Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 02:30 PM EDT

PDB ID	:	6P7G
Title	:	The co-crystal structure of BRAF(V600E) with PHI1
Authors	:	Agianian, B.; Gavathiotis, E.
Deposited on	:	2019-06-05
Resolution	:	2.65 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:

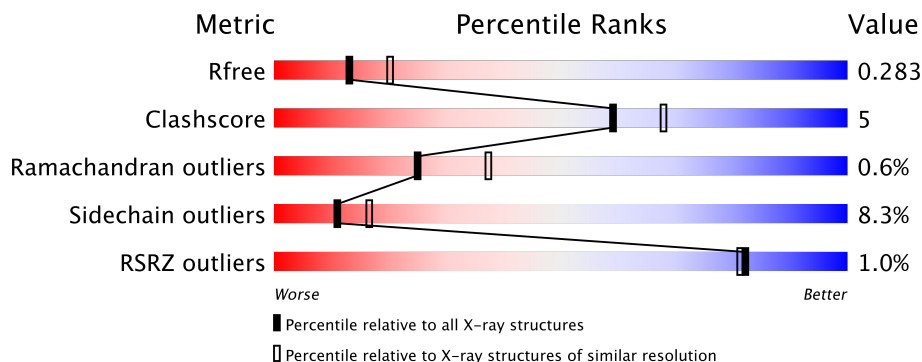|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4

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 2.65 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		5
Ramachandran outliers		0.6%
Sidechain outliers		8.3%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X–ray structures

▯ Percentile relative to X–ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	297	75% 9% • 14%
1	B	297	.% 80% 11% • 8%
1	C	297	74% 11% • 14%
1	D	297	.% 75% 7% • 14%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8543 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2046	1296	365	372	13			
1	B	273	Total	C	N	O	S	0	0	0
			2189	1385	391	400	13			
1	C	256	Total	C	N	O	S	0	0	0
			2050	1300	365	372	13			
1	D	254	Total	C	N	O	S	0	0	0
			2031	1290	362	366	13			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	MET	-	initiating methionine	UNP P15056
A	428	GLY	-	expression tag	UNP P15056
A	429	SER	-	expression tag	UNP P15056
A	430	SER	-	expression tag	UNP P15056
A	431	HIS	-	expression tag	UNP P15056
A	432	HIS	-	expression tag	UNP P15056
A	433	HIS	-	expression tag	UNP P15056
A	434	HIS	-	expression tag	UNP P15056
A	435	HIS	-	expression tag	UNP P15056
A	436	HIS	-	expression tag	UNP P15056
A	437	SER	-	expression tag	UNP P15056
A	438	SER	-	expression tag	UNP P15056
A	439	GLY	-	expression tag	UNP P15056
A	440	LEU	-	expression tag	UNP P15056
A	441	VAL	-	expression tag	UNP P15056
A	442	PRO	-	expression tag	UNP P15056
A	443	ARG	-	expression tag	UNP P15056
A	444	GLY	-	expression tag	UNP P15056
A	445	SER	-	expression tag	UNP P15056
A	446	LYS	-	expression tag	UNP P15056
A	447	MET	-	expression tag	UNP P15056

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	ALA	ILE	engineered mutation	UNP P15056
A	544	SER	ILE	engineered mutation	UNP P15056
A	551	LYS	ILE	engineered mutation	UNP P15056
A	562	ARG	GLN	engineered mutation	UNP P15056
A	588	ASN	LEU	engineered mutation	UNP P15056
A	600	GLU	VAL	engineered mutation	UNP P15056
A	630	SER	LYS	engineered mutation	UNP P15056
A	667	GLU	PHE	engineered mutation	UNP P15056
A	673	SER	TYR	engineered mutation	UNP P15056
A	688	ARG	ALA	engineered mutation	UNP P15056
A	706	SER	LEU	engineered mutation	UNP P15056
A	709	ARG	GLN	engineered mutation	UNP P15056
A	713	GLU	SER	engineered mutation	UNP P15056
A	716	GLU	LEU	engineered mutation	UNP P15056
A	720	GLU	SER	engineered mutation	UNP P15056
A	722	SER	PRO	engineered mutation	UNP P15056
A	723	GLY	LYS	engineered mutation	UNP P15056
B	427	MET	-	initiating methionine	UNP P15056
B	428	GLY	-	expression tag	UNP P15056
B	429	SER	-	expression tag	UNP P15056
B	430	SER	-	expression tag	UNP P15056
B	431	HIS	-	expression tag	UNP P15056
B	432	HIS	-	expression tag	UNP P15056
B	433	HIS	-	expression tag	UNP P15056
B	434	HIS	-	expression tag	UNP P15056
B	435	HIS	-	expression tag	UNP P15056
B	436	HIS	-	expression tag	UNP P15056
B	437	SER	-	expression tag	UNP P15056
B	438	SER	-	expression tag	UNP P15056
B	439	GLY	-	expression tag	UNP P15056
B	440	LEU	-	expression tag	UNP P15056
B	441	VAL	-	expression tag	UNP P15056
B	442	PRO	-	expression tag	UNP P15056
B	443	ARG	-	expression tag	UNP P15056
B	444	GLY	-	expression tag	UNP P15056
B	445	SER	-	expression tag	UNP P15056
B	446	LYS	-	expression tag	UNP P15056
B	447	MET	-	expression tag	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	588	ASN	LEU	engineered mutation	UNP P15056
B	600	GLU	VAL	engineered mutation	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	667	GLU	PHE	engineered mutation	UNP P15056
B	673	SER	TYR	engineered mutation	UNP P15056
B	688	ARG	ALA	engineered mutation	UNP P15056
B	706	SER	LEU	engineered mutation	UNP P15056
B	709	ARG	GLN	engineered mutation	UNP P15056
B	713	GLU	SER	engineered mutation	UNP P15056
B	716	GLU	LEU	engineered mutation	UNP P15056
B	720	GLU	SER	engineered mutation	UNP P15056
B	722	SER	PRO	engineered mutation	UNP P15056
B	723	GLY	LYS	engineered mutation	UNP P15056
C	427	MET	-	initiating methionine	UNP P15056
C	428	GLY	-	expression tag	UNP P15056
C	429	SER	-	expression tag	UNP P15056
C	430	SER	-	expression tag	UNP P15056
C	431	HIS	-	expression tag	UNP P15056
C	432	HIS	-	expression tag	UNP P15056
C	433	HIS	-	expression tag	UNP P15056
C	434	HIS	-	expression tag	UNP P15056
C	435	HIS	-	expression tag	UNP P15056
C	436	HIS	-	expression tag	UNP P15056
C	437	SER	-	expression tag	UNP P15056
C	438	SER	-	expression tag	UNP P15056
C	439	GLY	-	expression tag	UNP P15056
C	440	LEU	-	expression tag	UNP P15056
C	441	VAL	-	expression tag	UNP P15056
C	442	PRO	-	expression tag	UNP P15056
C	443	ARG	-	expression tag	UNP P15056
C	444	GLY	-	expression tag	UNP P15056
C	445	SER	-	expression tag	UNP P15056
C	446	LYS	-	expression tag	UNP P15056
C	447	MET	-	expression tag	UNP P15056
C	543	ALA	ILE	engineered mutation	UNP P15056
C	544	SER	ILE	engineered mutation	UNP P15056
C	551	LYS	ILE	engineered mutation	UNP P15056
C	562	ARG	GLN	engineered mutation	UNP P15056
C	588	ASN	LEU	engineered mutation	UNP P15056
C	600	GLU	VAL	engineered mutation	UNP P15056
C	630	SER	LYS	engineered mutation	UNP P15056
C	667	GLU	PHE	engineered mutation	UNP P15056

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	673	SER	TYR	engineered mutation	UNP P15056
C	688	ARG	ALA	engineered mutation	UNP P15056
C	706	SER	LEU	engineered mutation	UNP P15056
C	709	ARG	GLN	engineered mutation	UNP P15056
C	713	GLU	SER	engineered mutation	UNP P15056
C	716	GLU	LEU	engineered mutation	UNP P15056
C	720	GLU	SER	engineered mutation	UNP P15056
C	722	SER	PRO	engineered mutation	UNP P15056
C	723	GLY	LYS	engineered mutation	UNP P15056
D	427	MET	-	initiating methionine	UNP P15056
D	428	GLY	-	expression tag	UNP P15056
D	429	SER	-	expression tag	UNP P15056
D	430	SER	-	expression tag	UNP P15056
D	431	HIS	-	expression tag	UNP P15056
D	432	HIS	-	expression tag	UNP P15056
D	433	HIS	-	expression tag	UNP P15056
D	434	HIS	-	expression tag	UNP P15056
D	435	HIS	-	expression tag	UNP P15056
D	436	HIS	-	expression tag	UNP P15056
D	437	SER	-	expression tag	UNP P15056
D	438	SER	-	expression tag	UNP P15056
D	439	GLY	-	expression tag	UNP P15056
D	440	LEU	-	expression tag	UNP P15056
D	441	VAL	-	expression tag	UNP P15056
D	442	PRO	-	expression tag	UNP P15056
D	443	ARG	-	expression tag	UNP P15056
D	444	GLY	-	expression tag	UNP P15056
D	445	SER	-	expression tag	UNP P15056
D	446	LYS	-	expression tag	UNP P15056
D	447	MET	-	expression tag	UNP P15056
D	543	ALA	ILE	engineered mutation	UNP P15056
D	544	SER	ILE	engineered mutation	UNP P15056
D	551	LYS	ILE	engineered mutation	UNP P15056
D	562	ARG	GLN	engineered mutation	UNP P15056
D	588	ASN	LEU	engineered mutation	UNP P15056
D	600	GLU	VAL	engineered mutation	UNP P15056
D	630	SER	LYS	engineered mutation	UNP P15056
D	667	GLU	PHE	engineered mutation	UNP P15056
D	673	SER	TYR	engineered mutation	UNP P15056
D	688	ARG	ALA	engineered mutation	UNP P15056
D	706	SER	LEU	engineered mutation	UNP P15056
D	709	ARG	GLN	engineered mutation	UNP P15056

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	713	GLU	SER	engineered mutation	UNP P15056
D	716	GLU	LEU	engineered mutation	UNP P15056
D	720	GLU	SER	engineered mutation	UNP P15056
D	722	SER	PRO	engineered mutation	UNP P15056
D	723	GLY	LYS	engineered mutation	UNP P15056

- Molecule 2 is 3-[(imidazo[1,2-b]pyridazin-3-yl)ethynyl]-4-methyl-N-[4-({[2-(morpholin-4-yl)ethyl]amino}methyl)-3-(trifluoromethyl)phenyl]benzamide (three-letter code: E7M) (formula: $C_{30}H_{29}F_3N_6O_2$) (labeled as "Ligand of Interest" by author).
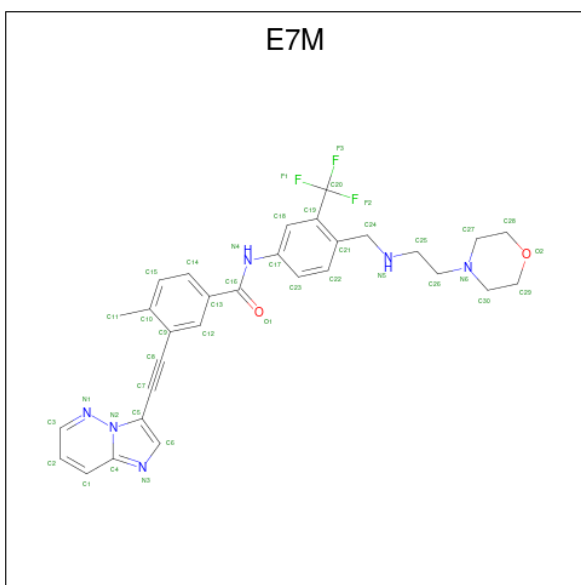
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			41	30	3	6	2		
2	B	1	Total	C	F	N	O	0	0
			41	30	3	6	2		
2	C	1	Total	C	F	N	O	0	0
			41	30	3	6	2		
2	D	1	Total	C	F	N	O	0	0
			41	30	3	6	2		

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).

NHE

O3
OH

O1 O = S = O O2
S

C1 C2

C6'
C5' C1' NH N

C4' C2'

C3'
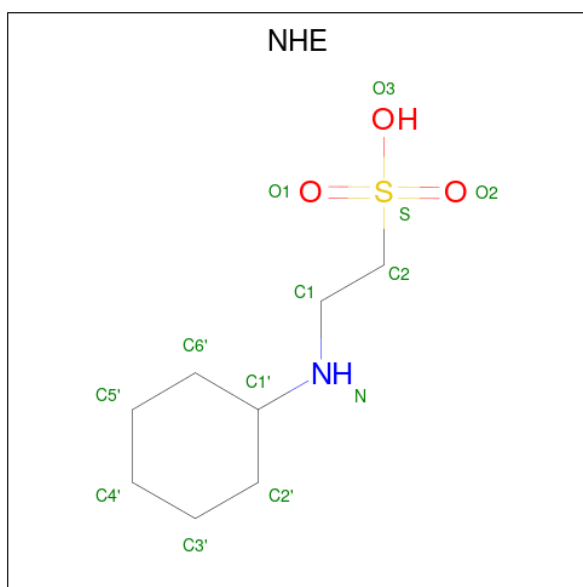
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total 12	O 12	0	0
4	B	20	Total 20	O 20	0	0
4	C	10	Total 10	O 10	0	0
4	D	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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.
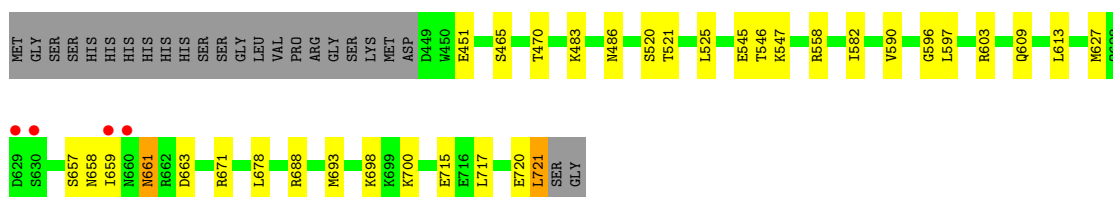
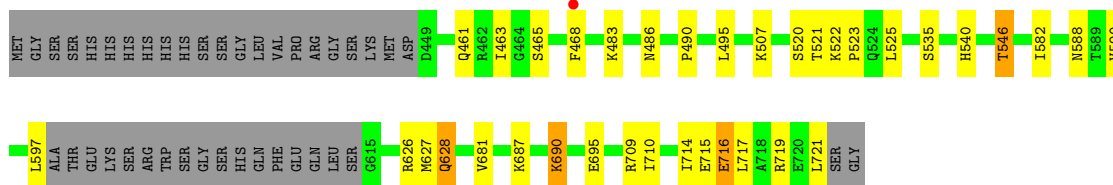- Molecule 1: Serine/threonine-protein kinase B-raf

Chain A:
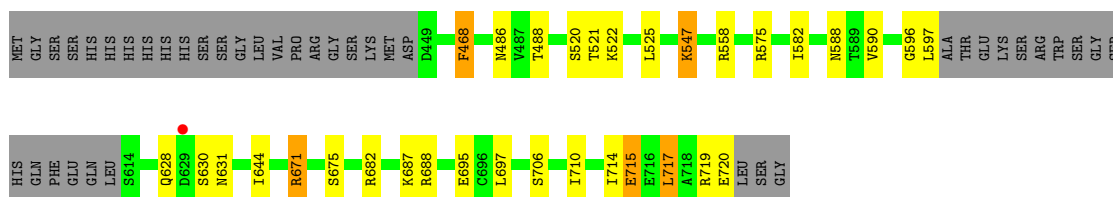
- Molecule 1: Serine/threonine-protein kinase B-raf

Chain B:

- Molecule 1: Serine/threonine-protein kinase B-raf

Chain C:

- Molecule 1: Serine/threonine-protein kinase B-raf

Chain D:

GLY SER HIS GLN PHE GLU GLN LEU **S614** **G615** **M627** GLN ASP SER **N631** **I659** **N660** **N661** **R662** **D663** **Q664** **I665** **M668** **L674** **S675** **K687** **E715** **E716** **L717** **A718** **L721** SER GLY

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.78Å 108.79Å 126.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.45 – 2.65 82.45 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.2 (82.45-2.65) 94.2 (82.45-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.29	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.248 , 0.279 0.251 , 0.283	Depositor DCC
R_{free} test set	1875 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.4	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8543	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NHE, E7M

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	0.61	0/2088	0.76	0/2812
1	B	0.58	0/2236	0.76	0/3013
1	C	0.57	0/2092	0.74	0/2818
1	D	0.55	0/2072	0.73	1/2789 (0.0%)
All	All	0.58	0/8488	0.75	1/11432 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	717	LEU	CA-CB-CG	5.01	126.82	115.30

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	2046	0	2059	20	0
1	B	2189	0	2196	15	0
1	C	2050	0	2069	20	0
1	D	2031	0	2052	27	0
2	A	41	0	0	0	0
2	B	41	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	41	0	0	0	0
2	D	41	0	0	1	0
3	B	13	0	17	0	0
4	A	12	0	0	0	0
4	B	20	0	0	1	0
4	C	10	0	0	1	0
4	D	8	0	0	0	0
All	All	8543	0	8393	80	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 (80) 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:D:659:ILE:HD11	1:D:665:ILE:CD1	1.77	1.15
1:D:659:ILE:HD11	1:D:665:ILE:HD13	1.39	1.04
1:C:687:LYS:HD2	1:C:690:LYS:HD2	1.41	1.02
1:C:716:GLU:O	1:C:719:ARG:HG2	1.62	0.99
1:D:721:LEU:HD23	1:D:721:LEU:H	1.29	0.98
1:B:661:ASN:HD21	1:B:663:ASP:HB2	1.35	0.90
1:D:659:ILE:HD11	1:D:665:ILE:HD11	1.54	0.89
1:A:575:ARG:NH2	1:A:631:ASN:HD21	1.80	0.80
1:C:687:LYS:CD	1:C:690:LYS:HD2	2.10	0.79
1:D:660:ASN:N	1:D:660:ASN:OD1	2.17	0.77
1:C:523:PRO:HG2	1:D:488:THR:HG22	1.69	0.74
1:A:717:LEU:O	1:A:717:LEU:HD12	1.91	0.70
1:D:661:ASN:H	1:D:661:ASN:HD22	1.38	0.69
1:A:717:LEU:C	1:A:717:LEU:HD12	2.15	0.66
1:D:659:ILE:CD1	1:D:665:ILE:HD13	2.20	0.65
1:C:687:LYS:HD2	1:C:690:LYS:CD	2.22	0.65
1:A:547:LYS:O	1:A:547:LYS:HG2	1.96	0.64
1:B:678:LEU:HD22	1:B:693:MET:CE	2.27	0.64
1:D:721:LEU:HD23	1:D:721:LEU:N	2.07	0.64
1:B:661:ASN:C	1:B:661:ASN:HD22	2.02	0.63
1:B:661:ASN:ND2	1:B:663:ASP:HB2	2.13	0.62
1:D:486:ASN:OD1	1:D:486:ASN:N	2.21	0.62
1:D:659:ILE:CD1	1:D:665:ILE:CD1	2.67	0.61
1:A:558:ARG:HD2	1:A:715:GLU:HG3	1.82	0.60
1:A:547:LYS:H	1:A:547:LYS:HE2	1.66	0.60
1:C:535:SER:HB3	4:C:1104:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLY:HA2	1:D:596:GLY:HA3	1.84	0.59
1:D:661:ASN:H	1:D:661:ASN:ND2	2.01	0.58
1:D:659:ILE:HG12	1:D:659:ILE:O	2.04	0.58
1:C:523:PRO:CG	1:D:488:THR:HG22	2.34	0.58
1:C:465:SER:O	1:C:597:LEU:N	2.37	0.57
1:A:575:ARG:NH2	1:A:631:ASN:ND2	2.50	0.57
1:C:681:VAL:HG21	1:C:690:LYS:HE3	1.86	0.56
1:D:668:MET:HB3	1:D:674:LEU:HB2	1.87	0.56
1:D:721:LEU:H	1:D:721:LEU:CD2	1.97	0.56
1:D:467:SER:O	1:D:467:SER:OG	2.20	0.55
1:A:582:ILE:HG23	1:A:590:VAL:HG13	1.89	0.55
1:B:698:LYS:HE3	4:B:904:HOH:O	2.07	0.54
1:B:582:ILE:HG23	1:B:590:VAL:HG13	1.89	0.54
1:C:582:ILE:HG23	1:C:590:VAL:HG13	1.90	0.54
1:D:582:ILE:HG23	1:D:590:VAL:HG13	1.90	0.54
1:C:687:LYS:HA	1:C:690:LYS:HD2	1.89	0.53
1:A:575:ARG:HH21	1:A:631:ASN:HD21	1.52	0.53
1:C:626:ARG:HE	1:C:628:GLN:NE2	2.08	0.52
1:A:671:ARG:HD2	1:A:671:ARG:O	2.09	0.52
1:A:706:SER:O	1:A:710:ILE:HG13	2.09	0.52
1:A:714:ILE:HG22	1:A:714:ILE:O	2.08	0.52
1:C:490:PRO:HB2	1:C:495:LEU:CD2	2.40	0.51
1:D:558:ARG:HD2	1:D:715:GLU:HG3	1.93	0.50
1:D:487:VAL:HG12	1:D:488:THR:N	2.26	0.49
1:A:468:PHE:CD1	1:A:468:PHE:C	2.86	0.49
1:D:487:VAL:CG1	1:D:488:THR:N	2.76	0.48
1:A:547:LYS:O	1:A:547:LYS:CG	2.62	0.48
1:B:465:SER:HA	1:B:470:THR:HA	1.96	0.47
1:B:661:ASN:ND2	1:B:663:ASP:H	2.12	0.47
1:C:463:ILE:HD13	1:C:463:ILE:N	2.30	0.47
1:C:710:ILE:O	1:C:714:ILE:HG13	2.16	0.46
1:B:661:ASN:HD22	1:B:663:ASP:H	1.64	0.45
1:B:688:ARG:NH2	1:B:720:GLU:OE1	2.50	0.45
1:B:721:LEU:CD2	1:B:721:LEU:C	2.85	0.45
1:C:468:PHE:O	1:C:468:PHE:CG	2.70	0.45
1:C:468:PHE:CD2	1:C:468:PHE:O	2.70	0.45
1:A:468:PHE:CG	1:A:468:PHE:O	2.70	0.44
1:B:558:ARG:HD2	1:B:715:GLU:HG3	2.00	0.44
1:B:658:ASN:C	1:B:659:ILE:HG13	2.39	0.43
1:A:575:ARG:HH21	1:A:631:ASN:ND2	2.13	0.43
1:A:644:ILE:CD1	1:A:697:LEU:HD21	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:ILE:HG21	1:D:718:ALA:HB2	2.01	0.43
1:A:558:ARG:CD	1:A:715:GLU:HG3	2.50	0.42
1:D:661:ASN:ND2	1:D:661:ASN:N	2.66	0.42
1:C:490:PRO:HB2	1:C:495:LEU:HD23	2.00	0.42
1:C:540:HIS:ND1	1:C:546:THR:HG21	2.35	0.42
1:D:662:ARG:HE	1:D:662:ARG:HB2	1.50	0.42
1:A:688:ARG:NH2	1:A:720:GLU:OE1	2.53	0.42
1:B:678:LEU:HD22	1:B:693:MET:HE2	2.00	0.41
1:D:500:ASN:HB3	2:D:801:E7M:C28	2.50	0.41
1:D:662:ARG:O	1:D:665:ILE:CG1	2.68	0.41
1:B:661:ASN:C	1:B:661:ASN:ND2	2.71	0.41
1:C:626:ARG:HE	1:C:628:GLN:HE21	1.68	0.40
1:A:644:ILE:HD13	1:A:697:LEU:HD21	2.02	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	252/297 (85%)	243 (96%)	7 (3%)	2 (1%)	19	29
1	B	271/297 (91%)	261 (96%)	9 (3%)	1 (0%)	34	48
1	C	252/297 (85%)	245 (97%)	7 (3%)	0	100	100
1	D	248/297 (84%)	236 (95%)	9 (4%)	3 (1%)	13	19
All	All	1023/1188 (86%)	985 (96%)	32 (3%)	6 (1%)	25	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	630	SER
1	A	596	GLY

Continued on next page...

WORLDWIDE wwPDB PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Res	Type
1	B	596	GLY
1	D	664	GLN
1	D	615	GLY
1	D	596	GLY

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	224/260 (86%)	205 (92%)	19 (8%)	10	15
1	B	240/260 (92%)	220 (92%)	20 (8%)	11	16
1	C	225/260 (86%)	206 (92%)	19 (8%)	11	16
1	D	222/260 (85%)	204 (92%)	18 (8%)	11	17
All	All	911/1040 (88%)	835 (92%)	76 (8%)	11	16

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	PHE
1	A	486	ASN
1	A	488	THR
1	A	520	SER
1	A	521	THR
1	A	522	LYS
1	A	525	LEU
1	A	547	LYS
1	A	588	ASN
1	A	597	LEU
1	A	628	GLN
1	A	671	ARG
1	A	675	SER
1	A	682	ARG
1	A	687	LYS
1	A	695	GLU
1	A	715	GLU

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	A	717	LEU
1	A	719	ARG
1	B	451	GLU
1	B	483	LYS
1	B	486	ASN
1	B	520	SER
1	B	521	THR
1	B	525	LEU
1	B	545	GLU
1	B	546	THR
1	B	547	LYS
1	B	597	LEU
1	B	603	ARG
1	B	609	GLN
1	B	613	LEU
1	B	627	MET
1	B	657	SER
1	B	661	ASN
1	B	671	ARG
1	B	700	LYS
1	B	717	LEU
1	B	721	LEU
1	C	461	GLN
1	C	483	LYS
1	C	486	ASN
1	C	507	LYS
1	C	520	SER
1	C	521	THR
1	C	522	LYS
1	C	525	LEU
1	C	546	THR
1	C	588	ASN
1	C	627	MET
1	C	628	GLN
1	C	690	LYS
1	C	695	GLU
1	C	709	ARG
1	C	715	GLU
1	C	716	GLU
1	C	717	LEU
1	C	721	LEU
1	D	468	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	486	ASN
1	D	488	THR
1	D	520	SER
1	D	525	LEU
1	D	546	THR
1	D	551	LYS
1	D	659	ILE
1	D	660	ASN
1	D	661	ASN
1	D	662	ARG
1	D	663	ASP
1	D	664	GLN
1	D	675	SER
1	D	687	LYS
1	D	715	GLU
1	D	717	LEU
1	D	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	GLN
1	A	580	ASN
1	A	631	ASN
1	B	494	GLN
1	B	658	ASN
1	B	661	ASN
1	B	664	GLN
1	C	524	GLN
1	C	628	GLN
1	D	661	ASN
1	D	664	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	E7M	A	801	-	42,45,45	0.61	1 (2%)	52,63,63	0.80	1 (1%)
3	NHE	B	802	-	13,13,13	2.65	2 (15%)	16,17,17	1.75	5 (31%)
2	E7M	B	801	-	42,45,45	0.54	1 (2%)	52,63,63	0.93	2 (3%)
2	E7M	C	1001	-	42,45,45	0.64	1 (2%)	52,63,63	0.77	1 (1%)
2	E7M	D	801	-	42,45,45	0.71	2 (4%)	52,63,63	0.88	1 (1%)

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
2	E7M	A	801	-	-	2/23/34/34	0/5/5/5
3	NHE	B	802	-	-	4/7/15/15	0/1/1/1
2	E7M	B	801	-	-	6/23/34/34	0/5/5/5
2	E7M	C	1001	-	-	5/23/34/34	0/5/5/5
2	E7M	D	801	-	-	4/23/34/34	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	NHE	C2-S	-8.04	1.66	1.77
3	B	802	NHE	O3-S	3.95	1.61	1.47
2	D	801	E7M	C4-N3	2.77	1.36	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	E7M	C2-C3	2.26	1.44	1.37
2	D	801	E7M	C2-C3	2.26	1.44	1.37
2	A	801	E7M	C2-C3	2.17	1.44	1.37
2	C	1001	E7M	C4-N3	2.16	1.35	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	NHE	C3'-C2'-C1'	-3.47	104.58	111.11
2	A	801	E7M	C2-C1-C4	-3.19	116.90	120.22
3	B	802	NHE	O3-S-C2	2.98	110.58	105.77
2	B	801	E7M	C2-C1-C4	-2.98	117.13	120.22
2	D	801	E7M	C2-C1-C4	-2.96	117.15	120.22
2	C	1001	E7M	C2-C1-C4	-2.87	117.24	120.22
3	B	802	NHE	O1-S-C2	2.78	110.26	106.92
2	B	801	E7M	C9-C8-C7	-2.20	169.16	175.91
3	B	802	NHE	C6'-C1'-C2'	-2.19	107.03	110.82
3	B	802	NHE	O3-S-O2	-2.14	106.05	111.27

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	NHE	N-C1-C2-S
2	B	801	E7M	C25-C26-N6-C27
2	C	1001	E7M	C21-C24-N5-C25
2	B	801	E7M	C21-C24-N5-C25
2	D	801	E7M	C21-C24-N5-C25
2	C	1001	E7M	C7-C8-C9-C10
3	B	802	NHE	C1-C2-S-O3
2	A	801	E7M	C7-C8-C9-C12
2	C	1001	E7M	C7-C8-C9-C12
2	A	801	E7M	C7-C8-C9-C10
2	C	1001	E7M	N5-C25-C26-N6
2	B	801	E7M	C23-C17-N4-C16
2	B	801	E7M	C7-C8-C9-C10
3	B	802	NHE	C1-C2-S-O1
3	B	802	NHE	C1-C2-S-O2
2	B	801	E7M	C7-C8-C9-C12
2	D	801	E7M	C7-C8-C9-C12
2	B	801	E7M	C18-C17-N4-C16
2	D	801	E7M	N5-C25-C26-N6

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	801	E7M	C7-C8-C9-C10
2	C	1001	E7M	C25-C26-N6-C27

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	E7M	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 then 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 E7M A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand E7M B 801

Bond lengths

Bond angles

Torsions

Rings

Ligand E7M C 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand E7M D 801

Bond lengths

Bond angles

Torsions

Rings
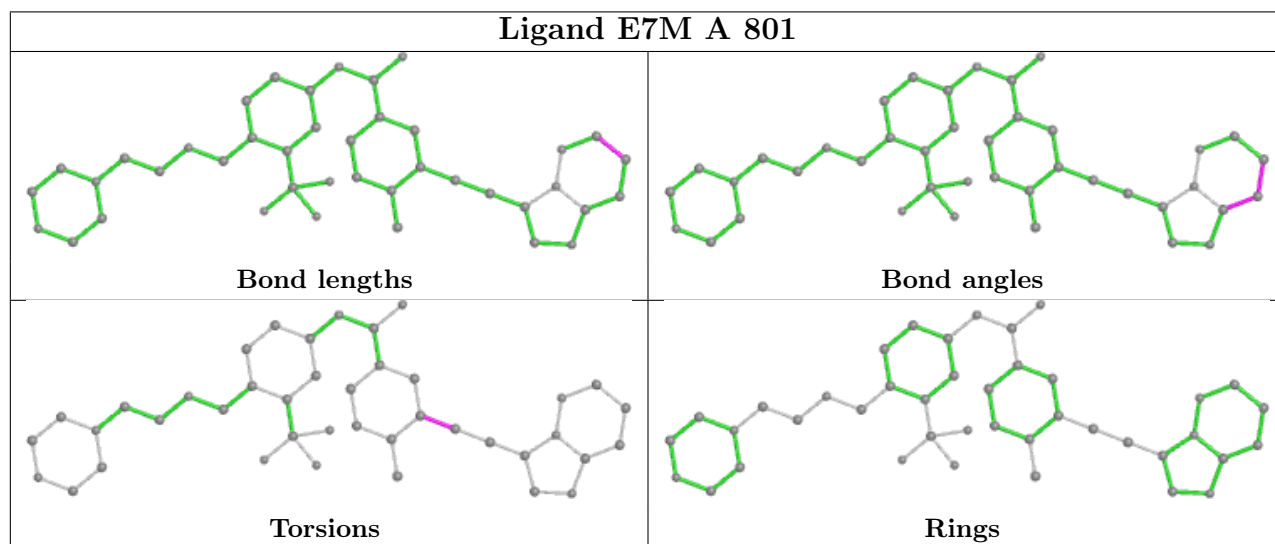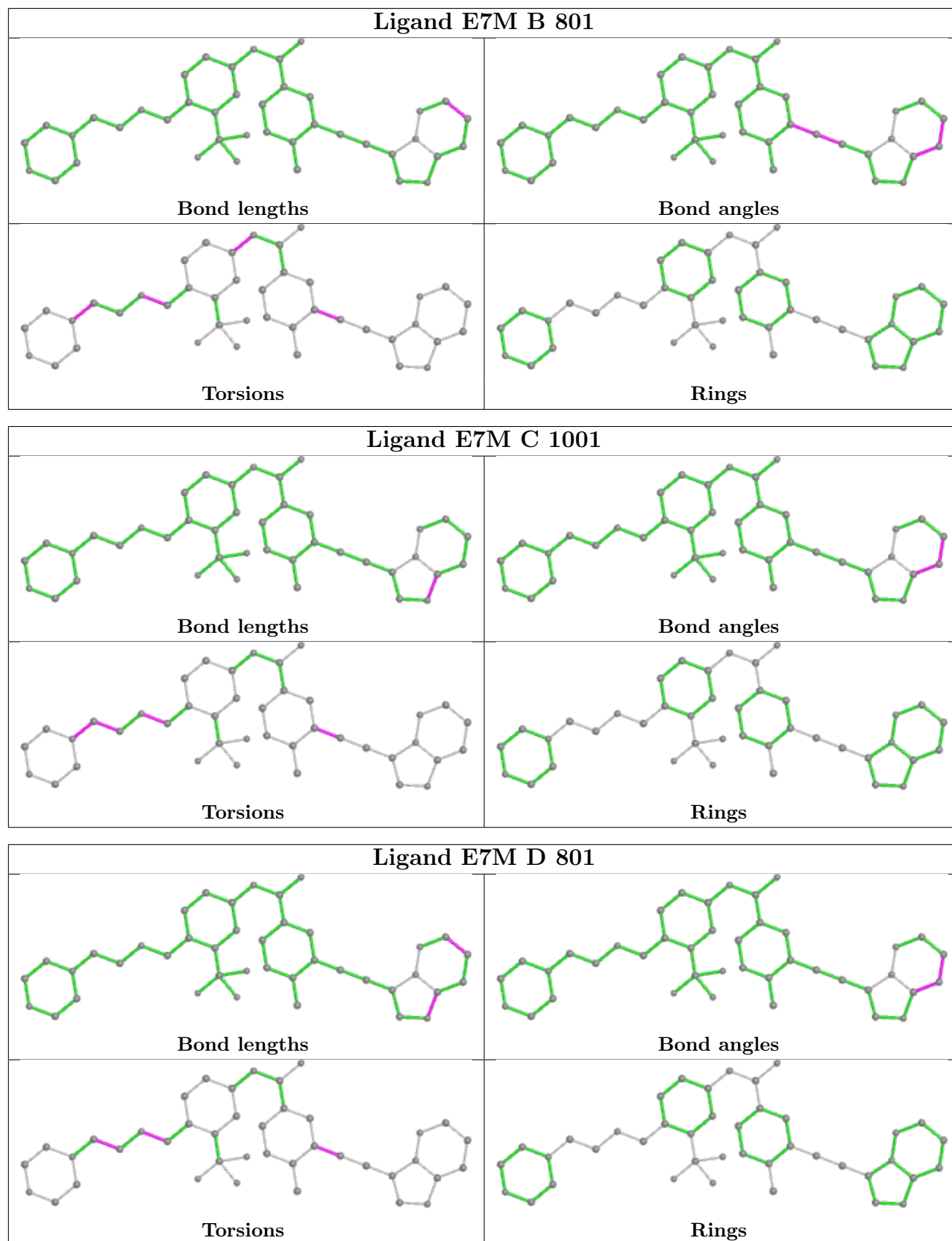
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	256/297 (86%)	0.04	1 (0%)	92	93	24, 43, 81, 104	0
1	B	273/297 (91%)	0.10	4 (1%)	73	71	23, 47, 84, 118	0
1	C	256/297 (86%)	0.06	1 (0%)	92	93	22, 46, 77, 96	0
1	D	254/297 (85%)	0.18	4 (1%)	72	69	25, 63, 101, 125	0
All	All	1039/1188 (87%)	0.09	10 (0%)	82	81	22, 50, 89, 125	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	630	SER	6.0
1	D	466	GLY	3.2
1	D	487	VAL	3.2
1	B	629	ASP	2.9
1	C	468	PHE	2.6
1	D	717	LEU	2.4
1	D	596	GLY	2.2
1	B	660	ASN	2.1
1	B	659	ILE	2.1
1	A	629	ASP	2.1

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

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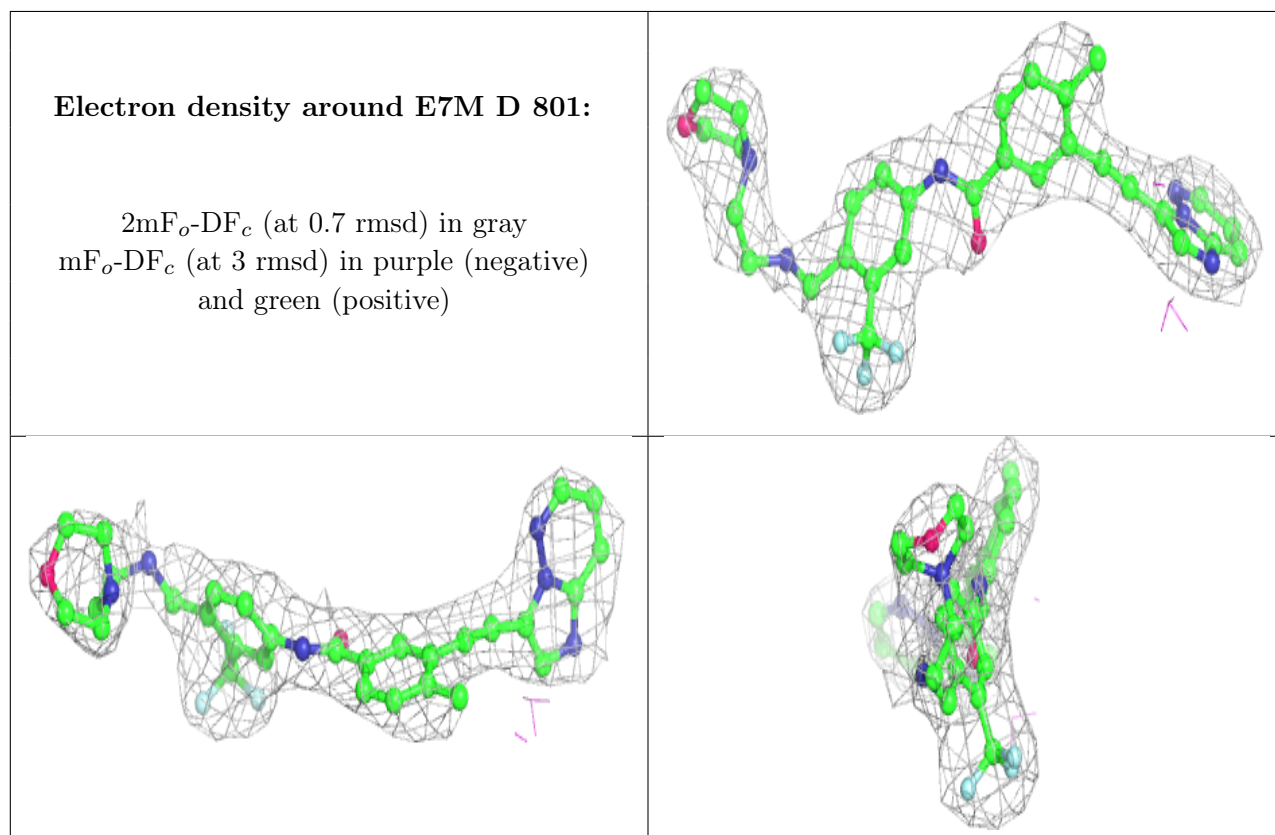
6.3   Carbohydrates   ⓘ

There are no 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
3	NHE	B	802	13/13	0.86	0.28	54,59,94,95	0
2	E7M	D	801	41/41	0.95	0.20	43,49,78,82	0
2	E7M	B	801	41/41	0.96	0.18	25,31,54,55	0
2	E7M	C	1001	41/41	0.96	0.21	30,33,54,55	0
2	E7M	A	801	41/41	0.96	0.19	26,29,56,60	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.
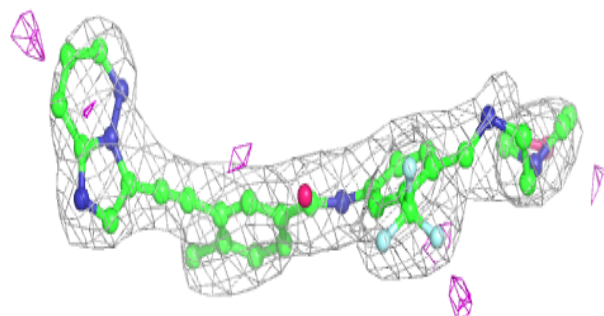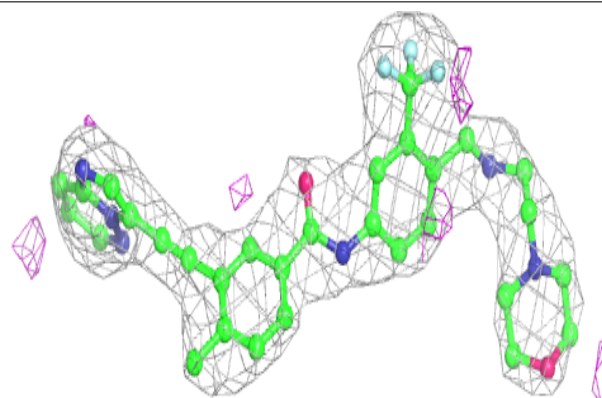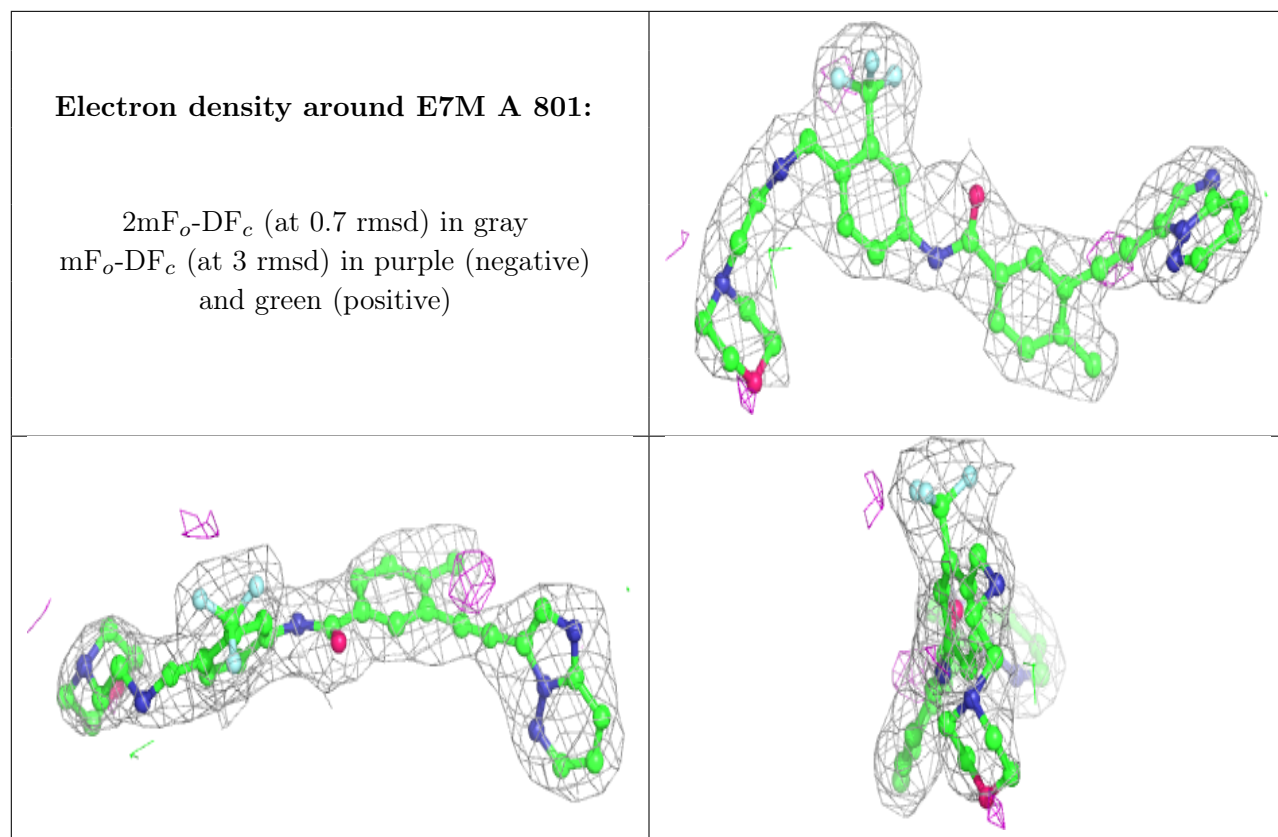

Electron density around E7M D 801:

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

Electron density around E7M B 801:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
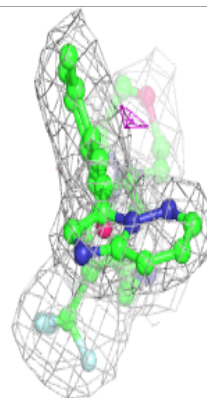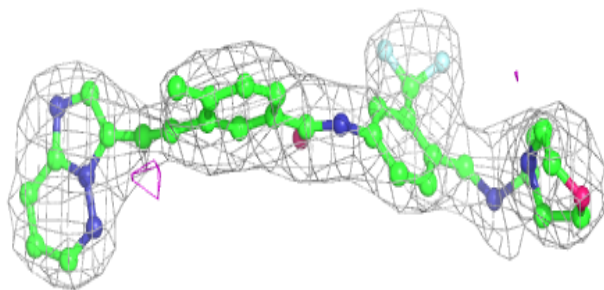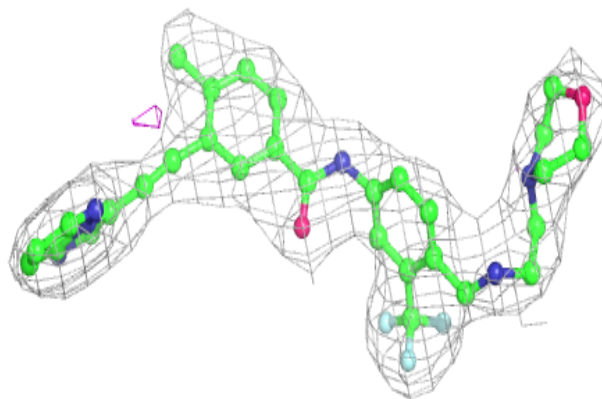
Electron density around E7M C 1001:

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

Electron density around E7M A 801:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.