



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:50 am BST

PDB ID : 3RV9
Title : Structure of a M. tuberculosis Salicylate Synthase, MbtI, in Complex with an Inhibitor with Ethyl R-Group
Authors : Chi, G.; Bulloch, E.M.M.; Manos-Turvey, A.; Payne, R.J.; Lott, J.S.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2011-05-06
Resolution : 2.14 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 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

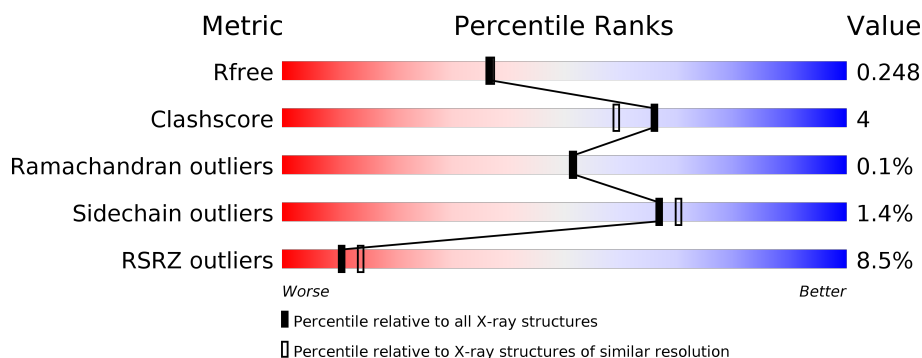
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	450	<div> <div>6%</div> <div>89% 7%</div> </div>
1	B	450	<div> <div>6%</div> <div>87% 6% 7%</div> </div>
1	C	450	<div> <div>5%</div> <div>83% 9% 8%</div> </div>
1	D	450	<div> <div>14%</div> <div>85% 9% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RVD	C	451	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13135 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.

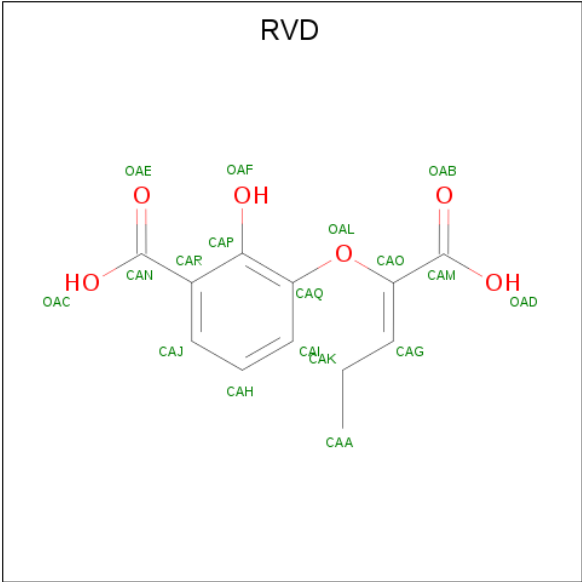
- Molecule 1 is a protein called Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	2	0
			3189	2001	570	608	10			
1	B	420	Total	C	N	O	S	5	2	0
			3188	2004	570	604	10			
1	C	413	Total	C	N	O	S	0	0	0
			3127	1960	557	600	10			
1	D	425	Total	C	N	O	S	0	0	0
			3184	1999	566	609	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	EXPRESSION TAG	UNP Q7D785
B	1	VAL	-	EXPRESSION TAG	UNP Q7D785
C	1	VAL	-	EXPRESSION TAG	UNP Q7D785
D	1	VAL	-	EXPRESSION TAG	UNP Q7D785

- Molecule 2 is 3-([(1Z)-1-carboxybut-1-en-1-yl]oxy)-2-hydroxybenzoic acid (three-letter code: RVD) (formula: C₁₂H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		
2	C	1	Total	C	O	0	0
			18	12	6		
2	D	1	Total	C	O	0	0
			18	12	6		

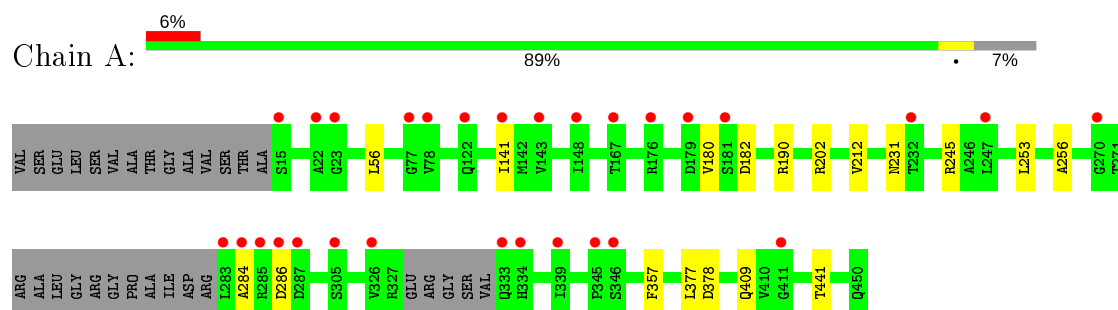
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	102	Total	O	0	0
			102	102		
3	C	102	Total	O	0	0
			102	102		
3	D	60	Total	O	0	0
			60	60		

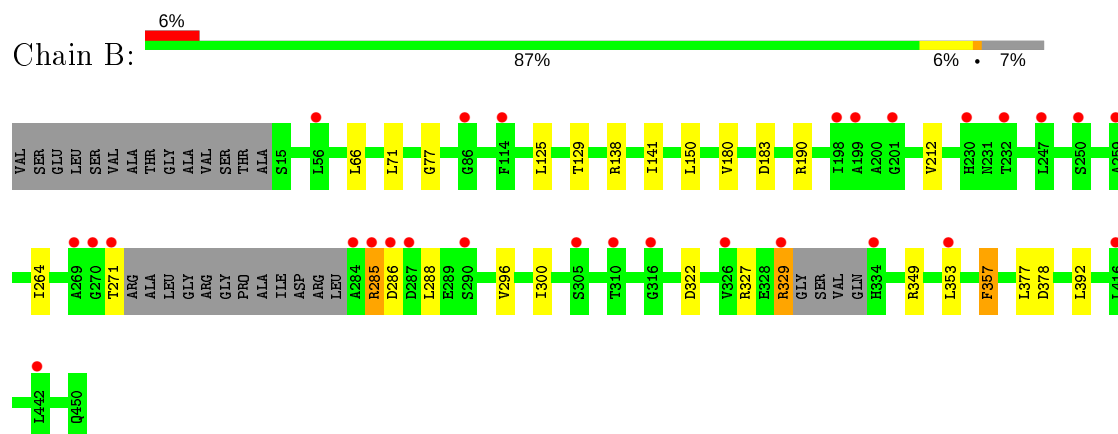
3 Residue-property plots [i](#)

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.

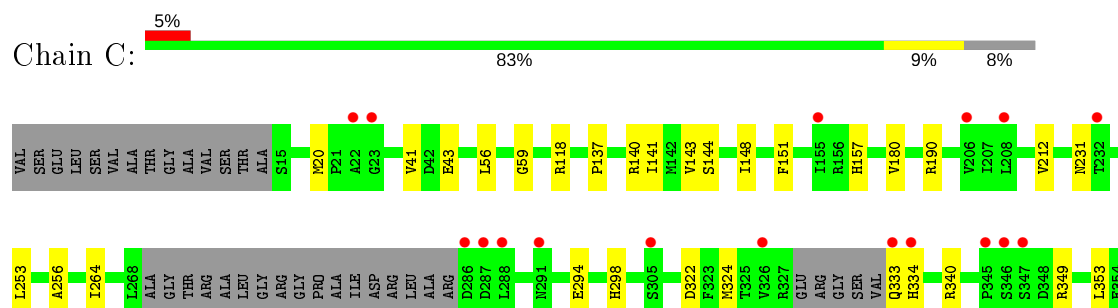
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI



- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI



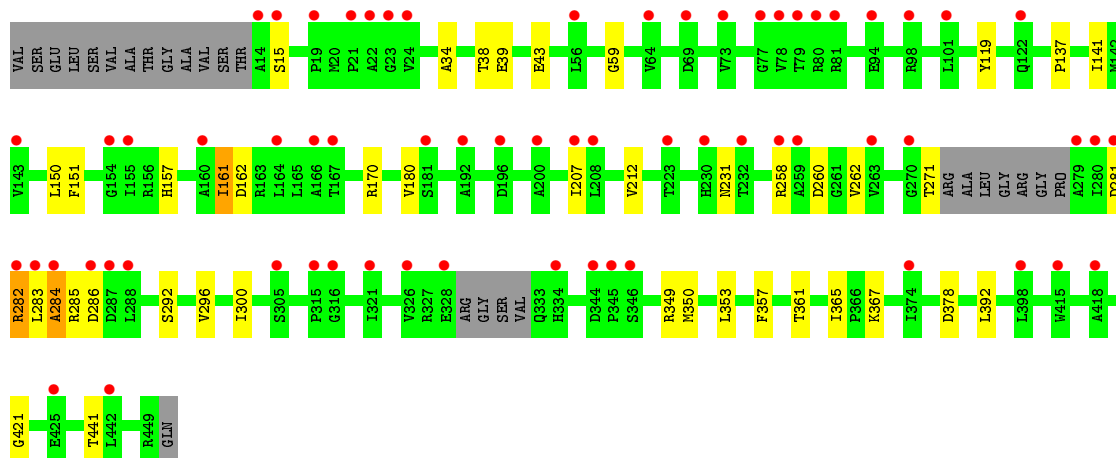
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI





- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain D: 14% 85% 9% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.27Å 115.47Å 95.47Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	19.84 – 2.14 19.84 – 2.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.84-2.14) 98.5 (19.84-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.15Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.207 , 0.229 0.225 , 0.248	Depositor DCC
R_{free} test set	5102 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13135	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: RVD

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	0.51	0/3246	0.67	0/4411
1	B	0.49	0/3249	0.72	3/4411 (0.1%)
1	C	0.50	0/3181	0.67	0/4325
1	D	0.56	0/3239	0.66	0/4405
All	All	0.52	0/12915	0.68	3/17552 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329[A]	ARG	CB-CA-C	10.17	130.74	110.40
1	B	329[B]	ARG	CB-CA-C	10.17	130.74	110.40
1	B	183	ASP	CB-CG-OD1	5.22	122.99	118.30

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	3189	0	3153	10	0
1	B	3188	0	3164	27	0
1	C	3127	0	3080	25	0
1	D	3184	0	3115	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	18	0	9	0	0
2	B	18	0	9	0	0
2	C	18	0	9	7	0
2	D	18	0	9	3	0
3	A	111	0	0	0	0
3	B	102	0	0	0	0
3	C	102	0	0	0	0
3	D	60	0	0	0	0
All	All	13135	0	12548	100	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 4.

All (100) 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:D:284:ALA:N	1:D:285:ARG:HB3	1.42	1.35
1:D:284:ALA:HA	1:D:286:ASP:N	1.44	1.31
1:D:284:ALA:H	1:D:285:ARG:CB	1.51	1.23
1:B:285:ARG:O	1:B:285:ARG:HD3	1.45	1.15
1:D:284:ALA:CA	1:D:286:ASP:H	1.60	1.12
1:D:284:ALA:HA	1:D:286:ASP:H	0.82	0.96
1:C:361:THR:HG21	2:C:451:RVD:HAAA	1.48	0.95
1:A:284:ALA:HA	1:A:286:ASP:H	1.31	0.93
1:C:361:THR:HG21	2:C:451:RVD:CAA	2.00	0.90
1:B:285:ARG:NH2	1:B:288:LEU:HB2	1.86	0.88
1:B:285:ARG:HD3	1:B:285:ARG:C	1.92	0.88
1:D:260:ASP:OD1	1:D:262:VAL:HG12	1.75	0.87
1:C:361:THR:CG2	2:C:451:RVD:HAAA	2.10	0.80
1:D:283:LEU:O	1:D:284:ALA:CB	2.30	0.80
1:B:77:GLY:HA3	1:D:170:ARG:HD3	1.63	0.79
1:B:285:ARG:HH22	1:B:288:LEU:CB	1.96	0.79
1:C:20:MET:HE3	1:C:144:SER:O	1.84	0.76
1:B:285:ARG:CD	1:B:285:ARG:C	2.53	0.76
1:B:285:ARG:O	1:B:285:ARG:CD	2.30	0.76
1:D:284:ALA:CA	1:D:286:ASP:N	2.32	0.74
1:B:285:ARG:NH2	1:B:288:LEU:H	1.86	0.73
1:D:157:HIS:O	1:D:161:ILE:HG23	1.90	0.71
1:C:20:MET:HE1	1:C:143:VAL:HG13	1.73	0.71
1:B:285:ARG:HH22	1:B:288:LEU:HB2	1.50	0.69
1:B:285:ARG:NH2	1:B:288:LEU:CB	2.52	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:LEU:O	1:D:284:ALA:HB3	1.95	0.66
1:D:281:ASP:O	1:D:282:ARG:HB2	1.98	0.62
1:D:141:ILE:HD12	1:D:150:LEU:HD22	1.82	0.62
1:B:141:ILE:HD12	1:B:150:LEU:HD22	1.82	0.61
1:B:285:ARG:O	1:B:285:ARG:NH1	2.34	0.60
2:D:451:RVD:HAI	2:D:451:RVD:CAM	2.33	0.58
1:C:361:THR:CG2	2:C:451:RVD:CAA	2.75	0.57
1:A:231:ASN:OD1	1:A:441:THR:HG23	2.05	0.57
1:D:284:ALA:N	1:D:286:ASP:H	2.04	0.55
1:A:284:ALA:HA	1:A:286:ASP:N	2.11	0.55
1:D:284:ALA:N	1:D:285:ARG:CB	2.30	0.55
1:B:66:LEU:HD13	1:B:71:LEU:HD12	1.89	0.55
1:D:207:ILE:HG13	1:D:421:GLY:HA2	1.89	0.54
1:C:353:LEU:O	1:C:357:PHE:HB2	2.09	0.52
1:B:285:ARG:HH21	1:B:288:LEU:H	1.57	0.52
1:C:41:VAL:HG21	1:C:157:HIS:CE1	2.44	0.52
1:B:180:VAL:HG12	1:B:212:VAL:HG11	1.92	0.52
1:D:284:ALA:H	1:D:285:ARG:HB3	0.57	0.51
1:C:231:ASN:OD1	1:C:441:THR:HG23	2.11	0.51
1:A:180:VAL:HG12	1:A:212:VAL:HG11	1.93	0.50
1:B:190:ARG:HD2	1:B:377:LEU:O	2.10	0.50
1:C:43:GLU:HB2	1:C:59:GLY:HA2	1.94	0.50
1:B:322:ASP:HB3	1:B:327:ARG:HH22	1.77	0.49
1:D:292:SER:O	1:D:296:VAL:HG12	2.12	0.49
1:C:20:MET:HE2	1:C:148:ILE:HG13	1.95	0.49
1:B:296:VAL:O	1:B:300:ILE:HG12	2.12	0.48
1:A:56:LEU:HD23	1:A:141:ILE:HD12	1.94	0.48
1:C:180:VAL:HG12	1:C:212:VAL:HG11	1.95	0.48
1:D:180:VAL:HG12	1:D:212:VAL:HG11	1.95	0.48
1:D:258:ARG:HG3	1:D:262:VAL:HG13	1.94	0.47
1:D:43:GLU:OE2	1:D:157:HIS:NE2	2.44	0.47
1:C:190:ARG:HD2	1:C:377:LEU:O	2.14	0.47
1:D:284:ALA:CA	1:D:285:ARG:HB3	2.35	0.47
1:C:361:THR:HG21	2:C:451:RVD:HAAB	1.91	0.47
1:C:298:HIS:HB3	1:C:324:MET:HE2	1.97	0.46
1:C:56:LEU:HD23	1:C:141:ILE:HD12	1.96	0.46
1:A:245[B]:ARG:HB2	1:A:409:GLN:HB3	1.97	0.46
1:C:264:ILE:CD1	1:C:340:ARG:HG3	2.45	0.46
2:C:451:RVD:HAI	2:C:451:RVD:CAM	2.45	0.46
1:D:161:ILE:HG13	1:D:162:ASP:N	2.31	0.46
1:B:285:ARG:HH22	1:B:288:LEU:HB3	1.76	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:O	1:B:357:PHE:HB2	2.16	0.46
1:A:245[A]:ARG:HB2	1:A:409:GLN:HB3	1.98	0.45
1:C:118:ARG:NH1	1:C:355:ALA:O	2.49	0.45
1:C:59:GLY:O	1:C:137:PRO:HA	2.16	0.45
1:D:34:ALA:O	1:D:38:THR:OG1	2.26	0.45
1:C:20:MET:CE	1:C:148:ILE:HG13	2.47	0.45
1:C:362:ALA:HB1	1:C:386:SER:HB2	1.99	0.45
1:D:15:SER:HB3	1:D:151:PHE:CE1	2.52	0.45
1:C:333:GLN:HG3	1:C:334:HIS:H	1.81	0.45
1:A:190:ARG:HD2	1:A:377:LEU:O	2.17	0.44
2:C:451:RVD:CAM	2:C:451:RVD:CAI	2.93	0.44
1:D:300:ILE:HG21	1:D:365:ILE:HG21	1.99	0.44
1:B:285:ARG:NH2	1:B:288:LEU:N	2.59	0.44
2:D:451:RVD:CAI	2:D:451:RVD:CAM	2.87	0.44
1:B:322:ASP:HB3	1:B:327:ARG:NH2	2.32	0.44
1:D:282:ARG:HB3	1:D:283:LEU:H	1.51	0.44
1:D:283:LEU:O	1:D:284:ALA:HB2	2.12	0.44
1:D:284:ALA:CA	1:D:285:ARG:CB	2.95	0.44
1:B:285:ARG:HH21	1:B:288:LEU:N	2.14	0.43
1:D:119:TYR:OH	1:D:367:LYS:HD2	2.18	0.43
1:D:361:THR:HG21	2:D:451:RVD:HAK	2.00	0.43
1:D:353:LEU:O	1:D:357:PHE:HB2	2.19	0.43
1:B:285:ARG:CZ	1:B:286:ASP:HA	2.49	0.42
1:B:138:ARG:NH2	1:D:39:GLU:OE2	2.46	0.42
1:C:140:ARG:HB2	1:C:151:PHE:HB2	2.02	0.41
1:B:125:LEU:HD22	1:B:129:THR:HG21	2.03	0.41
1:D:231:ASN:OD1	1:D:441:THR:HG23	2.20	0.41
1:A:253:LEU:HD21	1:A:256:ALA:HB2	2.03	0.41
1:D:349:ARG:HD2	1:D:392:LEU:HD23	2.03	0.41
1:A:245[B]:ARG:NH1	1:A:409:GLN:OE1	2.52	0.41
1:B:349:ARG:HD2	1:B:392:LEU:HD23	2.03	0.40
1:C:253:LEU:HD21	1:C:256:ALA:HB2	2.04	0.40
1:C:349:ARG:HD2	1:C:392:LEU:HD23	2.03	0.40
1:D:59:GLY:O	1:D:137:PRO:HA	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	416/450 (92%)	411 (99%)	5 (1%)	0	100	100
1	B	415/450 (92%)	410 (99%)	5 (1%)	0	100	100
1	C	407/450 (90%)	403 (99%)	4 (1%)	0	100	100
1	D	419/450 (93%)	411 (98%)	6 (1%)	2 (0%)	29	22
All	All	1657/1800 (92%)	1635 (99%)	20 (1%)	2 (0%)	51	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	282	ARG
1	D	284	ALA

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	327/358 (91%)	323 (99%)	4 (1%)	71	74
1	B	327/358 (91%)	320 (98%)	7 (2%)	53	54
1	C	323/358 (90%)	319 (99%)	4 (1%)	71	74
1	D	320/358 (89%)	316 (99%)	4 (1%)	69	73
All	All	1297/1432 (91%)	1278 (98%)	19 (2%)	67	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ASP
1	A	202	ARG
1	A	357	PHE
1	A	378	ASP
1	B	264	ILE
1	B	271	THR
1	B	285	ARG
1	B	329[A]	ARG
1	B	329[B]	ARG
1	B	357	PHE
1	B	378	ASP
1	C	294	GLU
1	C	322	ASP
1	C	360	VAL
1	C	378	ASP
1	D	161	ILE
1	D	271	THR
1	D	350	MET
1	D	378	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RVD	B	451	-	13,18,18	2.38	4 (30%)	14,24,24	1.01	0
2	RVD	C	451	-	13,18,18	2.82	5 (38%)	14,24,24	1.11	1 (7%)
2	RVD	A	451	-	13,18,18	2.97	7 (53%)	14,24,24	1.91	3 (21%)
2	RVD	D	451	-	13,18,18	2.54	5 (38%)	14,24,24	1.88	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RVD	B	451	-	-	0/7/15/15	0/1/1/1
2	RVD	C	451	-	-	0/7/15/15	0/1/1/1
2	RVD	A	451	-	-	1/7/15/15	0/1/1/1
2	RVD	D	451	-	-	0/7/15/15	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	RVD	OAL-CAQ	-6.06	1.29	1.41
2	B	451	RVD	CAK-CAG	-5.83	1.36	1.50
2	D	451	RVD	CAK-CAG	-5.75	1.37	1.50
2	A	451	RVD	CAR-CAN	5.43	1.52	1.47
2	C	451	RVD	CAK-CAG	-5.37	1.37	1.50
2	C	451	RVD	CAR-CAN	5.10	1.52	1.47
2	A	451	RVD	CAK-CAG	-4.72	1.39	1.50
2	C	451	RVD	OAL-CAQ	-4.65	1.31	1.41
2	B	451	RVD	OAL-CAQ	-3.96	1.33	1.41
2	D	451	RVD	OAL-CAQ	-3.77	1.33	1.41
2	D	451	RVD	CAR-CAN	3.59	1.50	1.47
2	C	451	RVD	CAQ-CAP	-3.54	1.35	1.40
2	D	451	RVD	CAG-CAO	-2.86	1.30	1.32
2	B	451	RVD	CAR-CAN	2.82	1.50	1.47
2	B	451	RVD	CAQ-CAP	-2.79	1.36	1.40
2	A	451	RVD	CAQ-CAP	-2.70	1.36	1.40
2	D	451	RVD	CAR-CAP	-2.40	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	RVD	CAR-CAP	-2.34	1.36	1.40
2	A	451	RVD	CAG-CAO	-2.15	1.31	1.32
2	C	451	RVD	OAF-CAP	-2.03	1.32	1.37
2	A	451	RVD	OAF-CAP	-2.00	1.32	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	451	RVD	CAK-CAG-CAO	-4.98	118.37	126.24
2	D	451	RVD	CAK-CAG-CAO	-4.84	118.59	126.24
2	D	451	RVD	CAQ-OAL-CAO	-4.39	111.54	118.50
2	A	451	RVD	CAQ-OAL-CAO	-3.29	113.28	118.50
2	A	451	RVD	CAI-CAQ-CAP	2.80	122.56	119.97
2	C	451	RVD	CAK-CAG-CAO	-2.17	122.81	126.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

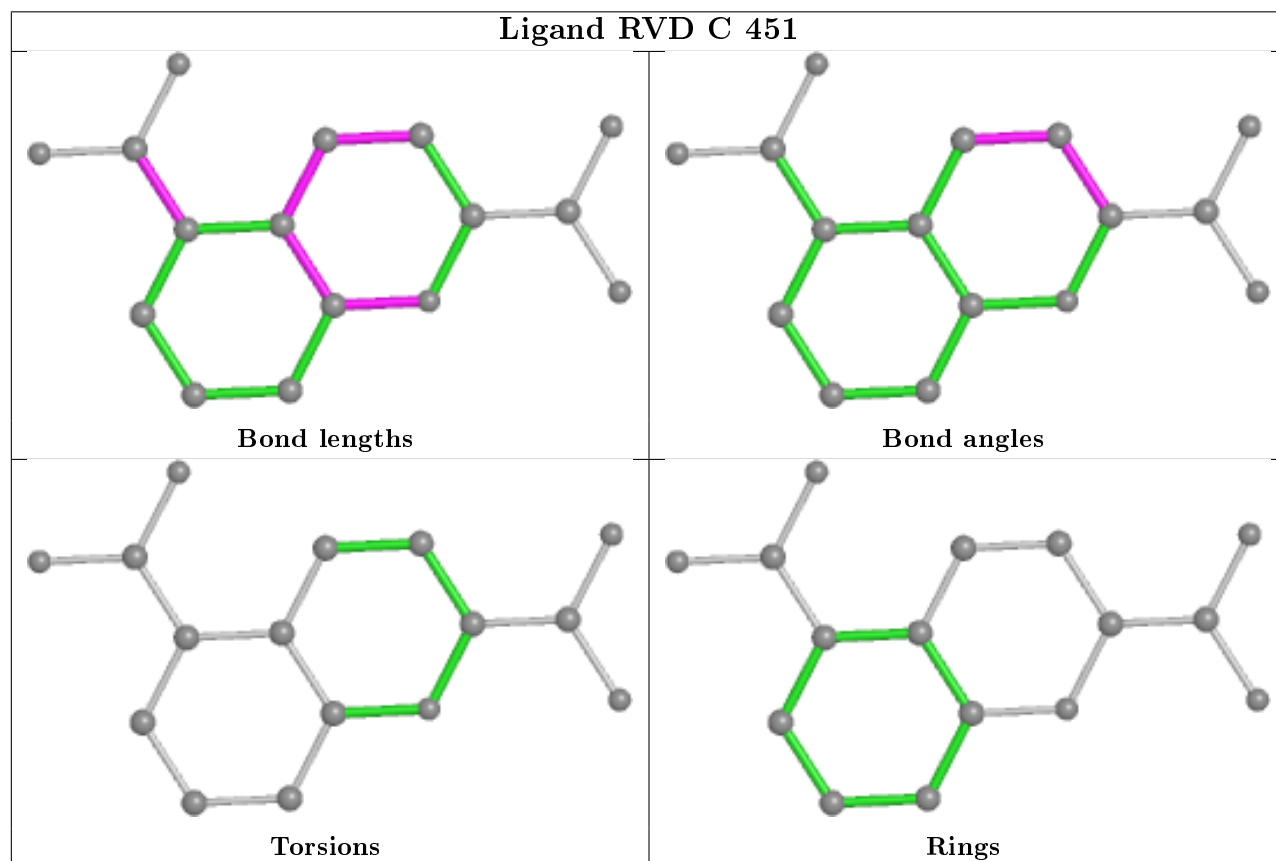
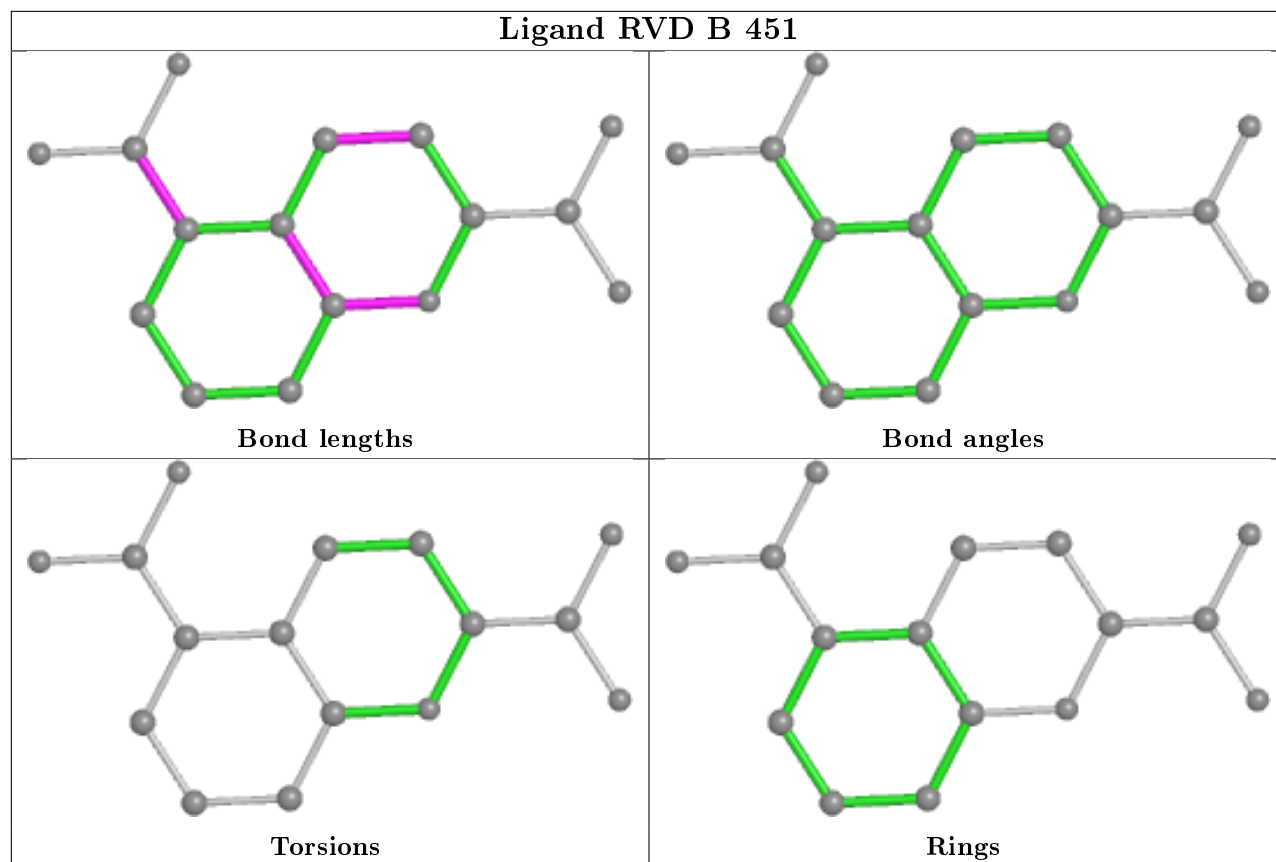
Mol	Chain	Res	Type	Atoms
2	A	451	RVD	CAK-CAG-CAO-CAM

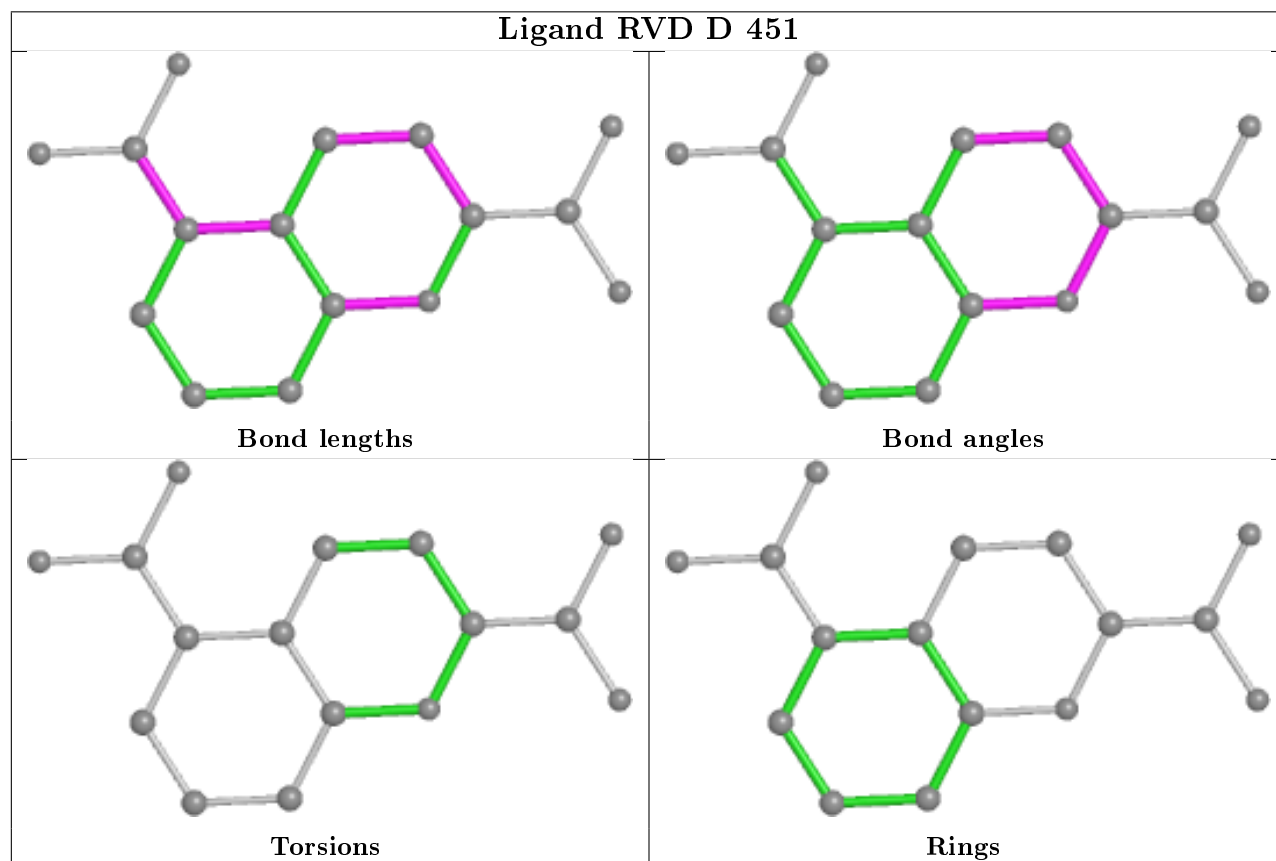
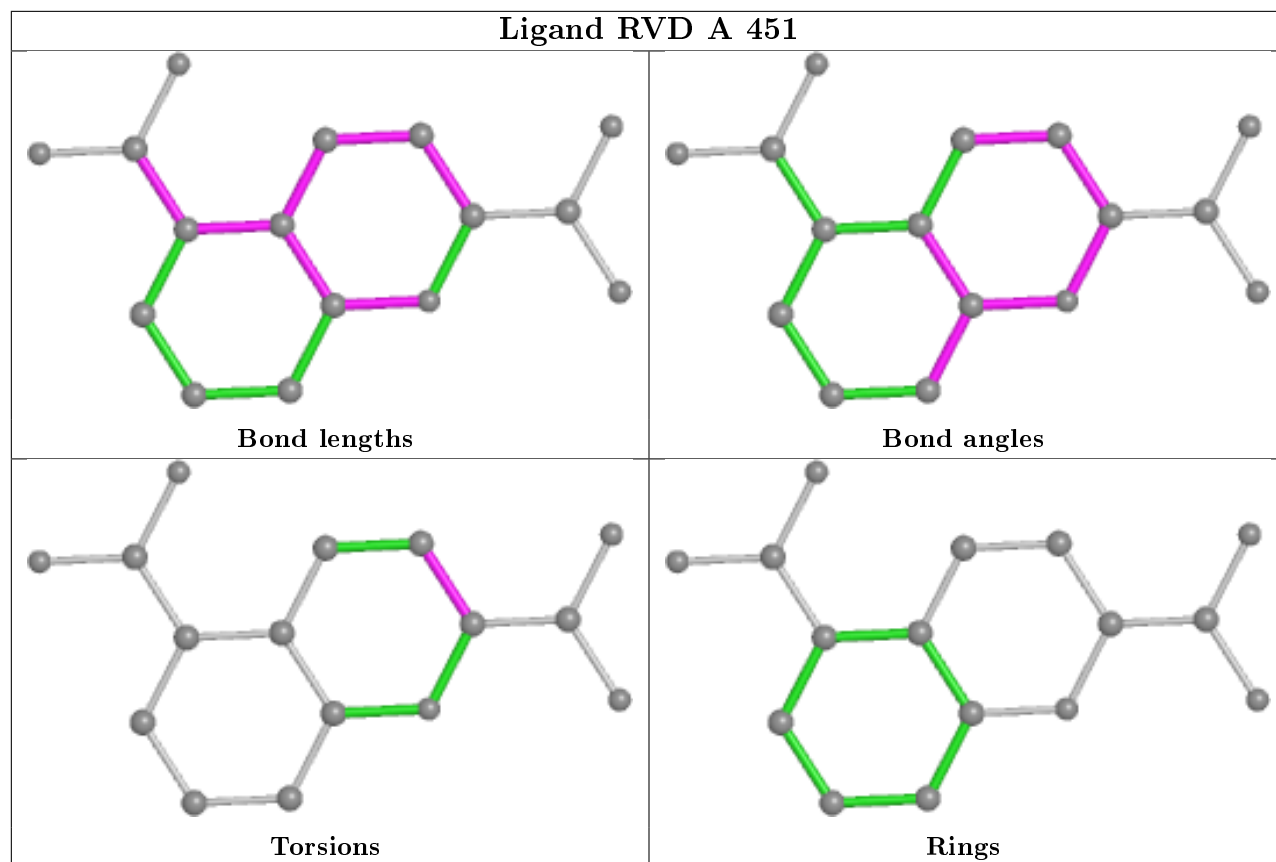
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	451	RVD	7	0
2	D	451	RVD	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

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

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	420/450 (93%)	0.45	29 (6%)	16 21	19, 37, 62, 90	8 (1%)
1	B	419/450 (93%)	0.41	28 (6%)	17 22	20, 37, 61, 82	8 (1%)
1	C	413/450 (91%)	0.45	21 (5%)	28 34	19, 39, 61, 87	8 (1%)
1	D	425/450 (94%)	0.83	65 (15%)	2 2	24, 48, 76, 91	8 (1%)
All	All	1677/1800 (93%)	0.54	143 (8%)	10 14	19, 40, 68, 91	32 (1%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	ILE	8.4
1	D	279	ALA	7.8
1	B	285	ARG	5.6
1	C	155	ILE	5.5
1	A	284	ALA	5.2
1	D	345	PRO	5.2
1	A	283	LEU	4.9
1	D	155	ILE	4.6
1	D	284	ALA	4.5
1	A	23	GLY	4.4
1	A	22	ALA	4.3
1	D	166	ALA	4.3
1	C	288	LEU	4.3
1	D	346	SER	4.3
1	B	326	VAL	4.3
1	B	86	GLY	4.2
1	D	281	ASP	4.2
1	D	23	GLY	4.1
1	C	333	GLN	4.0
1	D	79	THR	4.0
1	A	141	ILE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	263	VAL	4.0
1	D	288	LEU	3.9
1	C	346	SER	3.9
1	B	329[A]	ARG	3.9
1	C	347	SER	3.8
1	A	326	VAL	3.8
1	C	287	ASP	3.8
1	C	345	PRO	3.7
1	D	167	THR	3.6
1	D	208	LEU	3.6
1	C	326	VAL	3.5
1	C	22	ALA	3.5
1	D	22	ALA	3.5
1	D	14	ALA	3.5
1	D	81	ARG	3.4
1	D	154	GLY	3.4
1	D	232	THR	3.4
1	D	328	GLU	3.4
1	B	286	ASP	3.3
1	D	259	ALA	3.3
1	B	232	THR	3.3
1	A	333	GLN	3.3
1	A	305	SER	3.2
1	D	270	GLY	3.2
1	B	271	THR	3.1
1	B	270	GLY	3.1
1	B	442	LEU	3.1
1	D	415	TRP	3.0
1	D	374	ILE	3.0
1	D	287	ASP	3.0
1	D	73	VAL	3.0
1	A	15	SER	3.0
1	A	285[A]	ARG	2.9
1	D	326	VAL	2.9
1	A	334	HIS	2.9
1	D	230	HIS	2.8
1	B	199	ALA	2.8
1	C	291	ASN	2.8
1	C	208	LEU	2.8
1	B	198	ILE	2.8
1	D	321	ILE	2.8
1	A	143	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	286	ASP	2.8
1	A	176	ARG	2.8
1	D	196	ASP	2.7
1	C	232	THR	2.7
1	A	270	GLY	2.7
1	B	259	ALA	2.7
1	A	77	GLY	2.7
1	B	269	ALA	2.7
1	D	21	PRO	2.7
1	D	398	LEU	2.7
1	B	201	GLY	2.7
1	B	284	ALA	2.7
1	D	442	LEU	2.7
1	B	305	SER	2.7
1	A	78	VAL	2.6
1	A	148	ILE	2.6
1	A	411	GLY	2.6
1	A	181	SER	2.6
1	D	200	ALA	2.5
1	B	247	LEU	2.5
1	D	164	LEU	2.5
1	B	250	SER	2.5
1	C	286	ASP	2.5
1	D	305	SER	2.5
1	A	339	ILE	2.5
1	A	167	THR	2.4
1	B	416	LEU	2.4
1	D	315	PRO	2.4
1	D	122	GLN	2.4
1	D	282	ARG	2.4
1	C	442	LEU	2.4
1	D	24	VAL	2.4
1	D	19	PRO	2.4
1	A	346	SER	2.4
1	B	290	SER	2.4
1	A	232	THR	2.3
1	C	411	GLY	2.3
1	D	77	GLY	2.3
1	D	160	ALA	2.3
1	D	258	ARG	2.3
1	D	101	LEU	2.3
1	D	80	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	316	GLY	2.3
1	D	56	LEU	2.2
1	A	286	ASP	2.2
1	D	78	VAL	2.2
1	D	425	GLU	2.2
1	D	15	SER	2.2
1	B	287	ASP	2.2
1	D	316	GLY	2.2
1	D	94	GLU	2.2
1	B	334	HIS	2.2
1	A	122	GLN	2.2
1	D	192	ALA	2.2
1	D	223	THR	2.2
1	A	179	ASP	2.2
1	D	344	ASP	2.2
1	A	287	ASP	2.1
1	D	283	LEU	2.1
1	D	334	HIS	2.1
1	A	247	LEU	2.1
1	C	416	LEU	2.1
1	D	418	ALA	2.1
1	B	56	LEU	2.1
1	C	23	GLY	2.1
1	C	305	SER	2.1
1	D	181	SER	2.1
1	D	143	VAL	2.1
1	B	114	PHE	2.1
1	D	98	ARG	2.1
1	B	353	LEU	2.1
1	A	345	PRO	2.1
1	C	206	VAL	2.1
1	B	310	THR	2.1
1	C	374	ILE	2.0
1	C	334	HIS	2.0
1	D	69	ASP	2.0
1	D	207	ILE	2.0
1	B	230	HIS	2.0
1	D	64	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

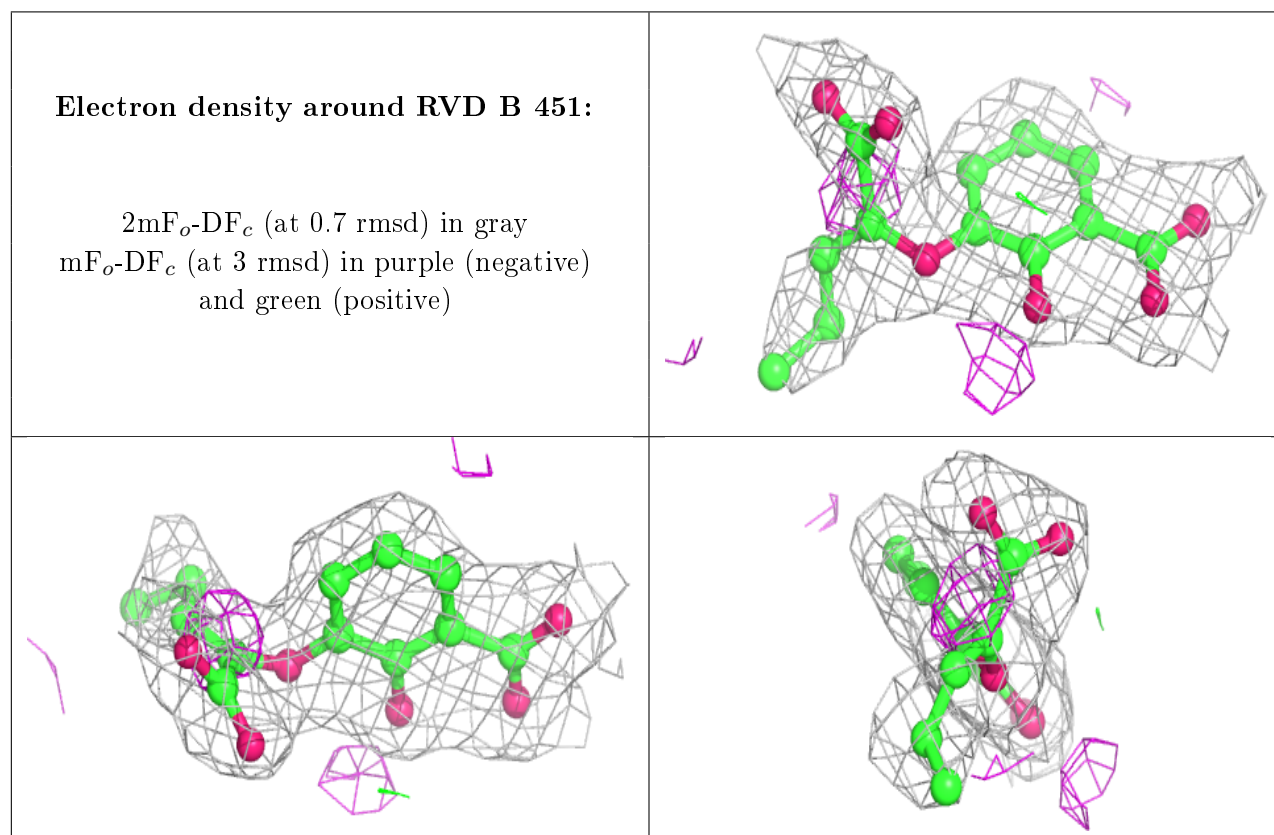
There are no carbohydrates in this entry.

6.4 Ligands [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, 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.

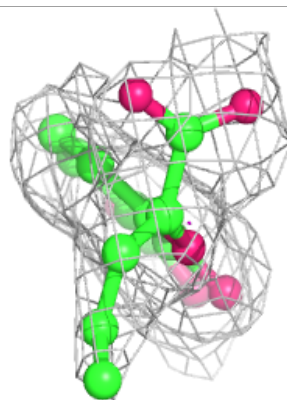
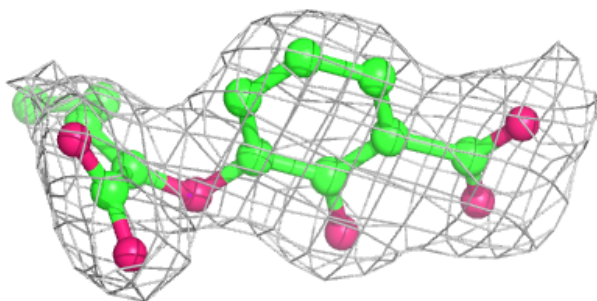
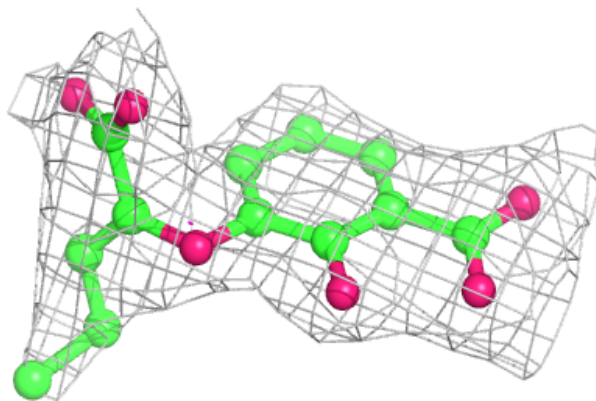
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RVD	B	451	18/18	0.84	0.21	33,38,51,51	0
2	RVD	D	451	18/18	0.86	0.18	37,46,62,64	0
2	RVD	C	451	18/18	0.89	0.16	32,34,50,51	0
2	RVD	A	451	18/18	0.93	0.14	23,33,45,47	0

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.

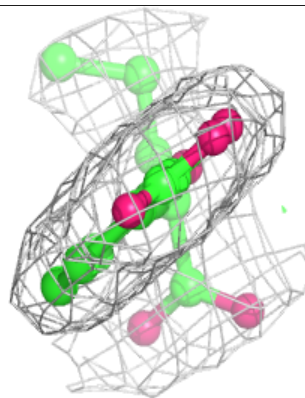
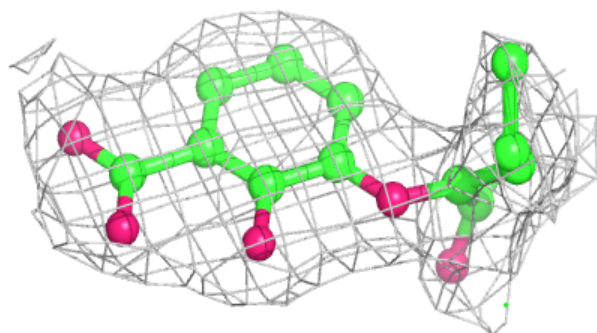
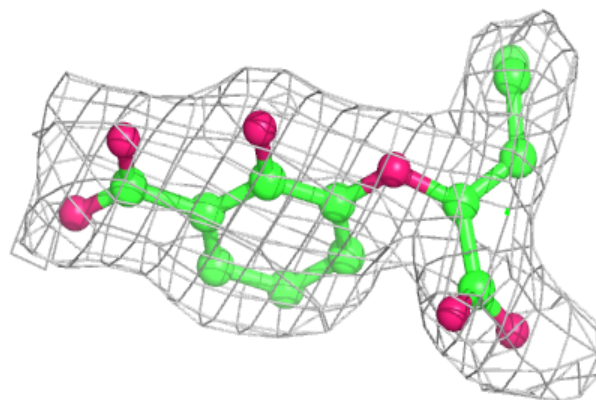


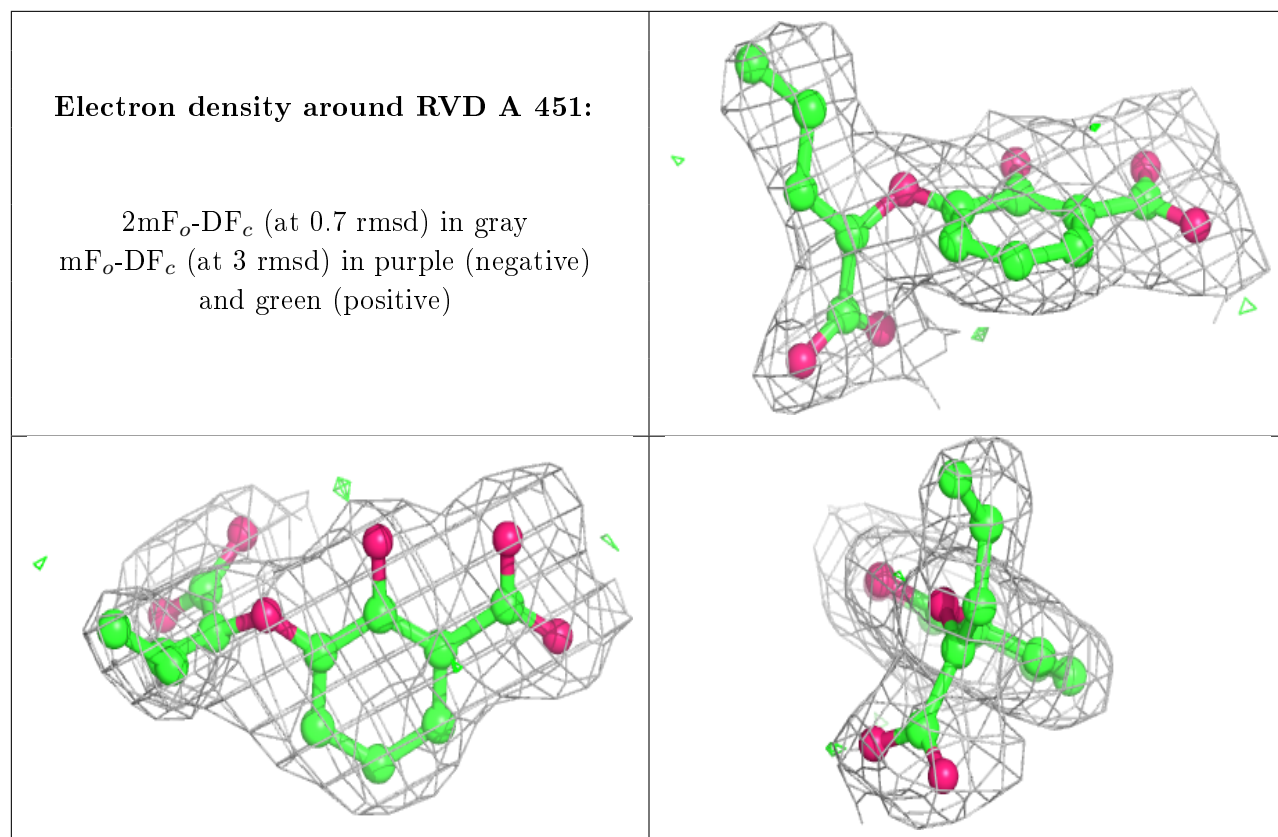
Electron density around RVD D 451:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around RVD C 451:**

$2mF_o-DF_c$ (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.