Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 11:07 am BST

PDB ID	:	1DP2
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN RHODANESE AND LIPOATE
Authors	:	Zanotti, G.; Cianci, M.
Deposited on	:	1999-12-23
Resolution	:	2.01 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 (i) symbol.

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

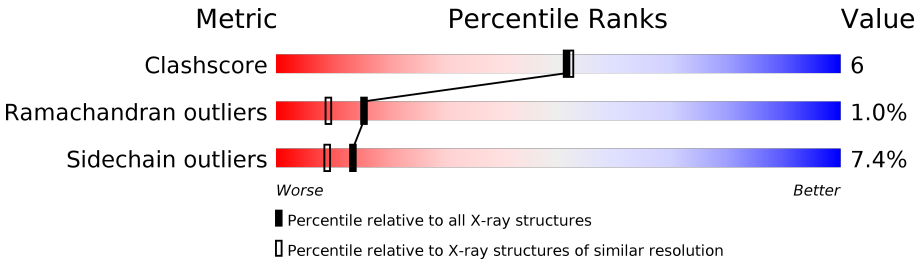
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.01 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	293	81% 16% •

2 Entry composition (i)

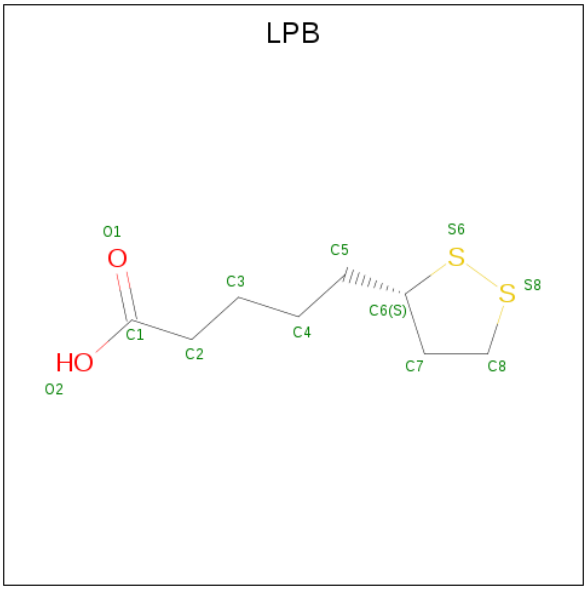
There are 3 unique types of molecules in this entry. The entry contains 2451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RHODANESE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2327	1486	405	426	10	0	0	0

- Molecule 2 is 5-[(3S)-1,2-dithiolan-3-yl]pentanoic acid (three-letter code: LPB) (formula: $C_8H_{14}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	12	8	2	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	112	112	112	0	0

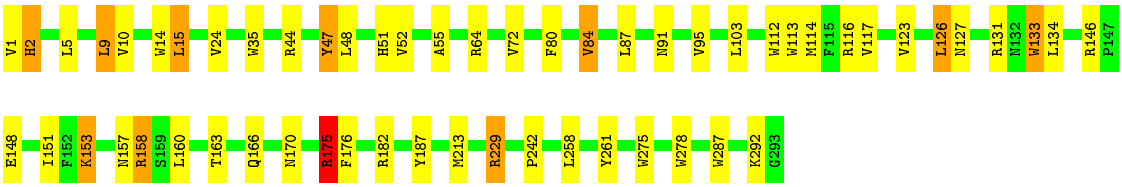
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

- Molecule 1: RHODANESE

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.36Å 49.31Å 41.68Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	55.00 – 2.01	Depositor
% Data completeness (in resolution range)	(Not available) (55.00-2.01)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.170 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2451	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

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: LPB, CSS

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	0.78	0/2386	1.41	38/3235 (1.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	A	35	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	A	287	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	14	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	275	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A	278	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	113	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	133	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	35	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	14	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	287	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	275	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	A	112	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	A	133	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	A	229	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	112	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	A	84	VAL	N-CA-CB	-6.34	97.56	111.50
1	A	131	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	187	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	113	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	35	TRP	CG-CD1-NE1	-6.08	104.02	110.10
1	A	182	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	287	TRP	CG-CD1-NE1	-5.99	104.11	110.10
1	A	14	TRP	CG-CD1-NE1	-5.94	104.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	275	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	A	175	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	14	TRP	CB-CG-CD1	-5.67	119.63	127.00
1	A	14	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	A	275	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	A	146	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	64	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	113	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	A	47	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	35	TRP	CB-CG-CD1	-5.19	120.26	127.00
1	A	275	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	A	84	VAL	CB-CA-C	5.14	121.16	111.40
1	A	261	TYR	CB-CG-CD2	-5.12	117.93	121.00

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	2327	0	2262	26	0
2	A	12	0	13	0	0
3	A	112	0	0	1	0
All	All	2451	0	2275	26	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 6.

All (26) 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:170:ASN:HD21	1:A:176:PHE:H	1.15	0.91
1:A:91:ASN:HD21	1:A:153:LYS:H	1.31	0.77
1:A:1:VAL:HB	1:A:116:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HG2	1:A:175:ARG:HH21	1.65	0.61
1:A:170:ASN:ND2	1:A:176:PHE:H	1.94	0.57
1:A:163:THR:H	1:A:166:GLN:HE21	1.56	0.52
1:A:44:ARG:NH2	1:A:48:LEU:HD11	2.25	0.52
1:A:80:PHE:O	1:A:84:VAL:HB	2.10	0.51
1:A:158:ARG:NH2	1:A:166:GLN:HE22	2.09	0.51
1:A:9:LEU:HG	1:A:127:ASN:HB2	1.93	0.51
1:A:1:VAL:HG11	3:A:906:HOH:O	2.13	0.49
1:A:170:ASN:HD22	1:A:175:ARG:HH21	1.62	0.48
1:A:91:ASN:HD21	1:A:153:LYS:N	2.08	0.47
1:A:52:VAL:HG22	1:A:55:ALA:HB2	1.97	0.47
1:A:158:ARG:HH22	1:A:166:GLN:NE2	2.12	0.46
1:A:114:MET:HA	1:A:117:VAL:HG12	1.97	0.46
1:A:47:TYR:O	1:A:51:HIS:HD2	1.98	0.46
1:A:95:VAL:O	1:A:123:VAL:HA	2.18	0.43
1:A:170:ASN:HD21	1:A:176:PHE:N	1.98	0.43
1:A:10:VAL:HG12	1:A:126:LEU:HD23	2.02	0.42
1:A:175:ARG:HG2	1:A:175:ARG:NH2	2.33	0.41
1:A:170:ASN:HD22	1:A:175:ARG:NH2	2.18	0.41
1:A:176:PHE:HA	1:A:242:PRO:HB2	2.02	0.41
1:A:15:LEU:HB3	1:A:133:TRP:HZ3	1.85	0.41
1:A:158:ARG:NH2	1:A:166:GLN:NE2	2.69	0.40
1:A:1:VAL:O	1:A:2:HIS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	290/293 (99%)	283 (98%)	4 (1%)	3 (1%)	15 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	72	VAL
1	A	292	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	244/244 (100%)	226 (93%)	18 (7%)	13 9

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LEU
1	A	15	LEU
1	A	24	VAL
1	A	87	LEU
1	A	103	LEU
1	A	126	LEU
1	A	134	LEU
1	A	148	GLU
1	A	151	ILE
1	A	153	LYS
1	A	157	ASN
1	A	158	ARG
1	A	160	LEU
1	A	175	ARG
1	A	213	MET
1	A	229	ARG
1	A	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	132	ASN
1	A	157	ASN
1	A	166	GLN
1	A	170	ASN
1	A	209	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSS	A	247	1	4,6,7	0.87	0	1,6,8	0.19	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
1	CSS	A	247	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	LPB	A	900	-	9,12,12	0.29	0	10,14,14	1.20	2 (20%)

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	LPB	A	900	-	-	5/5/14/14	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	LPB	C3-C4-C5	-2.14	106.04	113.62
2	A	900	LPB	C5-C6-S6	-2.12	106.10	113.63

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	LPB	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	900	LPB	C3-C4-C5-C6
2	A	900	LPB	C4-C5-C6-S6
2	A	900	LPB	C2-C3-C4-C5
2	A	900	LPB	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.