



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GPL
Title : RP2 LIPASE
Authors : Withers-Martinez, C.; Cambillau, C.
Deposited on : 1996-07-13
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

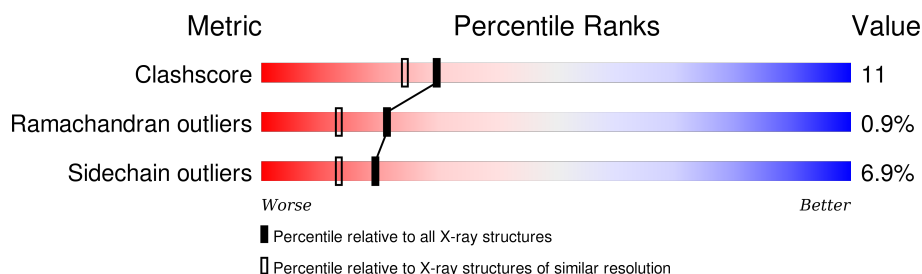
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	 76% 21% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4860 atoms, of which 1248 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 RP2 LIPASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	432	4118	2128	754	574	642	20	62	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	SER	THR	CONFLICT	UNP P16233
A	?	-	GLU	DELETION	UNP P16233
A	350	LYS	ASP	CONFLICT	UNP P16233
A	351	VAL	PRO	CONFLICT	UNP P16233
A	352	THR	SER	CONFLICT	UNP P16233
A	354	HIS	ASN	CONFLICT	UNP P16233
A	356	LEU	ASN	CONFLICT	UNP P16233
A	358	SER	ALA	CONFLICT	UNP P16233
A	360	PHE	LEU	CONFLICT	UNP P16233
A	362	ASN	LYS	CONFLICT	UNP P16233
A	363	LYS	ASN	CONFLICT	UNP P16233
A	367	LYS	ALA	CONFLICT	UNP P16233
A	370	GLU	GLN	CONFLICT	UNP P16233
A	371	ILE	VAL	CONFLICT	UNP P16233
A	380	SER	ALA	CONFLICT	UNP P16233
A	381	THR	SER	CONFLICT	UNP P16233
A	382	HIS	TYR	CONFLICT	UNP P16233
A	383	SER	THR	CONFLICT	UNP P16233
A	385	GLU	SER	CONFLICT	UNP P16233
A	386	PHE	ILE	CONFLICT	UNP P16233
A	388	SER	VAL	CONFLICT	UNP P16233
A	389	ASP	GLU	CONFLICT	UNP P16233
A	390	VAL	LEU	CONFLICT	UNP P16233
A	391	ASP	ASN	CONFLICT	UNP P16233
A	394	ASP	THR	CONFLICT	UNP P16233
A	395	LEU	ILE	CONFLICT	UNP P16233
A	397	MET	LYS	CONFLICT	UNP P16233

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Chain	Residue	Modelled	Actual	Comment	Reference
A	399	LYS	THR	CONFLICT	UNP P16233
A	401	ILE	LEU	CONFLICT	UNP P16233
A	403	TYR	LYS	CONFLICT	UNP P16233
A	404	ASN	ARG	CONFLICT	UNP P16233
A	406	ASN	SER	CONFLICT	UNP P16233
A	407	VAL	GLY	CONFLICT	UNP P16233
A	409	ASN	SER	CONFLICT	UNP P16233
A	410	PRO	VAL	CONFLICT	UNP P16233
A	411	THR	SER	CONFLICT	UNP P16233
A	412	LEU	LYS	CONFLICT	UNP P16233
A	414	ARG	LYS	CONFLICT	UNP P16233
A	415	VAL	MET	CONFLICT	UNP P16233
A	419	LYS	ARG	CONFLICT	UNP P16233
A	421	ILE	THR	CONFLICT	UNP P16233
A	?	-	GLN	DELETION	UNP P16233
A	423	GLU	SER	CONFLICT	UNP P16233
A	424	THR	GLY	CONFLICT	UNP P16233
A	425	ASN	LYS	CONFLICT	UNP P16233
A	426	VAL	ASP	CONFLICT	UNP P16233
A	428	LYS	THR	CONFLICT	UNP P16233
A	429	GLN	LYS	CONFLICT	UNP P16233
A	430	PHE	TYR	CONFLICT	UNP P16233
A	435	PRO	SER	CONFLICT	UNP P16233
A	436	GLU	ASP	CONFLICT	UNP P16233
A	437	THR	ILE	CONFLICT	UNP P16233
A	439	ARG	GLN	CONFLICT	UNP P16233
A	441	GLU	ASN	CONFLICT	UNP P16233
A	443	LEU	GLU	CONFLICT	UNP P16233
A	444	LEU	GLN	CONFLICT	UNP P16233
A	447	THR	SER	CONFLICT	UNP P16233

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is water.

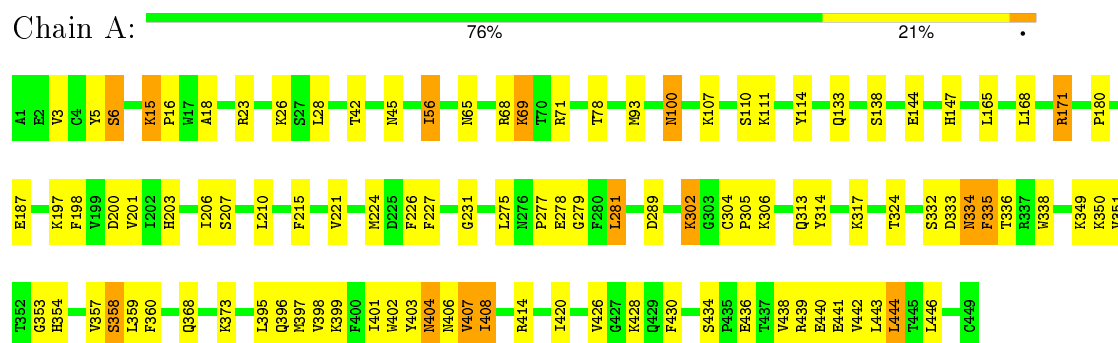
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	247	Total H O 741 494 247	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: RP2 LIPASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	62.00 Å 55.90 Å 144.00 Å 90.00° 93.20° 90.00°	Depositor
Resolution (Å)	6.00 – 2.01	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.01)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4860	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: CA

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	0.59	0/3449	0.77	2/4677 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	171	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	100	ASN	N-CA-C	-5.21	96.92	111.00

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	3364	754	3253	73	0
2	A	1	0	0	0	0
3	A	247	494	0	0	0
All	All	3612	1248	3253	73	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 11.

All (73) 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:279:GLY:HA3	1:A:336:THR:HG23	1.47	0.96
1:A:354:HIS:HB3	1:A:373:LYS:HG3	1.49	0.91
1:A:279:GLY:CA	1:A:336:THR:HG23	2.04	0.87
1:A:65:ASN:H	1:A:100:ASN:HD21	1.31	0.79
1:A:404:ASN:ND2	1:A:440:GLU:HB2	2.00	0.77
1:A:277:PRO:HB2	1:A:306:LYS:HD2	1.65	0.77
1:A:279:GLY:HA3	1:A:336:THR:CG2	2.16	0.73
1:A:404:ASN:H	1:A:404:ASN:ND2	1.84	0.72
1:A:353:GLY:HA3	1:A:403:TYR:O	1.90	0.71
1:A:398:VAL:HG11	1:A:420:ILE:HG21	1.73	0.69
1:A:201:VAL:HG21	1:A:221:VAL:HG23	1.74	0.69
1:A:404:ASN:OD1	1:A:408:ILE:HG12	1.93	0.68
1:A:354:HIS:HB3	1:A:373:LYS:CG	2.25	0.66
1:A:336:THR:HG22	1:A:338:TRP:CH2	2.32	0.64
1:A:15:LYS:HB3	1:A:15:LYS:NZ	2.12	0.64
1:A:404:ASN:ND2	1:A:440:GLU:CB	2.61	0.64
1:A:69:LYS:HE2	1:A:147:HIS:HB2	1.80	0.63
1:A:56:ILE:HD12	1:A:138:SER:HB3	1.81	0.62
1:A:147:HIS:CD2	1:A:171:ARG:HG2	2.33	0.62
1:A:434:SER:HB2	1:A:446:LEU:HG	1.81	0.62
1:A:403:TYR:CD2	1:A:441:GLU:HG2	2.35	0.62
1:A:351:VAL:HG21	1:A:402:TRP:CZ3	2.34	0.61
1:A:401:ILE:HB	1:A:443:LEU:HD23	1.81	0.61
1:A:65:ASN:H	1:A:100:ASN:ND2	1.97	0.61
1:A:302:LYS:HA	1:A:302:LYS:HE2	1.83	0.60
1:A:404:ASN:N	1:A:404:ASN:ND2	2.51	0.59
1:A:171:ARG:HD3	1:A:198:PHE:CD2	2.40	0.57
1:A:336:THR:CG2	1:A:338:TRP:CH2	2.88	0.56
1:A:439:ARG:HG2	1:A:440:GLU:OE1	2.07	0.54
1:A:224:MET:HG3	1:A:226:PHE:HE1	1.72	0.54
1:A:404:ASN:HD22	1:A:440:GLU:HB2	1.73	0.53
1:A:360:PHE:HB2	1:A:397:MET:HG2	1.90	0.53
1:A:203:HIS:HB3	1:A:206:ILE:CG2	2.39	0.53
1:A:336:THR:HG22	1:A:338:TRP:CZ3	2.45	0.52
1:A:403:TYR:CE2	1:A:441:GLU:HG2	2.45	0.51
1:A:358:SER:OG	1:A:368:GLN:HG2	2.11	0.51
1:A:107:LYS:HA	1:A:110:SER:OG	2.11	0.51
1:A:407:VAL:HG23	1:A:407:VAL:O	2.12	0.50
1:A:434:SER:OG	1:A:444:LEU:HD21	2.12	0.50
1:A:18:ALA:HB1	1:A:26:LYS:HA	1.93	0.50
1:A:171:ARG:HD2	1:A:200:ASP:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:HD3	1:A:414:ARG:H	1.77	0.49
1:A:305:PRO:HB3	1:A:314:TYR:CG	2.48	0.49
1:A:15:LYS:HB3	1:A:15:LYS:HZ2	1.78	0.49
1:A:438:VAL:HB	1:A:442:VAL:HB	1.95	0.48
1:A:78:THR:O	1:A:111:LYS:HE2	2.12	0.48
1:A:357:VAL:HA	1:A:399:LYS:O	2.13	0.48
1:A:224:MET:HE1	1:A:317:LYS:CB	2.43	0.48
1:A:357:VAL:HG13	1:A:398:VAL:HG13	1.96	0.47
1:A:168:LEU:HA	1:A:197:LYS:HE3	1.95	0.47
1:A:171:ARG:HD3	1:A:198:PHE:HD2	1.77	0.47
1:A:354:HIS:CD2	1:A:403:TYR:HB2	2.49	0.47
1:A:281:LEU:HG	1:A:304:CYS:HB2	1.96	0.47
1:A:201:VAL:HG21	1:A:221:VAL:CG2	2.42	0.47
1:A:227:PHE:CE1	1:A:324:THR:HG23	2.51	0.46
1:A:359:LEU:HB3	1:A:395:LEU:HD21	1.97	0.45
1:A:224:MET:HG3	1:A:226:PHE:CE1	2.52	0.45
1:A:65:ASN:HB3	1:A:68:ARG:HD2	1.99	0.45
1:A:408:ILE:HA	1:A:408:ILE:HD13	1.82	0.45
1:A:3:VAL:HG13	1:A:28:LEU:HD13	1.98	0.44
1:A:359:LEU:HD23	1:A:398:VAL:HG22	1.98	0.43
1:A:71:ARG:HD2	1:A:93:MET:SD	2.57	0.43
1:A:114:TYR:CE2	1:A:180:PRO:HB2	2.53	0.43
1:A:16:PRO:O	1:A:23:ARG:HD3	2.18	0.43
1:A:439:ARG:HG2	1:A:440:GLU:H	1.84	0.42
1:A:333:ASP:O	1:A:335:PHE:N	2.51	0.42
1:A:354:HIS:NE2	1:A:403:TYR:HB2	2.35	0.42
1:A:354:HIS:CB	1:A:373:LYS:HG3	2.36	0.42
1:A:42:THR:OG1	1:A:45:ASN:ND2	2.52	0.42
1:A:215:PHE:N	1:A:215:PHE:CD1	2.87	0.42
1:A:428:LYS:HD2	1:A:430:PHE:CZ	2.56	0.41
1:A:5:TYR:O	1:A:6:SER:C	2.59	0.41
1:A:206:ILE:HG12	1:A:231:GLY:O	2.21	0.40

There are no symmetry-related clashes.

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	A	430/432 (100%)	404 (94%)	22 (5%)	4 (1%)	21 13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	334	ASN
1	A	335	PHE
1	A	407	VAL

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	A	375/375 (100%)	349 (93%)	26 (7%)	19 13

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	56	ILE
1	A	69	LYS
1	A	133	GLN
1	A	144	GLU
1	A	165	LEU
1	A	187	GLU
1	A	207	SER
1	A	210	LEU
1	A	275	LEU
1	A	278	GLU
1	A	281	LEU
1	A	289	ASP

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Mol	Chain	Res	Type
1	A	302	LYS
1	A	313	GLN
1	A	332	SER
1	A	334	ASN
1	A	350	LYS
1	A	358	SER
1	A	396	GLN
1	A	404	ASN
1	A	406	ASN
1	A	408	ILE
1	A	426	VAL
1	A	436	GLU
1	A	444	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	35	ASN
1	A	45	ASN
1	A	63	ASN
1	A	95	GLN
1	A	100	ASN
1	A	276	ASN
1	A	328	ASN
1	A	404	ASN
1	A	431	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

5.7 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.