



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:46 am BST

PDB ID : 2P0M  
Title : Revised structure of rabbit reticulocyte 15S-lipoxygenase  
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Deposited on : 2007-02-28  
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](mailto: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.

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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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

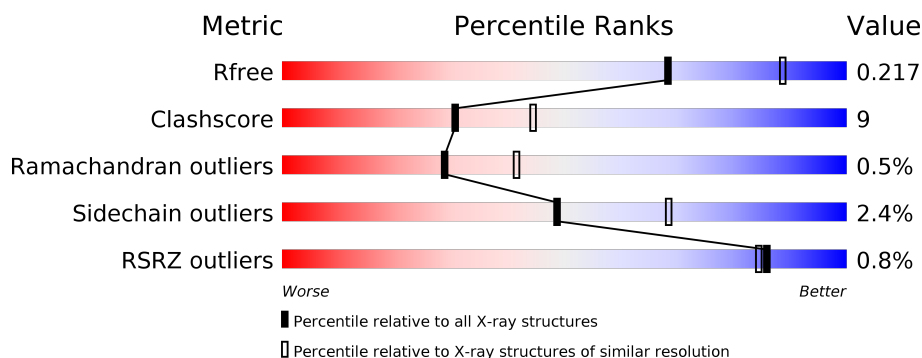
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>76%</span> <span>24%</span> </div> </div>
1	B	662	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> <span>%</span> <span>77%</span> <span>22%</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10831 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.

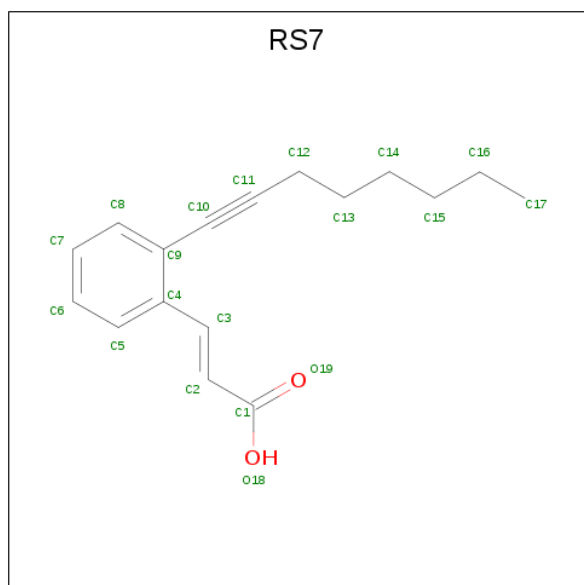
- Molecule 1 is a protein called Arachidonate 15-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5296	3406	906	953	31			
1	B	662	Total	C	N	O	S	0	0	0
			5296	3406	906	953	31			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is (2E)-3-(2-OCT-1-YN-1-YLPHENYL)ACRYLIC ACID (three-letter code: RS7) (formula: C<sub>17</sub>H<sub>20</sub>O<sub>2</sub>).



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

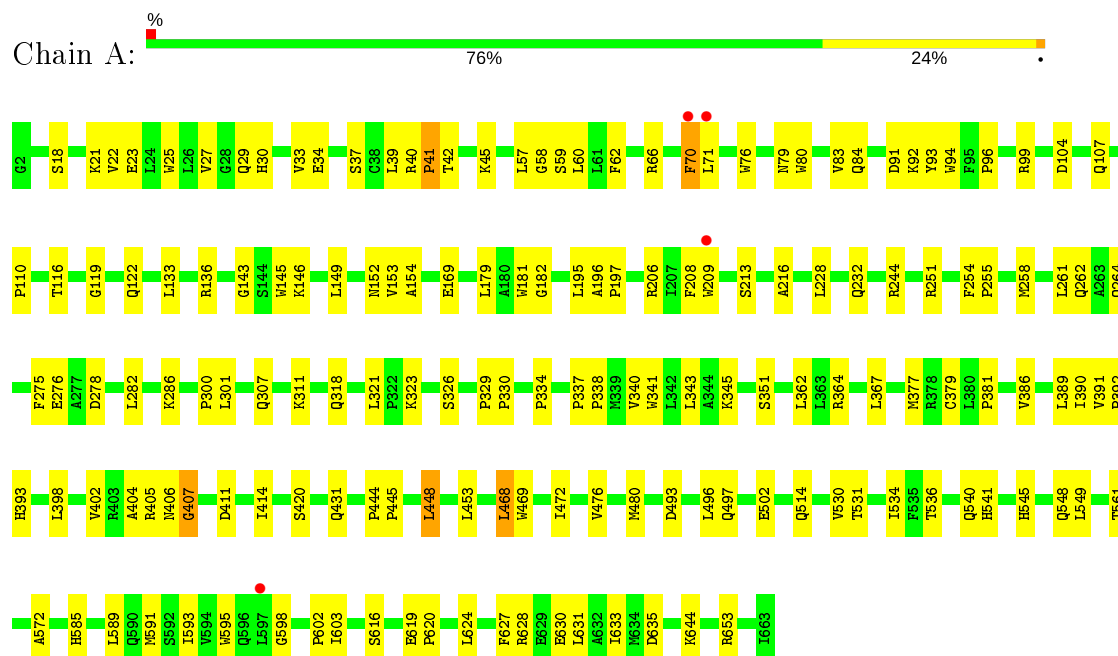
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	98	Total	O	0	0
			98	98		

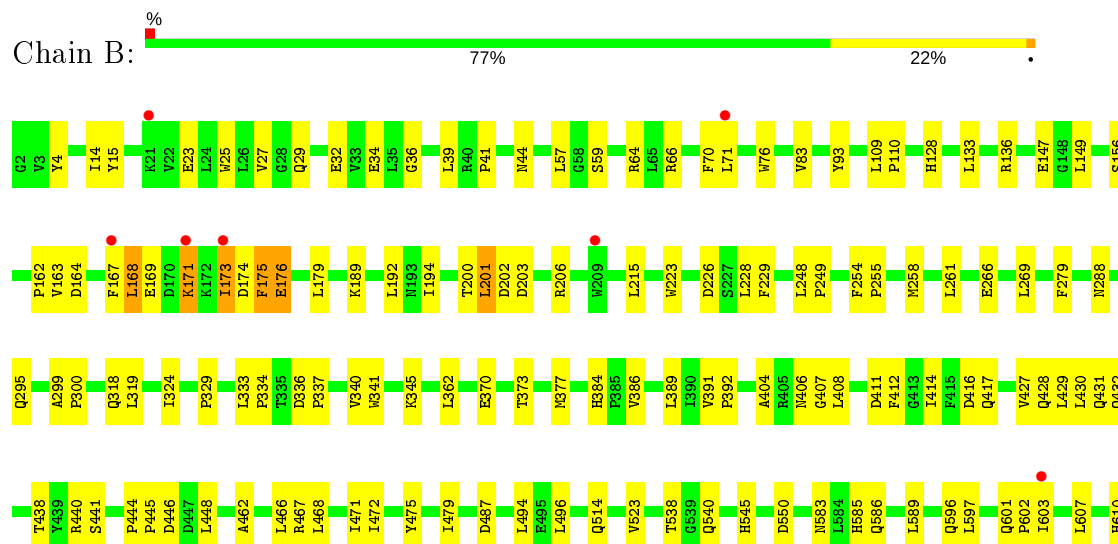
### 3 Residue-property plots [i](#)

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 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: Arachidonate 15-lipoxygenase



#### • Molecule 1: Arachidonate 15-lipoxygenase



E619	P620	V623	P627	M634	D635	I638	E639	N642	E643	K644	E650	R653	I656	N659	I663
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.90Å 198.90Å 136.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.99 – 2.40 24.21 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.99-2.40) 98.0 (24.21-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.193 , 0.230 0.186 , 0.217	Depositor DCC
$R_{free}$ test set	7408 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: RS7, FE2

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	0.53	0/5432	0.69	0/7373
1	B	0.54	0/5432	0.72	2/7373 (0.0%)
All	All	0.54	0/10864	0.71	2/14746 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LYS	N-CA-C	-6.20	94.27	111.00
1	B	173	ILE	N-CA-C	-5.09	97.27	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	5296	0	5286	105	0
1	B	5296	0	5286	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	19	0	19	3	0
4	A	120	0	0	8	0
4	B	98	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10831	0	10591	196	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 9.

All (196) 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:197:PRO:HD2	1:A:206:ARG:HH12	1.42	0.83
1:A:391:VAL:HG23	1:A:392:PRO:HD3	1.63	0.81
1:B:179:LEU:HD22	1:B:417:GLN:HE22	1.49	0.76
1:B:300:PRO:HB3	1:B:319:LEU:HD23	1.69	0.75
1:A:110:PRO:HD2	4:A:945:HOH:O	1.88	0.73
1:B:540:GLN:NE2	4:B:931:HOH:O	2.21	0.72
1:A:255:PRO:HD2	1:A:258:MET:HG3	1.71	0.70
1:B:147:GLU:O	1:B:431:GLN:NE2	2.25	0.66
1:B:189:LYS:HE3	4:B:912:HOH:O	1.95	0.65
1:A:33:VAL:HG13	1:A:57:LEU:HD21	1.77	0.65
1:A:549:LEU:HD12	1:A:549:LEU:H	1.61	0.65
1:B:619:GLU:HB2	1:B:620:PRO:HD3	1.79	0.65
1:B:201:LEU:HD23	1:B:201:LEU:H	1.62	0.64
1:B:324:ILE:HG13	4:B:926:HOH:O	1.97	0.64
1:A:472:ILE:HG22	1:A:531:THR:HG23	1.80	0.64
1:A:94:TRP:HB3	1:A:616:SER:HB3	1.80	0.64
1:B:200:THR:HG22	1:B:202:ASP:H	1.63	0.64
1:B:444:PRO:HB2	1:B:445:PRO:HD3	1.80	0.63
1:A:116:THR:HG23	1:A:119:GLY:H	1.62	0.63
1:A:323:LYS:HB3	1:A:326:SER:HB3	1.80	0.62
1:A:145:TRP:CG	1:A:405:ARG:HD2	2.34	0.62
1:A:149:LEU:HD23	4:A:889:HOH:O	1.98	0.62
1:B:279:PHE:O	1:B:299:ALA:HB1	2.01	0.61
1:B:341:TRP:CD1	1:B:345:LYS:HE2	2.35	0.61
1:A:208:PHE:HA	1:A:591:MET:CE	2.31	0.60
1:A:545:HIS:O	1:A:548:GLN:HG3	2.02	0.60
1:B:634:MET:O	1:B:638:ILE:HG13	2.02	0.60
1:A:530:VAL:O	1:A:534:ILE:HG12	2.03	0.59
1:B:597:LEU:HD21	3:B:841:RS7:O18	2.01	0.59
1:B:25:TRP:HB2	1:B:64:ARG:HB2	1.83	0.59
1:A:181:TRP:CZ3	1:B:206:ARG:HD2	2.39	0.58
1:B:404:ALA:HB2	3:B:841:RS7:H172	1.84	0.58
1:A:99:ARG:HH22	1:A:107:GLN:HG2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:HIS:HB2	4:A:920:HOH:O	2.06	0.56
1:A:146:LYS:HB2	1:A:149:LEU:HD12	1.87	0.56
1:A:541:HIS:HA	4:A:896:HOH:O	2.05	0.55
1:A:60:LEU:HD12	1:A:93:TYR:CD2	2.41	0.55
1:A:197:PRO:HD2	1:A:206:ARG:NH1	2.19	0.55
1:A:300:PRO:HA	1:A:318:GLN:O	2.07	0.55
1:A:603:ILE:HG13	1:A:603:ILE:O	2.07	0.55
1:B:538:THR:HG21	1:B:607:LEU:HD13	1.88	0.54
1:A:213:SER:H	1:A:216:ALA:HB3	1.72	0.54
1:B:223:TRP:HA	1:B:228:LEU:HD23	1.88	0.54
1:A:545:HIS:HA	1:A:548:GLN:HE21	1.71	0.54
1:A:23:GLU:HG3	1:A:66:ARG:HB3	1.88	0.54
1:A:94:TRP:CD1	1:A:96:PRO:HD3	2.43	0.54
1:B:407:GLY:O	1:B:414:ILE:HG13	2.08	0.54
1:B:585:HIS:CE1	1:B:589:LEU:HD11	2.43	0.54
1:A:196:ALA:HB1	1:A:206:ARG:HH11	1.73	0.53
1:A:27:VAL:HG13	1:A:62:PHE:HB2	1.90	0.53
1:A:379:CYS:SG	1:A:502:GLU:HB2	2.49	0.53
1:A:84:GLN:HB2	1:A:92:LYS:HG3	1.89	0.53
1:B:642:ASN:ND2	1:B:650:GLU:HG2	2.25	0.53
1:B:156:SER:O	1:B:406:ASN:ND2	2.42	0.52
1:B:215:LEU:HD23	1:B:550:ASP:HB3	1.91	0.52
1:A:261:LEU:HA	1:A:264:GLN:NE2	2.25	0.52
1:B:149:LEU:HD22	1:B:430:LEU:HB3	1.90	0.52
1:B:288:ASN:O	1:B:295:GLN:HB2	2.10	0.52
1:A:209:TRP:H	1:A:591:MET:HE1	1.76	0.51
1:B:25:TRP:HE1	1:B:34:GLU:HG2	1.76	0.51
1:A:444:PRO:HB2	1:A:445:PRO:HD3	1.94	0.50
1:A:42:THR:HB	1:A:45:LYS:HB2	1.94	0.50
1:B:300:PRO:HA	1:B:318:GLN:O	2.12	0.50
1:A:21:LYS:HA	1:A:40:ARG:HG2	1.94	0.50
1:B:362:LEU:HD13	3:B:841:RS7:H132	1.95	0.49
1:B:370:GLU:HB3	4:B:850:HOH:O	2.13	0.49
1:A:398:LEU:O	1:A:402:VAL:HG23	2.11	0.49
1:A:30:HIS:HD2	1:A:58:GLY:HA3	1.77	0.49
1:B:192:LEU:HB3	1:B:194:ILE:HG12	1.94	0.49
1:A:25:TRP:HD1	1:A:34:GLU:HA	1.78	0.49
1:B:545:HIS:CE1	1:B:663:ILE:HG23	2.47	0.49
1:B:479:ILE:HD12	1:B:623:VAL:HG11	1.95	0.49
1:B:438:THR:O	1:B:441:SER:OG	2.26	0.48
1:A:195:LEU:HD21	1:B:174:ASP:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:O	1:B:471:ILE:HG13	2.14	0.48
1:A:39:LEU:H	1:A:39:LEU:HD23	1.79	0.48
1:A:635:ASP:OD1	1:A:653:ARG:HB3	2.13	0.48
1:B:391:VAL:CG1	1:B:392:PRO:HD3	2.44	0.48
1:B:179:LEU:HD22	1:B:417:GLN:NE2	2.22	0.48
1:B:334:PRO:HG3	1:B:341:TRP:CZ2	2.49	0.48
1:A:179:LEU:HA	1:A:595:TRP:HZ3	1.79	0.48
1:A:334:PRO:HG3	1:A:341:TRP:CZ2	2.49	0.47
1:A:593:ILE:CG2	1:A:593:ILE:O	2.61	0.47
1:B:468:LEU:O	1:B:472:ILE:HG13	2.14	0.47
1:A:340:VAL:HG22	1:A:572:ALA:H	1.79	0.47
1:A:25:TRP:CD1	1:A:34:GLU:HA	2.50	0.47
1:A:448:LEU:HD12	1:A:453:LEU:HB2	1.97	0.47
1:A:619:GLU:HB2	1:A:620:PRO:HD3	1.97	0.47
1:B:583:ASN:OD1	1:B:586:GLN:HG3	2.14	0.47
1:A:18:SER:HB2	1:A:76:TRP:HB2	1.97	0.47
1:A:468:LEU:HD22	1:A:472:ILE:HD11	1.97	0.47
1:A:468:LEU:O	1:A:472:ILE:HG13	2.14	0.47
1:B:601:GLN:HA	1:B:602:PRO:HD3	1.77	0.47
1:A:345:LYS:HD2	4:A:928:HOH:O	2.15	0.46
1:B:391:VAL:HG12	1:B:392:PRO:HD3	1.96	0.46
1:A:152:ASN:ND2	1:A:153:VAL:O	2.48	0.46
1:B:41:PRO:HB3	1:B:76:TRP:CD1	2.50	0.46
1:A:22:VAL:HG13	1:A:22:VAL:O	2.16	0.46
1:B:179:LEU:HD13	1:B:179:LEU:C	2.36	0.46
1:B:487:ASP:HA	1:B:523:VAL:HG23	1.96	0.46
1:B:168:LEU:HD21	1:B:603:ILE:HG21	1.97	0.46
1:A:282:LEU:CD1	1:A:351:SER:HB3	2.47	0.45
1:B:384:HIS:CE1	1:B:386:VAL:HG23	2.51	0.45
1:B:39:LEU:N	1:B:39:LEU:HD23	2.30	0.45
1:B:336:ASP:HB3	1:B:337:PRO:CD	2.47	0.45
1:B:336:ASP:HB3	1:B:337:PRO:HD2	1.97	0.45
1:A:420:SER:HB3	1:A:561:THR:HA	1.98	0.45
1:B:27:VAL:HB	1:B:32:GLU:HB3	1.99	0.45
1:B:440:ARG:CZ	1:B:446:ASP:HB3	2.46	0.45
1:A:407:GLY:O	1:A:414:ILE:HG12	2.16	0.45
1:B:162:PRO:C	1:B:164:ASP:H	2.20	0.45
1:A:29:GLN:N	1:A:59:SER:O	2.50	0.45
1:B:83:VAL:HG13	1:B:93:TYR:HB2	1.98	0.45
1:B:23:GLU:HG3	1:B:36:GLY:C	2.37	0.45
1:B:29:GLN:HE21	1:B:59:SER:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HD2	1:B:377:MET:O	2.16	0.45
1:A:391:VAL:CG2	1:A:392:PRO:HD3	2.41	0.45
1:A:476:VAL:O	1:A:480:MET:HG2	2.17	0.45
1:A:60:LEU:HB2	1:A:93:TYR:CD1	2.52	0.45
1:A:70:PHE:HD1	1:A:71:LEU:H	1.64	0.45
1:B:337:PRO:HB2	1:B:340:VAL:HG23	1.99	0.44
1:A:472:ILE:CG2	1:A:531:THR:HG23	2.44	0.44
1:B:110:PRO:HG3	1:B:128:HIS:CD2	2.52	0.44
1:B:162:PRO:C	1:B:164:ASP:N	2.71	0.44
1:B:384:HIS:HE1	1:B:386:VAL:HG23	1.82	0.44
1:A:393:HIS:CD2	1:A:534:ILE:HD12	2.52	0.44
1:B:428:GLN:HG2	1:B:432:GLN:HE21	1.82	0.44
1:A:143:GLY:HA3	1:A:154:ALA:HA	2.00	0.44
1:B:226:ASP:O	1:B:229:PHE:HB3	2.18	0.44
1:A:337:PRO:HA	1:A:338:PRO:HD3	1.92	0.44
1:B:610:HIS:CD2	1:B:659:ASN:HD21	2.35	0.43
1:A:536:THR:HA	1:A:540:GLN:HB3	2.00	0.43
1:B:619:GLU:O	1:B:623:VAL:HG23	2.17	0.43
1:A:39:LEU:HD23	1:A:39:LEU:N	2.34	0.43
1:A:493:ASP:O	1:A:497:GLN:HG2	2.18	0.43
1:A:630:GLU:O	1:A:633:ILE:HG22	2.19	0.43
1:A:79:ASN:HB3	1:A:80:TRP:CD1	2.54	0.43
1:B:254:PHE:HA	1:B:255:PRO:HD3	1.75	0.43
1:B:4:TYR:CE2	1:B:57:LEU:HD12	2.54	0.43
1:B:639:GLU:HB2	1:B:653:ARG:HH21	1.83	0.43
1:A:21:LYS:HG2	1:A:37:SER:HB3	1.99	0.43
1:A:389:LEU:HD23	1:A:389:LEU:O	2.18	0.43
1:A:545:HIS:NE2	1:A:598:GLY:HA2	2.34	0.43
1:A:66:ARG:NH2	1:A:104:ASP:HB2	2.34	0.43
1:A:364:ARG:HD3	4:A:852:HOH:O	2.18	0.43
1:A:195:LEU:HD21	1:B:174:ASP:N	2.34	0.43
1:A:624:LEU:O	1:A:628:ARG:HG3	2.19	0.43
1:B:175:PHE:HB2	1:B:176:GLU:H	1.56	0.43
1:A:307:GLN:HE21	1:A:311:LYS:HB3	1.84	0.42
1:A:404:ALA:C	1:A:406:ASN:H	2.21	0.42
1:A:444:PRO:HD2	1:A:469:TRP:CE3	2.54	0.42
1:A:182:GLY:HA3	1:A:595:TRP:CZ3	2.54	0.42
1:A:514:GLN:NE2	1:A:514:GLN:HA	2.35	0.42
1:A:181:TRP:HH2	1:B:203:ASP:HB3	1.84	0.42
1:A:329:PRO:HA	1:A:330:PRO:HD3	1.73	0.42
1:A:493:ASP:CG	1:A:496:LEU:HB2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HD22	1:B:494:LEU:N	2.34	0.42
1:A:391:VAL:HG23	1:A:392:PRO:CD	2.43	0.42
1:A:593:ILE:O	1:A:593:ILE:HG23	2.19	0.42
1:A:244:ARG:HA	1:A:275:PHE:CD2	2.55	0.42
1:B:14:ILE:HG13	1:B:15:TYR:CD1	2.55	0.42
1:B:438:THR:HA	1:B:514:GLN:HB3	2.01	0.42
1:B:635:ASP:OD1	1:B:653:ARG:HB3	2.19	0.42
1:B:70:PHE:HD1	1:B:71:LEU:H	1.64	0.42
1:A:627:PHE:CZ	1:A:631:LEU:HD11	2.55	0.42
1:B:171:LYS:HA	1:B:601:GLN:OE1	2.20	0.42
1:B:448:LEU:HD21	1:B:462:ALA:HA	2.01	0.42
1:A:27:VAL:CG1	1:A:62:PHE:HB2	2.50	0.42
1:A:136:ARG:HD2	1:A:377:MET:O	2.20	0.41
1:B:255:PRO:HD2	1:B:258:MET:SD	2.60	0.41
1:B:269:LEU:C	1:B:269:LEU:HD13	2.40	0.41
1:B:427:VAL:O	1:B:431:GLN:HG3	2.20	0.41
1:A:362:LEU:HG	1:A:367:LEU:HD13	2.02	0.41
1:B:14:ILE:HG13	1:B:15:TYR:HD1	1.85	0.41
1:B:596:GLN:HE21	1:B:596:GLN:HB2	1.54	0.41
1:B:475:TYR:HB2	1:B:627:PHE:CD1	2.55	0.41
1:A:133:LEU:HD11	1:A:381:PRO:HD3	2.02	0.41
1:A:228:LEU:O	1:A:232:GLN:HG3	2.20	0.41
1:A:254:PHE:CE2	1:A:262:GLN:HG2	2.55	0.41
1:B:333:LEU:HA	1:B:334:PRO:HD3	1.94	0.41
1:A:589:LEU:HD23	1:A:589:LEU:O	2.21	0.41
1:B:329:PRO:HG2	4:B:901:HOH:O	2.21	0.41
1:B:411:ASP:O	1:B:412:PHE:HB2	2.20	0.41
1:B:429:LEU:HD23	1:B:429:LEU:O	2.21	0.41
1:B:448:LEU:N	1:B:448:LEU:HD12	2.35	0.41
1:A:286:LYS:HE3	4:A:898:HOH:O	2.20	0.41
1:B:163:VAL:HG22	1:B:163:VAL:O	2.21	0.41
1:B:173:ILE:HG13	1:B:173:ILE:O	2.20	0.41
1:B:373:THR:O	1:B:377:MET:HG2	2.21	0.41
1:A:251:ARG:NH1	1:A:278:ASP:OD1	2.54	0.41
1:A:40:ARG:HA	1:A:41:PRO:HD3	1.83	0.41
1:A:83:VAL:HG13	1:A:93:TYR:HB2	2.03	0.41
1:B:248:LEU:HA	1:B:249:PRO:HD3	1.91	0.41
1:A:323:LYS:HG3	4:A:876:HOH:O	2.20	0.41
1:A:386:VAL:O	1:A:390:ILE:HG13	2.21	0.40
1:B:109:LEU:HA	1:B:110:PRO:HD3	1.92	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	660/662 (100%)	615 (93%)	43 (6%)	2 (0%)	41	55
1	B	660/662 (100%)	611 (93%)	45 (7%)	4 (1%)	25	36
All	All	1320/1324 (100%)	1226 (93%)	88 (7%)	6 (0%)	29	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	PHE
1	B	168	LEU
1	B	176	GLU
1	A	407	GLY
1	B	169	GLU
1	A	41	PRO

### 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	576/576 (100%)	562 (98%)	14 (2%)	49	68
1	B	576/576 (100%)	562 (98%)	14 (2%)	49	68
All	All	1152/1152 (100%)	1124 (98%)	28 (2%)	49	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	PHE
1	A	91	ASP
1	A	122	GLN
1	A	169	GLU
1	A	276	GLU
1	A	301	LEU
1	A	321	LEU
1	A	343	LEU
1	A	411	ASP
1	A	431	GLN
1	A	448	LEU
1	A	468	LEU
1	A	602	PRO
1	A	644	LYS
1	B	44	ASN
1	B	66	ARG
1	B	133	LEU
1	B	167	PHE
1	B	201	LEU
1	B	261	LEU
1	B	266	GLU
1	B	389	LEU
1	B	408	LEU
1	B	416	ASP
1	B	466	LEU
1	B	496	LEU
1	B	644	LYS
1	B	656	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	107	GLN
1	A	122	GLN
1	A	190	ASN
1	A	264	GLN
1	A	307	GLN
1	A	359	ASN
1	A	406	ASN
1	A	432	GLN
1	A	514	GLN
1	A	548	GLN

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Mol	Chain	Res	Type
1	A	585	HIS
1	B	29	GLN
1	B	44	ASN
1	B	52	ASN
1	B	128	HIS
1	B	262	GLN
1	B	264	GLN
1	B	307	GLN
1	B	417	GLN
1	B	432	GLN
1	B	477	GLN
1	B	540	GLN
1	B	545	HIS
1	B	548	GLN
1	B	585	HIS
1	B	596	GLN
1	B	610	HIS
1	B	611	GLN

### 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 [i](#)

Of 3 ligands modelled in this entry, 2 are 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	B	841	-	16,19,19	2.76	9 (56%)	19,22,22	1.57	6 (31%)

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	B	841	-	-	5/11/13/13	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	841	RS7	C4-C9	7.18	1.48	1.41
3	B	841	RS7	C4-C3	3.53	1.52	1.47
3	B	841	RS7	C10-C11	3.35	1.24	1.19
3	B	841	RS7	C7-C8	3.25	1.45	1.38
3	B	841	RS7	C7-C6	3.03	1.46	1.38
3	B	841	RS7	C13-C12	2.60	1.66	1.51
3	B	841	RS7	C8-C9	2.42	1.44	1.40
3	B	841	RS7	C9-C10	-2.42	1.39	1.43
3	B	841	RS7	C14-C13	2.14	1.63	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	841	RS7	C12-C11-C10	-2.91	167.61	176.09
3	B	841	RS7	C8-C9-C4	-2.47	117.92	120.49
3	B	841	RS7	C4-C3-C2	-2.45	119.06	126.46
3	B	841	RS7	C9-C4-C3	-2.36	115.56	120.55
3	B	841	RS7	C4-C9-C10	2.34	123.58	121.09
3	B	841	RS7	C5-C4-C9	2.30	120.21	117.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	841	RS7	C12-C13-C14-C15

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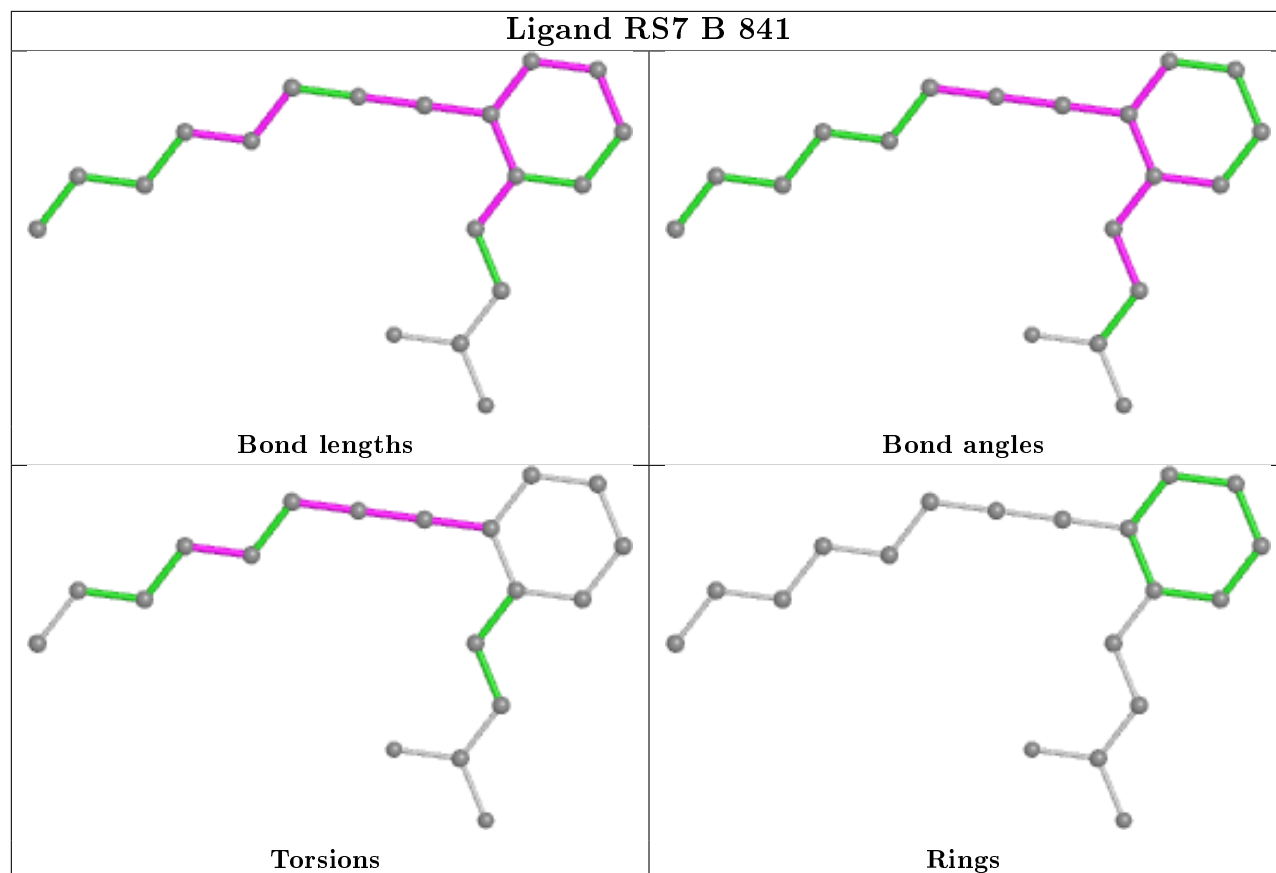
Mol	Chain	Res	Type	Atoms
3	B	841	RS7	C11-C10-C9-C4
3	B	841	RS7	C9-C10-C11-C12
3	B	841	RS7	C10-C11-C12-C13
3	B	841	RS7	C11-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	841	RS7	3	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	662/662 (100%)	-0.27	4 (0%) <a href="#">89</a> <a href="#">88</a>	25, 46, 71, 93	0
1	B	662/662 (100%)	-0.22	7 (1%) <a href="#">80</a> <a href="#">79</a>	19, 47, 77, 97	0
All	All	1324/1324 (100%)	-0.24	11 (0%) <a href="#">86</a> <a href="#">84</a>	19, 46, 74, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	TRP	5.5
1	A	71	LEU	5.4
1	B	173	ILE	3.8
1	B	71	LEU	3.4
1	A	70	PHE	2.6
1	B	603	ILE	2.5
1	B	21	LYS	2.3
1	B	209	TRP	2.3
1	B	171	LYS	2.2
1	A	597	LEU	2.2
1	B	167	PHE	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

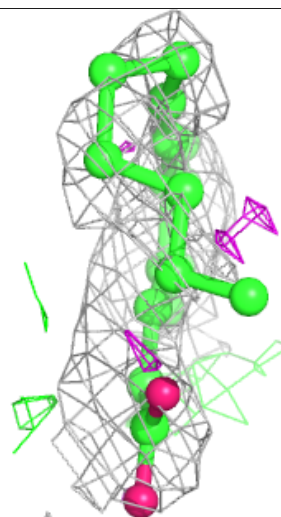
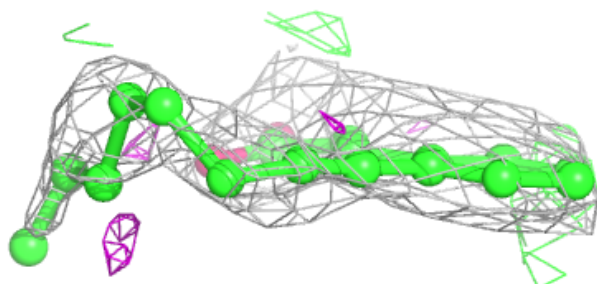
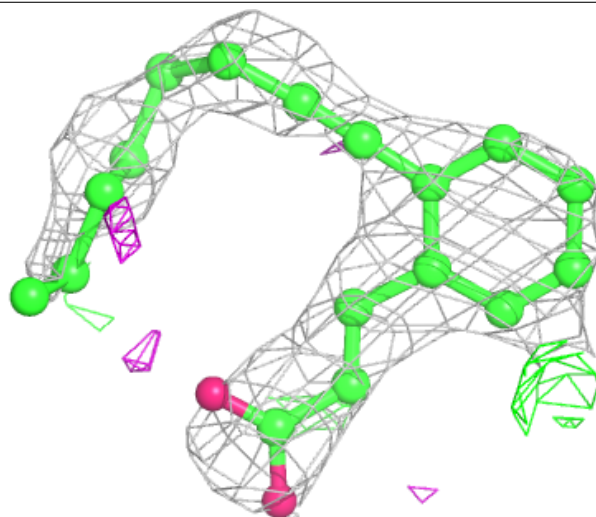
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	RS7	B	841	19/19	0.85	0.40	66,74,83,83	0
2	FE2	B	840	1/1	0.95	0.17	40,40,40,40	0
2	FE2	A	840	1/1	0.95	0.19	36,36,36,36	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 B 841:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.