



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:09 AM UTC

PDB ID : 6FUJ / pdb_00006fuj
Title : Complement factor D in complex with the inhibitor N-(3'-(aminomethyl)-[1,1'-biphenyl]-3-yl)-3-methylbutanamide
Authors : Mac Sweeney, A.; Ostermann, N.; Vulpetti, A.; Maibaum, J.; Erbel, P.; Lorthiois, E.; Yoon, T.; Randl, S.; Ruedisser, S.
Deposited on : 2018-02-27
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

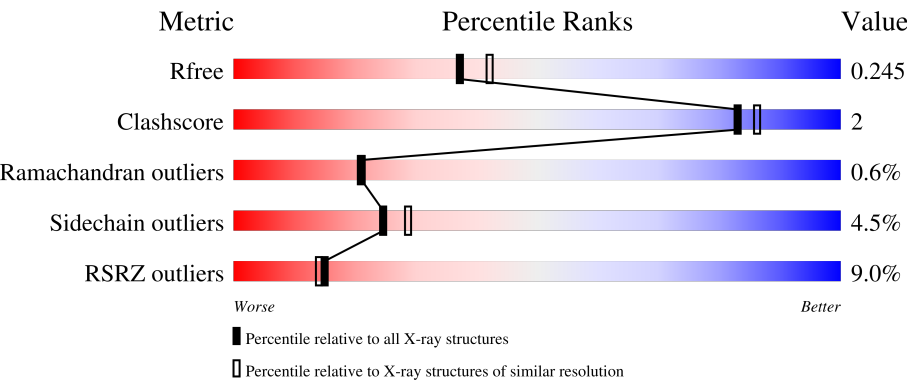
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	232	% 92%6%.
1	B	232	% 89%8%..
1	C	232	2% 90%8%.
1	D	232	7% 89%8%..

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Mol	Chain	Length	Quality of chain
1	E	232	9% 90% 6% . .
1	F	232	33% 88% 7% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10684 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 Complement factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	2	0
			1728	1067	330	321	10			
1	B	228	Total	C	N	O	S	0	0	0
			1711	1058	325	318	10			
1	C	228	Total	C	N	O	S	0	0	0
			1711	1058	325	318	10			
1	D	228	Total	C	N	O	S	0	3	0
			1734	1071	331	321	11			
1	E	223	Total	C	N	O	S	0	6	0
			1714	1064	328	310	12			
1	F	228	Total	C	N	O	S	0	2	0
			1724	1066	327	321	10			

There are 24 discrepancies between the modelled and reference sequences:

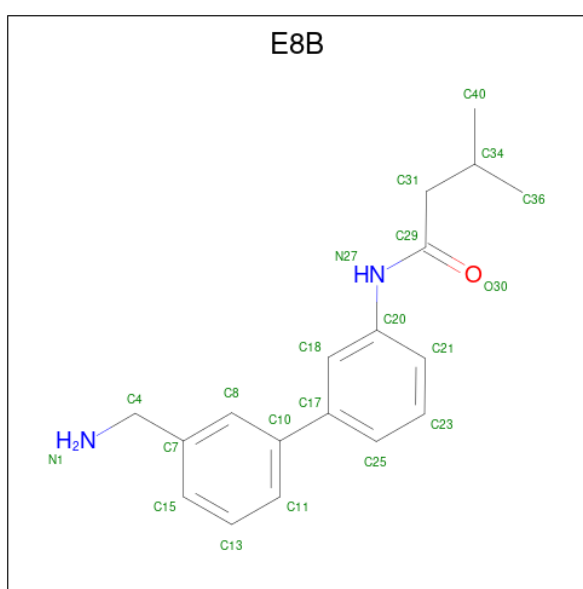
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	SER	-	expression tag	UNP P00746
A	245	ALA	-	expression tag	UNP P00746
A	246	ALA	-	expression tag	UNP P00746
A	247	ALA	-	expression tag	UNP P00746
B	244	SER	-	expression tag	UNP P00746
B	245	ALA	-	expression tag	UNP P00746
B	246	ALA	-	expression tag	UNP P00746
B	247	ALA	-	expression tag	UNP P00746
C	244	SER	-	expression tag	UNP P00746
C	245	ALA	-	expression tag	UNP P00746
C	246	ALA	-	expression tag	UNP P00746
C	247	ALA	-	expression tag	UNP P00746
D	244	SER	-	expression tag	UNP P00746
D	245	ALA	-	expression tag	UNP P00746
D	246	ALA	-	expression tag	UNP P00746
D	247	ALA	-	expression tag	UNP P00746
E	244	SER	-	expression tag	UNP P00746

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Chain	Residue	Modelled	Actual	Comment	Reference
E	245	ALA	-	expression tag	UNP P00746
E	246	ALA	-	expression tag	UNP P00746
E	247	ALA	-	expression tag	UNP P00746
F	244	SER	-	expression tag	UNP P00746
F	245	ALA	-	expression tag	UNP P00746
F	246	ALA	-	expression tag	UNP P00746
F	247	ALA	-	expression tag	UNP P00746

- Molecule 2 is {N}-[3-[3-(aminomethyl)phenyl]phenyl]-3-methyl-butanamide (CCD ID: E8B) (formula: C₁₈H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	18	2	1		
2	B	1	Total	C	N	O	0	1
			42	36	4	2		
2	C	1	Total	C	N	O	0	1
			42	36	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	59	Total	O	0	0
			59	59		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	46	Total 46	O 46	0	0
3	D	33	Total 33	O 33	0	0
3	E	29	Total 29	O 29	0	0
3	F	8	Total 8	O 8	0	0

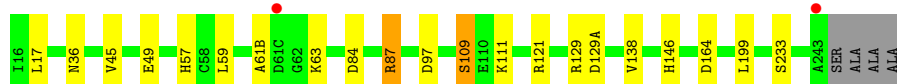
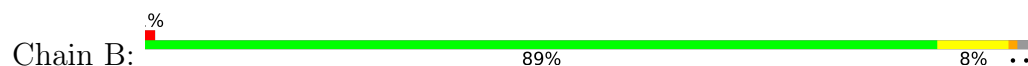
3 Residue-property plots [i](#)

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.

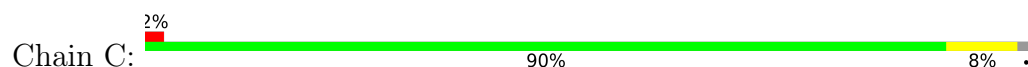
• Molecule 1: Complement factor D



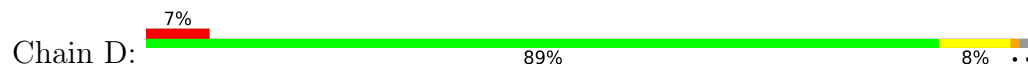
• Molecule 1: Complement factor D



• Molecule 1: Complement factor D



• Molecule 1: Complement factor D

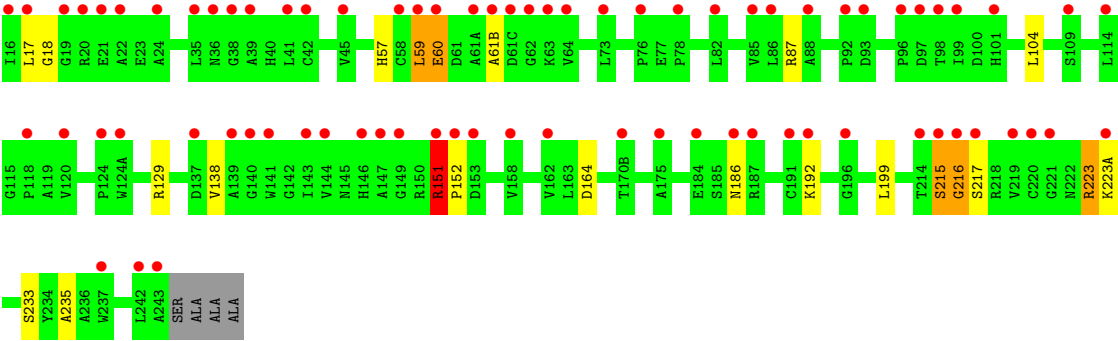
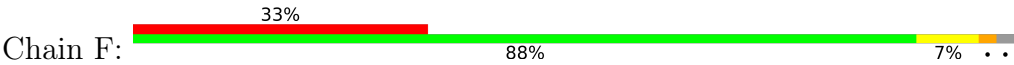


• Molecule 1: Complement factor D



SER
ALA
ALA
ALA

● Molecule 1: Complement factor D



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.66Å 210.53Å 143.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.76 – 2.25 71.76 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.76-2.25) 99.9 (71.76-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.218 , 0.244 0.222 , 0.245	Depositor DCC
R_{free} test set	4190 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.058 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.067 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10684	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: E8B

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	1.06	1/1763 (0.1%)	0.99	1/2399 (0.0%)
1	B	0.99	0/1746	0.97	0/2377
1	C	0.95	0/1746	0.98	2/2377 (0.1%)
1	D	0.94	0/1772	0.98	0/2412
1	E	0.90	0/1761	0.92	0/2395
1	F	0.88	0/1759	0.99	4/2395 (0.2%)
All	All	0.96	1/10547 (0.0%)	0.97	7/14355 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	VAL	N-CA	5.53	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	60	GLU	CB-CA-C	9.29	124.39	109.90
1	F	60	GLU	N-CA-C	-7.56	98.83	110.10
1	C	129	ARG	CB-CG-CD	5.86	124.78	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	GLU	N-CA-C	-5.62	101.73	110.10
1	F	151	ARG	CB-CG-CD	5.57	124.11	111.30
1	F	60	GLU	CA-CB-CG	5.50	125.10	114.10
1	A	60	GLU	N-CA-C	-5.32	102.17	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	217	SER	Peptide
1	E	217	SER	Peptide
1	F	217	SER	Peptide

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	1728	0	1711	6	0
1	B	1711	0	1695	12	0
1	C	1711	0	1695	11	0
1	D	1734	0	1719	10	0
1	E	1714	0	1711	7	0
1	F	1724	0	1707	11	0
2	A	21	0	0	0	0
2	B	42	0	0	0	0
2	C	42	0	0	1	0
3	A	82	0	0	2	0
3	B	59	0	0	2	0
3	C	46	0	0	1	0
3	D	33	0	0	5	0
3	E	29	0	0	2	0
3	F	8	0	0	0	0
All	All	10684	0	10238	50	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 2.

All (50) 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:B:87:ARG:HD3	3:D:309:HOH:O	1.76	0.85
2:C:301[B]:E8B:C36	2:C:301[B]:E8B:O30	2.29	0.78
1:C:75:GLN:HE22	1:D:157:HIS:CE1	2.07	0.72
1:F:59:LEU:HD22	1:F:104:LEU:HD13	1.72	0.71
1:B:138:VAL:HG22	1:B:199:LEU:HD12	1.74	0.69
1:C:75:GLN:HE22	1:D:157:HIS:HE1	1.43	0.66
1:E:138[B]:VAL:HG22	1:E:199:LEU:HD12	1.80	0.63
1:A:138:VAL:HG22	1:A:199:LEU:HD12	1.80	0.63
1:C:75:GLN:NE2	1:D:157:HIS:HE1	1.98	0.62
1:C:138:VAL:HG22	1:C:199:LEU:HD12	1.82	0.61
1:B:36:ASN:HD21	1:C:36:ASN:HD21	1.47	0.60
1:B:97:ASP:OD2	1:C:146:HIS:HD2	1.85	0.60
1:F:151:ARG:HG3	1:F:152:PRO:HD2	1.85	0.58
1:F:186:ASN:ND2	1:F:223:ARG:HG2	2.20	0.57
1:B:87:ARG:CD	3:D:309:HOH:O	2.44	0.55
1:F:138[B]:VAL:HG22	1:F:199:LEU:HD12	1.88	0.54
1:B:87:ARG:HG2	3:D:307:HOH:O	2.08	0.53
1:B:84:ASP:HB2	1:B:109:SER:OG	2.08	0.53
1:B:138:VAL:CG2	1:B:199:LEU:HD12	2.38	0.52
1:C:138:VAL:CG2	1:C:199:LEU:HD12	2.40	0.52
1:A:138:VAL:CG2	1:A:199:LEU:HD12	2.40	0.51
1:E:215:SER:O	1:E:216:GLY:C	2.54	0.51
1:A:214:THR:CG2	3:A:407:HOH:O	2.59	0.50
1:D:215:SER:O	1:D:216:GLY:C	2.54	0.50
1:F:57:HIS:HB2	1:F:215:SER:HB2	1.93	0.50
1:F:215:SER:O	1:F:216:GLY:C	2.55	0.50
1:D:94:SER:HB2	3:D:326:HOH:O	2.12	0.49
1:F:138[B]:VAL:CG2	1:F:199:LEU:HD12	2.43	0.49
1:D:129:ARG:HD3	3:D:315:HOH:O	2.13	0.48
1:E:138[B]:VAL:CG2	1:E:199:LEU:HD12	2.42	0.48
1:D:57:HIS:HB2	1:D:215:SER:HB2	1.95	0.48
1:D:151:ARG:CZ	1:D:151:ARG:HB2	2.44	0.47
1:B:57:HIS:CE1	3:B:431:HOH:O	2.67	0.47
1:E:124:PRO:O	3:E:301:HOH:O	2.20	0.46
1:B:49:GLU:CD	1:B:111:LYS:HD3	2.41	0.46
1:E:57:HIS:HB2	1:E:215:SER:HB2	1.98	0.45
1:C:94:SER:O	1:F:129:ARG:NH2	2.36	0.45
1:B:146:HIS:HD2	1:C:97:ASP:OD2	2.00	0.44
1:C:38:GLY:HA2	3:C:422:HOH:O	2.16	0.44
1:A:20:ARG:CZ	1:A:20:ARG:HB3	2.48	0.42
1:B:121:ARG:HD2	3:B:456:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ARG:NH2	3:E:305:HOH:O	2.52	0.42
1:C:87:ARG:CG	1:F:235:ALA:HB3	2.50	0.41
1:D:17:LEU:HD12	1:D:18:GLY:N	2.35	0.41
1:E:17:LEU:HD12	1:E:18:GLY:N	2.35	0.41
1:D:57:HIS:HB2	1:D:215:SER:CB	2.51	0.41
1:F:57:HIS:HB2	1:F:215:SER:CB	2.50	0.41
1:F:17:LEU:HD12	1:F:18:GLY:N	2.35	0.41
1:A:151:ARG:HD3	3:A:419:HOH:O	2.21	0.40
1:A:211:GLY:HA2	1:A:229:THR:O	2.21	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	228/232 (98%)	220 (96%)	7 (3%)	1 (0%)	30	31
1	B	226/232 (97%)	219 (97%)	6 (3%)	1 (0%)	30	31
1	C	226/232 (97%)	218 (96%)	7 (3%)	1 (0%)	30	31
1	D	229/232 (99%)	222 (97%)	5 (2%)	2 (1%)	14	12
1	E	225/232 (97%)	219 (97%)	5 (2%)	1 (0%)	30	31
1	F	228/232 (98%)	220 (96%)	6 (3%)	2 (1%)	14	12
All	All	1362/1392 (98%)	1318 (97%)	36 (3%)	8 (1%)	21	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61(B)	ALA
1	B	61(B)	ALA
1	C	61(B)	ALA

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Mol	Chain	Res	Type
1	F	61(B)	ALA
1	D	61(B)	ALA
1	E	216	GLY
1	D	216	GLY
1	F	216	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	184/183 (100%)	180 (98%)	4 (2%)	45	56
1	B	182/183 (100%)	172 (94%)	10 (6%)	19	20
1	C	182/183 (100%)	174 (96%)	8 (4%)	25	29
1	D	185/183 (101%)	174 (94%)	11 (6%)	18	18
1	E	184/183 (100%)	178 (97%)	6 (3%)	33	42
1	F	184/183 (100%)	174 (95%)	10 (5%)	20	21
All	All	1101/1098 (100%)	1052 (96%)	49 (4%)	24	29

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	87	ARG
1	A	159	LEU
1	A	233	SER
1	B	17	LEU
1	B	45	VAL
1	B	59	LEU
1	B	63	LYS
1	B	87	ARG
1	B	109	SER
1	B	129	ARG
1	B	129(A)	ASP
1	B	164	ASP

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Mol	Chain	Res	Type
1	B	233	SER
1	C	17	LEU
1	C	20	ARG
1	C	59	LEU
1	C	87	ARG
1	C	121	ARG
1	C	164	ASP
1	C	192	LYS
1	C	233	SER
1	D	23	GLU
1	D	59	LEU
1	D	61	ASP
1	D	61(C)	ASP
1	D	87	ARG
1	D	95	GLN
1	D	164	ASP
1	D	192	LYS
1	D	215	SER
1	D	233	SER
1	D	239	ASP
1	E	87	ARG
1	E	95	GLN
1	E	164	ASP
1	E	215	SER
1	E	233	SER
1	E	239	ASP
1	F	59	LEU
1	F	60	GLU
1	F	87	ARG
1	F	151	ARG
1	F	164	ASP
1	F	192	LYS
1	F	215	SER
1	F	223	ARG
1	F	223(A)	LYS
1	F	233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	B	34	GLN

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Mol	Chain	Res	Type
1	B	65	GLN
1	B	146	HIS
1	C	34	GLN
1	C	36	ASN
1	C	65	GLN
1	C	75	GLN
1	C	146	HIS
1	D	36	ASN
1	D	157	HIS
1	E	36	ASN
1	F	34	GLN
1	F	65	GLN
1	F	186	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E8B	B	301[A]	-	22,22,22	0.84	1 (4%)	29,29,29	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	E8B	C	301[A]	-	22,22,22	0.96	1 (4%)	29,29,29	1.37	4 (13%)
2	E8B	A	301	-	22,22,22	1.22	1 (4%)	29,29,29	0.93	1 (3%)
2	E8B	B	301[B]	-	22,22,22	0.94	1 (4%)	29,29,29	1.31	2 (6%)
2	E8B	C	301[B]	-	22,22,22	0.95	1 (4%)	29,29,29	1.22	3 (10%)

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	E8B	B	301[A]	-	-	1/14/14/14	0/2/2/2
2	E8B	C	301[A]	-	-	2/14/14/14	0/2/2/2
2	E8B	A	301	-	-	2/14/14/14	0/2/2/2
2	E8B	B	301[B]	-	-	2/14/14/14	0/2/2/2
2	E8B	C	301[B]	-	-	3/14/14/14	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	E8B	C29-N27	-4.58	1.25	1.35
2	C	301[B]	E8B	C29-N27	-4.02	1.27	1.35
2	C	301[A]	E8B	C29-N27	-3.84	1.27	1.35
2	B	301[A]	E8B	C29-N27	-3.48	1.28	1.35
2	B	301[B]	E8B	C29-N27	-3.41	1.28	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	E8B	C34-C31-C29	-4.34	106.80	113.29
2	B	301[B]	E8B	C34-C31-C29	3.97	119.22	113.29
2	A	301	E8B	C13-C11-C10	-3.21	116.88	120.54
2	C	301[B]	E8B	C20-N27-C29	-3.21	121.84	127.52
2	C	301[A]	E8B	C11-C10-C17	-3.17	115.78	121.25
2	B	301[B]	E8B	C11-C10-C17	-2.77	116.47	121.25
2	C	301[B]	E8B	C31-C29-N27	2.56	117.78	114.62
2	C	301[A]	E8B	C8-C10-C17	2.24	124.59	120.84
2	C	301[B]	E8B	C25-C17-C10	-2.19	117.47	121.25
2	B	301[A]	E8B	C23-C25-C17	-2.12	118.12	120.54
2	B	301[A]	E8B	C11-C10-C17	-2.07	117.69	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	E8B	C21-C20-C18	-2.03	117.20	119.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301[A]	E8B	C29-C31-C34-C36
2	B	301[B]	E8B	C29-C31-C34-C40
2	B	301[B]	E8B	C29-C31-C34-C36
2	C	301[B]	E8B	C29-C31-C34-C40
2	C	301[B]	E8B	C29-C31-C34-C36
2	C	301[A]	E8B	O30-C29-C31-C34
2	A	301	E8B	N27-C29-C31-C34
2	C	301[A]	E8B	N27-C29-C31-C34
2	C	301[B]	E8B	C21-C20-N27-C29
2	A	301	E8B	O30-C29-C31-C34

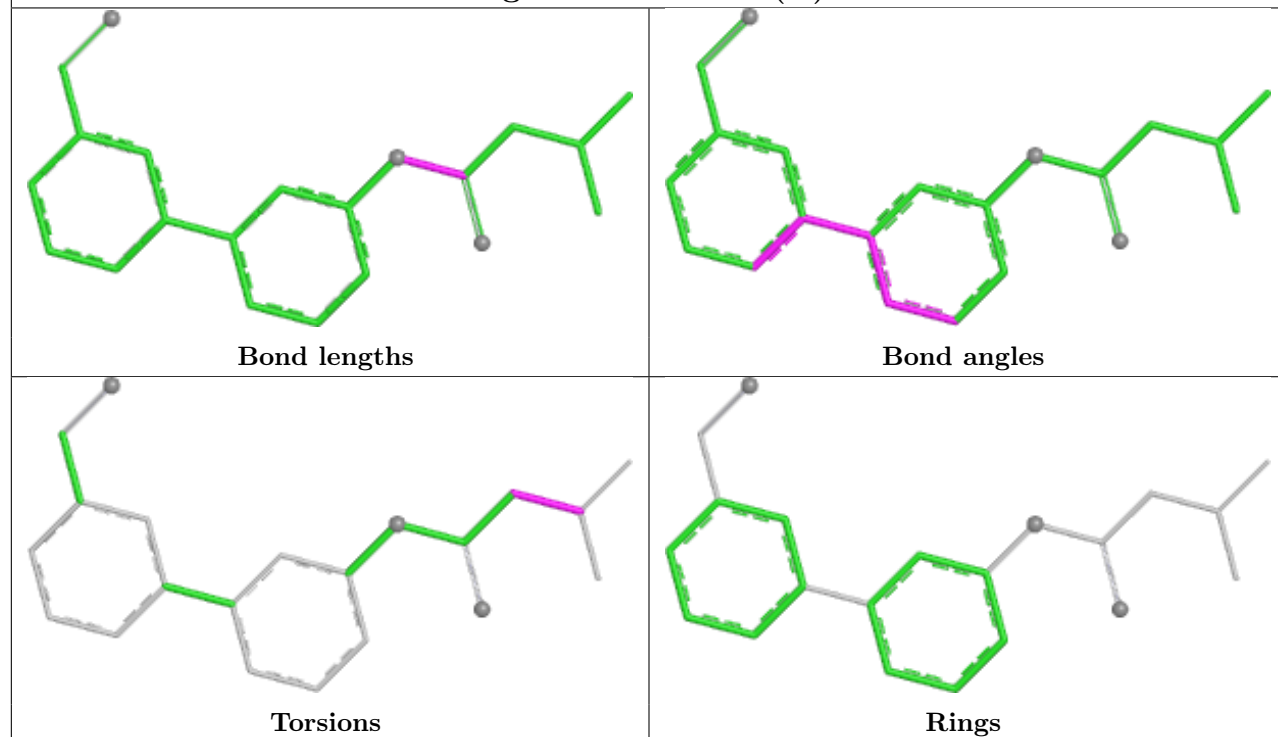
There are no ring outliers.

1 monomer is involved in 1 short contact:

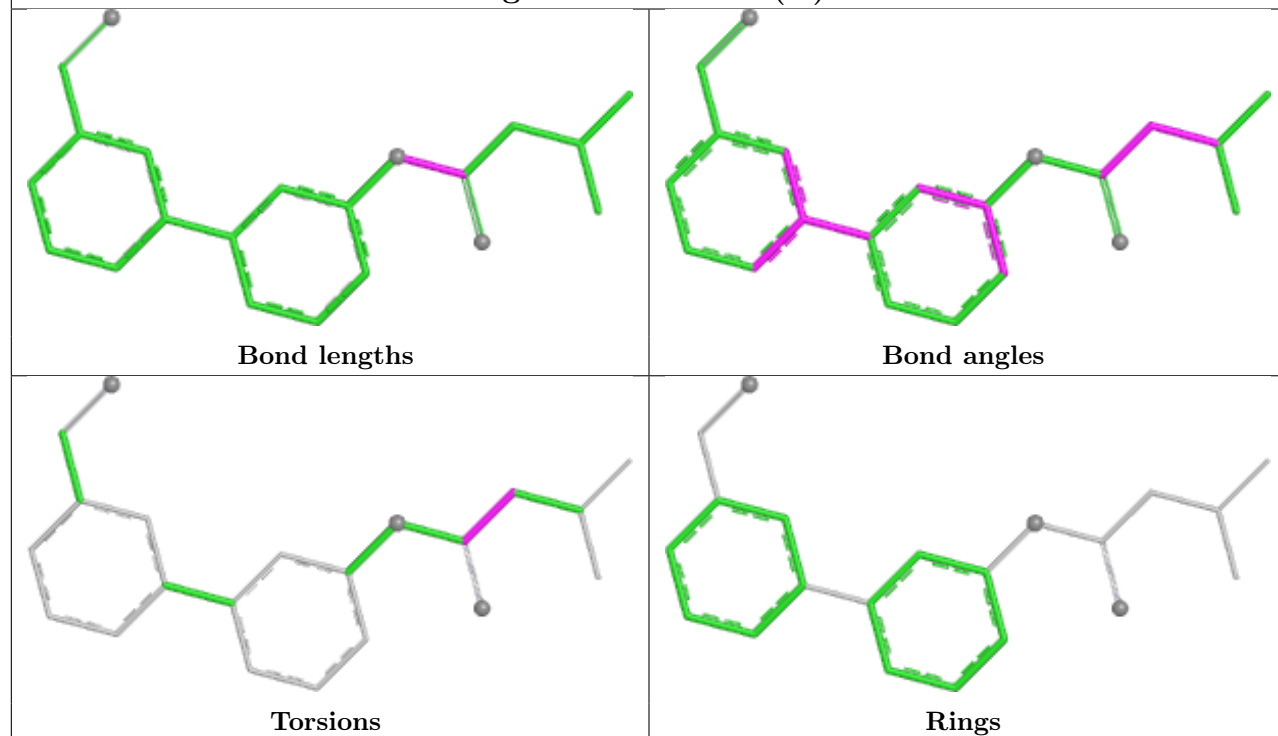
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301[B]	E8B	1	0

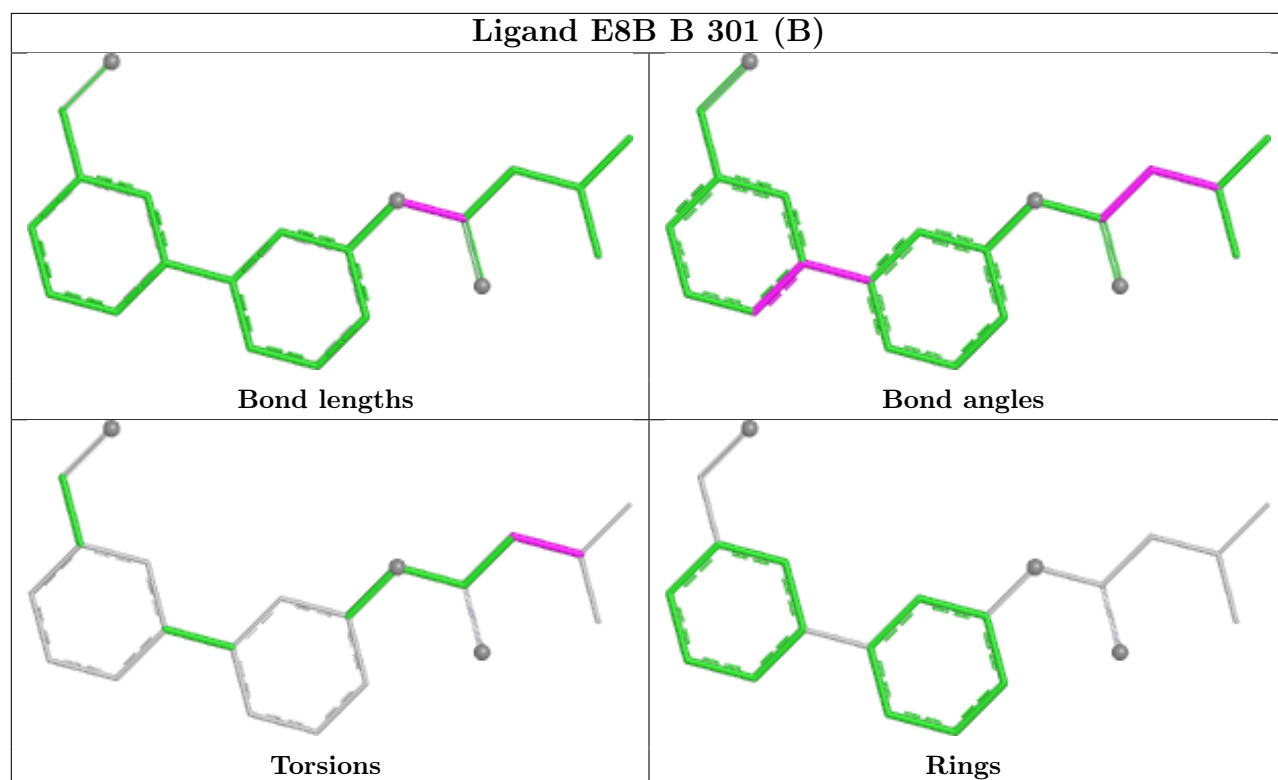
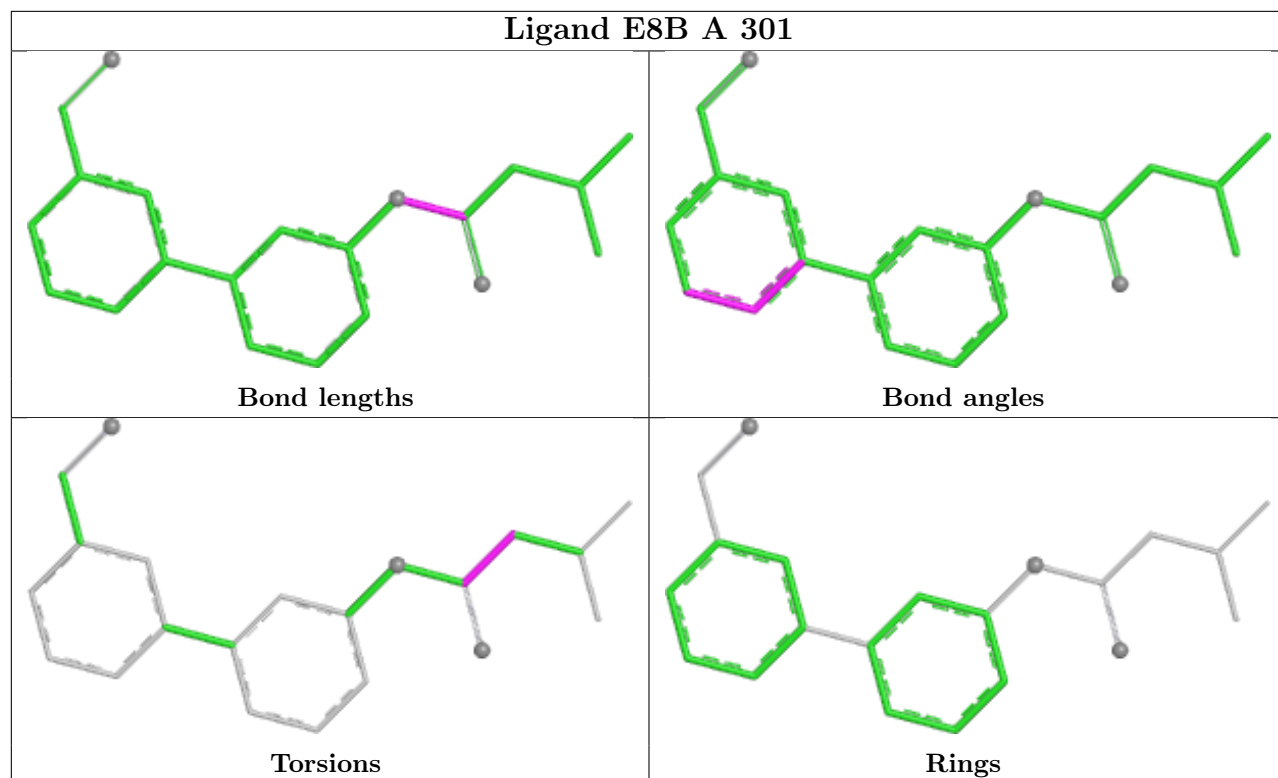
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

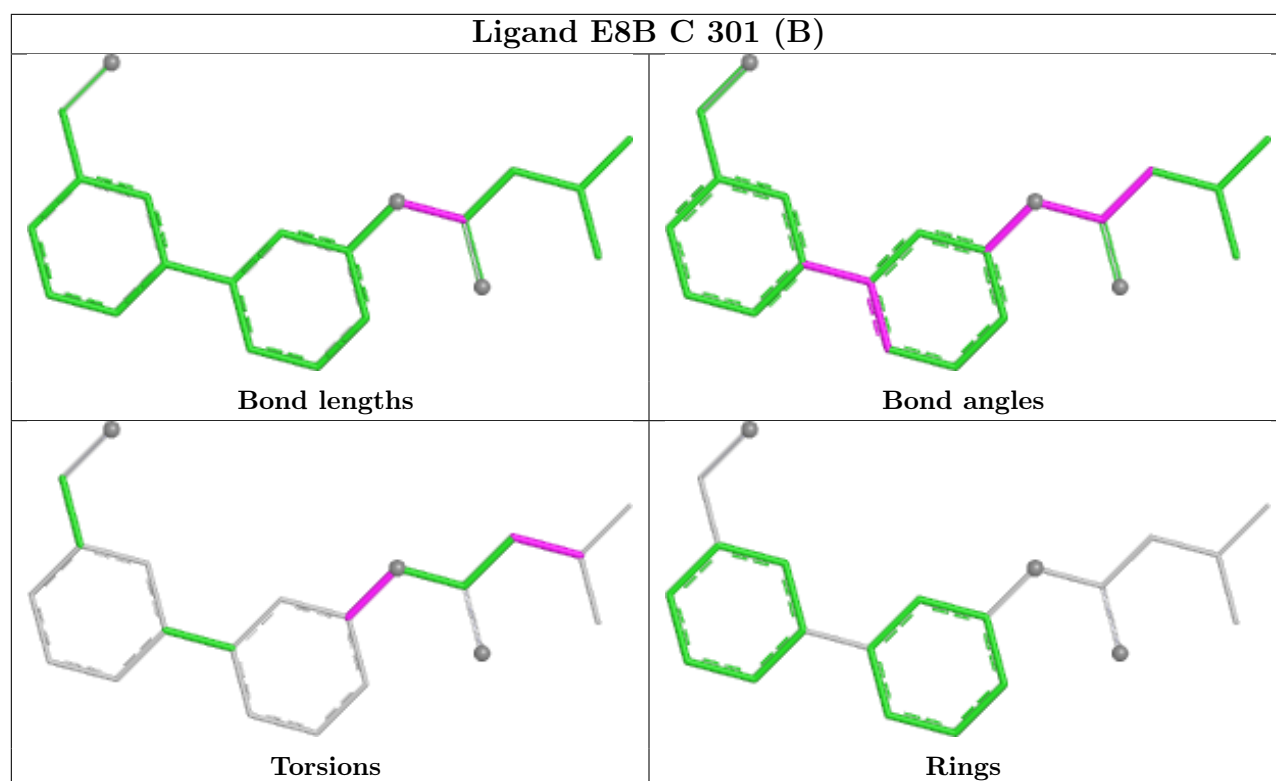
Ligand E8B B 301 (A)



Ligand E8B C 301 (A)







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/232 (98%)	-0.28	2 (0%) 81 82	11, 23, 48, 71	2 (0%)
1	B	228/232 (98%)	-0.12	2 (0%) 81 82	14, 29, 55, 86	0
1	C	228/232 (98%)	0.16	4 (1%) 67 68	21, 36, 68, 102	0
1	D	228/232 (98%)	0.61	16 (7%) 22 21	12, 45, 100, 140	3 (1%)
1	E	223/232 (96%)	0.69	22 (9%) 13 12	14, 48, 84, 129	6 (2%)
1	F	228/232 (98%)	1.76	76 (33%) 1 0	24, 76, 120, 145	2 (0%)
All	All	1363/1392 (97%)	0.47	122 (8%) 15 14	11, 40, 98, 145	13 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	219	VAL	7.8
1	F	59	LEU	6.8
1	E	243	ALA	6.6
1	F	243	ALA	6.2
1	F	63	LYS	5.4
1	D	219	VAL	4.9
1	D	63	LYS	4.9
1	E	62	GLY	4.9
1	C	243	ALA	4.9
1	E	216	GLY	4.7
1	E	59	LEU	4.6
1	F	99	ILE	4.5
1	D	243	ALA	4.4
1	F	61(B)	ALA	4.3
1	F	39	ALA	4.2
1	F	216	GLY	4.1
1	E	219	VAL	4.1
1	F	17	LEU	4.1
1	D	216	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	59	LEU	4.0
1	F	147	ALA	4.0
1	F	41	LEU	4.0
1	F	16	ILE	3.9
1	F	19	GLY	3.7
1	F	58	CYS	3.6
1	F	22	ALA	3.6
1	F	143	ILE	3.6
1	F	35	LEU	3.6
1	F	38	GLY	3.5
1	D	220	CYS	3.4
1	E	82	LEU	3.3
1	F	114	LEU	3.3
1	D	61(B)	ALA	3.3
1	E	215	SER	3.3
1	F	192	LYS	3.3
1	F	149	GLY	3.3
1	C	61(B)	ALA	3.2
1	F	144	VAL	3.3
1	F	86	LEU	3.2
1	E	187	ARG	3.2
1	B	243	ALA	3.2
1	E	38	GLY	3.2
1	D	61(A)	ALA	3.1
1	F	124	PRO	3.1
1	F	98	THR	3.1
1	E	217	SER	3.1
1	C	61(C)	ASP	3.1
1	D	62	GLY	3.1
1	D	215	SER	3.0
1	F	151	ARG	3.0
1	F	221	GLY	3.0
1	F	186	ASN	3.0
1	F	118	PRO	3.0
1	F	152	PRO	3.0
1	F	158	VAL	3.0
1	F	146	HIS	2.9
1	F	220	CYS	2.9
1	F	153	ASP	2.9
1	F	76	PRO	2.9
1	F	92	PRO	2.9
1	F	82	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	109[A]	SER	2.8
1	F	137	ASP	2.9
1	F	78	PRO	2.8
1	F	124(A)	TRP	2.8
1	D	221	GLY	2.8
1	D	86	LEU	2.8
1	E	86	LEU	2.8
1	F	61(A)	ALA	2.8
1	D	151	ARG	2.8
1	E	147	ALA	2.7
1	F	42	CYS	2.7
1	F	62	GLY	2.6
1	F	217	SER	2.6
1	F	141	TRP	2.6
1	F	85	VAL	2.6
1	A	243	ALA	2.5
1	E	63	LYS	2.5
1	F	36	ASN	2.5
1	F	191	CYS	2.5
1	F	215	SER	2.5
1	C	129	ARG	2.5
1	B	61(C)	ASP	2.5
1	D	192	LYS	2.4
1	E	214	THR	2.4
1	F	214	THR	2.4
1	F	170(B)	THR	2.4
1	F	237	TRP	2.4
1	A	61(B)	ALA	2.4
1	F	73	LEU	2.3
1	F	64	VAL	2.3
1	D	61(C)	ASP	2.3
1	E	96	PRO	2.3
1	F	140	GLY	2.3
1	F	20	ARG	2.3
1	F	187	ARG	2.3
1	D	217	SER	2.3
1	E	192	LYS	2.3
1	F	196	GLY	2.2
1	F	88	ALA	2.2
1	F	101	HIS	2.2
1	F	162	VAL	2.2
1	F	223(A)	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	20	ARG	2.2
1	F	93	ASP	2.2
1	F	96	PRO	2.2
1	F	184	GLU	2.2
1	F	139	ALA	2.2
1	F	21	GLU	2.2
1	F	175	ALA	2.2
1	E	151	ARG	2.1
1	F	97	ASP	2.1
1	F	24	ALA	2.1
1	E	149	GLY	2.1
1	F	60	GLU	2.1
1	F	242	LEU	2.1
1	F	120	VAL	2.1
1	E	223	ARG	2.1
1	E	97	ASP	2.0
1	F	45	VAL	2.0
1	E	223(A)	LYS	2.0
1	F	61(C)	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	E8B	B	301[A]	21/21	0.87	0.18	35,37,47,48	21
2	E8B	B	301[B]	21/21	0.87	0.18	28,32,43,48	21
2	E8B	C	301[A]	21/21	0.90	0.14	31,34,39,43	21
2	E8B	C	301[B]	21/21	0.90	0.14	27,33,45,46	21

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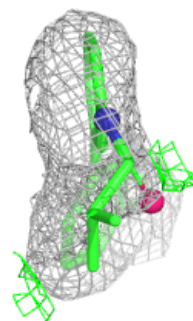
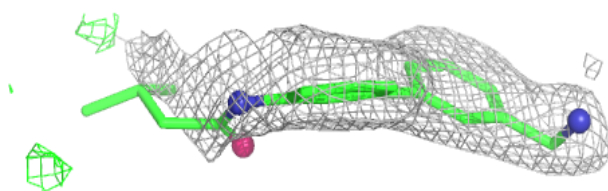
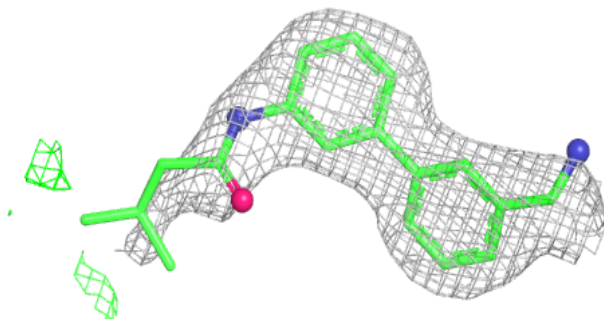
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	E8B	A	301	21/21	0.95	0.13	19,30,88,93	0

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.

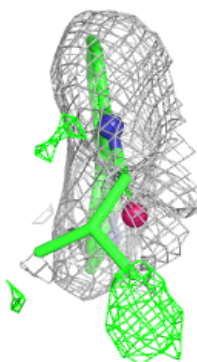
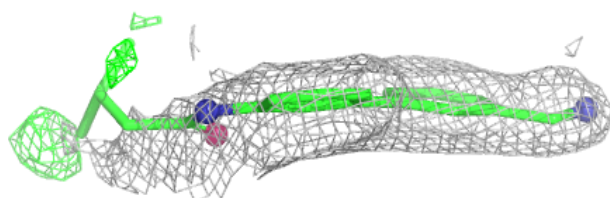
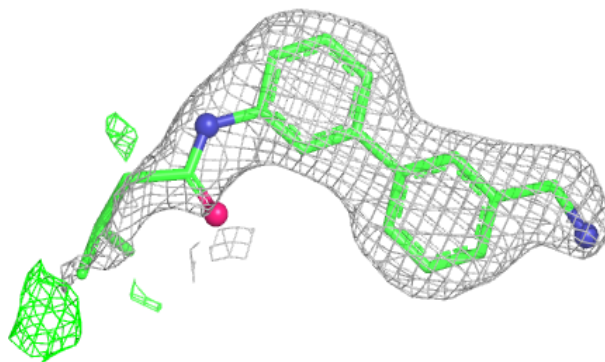
Electron density around E8B B 301 (A):

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

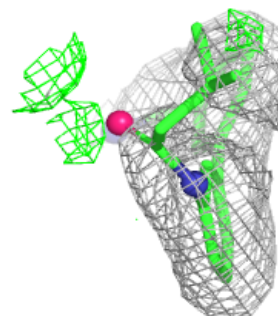
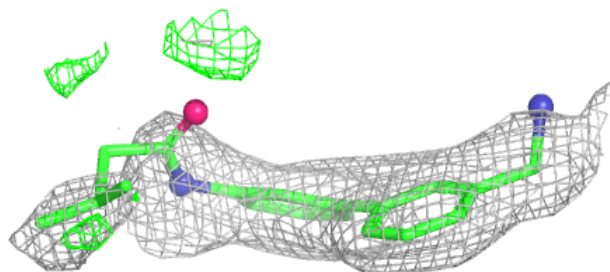
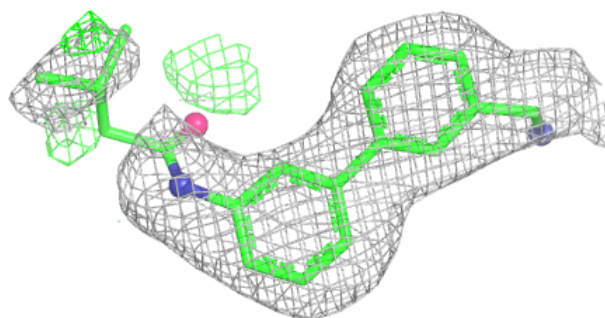


Electron density around E8B B 301 (B):

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

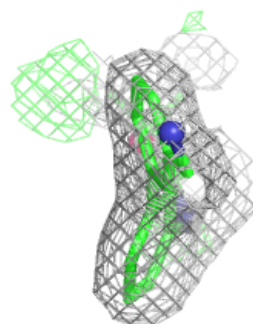
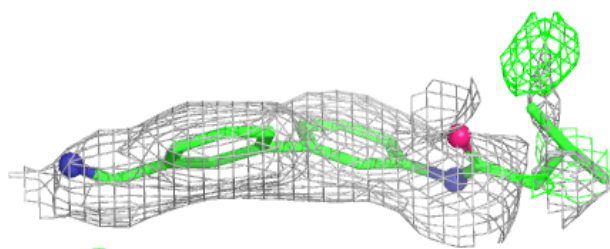
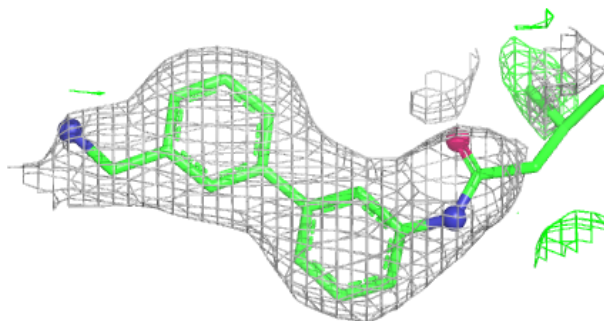
**Electron density around E8B C 301 (A):**

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

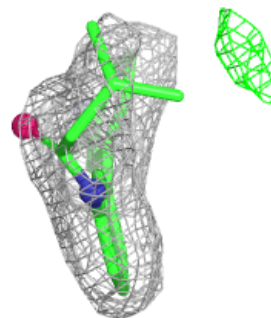
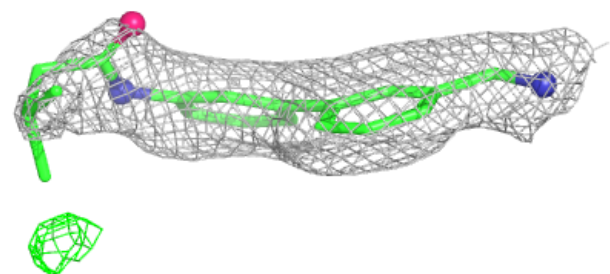
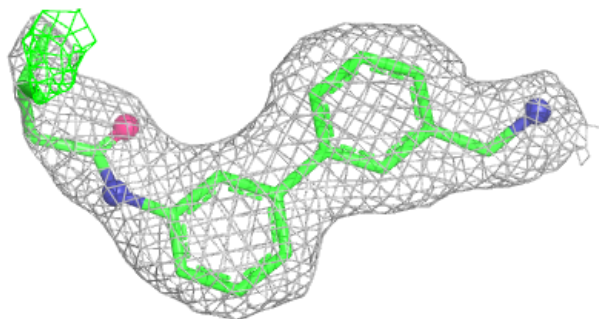


Electron density around E8B C 301 (B):

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

**Electron density around E8B A 301:**

$2mF_o-DF_c$ (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.