



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:42 PM UTC

PDB ID : 3RV7 / pdb_00003rv7
Title : Structure of a M. tuberculosis Salicylate Synthase, MbtI, in Complex with an Inhibitor with Isopropyl 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 : 2.50 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

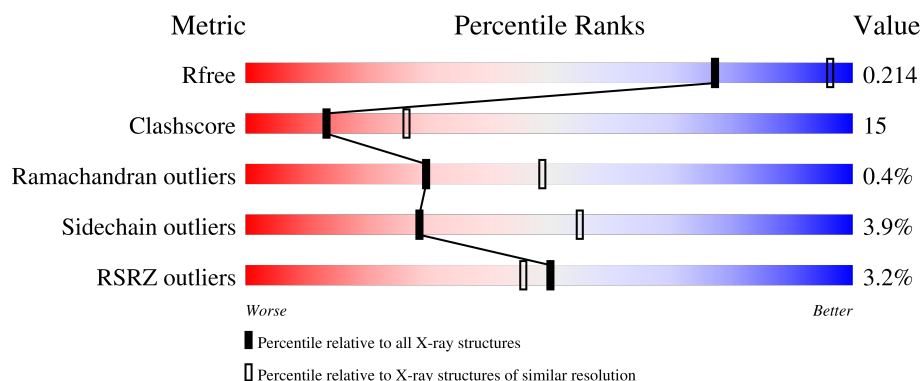
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	450	3% 56% 32% • 8%
1	B	450	3% 61% 29% • 6%
1	C	450	4% 61% 29% 5% •
1	D	450	3% 67% 25% • 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RVB	A	451	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13371 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.

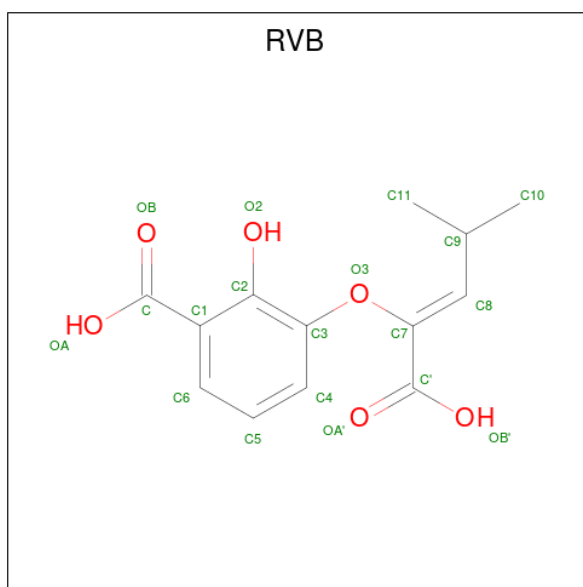
- Molecule 1 is a protein called Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	2	0
			3151	1981	559	601	10			
1	B	423	Total	C	N	O	S	0	1	0
			3211	2012	580	609	10			
1	C	431	Total	C	N	O	S	0	0	0
			3254	2036	588	620	10			
1	D	428	Total	C	N	O	S	0	0	0
			3222	2021	571	620	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-carboxy-3-methylbut-1-en-1-yl]oxy}-2-hydroxybenzoic acid (CCD ID: RVB) (formula: C₁₃H₁₄O₆).



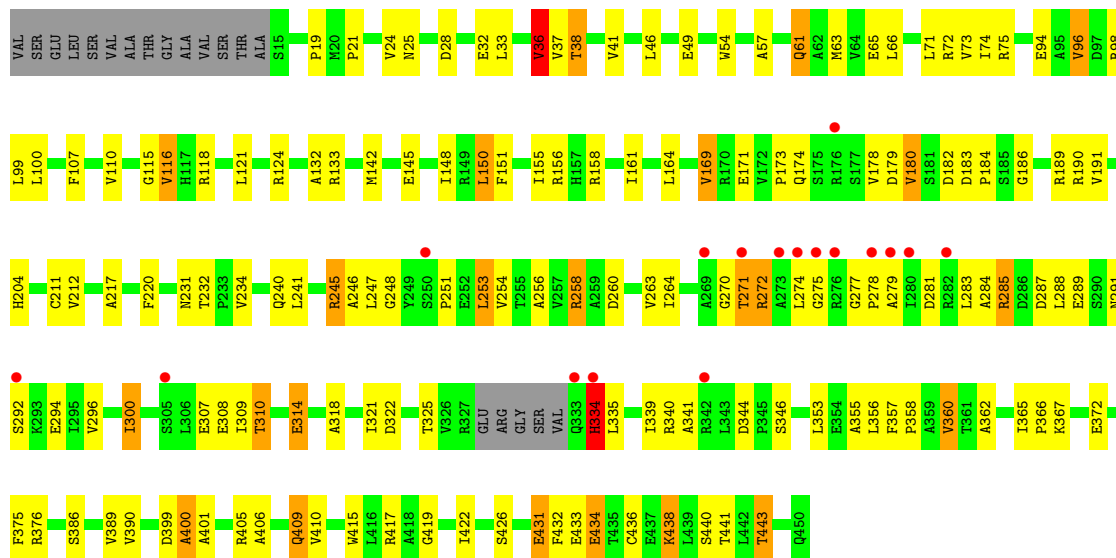
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	13	6		
2	B	1	Total	C	O	0	0
			19	13	6		
2	C	1	Total	C	O	4	0
			19	13	6		
2	D	1	Total	C	O	0	0
			19	13	6		

- Molecule 3 is water.

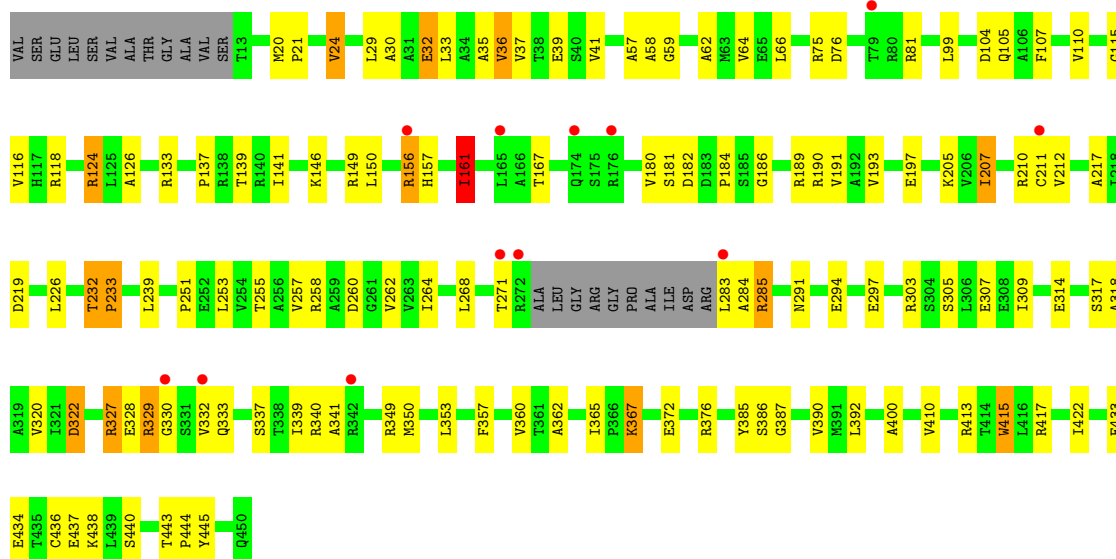
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total	O	0	0
			121	121		
3	B	118	Total	O	0	0
			118	118		
3	C	115	Total	O	0	0
			115	115		
3	D	103	Total	O	0	0
			103	103		



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.67Å 113.94Å 95.23Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	19.78 – 2.50 19.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.78-2.50) 99.5 (19.78-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.184 , 0.222 0.198 , 0.214	Depositor DCC
R_{free} test set	3224 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13371	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RVB

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	2.03	51/3213 (1.6%)	1.17	11/4370 (0.3%)
1	B	1.98	35/3270 (1.1%)	1.17	17/4444 (0.4%)
1	C	1.95	39/3311 (1.2%)	1.15	13/4501 (0.3%)
1	D	1.92	29/3278 (0.9%)	1.18	14/4459 (0.3%)
All	All	1.97	154/13072 (1.2%)	1.17	55/17774 (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	2

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	VAL	C-O	-6.91	1.17	1.24
1	C	220	PHE	C-O	-6.68	1.18	1.24
1	A	126	ALA	CA-CB	-6.62	1.44	1.53
1	C	438	LYS	C-O	-6.55	1.16	1.24
1	B	136	SER	C-O	-6.46	1.17	1.24
1	A	232	THR	C-O	-6.44	1.19	1.25
1	A	107	PHE	C-O	-6.41	1.16	1.23
1	A	387	GLY	C-O	-6.40	1.17	1.23
1	C	110	VAL	C-O	-6.39	1.17	1.24
1	B	398	LEU	C-O	-6.36	1.16	1.23
1	C	410	VAL	C-O	-6.32	1.17	1.24
1	B	58	ALA	CA-CB	-6.30	1.44	1.53
1	C	232	THR	C-O	-6.26	1.19	1.25
1	B	134	VAL	C-O	-6.23	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	LEU	C-O	-6.12	1.16	1.24
1	D	126	ALA	CA-CB	-6.12	1.44	1.53
1	B	410	VAL	C-O	-6.11	1.17	1.24
1	D	232	THR	C-O	-6.07	1.20	1.25
1	D	219	ASP	C-O	-6.07	1.16	1.24
1	A	48	TYR	C-O	-6.02	1.16	1.24
1	A	30	ALA	CA-CB	-5.99	1.44	1.53
1	A	96	VAL	C-O	-5.96	1.17	1.24
1	B	133	ARG	C-O	-5.96	1.17	1.24
1	D	320	VAL	C-O	-5.92	1.17	1.24
1	A	133	ARG	C-O	-5.92	1.17	1.24
1	C	389	VAL	C-O	-5.91	1.17	1.24
1	C	133	ARG	C-O	-5.90	1.17	1.24
1	B	400	ALA	C-O	-5.90	1.17	1.24
1	B	387	GLY	C-O	-5.89	1.18	1.24
1	A	32	GLU	C-O	-5.85	1.17	1.24
1	A	247	LEU	C-O	-5.81	1.16	1.23
1	D	107	PHE	C-O	-5.80	1.16	1.23
1	D	133	ARG	C-O	-5.79	1.17	1.24
1	B	46	LEU	C-O	-5.79	1.17	1.23
1	A	140	ARG	C-O	-5.79	1.17	1.24
1	A	143	VAL	C-O	-5.76	1.17	1.24
1	C	73	VAL	C-O	-5.75	1.18	1.24
1	A	400	ALA	CA-CB	-5.75	1.44	1.53
1	A	64	VAL	C-O	-5.75	1.17	1.24
1	C	217	ALA	CA-CB	-5.73	1.43	1.53
1	B	264	ILE	C-O	-5.71	1.18	1.24
1	C	390	VAL	C-O	-5.70	1.18	1.24
1	A	399	ASP	C-O	-5.69	1.17	1.24
1	B	132	ALA	C-O	-5.69	1.17	1.23
1	A	47	LEU	C-O	-5.69	1.17	1.24
1	A	46	LEU	C-O	-5.68	1.17	1.23
1	D	64	VAL	C-O	-5.68	1.17	1.24
1	D	58	ALA	C-O	-5.67	1.17	1.24
1	C	246	ALA	CA-CB	-5.67	1.43	1.53
1	C	355	ALA	CA-CB	-5.67	1.44	1.53
1	D	387	GLY	C-O	-5.66	1.18	1.24
1	A	54	TRP	C-O	-5.63	1.17	1.24
1	C	240	GLN	C-O	-5.62	1.17	1.23
1	A	82	GLN	C-O	-5.60	1.17	1.23
1	D	139	THR	C-O	-5.59	1.16	1.23
1	D	255	THR	C-O	-5.59	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	ALA	C-O	-5.59	1.17	1.23
1	C	443	THR	C-O	-5.59	1.19	1.24
1	D	367	LYS	C-O	-5.57	1.17	1.24
1	A	134	VAL	C-O	-5.56	1.18	1.24
1	A	148	ILE	C-O	-5.56	1.18	1.24
1	C	46	LEU	C-O	-5.56	1.17	1.23
1	A	141	ILE	C-O	-5.55	1.18	1.24
1	B	255	THR	C-O	-5.54	1.17	1.23
1	C	65	GLU	C-O	-5.53	1.17	1.24
1	C	401	ALA	C-O	-5.52	1.17	1.24
1	A	162	ASP	C-O	-5.51	1.17	1.24
1	D	410	VAL	C-O	-5.50	1.18	1.24
1	C	401	ALA	CA-CB	-5.49	1.45	1.53
1	B	116	VAL	C-O	-5.49	1.17	1.24
1	B	390	VAL	C-O	-5.49	1.18	1.24
1	C	314	GLU	CA-C	-5.48	1.47	1.53
1	A	136	SER	C-O	-5.48	1.16	1.24
1	A	67	ASP	C-O	-5.47	1.16	1.23
1	D	390	VAL	C-O	-5.46	1.18	1.24
1	B	338	THR	C-O	-5.46	1.17	1.24
1	C	234	VAL	C-O	-5.46	1.17	1.24
1	C	251	PRO	C-O	-5.46	1.17	1.24
1	A	209	SER	C-O	-5.45	1.16	1.23
1	A	60	VAL	C-O	-5.45	1.17	1.24
1	D	57	ALA	CA-CB	-5.45	1.46	1.53
1	A	73	VAL	C-O	-5.43	1.18	1.24
1	C	248	GLY	C-O	-5.42	1.18	1.24
1	A	257	VAL	C-O	-5.40	1.18	1.24
1	B	256	ALA	C-O	-5.39	1.17	1.24
1	A	220	PHE	C-O	-5.39	1.19	1.24
1	A	58	ALA	C-O	-5.39	1.17	1.24
1	B	196	ASP	C-O	-5.38	1.17	1.24
1	A	402	LEU	C-O	-5.37	1.17	1.24
1	B	73	VAL	C-O	-5.36	1.18	1.24
1	A	139	THR	C-O	-5.34	1.17	1.23
1	C	107	PHE	C-O	-5.34	1.17	1.23
1	A	414	THR	C-O	-5.33	1.17	1.24
1	B	66	LEU	C-O	-5.32	1.17	1.24
1	C	96	VAL	C-O	-5.32	1.18	1.24
1	C	132	ALA	C-O	-5.32	1.17	1.23
1	A	401	ALA	CA-CB	-5.32	1.44	1.53
1	A	33	LEU	C-O	-5.31	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	LEU	C-O	-5.30	1.17	1.24
1	A	56	LEU	C-O	-5.30	1.17	1.24
1	B	340	ARG	CA-C	-5.29	1.46	1.52
1	C	400	ALA	C-O	-5.28	1.18	1.24
1	B	110	VAL	C-O	-5.28	1.18	1.24
1	A	233	PRO	C-O	-5.27	1.17	1.24
1	A	150	LEU	C-O	-5.27	1.18	1.24
1	C	245	ARG	C-O	-5.27	1.17	1.24
1	D	207	ILE	C-O	-5.27	1.18	1.24
1	B	55	VAL	C-O	-5.26	1.18	1.24
1	D	257	VAL	C-O	-5.26	1.18	1.24
1	B	143	VAL	C-O	-5.25	1.18	1.24
1	B	212	VAL	C-O	-5.24	1.18	1.24
1	B	399	ASP	C-O	-5.24	1.18	1.24
1	B	18	ILE	C-O	-5.21	1.17	1.24
1	B	32	GLU	C-O	-5.21	1.18	1.24
1	D	239	LEU	C-O	-5.20	1.17	1.23
1	A	301	SER	C-O	-5.19	1.18	1.24
1	C	339	ILE	C-O	-5.18	1.18	1.24
1	C	150	LEU	C-O	-5.18	1.17	1.24
1	C	263	VAL	C-O	-5.18	1.18	1.24
1	D	32	GLU	C-O	-5.18	1.18	1.24
1	D	217	ALA	CA-CB	-5.18	1.45	1.53
1	C	399	ASP	C-O	-5.17	1.18	1.24
1	B	402	LEU	C-O	-5.16	1.17	1.23
1	B	388	ALA	C-O	-5.16	1.17	1.23
1	A	253	LEU	C-O	-5.15	1.17	1.24
1	A	227	GLY	C-O	-5.14	1.17	1.23
1	B	265	THR	C-O	-5.14	1.17	1.23
1	C	148	ILE	C-O	-5.14	1.18	1.24
1	B	235	ARG	C-O	-5.14	1.17	1.23
1	C	72	ARG	C-O	-5.13	1.17	1.23
1	D	35	ALA	C-O	-5.13	1.18	1.24
1	D	30	ALA	C-O	-5.13	1.18	1.24
1	A	391	MET	C-O	-5.13	1.18	1.24
1	A	55	VAL	C-O	-5.12	1.18	1.24
1	D	115	GLY	C-O	-5.12	1.18	1.24
1	A	24	VAL	CA-CB	-5.11	1.48	1.54
1	D	141	ILE	CA-CB	-5.11	1.48	1.54
1	B	206	VAL	C-O	-5.09	1.18	1.23
1	D	264	ILE	C-O	-5.08	1.19	1.24
1	C	57	ALA	CA-CB	-5.07	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ARG	C-O	-5.07	1.17	1.24
1	A	78	VAL	C-O	-5.05	1.18	1.24
1	C	212	VAL	C-O	-5.05	1.18	1.24
1	D	322	ASP	C-O	-5.05	1.18	1.23
1	D	297	GLU	C-O	-5.05	1.18	1.24
1	C	36	VAL	C-O	-5.05	1.18	1.24
1	C	61	GLN	C-O	-5.05	1.18	1.24
1	A	159	GLU	C-O	-5.03	1.18	1.24
1	B	320	VAL	CA-CB	-5.03	1.48	1.53
1	B	148	ILE	C-O	-5.03	1.18	1.24
1	D	110	VAL	C-O	-5.01	1.18	1.24
1	A	409	GLN	C-O	-5.01	1.18	1.24
1	C	409	GLN	C-O	-5.01	1.18	1.24
1	A	235	ARG	C-O	-5.00	1.17	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	VAL	N-CA-C	11.02	120.89	110.53
1	A	146	LYS	N-CA-C	9.22	121.10	111.14
1	D	36	VAL	N-CA-C	8.16	118.20	110.53
1	B	102	GLU	N-CA-C	7.70	119.76	111.36
1	B	204	HIS	N-CA-C	7.58	119.33	111.14
1	B	286	ASP	N-CA-C	-7.55	103.87	113.23
1	A	204	HIS	N-CA-C	7.37	119.10	111.14
1	B	368	ALA	N-CA-C	-7.24	103.47	111.36
1	C	334	HIS	N-CA-C	7.20	119.08	108.14
1	B	376	ARG	N-CA-C	7.13	119.13	111.36
1	D	104	ASP	N-CA-C	7.11	119.11	111.36
1	D	161	ILE	N-CA-C	-6.88	103.77	110.72
1	D	116	VAL	N-CA-C	6.83	119.63	111.09
1	D	376	ARG	N-CA-C	6.75	118.71	111.36
1	C	145	GLU	N-CA-C	-6.64	104.08	111.71
1	A	390	VAL	N-CA-C	6.49	119.44	108.86
1	C	308	GLU	N-CA-C	6.45	117.97	111.07
1	C	204	HIS	N-CA-C	6.32	117.96	111.14
1	D	271	THR	N-CA-C	6.29	117.83	110.41
1	B	254	VAL	N-CA-C	6.28	116.32	110.42
1	A	155	ILE	N-CA-C	6.23	117.80	111.00
1	C	36	VAL	CB-CA-C	-6.16	104.08	111.97
1	D	285	ARG	N-CA-C	-6.16	104.57	111.28
1	B	167	THR	N-CA-C	6.16	117.79	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	181	SER	N-CA-C	6.13	118.93	111.82
1	A	415	TRP	N-CA-C	6.00	117.36	108.60
1	A	376	ARG	N-CA-C	6.00	117.90	111.36
1	C	376	ARG	N-CA-C	5.99	117.89	111.36
1	C	38	THR	N-CA-C	-5.96	104.70	111.07
1	B	390	VAL	N-CA-C	5.76	116.77	108.48
1	B	122	GLN	N-CA-C	5.74	119.90	113.01
1	D	146	LYS	N-CA-C	5.73	117.33	111.14
1	A	104	ASP	N-CA-C	5.67	117.54	111.36
1	B	35	ALA	N-CA-C	5.67	117.32	111.03
1	B	123[A]	GLN	N-CA-C	-5.57	106.25	113.16
1	B	123[B]	GLN	N-CA-C	-5.57	106.25	113.16
1	D	415	TRP	N-CA-C	5.57	117.54	109.07
1	A	40	SER	N-CA-C	5.57	117.15	111.14
1	C	254	VAL	N-CA-C	5.51	115.71	110.53
1	A	36	VAL	N-CA-C	5.51	115.71	110.42
1	D	81	ARG	N-CA-C	5.47	118.38	110.28
1	D	167	THR	N-CA-C	5.46	117.23	111.28
1	B	147	GLU	N-CA-C	5.43	117.45	109.24
1	C	415	TRP	N-CA-C	5.42	117.08	108.79
1	A	95	ALA	N-CA-C	5.39	117.15	111.28
1	A	377	LEU	N-CA-C	5.35	120.47	113.30
1	C	426	SER	N-CA-C	5.26	117.86	110.23
1	C	390	VAL	N-CA-C	5.24	116.26	108.46
1	C	99	LEU	N-CA-C	-5.23	105.58	111.28
1	B	67	ASP	N-CA-C	-5.20	101.85	109.81
1	D	390	VAL	N-CA-C	5.20	116.21	108.46
1	D	318	ALA	N-CA-C	5.17	117.16	109.25
1	B	329	ARG	N-CA-C	5.14	114.82	108.19
1	B	331	SER	N-CA-C	5.09	116.92	107.60
1	C	74	ILE	N-CA-C	5.02	115.08	107.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182[A]	ASP	Mainchain
1	A	182[B]	ASP	Mainchain

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	3151	0	3107	91	0
1	B	3211	0	3191	95	0
1	C	3254	0	3209	112	0
1	D	3222	0	3164	81	0
2	A	19	0	11	11	0
2	B	19	0	11	4	0
2	C	19	0	11	2	0
2	D	19	0	11	6	0
3	A	121	0	0	4	0
3	B	118	0	0	5	0
3	C	115	0	0	0	0
3	D	103	0	0	0	0
All	All	13371	0	12715	379	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 15.

All (379) 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:361:THR:HG21	2:A:451:RVB:C10	1.62	1.27
1:A:361:THR:CG2	2:A:451:RVB:H10	1.69	1.21
1:C:291:ASN:HD22	1:C:294:GLU:HG2	1.05	1.17
1:C:272:ARG:HG3	1:C:284:ALA:HB1	1.24	1.16
1:A:291:ASN:HD22	1:A:294:GLU:HG2	1.12	1.13
1:C:271:THR:H	1:C:334:HIS:HB3	1.13	1.13
1:B:20:MET:HE2	1:B:148:ILE:HD11	1.31	1.09
1:C:274:LEU:HD23	1:C:275:GLY:N	1.68	1.07
1:B:331:SER:HA	1:B:332:VAL:HG22	1.32	1.06
1:C:431:GLU:OE1	1:C:431:GLU:HA	1.54	1.02
1:A:361:THR:HG21	2:A:451:RVB:H10	1.03	1.02
1:C:274:LEU:HD23	1:C:275:GLY:H	1.19	1.01
1:A:233:PRO:HG3	1:A:249:TYR:HB3	1.39	1.00
2:D:451:RVB:H10	2:D:451:RVB:O3	1.63	0.98
1:B:20:MET:HE2	1:B:148:ILE:CD1	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:HG12	1:C:37:VAL:N	1.78	0.95
1:C:271:THR:O	1:C:271:THR:HG23	1.64	0.95
1:C:291:ASN:ND2	1:C:294:GLU:HG2	1.83	0.93
1:A:358:PRO:O	1:A:367:LYS:HE3	1.69	0.93
1:A:448:ALA:O	1:A:449:ARG:HB2	1.68	0.92
1:A:205:LYS:HE2	3:A:564:HOH:O	1.68	0.91
1:B:20:MET:CE	1:B:148:ILE:CG1	2.50	0.90
1:D:283:LEU:O	1:D:284:ALA:HB3	1.71	0.90
1:B:340:ARG:HG3	1:B:340:ARG:HH11	1.36	0.89
1:A:291:ASN:ND2	1:A:294:GLU:HG2	1.89	0.87
1:B:303:ARG:O	1:B:307:GLU:HG3	1.74	0.87
1:A:271:THR:HB	1:A:334:HIS:CD2	2.10	0.86
1:C:270:GLY:O	1:C:271:THR:HG22	1.74	0.86
1:B:331:SER:HA	1:B:332:VAL:CG2	2.06	0.85
1:D:20:MET:HE3	1:D:24:VAL:HG22	1.58	0.85
1:B:361:THR:HG21	2:B:451:RVB:H10	1.58	0.85
1:D:291:ASN:HD22	1:D:294:GLU:HG2	1.40	0.84
1:A:358:PRO:O	1:A:367:LYS:CE	2.24	0.84
1:A:380:CYS:HB3	1:A:381:PRO:HA	1.60	0.84
1:C:271:THR:N	1:C:334:HIS:HB3	1.93	0.84
1:D:75:ARG:HG2	1:D:76:ASP:OD2	1.77	0.83
1:C:272:ARG:HG3	1:C:284:ALA:CB	2.08	0.83
1:C:142:MET:HE3	1:C:151:PHE:CE2	2.14	0.82
1:B:20:MET:HE2	1:B:148:ILE:CG1	2.08	0.82
1:B:285:ARG:HB2	1:B:333:GLN:OE1	1.80	0.81
1:C:272:ARG:CG	1:C:284:ALA:HB1	2.09	0.81
1:C:270:GLY:HA3	1:C:335:LEU:H	1.47	0.80
1:C:284:ALA:O	1:C:288:LEU:HB3	1.80	0.80
1:C:271:THR:O	1:C:271:THR:CG2	2.28	0.79
1:B:340:ARG:HG3	1:B:340:ARG:NH1	1.89	0.79
1:C:434:GLU:O	1:C:434:GLU:OE1	2.01	0.78
1:D:118:ARG:HH21	1:D:118:ARG:HG3	1.48	0.78
1:C:36:VAL:CG1	1:C:37:VAL:N	2.46	0.78
1:D:20:MET:CE	1:D:24:VAL:HG22	2.12	0.78
1:A:448:ALA:O	1:A:449:ARG:CB	2.32	0.76
1:B:419:GLY:N	2:B:451:RVB:OA	2.18	0.76
1:B:328:GLU:CD	1:B:328:GLU:O	2.29	0.76
1:B:20:MET:CE	1:B:148:ILE:HG13	2.15	0.76
2:D:451:RVB:O3	2:D:451:RVB:C10	2.29	0.76
1:A:270:GLY:HA3	1:A:335:LEU:H	1.50	0.76
1:C:360:VAL:HG23	1:C:367:LYS:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LYS:HG3	1:D:422:ILE:O	1.85	0.75
1:A:270:GLY:O	1:A:271:THR:HG22	1.86	0.75
1:D:303:ARG:O	1:D:307:GLU:HG3	1.87	0.74
1:D:327:ARG:HH21	1:D:327:ARG:HG3	1.51	0.74
1:D:156:ARG:HG2	1:D:157:HIS:N	2.02	0.73
1:C:291:ASN:HD22	1:C:294:GLU:CG	1.94	0.72
1:C:431:GLU:OE1	1:C:431:GLU:CA	2.34	0.71
1:B:362:ALA:HB1	1:B:386:SER:HB2	1.72	0.71
1:C:274:LEU:CD2	1:C:275:GLY:N	2.52	0.71
1:A:233:PRO:CG	1:A:249:TYR:HB3	2.20	0.71
1:B:20:MET:CE	1:B:148:ILE:HD11	2.17	0.70
1:D:283:LEU:C	1:D:285:ARG:H	1.97	0.70
1:B:294:GLU:OE2	1:B:294:GLU:HA	1.91	0.70
1:D:32:GLU:O	1:D:36:VAL:HG12	1.90	0.70
1:D:413:ARG:HG2	1:D:415:TRP:HE3	1.57	0.70
1:D:20:MET:HE3	1:D:24:VAL:CG2	2.22	0.69
1:D:413:ARG:HG2	1:D:415:TRP:CE3	2.26	0.69
1:B:233:PRO:HG3	1:B:249:TYR:HB3	1.74	0.69
1:B:20:MET:HE3	1:B:148:ILE:HG13	1.74	0.69
1:A:271:THR:HB	1:A:334:HIS:NE2	2.06	0.69
1:B:413:ARG:HG2	1:B:415:TRP:CE3	2.27	0.68
1:D:253:LEU:HD12	1:D:400:ALA:O	1.94	0.68
1:B:378:ASP:OD2	1:B:382:ARG:NH2	2.27	0.68
1:A:227:GLY:HA3	1:A:249:TYR:OH	1.94	0.67
1:B:340:ARG:HH11	1:B:340:ARG:CG	2.06	0.67
1:A:180:VAL:HG12	1:A:212:VAL:HG11	1.76	0.66
1:D:211:CYS:SG	1:D:417:ARG:HG3	2.35	0.66
1:D:283:LEU:C	1:D:285:ARG:N	2.53	0.66
1:A:298:HIS:O	1:A:302:VAL:HG23	1.97	0.64
1:A:113:GLU:O	1:A:116:VAL:HG22	1.98	0.64
1:A:362:ALA:HB1	1:A:386:SER:HB2	1.77	0.64
1:C:253:LEU:HD12	1:C:400:ALA:O	1.98	0.64
1:C:284:ALA:O	1:C:288:LEU:CB	2.45	0.64
1:A:361:THR:CG2	2:A:451:RVB:C10	2.48	0.63
1:A:398:LEU:HD12	1:A:399:ASP:N	2.12	0.63
1:C:277:GLY:C	1:C:279:ALA:H	2.05	0.63
1:B:353:LEU:O	1:B:357:PHE:HB2	1.99	0.63
1:B:80:ARG:NH2	3:B:457:HOH:O	2.31	0.63
1:C:321:ILE:HD13	1:C:340:ARG:HD2	1.80	0.63
1:C:277:GLY:O	1:C:279:ALA:N	2.31	0.63
1:D:340:ARG:HG2	1:D:341:ALA:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ILE:HD12	1:C:341:ALA:HB2	1.81	0.63
1:A:211:CYS:SG	1:A:417:ARG:HD2	2.39	0.62
1:C:155:ILE:HG13	1:C:158:ARG:NH1	2.15	0.62
1:B:233:PRO:HB3	1:B:249:TYR:HB3	1.81	0.62
1:B:413:ARG:HG2	1:B:415:TRP:HE3	1.64	0.62
1:B:117:HIS:CD2	1:B:117:HIS:H	2.17	0.62
1:C:353:LEU:O	1:C:357:PHE:HB2	2.00	0.62
1:A:367:LYS:O	1:A:371:VAL:HG23	2.00	0.61
1:A:438:LYS:HE2	2:A:451:RVB:C2	2.30	0.61
1:C:292:SER:O	1:C:296:VAL:HG23	2.00	0.61
1:B:20:MET:CE	1:B:148:ILE:HG12	2.29	0.61
1:D:193:VAL:O	1:D:197:GLU:HG3	2.01	0.61
1:B:43:GLU:HG2	1:B:59:GLY:HA2	1.83	0.61
1:C:284:ALA:O	1:C:288:LEU:N	2.30	0.61
1:B:325:THR:HG22	1:B:326:VAL:N	2.16	0.61
1:A:80:ARG:HD3	1:A:80:ARG:C	2.26	0.61
1:C:258:ARG:NH2	1:C:260:ASP:OD2	2.33	0.60
1:B:20:MET:HE3	1:B:148:ILE:CG1	2.28	0.60
1:B:182:ASP:OD2	1:B:183:ASP:N	2.32	0.60
1:C:231:ASN:OD1	1:C:441:THR:CG2	2.49	0.60
1:A:115:GLY:HA3	1:A:358:PRO:HD3	1.84	0.60
1:B:26:PRO:HB2	1:B:54:TRP:CZ3	2.37	0.60
1:A:193:VAL:O	1:A:197:GLU:HG3	2.02	0.59
1:D:291:ASN:ND2	1:D:294:GLU:HG2	2.14	0.59
1:D:283:LEU:O	1:D:284:ALA:CB	2.39	0.59
1:B:32:GLU:OE2	1:B:225:ARG:NH1	2.34	0.59
1:B:292:SER:O	1:B:296:VAL:HG23	2.03	0.59
1:D:226:LEU:HG	1:D:445:TYR:HB3	1.84	0.59
1:A:116:VAL:HG21	1:A:125:LEU:HD11	1.84	0.59
1:D:362:ALA:HB1	1:D:386:SER:HB2	1.84	0.59
1:D:189:ARG:O	1:D:193:VAL:HG23	2.03	0.59
1:C:362:ALA:HB1	1:C:386:SER:HB2	1.85	0.58
1:B:430:ARG:HD2	1:B:430:ARG:O	2.03	0.58
1:C:115:GLY:HA3	1:C:358:PRO:HD3	1.83	0.58
1:B:233:PRO:CG	1:B:249:TYR:HB3	2.32	0.58
1:B:226:LEU:HG	1:B:445:TYR:HB3	1.84	0.58
1:A:80:ARG:HH21	1:A:81:ARG:H	1.50	0.58
1:A:186:GLY:O	1:A:190:ARG:HG3	2.04	0.58
1:C:296:VAL:HG12	1:C:300:ILE:HD12	1.86	0.57
1:D:191:VAL:HG13	1:D:422:ILE:HD12	1.85	0.57
1:A:37:VAL:O	1:A:41:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:SER:HA	1:C:443:THR:OG1	2.04	0.57
1:D:20:MET:CE	1:D:24:VAL:CG2	2.81	0.57
1:B:358:PRO:O	1:B:367:LYS:HE2	2.05	0.57
1:C:270:GLY:O	1:C:271:THR:CG2	2.50	0.57
1:C:277:GLY:C	1:C:279:ALA:N	2.62	0.57
1:B:32:GLU:HG3	1:B:169:VAL:HG12	1.85	0.57
1:C:49:GLU:HB2	1:C:54:TRP:NE1	2.19	0.57
1:C:419:GLY:N	2:C:451:RVB:OA	2.37	0.56
1:A:220:PHE:CD2	1:A:247:LEU:HD23	2.40	0.56
1:D:283:LEU:O	1:D:285:ARG:N	2.35	0.56
1:A:326:VAL:HA	1:A:334:HIS:O	2.05	0.56
1:C:307:GLU:O	1:C:310:THR:HB	2.06	0.56
1:C:19:PRO:O	1:C:21:PRO:HD3	2.05	0.56
1:D:124:ARG:NH2	1:D:372:GLU:OE2	2.38	0.56
1:A:84:TRP:HH2	1:A:117[B]:HIS:CE1	2.23	0.56
1:A:379:GLU:HG3	3:A:548:HOH:O	2.05	0.56
1:B:20:MET:HE1	1:B:29:LEU:CD2	2.36	0.56
1:D:443:THR:N	1:D:444:PRO:CD	2.69	0.55
1:C:309:ILE:HG22	1:C:356:LEU:HD21	1.88	0.55
1:B:385:TYR:CG	1:B:417:ARG:HD3	2.41	0.55
1:D:149:ARG:C	1:D:150:LEU:HD23	2.31	0.55
1:C:36:VAL:HG12	1:C:37:VAL:H	1.65	0.55
1:B:126:ALA:O	1:B:129:THR:OG1	2.22	0.54
1:D:118:ARG:HG3	1:D:118:ARG:NH2	2.21	0.54
1:B:233:PRO:CB	1:B:249:TYR:HB3	2.38	0.54
1:B:57:ALA:HB1	1:B:137:PRO:HB3	1.90	0.54
1:C:33:LEU:HD11	1:C:161:ILE:HG12	1.88	0.54
1:C:285:ARG:O	1:C:289:GLU:HB2	2.08	0.54
1:A:189:ARG:HH21	1:C:118:ARG:HA	1.72	0.54
1:B:123[B]:GLN:H	1:B:123[B]:GLN:CD	2.16	0.53
1:A:113:GLU:HA	1:A:116:VAL:HG13	1.91	0.53
1:A:433:GLU:O	1:A:437:GLU:HG3	2.08	0.53
1:D:62:ALA:HB3	1:D:99:LEU:HD22	1.89	0.53
1:D:156:ARG:HG2	1:D:157:HIS:H	1.72	0.53
1:A:157:HIS:O	1:A:161:ILE:HG13	2.08	0.53
1:D:349:ARG:HG3	1:D:350:MET:N	2.23	0.53
1:B:394:ALA:HB1	1:C:189:ARG:HD3	1.92	0.52
1:C:142:MET:HG3	1:C:151:PHE:HE2	1.75	0.52
1:B:159:GLU:O	1:B:163:ARG:HG3	2.09	0.52
1:A:322:ASP:O	1:A:337:SER:HA	2.10	0.52
1:D:186:GLY:O	1:D:190:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:O	1:C:406:ALA:HA	2.10	0.52
1:B:26:PRO:HG3	1:B:145:GLU:HA	1.92	0.51
1:B:433:GLU:O	1:B:436:CYS:HB2	2.10	0.51
1:B:49:GLU:HB2	1:B:54:TRP:CD1	2.45	0.51
1:B:361:THR:CG2	2:B:451:RVB:H10	2.35	0.51
1:C:334:HIS:ND1	1:C:334:HIS:N	2.57	0.51
1:A:80:ARG:HD3	1:A:81:ARG:N	2.26	0.51
1:A:189:ARG:NH2	1:C:118:ARG:HA	2.25	0.51
1:D:443:THR:N	1:D:444:PRO:HD3	2.26	0.51
1:C:309:ILE:CG2	1:C:356:LEU:HD21	2.41	0.51
1:D:260:ASP:OD1	1:D:262:VAL:HG23	2.10	0.51
1:D:33:LEU:HD11	1:D:161:ILE:HG12	1.92	0.51
2:D:451:RVB:H10	2:D:451:RVB:C3	2.38	0.51
1:C:360:VAL:CG2	1:C:367:LYS:HE3	2.36	0.51
1:C:61:GLN:HE21	1:C:75:ARG:NH1	2.08	0.51
1:B:382:ARG:HG2	1:B:385:TYR:HD2	1.76	0.50
1:D:332:VAL:HG22	1:D:333:GLN:H	1.76	0.50
1:C:231:ASN:OD1	1:C:441:THR:HG22	2.12	0.50
1:B:233:PRO:HB3	1:B:249:TYR:CB	2.41	0.50
1:C:49:GLU:CD	1:C:54:TRP:CZ2	2.89	0.50
1:A:37:VAL:O	1:A:41:VAL:CG1	2.59	0.50
1:A:251:PRO:HB2	2:A:451:RVB:H11A	1.93	0.50
1:B:437:GLU:O	1:B:440:SER:OG	2.30	0.50
1:A:437:GLU:O	1:A:440:SER:OG	2.29	0.50
1:B:298:HIS:CD2	1:B:324:MET:HG3	2.46	0.50
1:C:32:GLU:HG3	1:C:169:VAL:HB	1.92	0.50
1:C:66:LEU:HD13	1:C:71:LEU:HD13	1.94	0.50
1:D:180:VAL:HG12	1:D:212:VAL:HG11	1.94	0.50
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.77	0.49
1:B:233:PRO:HB2	1:B:235:ARG:O	2.12	0.49
1:C:372:GLU:O	1:C:375:PHE:HB2	2.12	0.49
1:A:353:LEU:O	1:A:357:PHE:HB2	2.12	0.49
1:A:378:ASP:OD2	1:A:382:ARG:NH2	2.36	0.49
1:D:353:LEU:O	1:D:357:PHE:HB2	2.12	0.49
1:D:362:ALA:CB	1:D:386:SER:HB2	2.41	0.49
1:A:268:LEU:HD23	2:A:451:RVB:H11B	1.94	0.49
1:A:306:LEU:O	1:A:309:ILE:HG22	2.13	0.49
1:A:103:THR:HB	3:A:504:HOH:O	2.12	0.49
1:B:328:GLU:O	1:B:328:GLU:OE1	2.30	0.49
1:C:283:LEU:O	1:C:287:ASP:HB3	2.13	0.49
1:D:21:PRO:O	1:D:24:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLU:O	1:A:436:CYS:HB2	2.12	0.49
1:A:361:THR:HG21	2:A:451:RVB:H10B	1.80	0.49
1:C:41:VAL:HG22	1:C:156:ARG:CZ	2.43	0.48
1:C:49:GLU:HB2	1:C:54:TRP:CD1	2.47	0.48
1:A:253:LEU:HD12	1:A:400:ALA:O	2.13	0.48
1:B:75:ARG:O	1:B:76:ASP:HB2	2.12	0.48
1:B:295:ILE:HG23	1:B:324:MET:HE1	1.94	0.48
1:B:325:THR:CG2	1:B:326:VAL:N	2.75	0.48
1:D:24:VAL:HG21	1:D:29:LEU:HB2	1.94	0.48
1:B:25:ASN:ND2	3:B:547:HOH:O	2.33	0.48
1:D:20:MET:HE3	1:D:24:VAL:HG13	1.95	0.48
1:D:21:PRO:O	1:D:24:VAL:CG1	2.61	0.48
1:D:437:GLU:O	1:D:440:SER:OG	2.30	0.48
1:C:288:LEU:HD21	1:C:334:HIS:HA	1.96	0.48
1:B:142:MET:HE3	1:B:151:PHE:CE2	2.49	0.48
1:C:344:ASP:OD1	1:C:346:SER:OG	2.30	0.48
1:C:432:PHE:C	1:C:432:PHE:CD2	2.91	0.48
1:B:117:HIS:CD2	1:B:117:HIS:N	2.81	0.47
1:D:305:SER:HB2	1:D:339:ILE:HD13	1.96	0.47
1:C:322:ASP:OD2	1:C:325:THR:HB	2.13	0.47
1:D:305:SER:HB2	1:D:339:ILE:CD1	2.45	0.47
1:A:405:ARG:NH1	1:A:441:THR:HG21	2.29	0.47
1:D:59:GLY:O	1:D:137:PRO:HA	2.15	0.47
1:D:182:ASP:CG	1:D:184:PRO:HD3	2.40	0.47
1:D:211:CYS:SG	1:D:417:ARG:CD	3.03	0.47
1:A:268:LEU:HD23	2:A:451:RVB:C11	2.44	0.47
1:C:98:ARG:HD3	1:C:98:ARG:N	2.30	0.47
1:C:186:GLY:O	1:C:190:ARG:HG3	2.15	0.47
1:D:118:ARG:HH21	1:D:118:ARG:CG	2.23	0.47
1:D:327:ARG:HG3	1:D:327:ARG:NH2	2.21	0.47
1:B:327:ARG:O	1:B:334:HIS:N	2.38	0.47
1:B:370:GLY:O	1:B:374:ILE:HG13	2.15	0.47
1:C:94:GLU:O	1:C:98:ARG:HG2	2.14	0.47
1:A:440:SER:HA	1:A:443:THR:OG1	2.15	0.47
1:D:37:VAL:O	1:D:41:VAL:HG22	2.15	0.47
1:C:211:CYS:SG	1:C:417:ARG:HD2	2.55	0.46
1:C:155:ILE:HG13	1:C:158:ARG:HH12	1.80	0.46
1:C:245:ARG:HB2	1:C:409:GLN:HB3	1.98	0.46
1:C:321:ILE:CD1	1:C:340:ARG:HD2	2.44	0.46
1:D:75:ARG:CG	1:D:76:ASP:OD2	2.57	0.46
1:D:385:TYR:CG	1:D:417:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:GLU:O	1:C:436:CYS:HB2	2.15	0.46
1:A:266:GLU:OE1	1:A:327:ARG:NH1	2.47	0.46
1:B:443:THR:N	1:B:444:PRO:CD	2.79	0.46
1:A:358:PRO:O	1:A:367:LYS:HE2	2.09	0.46
1:B:334:HIS:CE1	2:B:451:RVB:H11	2.51	0.46
1:C:314:GLU:HG3	1:C:344:ASP:HA	1.97	0.46
1:C:321:ILE:HD13	1:C:340:ARG:CD	2.46	0.46
1:C:124:ARG:NH2	1:C:372:GLU:OE2	2.49	0.46
1:D:360:VAL:HG23	1:D:367:LYS:HE2	1.97	0.46
1:A:251:PRO:HB2	2:A:451:RVB:C11	2.46	0.46
1:C:183:ASP:N	1:C:184:PRO:CD	2.79	0.46
1:D:258:ARG:HB2	1:D:260:ASP:OD1	2.16	0.46
1:B:285:ARG:CB	1:B:333:GLN:OE1	2.58	0.46
1:B:286:ASP:O	1:B:290:SER:OG	2.30	0.46
1:A:296:VAL:O	1:A:300:ILE:HG13	2.16	0.45
1:D:332:VAL:HG22	1:D:333:GLN:N	2.31	0.45
1:A:119:TYR:OH	1:A:367:LYS:HD2	2.16	0.45
1:B:328:GLU:OE1	1:B:328:GLU:C	2.59	0.45
1:D:253:LEU:CD1	1:D:400:ALA:O	2.63	0.45
2:D:451:RVB:OB	2:D:451:RVB:O2	2.32	0.45
1:C:365:ILE:HA	1:C:366:PRO:C	2.40	0.45
1:D:314:GLU:O	1:D:317:SER:OG	2.30	0.45
2:A:451:RVB:O2	2:A:451:RVB:OA	2.30	0.45
1:B:20:MET:HE1	1:B:29:LEU:HD22	1.99	0.45
1:D:329:ARG:HA	1:D:330:GLY:HA2	1.50	0.45
1:B:107:PHE:N	1:B:107:PHE:CD2	2.85	0.45
1:B:253:LEU:HD12	1:B:400:ALA:O	2.17	0.45
1:C:272:ARG:HA	1:C:272:ARG:HD3	1.55	0.45
1:A:25:ASN:HB3	1:A:28:ASP:OD2	2.17	0.45
1:A:18:ILE:O	1:A:19:PRO:C	2.60	0.45
1:C:258:ARG:HB2	1:C:260:ASP:OD1	2.18	0.44
1:D:251:PRO:HB2	2:D:451:RVB:H10B	2.00	0.44
1:A:122:GLN:OE1	1:A:122:GLN:N	2.30	0.44
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.89	0.44
1:C:191:VAL:HG13	1:C:422:ILE:HD12	2.00	0.44
1:C:322:ASP:OD2	1:C:325:THR:CB	2.65	0.44
1:C:438:LYS:HE2	2:C:451:RVB:C'	2.48	0.44
1:C:25:ASN:HB3	1:C:28:ASP:OD2	2.17	0.44
1:C:171:GLU:O	1:C:173:PRO:HD3	2.18	0.44
1:C:309:ILE:HG13	1:C:310:THR:N	2.32	0.44
1:C:422:ILE:CD1	1:C:431:GLU:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ARG:HD2	1:D:327:ARG:HA	1.83	0.44
1:B:180:VAL:HG11	1:B:443:THR:HG21	1.99	0.44
1:A:18:ILE:O	1:A:18:ILE:HG13	2.18	0.44
1:B:43:GLU:HG2	1:B:59:GLY:CA	2.47	0.44
1:C:272:ARG:HG2	1:C:288:LEU:HD13	2.00	0.44
1:A:140:ARG:HB2	1:A:151:PHE:HB2	1.99	0.43
1:A:207:ILE:HG13	1:A:421:GLY:HA2	2.00	0.43
1:B:202:ARG:HG2	1:B:203:TYR:CD2	2.53	0.43
1:B:297:GLU:OE1	1:B:297:GLU:HA	2.17	0.43
1:A:117[B]:HIS:CD2	1:A:117[B]:HIS:H	2.35	0.43
1:D:24:VAL:CG2	1:D:29:LEU:HB2	2.48	0.43
1:B:211:CYS:SG	1:B:417:ARG:HD2	2.59	0.43
1:B:288:LEU:HD12	1:B:294:GLU:HG3	2.00	0.43
1:C:182:ASP:HB3	1:C:184:PRO:HD3	2.00	0.43
1:C:245:ARG:HH21	1:C:409:GLN:HE22	1.65	0.43
1:C:256:ALA:HB3	1:C:264:ILE:HB	2.00	0.43
1:C:274:LEU:HA	1:C:281:ASP:OD2	2.19	0.43
1:D:20:MET:HE3	1:D:24:VAL:CG1	2.49	0.43
1:D:150:LEU:HD23	1:D:150:LEU:N	2.33	0.43
1:B:20:MET:HE2	1:B:148:ILE:HG13	1.84	0.43
1:C:180:VAL:O	1:C:180:VAL:HG23	2.19	0.43
1:C:300:ILE:CG2	1:C:365:ILE:HD13	2.49	0.43
1:A:327:ARG:N	1:A:334:HIS:O	2.38	0.43
1:B:328:GLU:CD	1:B:328:GLU:C	2.87	0.43
1:C:334:HIS:N	1:C:334:HIS:HD1	2.16	0.43
1:A:138:ARG:NH2	1:D:39:GLU:OE2	2.39	0.43
1:C:155:ILE:CG1	1:C:158:ARG:NH1	2.82	0.43
1:D:327:ARG:O	1:D:328:GLU:CB	2.65	0.43
1:C:270:GLY:O	1:C:271:THR:CB	2.67	0.42
1:B:253:LEU:HD21	1:B:256:ALA:HB2	2.01	0.42
1:B:207:ILE:HG13	1:B:421:GLY:HA2	2.01	0.42
1:B:332:VAL:HG12	3:B:452:HOH:O	2.19	0.42
1:A:83:GLN:NE2	1:A:85:SER:OG	2.49	0.42
1:D:433:GLU:O	1:D:436:CYS:HB2	2.19	0.42
1:A:233:PRO:CB	1:A:249:TYR:HB3	2.50	0.42
1:A:305:SER:HB2	1:A:339:ILE:HD13	2.00	0.42
1:B:106:ALA:C	1:B:107:PHE:CD2	2.97	0.42
1:D:105:GLN:HA	1:D:392:LEU:O	2.20	0.42
1:D:211:CYS:SG	1:D:417:ARG:CG	3.06	0.42
1:D:322:ASP:O	1:D:337:SER:HA	2.20	0.42
1:A:344:ASP:OD1	1:A:346:SER:OG	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:GLU:O	1:D:329:ARG:CB	2.66	0.42
1:A:405:ARG:HH11	1:A:441:THR:HG21	1.85	0.42
1:A:18:ILE:O	1:A:18:ILE:CG1	2.68	0.42
1:C:32:GLU:HB3	1:C:164:LEU:HD11	2.01	0.42
1:C:36:VAL:HG12	1:C:37:VAL:HG13	2.01	0.42
1:C:63:MET:HE1	1:C:241:LEU:HD11	2.01	0.41
1:C:116:VAL:HB	1:C:121:LEU:HB2	2.02	0.41
1:B:213:GLU:OE1	1:B:413:ARG:NE	2.36	0.41
1:D:210:ARG:O	1:D:210:ARG:HG3	2.19	0.41
1:A:80:ARG:HD2	1:B:83:GLN:HG2	2.03	0.41
1:A:349:ARG:HD2	1:A:392:LEU:HD23	2.02	0.41
1:D:41:VAL:HG11	1:D:156:ARG:HG3	2.01	0.41
1:A:22:ALA:O	3:A:453:HOH:O	2.22	0.41
1:A:314:GLU:O	1:A:317:SER:OG	2.34	0.41
1:A:344:ASP:HA	1:A:345:PRO:HD3	1.89	0.41
1:B:140:ARG:HB2	1:B:151:PHE:HB2	2.03	0.41
1:C:287:ASP:O	1:C:291:ASN:HB2	2.21	0.41
1:B:326:VAL:HG12	3:B:544:HOH:O	2.19	0.41
1:B:380:CYS:HA	1:B:381:PRO:C	2.45	0.41
1:C:309:ILE:HD11	1:C:318:ALA:HB1	2.01	0.41
1:D:232:THR:HA	1:D:233:PRO:HD2	1.85	0.41
1:A:32:GLU:HG3	1:A:169:VAL:HG12	2.02	0.41
1:A:66:LEU:HD13	1:A:71:LEU:HD12	2.01	0.41
1:A:87:ARG:HB3	1:A:354:GLU:OE1	2.20	0.41
1:B:157:HIS:O	1:B:161:ILE:HG13	2.20	0.41
1:C:178:VAL:HG22	1:C:179:ASP:N	2.36	0.41
1:A:172:VAL:HA	1:A:173:PRO:HD3	1.92	0.41
1:B:245:ARG:HB2	1:B:409:GLN:HB3	2.02	0.41
1:A:189:ARG:O	1:A:193:VAL:HG23	2.21	0.40
1:B:413:ARG:NH2	3:B:567:HOH:O	2.30	0.40
1:A:113:GLU:HA	1:A:116:VAL:CG1	2.51	0.40
1:D:434:GLU:O	1:D:438:LYS:HG3	2.20	0.40
1:B:314:GLU:O	1:B:317:SER:OG	2.29	0.40
1:C:271:THR:O	1:C:272:ARG:NH1	2.54	0.40
1:D:268:LEU:HB2	2:D:451:RVB:C11	2.51	0.40
1:C:41:VAL:O	1:C:41:VAL:CG1	2.68	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	412/450 (92%)	405 (98%)	4 (1%)	3 (1%)	18	34
1	B	420/450 (93%)	411 (98%)	9 (2%)	0	100	100
1	C	427/450 (95%)	421 (99%)	4 (1%)	2 (0%)	24	43
1	D	424/450 (94%)	415 (98%)	7 (2%)	2 (0%)	24	43
All	All	1683/1800 (94%)	1652 (98%)	24 (1%)	7 (0%)	30	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	THR
1	D	329	ARG
1	A	19	PRO
1	C	278	PRO
1	A	271	THR
1	D	233	PRO
1	A	233	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	324/358 (90%)	314 (97%)	10 (3%)	35	62
1	B	332/358 (93%)	318 (96%)	14 (4%)	26	52
1	C	332/358 (93%)	313 (94%)	19 (6%)	18	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	329/358 (92%)	321 (98%)	8 (2%)	43 70
All	All	1317/1432 (92%)	1266 (96%)	51 (4%)	28 55

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	41	VAL
1	A	80	ARG
1	A	82	GLN
1	A	229	ARG
1	A	297	GLU
1	A	309	ILE
1	A	326	VAL
1	A	367	LYS
1	A	426	SER
1	B	25	ASN
1	B	80	ARG
1	B	116	VAL
1	B	174	GLN
1	B	268	LEU
1	B	285	ARG
1	B	309	ILE
1	B	324	MET
1	B	340	ARG
1	B	349	ARG
1	B	360	VAL
1	B	365	ILE
1	B	367	LYS
1	B	382	ARG
1	C	24	VAL
1	C	36	VAL
1	C	38	THR
1	C	96	VAL
1	C	116	VAL
1	C	150	LEU
1	C	169	VAL
1	C	174	GLN
1	C	180	VAL
1	C	258	ARG
1	C	272	ARG
1	C	285	ARG

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Mol	Chain	Res	Type
1	C	300	ILE
1	C	310	THR
1	C	334	HIS
1	C	360	VAL
1	C	405	ARG
1	C	431	GLU
1	C	434	GLU
1	D	24	VAL
1	D	124	ARG
1	D	156	ARG
1	D	161	ILE
1	D	207	ILE
1	D	309	ILE
1	D	327	ARG
1	D	365	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	240	GLN
1	A	291	ASN
1	B	25	ASN
1	B	83	GLN
1	B	117	HIS
1	B	230	HIS
1	B	334	HIS
1	C	61	GLN
1	C	122	GLN
1	C	230	HIS
1	C	291	ASN
1	C	409	GLN
1	D	25	ASN
1	D	123	GLN
1	D	230	HIS
1	D	291	ASN
1	D	333	GLN

5.3.3 RNA ⓘ

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](#)

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	RVB	C	451	-	19,19,19	2.08	6 (31%)	23,26,26	1.77	4 (17%)
2	RVB	A	451	-	19,19,19	1.91	5 (26%)	23,26,26	1.84	4 (17%)
2	RVB	B	451	-	19,19,19	1.95	7 (36%)	23,26,26	2.09	6 (26%)
2	RVB	D	451	-	19,19,19	2.24	7 (36%)	23,26,26	2.08	3 (13%)

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	RVB	C	451	-	-	6/16/16/16	0/1/1/1
2	RVB	A	451	-	-	3/16/16/16	0/1/1/1
2	RVB	B	451	-	-	6/16/16/16	0/1/1/1
2	RVB	D	451	-	-	7/16/16/16	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	451	RVB	C1-C	-6.54	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	451	RVB	C1-C	-5.83	1.37	1.49
2	A	451	RVB	C1-C	-5.68	1.37	1.49
2	B	451	RVB	C1-C	-4.69	1.39	1.49
2	C	451	RVB	O3-C3	-3.23	1.34	1.41
2	D	451	RVB	OA-C	-3.04	1.21	1.30
2	D	451	RVB	C8-C7	-3.02	1.28	1.33
2	B	451	RVB	O3-C3	-3.00	1.35	1.41
2	A	451	RVB	C3-C2	-2.78	1.36	1.40
2	D	451	RVB	O3-C3	-2.77	1.35	1.41
2	B	451	RVB	OA-C	-2.75	1.22	1.30
2	D	451	RVB	OB'-C'	-2.63	1.23	1.30
2	C	451	RVB	OA-C	-2.61	1.22	1.30
2	A	451	RVB	OA-C	-2.56	1.22	1.30
2	D	451	RVB	C1-C2	-2.55	1.37	1.41
2	C	451	RVB	O3-C7	-2.51	1.33	1.38
2	A	451	RVB	C1-C2	-2.49	1.37	1.41
2	B	451	RVB	OB'-C'	-2.48	1.23	1.30
2	B	451	RVB	O3-C7	-2.40	1.33	1.38
2	C	451	RVB	C1-C2	-2.24	1.37	1.41
2	D	451	RVB	C3-C2	-2.24	1.37	1.40
2	B	451	RVB	C1-C2	-2.21	1.37	1.41
2	B	451	RVB	C8-C7	-2.21	1.30	1.33
2	C	451	RVB	C3-C2	-2.09	1.37	1.40
2	A	451	RVB	O3-C3	-2.02	1.37	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	451	RVB	C3-O3-C7	-7.95	105.40	118.49
2	B	451	RVB	C3-O3-C7	-5.15	110.00	118.49
2	B	451	RVB	C1-C2-C3	5.13	123.75	119.56
2	A	451	RVB	C1-C2-C3	5.08	123.71	119.56
2	C	451	RVB	C3-O3-C7	-4.19	111.58	118.49
2	C	451	RVB	C1-C2-C3	3.85	122.70	119.56
2	A	451	RVB	O3-C3-C4	3.56	127.46	118.89
2	B	451	RVB	OA-C-OB	-3.20	116.47	123.35
2	C	451	RVB	OB'-C'-C7	3.19	121.28	114.06
2	D	451	RVB	OB'-C'-C7	2.85	120.52	114.06
2	A	451	RVB	OB'-C'-C7	2.53	119.80	114.06
2	B	451	RVB	OA-C-C1	2.50	122.40	115.28
2	D	451	RVB	C1-C2-C3	2.45	121.56	119.56
2	B	451	RVB	C6-C1-C2	-2.39	116.44	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	451	RVB	OB'-C'-C7	2.18	119.00	114.06
2	A	451	RVB	OA-C-OB	-2.12	118.80	123.35
2	C	451	RVB	O3-C3-C4	2.01	123.74	118.89

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	451	RVB	C'-C7-C8-C9
2	A	451	RVB	OB'-C'-C7-O3
2	B	451	RVB	C'-C7-C8-C9
2	B	451	RVB	OB'-C'-C7-O3
2	C	451	RVB	C'-C7-C8-C9
2	C	451	RVB	OA'-C'-C7-O3
2	C	451	RVB	OB'-C'-C7-O3
2	D	451	RVB	C'-C7-C8-C9
2	D	451	RVB	C7-C8-C9-C10
2	B	451	RVB	OA'-C'-C7-C8
2	D	451	RVB	OA'-C'-C7-C8
2	D	451	RVB	OB'-C'-C7-C8
2	C	451	RVB	OA-C-C1-C2
2	A	451	RVB	OA'-C'-C7-O3
2	B	451	RVB	OA'-C'-C7-O3
2	D	451	RVB	OA'-C'-C7-O3
2	C	451	RVB	OB-C-C1-C2
2	D	451	RVB	OB'-C'-C7-O3
2	B	451	RVB	OB'-C'-C7-C8
2	B	451	RVB	C8-C7-O3-C3
2	C	451	RVB	C8-C7-O3-C3
2	D	451	RVB	C8-C7-O3-C3

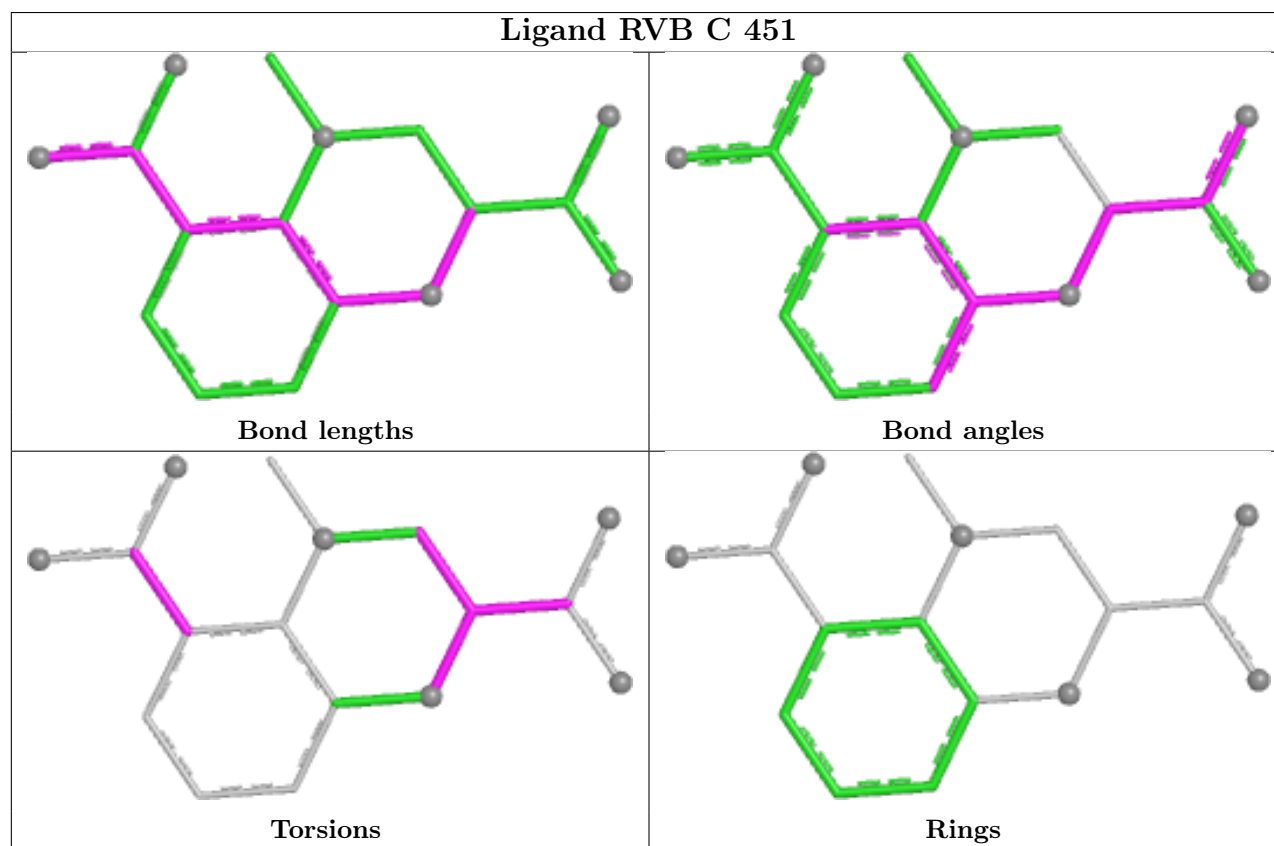
There are no ring outliers.

4 monomers are involved in 23 short contacts:

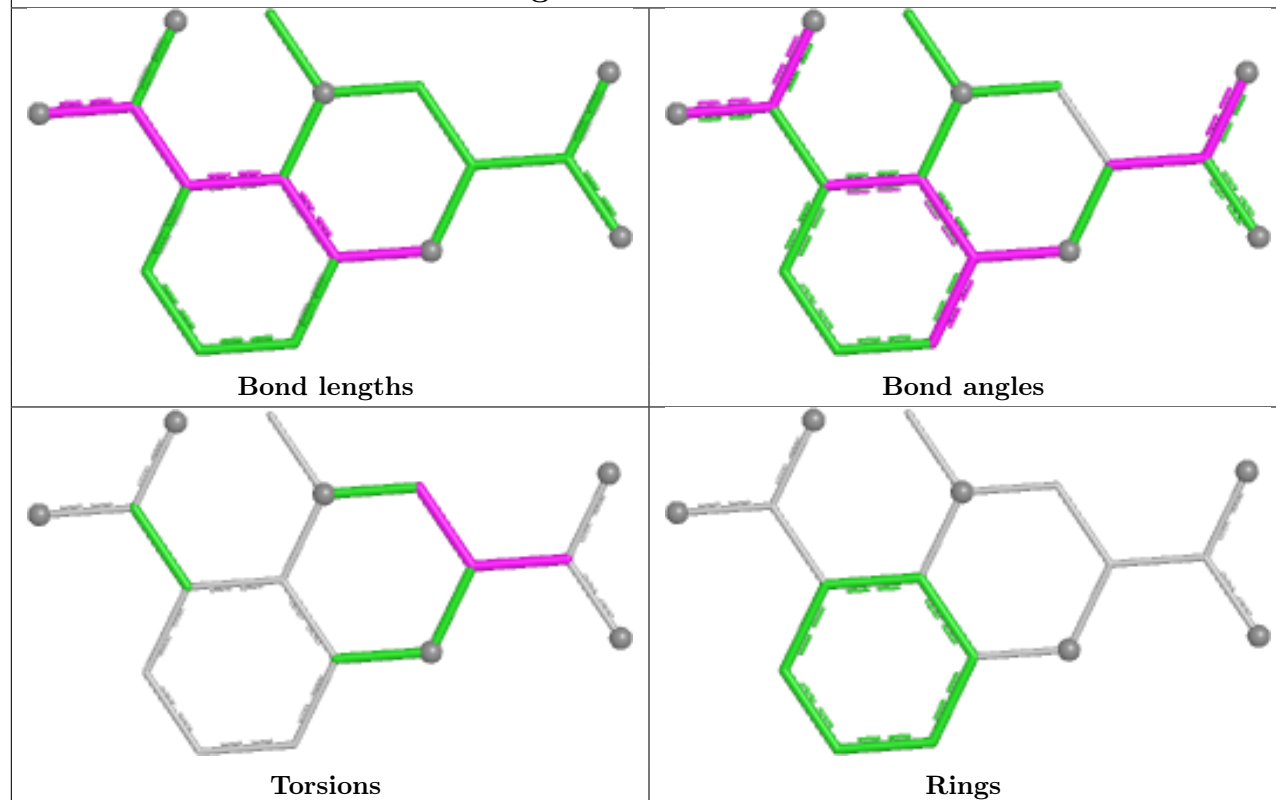
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	451	RVB	2	0
2	A	451	RVB	11	0
2	B	451	RVB	4	0
2	D	451	RVB	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

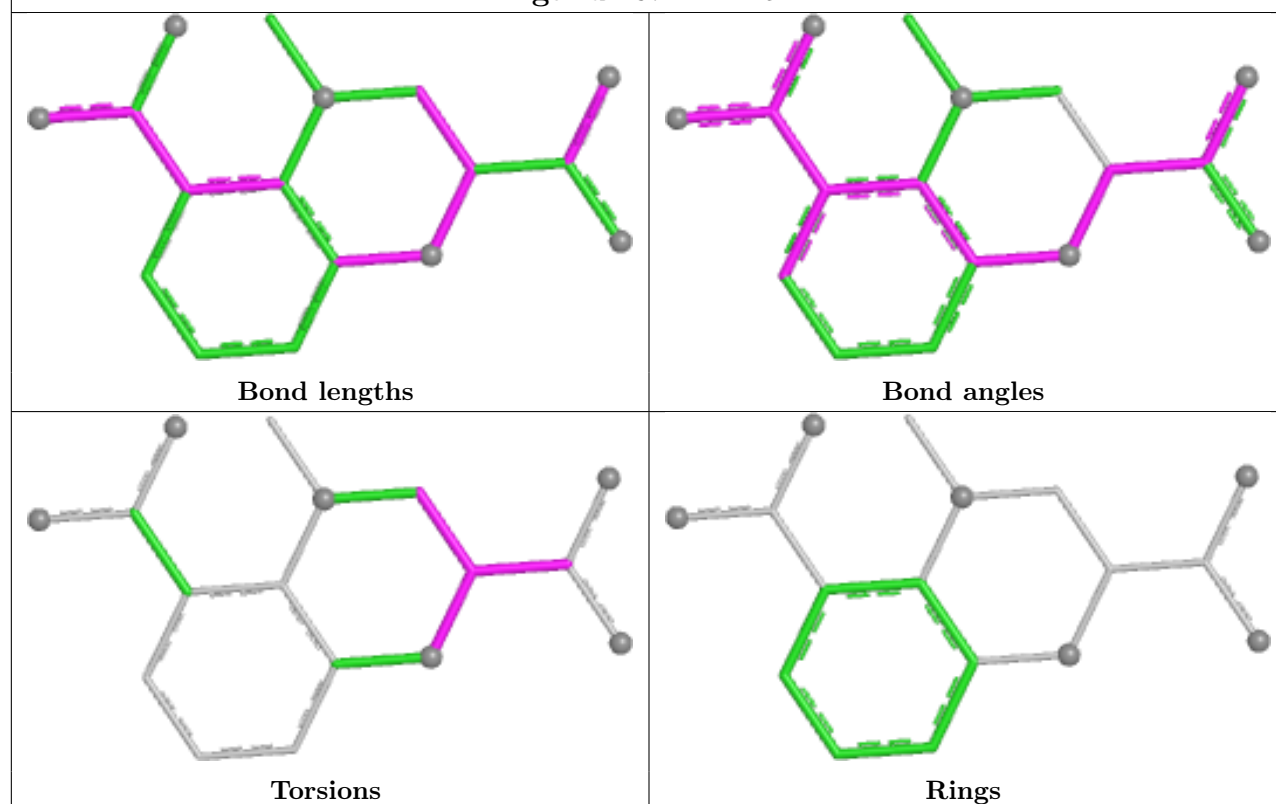
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

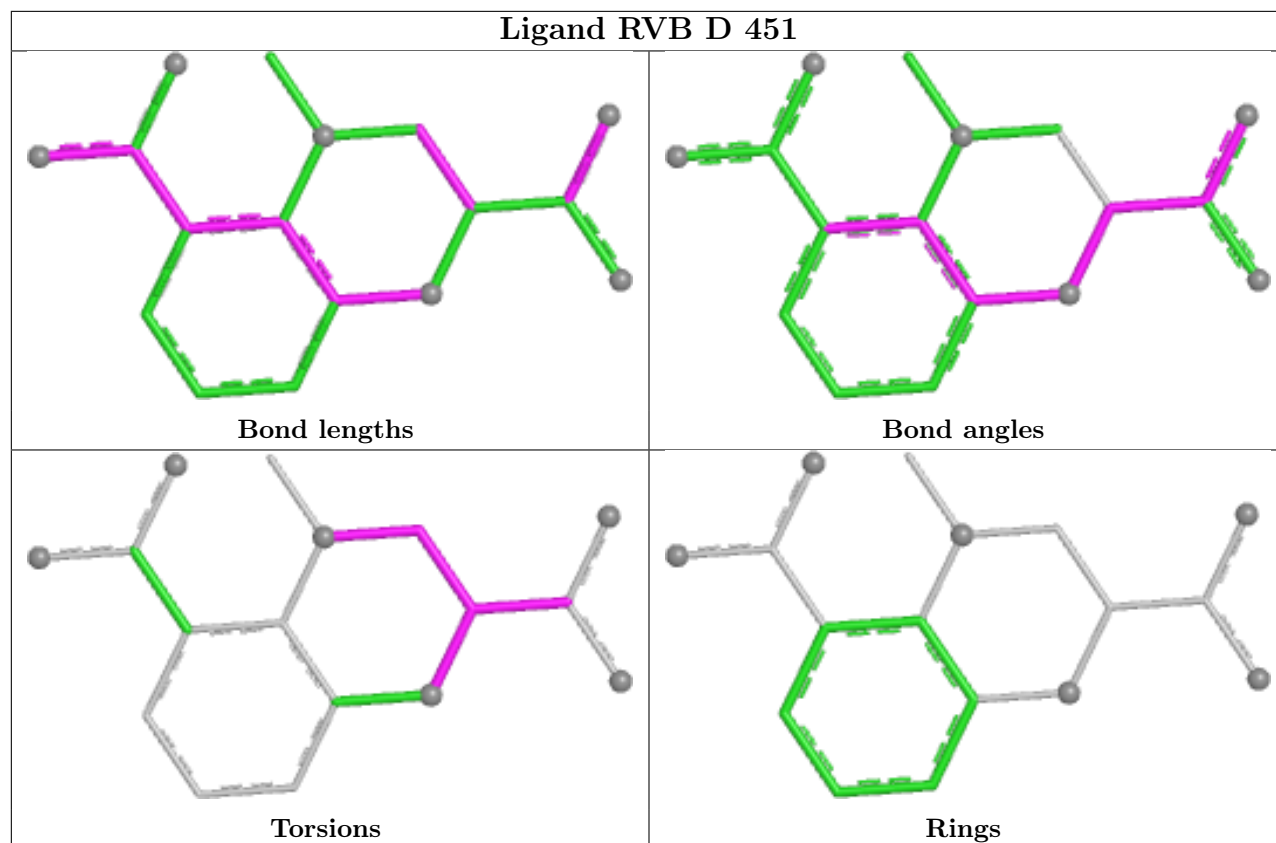


Ligand RVB A 451



Ligand RVB B 451





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	416/450 (92%)	-0.22	12 (2%)	53	49	17, 37, 62, 74	10 (2%)
1	B	423/450 (94%)	-0.21	13 (3%)	51	47	13, 38, 66, 89	9 (2%)
1	C	431/450 (95%)	-0.08	17 (3%)	43	38	9, 42, 77, 105	8 (1%)
1	D	428/450 (95%)	-0.11	12 (2%)	55	50	12, 44, 74, 88	8 (1%)
All	All	1698/1800 (94%)	-0.15	54 (3%)	50	46	9, 40, 71, 105	35 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ARG	4.8
1	A	176	ARG	3.8
1	C	274	LEU	3.7
1	D	342	ARG	3.6
1	B	330	GLY	3.5
1	B	249	TYR	3.4
1	B	271	THR	3.3
1	B	331	SER	3.2
1	D	176	ARG	3.2
1	D	332	VAL	3.1
1	A	272	ARG	3.1
1	B	332	VAL	3.1
1	C	280	ILE	3.1
1	D	211	CYS	3.1
1	A	115	GLY	3.0
1	B	176	ARG	2.9
1	A	269	ALA	2.9
1	C	305	SER	2.9
1	C	278	PRO	2.8
1	B	292	SER	2.7
1	D	330	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	116	VAL	2.7
1	A	271	THR	2.6
1	A	286	ASP	2.6
1	C	273	ALA	2.6
1	D	283	LEU	2.6
1	C	279	ALA	2.6
1	C	176	ARG	2.5
1	D	271	THR	2.5
1	B	122	GLN	2.5
1	A	292	SER	2.5
1	A	18	ILE	2.4
1	C	292	SER	2.4
1	D	156	ARG	2.4
1	A	249	TYR	2.4
1	C	269	ALA	2.4
1	C	275	GLY	2.3
1	D	79	THR	2.3
1	D	272	ARG	2.3
1	D	174	GLN	2.3
1	B	305	SER	2.3
1	B	211	CYS	2.3
1	C	271	THR	2.2
1	A	250	SER	2.2
1	C	334	HIS	2.1
1	C	333	GLN	2.1
1	C	250	SER	2.1
1	B	326	VAL	2.1
1	C	342	ARG	2.1
1	D	165	LEU	2.1
1	A	122	GLN	2.1
1	B	342	ARG	2.0
1	C	282	ARG	2.0
1	B	250	SER	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 ⓘ

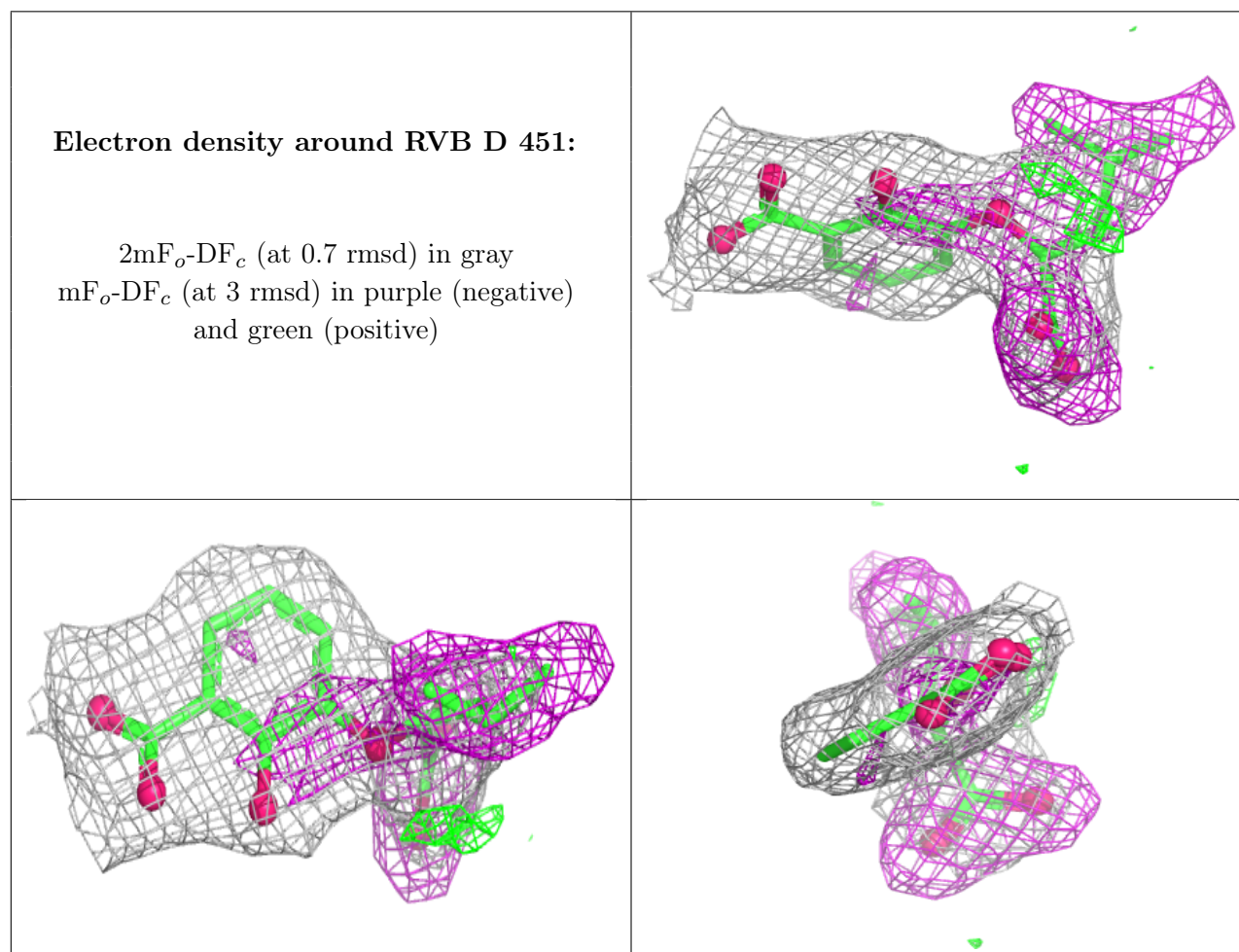
There are no oligosaccharides in this entry.

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.

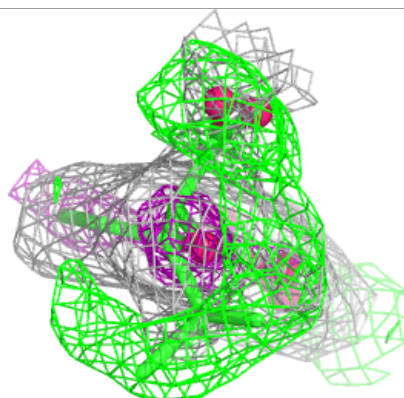
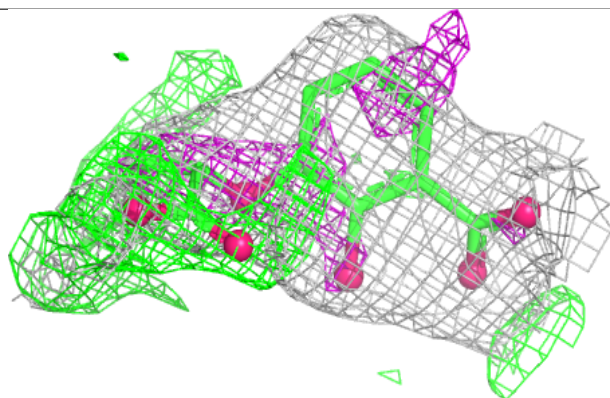
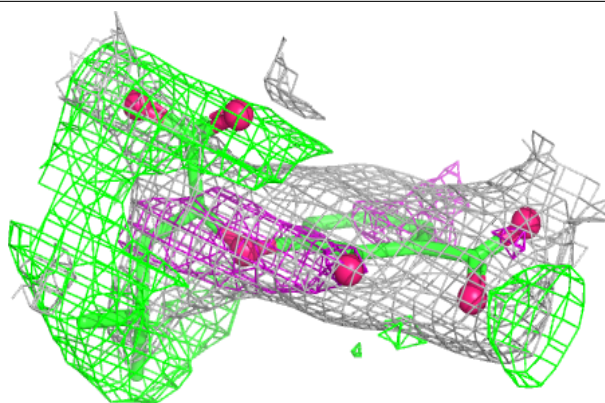
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	RVB	D	451	19/19	0.82	0.11	20,20,20,20	0
2	RVB	C	451	19/19	0.84	0.15	20,20,20,20	6
2	RVB	A	451	19/19	0.89	0.10	39,46,64,64	0
2	RVB	B	451	19/19	0.94	0.08	38,45,62,63	0

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.

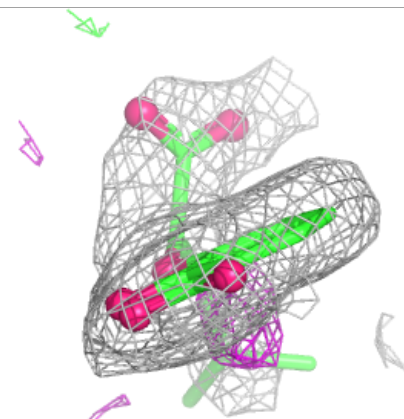
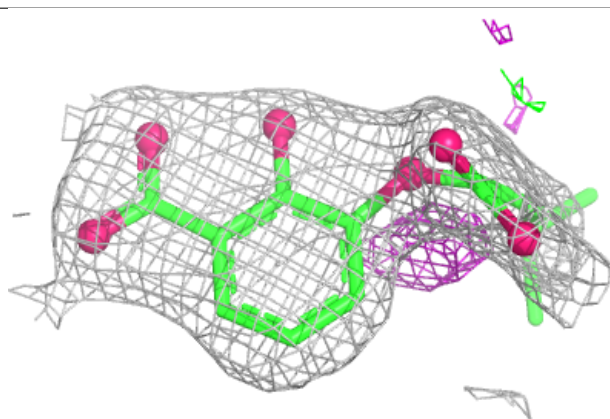
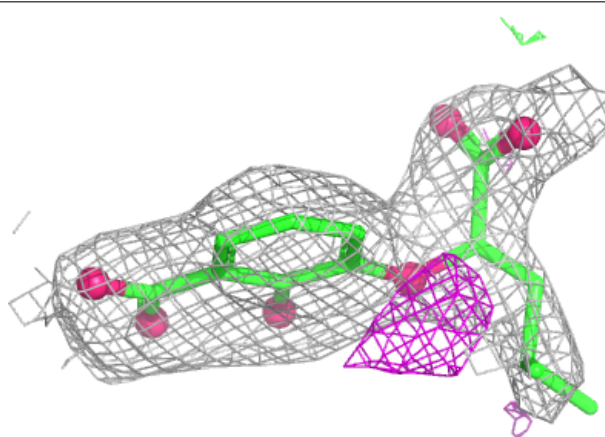


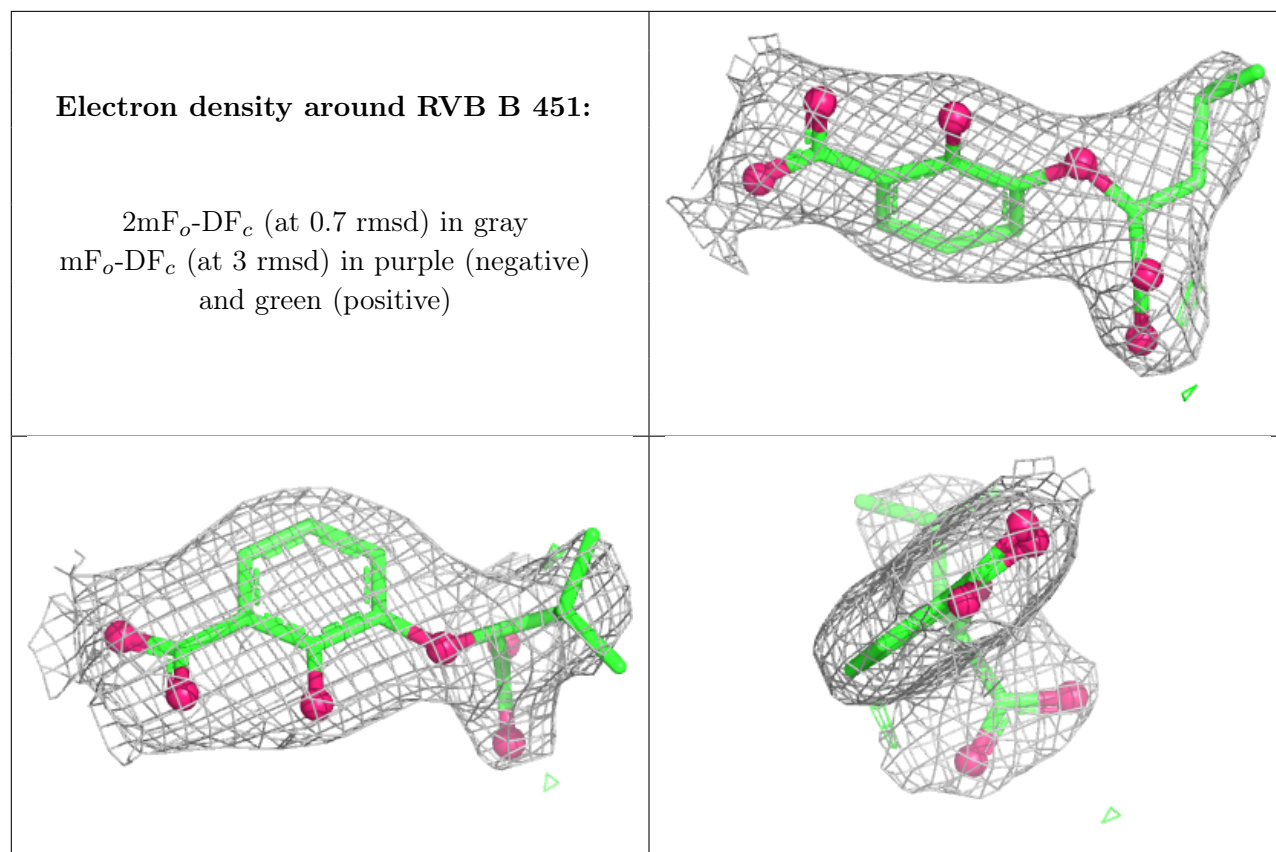
Electron density around RVB C 451:

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

**Electron density around RVB A 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.