



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:05 am GMT

PDB ID : 3VEH  
Title : Structure of a M. tuberculosis salicylate synthase, MbtI, in complex with an inhibitor methylAMT  
Authors : Bulloch, E.M.; Chi, G.; Manos-Turvey, A.; Johnston, J.M.; Baker, E.N.; Payne, R.J.; Lott, J.S.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2012-01-08  
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

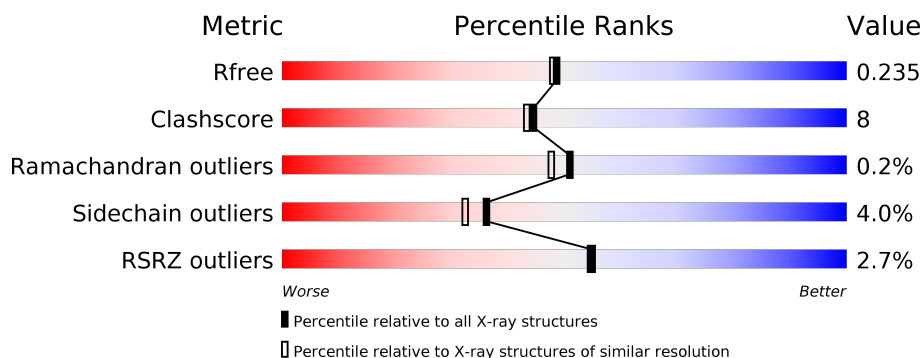
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	451	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div> </div>
1	B	451	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>••</div> </div> </div>
1	D	451	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>••</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	503	-	-	-	X
4	GOL	C	504	-	-	-	X
4	GOL	C	506	-	-	-	X
5	K	B	504	-	-	-	X
6	PEG	C	503	-	-	X	-
6	PEG	C	505	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14566 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.

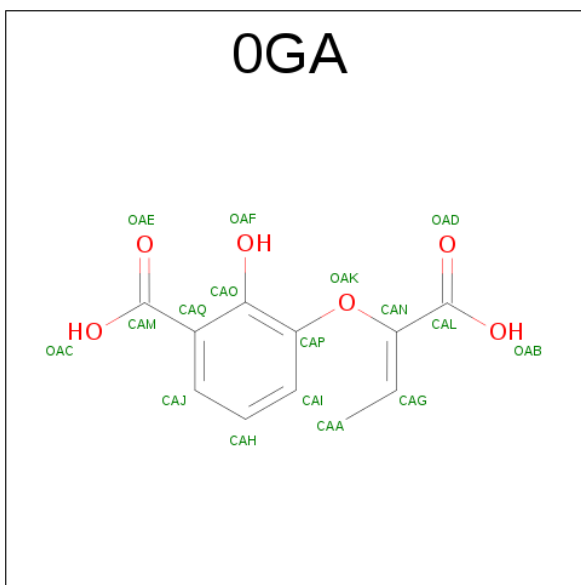
- Molecule 1 is a protein called Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	3	2	0
			3333	2086	604	633	10			
1	B	451	Total	C	N	O	S	3	3	0
			3438	2145	623	659	11			
1	C	435	Total	C	N	O	S	20	6	0
			3350	2098	612	630	10			
1	D	439	Total	C	N	O	S	3	2	0
			3347	2090	607	640	10			

There are 8 discrepancies between the modelled and reference sequences:

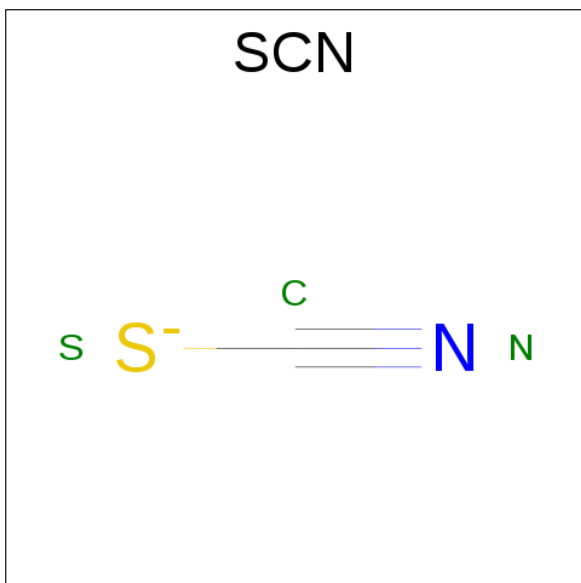
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q7D785
A	0	SER	-	EXPRESSION TAG	UNP Q7D785
B	-1	GLY	-	EXPRESSION TAG	UNP Q7D785
B	0	SER	-	EXPRESSION TAG	UNP Q7D785
C	-1	GLY	-	EXPRESSION TAG	UNP Q7D785
C	0	SER	-	EXPRESSION TAG	UNP Q7D785
D	-1	GLY	-	EXPRESSION TAG	UNP Q7D785
D	0	SER	-	EXPRESSION TAG	UNP Q7D785

- Molecule 2 is 3-[[[(1Z)-1-CARBOXYPROP-1-EN-1-YL]OXY}-2-HYDROXYBENZOIC ACID (three-letter code: 0GA) (formula: C<sub>11</sub>H<sub>10</sub>O<sub>6</sub>).



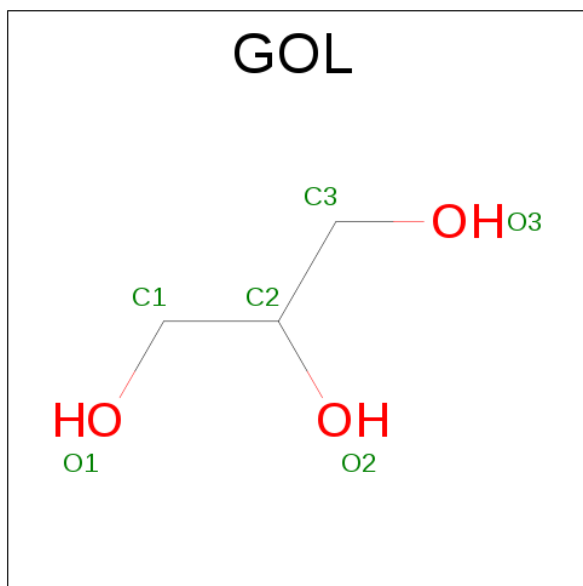
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	11	6		
2	B	1	Total	C	O	0	0
			17	11	6		
2	C	1	Total	C	O	0	0
			17	11	6		
2	D	1	Total	C	O	0	0
			17	11	6		

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		
3	C	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

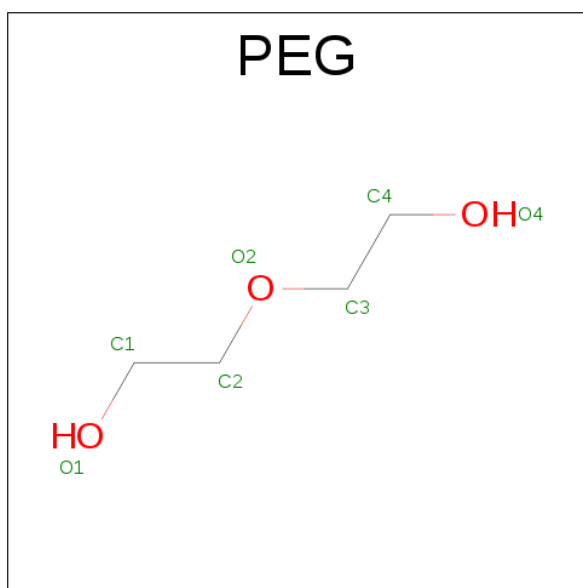


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		

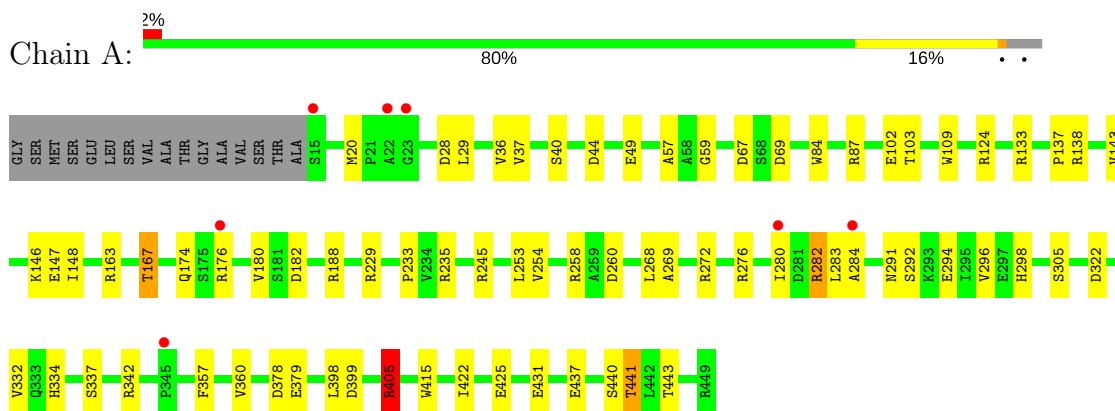
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	226	Total	O	0	0
			226	226		
7	B	284	Total	O	0	0
			284	284		
7	C	252	Total	O	0	0
			252	252		
7	D	219	Total	O	0	0
			219	219		

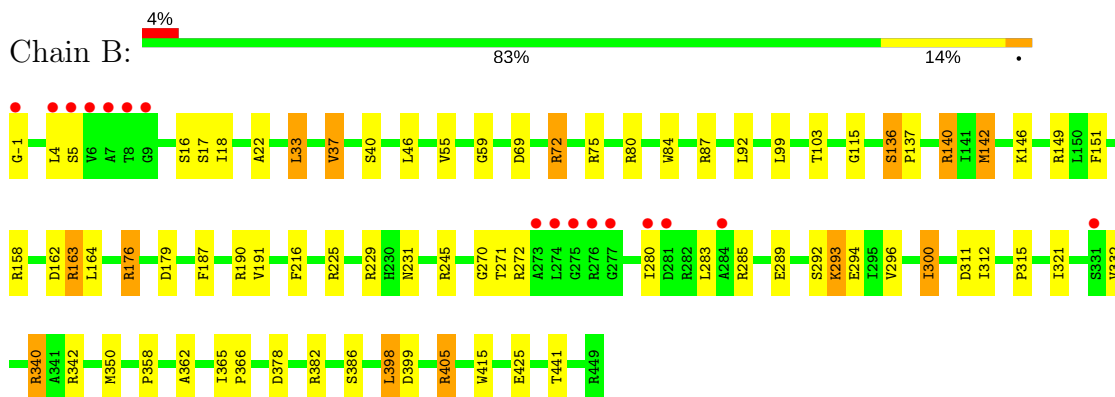
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

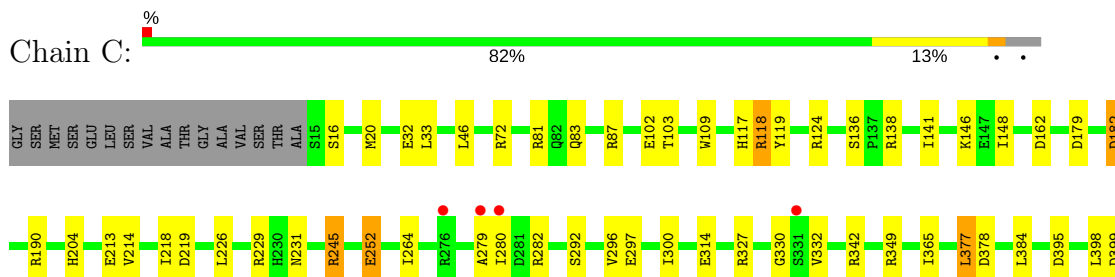
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI



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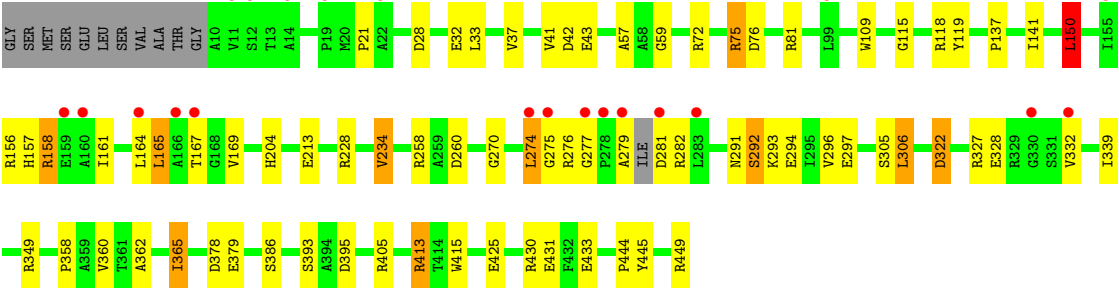
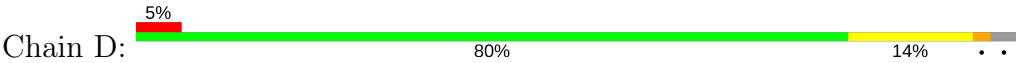


- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI





● Molecule 1: Isochorismate synthase/ischorismate-pyruvate lyase mbtI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.67Å 115.95Å 94.72Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	47.34 – 2.00 47.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.34-2.00) 99.7 (47.34-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.175 , 0.236 0.174 , 0.235	Depositor DCC
$R_{free}$ test set	6397 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.333 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: PEG, GOL, K, SCN, OGA

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	1.08	4/3397 (0.1%)	1.08	17/4613 (0.4%)
1	B	1.08	4/3505 (0.1%)	1.11	16/4759 (0.3%)
1	C	1.08	4/3425 (0.1%)	1.10	16/4646 (0.3%)
1	D	1.02	3/3410 (0.1%)	1.01	6/4631 (0.1%)
All	All	1.06	15/13737 (0.1%)	1.08	55/18649 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	415	TRP	CD2-CE2	7.90	1.50	1.41
1	A	109	TRP	CD2-CE2	7.75	1.50	1.41
1	B	415	TRP	CD2-CE2	7.56	1.50	1.41
1	D	109	TRP	CD2-CE2	7.52	1.50	1.41
1	B	136	SER	CB-OG	-6.95	1.33	1.42
1	A	379	GLU	CD-OE1	6.93	1.33	1.25
1	A	415	TRP	CD2-CE2	6.33	1.49	1.41
1	D	379	GLU	CD-OE1	6.19	1.32	1.25
1	B	84	TRP	CD2-CE2	6.08	1.48	1.41
1	C	252	GLU	CD-OE2	-5.63	1.19	1.25
1	C	117	HIS	CG-CD2	5.54	1.45	1.35
1	C	109	TRP	CD2-CE2	5.44	1.47	1.41
1	B	190	ARG	CZ-NH1	5.40	1.40	1.33
1	C	32	GLU	CD-OE1	5.06	1.31	1.25
1	A	84	TRP	CD2-CE2	5.04	1.47	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	C	349	ARG	NE-CZ-NH2	-9.35	115.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	124	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	72	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	28	ASP	CB-CG-OD1	7.42	124.98	118.30
1	C	87	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	67	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	87	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	225	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	402	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	C	245	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	C	179	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	176	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	B	245	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	C	179	ASP	CB-CG-OD1	6.35	124.02	118.30
1	D	306	LEU	CB-CG-CD2	6.34	121.79	111.00
1	B	69	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	140	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	87	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	190	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	176	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	140	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	28	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	179	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	395	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	234	VAL	CB-CA-C	-5.79	100.41	111.40
1	A	245	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	229	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	D	150	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	133	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	69	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	253	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	382	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	C	327	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	87	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	229	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	228	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	87	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	42	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	81	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	440	SER	CB-CA-C	-5.34	99.96	110.10
1	C	405	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	413	ARG	NE-CZ-NH1	5.25	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	A	44	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	405	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	377	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	B	405	ARG	CB-CG-CD	-5.13	98.26	111.60
1	B	72	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	158	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	413	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	49	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	305	SER	CB-CA-C	5.04	119.68	110.10
1	A	67	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	3333	0	3341	40	0
1	B	3438	0	3440	55	1
1	C	3350	0	3373	57	0
1	D	3347	0	3335	49	1
2	A	17	0	7	0	0
2	B	17	0	8	0	0
2	C	17	0	8	0	0
2	D	17	0	8	0	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	12	0	16	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	C	14	0	20	9	0
7	A	226	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	284	0	0	7	0
7	C	252	0	0	8	0
7	D	219	0	0	2	0
All	All	14566	0	13572	203	1

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 8.

All (203) 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:C:218:ILE:CA	1:C:219:ASP:N	2.11	1.14
1:B:342:ARG:HB3	7:B:838:HOH:O	1.56	1.02
1:B:405:ARG:HD3	1:B:441:THR:HG21	1.40	1.00
1:C:138:ARG:HB3	6:C:503:PEG:H12	1.43	0.99
1:C:292:SER:O	1:C:296:VAL:HG23	1.62	0.96
1:C:118:ARG:HH21	1:C:118:ARG:HG3	1.31	0.95
1:A:163:ARG:O	1:A:167:THR:HG22	1.68	0.94
1:C:103:THR:HG21	1:C:136:SER:HB2	1.50	0.93
6:C:503:PEG:H22	7:C:808:HOH:O	1.74	0.86
1:D:75:ARG:HH11	1:D:75:ARG:HB2	1.43	0.83
1:B:271:THR:CG2	1:B:332:VAL:HG21	2.09	0.81
1:D:75:ARG:HB2	1:D:75:ARG:NH1	1.95	0.81
1:C:405:ARG:HD3	1:C:441:THR:HG21	1.62	0.80
1:A:292:SER:O	1:A:296:VAL:HG23	1.82	0.79
1:C:138:ARG:CB	6:C:503:PEG:H12	2.13	0.79
1:D:204:HIS:HE1	1:D:297:GLU:OE1	1.68	0.77
1:D:291:ASN:HD22	1:D:294:GLU:HG2	1.48	0.77
1:C:20:MET:HA	1:C:20:MET:HE2	1.67	0.77
1:B:280:ILE:HD12	1:B:280:ILE:H	1.49	0.76
1:C:213:GLU:OE2	1:C:413:ARG:HD2	1.86	0.74
1:C:102:GLU:OE1	1:C:102:GLU:HA	1.90	0.72
1:C:103:THR:HG21	1:C:136:SER:CB	2.20	0.71
1:C:20:MET:CE	1:C:148:ILE:HG13	2.21	0.71
1:C:280:ILE:H	1:C:280:ILE:HD12	1.57	0.70
1:C:20:MET:HE1	1:C:148:ILE:CG1	2.22	0.69
1:C:213:GLU:OE1	1:C:413:ARG:NH1	2.26	0.69
1:B:271:THR:HG23	1:B:332:VAL:HG21	1.73	0.69
1:C:118:ARG:NH2	1:C:118:ARG:HG3	2.00	0.68
1:C:231:ASN:HD21	1:C:441:THR:HG23	1.59	0.68
1:B:271:THR:CG2	1:B:332:VAL:CG2	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:HIS:O	1:D:161:ILE:HG13	1.95	0.66
1:B:271:THR:HG23	1:B:332:VAL:CG2	2.26	0.65
1:B:158:ARG:NH1	1:B:162:ASP:OD2	2.28	0.65
1:D:293:LYS:NZ	1:D:425:GLU:HG3	2.13	0.64
1:A:425:GLU:HG3	7:A:782:HOH:O	1.97	0.64
1:B:342:ARG:NH2	7:B:830:HOH:O	2.30	0.64
1:D:213:GLU:OE2	1:D:413:ARG:NH1	2.31	0.63
1:B:17:SER:OG	1:B:149:ARG:NH1	2.32	0.63
1:B:398:LEU:HD12	1:B:399:ASP:N	2.14	0.63
1:A:36:VAL:CG1	1:A:37:VAL:N	2.62	0.62
1:A:176:ARG:NH2	7:A:680:HOH:O	2.26	0.62
1:A:146:LYS:HG3	1:A:147:GLU:HG2	1.81	0.61
1:A:36:VAL:HG13	1:A:37:VAL:N	2.14	0.61
1:A:291:ASN:HD22	1:A:294:GLU:H	1.48	0.61
1:C:20:MET:CE	1:C:148:ILE:CG1	2.79	0.61
1:D:158:ARG:HA	1:D:161:ILE:HD12	1.81	0.61
1:A:57:ALA:HB1	1:A:137:PRO:HB3	1.83	0.60
1:B:362:ALA:HB1	1:B:386:SER:HB2	1.83	0.60
1:A:398:LEU:HD12	1:A:399:ASP:N	2.16	0.60
1:B:270:GLY:HA2	1:B:294:GLU:OE2	2.02	0.60
1:B:33:LEU:O	1:B:37:VAL:HB	2.03	0.59
1:A:332:VAL:CG2	1:A:405:ARG:HH21	2.15	0.59
1:C:138:ARG:HD3	6:C:503:PEG:H11	1.84	0.59
1:A:298:HIS:NE2	1:A:337:SER:OG	2.28	0.58
1:C:231:ASN:ND2	1:C:441:THR:HG23	2.16	0.58
6:C:503:PEG:H41	7:C:851:HOH:O	2.01	0.58
1:D:291:ASN:ND2	1:D:294:GLU:HG2	2.18	0.58
1:B:176:ARG:HG2	1:B:216:PHE:CZ	2.39	0.57
1:A:405:ARG:HG2	1:A:441:THR:HG21	1.86	0.57
1:B:17:SER:C	1:B:18:ILE:HG13	2.23	0.57
1:C:245:ARG:HD3	7:C:784:HOH:O	2.02	0.57
1:B:92:LEU:HD23	1:B:350:MET:HE1	1.86	0.57
1:C:20:MET:HE2	1:C:148:ILE:HD11	1.86	0.57
1:B:-1:GLY:O	1:B:16:SER:HB3	2.05	0.57
1:B:55:VAL:HG22	1:B:142:MET:HG3	1.85	0.57
1:C:33:LEU:HD21	1:C:141:ILE:HD13	1.87	0.56
1:C:20:MET:HE1	1:C:148:ILE:HG13	1.86	0.56
1:C:437:GLU:O	1:C:440:SER:HB2	2.05	0.56
1:B:149:ARG:HG2	1:B:151:PHE:CZ	2.41	0.55
1:C:190:ARG:HD2	1:C:377:LEU:O	2.06	0.55
1:B:176:ARG:HG2	1:B:216:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ASP:C	1:D:322:ASP:OD1	2.45	0.54
1:B:300:ILE:CG1	1:B:365:ILE:HD13	2.38	0.54
1:B:103:THR:HG21	1:B:136:SER:HB2	1.90	0.54
1:D:430:ARG:NH1	1:D:433:GLU:HB3	2.22	0.54
1:C:213:GLU:CD	1:C:413:ARG:HH11	2.11	0.53
1:D:362:ALA:HB1	1:D:386:SER:HB2	1.91	0.53
1:D:33:LEU:HD23	1:D:164:LEU:HD23	1.90	0.53
1:C:182:ASP:HB2	7:C:777:HOH:O	2.06	0.53
1:A:20:MET:HE1	1:A:143:VAL:HG13	1.90	0.53
1:A:188:ARG:HD2	7:A:729:HOH:O	2.08	0.52
1:C:384:LEU:H	6:C:505:PEG:H22	1.74	0.52
1:D:279:ALA:N	1:D:282:ARG:HB3	2.25	0.52
1:B:321:ILE:CD1	1:B:340:ARG:NH2	2.73	0.52
1:D:279:ALA:H	1:D:282:ARG:HB3	1.74	0.52
1:B:321:ILE:HD13	1:B:340:ARG:NH2	2.25	0.52
1:C:410:VAL:HG21	6:C:505:PEG:H32	1.93	0.51
1:B:140:ARG:HD3	7:B:803:HOH:O	2.11	0.51
1:C:405:ARG:HB3	1:C:441:THR:HG21	1.93	0.51
1:B:158:ARG:HD2	1:B:162:ASP:OD2	2.10	0.51
1:B:231:ASN:OD1	1:B:441:THR:HG23	2.10	0.51
1:D:115:GLY:HA3	1:D:358:PRO:HD3	1.93	0.51
1:D:270:GLY:HA2	1:D:294:GLU:OE2	2.10	0.51
1:B:187:PHE:O	1:B:191:VAL:HG23	2.11	0.50
1:C:292:SER:O	1:C:296:VAL:CG2	2.49	0.50
1:D:57:ALA:HB1	1:D:137:PRO:HB3	1.93	0.50
1:D:258:ARG:NH2	1:D:260:ASP:OD2	2.43	0.50
1:A:20:MET:CE	1:A:148:ILE:HG13	2.42	0.50
1:A:36:VAL:CG1	1:A:37:VAL:HG23	2.41	0.50
1:C:300:ILE:CG2	1:C:365:ILE:HD13	2.41	0.50
1:D:431:GLU:HA	1:D:431:GLU:OE1	2.11	0.50
1:B:115:GLY:HA3	1:B:358:PRO:HD3	1.92	0.50
1:D:33:LEU:O	1:D:37:VAL:HB	2.12	0.50
1:A:36:VAL:HG13	1:A:37:VAL:HG23	1.94	0.50
1:C:415:TRP:HZ2	6:C:505:PEG:H11	1.77	0.50
1:C:20:MET:CE	1:C:148:ILE:HD11	2.42	0.49
1:A:398:LEU:HD12	1:A:399:ASP:H	1.77	0.49
1:D:59:GLY:O	1:D:137:PRO:HA	2.12	0.49
1:B:315:PRO:HA	7:B:734:HOH:O	2.12	0.49
1:D:430:ARG:HH11	1:D:433:GLU:HB3	1.78	0.49
1:A:405:ARG:NH1	3:A:502:SCN:S	2.86	0.48
1:C:118:ARG:HD3	1:C:119:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:GLY:C	1:D:277:GLY:H	2.17	0.48
1:B:285:ARG:O	1:B:289:GLU:HG3	2.14	0.48
1:C:138:ARG:HD3	6:C:503:PEG:C1	2.42	0.48
1:C:229:ARG:NH2	7:C:748:HOH:O	2.35	0.48
1:A:437:GLU:O	1:A:440:SER:HB2	2.13	0.48
1:D:360:VAL:HG13	1:D:365:ILE:HD12	1.96	0.48
1:B:149:ARG:HG2	1:B:151:PHE:CE2	2.49	0.48
1:D:164:LEU:HD12	1:D:164:LEU:O	2.14	0.48
1:C:118:ARG:HD3	1:C:119:TYR:CZ	2.48	0.48
1:D:327:ARG:HD2	7:D:722:HOH:O	2.13	0.48
1:D:444:PRO:HG2	1:D:445:TYR:CZ	2.49	0.48
1:C:20:MET:CE	1:C:20:MET:HA	2.40	0.48
1:A:233:PRO:HB2	1:A:235:ARG:O	2.14	0.47
1:C:214:VAL:O	4:C:504:GOL:H32	2.13	0.47
1:D:204:HIS:CE1	1:D:297:GLU:OE1	2.57	0.47
1:B:137:PRO:HG2	1:B:140:ARG:HD2	1.97	0.47
1:A:258:ARG:NH2	1:A:260:ASP:OD2	2.35	0.47
1:B:398:LEU:HD12	1:B:399:ASP:H	1.78	0.47
1:D:305:SER:HB2	1:D:339:ILE:HD13	1.97	0.47
1:D:213:GLU:CD	1:D:413:ARG:HH11	2.18	0.47
1:C:431:GLU:OE1	1:C:431:GLU:HA	2.16	0.46
1:D:292:SER:O	1:D:296:VAL:HG23	2.15	0.46
1:A:20:MET:HE2	1:A:148:ILE:HG13	1.96	0.46
1:A:422:ILE:HD12	1:A:431:GLU:HG3	1.97	0.46
1:C:314:GLU:OE1	1:C:342[B]:ARG:HD2	2.15	0.46
1:A:276:ARG:NH1	1:A:280:ILE:HG21	2.31	0.46
1:B:332:VAL:CG1	1:B:405:ARG:NH2	2.79	0.46
1:B:46:LEU:HD23	1:B:46:LEU:C	2.36	0.46
1:B:103:THR:HG21	1:B:136:SER:CB	2.46	0.46
1:A:59:GLY:O	1:A:137:PRO:HA	2.16	0.45
1:C:226:LEU:HG	1:C:445:TYR:HB3	1.98	0.45
1:D:213:GLU:CD	1:D:413:ARG:NH1	2.70	0.45
1:D:293:LYS:HZ3	1:D:425:GLU:HG3	1.82	0.45
1:B:158:ARG:NH1	1:B:162:ASP:CG	2.69	0.44
1:C:16:SER:CB	7:C:815:HOH:O	2.65	0.44
1:D:393:SER:HB3	1:D:395:ASP:OD1	2.17	0.44
1:D:274:LEU:HA	1:D:281:ASP:HB2	1.98	0.44
1:B:293:LYS:NZ	1:B:425:GLU:HG3	2.31	0.44
1:C:405:ARG:CD	1:C:441:THR:HG21	2.41	0.44
1:D:21:PRO:HG3	1:D:165:LEU:HD21	1.99	0.44
1:C:102:GLU:OE1	1:C:102:GLU:CA	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD12	1:C:399:ASP:N	2.32	0.44
1:A:269:ALA:HB3	1:A:298:HIS:HA	1.99	0.44
1:A:276:ARG:O	1:A:280:ILE:HD12	2.18	0.44
1:C:279:ALA:HB3	1:C:280:ILE:HD12	2.00	0.44
1:B:296:VAL:O	1:B:300:ILE:HG23	2.18	0.43
1:C:280:ILE:H	1:C:280:ILE:CD1	2.28	0.43
1:D:332:VAL:CG2	1:D:405:ARG:HH22	2.32	0.43
1:C:20:MET:HE2	1:C:148:ILE:CD1	2.48	0.43
1:C:20:MET:CE	1:C:148:ILE:CD1	2.97	0.43
1:C:332:VAL:HG23	1:C:405:ARG:NH2	2.34	0.43
1:D:293:LYS:HZ1	1:D:425:GLU:HG3	1.82	0.43
1:A:322:ASP:O	1:A:337:SER:HB3	2.19	0.43
1:B:22:ALA:HA	7:B:797:HOH:O	2.18	0.43
1:D:75:ARG:NH1	1:D:75:ARG:CB	2.74	0.43
1:A:272:ARG:HA	1:A:272:ARG:HD3	1.75	0.42
1:D:156:ARG:HB2	7:D:661:HOH:O	2.19	0.42
1:A:332:VAL:HG22	1:A:405:ARG:HH21	1.83	0.42
1:A:282:ARG:NH2	7:A:716:HOH:O	2.53	0.42
1:C:16:SER:HB3	7:C:815:HOH:O	2.18	0.42
1:D:141:ILE:HG23	1:D:150:LEU:HD12	2.01	0.42
1:B:272:ARG:O	1:B:332:VAL:HG23	2.19	0.42
1:B:59:GLY:O	1:B:137:PRO:HA	2.20	0.42
1:B:176:ARG:HH11	1:B:176:ARG:HD2	1.55	0.42
1:B:340:ARG:HD2	7:B:770:HOH:O	2.19	0.42
1:A:268:LEU:HD23	1:A:334:HIS:CD2	2.55	0.42
1:C:252:GLU:HA	7:C:683:HOH:O	2.19	0.42
1:B:365:ILE:HA	1:B:366:PRO:C	2.39	0.42
1:D:28:ASP:O	1:D:32:GLU:HG2	2.20	0.41
1:D:32:GLU:HG3	1:D:169:VAL:HB	2.02	0.41
1:D:43:GLU:HB2	1:D:59:GLY:HA2	2.00	0.41
1:B:312:ILE:C	1:B:312:ILE:HD12	2.41	0.41
1:A:138:ARG:HH11	1:A:138:ARG:HG2	1.86	0.41
1:B:332:VAL:HG12	1:B:405:ARG:NH2	2.36	0.41
1:B:55:VAL:HG23	7:B:878:HOH:O	2.20	0.41
1:C:204:HIS:NE2	1:C:297:GLU:OE2	2.42	0.41
1:A:180:VAL:HG11	1:A:443:THR:HG21	2.02	0.41
1:A:332:VAL:HG22	1:A:405:ARG:NH2	2.35	0.41
1:B:280:ILE:H	1:B:280:ILE:CD1	2.24	0.41
1:D:118:ARG:HD3	1:D:119:TYR:CZ	2.55	0.41
1:D:444:PRO:HG2	1:D:445:TYR:CE2	2.56	0.41
1:A:138:ARG:HG2	7:A:631:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD13	1:B:164:LEU:HD12	2.01	0.40
1:A:284:ALA:HA	7:A:784:HOH:O	2.20	0.40
1:B:72:ARG:HA	1:B:80:ARG:O	2.21	0.40
1:D:72:ARG:HG2	1:D:81:ARG:HG2	2.03	0.40
1:A:20:MET:HE1	1:A:148:ILE:CG1	2.51	0.40
1:D:279:ALA:CA	1:D:282:ARG:HB3	2.52	0.40
1:B:300:ILE:HG12	1:B:365:ILE:HD13	2.02	0.40
1:B:292:SER:O	1:B:296:VAL:HG23	2.21	0.40
1:C:46:LEU:C	1:C:46:LEU:HD23	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:NH1	1:D:76:ASP:OD2[2_655]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	424 (98%)	10 (2%)	1 (0%)	51	48
1	B	452/451 (100%)	442 (98%)	10 (2%)	0	100	100
1	C	437/451 (97%)	426 (98%)	10 (2%)	1 (0%)	51	48
1	D	437/451 (97%)	427 (98%)	9 (2%)	1 (0%)	51	48
All	All	1761/1804 (98%)	1719 (98%)	39 (2%)	3 (0%)	51	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	276	ARG

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Mol	Chain	Res	Type
1	A	40	SER
1	C	330	GLY

### 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	348/358 (97%)	333 (96%)	15 (4%)	33	29
1	B	359/358 (100%)	343 (96%)	16 (4%)	32	27
1	C	350/358 (98%)	342 (98%)	8 (2%)	56	58
1	D	348/358 (97%)	332 (95%)	16 (5%)	31	27
All	All	1405/1432 (98%)	1350 (96%)	55 (4%)	36	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	102	GLU
1	A	103	THR
1	A	167	THR
1	A	174	GLN
1	A	182	ASP
1	A	254	VAL
1	A	282	ARG
1	A	283	LEU
1	A	342	ARG
1	A	357	PHE
1	A	360	VAL
1	A	378	ASP
1	A	405	ARG
1	A	441	THR
1	B	4	LEU
1	B	5	SER
1	B	33	LEU
1	B	37	VAL

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Mol	Chain	Res	Type
1	B	40	SER
1	B	75	ARG
1	B	99	LEU
1	B	142	MET
1	B	146	LYS
1	B	163	ARG
1	B	283	LEU
1	B	293	LYS
1	B	300	ILE
1	B	311	ASP
1	B	340	ARG
1	B	378	ASP
1	C	83	GLN
1	C	118	ARG
1	C	146	LYS
1	C	162	ASP
1	C	182	ASP
1	C	264	ILE
1	C	282	ARG
1	C	378	ASP
1	D	41	VAL
1	D	75	ARG
1	D	150	LEU
1	D	165	LEU
1	D	167	THR
1	D	234	VAL
1	D	274	LEU
1	D	292	SER
1	D	306	LEU
1	D	322	ASP
1	D	328	GLU
1	D	349	ARG
1	D	365	ILE
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	230	HIS

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Mol	Chain	Res	Type
1	A	291	ASN
1	B	83	GLN
1	B	230	HIS
1	C	25	ASN
1	C	83	GLN
1	C	231	ASN
1	D	204	HIS
1	D	291	ASN

### 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](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	0GA	A	501	-	10,17,17	2.06	3 (30%)	12,23,23	1.98	4 (33%)
3	SCN	A	502	-	1,2,2	0.37	0	0,1,1	0.00	-
4	GOL	A	503	-	5,5,5	0.28	0	5,5,5	0.64	0
2	0GA	B	501	-	10,17,17	2.20	3 (30%)	12,23,23	3.00	4 (33%)
3	SCN	B	502	-	1,2,2	0.16	0	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	503	-	5,5,5	0.48	0	5,5,5	0.32	0
2	OGA	C	501	-	10,17,17	2.14	2 (20%)	12,23,23	3.32	5 (41%)
3	SCN	C	502	-	1,2,2	0.10	0	0,1,1	0.00	-
6	PEG	C	503	-	6,6,6	0.68	0	5,5,5	1.32	0
4	GOL	C	504	-	5,5,5	0.69	0	5,5,5	1.43	1 (20%)
6	PEG	C	505	-	6,6,6	1.14	0	5,5,5	1.66	1 (20%)
4	GOL	C	506	-	5,5,5	0.57	0	5,5,5	0.49	0
2	OGA	D	501	-	10,17,17	2.25	2 (20%)	12,23,23	2.37	1 (8%)

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	OGA	A	501	-	-	0/6/14/14	0/1/1/1
3	SCN	A	502	-	-	0/0/0/0	0/0/0/0
4	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	OGA	B	501	-	-	0/6/14/14	0/1/1/1
3	SCN	B	502	-	-	0/0/0/0	0/0/0/0
4	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	OGA	C	501	-	-	0/6/14/14	0/1/1/1
3	SCN	C	502	-	-	0/0/0/0	0/0/0/0
6	PEG	C	503	-	-	0/4/4/4	0/0/0/0
4	GOL	C	504	-	-	0/4/4/4	0/0/0/0
6	PEG	C	505	-	-	0/4/4/4	0/0/0/0
4	GOL	C	506	-	-	0/4/4/4	0/0/0/0
2	OGA	D	501	-	-	0/6/14/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	OGA	CAH-CAJ	2.28	1.43	1.38
2	A	501	OGA	CAH-CAJ	2.81	1.44	1.38
2	A	501	OGA	CAQ-CAO	3.48	1.46	1.40
2	C	501	OGA	CAP-CAO	3.78	1.45	1.40
2	B	501	OGA	CAP-CAO	3.94	1.45	1.40
2	D	501	OGA	CAQ-CAO	4.23	1.48	1.40
2	B	501	OGA	CAQ-CAO	4.26	1.48	1.40
2	A	501	OGA	CAP-CAO	4.46	1.46	1.40
2	C	501	OGA	CAQ-CAO	5.01	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	0GA	CAP-CAO	5.28	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	0GA	CAQ-CAO-CAP	-9.94	115.38	120.30
2	B	501	0GA	CAQ-CAO-CAP	-8.57	116.05	120.30
2	D	501	0GA	CAQ-CAO-CAP	-7.21	116.73	120.30
2	A	501	0GA	CAA-CAG-CAN	-3.99	117.11	125.08
2	A	501	0GA	CAQ-CAO-CAP	-2.73	118.94	120.30
2	C	501	0GA	CAA-CAG-CAN	-2.19	120.70	125.08
4	C	504	GOL	O1-C1-C2	-2.01	99.94	110.07
2	B	501	0GA	OAF-CAO-CAP	2.03	123.75	119.31
2	C	501	0GA	OAK-CAP-CAI	2.04	123.84	118.81
2	C	501	0GA	CAI-CAP-CAO	2.27	122.26	120.00
6	C	505	PEG	O2-C3-C4	2.41	121.26	110.15
2	B	501	0GA	CAJ-CAQ-CAM	2.66	124.32	120.23
2	C	501	0GA	CAJ-CAQ-CAM	2.67	124.33	120.23
2	A	501	0GA	CAJ-CAQ-CAM	2.84	124.60	120.23
2	A	501	0GA	OAK-CAP-CAI	2.92	126.02	118.81
2	B	501	0GA	CAJ-CAQ-CAO	3.74	121.88	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	SCN	1	0
6	C	503	PEG	6	0
4	C	504	GOL	1	0
6	C	505	PEG	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	435/451 (96%)	-0.22	7 (1%) 72 71	13, 27, 50, 73	8 (1%)
1	B	451/451 (100%)	-0.17	16 (3%) 44 45	11, 26, 53, 76	9 (1%)
1	C	435/451 (96%)	-0.27	4 (0%) 84 83	13, 25, 44, 68	9 (2%)
1	D	439/451 (97%)	0.03	21 (4%) 31 31	15, 28, 59, 83	7 (1%)
All	All	1760/1804 (97%)	-0.16	48 (2%) 55 54	11, 27, 53, 83	33 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ILE	7.2
1	B	6	VAL	6.0
1	A	15	SER	5.7
1	B	280	ILE	5.4
1	D	155	ILE	5.2
1	D	278	PRO	4.4
1	B	-1	GLY	4.4
1	B	275	GLY	4.3
1	D	22	ALA	3.8
1	B	273	ALA	3.7
1	B	9	GLY	3.7
1	C	331	SER	3.7
1	B	277	GLY	3.6
1	B	5	SER	3.6
1	A	23	GLY	3.5
1	A	22	ALA	3.5
1	D	167	THR	3.4
1	B	8	THR	3.3
1	D	166	ALA	3.3
1	B	284	ALA	3.3
1	D	274	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	332	VAL	3.1
1	D	164	LEU	3.0
1	A	284	ALA	3.0
1	B	274	LEU	2.9
1	D	283	LEU	2.9
1	D	12	SER	2.8
1	B	276	ARG	2.8
1	B	7	ALA	2.8
1	D	160	ALA	2.7
1	D	275	GLY	2.7
1	B	331	SER	2.7
1	D	99	LEU	2.7
1	B	281	ASP	2.6
1	D	14	ALA	2.6
1	D	279	ALA	2.5
1	D	281	ASP	2.5
1	D	277	GLY	2.4
1	C	279	ALA	2.3
1	D	330	GLY	2.3
1	A	176	ARG	2.3
1	D	159	GLU	2.2
1	C	280	ILE	2.1
1	C	276	ARG	2.1
1	A	345	PRO	2.1
1	D	11	VAL	2.1
1	D	19	PRO	2.1
1	B	4	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(Å <sup>2</sup> )	Q<0.9
6	PEG	C	505	7/7	0.90	0.18	6.88	25,39,42,43	0
4	GOL	A	503	6/6	0.91	0.26	5.95	40,47,53,56	0
4	GOL	C	504	6/6	0.95	0.21	4.98	32,39,42,46	0
5	K	B	504	1/1	0.98	0.18	4.35	50,50,50,50	0
4	GOL	C	506	6/6	0.81	0.21	3.92	50,53,56,56	0
4	GOL	B	503	6/6	0.84	0.18	1.39	46,52,58,63	0
6	PEG	C	503	7/7	0.90	0.15	1.16	29,38,46,47	0
5	K	D	502	1/1	0.97	0.12	0.33	56,56,56,56	0
2	0GA	C	501	17/17	0.96	0.10	-0.27	19,22,28,28	0
2	0GA	B	501	17/17	0.96	0.09	-0.51	21,27,32,34	0
2	0GA	A	501	17/17	0.97	0.08	-0.65	19,22,33,35	0
2	0GA	D	501	17/17	0.97	0.08	-0.69	23,28,44,46	0
3	SCN	B	502	3/3	0.97	0.10	-0.76	28,28,31,35	0
3	SCN	C	502	3/3	0.99	0.08	-0.94	27,27,27,33	0
3	SCN	A	502	3/3	0.99	0.06	-1.42	27,27,29,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.