



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:44 PM GMT

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

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

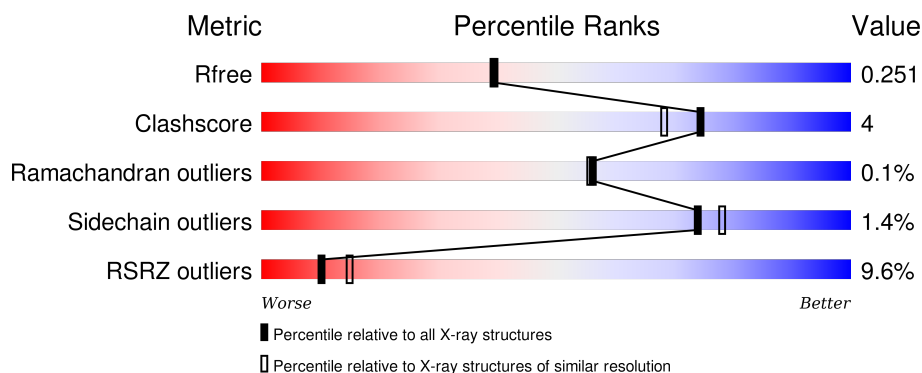
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>7%</div> <div>89%</div> <div>7%</div> </div>
1	B	450	<div> <div>7%</div> <div>87%</div> <div>6% • 7%</div> </div>
1	C	450	<div> <div>6%</div> <div>83%</div> <div>9% 8%</div> </div>
1	D	450	<div> <div>16%</div> <div>85%</div> <div>9% • 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

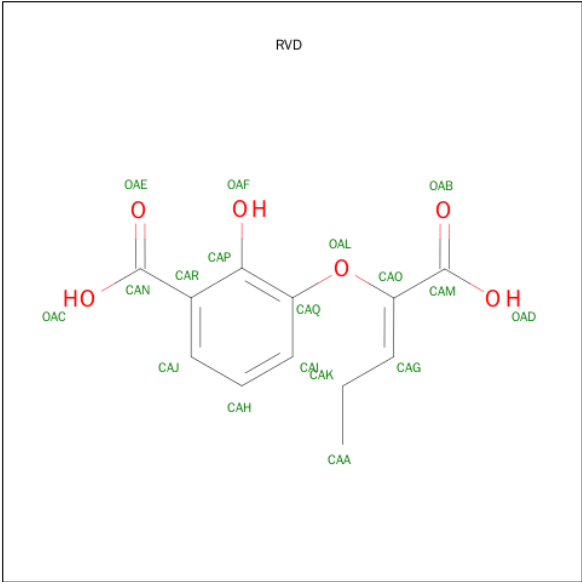
- Molecule 1 is a protein called Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 3-{[(1Z)-1-CARBOXYBUT-1-EN-1-YL]OXY}-2-HYDROXYBENZOIC ACID (three-letter code: RVD) (formula: C₁₂H₁₂O₆).

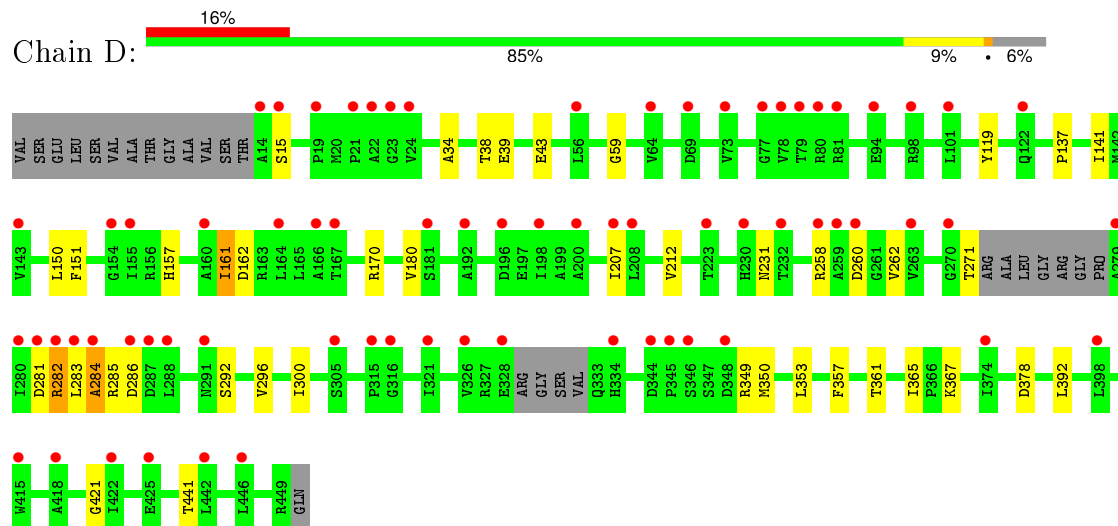


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		
2	C	1	Total	C	O	0	0
			18	12	6		
2	D	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is water.

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

• 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	87.27Å 115.47Å 95.47Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	19.84 – 2.14 19.84 – 2.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.84-2.14) 98.5 (19.84-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.15Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.207 , 0.229 0.227 , 0.251	Depositor DCC
R_{free} test set	5102 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
Estimated twinning fraction	0.006 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	4 of 101828 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13135	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: RVD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3246	0.67	0/4411
1	B	0.49	0/3249	0.72	3/4411 (0.1%)
1	C	0.50	0/3181	0.67	0/4325
1	D	0.56	0/3239	0.66	0/4405
All	All	0.52	0/12915	0.68	3/17552 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3189	0	3153	10	0
1	B	3188	0	3164	27	0
1	C	3127	0	3080	25	0
1	D	3184	0	3115	36	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:O	1:B:357:PHE:HB2	2.16	0.46
1:A:245[A]:ARG:HB2	1:A:409:GLN:HB3	1.98	0.45
1:C:118:ARG:NH1	1:C:355:ALA:O	2.49	0.45
1:C:59:GLY:O	1:C:137:PRO:HA	2.16	0.45
1:D:34:ALA:O	1:D:38:THR:OG1	2.26	0.45
1:C:20:MET:CE	1:C:148:ILE:HG13	2.47	0.45
1:C:362:ALA:HB1	1:C:386:SER:HB2	1.99	0.45
1:D:15:SER:HB3	1:D:151:PHE:CE1	2.52	0.45
1:C:333:GLN:HG3	1:C:334:HIS:H	1.81	0.45
2:C:451:RVD:CAM	2:C:451:RVD:CAI	2.93	0.44
1:A:190:ARG:HD2	1:A:377:LEU:O	2.17	0.44
1:D:300:ILE:HG21	1:D:365:ILE:HG21	1.99	0.44
1:B:285:ARG:NH2	1:B:288:LEU:N	2.59	0.44
2:D:451:RVD:CAI	2:D:451:RVD:CAM	2.87	0.44
1:D:282:ARG:HB3	1:D:283:LEU:H	1.51	0.44
1:D:283:LEU:O	1:D:284:ALA:HB2	2.12	0.44
1:B:322:ASP:HB3	1:B:327:ARG:NH2	2.32	0.44
1:D:284:ALA:CA	1:D:285:ARG:CB	2.95	0.44
1:B:285:ARG:HH21	1:B:288:LEU:N	2.14	0.43
1:D:361:THR:HG21	2:D:451:RVD:HAK	2.00	0.43
1:D:119:TYR:OH	1:D:367:LYS:HD2	2.18	0.43
1:D:353:LEU:O	1:D:357:PHE:HB2	2.19	0.43
1:B:285:ARG:CZ	1:B:286:ASP:HA	2.49	0.42
1:B:138:ARG:NH2	1:D:39:GLU:OE2	2.46	0.42
1:C:140:ARG:HB2	1:C:151:PHE:HB2	2.02	0.41
1:B:125:LEU:HD22	1:B:129:THR:HG21	2.03	0.41
1:D:231:ASN:OD1	1:D:441:THR:HG23	2.20	0.41
1:A:253:LEU:HD21	1:A:256:ALA:HB2	2.03	0.41
1:D:349:ARG:HD2	1:D:392:LEU:HD23	2.03	0.41
1:A:245[B]:ARG:NH1	1:A:409:GLN:OE1	2.52	0.41
1:B:349:ARG:HD2	1:B:392:LEU:HD23	2.03	0.40
1:D:59:GLY:O	1:D:137:PRO:HA	2.21	0.40
1:C:349:ARG:HD2	1:C:392:LEU:HD23	2.03	0.40
1:C:253:LEU:HD21	1:C:256:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/450 (92%)	411 (99%)	5 (1%)	0	100	100
1	B	415/450 (92%)	410 (99%)	5 (1%)	0	100	100
1	C	407/450 (90%)	403 (99%)	4 (1%)	0	100	100
1	D	419/450 (93%)	411 (98%)	6 (1%)	2 (0%)	34	26
All	All	1657/1800 (92%)	1635 (99%)	20 (1%)	2 (0%)	56	56

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/358 (91%)	323 (99%)	4 (1%)	78	81
1	B	327/358 (91%)	320 (98%)	7 (2%)	61	64
1	C	323/358 (90%)	319 (99%)	4 (1%)	78	81
1	D	320/358 (89%)	316 (99%)	4 (1%)	76	80
All	All	1297/1432 (91%)	1278 (98%)	19 (2%)	74	76

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RVD	A	451	-	11,18,18	2.90	5 (45%)	12,24,24	1.09	1 (8%)
2	RVD	B	451	-	11,18,18	2.78	3 (27%)	12,24,24	0.89	1 (8%)
2	RVD	C	451	-	11,18,18	2.88	4 (36%)	12,24,24	0.92	0
2	RVD	D	451	-	11,18,18	2.72	3 (27%)	12,24,24	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RVD	A	451	-	-	0/6/15/15	0/1/1/1
2	RVD	B	451	-	-	0/6/15/15	0/1/1/1
2	RVD	C	451	-	-	0/6/15/15	0/1/1/1
2	RVD	D	451	-	-	0/6/15/15	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	451	RVD	CAK-CAG	-7.44	1.36	1.50
2	D	451	RVD	CAK-CAG	-7.33	1.37	1.50
2	C	451	RVD	CAK-CAG	-6.87	1.37	1.50
2	A	451	RVD	CAK-CAG	-6.05	1.39	1.50
2	A	451	RVD	OAL-CAQ	-5.85	1.29	1.41
2	C	451	RVD	OAL-CAQ	-4.50	1.31	1.41
2	B	451	RVD	OAL-CAQ	-3.82	1.33	1.41
2	D	451	RVD	OAL-CAQ	-3.64	1.33	1.41
2	C	451	RVD	CAQ-CAP	-3.35	1.35	1.40
2	B	451	RVD	CAQ-CAP	-2.62	1.36	1.40
2	A	451	RVD	CAQ-CAP	-2.54	1.36	1.40
2	D	451	RVD	CAR-CAP	-2.19	1.36	1.40
2	A	451	RVD	CAR-CAP	-2.14	1.36	1.40
2	C	451	RVD	OAF-CAP	-2.05	1.32	1.37
2	A	451	RVD	OAF-CAP	-2.02	1.32	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	451	RVD	CAJ-CAR-CAP	2.00	119.81	118.04
2	A	451	RVD	CAI-CAQ-CAP	2.38	122.56	120.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	451	RVD	7	0
2	D	451	RVD	3	0

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	420/450 (93%)	0.51	32 (7%) 17 22	19, 37, 62, 90	8 (1%)
1	B	419/450 (93%)	0.48	30 (7%) 18 24	20, 37, 61, 82	8 (1%)
1	C	413/450 (91%)	0.52	28 (6%) 20 27	19, 39, 61, 87	8 (1%)
1	D	425/450 (94%)	0.91	71 (16%) 2 4	24, 48, 76, 91	8 (1%)
All	All	1677/1800 (93%)	0.61	161 (9%) 10 15	19, 40, 68, 91	32 (1%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	ILE	8.8
1	D	279	ALA	8.2
1	B	285	ARG	5.8
1	C	155	ILE	5.7
1	A	284	ALA	5.5
1	D	345	PRO	5.3
1	A	283	LEU	5.1
1	D	155	ILE	4.9
1	D	284	ALA	4.8
1	A	23	GLY	4.6
1	D	166	ALA	4.5
1	A	22	ALA	4.5
1	C	288	LEU	4.5
1	B	326	VAL	4.5
1	D	346	SER	4.4
1	D	281	ASP	4.4
1	B	86	GLY	4.3
1	D	23	GLY	4.3
1	A	141	ILE	4.3
1	D	263	VAL	4.3
1	C	333	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	79	THR	4.2
1	D	288	LEU	4.2
1	C	346	SER	4.1
1	B	329[A]	ARG	4.0
1	A	326	VAL	4.0
1	C	347	SER	4.0
1	C	345	PRO	3.9
1	C	287	ASP	3.9
1	D	208	LEU	3.7
1	D	22	ALA	3.7
1	D	167	THR	3.7
1	C	326	VAL	3.7
1	C	22	ALA	3.7
1	D	14	ALA	3.7
1	D	259	ALA	3.6
1	D	81	ARG	3.6
1	D	232	THR	3.6
1	B	286	ASP	3.5
1	D	154	GLY	3.5
1	D	328	GLU	3.5
1	B	232	THR	3.4
1	A	333	GLN	3.4
1	A	305	SER	3.4
1	D	270	GLY	3.3
1	B	271	THR	3.3
1	D	73	VAL	3.2
1	B	442	LEU	3.2
1	B	270	GLY	3.2
1	D	374	ILE	3.2
1	D	415	TRP	3.2
1	D	287	ASP	3.1
1	D	326	VAL	3.1
1	A	15	SER	3.1
1	A	334	HIS	3.0
1	B	199	ALA	3.0
1	B	198	ILE	3.0
1	A	143	VAL	3.0
1	A	285[A]	ARG	3.0
1	D	321	ILE	3.0
1	C	208	LEU	3.0
1	D	230	HIS	2.9
1	B	259	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	232	THR	2.9
1	C	291	ASN	2.9
1	D	398	LEU	2.9
1	B	269	ALA	2.9
1	D	21	PRO	2.9
1	D	196	ASP	2.9
1	D	286	ASP	2.9
1	A	270	GLY	2.9
1	A	176	ARG	2.9
1	A	77	GLY	2.9
1	B	284	ALA	2.9
1	D	442	LEU	2.8
1	A	78	VAL	2.8
1	B	201	GLY	2.8
1	B	305	SER	2.8
1	A	148	ILE	2.8
1	D	200	ALA	2.8
1	A	411	GLY	2.7
1	A	181	SER	2.7
1	B	247	LEU	2.7
1	D	164	LEU	2.7
1	B	250	SER	2.7
1	D	305	SER	2.7
1	A	339	ILE	2.6
1	C	286	ASP	2.6
1	B	416	LEU	2.6
1	D	24	VAL	2.5
1	A	167	THR	2.5
1	C	442	LEU	2.5
1	B	290	SER	2.5
1	D	315	PRO	2.5
1	D	160	ALA	2.5
1	D	101	LEU	2.5
1	A	346	SER	2.5
1	C	411	GLY	2.5
1	D	77	GLY	2.5
1	D	19	PRO	2.5
1	D	122	GLN	2.5
1	A	232	THR	2.5
1	D	282	ARG	2.4
1	D	78	VAL	2.4
1	D	258	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	316	GLY	2.4
1	A	286	ASP	2.4
1	D	56	LEU	2.4
1	D	80	ARG	2.4
1	D	15	SER	2.4
1	B	334	HIS	2.3
1	B	287	ASP	2.3
1	D	425	GLU	2.3
1	D	316	GLY	2.3
1	D	283	LEU	2.3
1	D	192	ALA	2.3
1	A	179	ASP	2.3
1	D	344	ASP	2.3
1	D	94	GLU	2.3
1	D	223	THR	2.3
1	A	122	GLN	2.3
1	D	143	VAL	2.3
1	D	418	ALA	2.3
1	D	334	HIS	2.3
1	C	206	VAL	2.2
1	C	374	ILE	2.2
1	B	56	LEU	2.2
1	C	416	LEU	2.2
1	B	114	PHE	2.2
1	A	287	ASP	2.2
1	D	64	VAL	2.2
1	C	23	GLY	2.2
1	C	305	SER	2.2
1	D	207	ILE	2.2
1	A	247	LEU	2.2
1	B	353	LEU	2.2
1	D	181	SER	2.2
1	A	345	PRO	2.2
1	B	310	THR	2.2
1	D	98	ARG	2.1
1	A	56	LEU	2.1
1	A	19	PRO	2.1
1	B	230	HIS	2.1
1	C	334	HIS	2.1
1	D	69	ASP	2.1
1	D	260	ASP	2.1
1	C	264	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	422	ILE	2.1
1	C	78	VAL	2.1
1	D	198	ILE	2.1
1	C	21	PRO	2.1
1	C	424	GLU	2.1
1	D	291	ASN	2.1
1	C	292	SER	2.1
1	B	117	HIS	2.0
1	D	446	LEU	2.0
1	A	311	ASP	2.0
1	B	311	ASP	2.0
1	C	167	THR	2.0
1	C	427	GLU	2.0
1	D	348	ASP	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	RVD	B	451	18/18	0.85	0.21	1.05	33,38,51,51	0
2	RVD	C	451	18/18	0.89	0.16	1.03	32,34,50,51	0
2	RVD	D	451	18/18	0.86	0.18	0.29	37,46,62,64	0
2	RVD	A	451	18/18	0.93	0.14	-0.12	23,33,45,47	0

6.5 Other polymers

There are no such residues in this entry.