Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 04:06 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

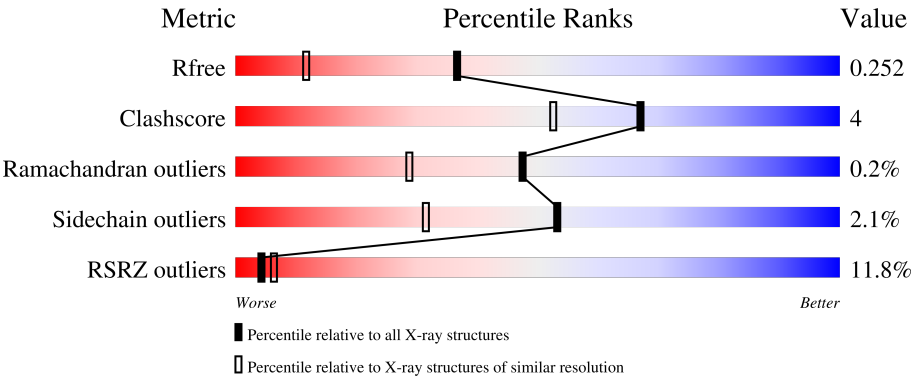
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 <=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% 94% . .
1	B	450	4% 90% 7% .
1	C	450	10% 87% 7% 6%
1	D	450	28% 73% 16% . 9%

2 Entry composition

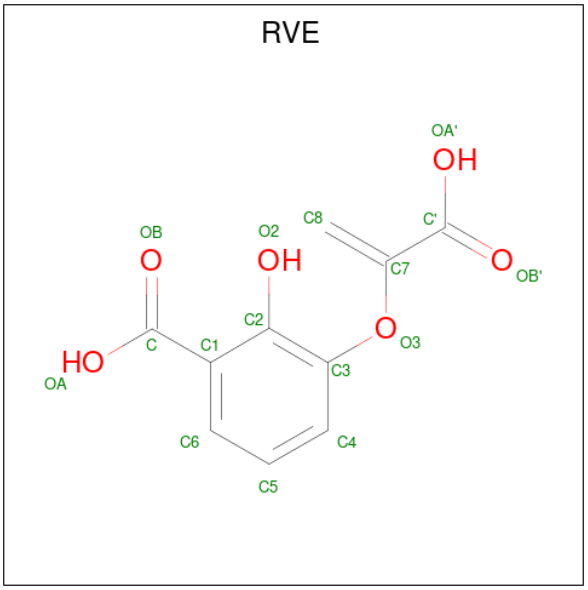
There are 3 unique types of molecules in this entry. The entry contains 13876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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/isochorismate-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: $C_{10}H_8O_6$).



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.

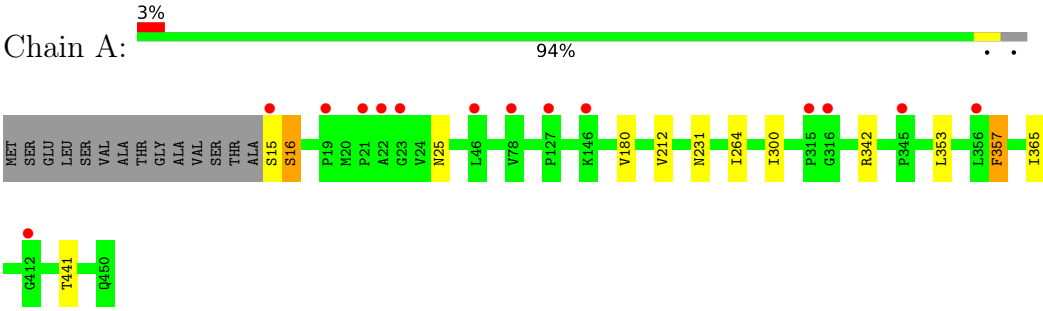
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	364	Total O 364 364	0	0
3	B	299	Total O 299 299	0	0
3	C	227	Total O 227 227	0	0
3	D	112	Total O 112 112	0	0

3 Residue-property plots (i)

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

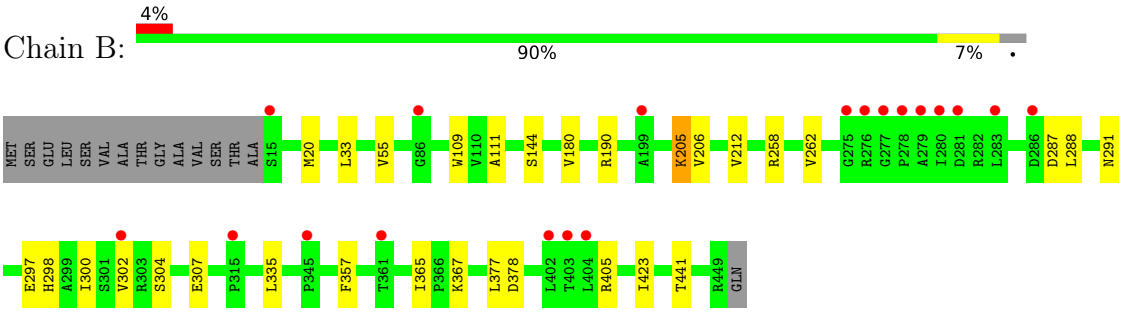
• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain A:



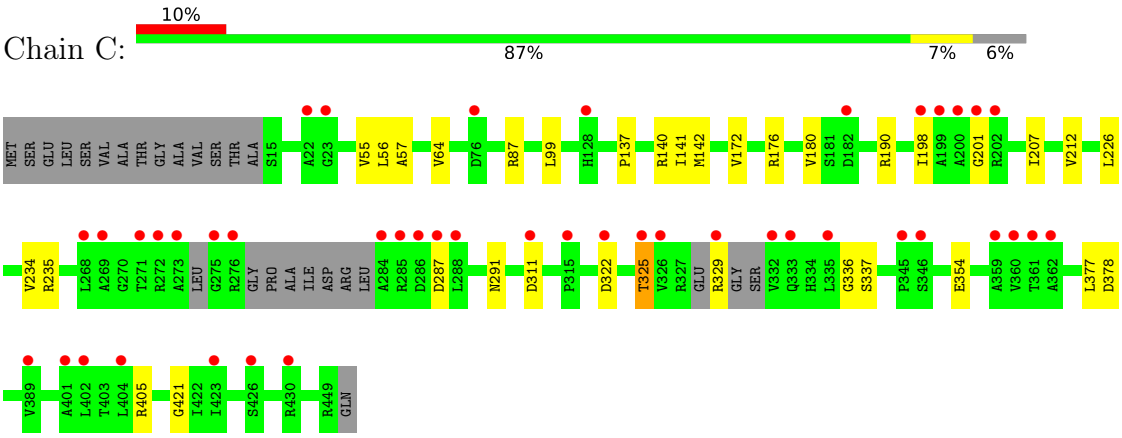
• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain B:



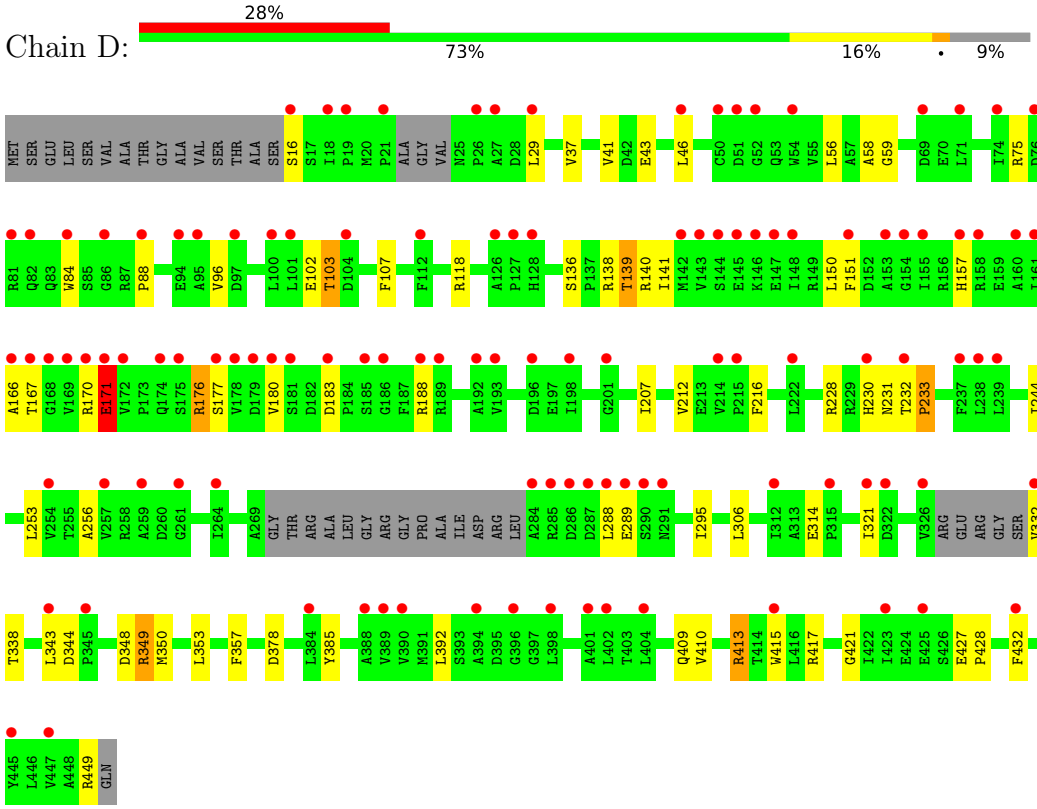
• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain C:



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

Chain D:


28%
73%
16%
9%
MET SER GLU LEU SER VAL ALA ALA THR GLY ALA ALA VAL SER THR ALA SER S16 S17 I18 P19 M20 P21 ALA GLY VAL N25 P26 A27 D28 L29 V37 V41 D42 E43 L46 C50 D51 G52 Q53 W54 V55 L56 A57 A58 G59 D69 E70 L71 I74 R75 D76 G77 V78 T79 R80
R81 Q82 Q83 W84 S85 G86 R87 P88 E94 A95 V96 D97 L100 L101 E102 T103 D104 F107 F112 R118 A126 P127 H128 S136 P137 R138 T139 R140 I141 M142 V143 S144 E145 K146 E147 I148 R149 L150 F151 D152 A153 G154 I155 R156 H157 R158 E159 A160 I161 D162 R163 LEU L165
A166 T167 G168 V169 R170 E171 V172 P173 Q174 S175 R176 S177 V178 D179 V180 S181 D182 D183 P184 S185 G186 F187 R188 R189 A192 V193 D196 E197 I198 G201 I207 V212 E213 V214 P215 F216 L222 R228 R229 H230 N231 T232 P233 F237 L238 L239 I244 R245 Y249 S250
L253 V254 T255 A256 V257 R258 A259 D260 G261 I264 A269 GLY THR ARG ALA LEU GLY ARG GLY PRO ALA ILE ASP ARG LEU A284 R285 D286 D287 L288 E289 S290 N291 I295 L306 I312 A313 E314 P315 I321 D322 V326 ARG GLU ARG GLY SER V332 Q333 H334 L335
T338 L343 D344 P345 D348 R349 M350 L353 F357 D378 L384 Y385 A388 V389 V390 M391 L392 S393 A394 D395 G396 G397 L398 A401 L402 T403 L404 Q409 V410 R413 T414 W415 L416 R417 G421 I422 I423 E424 E425 S426 E427 P428 F432 T441 L442 T443 P444
Y445 L446 V447 A448 R449 GLN

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.34 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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

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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:165:LEU:C	1:D:167:THR:H	2.17	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:HZ3	1:B:205:LYS:HG2	1.33	0.46
1:B:205:LYS:HG3	1:B:206:VAL:N	2.30	0.45
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

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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: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
1:B:304:SER:O	1:B:307:GLU:HG2	2.17	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: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: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%)	47 29
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%)	22 8
All	All	1691/1800 (94%)	1655 (98%)	32 (2%)	4 (0%)	47 29

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	343/358 (96%)	339 (99%)	4 (1%)	71 56
1	B	340/358 (95%)	334 (98%)	6 (2%)	59 40
1	C	327/358 (91%)	322 (98%)	5 (2%)	65 49
1	D	294/358 (82%)	282 (96%)	12 (4%)	30 10
All	All	1304/1432 (91%)	1277 (98%)	27 (2%)	53 31

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	451	-	16,16,16	2.76	8 (50%)	20,22,22	2.00	6 (30%)
2	RVE	A	451	-	16,16,16	3.20	8 (50%)	20,22,22	2.22	6 (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	B	451	-	-	2/12/12/12	0/1/1/1
2	RVE	A	451	-	-	3/12/12/12	0/1/1/1

All (16) 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	-4.41	1.33	1.41
2	A	451	RVE	O3-C7	-4.23	1.33	1.41
2	A	451	RVE	O3-C3	-3.63	1.33	1.41
2	B	451	RVE	O3-C3	-3.49	1.34	1.41
2	A	451	RVE	OA'-C'	-3.39	1.20	1.30
2	B	451	RVE	OA'-C'	-3.20	1.21	1.30
2	B	451	RVE	C3-C2	-3.15	1.36	1.40
2	A	451	RVE	O2-C2	-2.83	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	RVE	OA-C	-2.75	1.22	1.30
2	A	451	RVE	C3-C2	-2.69	1.36	1.40
2	B	451	RVE	OA-C	-2.56	1.22	1.30
2	B	451	RVE	O2-C2	-2.38	1.31	1.37
2	B	451	RVE	C8-C7	2.18	1.37	1.31
2	A	451	RVE	C8-C7	2.01	1.37	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	451	RVE	C3-O3-C7	6.54	131.71	118.43
2	A	451	RVE	C3-O3-C7	5.48	129.55	118.43
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	2.70	122.83	117.65
2	B	451	RVE	O3-C3-C2	2.43	122.30	117.65
2	B	451	RVE	C4-C3-C2	-2.29	117.86	119.97
2	B	451	RVE	C6-C5-C4	-2.15	117.20	120.25
2	A	451	RVE	C2-C1-C	2.06	122.11	119.83
2	B	451	RVE	C5-C4-C3	2.04	123.45	119.71
2	A	451	RVE	OB-C-C1	-2.01	117.05	121.94

There are no chirality outliers.

All (5) 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	A	451	RVE	C2-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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	436/450 (96%)	0.40	14 (3%) 47 54	11, 24, 44, 62	0
1	B	435/450 (96%)	0.36	19 (4%) 34 40	12, 25, 44, 59	0
1	C	424/450 (94%)	0.76	44 (10%) 6 9	10, 30, 50, 84	0
1	D	411/450 (91%)	1.50	125 (30%) 0 0	19, 44, 72, 100	1 (0%)
All	All	1706/1800 (94%)	0.74	202 (11%) 4 6	10, 29, 59, 100	1 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	ALA	8.0
1	C	288	LEU	7.8
1	C	326	VAL	7.6
1	D	160	ALA	6.2
1	C	275	GLY	6.0
1	D	288	LEU	5.8
1	D	19	PRO	5.8
1	D	155	ILE	5.8
1	D	332	VAL	5.6
1	C	335	LEU	5.4
1	D	172	VAL	5.3
1	D	161	ILE	5.1
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	C	284	ALA	4.8
1	B	283	LEU	4.8
1	D	145	GLU	4.7
1	B	279	ALA	4.7
1	D	287	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	22[A]	ALA	4.7
1	D	445	TYR	4.6
1	D	186	GLY	4.6
1	D	178	VAL	4.6
1	D	345	PRO	4.5
1	D	21	PRO	4.4
1	D	128	HIS	4.3
1	C	276	ARG	4.3
1	D	389	VAL	4.2
1	D	447	VAL	4.2
1	D	192	ALA	4.2
1	D	169	VAL	4.2
1	D	167	THR	4.2
1	D	180	VAL	4.1
1	C	22	ALA	4.0
1	B	278	PRO	4.0
1	D	162	ASP	4.0
1	D	333	GLN	4.0
1	D	423	ILE	3.9
1	D	26	PRO	3.9
1	D	432	PHE	3.8
1	D	80	ARG	3.8
1	D	158	ARG	3.8
1	D	214	VAL	3.7
1	A	23[A]	GLY	3.7
1	D	154	GLY	3.7
1	C	362	ALA	3.7
1	D	84	TRP	3.6
1	C	23	GLY	3.6
1	C	201	GLY	3.6
1	D	181	SER	3.6
1	D	166	ALA	3.6
1	C	345	PRO	3.6
1	D	444	PRO	3.6
1	D	196	ASP	3.6
1	D	175	SER	3.5
1	B	277	GLY	3.5
1	C	199	ALA	3.5
1	D	257	VAL	3.5
1	B	280	ILE	3.4
1	B	315	PRO	3.4
1	D	151	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	321	ILE	3.4
1	D	237	PHE	3.3
1	D	101	LEU	3.3
1	A	146	LYS	3.3
1	D	394	ALA	3.3
1	D	148	ILE	3.3
1	D	264	ILE	3.3
1	D	163	ARG	3.2
1	D	177	SER	3.2
1	C	360	VAL	3.2
1	D	415	TRP	3.2
1	C	200	ALA	3.1
1	D	259	ALA	3.1
1	C	198	ILE	3.1
1	D	230	HIS	3.1
1	D	222	LEU	3.1
1	D	390	VAL	3.1
1	D	52	GLY	3.1
1	D	95	ALA	3.1
1	D	170	ARG	3.0
1	D	402	LEU	3.0
1	D	334	HIS	3.0
1	C	272	ARG	3.0
1	D	54	TRP	3.0
1	C	311	ASP	2.9
1	D	326	VAL	2.9
1	D	165	LEU	2.9
1	D	388	ALA	2.9
1	D	384	LEU	2.9
1	C	182	ASP	2.9
1	D	238	LEU	2.8
1	D	69	ASP	2.8
1	D	171	GLU	2.8
1	B	86	GLY	2.8
1	D	174	GLN	2.8
1	A	315	PRO	2.8
1	D	127	PRO	2.8
1	D	343	LEU	2.8
1	A	127	PRO	2.8
1	D	168	GLY	2.7
1	D	183	ASP	2.7
1	D	201	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	315	PRO	2.7
1	D	51	ASP	2.7
1	C	271	THR	2.7
1	D	285	ARG	2.7
1	D	146	LYS	2.7
1	D	404	LEU	2.7
1	C	346	SER	2.7
1	C	286	ASP	2.6
1	A	15	SER	2.6
1	D	290	SER	2.6
1	D	179	ASP	2.6
1	D	401	ALA	2.6
1	C	430	ARG	2.6
1	A	356	LEU	2.6
1	D	82	GLN	2.6
1	C	423	ILE	2.6
1	C	404	LEU	2.6
1	A	412	GLY	2.5
1	C	361	THR	2.5
1	D	126	ALA	2.5
1	C	389	VAL	2.5
1	A	345	PRO	2.5
1	D	86	GLY	2.5
1	D	142	MET	2.5
1	B	281	ASP	2.5
1	D	74	ILE	2.5
1	D	97	ASP	2.5
1	D	143	VAL	2.5
1	D	29	LEU	2.5
1	D	239	LEU	2.5
1	D	76	ASP	2.5
1	A	46	LEU	2.5
1	D	261	GLY	2.5
1	D	16	SER	2.5
1	C	401	ALA	2.4
1	D	157	HIS	2.4
1	C	268	LEU	2.4
1	C	322	ASP	2.4
1	C	426	SER	2.4
1	D	250	SER	2.4
1	D	232	THR	2.4
1	D	312	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	188	ARG	2.4
1	D	153	ALA	2.4
1	D	100	LEU	2.3
1	C	315	PRO	2.3
1	B	286	ASP	2.3
1	C	402	LEU	2.3
1	D	46	LEU	2.3
1	B	199	ALA	2.3
1	C	269	ALA	2.3
1	D	50	CYS	2.3
1	B	403	THR	2.3
1	D	185	SER	2.3
1	A	316	GLY	2.3
1	D	71	LEU	2.3
1	C	333	GLN	2.2
1	B	302	VAL	2.2
1	D	291	ASN	2.2
1	D	286	ASP	2.2
1	D	78	VAL	2.2
1	D	254	VAL	2.2
1	B	404	LEU	2.2
1	C	202	ARG	2.2
1	D	189	ARG	2.2
1	B	15	SER	2.2
1	A	21[A]	PRO	2.2
1	D	215	PRO	2.2
1	C	359	ALA	2.2
1	D	27	ALA	2.2
1	D	18	ILE	2.2
1	D	104	ASP	2.2
1	B	345	PRO	2.2
1	B	275	GLY	2.2
1	D	425	GLU	2.1
1	C	76	ASP	2.1
1	D	442	LEU	2.1
1	D	322	ASP	2.1
1	B	402	LEU	2.1
1	D	144	SER	2.1
1	A	19	PRO	2.1
1	D	88	PRO	2.1
1	D	147	GLU	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	396	GLY	2.1
1	D	398	LEU	2.1
1	C	128	HIS	2.1
1	C	329	ARG	2.0
1	D	81	ARG	2.0
1	B	361	THR	2.0
1	D	193	VAL	2.0
1	B	276	ARG	2.0
1	D	94	GLU	2.0
1	D	198	ILE	2.0
1	D	289	GLU	2.0
1	A	78	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	RVE	B	451	16/16	0.94	0.11	19,26,32,33	0
2	RVE	A	451	16/16	0.95	0.10	15,23,29,31	0

6.5 Other polymers (i)

There are no such residues in this entry.