



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2023 – 10:43 AM JST

PDB ID : 8HLE
Title : Structure of DddY-DMSOP complex
Deposited on : 2022-11-30
Resolution : 1.91 Å (reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

<https://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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
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)	:	2.33

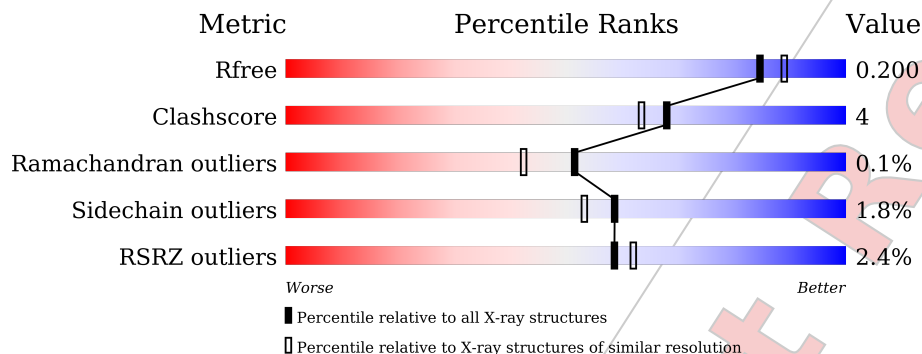
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	407	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 86% 6% • 7%</p>
1	B	407	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 88% 5% 7%</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7308 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 DMSF lyase DddY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	3069	1943	524	585	17	0	1	0
1	B	380	3069	1943	524	585	17	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

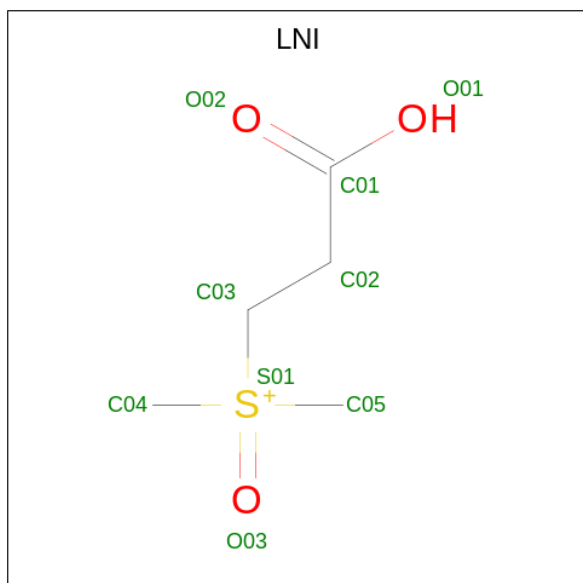
Chain	Residue	Modelled	Actual	Comment	Reference
A	260	ALA	TYR	engineered mutation	UNP N8X9V6
A	402	HIS	-	expression tag	UNP N8X9V6
A	403	HIS	-	expression tag	UNP N8X9V6
A	404	HIS	-	expression tag	UNP N8X9V6
A	405	HIS	-	expression tag	UNP N8X9V6
A	406	HIS	-	expression tag	UNP N8X9V6
A	407	HIS	-	expression tag	UNP N8X9V6
B	260	ALA	TYR	engineered mutation	UNP N8X9V6
B	402	HIS	-	expression tag	UNP N8X9V6
B	403	HIS	-	expression tag	UNP N8X9V6
B	404	HIS	-	expression tag	UNP N8X9V6
B	405	HIS	-	expression tag	UNP N8X9V6
B	406	HIS	-	expression tag	UNP N8X9V6
B	407	HIS	-	expression tag	UNP N8X9V6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 3-[dimethyl(oxidanyl)-sulfanyl]propanoic acid (three-letter code: LNI)

(formula: C₅H₁₁O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	9	5	3	1	0	0
3	B	1	9	5	3	1	0	0

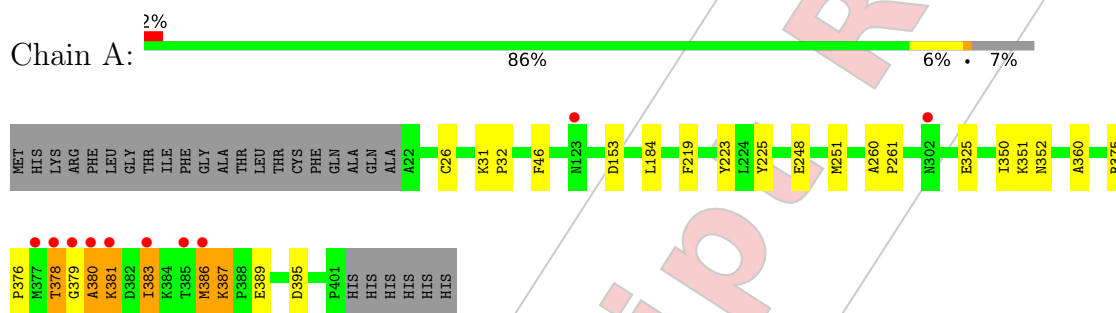
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	561	561	561	0	0
4	B	589	589	589	0	0

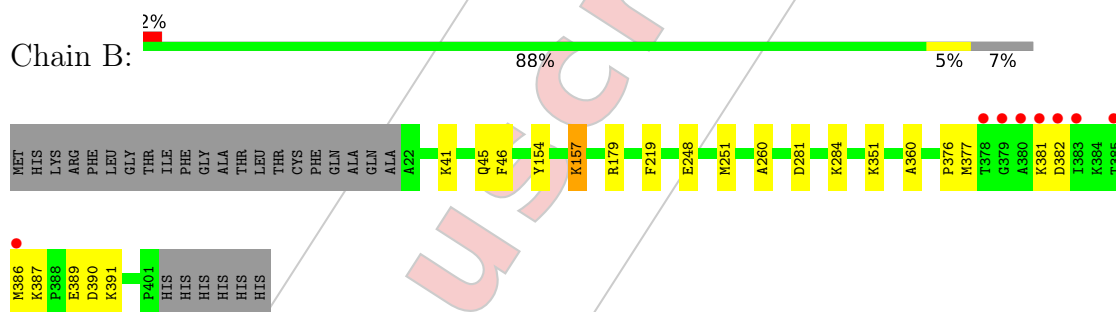
3 Residue-property plots [\(i\)](#)

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: DMSP lyase DddY



- Molecule 1: DMSP lyase DddY



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 73.39Å 87.37Å 90.00° 91.14° 90.00°	Depositor
Resolution (Å)	36.72 – 1.91 48.99 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.72-1.91) 97.3 (48.99-1.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.63 (at 1.91Å)	Xtrriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.160 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	3197 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtrriage
Anisotropy	0.450	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7308	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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 centric 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: LNI, ZN

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	0.38	0/3153	0.55	0/4280
1	B	0.37	0/3153	0.55	0/4280
All	All	0.38	0/6306	0.55	0/8560

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 [i](#)

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	3069	0	2958	26	0
1	B	3069	0	2958	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	9	0	0	2	0
3	B	9	0	0	0	0
4	A	561	0	0	3	0
4	B	589	0	0	3	0
All	All	7308	0	5916	46	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 4.

All (46) 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:376:PRO:HB3	1:B:381:LYS:CG	2.12	0.80
1:B:376:PRO:HB3	1:B:381:LYS:HG2	1.65	0.77
1:A:350:ILE:C	1:A:351:LYS:HD3	2.05	0.76
1:B:381:LYS:NZ	1:B:390:ASP:OD1	2.20	0.75
1:B:387:LYS:HG3	1:B:389:GLU:HG2	1.70	0.73
1:A:350:ILE:O	1:A:351:LYS:HD3	1.91	0.70
1:A:387:LYS:HG3	1:A:389:GLU:HG2	1.79	0.65
1:A:261:PRO:HB3	1:A:386:MET:SD	2.37	0.64
1:B:377:MET:HE2	1:B:391:LYS:HD3	1.85	0.58
1:B:387:LYS:HG2	1:B:390:ASP:OD2	2.03	0.57
1:A:381:LYS:H	1:A:381:LYS:CD	2.18	0.57
1:A:381:LYS:H	1:A:381:LYS:HD2	1.70	0.56
1:B:387:LYS:NZ	1:B:389:GLU:OE2	2.34	0.55
1:A:376:PRO:HD3	1:A:386:MET:CE	2.37	0.55
1:B:377:MET:CE	1:B:391:LYS:HD3	2.38	0.54
1:B:376:PRO:HG3	1:B:386:MET:SD	2.49	0.53
1:A:376:PRO:HD3	1:A:386:MET:HE3	1.91	0.52
1:A:379:GLY:HA3	1:A:381:LYS:HD3	1.92	0.52
1:B:157:LYS:HE2	4:B:1036:HOH:O	2.09	0.51
1:A:379:GLY:CA	1:A:381:LYS:HD3	2.41	0.51
1:A:379:GLY:C	1:A:381:LYS:HD3	2.32	0.49
1:A:26:CYS:HB2	4:A:1061:HOH:O	2.13	0.48
1:A:184:LEU:HD22	1:A:325:GLU:OE2	2.16	0.45
1:A:31:LYS:HD2	1:A:31:LYS:HA	1.53	0.45
1:B:41:LYS:O	1:B:45:GLN:HG2	2.15	0.45
1:A:225:TYR:CD2	3:A:502:LNI:C04	3.00	0.44
1:A:223:TYR:OH	3:A:502:LNI:C05	2.64	0.44
1:A:352:ASN:OD1	4:A:601:HOH:O	2.21	0.44
1:B:154:TYR:O	1:B:157:LYS:HE3	2.18	0.43
1:A:376:PRO:HB2	1:A:379:GLY:H	1.83	0.43
1:B:281:ASP:OD2	4:B:601:HOH:O	2.21	0.43
1:A:219:PHE:CE1	1:A:260:ALA:HB2	2.53	0.43
1:B:376:PRO:HB3	1:B:381:LYS:CB	2.48	0.43
1:A:375:ARG:NH1	1:A:395:ASP:OD2	2.52	0.43
1:B:376:PRO:HB3	1:B:381:LYS:HB3	2.01	0.42
1:A:31:LYS:HE3	1:A:32:PRO:HD2	2.00	0.42
1:B:157:LYS:HE3	1:B:157:LYS:HB3	1.67	0.42
1:B:351:LYS:HA	1:B:351:LYS:HD3	1.80	0.41
1:A:380:ALA:O	1:A:383:ILE:HB	2.20	0.41
1:A:378:THR:O	1:A:381:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:OD1	4:A:602:HOH:O	2.22	0.41
1:A:350:ILE:C	1:A:351:LYS:CD	2.85	0.41
1:A:248:GLU:O	1:A:360:ALA:HA	2.21	0.40
1:B:219:PHE:CE1	1:B:260:ALA:HB2	2.56	0.40
1:B:248:GLU:O	1:B:360:ALA:HA	2.21	0.40
1:B:284:LYS:NZ	4:B:629:HOH:O	2.49	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	379/407 (93%)	370 (98%)	8 (2%)	1 (0%)	41	31
1	B	379/407 (93%)	370 (98%)	9 (2%)	0	100	100
All	All	758/814 (93%)	740 (98%)	17 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ALA

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	333/354 (94%)	326 (98%)	7 (2%)	53	46
1	B	333/354 (94%)	328 (98%)	5 (2%)	65	61
All	All	666/708 (94%)	654 (98%)	12 (2%)	59	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	251	MET
1	A	378	THR
1	A	381	LYS
1	A	383	ILE
1	A	386	MET
1	A	387	LYS
1	B	46	PHE
1	B	157	LYS
1	B	179	ARG
1	B	251	MET
1	B	382	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](#)

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	LNI	A	502	2	6,8,8	1.44	0	9,11,11	2.30	3 (33%)
3	LNI	B	502	2	6,8,8	1.57	1 (16%)	9,11,11	1.91	4 (44%)

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
3	LNI	A	502	2	-	3/4/6/6	-
3	LNI	B	502	2	-	4/4/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	LNI	O03-S01	2.08	1.47	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	LNI	C05-S01-C04	4.57	111.11	105.92
3	A	502	LNI	C03-C02-C01	-3.31	108.57	113.14
3	B	502	LNI	C05-S01-C04	3.14	109.48	105.92
3	B	502	LNI	C03-C02-C01	-2.65	109.48	113.14
3	A	502	LNI	O03-S01-C05	-2.56	108.97	112.15
3	B	502	LNI	O03-S01-C05	-2.17	109.46	112.15
3	B	502	LNI	O03-S01-C04	-2.16	109.48	112.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	LNI	C02-C03-S01-O03

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Mol	Chain	Res	Type	Atoms
3	A	502	LNI	O01-C01-C02-C03
3	A	502	LNI	O02-C01-C02-C03
3	B	502	LNI	O02-C01-C02-C03
3	B	502	LNI	C01-C02-C03-S01
3	B	502	LNI	C02-C03-S01-O03
3	B	502	LNI	O01-C01-C02-C03

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	LNI	2	0

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 [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	A	380/407 (93%)	-0.03	10 (2%) 56 59	9, 17, 34, 64	0
1	B	380/407 (93%)	-0.11	8 (2%) 63 66	9, 15, 32, 59	0
All	All	760/814 (93%)	-0.07	18 (2%) 59 62	9, 16, 33, 64	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	ALA	8.5
1	B	380	ALA	8.0
1	B	379	GLY	6.4
1	B	381	LYS	6.0
1	B	378	THR	5.5
1	B	383	ILE	4.6
1	A	379	GLY	4.5
1	A	381	LYS	4.5
1	A	386	MET	4.5
1	B	382	ASP	4.2
1	A	383	ILE	3.7
1	A	378	THR	3.5
1	B	385	THR	2.9
1	A	377	MET	2.6
1	A	302	ASN	2.5
1	B	386	MET	2.3
1	A	123	ASN	2.1
1	A	385	THR	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LNI	A	502	9/9	0.88	0.22	16,23,36,46	0
3	LNI	B	502	9/9	0.91	0.18	12,23,30,49	0
2	ZN	A	501	1/1	1.00	0.07	14,14,14,14	0
2	ZN	B	501	1/1	1.00	0.06	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.