



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2021 – 09:06 pm BST

PDB ID : 6G8H
Title : Flavonoid-responsive Regulator FrrA in complex with (R,S)-Naringenin
Authors : Werner, N.; Hoppen, J.; Palm, G.; Werten, S.; Goettfert, M.; Hinrichs, W.
Deposited on : 2018-04-08
Resolution : 2.60 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 : 2.23.1
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) : 2.23.1

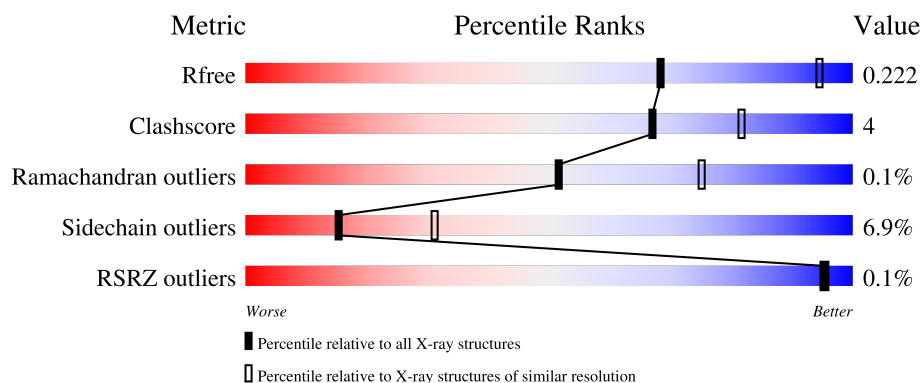
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	AAA	195	<div> <div style="width: 82%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>82% 16% ..</div>
1	BBB	195	<div> <div style="width: 82%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>82% 16% ..</div>
1	CCC	195	<div> <div style="width: 86%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>86% 11% ..</div>
1	DDD	195	<div> <div style="width: 88%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>88% 12% .</div>

2 Entry composition [i](#)

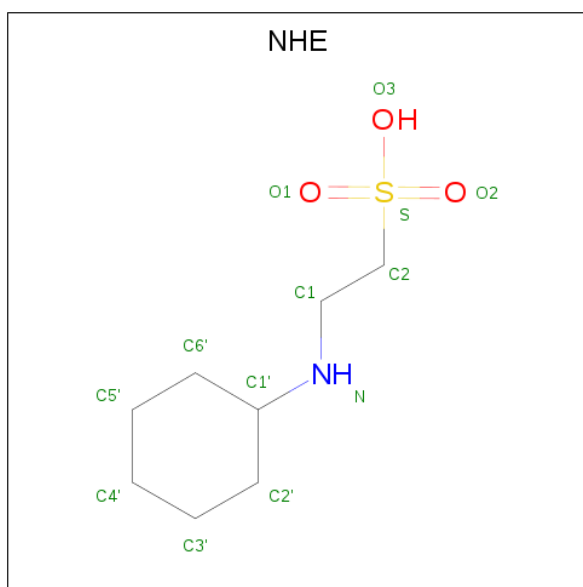
There are 4 unique types of molecules in this entry. The entry contains 6199 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcriptional regulatory protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	CCC	194	Total	C	N	O	S	Se	0	0	0
			1522	981	259	277	2	3			
1	DDD	195	Total	C	N	O	S	Se	0	0	0
			1527	984	260	278	2	3			
1	AAA	193	Total	C	N	O	S	Se	0	0	0
			1514	976	257	276	2	3			
1	BBB	193	Total	C	N	O	S	Se	0	0	0
			1505	972	252	276	2	3			

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).



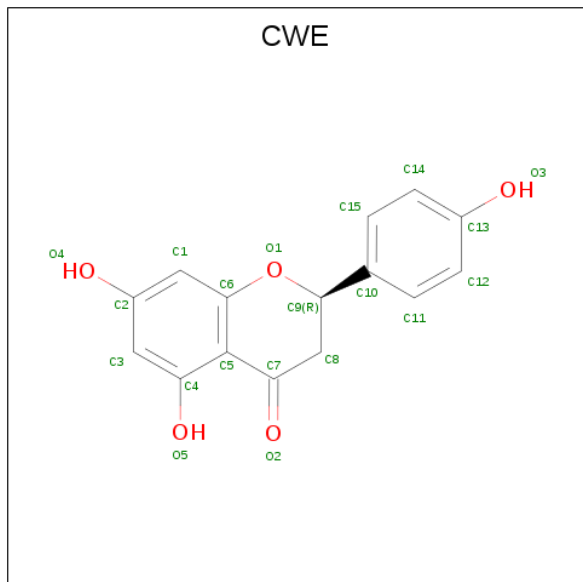
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	CCC	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	DDD	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

Continued on next page...

Continued from previous page...

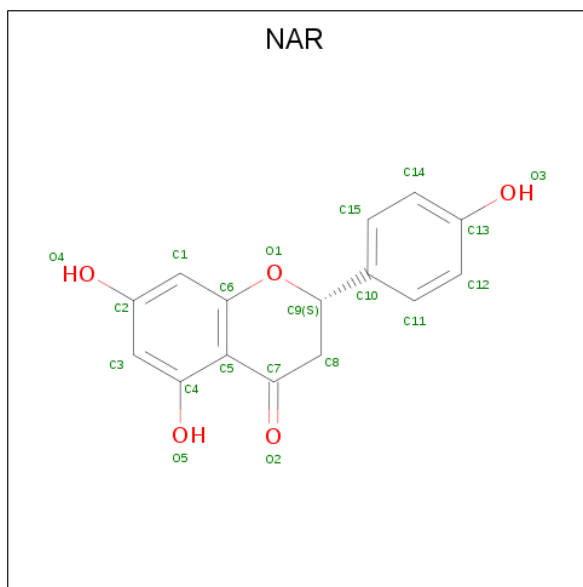
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	DDD	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	AAA	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	AAA	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	AAA	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	BBB	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is R-naringenin (three-letter code: CWE) (formula: C₁₅H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	DDD	1	Total	C	O	0	0
			20	15	5		

- Molecule 4 is NARINGENIN (three-letter code: NAR) (formula: C₁₅H₁₂O₅).



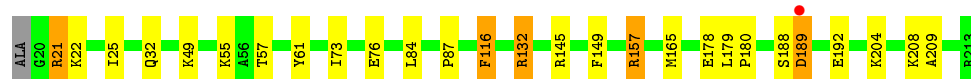
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	C	O	0	0
			20	15	5		

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: Transcriptional regulatory protein

Chain CCC: 



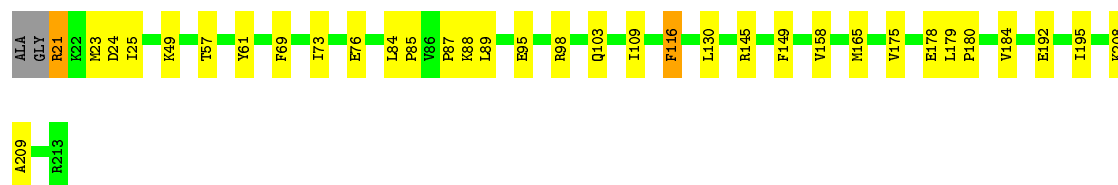
- Molecule 1: Transcriptional regulatory protein

Chain DDD: 




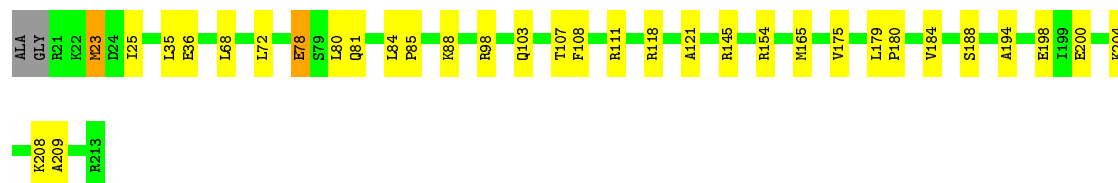
- Molecule 1: Transcriptional regulatory protein

Chain AAA: 



- Molecule 1: Transcriptional regulatory protein

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	118.71Å 118.71Å 78.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.71 – 2.60 118.71 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (118.71-2.60) 98.6 (118.71-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.219 0.188 , 0.222	Depositor DCC
R_{free} test set	2253 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6199	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: NAR, NHE, CWE

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	AAA	0.78	0/1540	0.93	2/2077 (0.1%)
1	BBB	0.79	1/1531 (0.1%)	1.01	4/2066 (0.2%)
1	CCC	0.76	0/1548	0.97	3/2086 (0.1%)
1	DDD	0.75	0/1553	0.98	2/2093 (0.1%)
All	All	0.77	1/6172 (0.0%)	0.97	11/8322 (0.1%)

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	DDD	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	188	SER	CA-CB	-5.38	1.44	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	165	MSE	CG-SE-CE	9.36	119.49	98.90
1	AAA	165	MSE	CG-SE-CE	7.54	115.50	98.90
1	AAA	23	MSE	CG-SE-CE	7.26	114.86	98.90
1	CCC	132	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	DDD	118	ARG	CG-CD-NE	5.82	124.03	111.80
1	DDD	126	ARG	CB-CA-C	-5.53	99.33	110.40
1	CCC	165	MSE	CG-SE-CE	5.45	110.89	98.90
1	BBB	23	MSE	CG-SE-CE	5.28	110.51	98.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	36	GLU	CB-CA-C	5.15	120.69	110.40
1	BBB	154	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	CCC	189	ASP	CB-CA-C	5.02	120.45	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DDD	19	ALA	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	AAA	1514	0	1527	15	0
1	BBB	1505	0	1511	16	0
1	CCC	1522	0	1541	11	1
1	DDD	1527	0	1546	10	0
2	AAA	39	0	48	1	0
2	BBB	13	0	16	0	0
2	CCC	13	0	16	0	0
2	DDD	26	0	32	0	0
3	DDD	20	0	0	0	0
4	BBB	20	0	12	0	0
All	All	6199	0	6249	49	1

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 4.

All (49) 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:DDD:118:ARG:HG2	1:DDD:118:ARG:HH11	1.36	0.90
1:CCC:178:GLU:OE2	1:DDD:135:TYR:OH	2.02	0.77
1:AAA:209:ALA:HB2	1:BBB:209:ALA:HB2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:103:GLN:O	1:BBB:107:THR:HG23	1.92	0.70
1:DDD:103:GLN:O	1:DDD:107:THR:HG23	1.95	0.67
1:AAA:21:ARG:HG2	1:AAA:24:ASP:OD2	1.94	0.65
1:AAA:109:ILE:HD13	1:AAA:195:ILE:HD11	1.80	0.64
1:CCC:76:GLU:HB3	1:CCC:116:PHE:CE2	2.35	0.62
1:BBB:84:LEU:O	1:BBB:145:ARG:NH1	2.34	0.60
1:BBB:78:GLU:OE1	1:BBB:78:GLU:HA	2.03	0.59
1:CCC:73:ILE:HA	1:CCC:116:PHE:CZ	2.40	0.57
1:DDD:107:THR:O	1:DDD:111:ARG:HB2	2.06	0.56
1:AAA:184:VAL:HG13	1:BBB:121:ALA:HB2	1.88	0.54
1:BBB:81:GLN:OE1	1:BBB:145:ARG:HD3	2.08	0.54
1:BBB:107:THR:O	1:BBB:111:ARG:HB2	2.08	0.54
1:CCC:76:GLU:HB3	1:CCC:116:PHE:HE2	1.73	0.52
1:BBB:78:GLU:OE1	1:BBB:78:GLU:CA	2.57	0.52
1:CCC:209:ALA:HB2	1:DDD:209:ALA:HB2	1.92	0.52
1:AAA:85:PRO:HD3	1:AAA:103:GLN:HG3	1.92	0.52
1:BBB:85:PRO:O	1:BBB:145:ARG:NH1	2.43	0.51
1:AAA:76:GLU:HB2	1:AAA:116:PHE:CE2	2.47	0.50
1:CCC:25:ILE:HD12	1:CCC:25:ILE:H	1.77	0.49
1:AAA:25:ILE:H	1:AAA:25:ILE:HD12	1.76	0.49
1:AAA:109:ILE:HD13	1:AAA:195:ILE:CD1	2.40	0.49
1:AAA:73:ILE:HA	1:AAA:116:PHE:CZ	2.46	0.49
1:BBB:25:ILE:H	1:BBB:25:ILE:HD12	1.79	0.47
1:DDD:85:PRO:HD3	1:DDD:103:GLN:HG3	1.97	0.46
2:AAA:1001:NHE:HC12	2:AAA:1001:NHE:H6'1	1.83	0.46
1:DDD:118:ARG:HH11	1:DDD:118:ARG:CG	2.16	0.45
1:BBB:80:LEU:C	1:BBB:80:LEU:HD23	2.37	0.45
1:CCC:87:PRO:HB2	1:CCC:149:PHE:CD1	2.52	0.45
1:CCC:157:ARG:HH11	1:CCC:157:ARG:HA	1.83	0.44
1:AAA:87:PRO:HB2	1:AAA:149:PHE:CD1	2.52	0.44
1:DDD:80:LEU:HD23	1:DDD:80:LEU:C	2.38	0.44
1:AAA:57:THR:O	1:AAA:61:TYR:HD2	2.01	0.43
1:CCC:84:LEU:O	1:CCC:145:ARG:NH2	2.50	0.43
1:AAA:95:GLU:OE2	1:AAA:98:ARG:NH1	2.51	0.43
1:DDD:69:PHE:HD2	1:DDD:130:LEU:HD13	1.84	0.43
1:CCC:179:LEU:N	1:CCC:180:PRO:CD	2.82	0.43
1:BBB:98:ARG:NH1	1:BBB:200:GLU:OE1	2.51	0.43
1:AAA:84:LEU:O	1:AAA:145:ARG:NH2	2.51	0.43
1:AAA:179:LEU:N	1:AAA:180:PRO:CD	2.82	0.43
1:AAA:69:PHE:HD2	1:AAA:130:LEU:HD13	1.84	0.42
1:BBB:194:ALA:O	1:BBB:198:GLU:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:87:PRO:HB2	1:DDD:149:PHE:CD1	2.55	0.41
1:CCC:57:THR:O	1:CCC:61:TYR:HD2	2.04	0.41
1:BBB:68:LEU:C	1:BBB:68:LEU:HD23	2.41	0.41
1:BBB:84:LEU:C	1:BBB:145:ARG:HH12	2.24	0.40
1:BBB:179:LEU:N	1:BBB:180:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:32:GLN:OE1	1:CCC:55:LYS:NZ[4_555]	2.13	0.07

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	AAA	191/195 (98%)	188 (98%)	3 (2%)	0	100	100
1	BBB	191/195 (98%)	189 (99%)	2 (1%)	0	100	100
1	CCC	192/195 (98%)	190 (99%)	1 (0%)	1 (0%)	29	52
1	DDD	193/195 (99%)	192 (100%)	1 (0%)	0	100	100
All	All	767/780 (98%)	759 (99%)	7 (1%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	21	ARG

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	AAA	155/154 (101%)	145 (94%)	10 (6%)	17	34
1	BBB	153/154 (99%)	142 (93%)	11 (7%)	14	29
1	CCC	156/154 (101%)	145 (93%)	11 (7%)	14	29
1	DDD	156/154 (101%)	145 (93%)	11 (7%)	14	29
All	All	620/616 (101%)	577 (93%)	43 (7%)	15	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	21	ARG
1	CCC	22	LYS
1	CCC	49	LYS
1	CCC	116	PHE
1	CCC	132	ARG
1	CCC	157	ARG
1	CCC	188	SER
1	CCC	189	ASP
1	CCC	192	GLU
1	CCC	204	LYS
1	CCC	208	LYS
1	DDD	21	ARG
1	DDD	23	MSE
1	DDD	35	LEU
1	DDD	71	SER
1	DDD	72	LEU
1	DDD	84	LEU
1	DDD	108	PHE
1	DDD	113	ASP
1	DDD	118	ARG
1	DDD	184	VAL
1	DDD	204	LYS
1	AAA	21	ARG
1	AAA	49	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AAA	88	LYS
1	AAA	89	LEU
1	AAA	116	PHE
1	AAA	158	VAL
1	AAA	175	VAL
1	AAA	178	GLU
1	AAA	192	GLU
1	AAA	208	LYS
1	BBB	23	MSE
1	BBB	35	LEU
1	BBB	72	LEU
1	BBB	78	GLU
1	BBB	88	LYS
1	BBB	108	PHE
1	BBB	118	ARG
1	BBB	175	VAL
1	BBB	184	VAL
1	BBB	204	LYS
1	BBB	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

9 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	NHE	AAA	1003	-	13,13,13	1.10	1 (7%)	16,17,17	2.08	3 (18%)
4	NAR	BBB	1001	-	22,22,22	0.70	1 (4%)	32,32,32	0.75	1 (3%)
2	NHE	DDD	303	-	13,13,13	1.16	1 (7%)	16,17,17	1.24	1 (6%)
2	NHE	DDD	302	-	13,13,13	1.20	1 (7%)	16,17,17	1.43	2 (12%)
2	NHE	AAA	1001	-	13,13,13	1.05	1 (7%)	16,17,17	1.45	3 (18%)
2	NHE	AAA	1002	-	13,13,13	1.22	1 (7%)	16,17,17	0.98	1 (6%)
2	NHE	CCC	301	-	13,13,13	1.06	1 (7%)	16,17,17	1.48	2 (12%)
2	NHE	BBB	1002	-	13,13,13	1.27	1 (7%)	16,17,17	0.99	1 (6%)
3	CWE	DDD	301	-	22,22,22	0.72	0	32,32,32	1.32	5 (15%)

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	NHE	AAA	1003	-	-	4/7/15/15	0/1/1/1
4	NAR	BBB	1001	-	-	2/4/16/16	0/3/3/3
2	NHE	DDD	303	-	-	1/7/15/15	0/1/1/1
2	NHE	DDD	302	-	-	1/7/15/15	0/1/1/1
2	NHE	AAA	1001	-	-	5/7/15/15	0/1/1/1
2	NHE	AAA	1002	-	-	1/7/15/15	0/1/1/1
2	NHE	CCC	301	-	-	3/7/15/15	0/1/1/1
2	NHE	BBB	1002	-	-	3/7/15/15	0/1/1/1
3	CWE	DDD	301	-	-	1/4/16/16	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	1002	NHE	O1-S	4.25	1.57	1.45
2	AAA	1002	NHE	O2-S	4.16	1.57	1.45
2	DDD	302	NHE	O2-S	4.04	1.56	1.45
2	DDD	303	NHE	O1-S	3.77	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1003	NHE	O1-S	3.50	1.55	1.45
2	AAA	1001	NHE	O1-S	3.47	1.55	1.45
2	CCC	301	NHE	O1-S	3.35	1.54	1.45
4	BBB	1001	NAR	O2-C7	2.30	1.26	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1003	NHE	O1-S-C2	-7.14	98.32	106.92
2	CCC	301	NHE	O1-S-C2	-4.20	101.86	106.92
2	DDD	302	NHE	O3-S-O1	3.99	121.02	111.27
2	AAA	1001	NHE	O3-S-O2	3.94	120.91	111.27
3	DDD	301	CWE	C6-O1-C9	-3.50	109.62	115.50
2	DDD	303	NHE	O3-S-O2	3.41	119.60	111.27
3	DDD	301	CWE	C4-C5-C7	2.86	124.82	120.81
2	AAA	1002	NHE	O3-S-O1	2.79	118.08	111.27
3	DDD	301	CWE	O1-C6-C5	-2.76	118.71	121.56
2	CCC	301	NHE	O3-S-O2	2.76	118.02	111.27
3	DDD	301	CWE	C6-C5-C7	-2.69	117.89	120.33
3	DDD	301	CWE	O1-C9-C10	2.49	112.17	107.66
2	BBB	1002	NHE	O3-S-O2	2.47	117.31	111.27
2	AAA	1003	NHE	O3-S-O2	2.39	117.12	111.27
2	DDD	302	NHE	O2-S-C2	2.32	109.71	106.92
2	AAA	1003	NHE	O2-S-C2	2.31	109.70	106.92
2	AAA	1001	NHE	O1-S-C2	2.29	109.67	106.92
2	AAA	1001	NHE	O2-S-O1	-2.23	106.23	113.95
4	BBB	1001	NAR	O1-C9-C10	2.16	111.57	107.66

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	301	NHE	C6'-C1'-N-C1
2	AAA	1001	NHE	C6'-C1'-N-C1
2	AAA	1001	NHE	C1-C2-S-O1
2	AAA	1002	NHE	N-C1-C2-S
2	AAA	1003	NHE	C1-C2-S-O3
2	DDD	302	NHE	C2-C1-N-C1'
2	AAA	1001	NHE	C1-C2-S-O3
2	BBB	1002	NHE	C6'-C1'-N-C1
2	AAA	1001	NHE	C2-C1-N-C1'
2	AAA	1003	NHE	C2-C1-N-C1'

Continued on next page...

Continued from previous page...

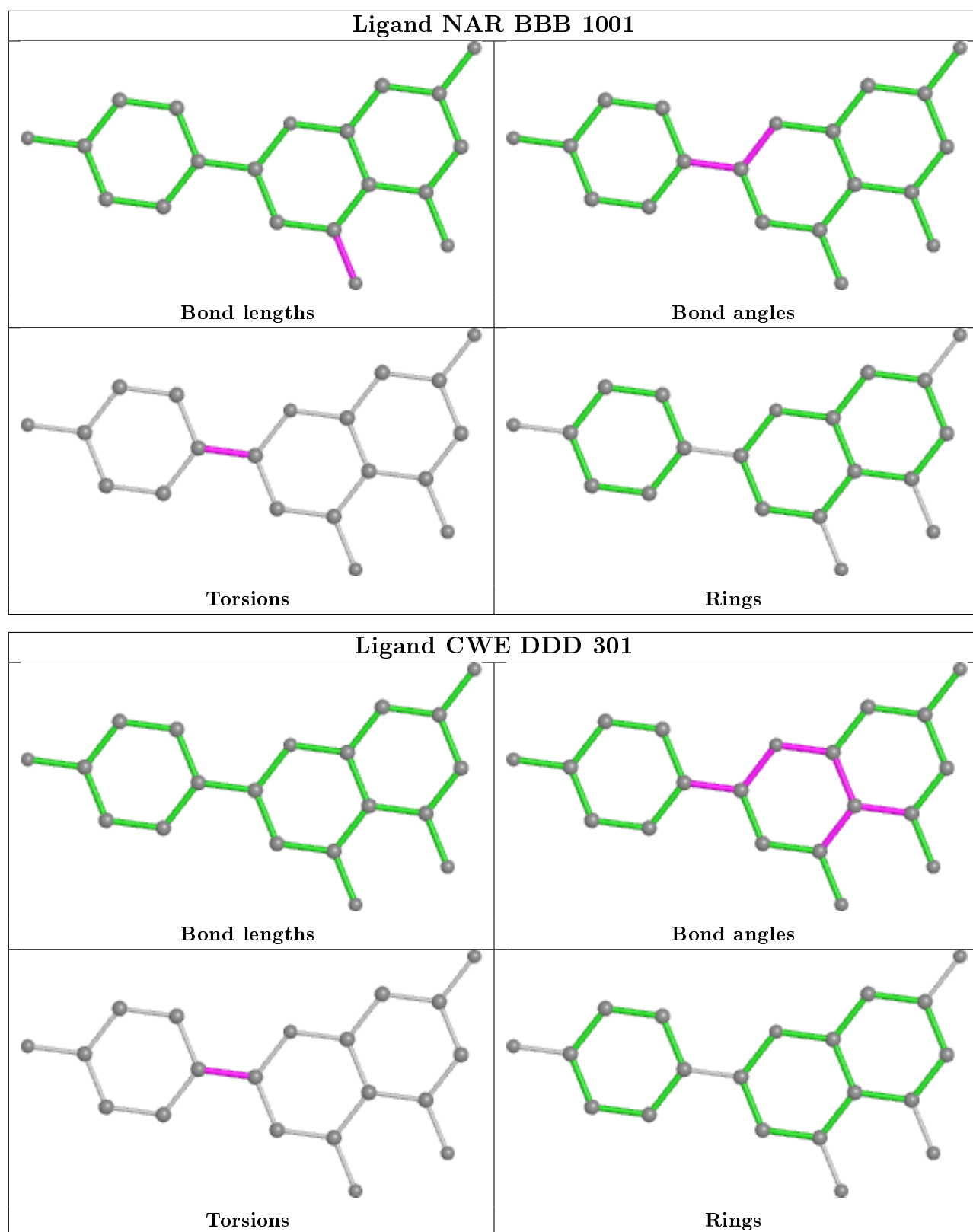
Mol	Chain	Res	Type	Atoms
2	CCC	301	NHE	C1-C2-S-O2
2	DDD	303	NHE	C2-C1-N-C1'
2	AAA	1001	NHE	C1-C2-S-O2
2	AAA	1003	NHE	C1-C2-S-O1
2	AAA	1003	NHE	C1-C2-S-O2
2	BBB	1002	NHE	C2-C1-N-C1'
4	BBB	1001	NAR	C15-C10-C9-C8
2	BBB	1002	NHE	C2'-C1'-N-C1
4	BBB	1001	NAR	C11-C10-C9-C8
3	DDD	301	CWE	C15-C10-C9-O1
2	CCC	301	NHE	C1-C2-S-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	1001	NHE	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 ⓘ

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	190/195 (97%)	-0.53	0 100 100	55, 78, 105, 151	0
1	BBB	190/195 (97%)	-0.51	0 100 100	54, 78, 115, 131	0
1	CCC	191/195 (97%)	-0.49	1 (0%) 91 89	51, 79, 115, 130	0
1	DDD	192/195 (98%)	-0.48	0 100 100	54, 71, 108, 131	0
All	All	763/780 (97%)	-0.50	1 (0%) 95 95	51, 77, 111, 151	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	189	ASP	2.6

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
2	NHE	BBB	1002	13/13	0.84	0.17	87,139,149,152	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CWE	DDD	301	20/20	0.88	0.21	97,109,119,122	0
4	NAR	BBB	1001	20/20	0.90	0.15	82,96,121,122	0
2	NHE	CCC	301	13/13	0.91	0.36	110,126,139,151	0
2	NHE	DDD	303	13/13	0.92	0.13	113,128,149,151	0
2	NHE	AAA	1002	13/13	0.95	0.24	94,121,135,138	0
2	NHE	AAA	1003	13/13	0.96	0.18	80,99,106,107	0
2	NHE	AAA	1001	13/13	0.98	0.13	62,74,82,85	0
2	NHE	DDD	302	13/13	0.98	0.14	72,90,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.