



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:08 PM GMT

PDB ID : 3ST6  
Title : Structure of a M. tuberculosis Synthase, MbtI, in Complex with an Isochorismate Analogue Inhibitor  
Authors : Chi, G.; Bulloch, E.M.M.; Manos-Turvey, A.; Payne, R.J.; Lott, J.S.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2011-07-08  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

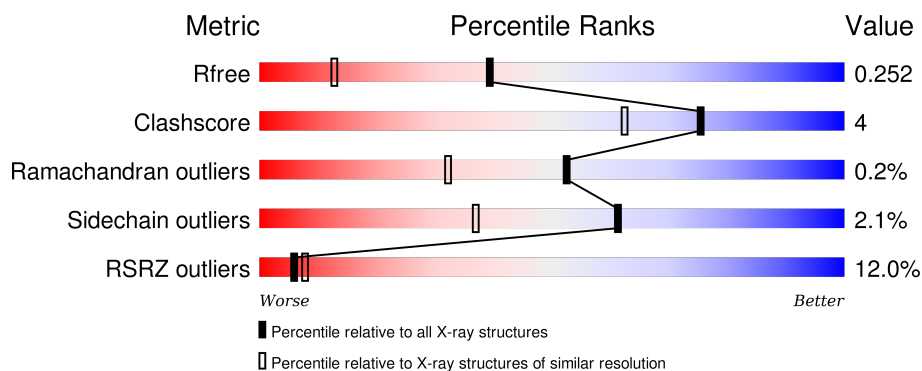
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>3%</div> <div>94%</div> <div>• •</div> </div>
1	B	450	<div> <div>4%</div> <div>90%</div> <div>7% •</div> </div>
1	C	450	<div> <div>10%</div> <div>87%</div> <div>7% 6%</div> </div>
1	D	450	<div> <div>28%</div> <div>73%</div> <div>16% • 9%</div> </div>

## 2 Entry composition [i](#)

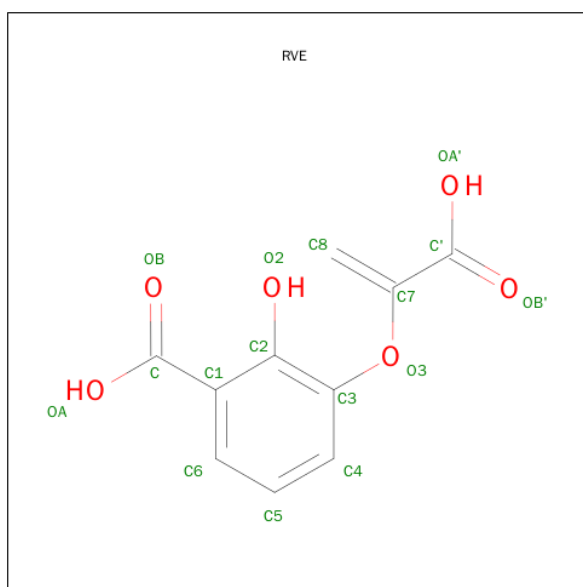
There are 3 unique types of molecules in this entry. The entry contains 13876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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/ischorismate-pyruvate lyase mbtI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	5	0
			3332	2088	606	628	10			
1	B	435	Total	C	N	O	S	0	1	0
			3301	2070	594	627	10			
1	C	424	Total	C	N	O	S	0	2	0
			3197	2006	574	607	10			
1	D	411	Total	C	N	O	S	0	0	0
			3012	1900	523	580	9			

- Molecule 2 is 3-[(1-CARBOXYETHENYL)OXY]-2-HYDROXYBENZOIC ACID (three-letter code: RVE) (formula: C<sub>10</sub>H<sub>8</sub>O<sub>6</sub>).

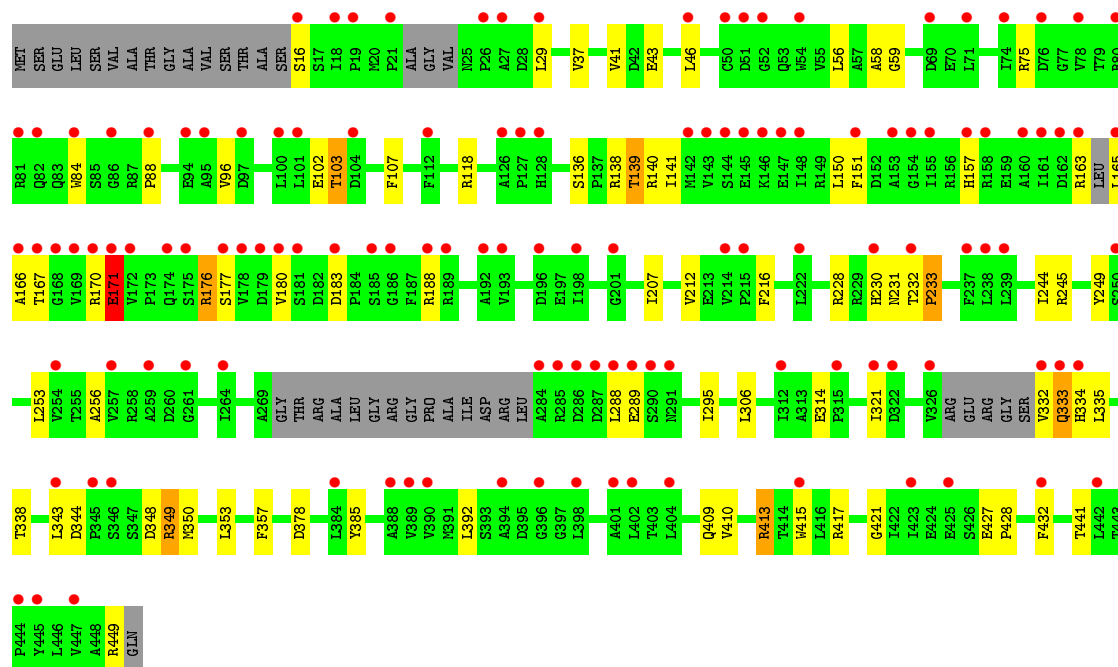


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	364	Total 364	O 364	0	0
3	B	299	Total 299	O 299	0	0
3	C	227	Total 227	O 227	0	0
3	D	112	Total 112	O 112	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.10Å 115.85Å 94.90Å 90.00° 91.25° 90.00°	Depositor
Resolution (Å)	29.36 – 1.75 29.36 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.36-1.75) 97.7 (29.36-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.217 , 0.243 0.225 , 0.252	Depositor DCC
$R_{free}$ test set	9407 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.6	EDS
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 187003 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: RVE

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	0.59	0/3397	0.68	0/4616
1	B	0.60	0/3362	0.70	0/4569
1	C	0.63	0/3256	0.71	0/4424
1	D	0.65	0/3065	0.76	2/4179 (0.0%)
All	All	0.62	0/13080	0.71	2/17788 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	29	LEU	CB-CG-CD1	5.00	119.51	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3332	0	3328	7	0
1	B	3301	0	3288	15	0
1	C	3197	0	3157	16	0
1	D	3012	0	2874	62	0
2	A	16	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	5	0	0
3	A	364	0	0	1	0
3	B	299	0	0	1	0
3	C	227	0	0	0	0
3	D	112	0	0	3	0
All	All	13876	0	12657	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:288:LEU:HD11	1:D:335:LEU:HB2	1.13	1.13
1:D:413:ARG:HH11	1:D:415:TRP:HB3	1.20	1.04
1:D:288:LEU:CD1	1:D:335:LEU:HB2	1.89	1.03
1:D:413:ARG:NH1	1:D:415:TRP:HB3	1.86	0.89
1:D:413:ARG:NH1	1:D:415:TRP:CB	2.41	0.82
1:D:102:GLU:HG3	1:D:102:GLU:O	1.79	0.81
1:D:349:ARG:HG3	1:D:350:MET:H	1.44	0.80
1:D:170:ARG:O	1:D:171:GLU:HB3	1.83	0.76
1:D:180:VAL:HG12	1:D:212:VAL:HG11	1.68	0.74
1:D:102:GLU:CG	1:D:102:GLU:O	2.34	0.72
1:C:137:PRO:HG2	1:C:140:ARG:HD2	1.71	0.71
1:D:413:ARG:HD2	1:D:415:TRP:CE3	2.31	0.64
1:B:300:ILE:HG22	1:B:365:ILE:HD13	1.80	0.64
1:D:183:ASP:CG	1:D:432:PHE:HE1	2.01	0.63
1:D:163:ARG:O	1:D:167:THR:HG22	1.99	0.63
1:D:165:LEU:O	1:D:167:THR:N	2.34	0.60
1:D:288:LEU:HD11	1:D:335:LEU:CB	2.09	0.60
1:D:288:LEU:HD12	1:D:335:LEU:HD12	1.83	0.59
1:D:176:ARG:HG2	1:D:177:SER:N	2.16	0.59
1:D:228:ARG:HD2	1:D:228:ARG:O	2.03	0.59
1:C:180:VAL:HG12	1:C:212:VAL:HG11	1.85	0.59
1:D:165:LEU:O	1:D:166:ALA:C	2.42	0.57
1:B:190:ARG:HD2	1:B:377:LEU:O	2.06	0.56
1:D:332:VAL:C	1:D:334:HIS:H	2.09	0.56
1:D:228:ARG:NH1	1:D:228:ARG:O	2.30	0.55
1:D:413:ARG:CD	1:D:415:TRP:CE3	2.89	0.55
1:D:84:TRP:CZ3	1:D:88:PRO:HA	2.43	0.54
1:D:231:ASN:OD1	1:D:441:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:ARG:HD2	1:D:216:PHE:CE2	2.43	0.53
1:A:15:SER:O	1:A:16:SER:HB3	2.08	0.53
1:C:56:LEU:HD23	1:C:141:ILE:HD12	1.90	0.53
1:D:165:LEU:C	1:D:167:THR:N	2.59	0.53
1:D:349:ARG:HG3	1:D:350:MET:N	2.18	0.52
1:D:207:ILE:HG13	1:D:421:GLY:HA2	1.92	0.52
1:C:325:THR:O	1:C:336:GLY:N	2.33	0.51
1:D:233:PRO:HG3	1:D:249:TYR:HB3	1.92	0.51
1:D:343:LEU:HD21	1:D:348:ASP:HA	1.92	0.51
1:D:253:LEU:HD21	1:D:256:ALA:HB2	1.92	0.51
1:C:287:ASP:O	1:C:291:ASN:HB2	2.10	0.51
1:D:171:GLU:OE1	1:D:171:GLU:O	2.30	0.51
1:D:118:ARG:NH1	3:D:965:HOH:O	2.40	0.51
1:B:288:LEU:HG	1:B:335:LEU:HG	1.94	0.50
1:D:75:ARG:NH1	3:D:505:HOH:O	2.30	0.49
1:B:405:ARG:HB3	1:B:441:THR:HG21	1.93	0.49
1:B:180:VAL:HG12	1:B:212:VAL:HG11	1.94	0.49
1:D:314:GLU:HG3	1:D:344:ASP:HA	1.95	0.49
1:D:43:GLU:OE2	1:D:157:HIS:NE2	2.42	0.48
1:D:103:THR:HG21	1:D:136:SER:HB2	1.95	0.48
1:D:332:VAL:O	1:D:334:HIS:N	2.43	0.48
1:C:198:ILE:O	1:C:201:GLY:N	2.41	0.48
1:D:245:ARG:HB2	1:D:409:GLN:HB3	1.95	0.48
1:D:183:ASP:OD1	1:D:432:PHE:HE1	1.97	0.48
1:D:165:LEU:C	1:D:167:THR:H	2.17	0.47
1:A:25:ASN:OD1	3:A:795:HOH:O	2.20	0.47
1:B:109:TRP:HZ3	1:B:111:ALA:HB2	1.80	0.47
1:D:96:VAL:HG11	1:D:392:LEU:HD13	1.96	0.47
1:C:64:VAL:HG23	1:C:99:LEU:HD11	1.97	0.47
1:C:57:ALA:HB1	1:C:137:PRO:HB3	1.97	0.47
1:D:58:ALA:HB3	1:D:139:THR:HG22	1.97	0.47
1:D:321:ILE:HG13	1:D:338:THR:HB	1.97	0.47
1:A:231:ASN:OD1	1:A:441:THR:HG23	2.15	0.47
1:D:138:ARG:HD2	3:D:996:HOH:O	2.16	0.46
1:C:234:VAL:HG23	1:C:235:ARG:HG2	1.98	0.46
1:B:205:LYS:HG2	1:B:205:LYS:HZ3	1.33	0.46
1:B:205:LYS:HG3	1:B:206:VAL:N	2.30	0.45
1:D:37:VAL:O	1:D:41:VAL:HG22	2.15	0.45
1:C:87:ARG:NH2	1:C:354:GLU:OE2	2.49	0.45
1:A:353:LEU:O	1:A:357:PHE:HB2	2.16	0.45
1:B:20:MET:HG3	1:B:144:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:LEU:CD1	1:D:335:LEU:CD1	2.95	0.45
1:D:140:ARG:HB2	1:D:151:PHE:HB2	1.99	0.44
1:C:172:VAL:HG11	1:C:226:LEU:HB2	1.98	0.44
1:B:55:VAL:HG23	3:B:492:HOH:O	2.17	0.44
1:D:228:ARG:HD2	1:D:228:ARG:HA	1.64	0.44
1:B:304:SER:O	1:B:307:GLU:HG2	2.17	0.44
1:D:288:LEU:CD1	1:D:335:LEU:HD12	2.46	0.44
1:D:176:ARG:HD2	1:D:216:PHE:CZ	2.52	0.44
1:C:55:VAL:HG22	1:C:142:MET:HG2	2.00	0.44
1:D:244:ILE:HG12	1:D:410:VAL:HG22	1.99	0.44
1:A:405:ARG:HB3	1:A:441:THR:HG21	2.00	0.44
1:C:234:VAL:HG12	1:C:329:ARG:NH2	2.33	0.43
1:D:353:LEU:O	1:D:357:PHE:HB2	2.19	0.43
1:D:413:ARG:NH1	1:D:415:TRP:CG	2.86	0.42
1:D:43:GLU:HB2	1:D:59:GLY:HA2	2.00	0.42
1:D:385:TYR:CG	1:D:417:ARG:HD3	2.54	0.42
1:D:188:ARG:HG3	1:D:432:PHE:CD1	2.55	0.42
1:B:298:HIS:O	1:B:302:VAL:HG23	2.19	0.42
1:B:287:ASP:O	1:B:291:ASN:HB2	2.20	0.42
1:C:322:ASP:O	1:C:337:SER:HA	2.20	0.42
1:D:289:GLU:O	1:D:295:ILE:HD11	2.20	0.41
1:C:190:ARG:HD2	1:C:377:LEU:O	2.20	0.41
1:D:427:GLU:HA	1:D:428:PRO:HD3	1.95	0.41
1:A:300:ILE:HG22	1:A:365:ILE:HD13	2.01	0.41
1:B:258:ARG:HE	1:B:262:VAL:HB	1.86	0.41
1:A:180:VAL:HG12	1:A:212:VAL:HG11	2.03	0.41
1:C:207:ILE:HG13	1:C:421:GLY:HA2	2.03	0.40
1:D:56:LEU:HD23	1:D:141:ILE:HD12	2.03	0.40
1:D:46:LEU:HD22	1:D:107:PHE:HB3	2.02	0.40
1:B:205:LYS:HD3	1:B:423:ILE:HG23	2.02	0.40
1:D:230:HIS:N	1:D:230:HIS:CD2	2.90	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	439/450 (98%)	431 (98%)	7 (2%)	1 (0%)	52	32
1	B	434/450 (96%)	430 (99%)	4 (1%)	0	100	100
1	C	417/450 (93%)	411 (99%)	6 (1%)	0	100	100
1	D	401/450 (89%)	383 (96%)	15 (4%)	3 (1%)	26	10
All	All	1691/1800 (94%)	1655 (98%)	32 (2%)	4 (0%)	52	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	D	171	GLU
1	D	333	GLN
1	D	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	343/358 (96%)	339 (99%)	4 (1%)	78	62
1	B	340/358 (95%)	334 (98%)	6 (2%)	66	46
1	C	327/358 (91%)	322 (98%)	5 (2%)	72	55
1	D	294/358 (82%)	282 (96%)	12 (4%)	37	13
All	All	1304/1432 (91%)	1277 (98%)	27 (2%)	61	37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ILE
1	A	342	ARG
1	A	357	PHE
1	A	378	ASP

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	205	LYS
1	B	297	GLU
1	B	357	PHE
1	B	367	LYS
1	B	378	ASP
1	C	176	ARG
1	C	311	ASP
1	C	325	THR
1	C	378	ASP
1	C	405	ARG
1	D	16	SER
1	D	103	THR
1	D	139	THR
1	D	150	LEU
1	D	171	GLU
1	D	232	THR
1	D	306	LEU
1	D	333	GLN
1	D	349	ARG
1	D	378	ASP
1	D	413	ARG
1	D	449	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	HIS
1	C	53	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

2 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	RVE	A	451	-	10,16,16	2.33	5 (50%)	13,22,22	2.12	2 (15%)
2	RVE	B	451	-	10,16,16	2.39	5 (50%)	13,22,22	2.54	4 (30%)

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	RVE	A	451	-	-	0/3/12/12	0/1/1/1
2	RVE	B	451	-	-	0/3/12/12	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	451	RVE	O3-C7	-4.32	1.33	1.41
2	A	451	RVE	O3-C7	-4.15	1.33	1.41
2	A	451	RVE	O3-C3	-3.50	1.33	1.41
2	B	451	RVE	O3-C3	-3.37	1.34	1.41
2	B	451	RVE	C3-C2	-2.97	1.36	1.40
2	A	451	RVE	O2-C2	-2.83	1.30	1.37
2	A	451	RVE	C3-C2	-2.52	1.36	1.40
2	B	451	RVE	O2-C2	-2.39	1.31	1.37
2	A	451	RVE	C8-C7	2.23	1.37	1.33
2	B	451	RVE	C8-C7	2.48	1.37	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	451	RVE	C6-C5-C4	-2.13	117.20	120.24
2	B	451	RVE	C4-C3-C2	-2.07	117.86	120.05
2	B	451	RVE	O3-C3-C2	2.83	122.30	117.66
2	A	451	RVE	O3-C3-C2	3.15	122.83	117.66
2	A	451	RVE	C3-O3-C7	6.37	129.55	118.01
2	B	451	RVE	C3-O3-C7	7.55	131.71	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	436/450 (96%)	0.42	15 (3%) 49 55	11, 24, 44, 62	0
1	B	435/450 (96%)	0.38	19 (4%) 38 44	12, 25, 44, 59	0
1	C	424/450 (94%)	0.78	45 (10%) 8 10	10, 30, 50, 84	0
1	D	411/450 (91%)	1.52	126 (30%) 1 1	19, 44, 72, 100	1 (0%)
All	All	1706/1800 (94%)	0.77	205 (12%) 6 8	10, 29, 59, 100	1 (0%)

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	ALA	8.0
1	C	288	LEU	7.7
1	C	326	VAL	7.6
1	D	160	ALA	6.3
1	C	275	GLY	6.1
1	D	155	ILE	5.9
1	D	288	LEU	5.8
1	D	19	PRO	5.8
1	D	332	VAL	5.6
1	C	335	LEU	5.5
1	D	172	VAL	5.4
1	D	161	ILE	5.2
1	C	273	ALA	5.1
1	C	287	ASP	4.9
1	C	332	VAL	4.9
1	C	285	ARG	4.9
1	B	283	LEU	4.9
1	C	284	ALA	4.9
1	B	279	ALA	4.8
1	D	186	GLY	4.8
1	A	22[A]	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	145	GLU	4.7
1	D	287	ASP	4.7
1	D	445	TYR	4.6
1	D	178	VAL	4.6
1	D	345	PRO	4.6
1	D	21	PRO	4.5
1	C	276	ARG	4.4
1	D	389	VAL	4.3
1	D	447	VAL	4.3
1	D	128	HIS	4.3
1	D	192	ALA	4.2
1	D	167	THR	4.2
1	D	169	VAL	4.2
1	D	180	VAL	4.1
1	C	22	ALA	4.1
1	B	278	PRO	4.0
1	D	162	ASP	4.0
1	D	423	ILE	4.0
1	D	333	GLN	3.9
1	D	26	PRO	3.9
1	D	432	PHE	3.8
1	D	158	ARG	3.8
1	D	84	TRP	3.8
1	D	80	ARG	3.8
1	D	154	GLY	3.8
1	C	362	ALA	3.7
1	D	214	VAL	3.7
1	A	23[A]	GLY	3.7
1	C	23	GLY	3.7
1	D	166	ALA	3.7
1	C	201	GLY	3.7
1	D	196	ASP	3.6
1	B	277	GLY	3.6
1	D	444	PRO	3.6
1	C	345	PRO	3.6
1	D	175	SER	3.6
1	C	199	ALA	3.6
1	D	181	SER	3.5
1	D	257	VAL	3.5
1	B	315	PRO	3.4
1	D	321	ILE	3.4
1	D	151	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	3.4
1	A	146	LYS	3.4
1	D	101	LEU	3.3
1	D	163	ARG	3.3
1	D	237	PHE	3.3
1	D	394	ALA	3.3
1	D	264	ILE	3.3
1	D	148	ILE	3.3
1	D	177	SER	3.2
1	D	259	ALA	3.2
1	C	360	VAL	3.2
1	D	415	TRP	3.2
1	D	222	LEU	3.2
1	C	198	ILE	3.2
1	D	230	HIS	3.1
1	D	390	VAL	3.1
1	C	200	ALA	3.1
1	D	95	ALA	3.1
1	D	402	LEU	3.1
1	D	334	HIS	3.1
1	D	52	GLY	3.1
1	D	326	VAL	3.1
1	D	170	ARG	3.1
1	C	272	ARG	3.0
1	D	54	TRP	3.0
1	C	311	ASP	3.0
1	D	238	LEU	2.9
1	D	388	ALA	2.9
1	D	165	LEU	2.9
1	D	384	LEU	2.9
1	D	127	PRO	2.9
1	C	182	ASP	2.9
1	D	171	GLU	2.8
1	D	174	GLN	2.8
1	D	69	ASP	2.8
1	B	86	GLY	2.8
1	D	168	GLY	2.8
1	A	315	PRO	2.8
1	D	343	LEU	2.8
1	D	183	ASP	2.8
1	C	271	THR	2.8
1	D	315	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	127	PRO	2.8
1	D	285	ARG	2.8
1	D	201	GLY	2.7
1	D	51	ASP	2.7
1	D	404	LEU	2.7
1	D	290	SER	2.7
1	C	346	SER	2.7
1	C	286	ASP	2.7
1	D	146	LYS	2.7
1	A	356	LEU	2.7
1	D	179	ASP	2.7
1	C	404	LEU	2.6
1	D	401	ALA	2.6
1	A	15	SER	2.6
1	C	430	ARG	2.6
1	C	423	ILE	2.6
1	D	86	GLY	2.6
1	D	126	ALA	2.6
1	D	82	GLN	2.6
1	A	345	PRO	2.6
1	D	97	ASP	2.6
1	C	389	VAL	2.6
1	D	74	ILE	2.6
1	D	142	MET	2.6
1	D	29	LEU	2.6
1	D	239	LEU	2.6
1	A	412	GLY	2.6
1	D	261	GLY	2.6
1	C	361	THR	2.5
1	A	46	LEU	2.5
1	B	281	ASP	2.5
1	C	401	ALA	2.5
1	D	143	VAL	2.5
1	D	76	ASP	2.5
1	D	16	SER	2.5
1	D	157	HIS	2.5
1	C	268	LEU	2.5
1	C	426	SER	2.5
1	C	322	ASP	2.4
1	D	188	ARG	2.4
1	D	232	THR	2.4
1	D	250	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	100	LEU	2.4
1	D	153	ALA	2.4
1	D	50	CYS	2.4
1	C	402	LEU	2.4
1	D	312	ILE	2.4
1	B	199	ALA	2.4
1	B	286	ASP	2.4
1	D	46	LEU	2.3
1	D	71	LEU	2.3
1	C	269	ALA	2.3
1	D	185	SER	2.3
1	C	315	PRO	2.3
1	B	403	THR	2.3
1	D	291	ASN	2.3
1	B	302	VAL	2.3
1	A	316	GLY	2.3
1	B	404	LEU	2.3
1	B	15	SER	2.3
1	D	254	VAL	2.3
1	A	21[A]	PRO	2.3
1	C	359	ALA	2.2
1	D	18	ILE	2.2
1	D	78	VAL	2.2
1	D	189	ARG	2.2
1	D	27	ALA	2.2
1	D	104	ASP	2.2
1	D	286	ASP	2.2
1	B	275	GLY	2.2
1	C	333	GLN	2.2
1	B	345	PRO	2.2
1	C	76	ASP	2.2
1	C	202	ARG	2.2
1	D	425	GLU	2.2
1	D	322	ASP	2.2
1	B	402	LEU	2.2
1	D	442	LEU	2.2
1	D	215	PRO	2.1
1	D	144	SER	2.1
1	D	398	LEU	2.1
1	A	19	PRO	2.1
1	B	361	THR	2.1
1	C	325	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	112	PHE	2.1
1	D	147	GLU	2.1
1	D	198	ILE	2.1
1	D	396	GLY	2.1
1	B	276	ARG	2.1
1	D	81	ARG	2.1
1	A	78	VAL	2.1
1	D	193	VAL	2.1
1	D	88	PRO	2.1
1	C	128	HIS	2.1
1	C	329	ARG	2.1
1	D	94	GLU	2.0
1	D	346	SER	2.0
1	D	289	GLU	2.0
1	A	103	THR	2.0
1	C	239	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RVE	B	451	16/16	0.94	0.11	-0.48	19,26,32,33	0
2	RVE	A	451	16/16	0.95	0.10	-0.58	15,23,29,31	0

## 6.5 Other polymers

There are no such residues in this entry.