ACP	A	401	4	27,33,33	0.81	1 (3%)	32,52,52	0.82	2 (6%)
5	BEF	B	202	2	0,3,3	-	-	-	-	-
6	SO4	E	203	-	4,4,4	0.20	0	6,6,6	0.10	0
3	ACP	D	401	4	27,33,33	0.84	1 (3%)	32,52,52	0.93	2 (6%)
5	BEF	E	202	2	0,3,3	-	-	-	-	-
5	BEF	F	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	D	401	4	-	3/15/38/38	0/3/3/3
3	ACP	A	401	4	-	3/15/38/38	0/3/3/3
3	ACP	C	401	4	-	3/15/38/38	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	3.08	1.61	1.58
3	A	401	ACP	PB-O3A	2.95	1.61	1.58
3	D	401	ACP	PB-O3A	2.77	1.61	1.58

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ACP	O1B-PB-C3B	3.15	117.40	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ACP	O1B-PB-C3B	2.92	116.79	109.07
3	A	401	ACP	O1B-PB-C3B	2.85	116.60	109.07
3	D	401	ACP	C5-C6-N6	2.49	124.14	120.35
3	A	401	ACP	C5-C6-N6	2.46	124.09	120.35
3	C	401	ACP	C5-C6-N6	2.39	123.98	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

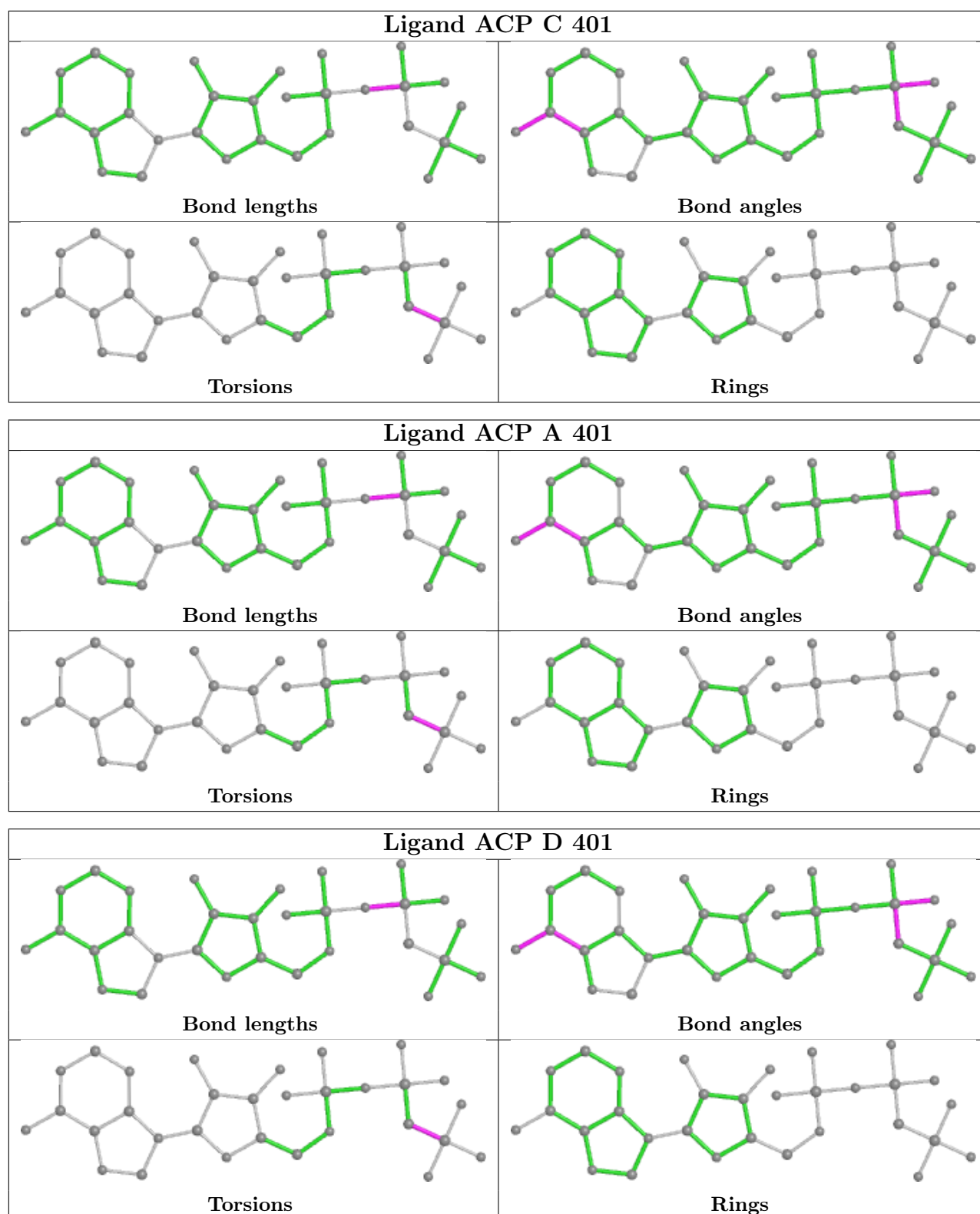
Mol	Chain	Res	Type	Atoms
3	A	401	ACP	PB-C3B-PG-O1G
3	A	401	ACP	PB-C3B-PG-O2G
3	C	401	ACP	PB-C3B-PG-O1G
3	C	401	ACP	PB-C3B-PG-O3G
3	D	401	ACP	PB-C3B-PG-O1G
3	D	401	ACP	PB-C3B-PG-O2G
3	D	401	ACP	PB-C3B-PG-O3G
3	A	401	ACP	PB-C3B-PG-O3G
3	C	401	ACP	PB-C3B-PG-O2G

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	A	401	ACP	1	0
3	D	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

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%)	0.52	10 (4%) 32 35	60, 85, 132, 140	11 (5%)
1	C	216/224 (96%)	0.89	35 (16%) 1 1	68, 132, 189, 212	0
1	D	218/224 (97%)	0.60	20 (9%) 9 9	70, 108, 138, 159	0
2	B	130/139 (93%)	0.37	5 (3%) 40 44	60, 78, 109, 123	0
2	E	131/139 (94%)	0.35	2 (1%) 73 76	63, 81, 103, 115	0
2	F	130/139 (93%)	1.08	28 (21%) 0 0	97, 119, 132, 136	0
All	All	1044/1089 (95%)	0.64	100 (9%) 8 8	60, 101, 150, 212	11 (1%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	331	PHE	8.2
1	D	333	LYS	5.6
1	C	246	LEU	4.7
2	F	98	GLY	4.4
1	C	290	ALA	4.4
1	C	211	LYS	4.3
2	F	128	MET	4.3
2	F	100	LEU	4.1
1	C	177	LEU	4.1
2	F	108	GLU	4.1
1	C	287	LEU	4.0
1	D	331	PHE	4.0
2	F	29	VAL	4.0
1	C	305	VAL	3.9
2	F	123	TYR	3.9
1	C	355	THR	3.7
2	F	50	VAL	3.6
1	D	149	GLY	3.6
1	C	350	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	174	LEU	3.5
2	F	63	LEU	3.5
2	F	113	ILE	3.4
1	C	278	LEU	3.4
1	C	361	LEU	3.3
1	A	163	LYS	3.3
2	F	99	TYR	3.3
1	C	291	VAL	3.3
2	E	127	LEU	3.3
1	C	307	ILE	3.2
1	C	314	VAL	3.2
1	C	150	ILE	3.2
2	F	109	LEU	3.1
2	F	1	MET	3.1
2	F	78	ILE	3.0
1	C	173	GLU	3.0
1	C	286	CYS	3.0
2	F	112	ALA	3.0
1	C	303	CYS	2.9
1	D	250	LEU	2.9
1	D	287	LEU	2.9
1	D	150	ILE	2.8
1	C	266	TYR	2.8
1	C	367	ASN	2.8
2	F	124	ALA	2.7
1	C	337	LEU	2.7
1	A	161	GLU	2.7
2	F	101	LEU	2.7
2	F	20	LEU	2.7
1	D	185	ARG	2.6
1	A	333	LYS	2.6
1	C	208	LEU	2.6
1	D	337	LEU	2.6
1	C	264	PHE	2.6
1	D	174	LEU	2.6
1	A	331	PHE	2.6
1	C	353	ILE	2.5
1	D	346	PHE	2.5
2	F	87	TYR	2.5
1	A	154	ARG	2.4
1	D	228	ARG	2.4
2	F	21	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	275	ILE	2.4
2	F	82	PHE	2.4
1	D	286	CYS	2.4
2	B	122	ILE	2.4
2	F	76	ILE	2.4
1	D	302	THR	2.4
1	A	151	ILE	2.4
1	D	176	LYS	2.4
1	C	364	ALA	2.4
1	C	180	ARG	2.3
2	B	69	LEU	2.3
1	A	329	ASN	2.3
1	C	311	TRP	2.3
1	C	315	VAL	2.3
1	D	175	VAL	2.3
2	B	77	ILE	2.3
1	C	253	ILE	2.3
2	F	122	ILE	2.3
2	F	69	LEU	2.3
1	D	314	VAL	2.2
1	D	171	ILE	2.2
2	F	2	ILE	2.2
1	A	187	LEU	2.2
1	D	151	ILE	2.2
1	C	169	GLU	2.2
1	C	265	ILE	2.2
1	D	237	ILE	2.2
1	C	351	LEU	2.2
1	D	283	LEU	2.2
2	B	79	LEU	2.2
2	F	83	ALA	2.1
2	F	11	GLN	2.1
2	F	40	VAL	2.1
1	A	192	GLY	2.1
1	C	283	LEU	2.1
2	E	46	ARG	2.1
1	A	183	ILE	2.0
2	F	14	LEU	2.0
2	B	43	VAL	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](#)

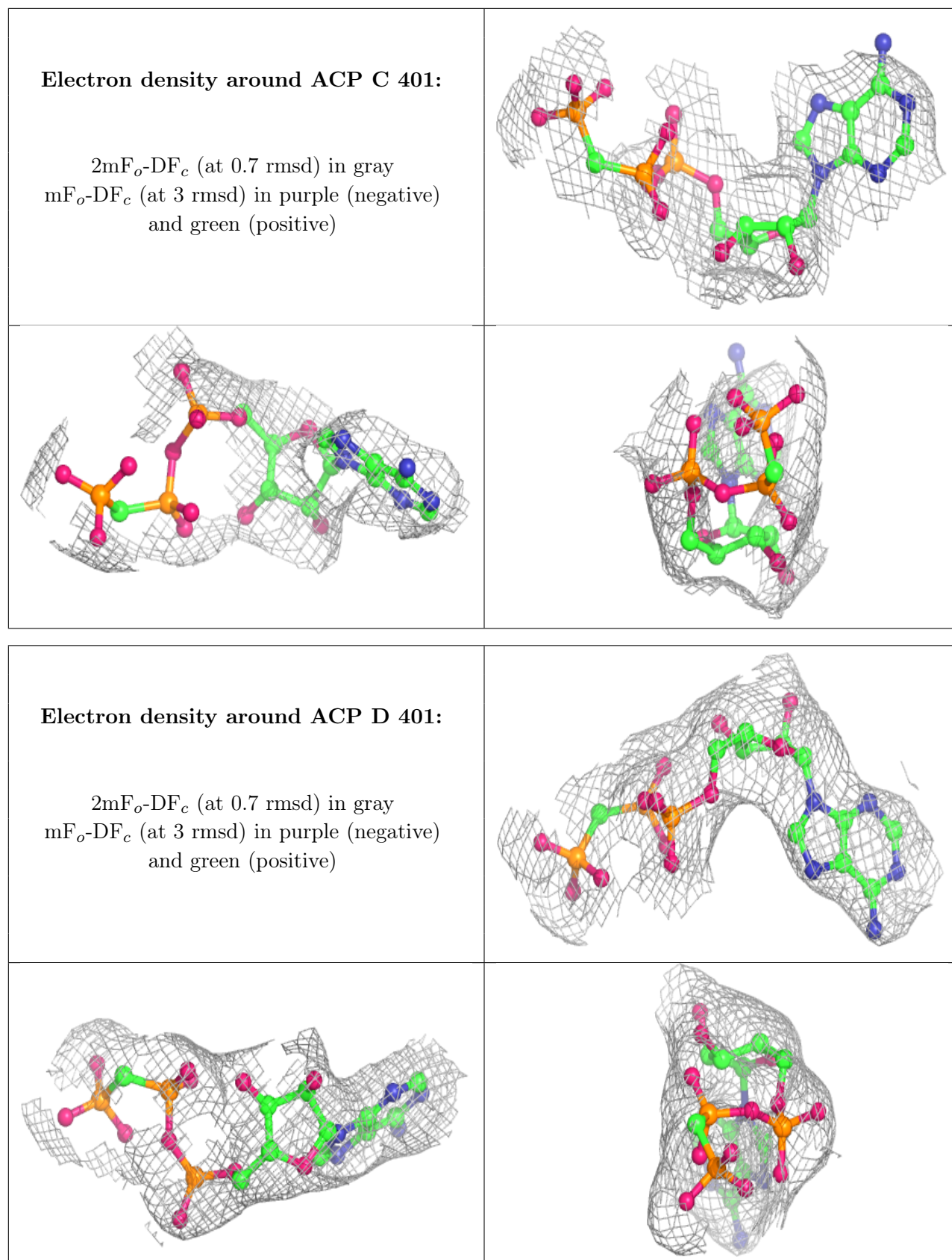
There are no monosaccharides in this entry.

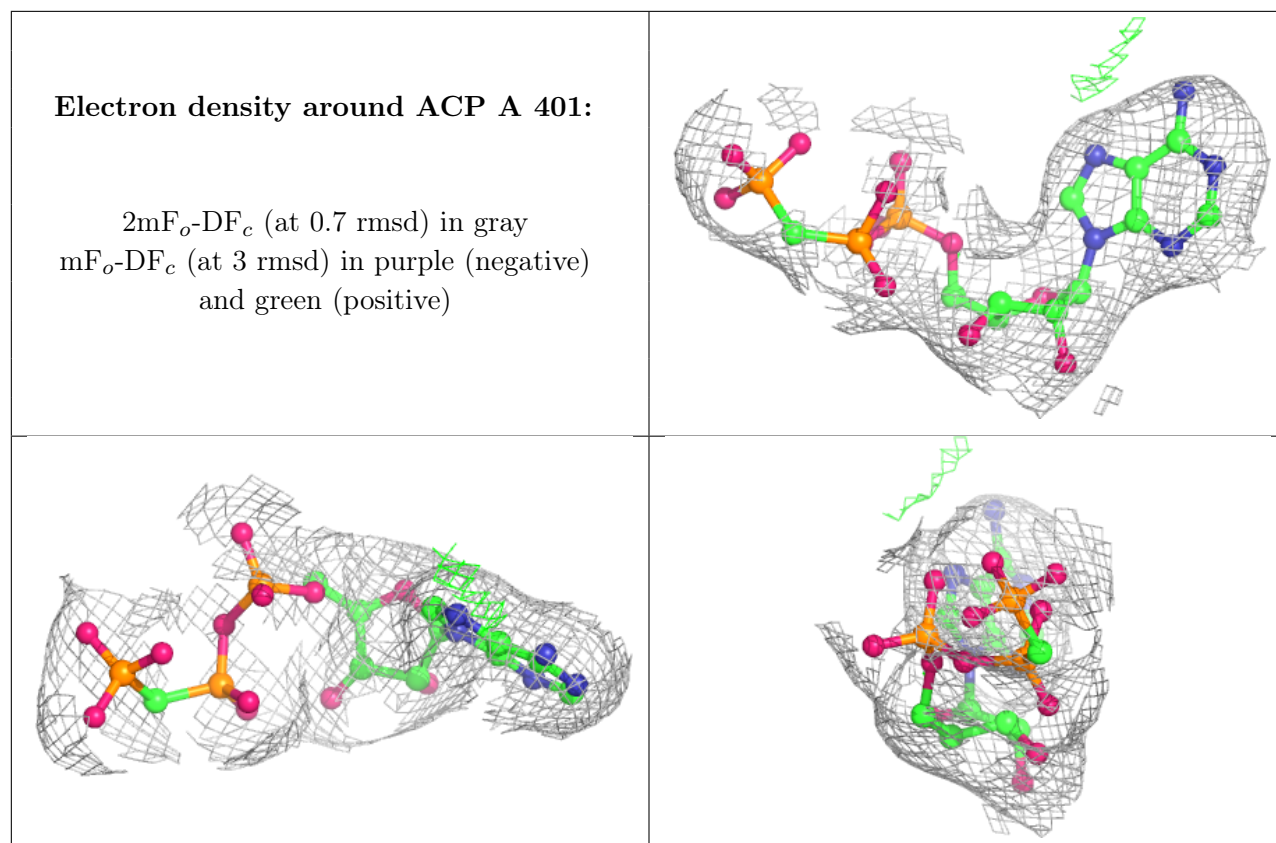
6.4 Ligands [i](#)

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
4	MG	C	402	1/1	0.68	0.16	188,188,188,188	0
4	MG	F	201	1/1	0.80	0.10	133,133,133,133	0
6	SO4	E	203	5/5	0.83	0.16	170,170,170,170	0
3	ACP	C	401	31/31	0.90	0.16	152,156,159,159	0
4	MG	D	402	1/1	0.93	0.12	89,89,89,89	0
5	BEF	F	202	4/4	0.94	0.14	122,122,122,123	0
5	BEF	E	202	4/4	0.95	0.16	74,75,75,77	0
3	ACP	D	401	31/31	0.95	0.14	87,89,91,91	0
5	BEF	B	202	4/4	0.95	0.13	72,72,73,73	0
4	MG	E	201	1/1	0.97	0.12	77,77,77,77	0
3	ACP	A	401	31/31	0.97	0.15	90,92,97,97	0
4	MG	A	402	1/1	0.98	0.19	84,84,84,84	0
4	MG	B	201	1/1	0.99	0.11	51,51,51,51	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.