



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:05 PM UTC

PDB ID : 3ST6 / pdb_00003st6
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

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
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

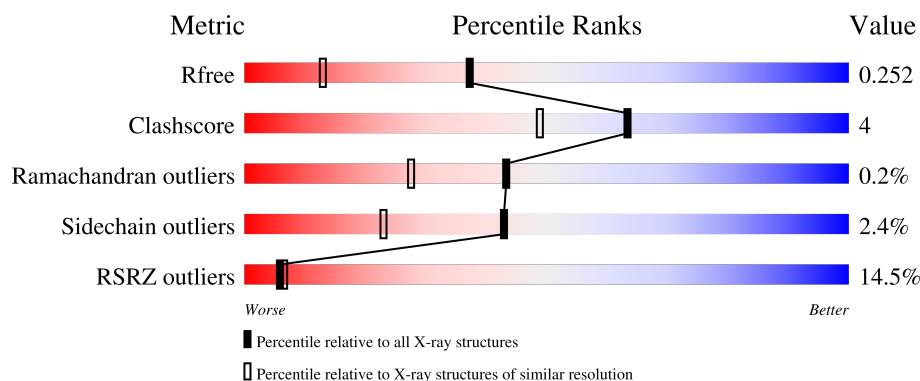
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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% 90% 6% .
1	B	450	2% 89% 8% .
1	C	450	14% 85% 9% . 6%
1	D	450	36% 72% 16% . 9%

2 Entry composition [i](#)

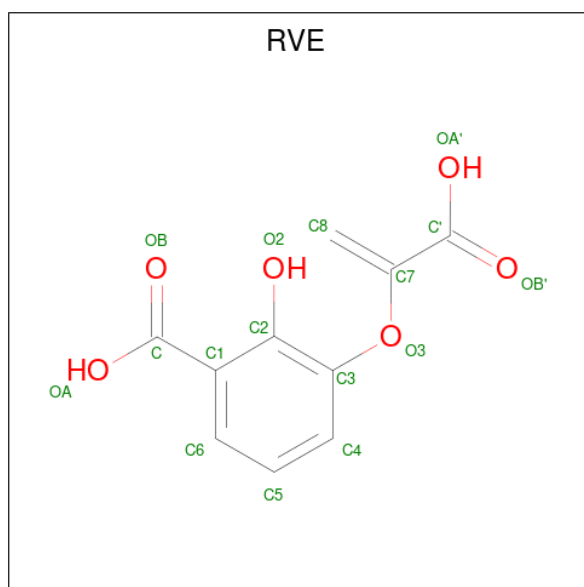
There are 3 unique types of molecules in this entry. The entry contains 13876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: RVE) (formula: C₁₀H₈O₆).



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		

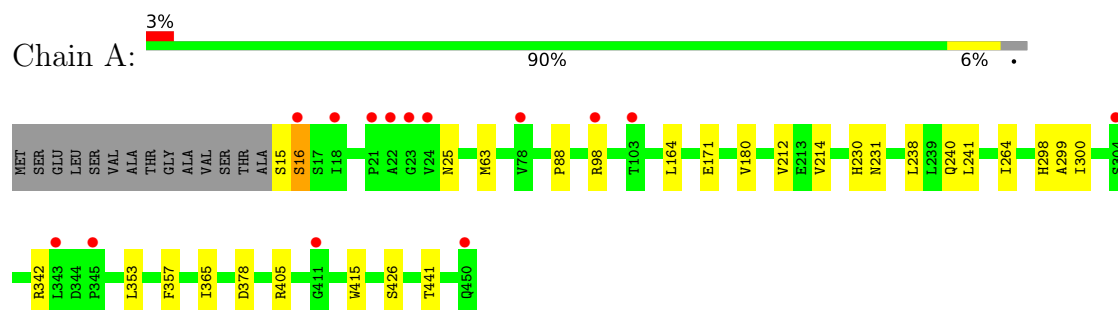
- Molecule 3 is water.

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

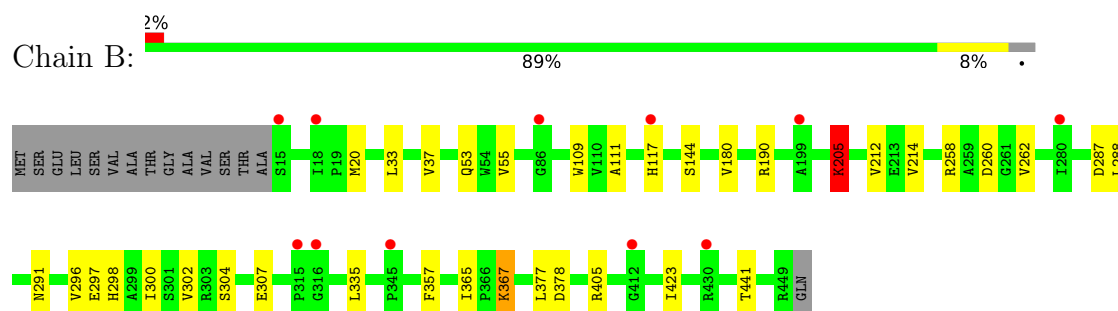
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

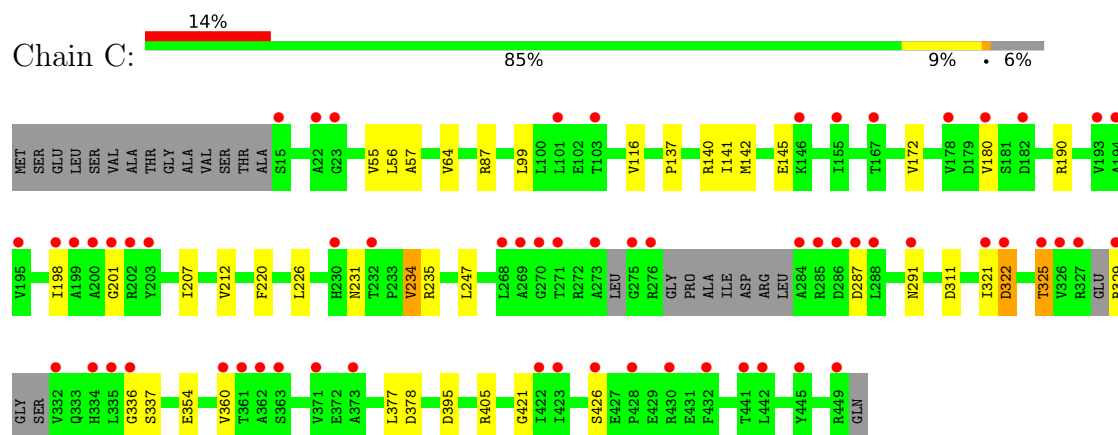
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI



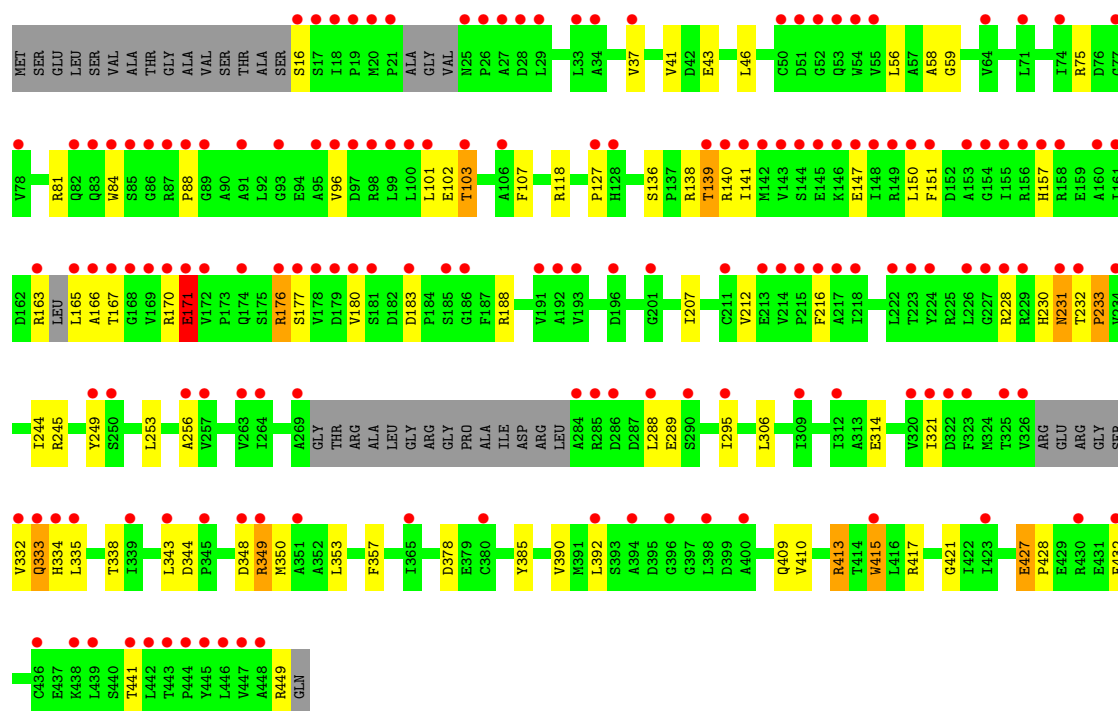
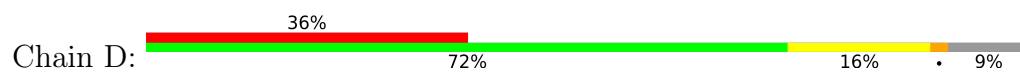
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13876	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.94	5/3397 (0.1%)	1.17	5/4616 (0.1%)
1	B	0.94	3/3362 (0.1%)	1.18	6/4569 (0.1%)
1	C	0.97	4/3256 (0.1%)	1.20	6/4424 (0.1%)
1	D	0.97	2/3065 (0.1%)	1.33	6/4179 (0.1%)
All	All	0.95	14/13080 (0.1%)	1.22	23/17788 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	LEU	C-O	-8.01	1.14	1.23
1	A	298	HIS	C-O	-6.53	1.16	1.24
1	B	53	GLN	C-O	-6.24	1.16	1.24
1	C	321	ILE	C-O	-5.71	1.17	1.24
1	B	205	LYS	C-O	-5.62	1.16	1.23
1	C	426	SER	C-O	-5.52	1.17	1.23
1	A	240	GLN	C-O	-5.49	1.17	1.23
1	C	231	ASN	C-O	-5.38	1.17	1.23
1	D	127	PRO	C-O	-5.33	1.17	1.23
1	C	220	PHE	C-O	-5.19	1.19	1.24
1	D	427	GLU	C-O	-5.11	1.18	1.24
1	A	299	ALA	C-O	-5.09	1.18	1.24
1	A	230	HIS	C-O	-5.06	1.17	1.24
1	B	117	HIS	C-O	-5.01	1.18	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	LEU	N-CA-C	-9.97	100.10	110.97
1	B	296	VAL	N-CA-CB	6.96	118.69	110.55
1	A	426	SER	N-CA-C	6.04	118.99	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	ARG	N-CA-C	5.97	119.20	109.59
1	C	116	VAL	CA-C-N	5.73	127.95	120.28
1	C	116	VAL	C-N-CA	5.73	127.95	120.28
1	A	88	PRO	CA-C-N	5.72	126.33	119.98
1	A	88	PRO	C-N-CA	5.72	126.33	119.98
1	B	214	VAL	N-CA-C	-5.67	101.94	107.55
1	C	360	VAL	CA-C-N	5.58	128.53	120.38
1	C	360	VAL	C-N-CA	5.58	128.53	120.38
1	C	322	ASP	N-CA-C	-5.47	98.29	108.02
1	D	415	TRP	N-CA-C	5.43	117.33	109.07
1	B	37	VAL	CA-C-N	5.42	127.55	120.28
1	B	37	VAL	C-N-CA	5.42	127.55	120.28
1	A	214	VAL	N-CA-C	-5.33	102.27	107.55
1	D	231	ASN	N-CA-C	-5.32	100.35	108.76
1	B	367	LYS	N-CA-C	5.30	116.74	111.07
1	D	147	GLU	N-CA-C	5.26	118.10	110.42
1	C	395	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	260	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	415	TRP	N-CA-C	5.05	116.75	109.07
1	D	390	VAL	N-CA-C	5.02	116.57	108.85

There are no chirality outliers.

There are no planarity outliers.

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	3332	0	3328	8	0
1	B	3301	0	3288	14	0
1	C	3197	0	3157	17	0
1	D	3012	0	2874	64	0
2	A	16	0	5	0	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	112	0	0	3	0
All	All	13876	0	12657	103	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 (103) 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:O	1:D:102:GLU:HG3	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:O	1:D:102:GLU:CG	2.34	0.72
1:C:137:PRO:HG2	1:C:140:ARG:HD2	1.71	0.71
1:D:183:ASP:CG	1:D:432:PHE:HE1	2.01	0.68
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:163:ARG:O	1:D:167:THR:HG22	1.99	0.63
1:D:165:LEU:O	1:D:166:ALA:C	2.42	0.62
1:D:165:LEU:O	1:D:167:THR:N	2.34	0.60
1:D:332:VAL:C	1:D:334:HIS:H	2.09	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:O	1:D:228:ARG:HD2	2.03	0.59
1:C:180:VAL:HG12	1:C:212:VAL:HG11	1.85	0.59
1:B:190:ARG:HD2	1:B:377:LEU:O	2.06	0.56
1:D:165:LEU:C	1:D:167:THR:N	2.59	0.56
1:D:228:ARG:O	1:D:228:ARG:NH1	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
1:A:15:SER:O	1:A:16:SER:HB3	2.08	0.53
1:D:176:ARG:HD2	1:D:216:PHE:CE2	2.43	0.53
1:C:56:LEU:HD23	1:C:141:ILE:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LEU:C	1:D:167:THR:H	2.17	0.52
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:118:ARG:NH1	3:D:965:HOH:O	2.40	0.51
1:D:171:GLU:OE1	1:D:171:GLU:O	2.30	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: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:D:228:ARG:HD2	1:D:228:ARG:C	2.35	0.46
1:C:87:ARG:NH2	1:C:354:GLU:OE2	2.49	0.45
1:D:37:VAL:O	1:D:41:VAL:HG22	2.15	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
1:D:288:LEU:CD1	1:D:335:LEU:CD1	2.95	0.45
1:C:172:VAL:HG11	1:C:226:LEU:HB2	1.98	0.44
1:D:140:ARG:HB2	1:D:151:PHE:HB2	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:SER:O	1:B:307:GLU:HG2	2.17	0.44
1:C:247:LEU:C	1:C:247:LEU:HD12	2.43	0.44
1:C:55:VAL:HG22	1:C:142:MET:HG2	2.00	0.44
1:D:176:ARG:HD2	1:D:216:PHE:CZ	2.52	0.44
1:D:288:LEU:CD1	1:D:335:LEU:HD12	2.46	0.44
1:B:205:LYS:HZ3	1:B:205:LYS:HG2	1.36	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: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:413:ARG:NH1	1:D:415:TRP:CG	2.86	0.42
1:D:188:ARG:HG3	1:D:432:PHE:CD1	2.55	0.42
1:B:287:ASP:O	1:B:291:ASN:HB2	2.20	0.42
1:B:298:HIS:O	1:B:302:VAL:HG23	2.19	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:D:183:ASP:CG	1:D:432:PHE:CE1	2.92	0.40
1:A:63:MET:HE1	1:A:241:LEU:HD11	2.04	0.40
1:B:205:LYS:HD3	1:B:423:ILE:HG23	2.02	0.40
1:D:230:HIS:CD2	1:D:230:HIS:N	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%)	43	27
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%)	18	7
All	All	1691/1800 (94%)	1655 (98%)	32 (2%)	4 (0%)	43	27

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%)	337 (98%)	6 (2%)	53	36
1	B	340/358 (95%)	334 (98%)	6 (2%)	51	33
1	C	327/358 (91%)	321 (98%)	6 (2%)	51	33
1	D	294/358 (82%)	281 (96%)	13 (4%)	25	7
All	All	1304/1432 (91%)	1273 (98%)	31 (2%)	43	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	A	164	LEU
1	A	171	GLU
1	A	264	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	342	ARG
1	A	378	ASP
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	145	GLU
1	C	234	VAL
1	C	311	ASP
1	C	325	THR
1	C	378	ASP
1	C	405	ARG
1	D	16	SER
1	D	81	ARG
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

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

Mol	Chain	Res	Type
1	A	25	ASN
1	A	83	GLN
1	C	61	GLN
1	C	83	GLN
1	C	291	ASN

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](#)

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	-	16,16,16	3.22	8 (50%)	19,22,22	1.90	5 (26%)
2	RVE	B	451	-	16,16,16	2.79	9 (56%)	19,22,22	1.43	5 (26%)

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	RVE	C7-C'	9.24	1.58	1.49
2	B	451	RVE	C7-C'	6.42	1.55	1.49
2	B	451	RVE	O3-C7	-4.34	1.33	1.41
2	A	451	RVE	O3-C7	-4.16	1.33	1.41
2	A	451	RVE	O3-C3	-3.63	1.33	1.41
2	A	451	RVE	OA'-C'	-3.63	1.20	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	451	RVE	O3-C3	-3.48	1.34	1.41
2	B	451	RVE	OA'-C'	-3.42	1.21	1.30
2	B	451	RVE	C3-C2	-3.02	1.36	1.40
2	A	451	RVE	O2-C2	-2.84	1.30	1.36
2	A	451	RVE	OA-C	-2.81	1.22	1.30
2	B	451	RVE	OA-C	-2.61	1.22	1.30
2	A	451	RVE	C3-C2	-2.59	1.36	1.40
2	B	451	RVE	O2-C2	-2.38	1.31	1.36
2	B	451	RVE	C8-C7	2.27	1.37	1.31
2	A	451	RVE	C8-C7	2.10	1.37	1.31
2	B	451	RVE	C6-C1	-2.06	1.36	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	451	RVE	OB'-C'-C7	-5.04	114.19	121.79
2	A	451	RVE	OA'-C'-C7	4.22	121.11	113.91
2	B	451	RVE	OA'-C'-C7	2.80	118.68	113.91
2	A	451	RVE	O3-C3-C2	2.64	122.83	117.50
2	B	451	RVE	O3-C3-C2	2.38	122.30	117.50
2	B	451	RVE	C6-C5-C4	-2.37	117.20	120.24
2	B	451	RVE	C4-C3-C2	-2.29	117.86	119.98
2	B	451	RVE	C5-C4-C3	2.12	123.45	119.60
2	A	451	RVE	OB-C-C1	-2.06	117.05	121.97
2	A	451	RVE	C2-C1-C	2.01	122.11	119.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	451	RVE	OB'-C'-C7-C8
2	A	451	RVE	C4-C3-O3-C7
2	B	451	RVE	C4-C3-O3-C7
2	B	451	RVE	C2-C3-O3-C7

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, 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	436/450 (96%)	0.24	14 (3%) 50 57	10, 24, 43, 62	5 (1%)
1	B	435/450 (96%)	0.31	11 (2%) 58 64	12, 25, 44, 59	1 (0%)
1	C	424/450 (94%)	0.90	61 (14%) 6 7	10, 30, 50, 84	2 (0%)
1	D	411/450 (91%)	1.86	161 (39%) 1 1	19, 44, 72, 100	1 (0%)
All	All	1706/1800 (94%)	0.81	247 (14%) 6 6	10, 29, 59, 100	9 (0%)

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	332	VAL	10.2
1	D	326	VAL	7.3
1	C	335	LEU	6.7
1	C	326	VAL	6.6
1	C	288	LEU	6.2
1	D	165	LEU	5.8
1	D	18	ILE	5.7
1	C	273	ALA	5.7
1	D	178	VAL	5.7
1	C	275	GLY	5.2
1	D	151	PHE	5.2
1	A	22[A]	ALA	5.1
1	D	21	PRO	5.1
1	D	100	LEU	5.0
1	C	269	ALA	4.9
1	D	269	ALA	4.9
1	D	161	ILE	4.8
1	D	84	TRP	4.8
1	D	160	ALA	4.7
1	D	447	VAL	4.6
1	C	271	THR	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	325	THR	4.6
1	D	148	ILE	4.6
1	D	172	VAL	4.6
1	D	101	LEU	4.6
1	D	288	LEU	4.5
1	D	321	ILE	4.5
1	D	99	LEU	4.4
1	D	446	LEU	4.4
1	D	155	ILE	4.4
1	D	144	SER	4.2
1	D	214	VAL	4.2
1	D	86	GLY	4.1
1	C	332	VAL	4.0
1	D	264	ILE	4.0
1	D	26	PRO	4.0
1	D	54	TRP	4.0
1	C	285	ARG	3.9
1	D	170	ARG	3.9
1	D	143	VAL	3.9
1	D	180	VAL	3.9
1	D	257	VAL	3.9
1	D	95	ALA	3.9
1	D	415	TRP	3.9
1	C	198	ILE	3.8
1	D	29	LEU	3.8
1	C	193	VAL	3.8
1	D	150	LEU	3.8
1	D	153	ALA	3.8
1	D	284	ALA	3.8
1	D	392	LEU	3.8
1	D	27	ALA	3.8
1	D	186	GLY	3.7
1	D	88	PRO	3.7
1	C	287	ASP	3.7
1	D	16	SER	3.7
1	C	268	LEU	3.7
1	D	167	THR	3.7
1	C	276	ARG	3.7
1	D	234	VAL	3.7
1	D	442	LEU	3.7
1	D	445	TYR	3.7
1	D	141	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	3.6
1	D	333	GLN	3.6
1	C	22	ALA	3.6
1	C	284	ALA	3.5
1	A	450	GLN	3.5
1	C	362	ALA	3.5
1	D	216	PHE	3.5
1	D	169	VAL	3.5
1	C	430	ARG	3.5
1	D	168	GLY	3.4
1	D	438	LYS	3.4
1	D	20	MET	3.4
1	D	443	THR	3.4
1	C	423	ILE	3.4
1	C	322	ASP	3.3
1	D	83	GLN	3.3
1	D	52	GLY	3.3
1	D	25	ASN	3.3
1	D	157	HIS	3.3
1	D	432	PHE	3.3
1	D	17	SER	3.3
1	D	217	ALA	3.3
1	D	396	GLY	3.2
1	C	449	ARG	3.2
1	C	195	VAL	3.2
1	C	361	THR	3.2
1	D	74	ILE	3.2
1	D	394	ALA	3.2
1	D	96	VAL	3.2
1	B	315	PRO	3.1
1	C	432	PHE	3.1
1	D	55	VAL	3.1
1	C	321	ILE	3.1
1	D	398	LEU	3.1
1	A	23[A]	GLY	3.0
1	D	400	ALA	3.0
1	D	19	PRO	3.0
1	C	360	VAL	3.0
1	D	53	GLN	3.0
1	D	423	ILE	3.0
1	D	263	VAL	2.9
1	D	71	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	199	ALA	2.9
1	D	181	SER	2.9
1	D	232	THR	2.9
1	C	203	TYR	2.9
1	D	163	ARG	2.9
1	C	101	LEU	2.9
1	D	335	LEU	2.9
1	D	87	ARG	2.8
1	D	78	VAL	2.8
1	D	147	GLU	2.8
1	D	154	GLY	2.8
1	D	146	LYS	2.8
1	D	322	ASP	2.8
1	D	50	CYS	2.8
1	D	174	GLN	2.8
1	C	23	GLY	2.8
1	C	270	GLY	2.8
1	D	166	ALA	2.8
1	D	285	ARG	2.8
1	A	103	THR	2.8
1	C	182	ASP	2.8
1	D	139	THR	2.8
1	D	227	GLY	2.8
1	C	155	ILE	2.7
1	C	426	SER	2.7
1	B	86	GLY	2.7
1	D	93	GLY	2.7
1	C	334	HIS	2.7
1	D	226	LEU	2.7
1	C	329	ARG	2.7
1	A	18	ILE	2.7
1	B	412	GLY	2.7
1	D	34	ALA	2.7
1	D	97	ASP	2.7
1	D	215	PRO	2.7
1	D	349	ARG	2.7
1	A	78	VAL	2.7
1	C	441	THR	2.7
1	D	158	ARG	2.6
1	C	232	THR	2.6
1	D	223	THR	2.6
1	D	231	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	327	ARG	2.6
1	D	325	THR	2.6
1	D	436	CYS	2.6
1	C	180	VAL	2.6
1	D	444	PRO	2.6
1	D	33	LEU	2.6
1	D	439	LEU	2.5
1	D	64	VAL	2.5
1	D	82	GLN	2.5
1	B	15	SER	2.5
1	D	142	MET	2.5
1	D	250	SER	2.5
1	D	171	GLU	2.5
1	C	178	VAL	2.5
1	C	371	VAL	2.5
1	D	191	VAL	2.5
1	D	365	ILE	2.5
1	D	334	HIS	2.5
1	D	85	SER	2.5
1	D	185	SER	2.5
1	D	448	ALA	2.5
1	A	411	GLY	2.5
1	B	117	HIS	2.4
1	D	213	GLU	2.4
1	D	256	ALA	2.4
1	B	18	ILE	2.4
1	C	15	SER	2.4
1	D	192	ALA	2.4
1	C	445	TYR	2.4
1	A	24	VAL	2.4
1	D	193	VAL	2.4
1	D	312	ILE	2.4
1	D	339	ILE	2.4
1	D	348	ASP	2.4
1	D	128	HIS	2.4
1	B	316	GLY	2.4
1	D	177	SER	2.4
1	D	343	LEU	2.4
1	C	194	ALA	2.4
1	D	179	ASP	2.4
1	D	149	ARG	2.4
1	C	336	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	77	GLY	2.3
1	A	345	PRO	2.3
1	D	140	ARG	2.3
1	D	183	ASP	2.3
1	D	145	GLU	2.3
1	C	428	PRO	2.3
1	D	91	ALA	2.3
1	D	218	ILE	2.3
1	D	98	ARG	2.3
1	C	286	ASP	2.3
1	B	199	ALA	2.3
1	C	200	ALA	2.3
1	D	176	ARG	2.3
1	D	228	ARG	2.3
1	D	430	ARG	2.3
1	D	295	ILE	2.3
1	D	103	THR	2.2
1	D	441	THR	2.2
1	D	106	ALA	2.2
1	A	98	ARG	2.2
1	D	345	PRO	2.2
1	C	422	ILE	2.2
1	C	103	THR	2.2
1	D	127	PRO	2.2
1	D	290	SER	2.2
1	C	373	ALA	2.2
1	C	201	GLY	2.2
1	D	156	ARG	2.2
1	C	146	LYS	2.2
1	C	291	ASN	2.2
1	D	309	ILE	2.2
1	C	363	SER	2.2
1	D	286	ASP	2.1
1	C	442	LEU	2.1
1	A	21[A]	PRO	2.1
1	D	224	TYR	2.1
1	A	16	SER	2.1
1	D	28	ASP	2.1
1	D	51	ASP	2.1
1	B	345	PRO	2.1
1	B	430	ARG	2.1
1	D	323	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	2.1
1	D	89	GLY	2.1
1	D	201	GLY	2.1
1	D	37	VAL	2.1
1	D	320	VAL	2.1
1	A	343	LEU	2.1
1	A	304	SER	2.0
1	C	202	ARG	2.0
1	D	229	ARG	2.0
1	D	211	CYS	2.0
1	C	167	THR	2.0
1	D	249	TYR	2.0
1	D	196	ASP	2.0
1	D	351	ALA	2.0
1	D	380	CYS	2.0
1	C	230	HIS	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 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	RVE	A	451	16/16	0.96	0.06	15,23,29,31	0
2	RVE	B	451	16/16	0.96	0.06	19,26,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.