Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2021 – 01:03 pm BST

PDB ID	:	7AH8
Title	:	NF-Y bound to suramin inhibitor
Authors	:	Nardone, V.; Chaves-Sanjuan, A.; Lapi, M.; Nardini, M.
Deposited on	:	2020-09-24
Resolution	:	2.70 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:

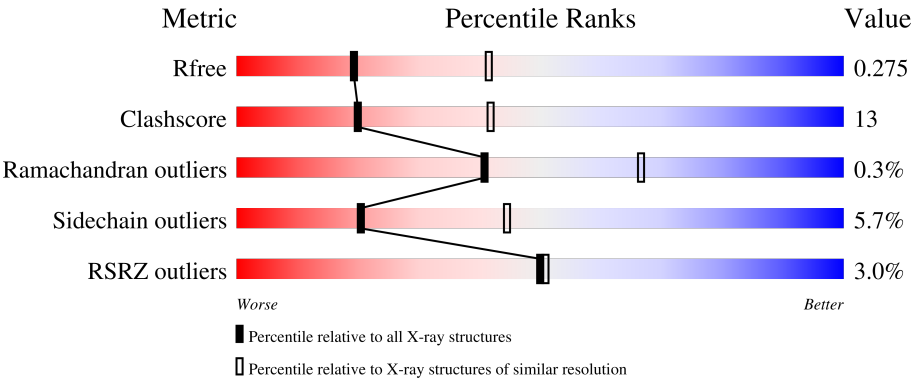
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	89	3% 79% 17%
1	C	89	2% 76% 19%
2	B	80	% 66% 32%
2	D	80	5% 71% 22% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2898 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.

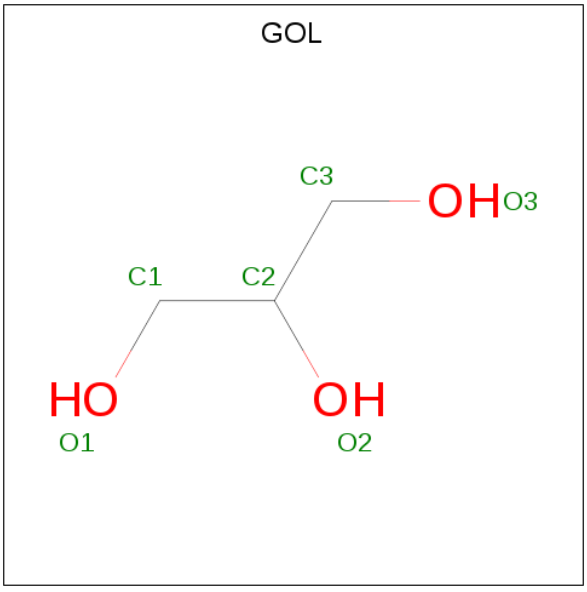
- Molecule 1 is a protein called Nuclear transcription factor Y subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	S	0	0	0
			704	448	118	133	5			
1	C	89	Total	C	N	O	S	0	1	0
			724	462	120	137	5			

- Molecule 2 is a protein called Isoform 6 of Nuclear transcription factor Y subunit gamma.

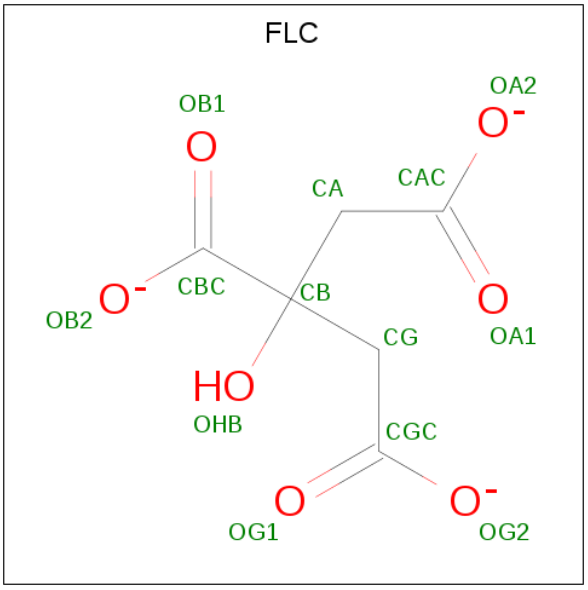
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	1	0
			659	425	115	116	3			
2	D	80	Total	C	N	O	S	0	0	0
			658	424	114	117	3			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



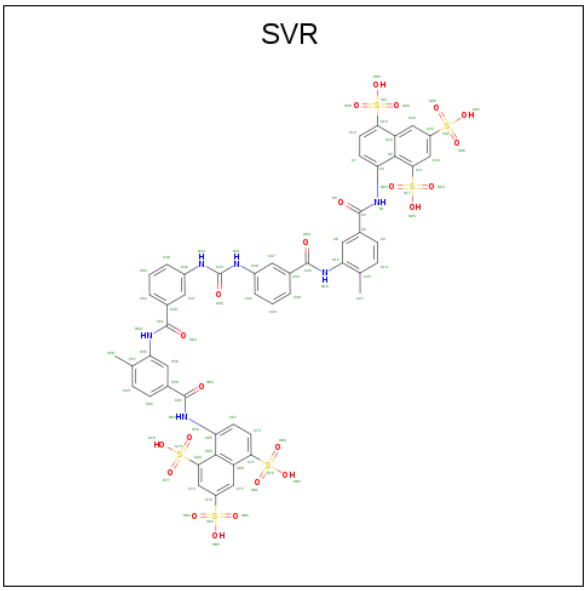
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 13 6 7	0	0

- Molecule 5 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFON IC ACID (three-letter code: SVR) (formula: $C_{51}H_{40}N_6O_{23}S_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			86	51	6	23	6		

- Molecule 6 is water.

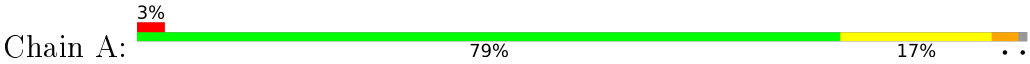
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	11	Total	O	0	0
			11	11		
6	C	11	Total	O	0	0
			11	11		
6	D	8	Total	O	0	1
			9	9		

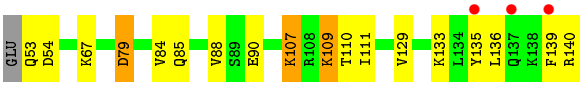
3 Residue-property plots (i)

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: Nuclear transcription factor Y subunit beta

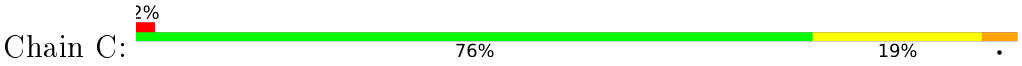
Chain A:

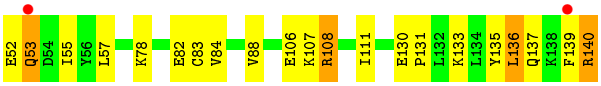




- Molecule 1: Nuclear transcription factor Y subunit beta

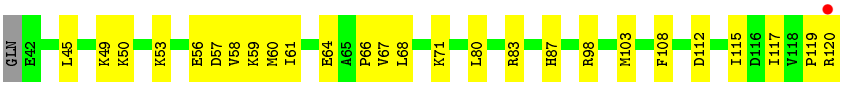
Chain C:





- Molecule 2: Isoform 6 of Nuclear transcription factor Y subunit gamma

Chain B:



- Molecule 2: Isoform 6 of Nuclear transcription factor Y subunit gamma

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.70Å 61.21Å 123.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.48 – 2.70 43.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.48-2.70) 100.0 (43.48-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.223 , 0.274 0.223 , 0.275	Depositor DCC
R_{free} test set	486 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2898	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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: SVR, FLC, GOL

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	0.45	0/715	0.54	0/960
1	C	0.55	1/736 (0.1%)	0.82	4/988 (0.4%)
2	B	0.28	0/670	0.55	0/901
2	D	0.50	1/668 (0.1%)	0.94	4/898 (0.4%)
All	All	0.46	2/2789 (0.1%)	0.73	8/3747 (0.2%)

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	C	0	1
2	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	GLU	CB-CG	5.12	1.61	1.52
2	D	94	ARG	CG-CD	5.00	1.64	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	120	ARG	NE-CZ-NH1	-13.27	113.67	120.30
1	C	53	GLN	CA-CB-CG	10.16	135.76	113.40
1	C	53	GLN	N-CA-CB	8.37	125.67	110.60
1	C	53	GLN	CB-CA-C	-8.26	93.89	110.40
2	D	120	ARG	CB-CG-CD	-7.25	92.76	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	120	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	C	136	LEU	CA-CB-CG	7.10	131.62	115.30
2	D	120	ARG	CG-CD-NE	5.83	124.05	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	ARG	Sidechain
2	D	56	GLU	Sidechain

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	704	0	713	13	0
1	C	724	0	727	17	0
2	B	659	0	688	26	0
2	D	658	0	690	25	0
3	B	6	0	8	4	0
4	C	13	0	5	1	0
5	D	86	0	40	2	0
6	A	17	0	0	0	0
6	B	11	0	0	1	0
6	C	11	0	0	0	0
6	D	9	0	0	0	0
All	All	2898	0	2871	72	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 13.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LYS:HG3	2:B:61:ILE:CD1	1.62	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LYS:HG3	2:B:61:ILE:HD11	1.32	1.10
2:B:49:LYS:CG	2:B:61:ILE:HD11	1.88	1.01
2:B:49:LYS:HG3	2:B:61:ILE:HD13	1.40	0.99
2:B:49:LYS:HD2	2:B:61:ILE:HD11	1.44	0.98
2:B:49:LYS:CD	2:B:61:ILE:HD11	1.95	0.95
1:C:111:ILE:H	1:C:111:ILE:HD12	1.33	0.92
2:D:99:ASN:ND2	2:D:120:ARG:NH1	2.23	0.87
2:B:49:LYS:CG	2:B:61:ILE:CD1	2.48	0.85
2:D:99:ASN:ND2	2:D:120:ARG:HH12	1.75	0.84
1:C:55:ILE:HD13	2:D:50:LYS:HE2	1.64	0.78
1:C:111:ILE:HD12	1:C:111:ILE:N	2.00	0.76
1:A:135:TYR:CE1	2:B:71:LYS:HE3	2.23	0.74
2:B:45:LEU:HD13	3:B:201:GOL:O2	1.89	0.72
1:A:129:VAL:HG12	1:A:133:LYS:HE2	1.72	0.71
2:B:98:ARG:HH22	2:B:119:PRO:HD2	1.53	0.71
1:C:78:LYS:NZ	1:C:82:GLU:OE2	2.23	0.71
2:B:66:PRO:HG2	5:D:201:SVR:H272	1.76	0.65
1:C:111:ILE:H	1:C:111:ILE:CD1	2.08	0.65
2:D:99:ASN:CG	2:D:120:ARG:NH1	2.49	0.65
1:A:109:LYS:HD3	1:A:110:THR:H	1.61	0.64
2:D:79:GLU:OE1	2:D:83:ARG:NH1	2.28	0.64
1:C:136:LEU:O	1:C:140:ARG:HD2	1.97	0.64
2:D:107:LYS:HG2	2:D:107:LYS:O	1.99	0.63
2:D:99:ASN:CG	2:D:120:ARG:HH12	2.02	0.62
1:A:136:LEU:HD23	1:A:136:LEU:O	2.00	0.62
2:D:112:ASP:O	2:D:115:ILE:HG23	2.01	0.60
1:A:136:LEU:HD21	1:A:140:ARG:CZ	2.33	0.59
2:B:64:GLU:O	2:B:67:VAL:HG22	2.02	0.58
2:D:56:GLU:N	2:D:56:GLU:OE1	2.31	0.58
2:B:45:LEU:HD21	2:B:67:VAL:HG12	1.86	0.58
1:A:90:GLU:HG2	2:B:117:ILE:HG13	1.84	0.58
1:C:84:VAL:O	1:C:88:VAL:HG23	2.04	0.57
1:A:109:LYS:CD	1:A:109:LYS:H	2.18	0.56
2:B:120:ARG:NE	2:B:120:ARG:HA	2.20	0.56
1:C:83:CYS:SG	2:D:118:VAL:HG11	2.46	0.56
3:B:201:GOL:H12	2:D:45:LEU:HD23	1.89	0.53
2:B:83:ARG:HG2	2:B:108:PHE:CZ	2.44	0.53
3:B:201:GOL:H11	2:D:41:GLN:N	2.25	0.52
2:D:115:ILE:HG13	2:D:116:ASP:OD1	2.10	0.52
2:B:58:VAL:O	2:B:59:LYS:HE2	2.10	0.51
2:B:53:LYS:NZ	2:B:59:LYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLU:HB2	1:C:108:ARG:HG3	1.91	0.51
2:D:56:GLU:HG2	2:D:57:ASP:OD1	2.10	0.50
2:D:118:VAL:O	2:D:118:VAL:HG23	2.12	0.50
2:D:53:LYS:NZ	5:D:201:SVR:O78	2.30	0.50
2:D:83:ARG:HG2	2:D:108:PHE:CE2	2.46	0.50
1:C:136:LEU:O	1:C:140:ARG:HG3	2.13	0.49
1:A:84:VAL:HG22	2:B:80:LEU:HD23	1.95	0.49
1:C:57:LEU:HD13	2:D:43:LEU:HD22	1.94	0.49
2:B:50:LYS:NZ	6:B:301:HOH:O	2.47	0.48
1:C:135:TYR:CZ	1:C:139[A]:PHE:HE2	2.33	0.47
1:A:109:LYS:HD3	1:A:109:LYS:H	1.80	0.46
1:C:136:LEU:HD21	2:D:68:LEU:HD21	1.96	0.46
2:D:60:MET:HE3	2:D:60:MET:HB3	1.89	0.46
1:A:135:TYR:CD1	2:B:71:LYS:HE3	2.50	0.45
2:B:112:ASP:O	2:B:115:ILE:HG12	2.16	0.45
4:C:201:FLC:OB1	4:C:201:FLC:CGC	2.64	0.45
1:A:79:ASP:OD1	1:A:79:ASP:N	2.48	0.45
1:C:136:LEU:O	1:C:140:ARG:CD	2.64	0.44
2:D:99:ASN:HD22	2:D:120:ARG:HH12	1.61	0.44
2:D:65:ALA:HB3	2:D:66:PRO:HD3	2.00	0.43
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.84	0.42
2:B:87[B]:HIS:CE1	2:B:103:MET:HG3	2.54	0.42
1:C:133:LYS:O	1:C:137:GLN:HG3	2.19	0.42
1:A:85:GLN:O	1:A:88:VAL:HG12	2.20	0.42
2:D:41:GLN:HB3	2:D:42:GLU:H	1.70	0.42
1:C:136:LEU:HD21	2:D:68:LEU:CD2	2.50	0.42
2:D:99:ASN:CB	2:D:120:ARG:HH12	2.33	0.42
1:C:130:GLU:HB3	1:C:131:PRO:HD3	2.02	0.41
2:B:45:LEU:HD13	3:B:201:GOL:HO2	1.84	0.41
1:A:111:ILE:HD11	2:B:58:VAL:HG22	2.02	0.41

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	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13 32
1	C	88/89 (99%)	85 (97%)	3 (3%)	0	100 100
2	B	78/80 (98%)	77 (99%)	1 (1%)	0	100 100
2	D	78/80 (98%)	77 (99%)	1 (1%)	0	100 100
All	All	330/338 (98%)	321 (97%)	8 (2%)	1 (0%)	41 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	LYS

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	78/79 (99%)	71 (91%)	7 (9%)	9 22
1	C	80/79 (101%)	77 (96%)	3 (4%)	33 62
2	B	71/71 (100%)	68 (96%)	3 (4%)	30 58
2	D	71/71 (100%)	67 (94%)	4 (6%)	21 45
All	All	300/300 (100%)	283 (94%)	17 (6%)	20 44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	54	ASP
1	A	67	LYS
1	A	79	ASP
1	A	107	LYS
1	A	109	LYS
1	A	139	PHE

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Mol	Chain	Res	Type
2	B	56	GLU
2	B	57	ASP
2	B	60	MET
1	C	53	GLN
1	C	107	LYS
1	C	108	ARG
2	D	83	ARG
2	D	94	ARG
2	D	116	ASP
2	D	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	ASN
2	D	99	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

3 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	$\#\|Z\|>2$
4	FLC	C	201	-	3,12,12	1.21	0	3,17,17	1.54	1 (33%)
3	GOL	B	201	-	5,5,5	0.27	0	5,5,5	0.53	0
5	SVR	D	201	-	89,93,93	1.83	23 (25%)	129,145,145	1.48	22 (17%)

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
4	FLC	C	201	-	-	3/6/16/16	-
3	GOL	B	201	-	-	4/4/4/4	-
5	SVR	D	201	-	-	10/76/76/76	0/8/8/8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	201	SVR	C43-N44	5.07	1.48	1.37
5	D	201	SVR	C43-N41	4.95	1.47	1.37
5	D	201	SVR	C61-N63	4.42	1.47	1.35
5	D	201	SVR	C2-N1	4.29	1.47	1.35
5	D	201	SVR	C26-N19	4.06	1.46	1.35
5	D	201	SVR	C51-N53	3.72	1.45	1.35
5	D	201	SVR	C39-N41	3.19	1.48	1.41
5	D	201	SVR	C13-N19	2.99	1.47	1.41
5	D	201	SVR	C46-N44	2.75	1.47	1.41
5	D	201	SVR	C68-C66	-2.75	1.37	1.42
5	D	201	SVR	C69-C66	-2.72	1.40	1.43
5	D	201	SVR	C76-S83	2.71	1.82	1.77
5	D	201	SVR	C22-S31	2.54	1.82	1.77
5	D	201	SVR	C10-C6	-2.46	1.37	1.42
5	D	201	SVR	C33-C26	2.38	1.55	1.50
5	D	201	SVR	C49-C51	2.29	1.55	1.50
5	D	201	SVR	O4-C2	-2.29	1.18	1.23
5	D	201	SVR	O64-C61	-2.28	1.18	1.23
5	D	201	SVR	C3-N1	2.27	1.47	1.41
5	D	201	SVR	O45-C43	-2.23	1.18	1.23
5	D	201	SVR	O54-C51	-2.12	1.19	1.23
5	D	201	SVR	C11-C6	-2.07	1.41	1.43
5	D	201	SVR	C5-C2	2.01	1.54	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	201	SVR	C69-C66-C68	4.23	120.32	116.34
5	D	201	SVR	C55-N53-C51	-4.08	115.73	126.93
5	D	201	SVR	C60-C57-C55	3.52	120.75	117.44
5	D	201	SVR	C14-C20-C13	3.49	120.73	117.44
5	D	201	SVR	N44-C43-N41	3.48	118.57	112.49
5	D	201	SVR	C65-N63-C61	-3.20	119.15	128.64
5	D	201	SVR	C11-C6-C10	2.83	119.00	116.34
5	D	201	SVR	O36-S31-C22	2.64	112.73	106.65
5	D	201	SVR	C33-C26-N19	2.58	121.61	115.92
5	D	201	SVR	C39-N41-C43	-2.56	121.38	126.61
5	D	201	SVR	O84-S83-C76	2.54	112.49	106.65
5	D	201	SVR	C72-C76-S83	2.54	124.25	119.89
5	D	201	SVR	C49-C51-N53	2.53	121.48	115.92
4	C	201	FLC	CB-CA-CAC	-2.50	110.98	114.98
5	D	201	SVR	O81-S75-C71	2.38	113.54	106.43
5	D	201	SVR	O29-S21-O28	-2.34	100.71	112.86
5	D	201	SVR	C74-C76-S83	-2.30	115.92	119.89
5	D	201	SVR	O36-S31-O35	-2.30	100.91	112.86
5	D	201	SVR	O84-S83-O86	-2.30	100.94	112.86
5	D	201	SVR	O24-S17-O23	-2.07	102.11	112.86
5	D	201	SVR	O81-S75-O80	-2.06	102.16	112.86
5	D	201	SVR	C16-C22-S31	2.03	123.38	119.89
5	D	201	SVR	C13-N19-C26	-2.01	121.42	126.93

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	GOL	O1-C1-C2-O2
3	B	201	GOL	O1-C1-C2-C3
3	B	201	GOL	C1-C2-C3-O3
4	C	201	FLC	CAC-CA-CB-CBC
4	C	201	FLC	CAC-CA-CB-OHB
5	D	201	SVR	C68-C71-S75-O82
4	C	201	FLC	CAC-CA-CB-CG
3	B	201	GOL	O2-C2-C3-O3
5	D	201	SVR	C7-C3-N1-C2
5	D	201	SVR	C68-C71-S75-O80
5	D	201	SVR	C70-C71-S75-O80
5	D	201	SVR	C56-C55-N53-C51
5	D	201	SVR	C67-C65-N63-C61

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Mol	Chain	Res	Type	Atoms
5	D	201	SVR	C57-C55-N53-C51
5	D	201	SVR	C6-C11-S17-O23
5	D	201	SVR	C68-C71-S75-O81
5	D	201	SVR	C18-C11-S17-O23

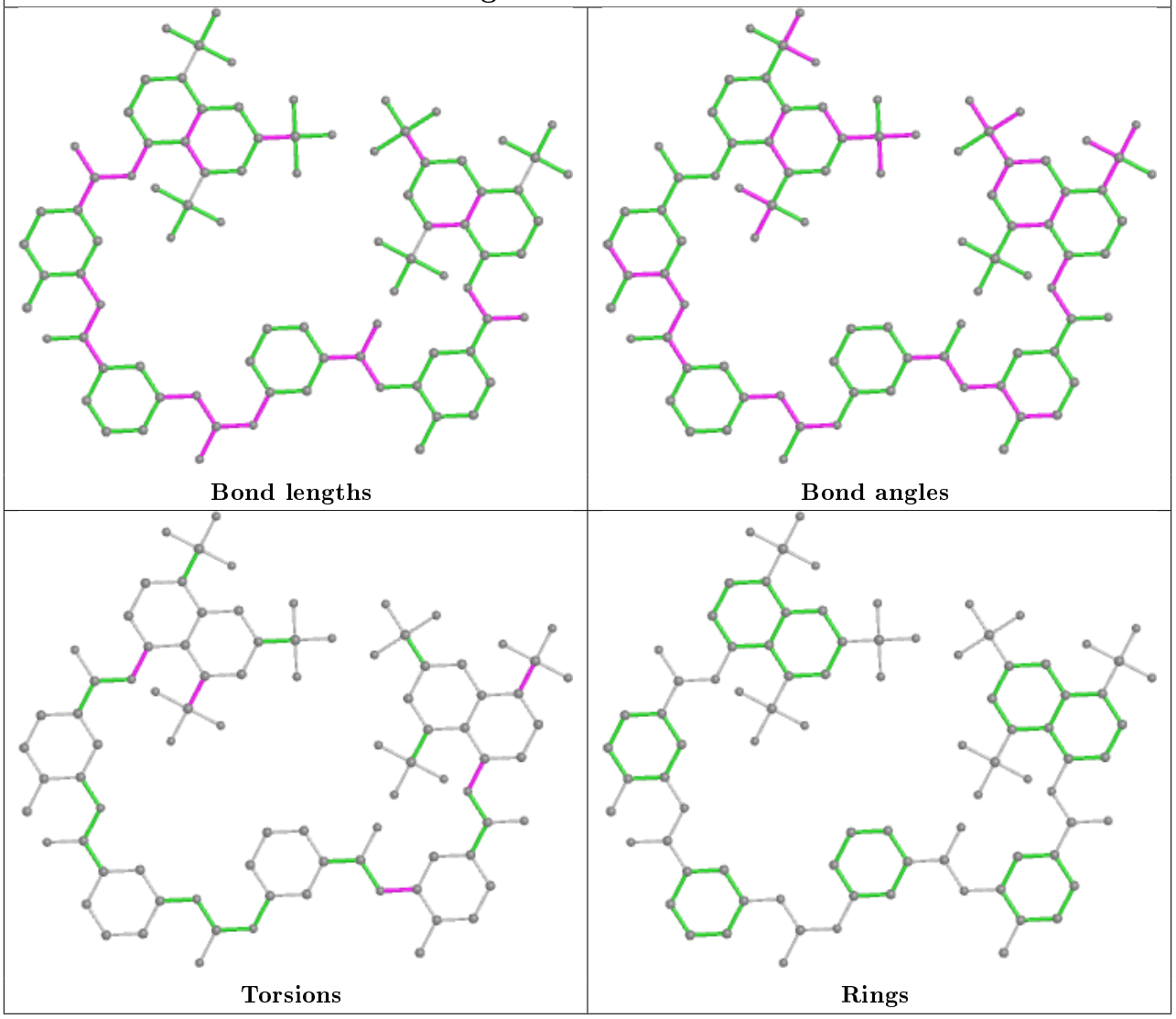
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	201	FLC	1	0
3	B	201	GOL	4	0
5	D	201	SVR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SVR D 201



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, 95^{th} 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	88/89 (98%)	-0.11	3 (3%)	45	45	30, 46, 86, 96	0
1	C	89/89 (100%)	-0.13	2 (2%)	62	63	30, 52, 92, 107	0
2	B	79/80 (98%)	-0.11	1 (1%)	77	78	27, 47, 84, 90	0
2	D	80/80 (100%)	0.01	4 (5%)	28	27	32, 53, 81, 104	0
All	All	336/338 (99%)	-0.08	10 (2%)	50	51	27, 49, 88, 107	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	GLN	4.9
2	D	120	ARG	4.8
2	B	120	ARG	4.2
2	D	56	GLU	3.3
2	D	103	MET	2.7
1	A	139	PHE	2.7
1	C	139[A]	PHE	2.5
1	A	135	TYR	2.1
2	D	119	PRO	2.0
1	A	137	GLN	2.0

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

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, 95^{th} 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	FLC	C	201	13/13	0.76	0.27	60,72,75,78	0
3	GOL	B	201	6/6	0.81	0.28	53,60,73,80	0
5	SVR	D	201	86/86	0.86	0.23	37,74,102,118	0

6.5 Other polymers

There are no such residues in this entry.