Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 08:47 PM EDT

PDB ID	:	2Q8I
Title	:	Pyruvate dehydrogenase kinase isoform 3 in complex with antitumor drug radicicol
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Deposited on	:	2007-06-10
Resolution	:	2.60 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:

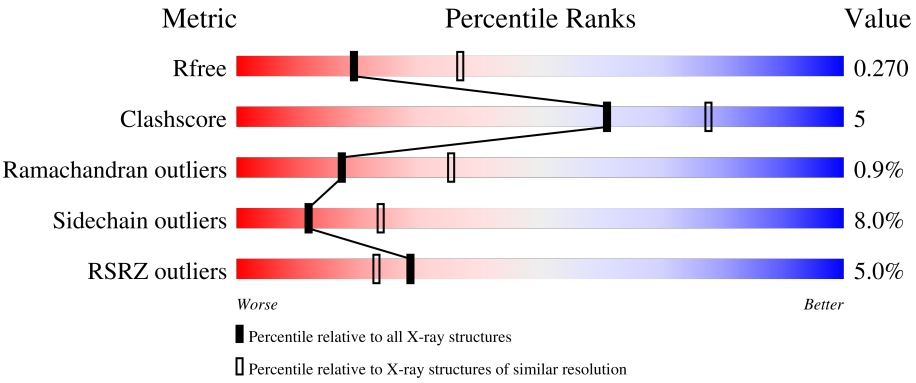
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	419	2% 73% 12% · 12%
2	B	128	10% 55% 15% · 27%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3863 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 [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	369	3023	1949	504	557	13	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	cloning artifact	UNP Q15120
A	-11	GLY	-	cloning artifact	UNP Q15120
A	-10	SER	-	cloning artifact	UNP Q15120
A	-9	HIS	-	expression tag	UNP Q15120
A	-8	HIS	-	expression tag	UNP Q15120
A	-7	HIS	-	expression tag	UNP Q15120
A	-6	HIS	-	expression tag	UNP Q15120
A	-5	HIS	-	expression tag	UNP Q15120
A	-4	HIS	-	expression tag	UNP Q15120
A	-3	GLY	-	cloning artifact	UNP Q15120
A	-2	MET	-	cloning artifact	UNP Q15120
A	-1	ALA	-	cloning artifact	UNP Q15120
A	0	ARG	-	cloning artifact	UNP Q15120
A	1	LEU	-	cloning artifact	UNP Q15120
A	2	GLU	-	cloning artifact	UNP Q15120
A	3	ASN	-	cloning artifact	UNP Q15120
A	4	LEU	-	cloning artifact	UNP Q15120
A	5	TYR	-	cloning artifact	UNP Q15120
A	6	PHE	-	cloning artifact	UNP Q15120
A	7	GLN	-	cloning artifact	UNP Q15120
A	8	GLY	-	cloning artifact	UNP Q15120

- Molecule 2 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	93	Total	C	N	O	S	0	0	0
			716	459	111	142	4			

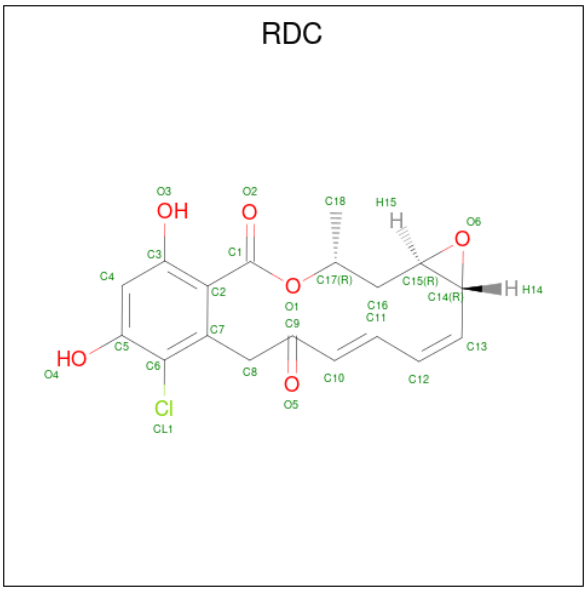
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	GLY	-	cloning artifact	UNP P10515
B	107	GLY	-	cloning artifact	UNP P10515
B	108	SER	-	cloning artifact	UNP P10515
B	109	HIS	-	expression tag	UNP P10515
B	110	HIS	-	expression tag	UNP P10515
B	111	HIS	-	expression tag	UNP P10515
B	112	HIS	-	expression tag	UNP P10515
B	113	HIS	-	expression tag	UNP P10515
B	114	HIS	-	expression tag	UNP P10515
B	115	GLY	-	cloning artifact	UNP P10515
B	116	MET	-	cloning artifact	UNP P10515
B	117	ALA	-	cloning artifact	UNP P10515
B	118	ARG	-	cloning artifact	UNP P10515
B	119	LEU	-	cloning artifact	UNP P10515
B	120	GLU	-	cloning artifact	UNP P10515
B	121	ASN	-	cloning artifact	UNP P10515
B	122	LEU	-	cloning artifact	UNP P10515
B	123	TYR	-	cloning artifact	UNP P10515
B	124	PHE	-	cloning artifact	UNP P10515
B	125	GLN	-	cloning artifact	UNP P10515

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

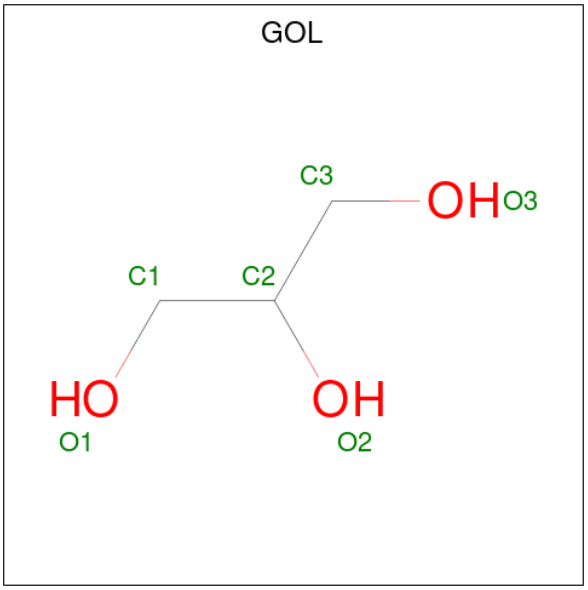
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is RADICICOL (three-letter code: RDC) (formula: $C_{18}H_{17}ClO_6$).



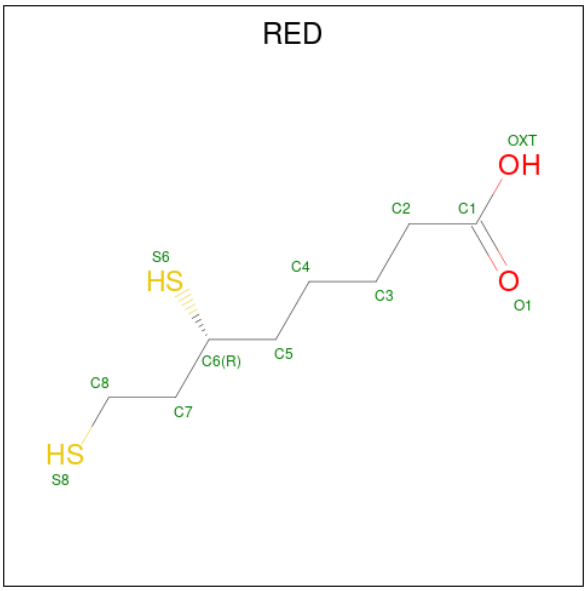
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
4	A	1	25	18	1	6	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	6	3	3		0	0

- Molecule 6 is DIHYDROLIPOIC ACID (three-letter code: RED) (formula: $C_8H_{16}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O S 11 8 1 2	0	0

- Molecule 7 is water.

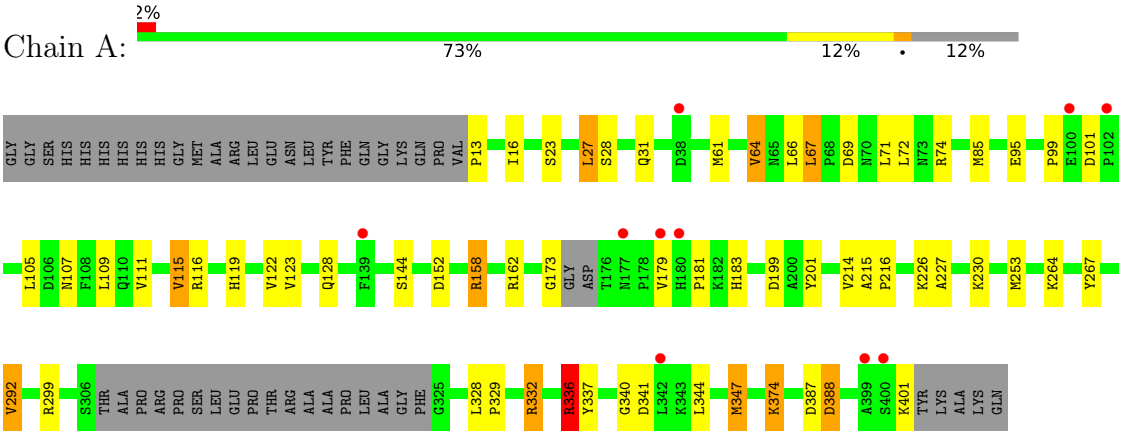
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	76	Total O 76 76	0	0
7	B	5	Total O 5 5	0	0

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.

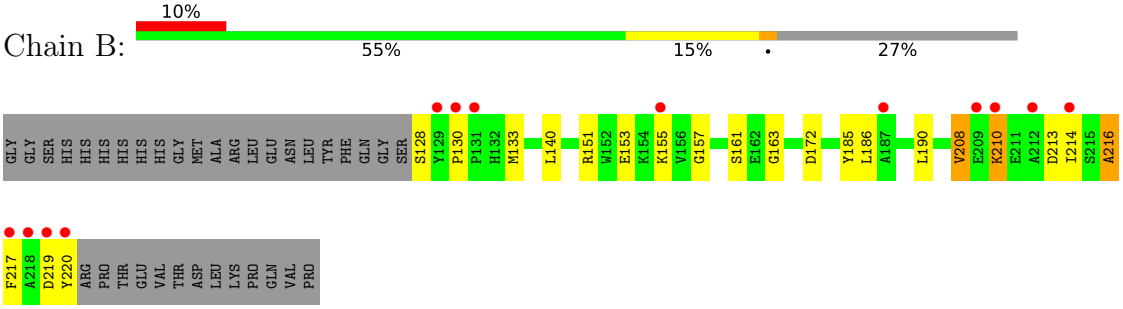
• Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

Chain A:



• Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.87Å 120.87Å 239.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.60) 100.0 (48.20-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.238 0.248 , 0.270	Depositor DCC
R_{free} test set	1647 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3863	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, RED, RDC

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	0.92	2/3100 (0.1%)	0.89	9/4196 (0.2%)
2	B	1.27	9/730 (1.2%)	0.97	6/992 (0.6%)
All	All	1.00	11/3830 (0.3%)	0.91	15/5188 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	PRO	N-CD	12.36	1.65	1.47
2	B	217	PHE	CE2-CZ	10.22	1.56	1.37
2	B	210	LYS	CE-NZ	9.68	1.73	1.49
2	B	128	SER	CB-OG	7.79	1.52	1.42
2	B	216	ALA	C-N	7.45	1.51	1.34
2	B	213	ASP	C-O	6.78	1.36	1.23
1	A	267	TYR	CE1-CZ	-6.22	1.30	1.38
2	B	217	PHE	CE1-CZ	5.57	1.48	1.37
2	B	217	PHE	CD2-CE2	-5.55	1.28	1.39
2	B	217	PHE	CG-CD1	5.55	1.47	1.38
1	A	337	TYR	CB-CG	-5.02	1.44	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	332	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	A	336	ARG	NE-CZ-NH2	-8.16	116.22	120.30
2	B	217	PHE	CD1-CG-CD2	6.86	127.22	118.30
2	B	217	PHE	CB-CG-CD1	-6.79	116.05	120.80
2	B	217	PHE	CB-CG-CD2	-6.73	116.09	120.80
2	B	210	LYS	CD-CE-NZ	-6.34	97.12	111.70
1	A	344	LEU	CA-CB-CG	6.31	129.82	115.30
2	B	172	ASP	N-CA-CB	-6.21	99.41	110.60
1	A	332	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	347	MET	CG-SD-CE	5.86	109.58	100.20
1	A	199	ASP	CB-CG-OD2	-5.76	113.11	118.30
2	B	130	PRO	N-CD-CG	-5.66	94.71	103.20
1	A	152	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	388	ASP	N-CA-CB	-5.27	101.11	110.60
1	A	292	VAL	CB-CA-C	-5.15	101.62	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	ASP	Peptide

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	3023	0	2985	25	0
2	B	716	0	718	9	0
3	A	1	0	0	0	0
4	A	25	0	15	1	0
5	A	6	0	8	0	0
6	B	11	0	15	0	0
7	A	76	0	0	1	0
7	B	5	0	0	0	0
All	All	3863	0	3741	34	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 5.

All (34) 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)
2:B:210:LYS:CE	2:B:210:LYS:NZ	1.73	1.52
1:A:332:ARG:HD2	7:A:410:HOH:O	1.76	0.84
1:A:28:SER:H	1:A:31:GLN:HE21	1.30	0.79
2:B:210:LYS:NZ	2:B:210:LYS:CD	2.51	0.73
1:A:201:TYR:CZ	1:A:253:MET:HE2	2.25	0.72
1:A:374:LYS:HG3	2:B:163:GLY:HA3	1.73	0.70
1:A:201:TYR:CZ	1:A:253:MET:CE	2.76	0.69
4:A:408:RDC:C9	4:A:408:RDC:CL1	2.87	0.59
1:A:336:ARG:HD3	1:A:341:ASP:OD1	2.03	0.58
1:A:201:TYR:CE1	1:A:253:MET:HE2	2.39	0.57
1:A:123:VAL:HG23	1:A:158:ARG:HE	1.70	0.55
1:A:16:ILE:HD11	1:A:85:MET:SD	2.47	0.54
1:A:67:LEU:HG	1:A:71:LEU:HD23	1.89	0.53
1:A:99:PRO:C	1:A:101:ASP:H	2.13	0.52
1:A:336:ARG:HA	1:A:340:GLY:O	2.11	0.51
2:B:157:GLY:HA2	2:B:214:ILE:HD13	1.93	0.50
1:A:107:ASN:O	1:A:111:VAL:HG23	2.12	0.49
2:B:219:ASP:O	2:B:220:TYR:C	2.50	0.49
1:A:61:MET:HA	1:A:64:VAL:HG13	1.95	0.49
1:A:64:VAL:HA	1:A:67:LEU:HD22	1.95	0.48
1:A:216:PRO:HD2	1:A:253:MET:HG2	1.95	0.48
2:B:151:ARG:HD3	2:B:153:GLU:OE2	2.14	0.48
1:A:328:LEU:N	1:A:329:PRO:HD2	2.31	0.45
2:B:208:VAL:HG13	2:B:210:LYS:O	2.16	0.45
1:A:201:TYR:CE1	1:A:253:MET:CE	2.98	0.45
2:B:220:TYR:CD2	2:B:220:TYR:O	2.70	0.45
1:A:332:ARG:O	1:A:336:ARG:HG2	2.18	0.44
1:A:27:LEU:HA	1:A:31:GLN:NE2	2.34	0.43
1:A:111:VAL:O	1:A:115:VAL:HG13	2.19	0.43
1:A:119:HIS:O	1:A:122:VAL:HB	2.19	0.42
2:B:185:TYR:HB3	2:B:214:ILE:HD11	2.02	0.42
1:A:109:LEU:HD21	1:A:173:GLY:HA2	2.03	0.41
1:A:227:ALA:HB1	1:A:230:LYS:HG3	2.02	0.41
1:A:214:VAL:HG22	1:A:215:ALA:H	1.86	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	364/419 (87%)	347 (95%)	14 (4%)	3 (1%)	19 39
2	B	91/128 (71%)	88 (97%)	2 (2%)	1 (1%)	14 30
All	All	455/547 (83%)	435 (96%)	16 (4%)	4 (1%)	17 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	A	388	ASP
2	B	216	ALA
1	A	181	PRO

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	335/374 (90%)	309 (92%)	26 (8%)	12 25
2	B	79/109 (72%)	72 (91%)	7 (9%)	9 19
All	All	414/483 (86%)	381 (92%)	33 (8%)	12 24

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	23	SER

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	64	VAL
1	A	66	LEU
1	A	67	LEU
1	A	69	ASP
1	A	72	LEU
1	A	74	ARG
1	A	95	GLU
1	A	105	LEU
1	A	115	VAL
1	A	116	ARG
1	A	128	GLN
1	A	144	SER
1	A	158	ARG
1	A	162	ARG
1	A	183	HIS
1	A	226	LYS
1	A	264	LYS
1	A	292	VAL
1	A	299	ARG
1	A	336	ARG
1	A	347	MET
1	A	374	LYS
1	A	401	LYS
2	B	133	MET
2	B	140	LEU
2	B	155	LYS
2	B	161	SER
2	B	186	LEU
2	B	190	LEU
2	B	208	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	70	ASN
1	A	73	ASN
1	A	107	ASN
1	A	128	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
6	RED	B	300	2	9,10,11	0.44	0	6,10,12	2.72	1 (16%)
5	GOL	A	409	-	5,5,5	0.68	0	5,5,5	1.23	0
4	RDC	A	408	-	26,27,27	2.17	4 (15%)	30,39,39	2.34	10 (33%)

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
6	RED	B	300	2	-	2/7/9/10	-
5	GOL	A	409	-	-	2/4/4/4	-
4	RDC	A	408	-	-	7/23/28/28	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	RDC	C5-C6	7.36	1.48	1.40
4	A	408	RDC	C2-C7	4.41	1.48	1.40
4	A	408	RDC	C2-C3	3.90	1.47	1.41
4	A	408	RDC	O1-C1	3.63	1.42	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	300	RED	C7-C8-S8	-6.27	107.21	113.74
4	A	408	RDC	C2-C7-C6	-5.69	112.48	118.33
4	A	408	RDC	O6-C15-C16	-4.65	106.49	116.33
4	A	408	RDC	C4-C5-C6	4.51	123.11	119.20
4	A	408	RDC	C7-C6-CL1	-4.07	113.70	119.87
4	A	408	RDC	O3-C3-C2	-3.92	113.80	121.14
4	A	408	RDC	C3-C2-C7	3.28	122.74	119.05
4	A	408	RDC	C5-C4-C3	-3.21	116.94	120.14
4	A	408	RDC	C5-C6-CL1	2.60	123.50	119.12
4	A	408	RDC	O6-C14-C13	-2.40	109.43	115.37
4	A	408	RDC	C15-C14-C13	-2.22	115.78	122.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	409	GOL	C1-C2-C3-O3
6	B	300	RED	C5-C6-C7-C8
5	A	409	GOL	O2-C2-C3-O3
4	A	408	RDC	C11-C10-C9-O5
4	A	408	RDC	C6-C7-C8-C9
4	A	408	RDC	C11-C10-C9-C8
4	A	408	RDC	C7-C8-C9-O5
4	A	408	RDC	O2-C1-C2-C3
4	A	408	RDC	O1-C1-C2-C3
6	B	300	RED	C6-C7-C8-S8
4	A	408	RDC	C12-C13-C14-C15

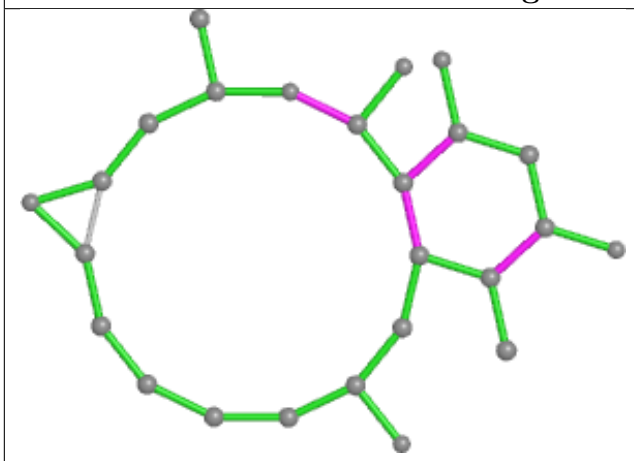
There are no ring outliers.

1 monomer is involved in 1 short contact:

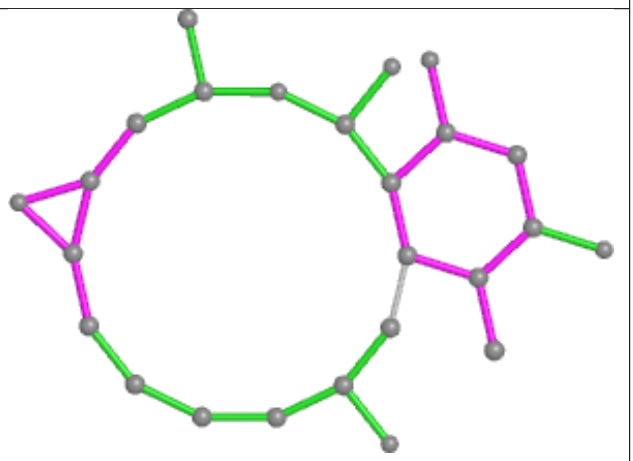
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	408	RDC	1	0

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 then 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.

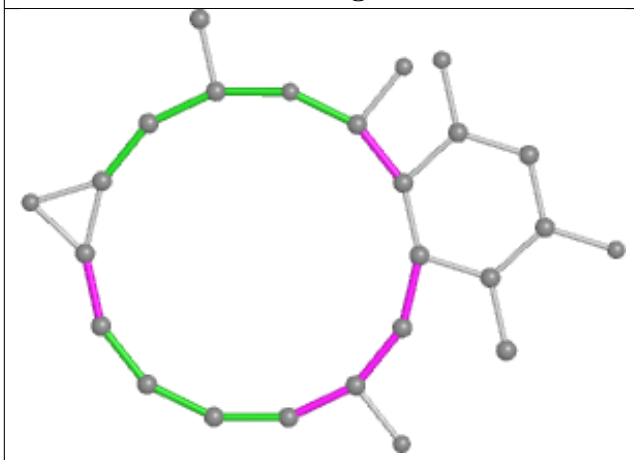
Ligand RDC A 408



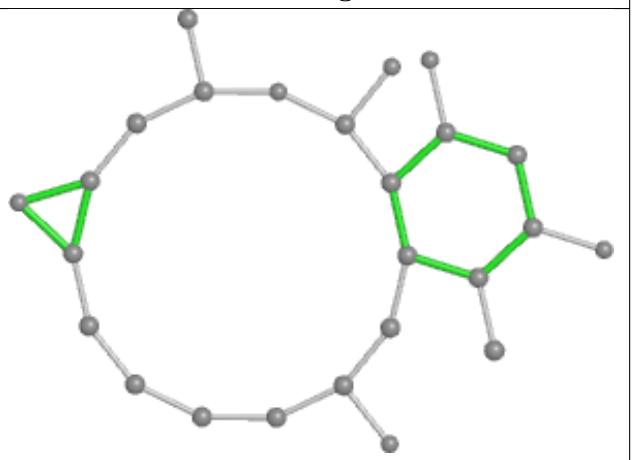
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	369/419 (88%)	0.32	10 (2%) 54 48	32, 53, 76, 126	0
2	B	93/128 (72%)	0.69	13 (13%) 2 1	45, 51, 63, 79	0
All	All	462/547 (84%)	0.39	23 (4%) 28 23	32, 53, 75, 126	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ASP	4.6
1	A	177	ASN	4.0
2	B	212	ALA	3.4
2	B	218	ALA	3.3
1	A	102	PRO	3.1
1	A	139	PHE	3.1
2	B	187	ALA	2.9
2	B	214	ILE	2.8
2	B	131	PRO	2.8
2	B	210	LYS	2.7
2	B	217	PHE	2.7
2	B	220	TYR	2.7
1	A	399	ALA	2.6
2	B	129	TYR	2.5
1	A	180	HIS	2.3
1	A	38	ASP	2.3
2	B	155	LYS	2.3
1	A	179	VAL	2.3
2	B	130	PRO	2.2
2	B	209	GLU	2.2
1	A	400	SER	2.1
1	A	100	GLU	2.0
1	A	342	LEU	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)

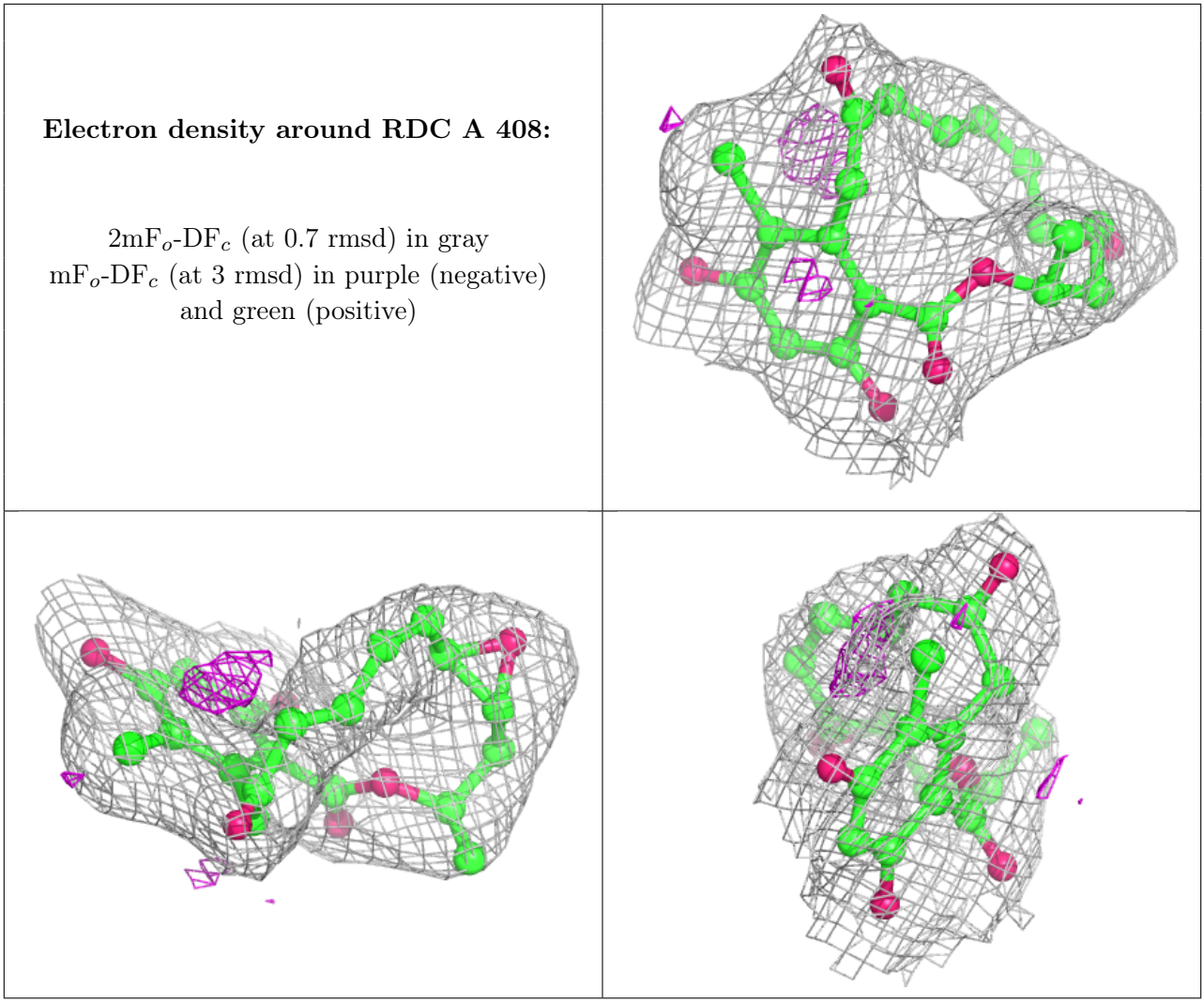
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	K	A	407	1/1	0.87	0.17	64,64,64,64	0
5	GOL	A	409	6/6	0.95	0.24	36,45,48,49	0
6	RED	B	300	11/12	0.95	0.21	46,53,62,66	0
4	RDC	A	408	25/25	0.98	0.18	33,42,47,50	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 RDC A 408:

$2mF_o$-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.