Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 01:14 pm BST

PDB ID	:	7YXL
Title	:	Drosophila melanogaster JMJD7 (dmJMJD7) in complex with Mn and N-oxalyl-D-phenylalanine (NOFD)
Authors	:	Chowdhury, R.; Schofield, C.J.
Deposited on	:	2022-02-16
Resolution	:	2.20 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:

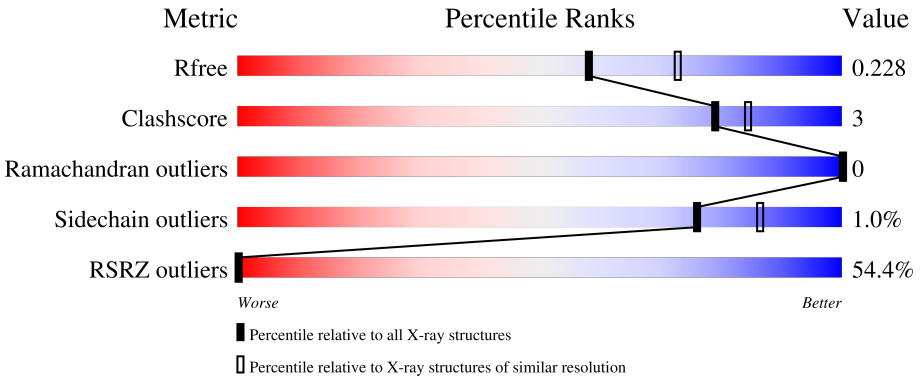
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	322	41% 88% 7% 5%
1	B	322	62% 89% 5% 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
6	ACT	A	509	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9846 atoms, of which 4633 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 GH14974p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	307	Total	C	H	N	O	S	0	3	0
			4792	1579	2327	408	467	11			
1	B	305	Total	C	H	N	O	S	0	4	0
			4645	1548	2240	393	453	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9VU77
A	-4	SER	-	expression tag	UNP Q9VU77
A	-3	HIS	-	expression tag	UNP Q9VU77
A	-2	MET	-	expression tag	UNP Q9VU77
A	-1	ALA	-	expression tag	UNP Q9VU77
A	0	SER	-	expression tag	UNP Q9VU77
B	-5	GLY	-	expression tag	UNP Q9VU77
B	-4	SER	-	expression tag	UNP Q9VU77
B	-3	HIS	-	expression tag	UNP Q9VU77
B	-2	MET	-	expression tag	UNP Q9VU77
B	-1	ALA	-	expression tag	UNP Q9VU77
B	0	SER	-	expression tag	UNP Q9VU77

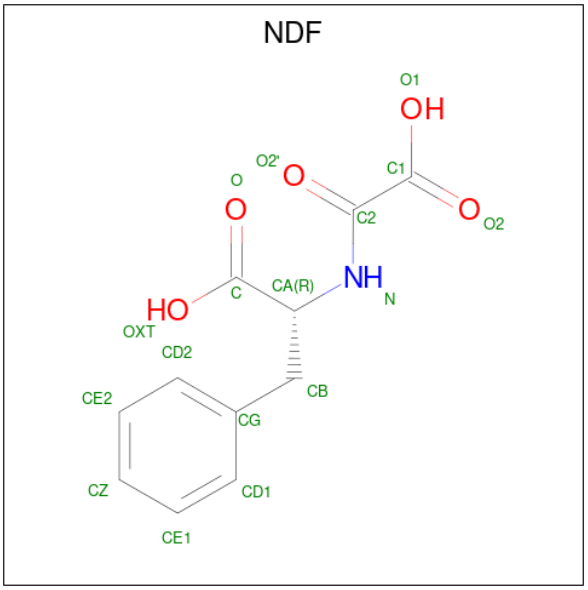
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

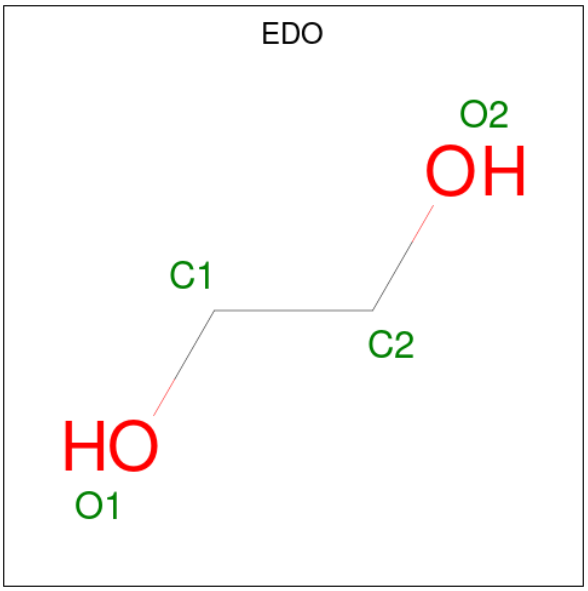
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is N-(CARBOXYCARBONYL)-D-PHENYLALANINE (three-letter code: NDF) (formula: $C_{11}H_{11}NO_5$) (labeled as "Ligand of Interest" by depositor).



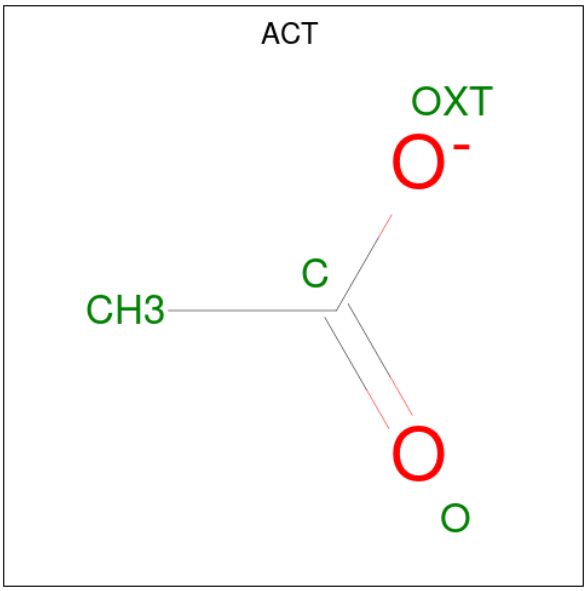
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N O 26 11 9 1 5	0	0
4	B	1	Total C H N O 26 11 9 1 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 7 2 3 2	0	0
6	A	1	Total C H O 7 2 3 2	0	0

- Molecule 7 is water.

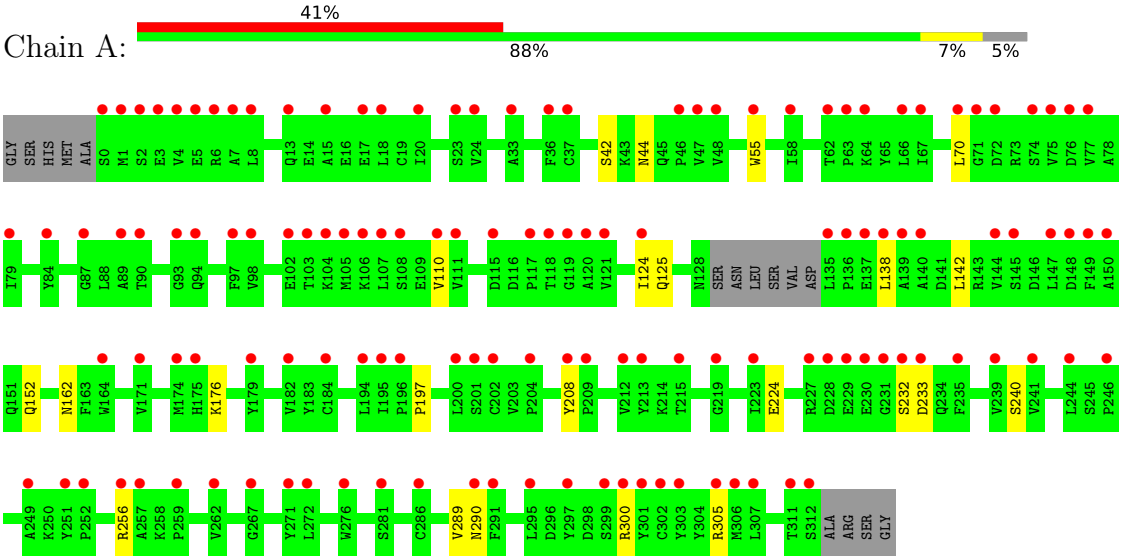
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	186	Total O 186 186	0	0
7	B	83	Total O 83 83	0	0

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.

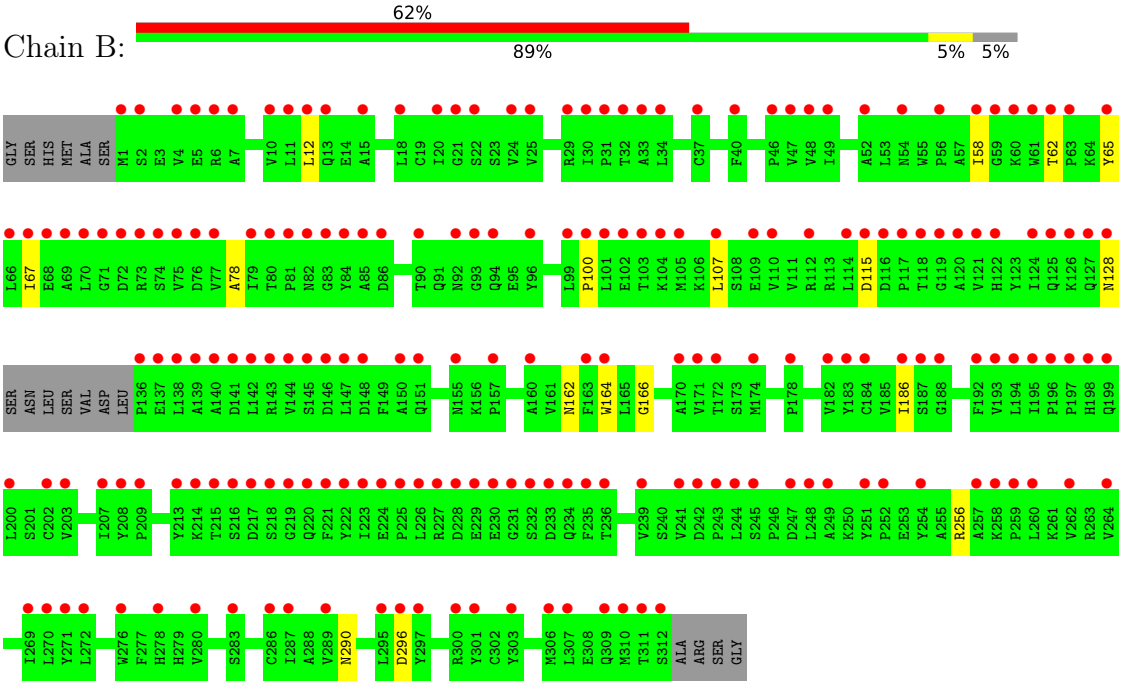
• Molecule 1: GH14974p

Chain A:



• Molecule 1: GH14974p

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.02Å 65.16Å 99.22Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	40.42 – 2.20 40.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.42-2.20) 99.8 (40.42-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.189 , 0.230 0.188 , 0.228	Depositor DCC
R_{free} test set	1758 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.95	EDS
Total number of atoms	9846	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 5.79% 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: CSO, EDO, MG, ACT, NDF, MN

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	0.28	0/2539	0.48	0/3466
1	B	0.26	0/2494	0.44	0/3412
All	All	0.27	0/5033	0.46	0/6878

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2465	2327	2320	15	0
1	B	2405	2240	2222	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	17	9	9	0	0
4	B	17	9	9	1	0
5	A	20	30	30	1	0
5	B	8	12	12	2	0
6	A	8	6	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	186	0	0	4	0
7	B	83	0	0	4	0
All	All	5213	4633	4608	27	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:O	1:A:300[A]:ARG:NH2	2.25	0.69
1:A:305:ARG:NH1	7:A:608:HOH:O	2.30	0.64
1:B:128:ASN:ND2	7:B:606:HOH:O	2.35	0.60
1:A:300[A]:ARG:HD3	6:A:509:ACT:H3	1.86	0.58
1:B:67:ILE:HA	1:B:107:LEU:HD23	1.89	0.53
1:B:65:TYR:N	7:B:601:HOH:O	2.20	0.52
1:B:164:TRP:CH2	1:B:166:GLY:HA3	2.46	0.50
1:A:44:ASN:OD1	7:A:601:HOH:O	2.20	0.50
4:B:503:NDF:HD2	5:B:504:EDO:C2	2.43	0.48
1:A:110:VAL:HG11	1:A:124:ILE:HD11	1.96	0.47
1:A:224[B]:GLU:OE2	7:A:602:HOH:O	2.20	0.47
1:B:164:TRP:HB2	5:B:504:EDO:C1	2.46	0.46
1:A:208:TYR:OH	1:A:240:SER:HB3	2.15	0.46
1:A:232:SER:OG	1:A:233:ASP:N	2.49	0.45
1:B:62:THR:OG1	7:B:601:HOH:O	2.21	0.45
1:A:70:LEU:HD11	1:A:138:LEU:HD11	1.99	0.44
1:A:152:GLN:OE1	7:A:603:HOH:O	2.21	0.44
1:A:55:TRP:CE3	1:A:142:LEU:HD22	2.53	0.43
1:A:162:ASN:HB2	1:A:290:ASN:OD1	2.19	0.43
1:B:65:TYR:HB2	7:B:601:HOH:O	2.19	0.42
1:B:162:ASN:HB2	1:B:290:ASN:OD1	2.19	0.42
1:A:162:ASN:O	1:A:289:VAL:HA	2.20	0.41
1:A:300[B]:ARG:NH2	5:A:508:EDO:O1	2.53	0.41
1:B:78:ALA:HB1	1:B:100:PRO:HB2	2.02	0.41
1:B:12:LEU:HD13	1:B:256:ARG:HD3	2.02	0.41
1:A:197:PRO:HG2	6:A:509:ACT:H2	2.02	0.41
1:B:58:ILE:HD13	1:B:186:ILE:HA	2.03	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	305/322 (95%)	300 (98%)	5 (2%)	0	100	100
1	B	304/322 (94%)	296 (97%)	8 (3%)	0	100	100
All	All	609/644 (95%)	596 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	262/283 (93%)	259 (99%)	3 (1%)	73	85
1	B	250/283 (88%)	248 (99%)	2 (1%)	81	90
All	All	512/566 (90%)	507 (99%)	5 (1%)	76	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	176	LYS
1	A	256	ARG
1	B	115	ASP
1	B	296	ASP

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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	B	19	1	3,6,7	0.65	0	0,6,8	-	-
1	CSO	A	19	1	3,6,7	0.59	0	0,6,8	-	-

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
1	CSO	B	19	1	-	0/1/5/7	-
1	CSO	A	19	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ACT	A	510	-	1,3,3	5.61	1 (100%)	0,3,3	-	-
6	ACT	A	509	-	1,3,3	5.96	1 (100%)	0,3,3	-	-
5	EDO	A	506	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.59	0
5	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	A	504	-	3,3,3	0.48	0	2,2,2	0.13	0
5	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.29	0
4	NDF	A	503	2	11,17,17	1.12	0	13,22,22	0.90	1 (7%)
4	NDF	B	503	2	11,17,17	1.15	0	13,22,22	1.30	3 (23%)
5	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.28	0
5	EDO	A	508	-	3,3,3	0.46	0	2,2,2	0.38	0

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
5	EDO	A	506	-	-	1/1/1/1	-
5	EDO	B	504	-	-	1/1/1/1	-
5	EDO	B	505	-	-	1/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-
4	NDF	A	503	2	-	0/8/16/16	0/1/1/1
4	NDF	B	503	2	-	2/8/16/16	0/1/1/1
5	EDO	A	505	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	508	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	ACT	CH3-C	5.96	1.56	1.48
6	A	510	ACT	CH3-C	5.61	1.55	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	503	NDF	CB-CA-N	3.11	114.67	109.01
4	B	503	NDF	CG-CB-CA	2.42	117.08	112.97
4	B	503	NDF	CA-N-C2	2.30	125.30	122.34
4	A	503	NDF	CA-N-C2	2.12	125.07	122.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	NDF	C-CA-CB-CG
4	B	503	NDF	N-CA-CB-CG
5	A	506	EDO	O1-C1-C2-O2
5	B	504	EDO	O1-C1-C2-O2
5	A	508	EDO	O1-C1-C2-O2
5	B	505	EDO	O1-C1-C2-O2

There are no ring outliers.

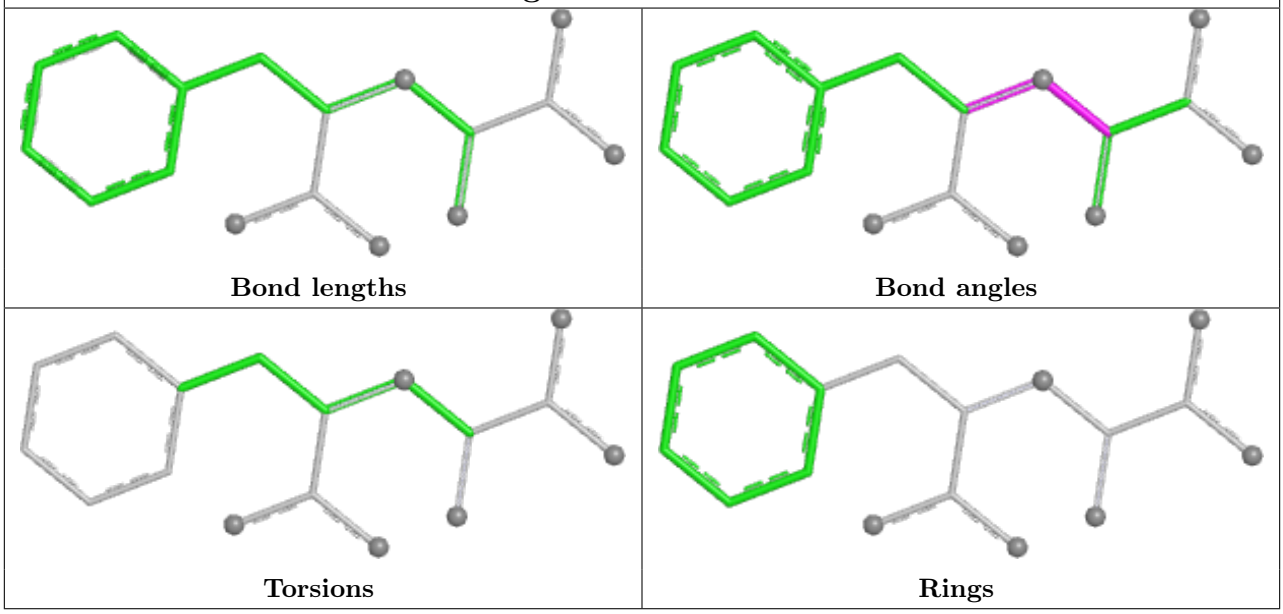
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	509	ACT	2	0
5	B	504	EDO	2	0
4	B	503	NDF	1	0
5	A	508	EDO	1	0

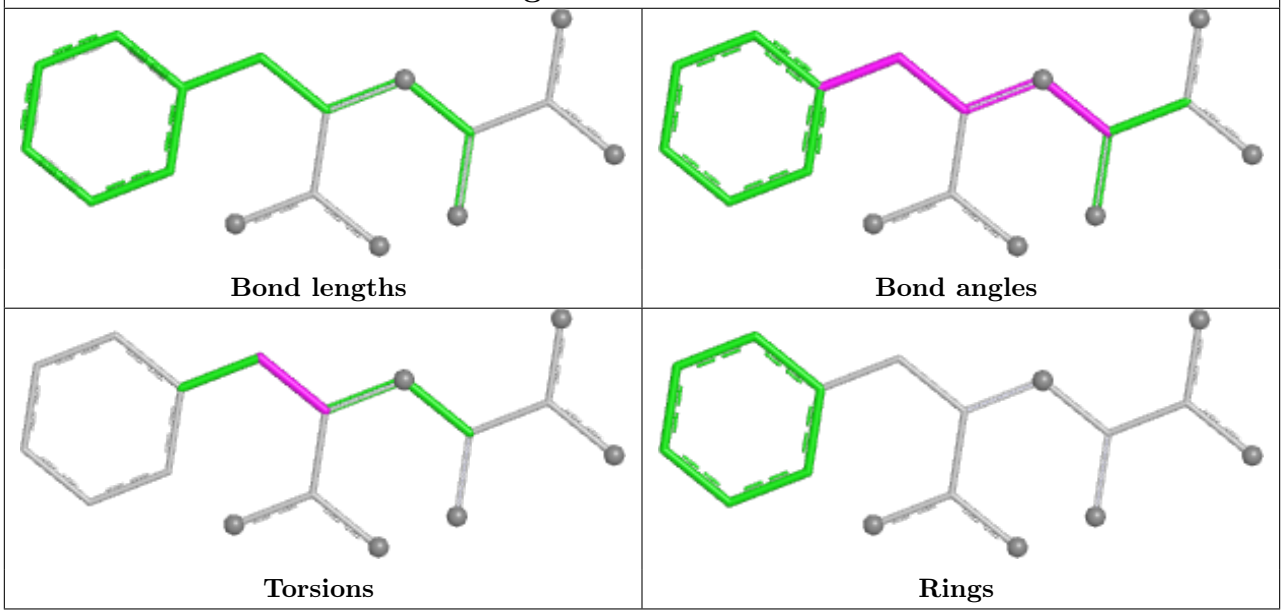
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NDF A 503



Ligand NDF B 503



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	306/322 (95%)	2.16	133 (43%)	0	0	24, 36, 71, 115	1 (0%)
1	B	304/322 (94%)	2.79	199 (65%)	0	0	28, 53, 103, 150	0
All	All	610/644 (94%)	2.48	332 (54%)	0	0	24, 43, 96, 150	1 (0%)

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ALA	12.3
1	B	71	GLY	10.8
1	B	220	GLN	9.8
1	A	232	SER	9.5
1	B	215	THR	8.4
1	B	118	THR	8.2
1	A	0	SER	8.2
1	B	228	ASP	7.7
1	B	67	ILE	7.5
1	B	136	PRO	7.5
1	A	230	GLU	7.3
1	B	144	VAL	7.2
1	B	233	ASP	7.1
1	B	69	ALA	7.0
1	B	139	ALA	6.9
1	A	117	PRO	6.7
1	A	231	GLY	6.7
1	B	231	GLY	6.6
1	B	138	LEU	6.5
1	A	118	THR	6.5
1	B	74	SER	6.5
1	A	74	SER	6.1
1	B	83	GLY	6.1
1	B	157	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	230	GLU	6.0
1	B	73	ARG	5.9
1	B	216	SER	5.9
1	B	232	SER	5.8
1	A	228	ASP	5.6
1	B	70	LEU	5.6
1	B	66	LEU	5.5
1	B	62	THR	5.5
1	B	77	VAL	5.4
1	A	70	LEU	5.3
1	B	121	VAL	5.3
1	B	252	PRO	5.3
1	B	92	ASN	5.0
1	B	94	GLN	5.0
1	A	103	THR	5.0
1	B	115	ASP	5.0
1	B	128	ASN	4.9
1	A	138	LEU	4.9
1	A	229	GLU	4.9
1	B	235	PHE	4.9
1	B	226	LEU	4.8
1	B	65	TYR	4.8
1	B	1	MET	4.8
1	B	287	ILE	4.7
1	B	116	ASP	4.7
1	B	217	ASP	4.6
1	B	75	VAL	4.6
1	A	24	VAL	4.6
1	B	101	LEU	4.6
1	B	219	GLY	4.6
1	B	119	GLY	4.5
1	B	58	ILE	4.5
1	B	145	SER	4.4
1	B	225	PRO	4.4
1	A	257	ALA	4.4
1	B	103	THR	4.4
1	B	61	TRP	4.4
1	A	135	LEU	4.3
1	B	105	MET	4.3
1	B	209	PRO	4.3
1	B	218	SER	4.3
1	B	56	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	PRO	4.3
1	B	222	TYR	4.2
1	A	223	ILE	4.2
1	B	142	LEU	4.2
1	A	3	GLU	4.2
1	B	93	GLY	4.1
1	B	141	ASP	4.1
1	B	229	GLU	4.1
1	A	144	VAL	4.1
1	B	6	ARG	4.0
1	A	115	ASP	4.0
1	B	151	GLN	3.9
1	B	262	VAL	3.9
1	B	117	PRO	3.9
1	B	243	PRO	3.9
1	B	122	HIS	3.9
1	B	102	GLU	3.8
1	B	272	LEU	3.8
1	A	8	LEU	3.8
1	B	224	GLU	3.8
1	B	249	ALA	3.8
1	B	120	ALA	3.7
1	A	90	THR	3.7
1	A	136	PRO	3.7
1	B	163	PHE	3.7
1	B	7	ALA	3.7
1	B	10	VAL	3.7
1	B	244	LEU	3.6
1	A	148	ASP	3.6
1	B	311	THR	3.6
1	B	52	ALA	3.6
1	B	114	LEU	3.6
1	B	221	PHE	3.6
1	B	214	LYS	3.6
1	A	252	PRO	3.6
1	B	296	ASP	3.5
1	A	239	VAL	3.5
1	B	295	LEU	3.5
1	B	227	ARG	3.5
1	A	4	VAL	3.5
1	B	80	THR	3.4
1	A	286	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	72	ASP	3.4
1	A	311	THR	3.4
1	A	140	ALA	3.4
1	A	1	MET	3.4
1	A	105	MET	3.4
1	B	137	GLU	3.4
1	B	203	VAL	3.4
1	A	2	SER	3.3
1	A	303	TYR	3.3
1	B	96	TYR	3.3
1	B	286	CYS	3.3
1	A	5	GLU	3.3
1	B	127	GLN	3.3
1	B	148[A]	ASP	3.3
1	B	79	ILE	3.3
1	B	146	ASP	3.3
1	B	170	ALA	3.3
1	B	223	ILE	3.3
1	A	121	VAL	3.3
1	A	233	ASP	3.2
1	B	251	TYR	3.2
1	B	20	ILE	3.2
1	A	64	LYS	3.2
1	A	62	THR	3.2
1	B	234	GLN	3.2
1	A	147	LEU	3.2
1	B	2	SER	3.2
1	B	30	ILE	3.1
1	A	111	VAL	3.1
1	B	140	ALA	3.1
1	A	184	CYS	3.1
1	B	29	ARG	3.1
1	A	124	ILE	3.1
1	A	89	ALA	3.1
1	B	59	GLY	3.1
1	B	307	LEU	3.1
1	B	202	CYS	3.1
1	B	85	ALA	3.1
1	B	109	GLU	3.0
1	A	71	GLY	3.0
1	A	302	CYS	3.0
1	A	312	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	68	GLU	3.0
1	A	119	GLY	3.0
1	B	248	LEU	3.0
1	B	124	ILE	3.0
1	A	48	VAL	3.0
1	A	251	TYR	3.0
1	B	90	THR	3.0
1	B	245	SER	3.0
1	B	54[A]	ASN	3.0
1	A	58	ILE	3.0
1	B	241	VAL	3.0
1	B	192	PHE	2.9
1	B	276	TRP	2.9
1	B	13	GLN	2.9
1	B	125	GLN	2.9
1	A	108	SER	2.9
1	A	15	ALA	2.9
1	A	84	TYR	2.9
1	A	67	ILE	2.9
1	A	201	SER	2.9
1	A	107	LEU	2.9
1	A	244	LEU	2.9
1	B	48	VAL	2.9
1	B	183	TYR	2.9
1	B	21	GLY	2.9
1	B	104	LYS	2.9
1	B	208	TYR	2.9
1	A	299	SER	2.8
1	B	107	LEU	2.8
1	A	104	LYS	2.8
1	B	280	VAL	2.8
1	A	256	ARG	2.8
1	B	46	PRO	2.8
1	B	32	THR	2.8
1	B	303	TYR	2.8
1	A	241	VAL	2.8
1	A	63	PRO	2.8
1	B	18	LEU	2.8
1	A	20	ILE	2.8
1	A	110	VAL	2.8
1	A	267	GLY	2.8
1	A	13	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	235	PHE	2.7
1	A	6	ARG	2.7
1	B	270	LEU	2.7
1	A	200	LEU	2.7
1	B	99	LEU	2.7
1	B	310	MET	2.7
1	B	155	ASN	2.7
1	A	179	TYR	2.7
1	B	100	PRO	2.7
1	A	149	PHE	2.7
1	A	202	CYS	2.7
1	B	207	ILE	2.7
1	A	17	GLU	2.7
1	B	81	PRO	2.6
1	A	7	ALA	2.6
1	B	257	ALA	2.6
1	A	75	VAL	2.6
1	B	40	PHE	2.6
1	B	271	TYR	2.6
1	B	312	SER	2.6
1	A	175	HIS	2.6
1	A	97	PHE	2.6
1	B	34	LEU	2.6
1	A	37	CYS	2.6
1	A	137	GLU	2.6
1	B	47	VAL	2.6
1	B	247	ASP	2.6
1	B	236	THR	2.6
1	A	23	SER	2.6
1	A	66	LEU	2.6
1	A	262	VAL	2.6
1	B	172	THR	2.6
1	B	184	CYS	2.6
1	A	305	ARG	2.5
1	B	239	VAL	2.5
1	A	195	ILE	2.5
1	A	259	PRO	2.5
1	A	164	TRP	2.5
1	A	171	VAL	2.5
1	B	84	TYR	2.5
1	B	197	PRO	2.5
1	A	182	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	106	LYS	2.5
1	A	307	LEU	2.5
1	B	199	GLN	2.5
1	A	33	ALA	2.5
1	B	150	ALA	2.5
1	A	290	ASN	2.4
1	B	260	LEU	2.4
1	A	36	PHE	2.4
1	B	82	ASN	2.4
1	A	18	LEU	2.4
1	B	15	ALA	2.4
1	A	196	PRO	2.4
1	B	297	TYR	2.4
1	B	12	LEU	2.4
1	A	219	GLY	2.4
1	B	4	VAL	2.4
1	B	258	LYS	2.4
1	B	213	TYR	2.4
1	B	300	ARG	2.4
1	A	227	ARG	2.4
1	B	11	LEU	2.4
1	A	79	ILE	2.3
1	A	46	PRO	2.3
1	B	147	LEU	2.3
1	A	47	VAL	2.3
1	B	182	VAL	2.3
1	B	195	ILE	2.3
1	A	208	TYR	2.3
1	B	309	GLN	2.3
1	B	171	VAL	2.3
1	B	37	CYS	2.3
1	A	272	LEU	2.3
1	B	33	ALA	2.3
1	A	72	ASP	2.3
1	A	145	SER	2.3
1	B	86	ASP	2.3
1	A	55	TRP	2.3
1	B	269	ILE	2.3
1	B	24	VAL	2.3
1	B	193	VAL	2.3
1	A	204	PRO	2.3
1	A	98	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	110	VAL	2.3
1	B	196	PRO	2.3
1	A	301[A]	TYR	2.2
1	B	76	ASP	2.2
1	B	264	VAL	2.2
1	B	289	VAL	2.2
1	B	259	PRO	2.2
1	B	187	SER	2.2
1	A	150	ALA	2.2
1	B	186	ILE	2.2
1	A	212	VAL	2.2
1	B	25	VAL	2.2
1	B	22	SER	2.2
1	A	76	ASP	2.2
1	A	246	PRO	2.2
1	B	278	HIS	2.2
1	A	194	LEU	2.2
1	A	297	TYR	2.2
1	B	5	GLU	2.2
1	A	120	ALA	2.2
1	A	300[A]	ARG	2.1
1	B	198	HIS	2.1
1	A	281	SER	2.1
1	B	178	PRO	2.1
1	B	143	ARG	2.1
1	B	254	TYR	2.1
1	B	60	LYS	2.1
1	B	31	PRO	2.1
1	A	93	GLY	2.1
1	B	188	GLY	2.1
1	B	306	MET	2.1
1	A	77	VAL	2.1
1	A	213	TYR	2.1
1	A	209	PRO	2.1
1	B	283	SER	2.1
1	A	306	MET	2.1
1	A	276	TRP	2.1
1	A	94	GLN	2.1
1	B	112	ARG	2.1
1	A	87	GLY	2.1
1	B	194	LEU	2.1
1	A	174	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	215	THR	2.1
1	A	271	TYR	2.1
1	B	126	LYS	2.1
1	B	301	TYR	2.1
1	B	49	ILE	2.1
1	B	164	TRP	2.1
1	B	200	LEU	2.0
1	A	249	ALA	2.0
1	A	295	LEU	2.0
1	A	102	GLU	2.0
1	B	160	ALA	2.0
1	A	291	PHE	2.0
1	B	174	MET	2.0
1	B	242	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	CSO	A	19	7/8	0.61	0.29	44,53,58,66	0
1	CSO	B	19	7/8	0.73	0.29	23,28,36,39	0

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, 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
5	EDO	A	507	4/4	0.17	0.37	69,83,87,87	0
6	ACT	A	510	4/4	0.58	0.30	78,82,93,93	0

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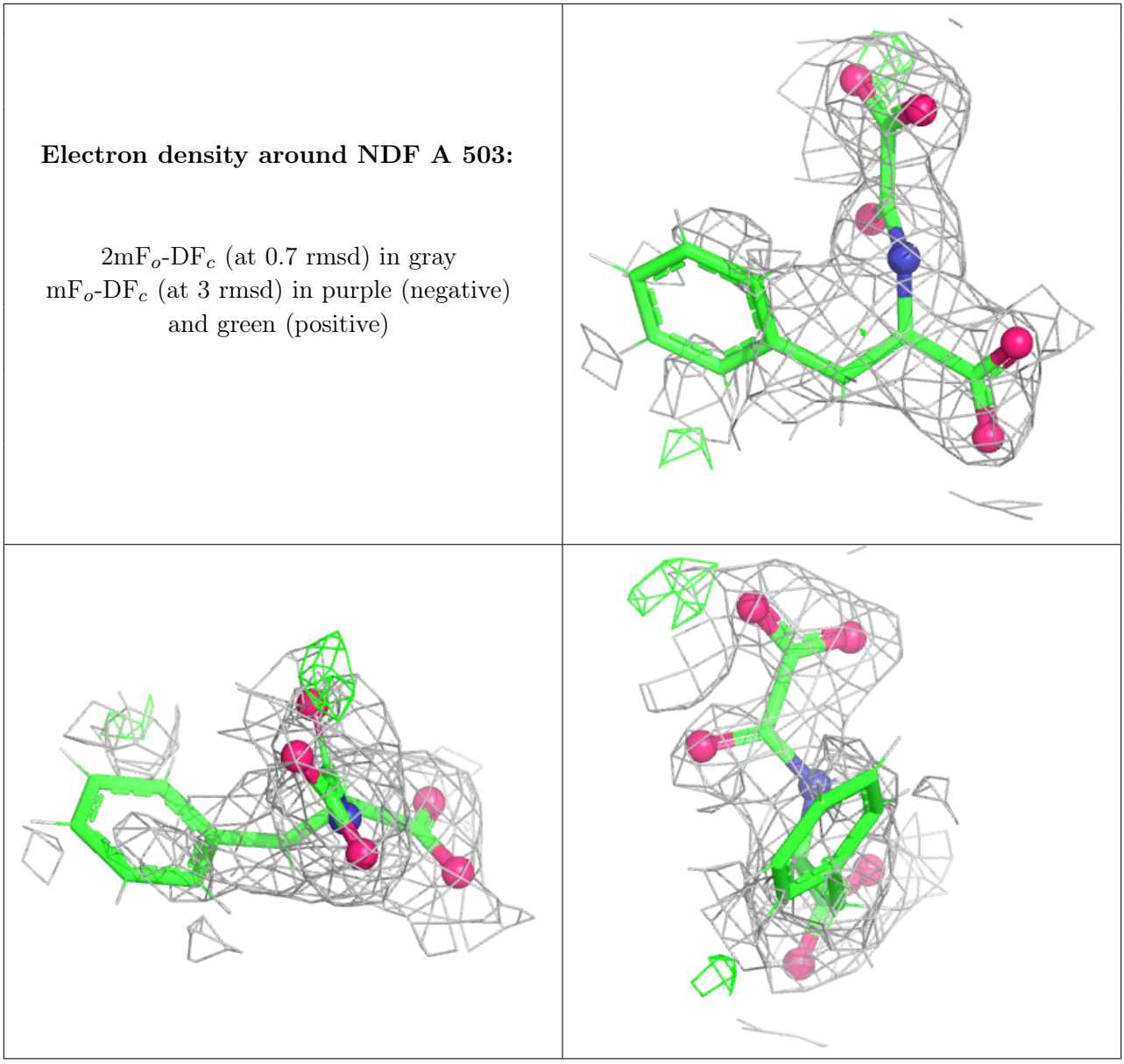
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	504	4/4	0.67	0.23	48,58,70,71	0
5	EDO	A	504	4/4	0.68	0.33	48,64,66,77	0
5	EDO	A	508	4/4	0.74	0.16	34,41,49,51	0
4	NDF	A	503	17/17	0.78	0.29	29,68,128,132	0
4	NDF	B	503	17/17	0.81	0.28	35,75,129,133	0
5	EDO	A	506	4/4	0.82	0.35	50,64,77,77	0
5	EDO	A	505	4/4	0.83	0.26	35,51,61,61	0
6	ACT	A	509	4/4	0.85	0.31	43,47,51,51	0
5	EDO	B	505	4/4	0.86	0.41	53,64,67,68	0
3	MG	B	502	1/1	0.91	0.43	47,47,47,47	0
2	MN	B	501	1/1	0.96	0.09	34,34,34,34	0
2	MN	A	501	1/1	0.97	0.13	24,24,24,24	0
3	MG	A	502	1/1	0.97	0.56	35,35,35,35	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.

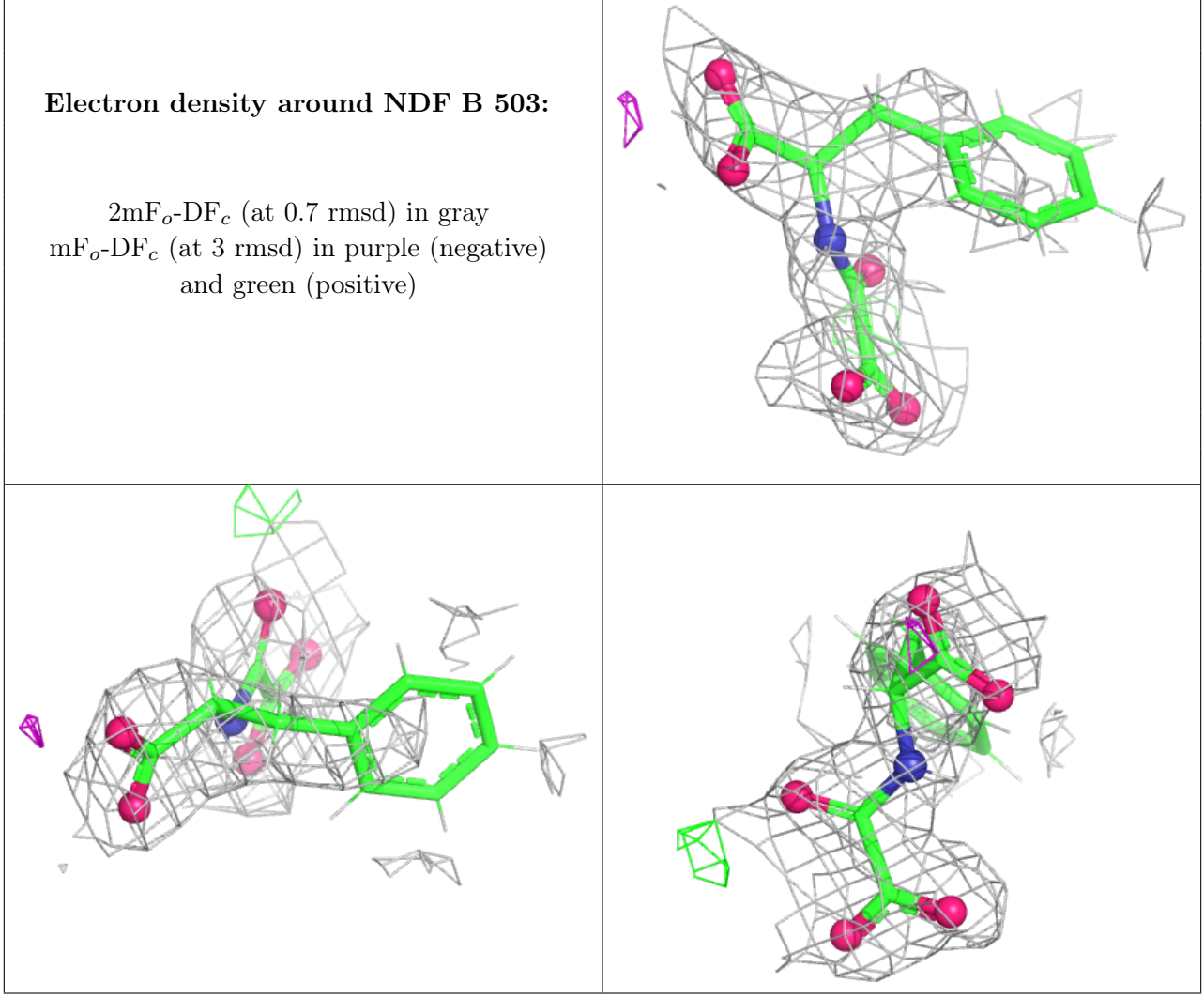
Electron density around NDF A 503:

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



Electron density around NDF B 503:

$2mF_o$-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

There are no such residues in this entry.