



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 1LOX / pdb_00001lox
Title : RABBIT RETICULOCYTE 15-LIPOXYGENASE
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Deposited on : 1997-10-06
Resolution : 2.40 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 types of validation reports are described at

<http://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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

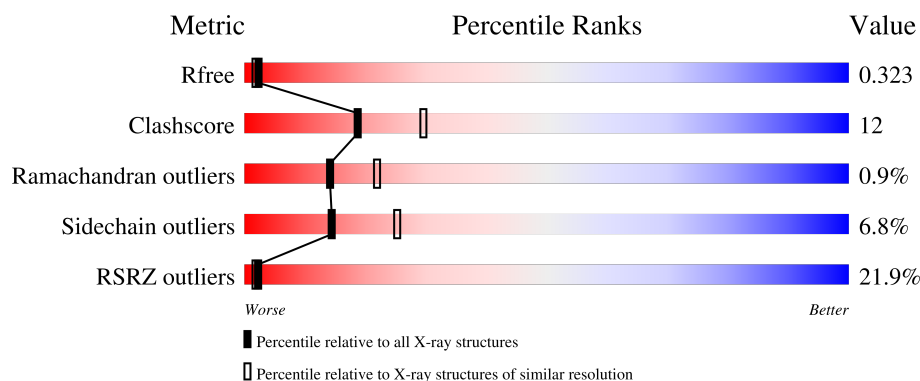
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	662	21% 71% 23% ...

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5223 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 15-LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	647	5109	3285	870	924	30	0	0	0

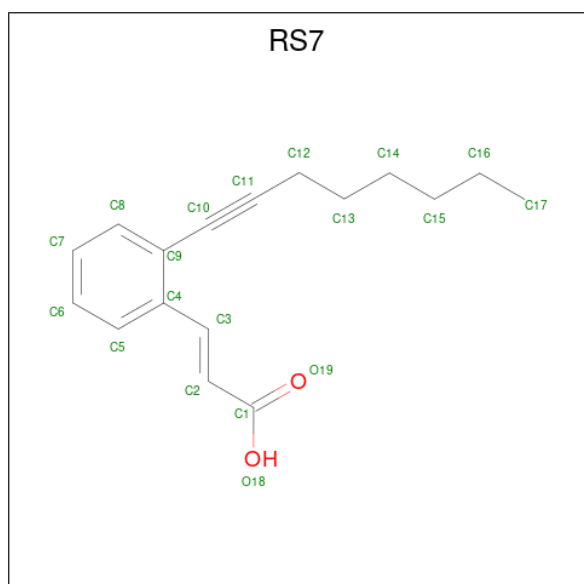
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	585	LYS	HIS	conflict	UNP P12530

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 3 is (2E)-3-(2-OCT-1-YN-1-YLPHENYL)ACRYLIC ACID (CCD ID: RS7) (formula: C₁₇H₂₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	17	2		

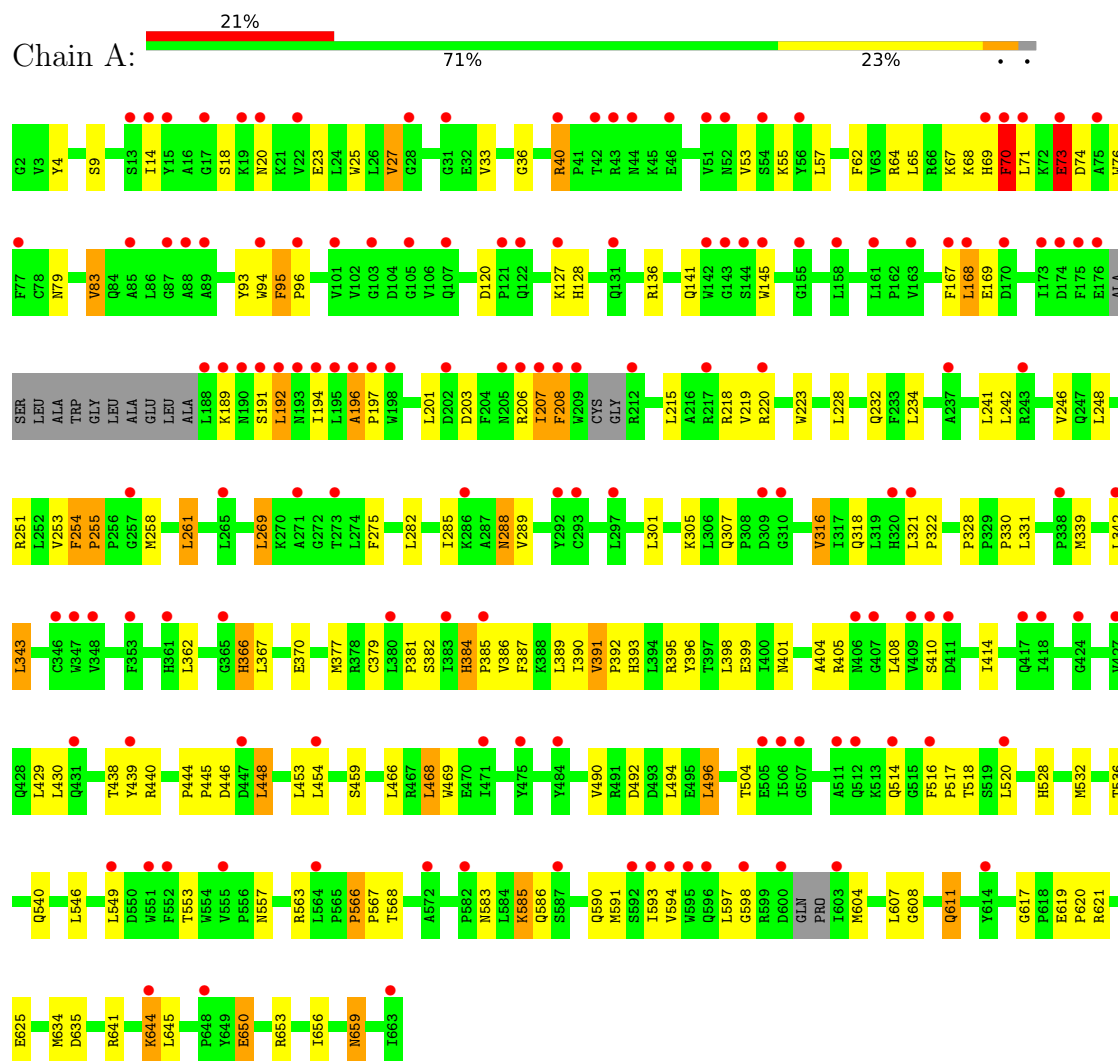
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		

3 Residue-property plots

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: 15-LIPOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	198.90Å 198.90Å 136.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.00 – 2.40 16.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (16.00-2.40) 97.4 (16.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.198 , 0.247 0.299 , 0.323	Depositor DCC
R_{free} test set	1967 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5223	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 acentric 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: FE2, RS7

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	0/5236	0.93	25/7111 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ILE	N-CA-C	8.00	120.06	111.58
1	A	189	LYS	N-CA-C	-7.83	102.74	111.82
1	A	40	ARG	CA-C-N	7.57	129.30	119.84
1	A	40	ARG	C-N-CA	7.57	129.30	119.84
1	A	246	VAL	N-CA-C	-7.31	103.83	111.58
1	A	95	PHE	CA-C-N	6.86	126.62	119.76
1	A	95	PHE	C-N-CA	6.86	126.62	119.76
1	A	196	ALA	CA-C-N	6.49	126.52	119.90
1	A	196	ALA	C-N-CA	6.49	126.52	119.90
1	A	254	PHE	N-CA-C	6.47	119.00	109.62
1	A	73	GLU	N-CA-C	6.31	119.14	111.82
1	A	192	LEU	N-CA-C	-6.20	104.45	111.14
1	A	384	HIS	CA-C-N	6.02	127.37	119.84
1	A	384	HIS	C-N-CA	6.02	127.37	119.84
1	A	504	THR	N-CA-C	5.96	117.47	110.97
1	A	546	LEU	N-CA-C	5.65	118.17	111.33
1	A	168	LEU	N-CA-C	-5.29	102.02	109.96
1	A	566	PRO	CA-C-N	5.28	125.22	119.78
1	A	566	PRO	C-N-CA	5.28	125.22	119.78
1	A	379	CYS	N-CA-C	5.27	120.37	113.88
1	A	120	ASP	CA-C-N	5.22	125.27	119.32
1	A	120	ASP	C-N-CA	5.22	125.27	119.32
1	A	255	PRO	N-CA-C	-5.18	104.38	110.70
1	A	366	HIS	N-CA-C	5.05	116.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	N-CA-C	5.03	117.84	110.30

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	5109	0	5021	121	0
2	A	1	0	0	0	0
3	A	19	0	19	6	0
4	A	94	0	0	3	0
All	All	5223	0	5040	121	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 12.

All (121) 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:362:LEU:HB2	3:A:841:RS7:H132	1.49	0.92
1:A:404:ALA:HB2	3:A:841:RS7:H173	1.65	0.79
1:A:343:LEU:HD13	1:A:567:PRO:HG2	1.66	0.77
1:A:232:GLN:HE22	1:A:557:ASN:HD21	1.32	0.77
1:A:25:TRP:HB2	1:A:64:ARG:HB2	1.66	0.75
1:A:391:VAL:HG23	1:A:392:PRO:HD3	1.70	0.74
1:A:387:PHE:O	1:A:391:VAL:HG22	1.90	0.70
1:A:608:GLY:H	1:A:659:ASN:ND2	1.90	0.70
1:A:33:VAL:HG13	1:A:57:LEU:HD21	1.74	0.68
1:A:253:VAL:HG23	1:A:328:PRO:HB3	1.75	0.68
1:A:255:PRO:HD2	1:A:258:MET:HG3	1.77	0.65
1:A:414:ILE:CG2	1:A:593:ILE:HD12	2.27	0.65
1:A:27:VAL:HG13	1:A:62:PHE:HB2	1.78	0.65
1:A:220:ARG:HG2	1:A:220:ARG:HH11	1.63	0.63
1:A:583:ASN:H	1:A:586:GLN:NE2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HE2	1:A:331:LEU:HD12	1.84	0.60
1:A:532:MET:O	1:A:536:THR:HG23	2.02	0.59
1:A:203:ASP:O	1:A:206:ARG:HG2	2.02	0.59
1:A:644:LYS:HE3	1:A:644:LYS:HA	1.83	0.59
1:A:362:LEU:CB	3:A:841:RS7:H132	2.30	0.58
1:A:414:ILE:HG21	1:A:593:ILE:HD12	1.85	0.58
1:A:611:GLN:HE21	1:A:611:GLN:HA	1.68	0.58
1:A:305:LYS:HE3	1:A:307:GLN:HE21	1.70	0.57
1:A:362:LEU:HB2	3:A:841:RS7:C13	2.30	0.56
1:A:207:ILE:CB	1:A:591:MET:HE3	2.34	0.56
1:A:27:VAL:CG1	1:A:62:PHE:HB2	2.35	0.56
1:A:288:ASN:ND2	1:A:289:VAL:H	2.03	0.56
1:A:384:HIS:CD2	1:A:385:PRO:HD2	2.41	0.55
1:A:583:ASN:H	1:A:586:GLN:HE21	1.54	0.55
1:A:384:HIS:HD2	1:A:386:VAL:H	1.55	0.55
1:A:223:TRP:HA	1:A:228:LEU:HD23	1.89	0.54
1:A:553:THR:O	1:A:591:MET:SD	2.66	0.54
1:A:563:ARG:HD3	1:A:586:GLN:HE22	1.74	0.53
1:A:253:VAL:CG2	1:A:328:PRO:HB3	2.39	0.53
1:A:381:PRO:HD2	1:A:384:HIS:HB2	1.91	0.53
1:A:536:THR:HG22	4:A:898:HOH:O	2.09	0.53
1:A:23:GLU:HA	1:A:36:GLY:O	2.09	0.52
1:A:282:LEU:HA	1:A:285:ILE:HD12	1.91	0.52
1:A:414:ILE:HG22	1:A:593:ILE:HD12	1.92	0.52
1:A:650:GLU:O	1:A:656:ILE:HD11	2.09	0.52
1:A:94:TRP:CD1	1:A:96:PRO:HG3	2.45	0.52
1:A:196:ALA:HB1	1:A:206:ARG:HH12	1.75	0.52
1:A:343:LEU:HD13	1:A:567:PRO:CG	2.38	0.52
1:A:20:ASN:HB3	1:A:68:LYS:O	2.10	0.51
1:A:127:LYS:HG3	1:A:128:HIS:N	2.25	0.51
1:A:619:GLU:HB2	1:A:620:PRO:HD3	1.93	0.51
1:A:288:ASN:HD22	1:A:289:VAL:H	1.59	0.51
1:A:440:ARG:NH1	1:A:446:ASP:HB3	2.26	0.51
1:A:496:LEU:CD1	1:A:520:LEU:HD12	2.40	0.51
1:A:597:LEU:HB3	3:A:841:RS7:C1	2.40	0.50
1:A:33:VAL:HG21	1:A:53:VAL:HG11	1.93	0.50
1:A:20:ASN:ND2	1:A:73:GLU:O	2.45	0.50
1:A:14:ILE:HD12	1:A:169:GLU:HG3	1.93	0.50
1:A:444:PRO:HD2	1:A:469:TRP:CE3	2.46	0.50
1:A:23:GLU:O	1:A:65:LEU:HA	2.12	0.49
1:A:219:VAL:O	1:A:223:TRP:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:HB3	1:A:79:ASN:HB2	1.95	0.49
1:A:196:ALA:HB1	1:A:206:ARG:NH1	2.28	0.49
1:A:70:PHE:HD1	1:A:71:LEU:H	1.61	0.49
1:A:167:PHE:CE1	1:A:399:GLU:HG2	2.47	0.48
1:A:440:ARG:HG3	4:A:880:HOH:O	2.13	0.48
1:A:496:LEU:HD11	1:A:520:LEU:HD12	1.95	0.48
1:A:248:LEU:HD13	1:A:269:LEU:HD12	1.95	0.48
1:A:261:LEU:HD21	1:A:316:VAL:HG22	1.95	0.48
1:A:384:HIS:CD2	1:A:386:VAL:H	2.32	0.48
1:A:261:LEU:HD11	1:A:316:VAL:HG21	1.95	0.48
1:A:191:SER:O	1:A:194:ILE:HB	2.13	0.48
1:A:40:ARG:NH2	1:A:70:PHE:HE2	2.12	0.47
1:A:285:ILE:HD13	1:A:429:LEU:HB2	1.95	0.47
1:A:607:LEU:HD12	1:A:659:ASN:HD22	1.80	0.47
1:A:136:ARG:HD2	1:A:377:MET:O	2.16	0.46
1:A:593:ILE:HG23	1:A:594:VAL:N	2.30	0.46
1:A:145:TRP:CG	1:A:405:ARG:HD2	2.50	0.46
1:A:536:THR:HA	1:A:540:GLN:HB3	1.97	0.46
1:A:590:GLN:O	1:A:593:ILE:HG22	2.16	0.46
1:A:494:LEU:H	1:A:494:LEU:HD22	1.79	0.46
1:A:136:ARG:HB3	1:A:377:MET:O	2.16	0.46
1:A:439:TYR:OH	1:A:528:HIS:HD2	1.99	0.46
1:A:251:ARG:HE	1:A:318:GLN:NE2	2.14	0.45
1:A:18:SER:HB2	1:A:76:TRP:HB2	1.99	0.45
1:A:251:ARG:HE	1:A:318:GLN:HE22	1.65	0.45
1:A:370:GLU:HG3	1:A:398:LEU:CD2	2.46	0.45
1:A:208:PHE:HE2	1:A:591:MET:HG3	1.81	0.44
1:A:220:ARG:HG2	1:A:220:ARG:NH1	2.29	0.44
1:A:516:PHE:HA	1:A:517:PRO:HD3	1.83	0.44
1:A:330:PRO:HG2	1:A:568:THR:O	2.17	0.44
1:A:607:LEU:HA	1:A:659:ASN:HD22	1.82	0.44
1:A:566:PRO:HA	1:A:567:PRO:HD3	1.84	0.44
1:A:366:HIS:HD1	1:A:401:ASN:HD21	1.65	0.43
1:A:251:ARG:O	1:A:322:PRO:HG2	2.18	0.43
1:A:387:PHE:CZ	1:A:391:VAL:HG11	2.53	0.43
1:A:382:SER:HA	1:A:387:PHE:CD1	2.54	0.43
1:A:254:PHE:HA	1:A:255:PRO:HD3	1.89	0.42
1:A:611:GLN:HE21	1:A:611:GLN:CA	2.32	0.42
1:A:448:LEU:HD12	1:A:453:LEU:HB2	2.01	0.42
1:A:444:PRO:HB2	1:A:445:PRO:HD3	2.01	0.42
1:A:232:GLN:HE22	1:A:557:ASN:ND2	2.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LEU:HD22	3:A:841:RS7:C3	2.50	0.42
1:A:261:LEU:HD21	1:A:316:VAL:CG2	2.49	0.42
1:A:384:HIS:HD2	1:A:386:VAL:N	2.16	0.42
1:A:468:LEU:HB2	1:A:634:MET:HE1	2.01	0.42
1:A:621:ARG:O	1:A:625:GLU:HG2	2.19	0.42
1:A:4:TYR:HB3	1:A:83:VAL:HG23	2.02	0.42
1:A:536:THR:HA	1:A:540:GLN:CB	2.50	0.41
1:A:93:TYR:HB3	1:A:95:PHE:CE2	2.55	0.41
1:A:192:LEU:C	1:A:194:ILE:H	2.27	0.41
1:A:635:ASP:OD1	1:A:653:ARG:HB3	2.21	0.41
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.92	0.41
1:A:339:MET:O	1:A:343:LEU:HB2	2.20	0.41
1:A:585:LYS:HB3	1:A:585:LYS:NZ	2.35	0.41
1:A:20:ASN:OD1	1:A:69:HIS:HA	2.21	0.41
1:A:393:HIS:HA	1:A:659:ASN:O	2.21	0.41
1:A:438:THR:HA	1:A:514:GLN:HB3	2.01	0.41
1:A:196:ALA:HA	1:A:197:PRO:HD3	1.89	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.80	0.41
1:A:215:LEU:O	1:A:218:ARG:HB3	2.21	0.41
1:A:234:LEU:HD22	1:A:459:SER:HB2	2.03	0.40
1:A:492:ASP:O	1:A:494:LEU:HD22	2.21	0.40
1:A:242:LEU:HD11	1:A:275:PHE:HB3	2.04	0.40
1:A:396:TYR:HA	4:A:875:HOH:O	2.22	0.40
1:A:405:ARG:O	1:A:410:SER:HB3	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	639/662 (96%)	607 (95%)	26 (4%)	6 (1%)	14 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	208	PHE
1	A	207	ILE
1	A	70	PHE
1	A	617	GLY
1	A	598	GLY

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	546/576 (95%)	509 (93%)	37 (7%)	14	25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	55	LYS
1	A	70	PHE
1	A	73	GLU
1	A	83	VAL
1	A	141	GLN
1	A	168	LEU
1	A	201	LEU
1	A	241	LEU
1	A	261	LEU
1	A	269	LEU
1	A	288	ASN
1	A	301	LEU
1	A	316	VAL
1	A	321	LEU
1	A	342	LEU
1	A	343	LEU
1	A	367	LEU
1	A	389	LEU

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Mol	Chain	Res	Type
1	A	391	VAL
1	A	408	LEU
1	A	430	LEU
1	A	448	LEU
1	A	466	LEU
1	A	468	LEU
1	A	490	VAL
1	A	496	LEU
1	A	518	THR
1	A	549	LEU
1	A	585	LYS
1	A	604	MET
1	A	611	GLN
1	A	641	ARG
1	A	644	LYS
1	A	645	LEU
1	A	650	GLU
1	A	659	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	30	HIS
1	A	126	GLN
1	A	128	HIS
1	A	131	GLN
1	A	238	ASN
1	A	247	GLN
1	A	284	ASN
1	A	288	ASN
1	A	307	GLN
1	A	318	GLN
1	A	384	HIS
1	A	401	ASN
1	A	417	GLN
1	A	426	HIS
1	A	463	GLN
1	A	528	HIS
1	A	557	ASN
1	A	586	GLN
1	A	610	HIS

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Mol	Chain	Res	Type
1	A	611	GLN
1	A	659	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	RS7	A	841	-	19,19,19	4.24	5 (26%)	22,22,22	0.88	1 (4%)

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	RS7	A	841	-	-	0/13/13/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	841	RS7	C10-C11	16.98	1.41	1.19
3	A	841	RS7	C4-C3	-4.63	1.39	1.47
3	A	841	RS7	C4-C9	3.42	1.44	1.41
3	A	841	RS7	C2-C3	2.52	1.39	1.33
3	A	841	RS7	O18-C1	-2.09	1.25	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	841	RS7	C4-C3-C2	-2.95	121.13	126.91

There are no chirality outliers.

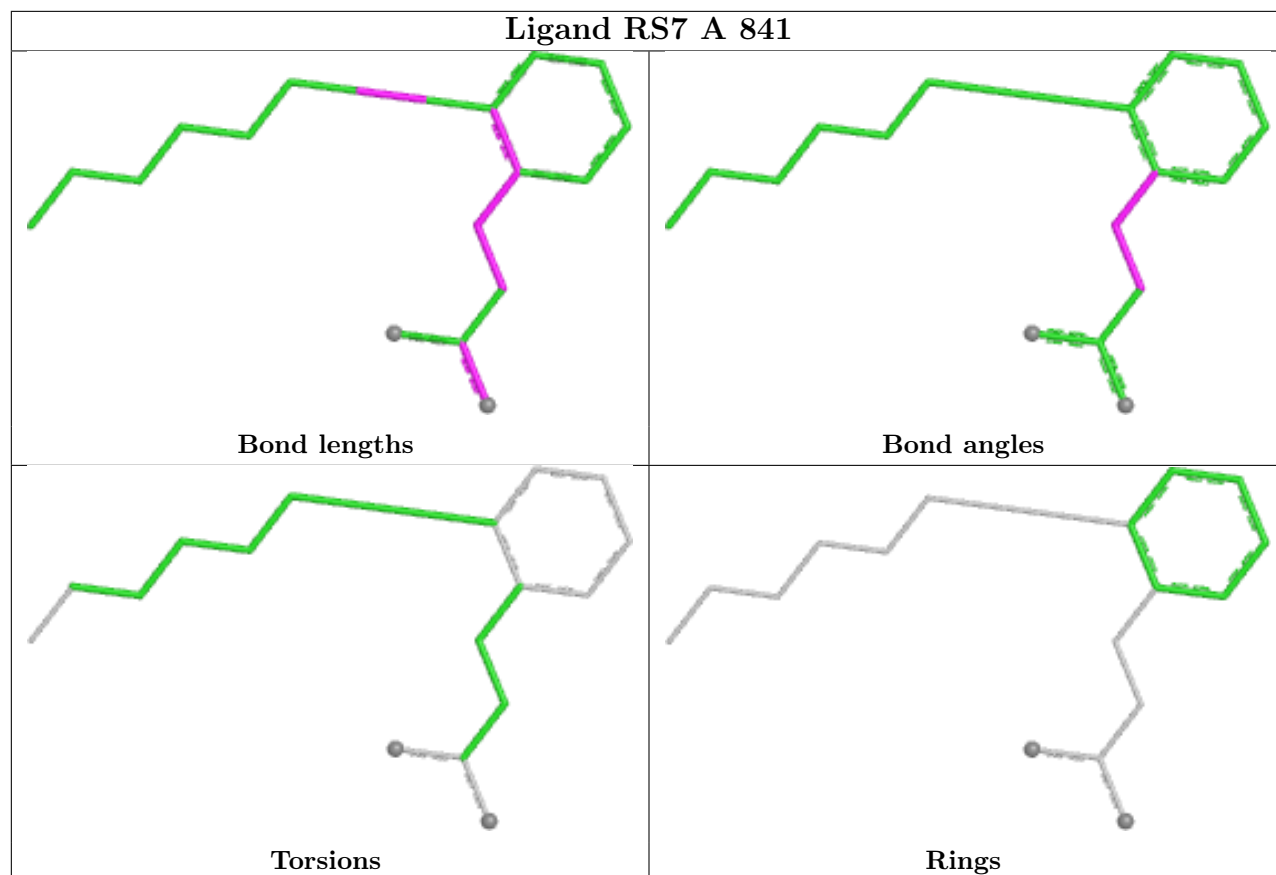
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	841	RS7	6	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 than 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.



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, 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	647/662 (97%)	1.48	142 (21%) 2 2	25, 45, 80, 112	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	7.6
1	A	209	TRP	7.1
1	A	197	PRO	5.0
1	A	595	TRP	4.2
1	A	195	LEU	3.9
1	A	572	ALA	3.8
1	A	188	LEU	3.8
1	A	506	ILE	3.7
1	A	176	GLU	3.6
1	A	191	SER	3.5
1	A	168	LEU	3.5
1	A	512	GLN	3.5
1	A	71	LEU	3.5
1	A	31	GLY	3.4
1	A	507	GLY	3.2
1	A	105	GLY	3.2
1	A	54	SER	3.2
1	A	257	GLY	3.2
1	A	198	TRP	3.1
1	A	122	GLN	3.1
1	A	342	LEU	3.1
1	A	431	GLN	3.1
1	A	293	CYS	3.1
1	A	310	GLY	3.1
1	A	88	ALA	3.0
1	A	475	TYR	3.0
1	A	161	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	70	PHE	3.0
1	A	56	TYR	3.0
1	A	552	PHE	3.0
1	A	173	ILE	2.9
1	A	194	ILE	2.9
1	A	320	HIS	2.9
1	A	167	PHE	2.9
1	A	505	GLU	2.9
1	A	237	ALA	2.9
1	A	427	VAL	2.8
1	A	383	ILE	2.8
1	A	603	ILE	2.8
1	A	516	PHE	2.8
1	A	644	LYS	2.8
1	A	51	VAL	2.8
1	A	15	TYR	2.8
1	A	410	SER	2.8
1	A	101	VAL	2.8
1	A	407	GLY	2.7
1	A	44	ASN	2.7
1	A	520	LEU	2.7
1	A	212	ARG	2.7
1	A	202	ASP	2.7
1	A	600	ASP	2.7
1	A	353	PHE	2.7
1	A	163	VAL	2.7
1	A	42	THR	2.7
1	A	271	ALA	2.7
1	A	69	HIS	2.7
1	A	144	SER	2.7
1	A	85	ALA	2.7
1	A	145	TRP	2.7
1	A	174	ASP	2.6
1	A	89	ALA	2.6
1	A	103	GLY	2.6
1	A	127	LYS	2.6
1	A	406	ASN	2.6
1	A	551	TRP	2.6
1	A	582	PRO	2.6
1	A	205	ASN	2.6
1	A	587	SER	2.6
1	A	143	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	2.6
1	A	297	LEU	2.6
1	A	13	SER	2.6
1	A	292	TYR	2.6
1	A	338	PRO	2.5
1	A	439	TYR	2.5
1	A	411	ASP	2.5
1	A	598	GLY	2.5
1	A	189	LYS	2.5
1	A	75	ALA	2.5
1	A	43	ARG	2.5
1	A	564	LEU	2.5
1	A	208	PHE	2.5
1	A	347	TRP	2.5
1	A	52	ASN	2.5
1	A	217	ARG	2.5
1	A	207	ILE	2.4
1	A	596	GLN	2.4
1	A	511	ALA	2.4
1	A	46	GLU	2.4
1	A	94	TRP	2.4
1	A	454	LEU	2.4
1	A	206	ARG	2.4
1	A	243	ARG	2.4
1	A	19	LYS	2.4
1	A	17	GLY	2.3
1	A	28	GLY	2.3
1	A	286	LYS	2.3
1	A	96	PRO	2.3
1	A	14	ILE	2.3
1	A	514	GLN	2.3
1	A	158	LEU	2.3
1	A	471	ILE	2.3
1	A	348	VAL	2.3
1	A	555	VAL	2.3
1	A	107	GLN	2.3
1	A	593	ILE	2.3
1	A	594	VAL	2.3
1	A	131	GLN	2.2
1	A	380	LEU	2.2
1	A	592	SER	2.2
1	A	648	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	309	ASP	2.2
1	A	447	ASP	2.2
1	A	385	PRO	2.2
1	A	20	ASN	2.2
1	A	265	LEU	2.2
1	A	321	LEU	2.2
1	A	365	GLY	2.2
1	A	614	TYR	2.2
1	A	193	ASN	2.1
1	A	196	ALA	2.1
1	A	73	GLU	2.1
1	A	77	PHE	2.1
1	A	417	GLN	2.1
1	A	40	ARG	2.1
1	A	175	PHE	2.1
1	A	22	VAL	2.1
1	A	409	VAL	2.1
1	A	190	ASN	2.1
1	A	170	ASP	2.1
1	A	192	LEU	2.1
1	A	220	ARG	2.1
1	A	424	GLY	2.1
1	A	484	TYR	2.1
1	A	346	CYS	2.1
1	A	142	TRP	2.0
1	A	273	THR	2.0
1	A	361	HIS	2.0
1	A	549	LEU	2.0
1	A	418	ILE	2.0
1	A	663	ILE	2.0
1	A	121	PRO	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

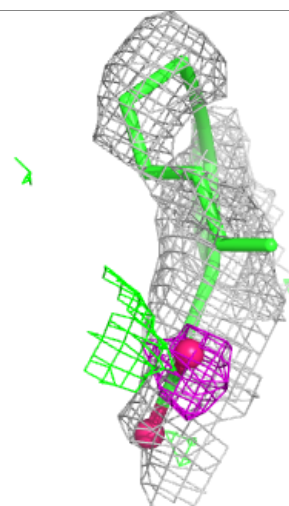
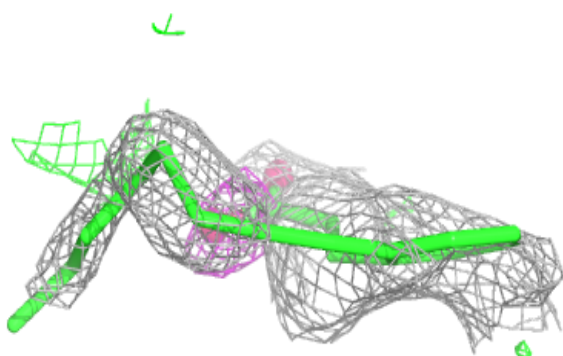
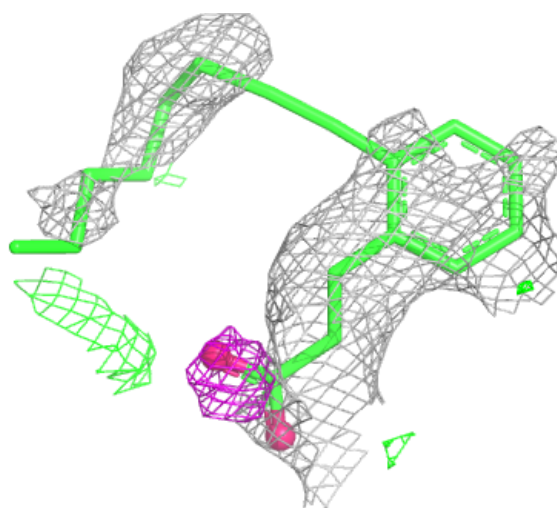
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	RS7	A	841	19/19	0.67	0.26	63,72,81,83	0
2	FE2	A	840	1/1	0.69	0.10	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 RS7 A 841:

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 [i](#)

There are no such residues in this entry.