



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:23 PM UTC

PDB ID : 3VEH / pdb_00003veh
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

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

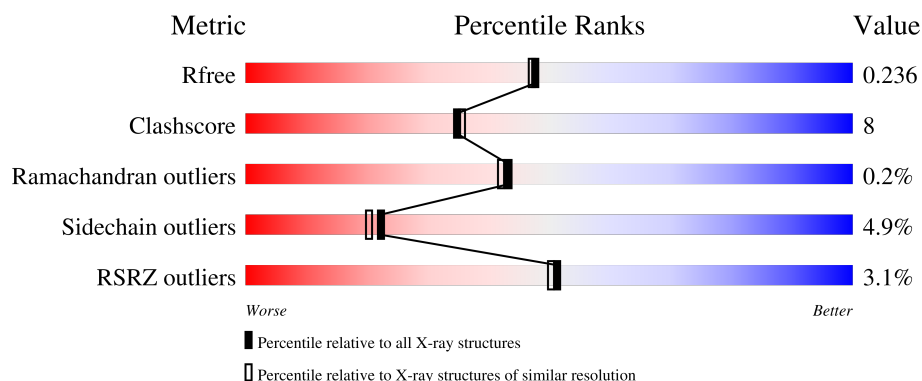
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	451	2% 79% 16% • •
1	B	451	4% 81% 16% •
1	C	451	• 80% 14% • •
1	D	451	4% 78% 16% • •

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
6	PEG	C	503	-	-	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.

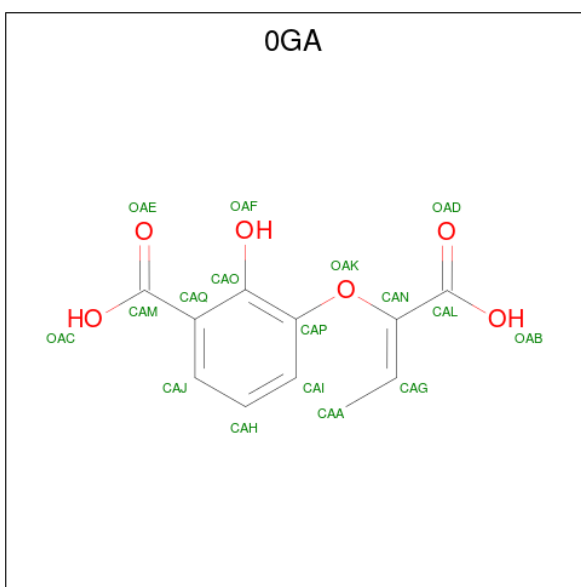
- Molecule 1 is a protein called Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

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:

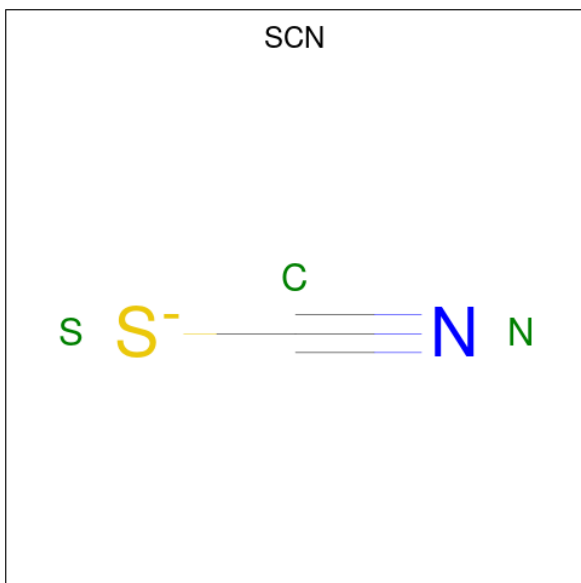
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7D785
A	0	SER	-	expression tag	UNP Q7D785
B	-1	GLY	-	expression tag	UNP Q7D785
B	0	SER	-	expression tag	UNP Q7D785
C	-1	GLY	-	expression tag	UNP Q7D785
C	0	SER	-	expression tag	UNP Q7D785
D	-1	GLY	-	expression tag	UNP Q7D785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

- Molecule 2 is 3-{{(1Z)-1-carboxyprop-1-en-1-yl}oxy}-2-hydroxybenzoic acid (CCD ID: 0GA) (formula: C₁₁H₁₀O₆).



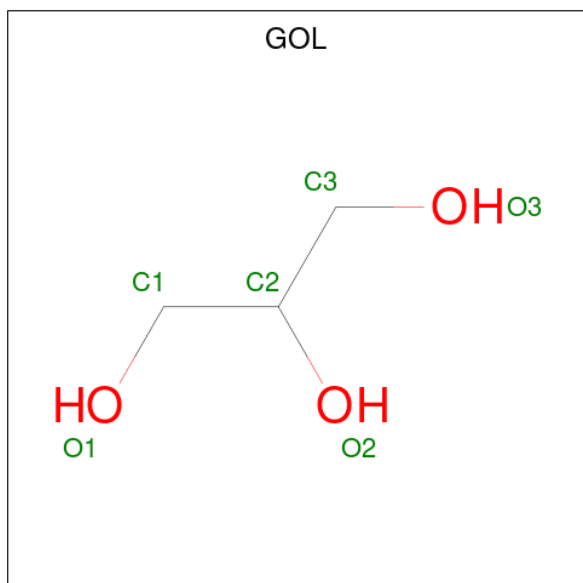
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	11	6		
2	B	1	Total	C	O	0	0
			17	11	6		
2	C	1	Total	C	O	0	0
			17	11	6		
2	D	1	Total	C	O	0	0
			17	11	6		

- Molecule 3 is THIOCYANATE ION (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).

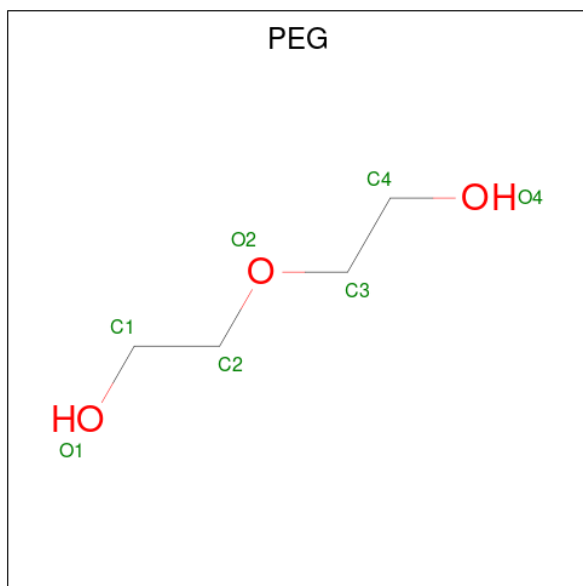


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (CCD ID: 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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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		

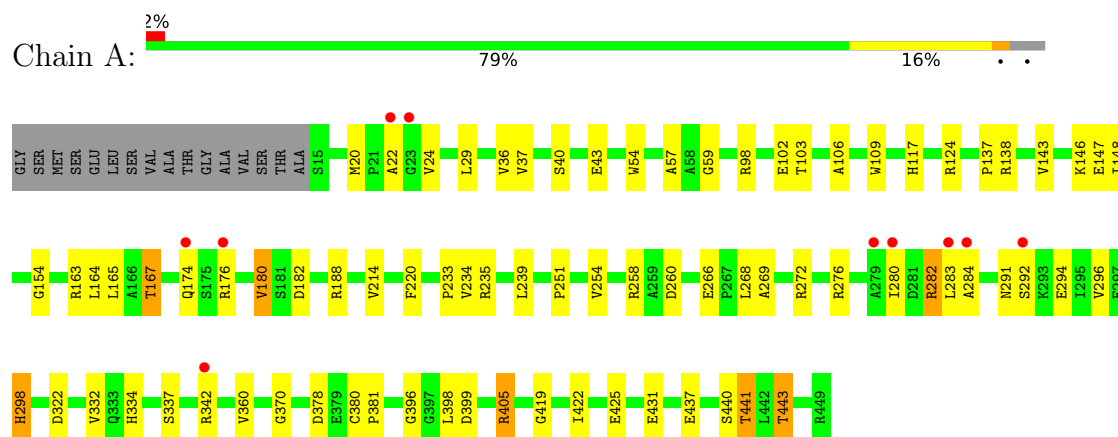
- Molecule 7 is water.

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		

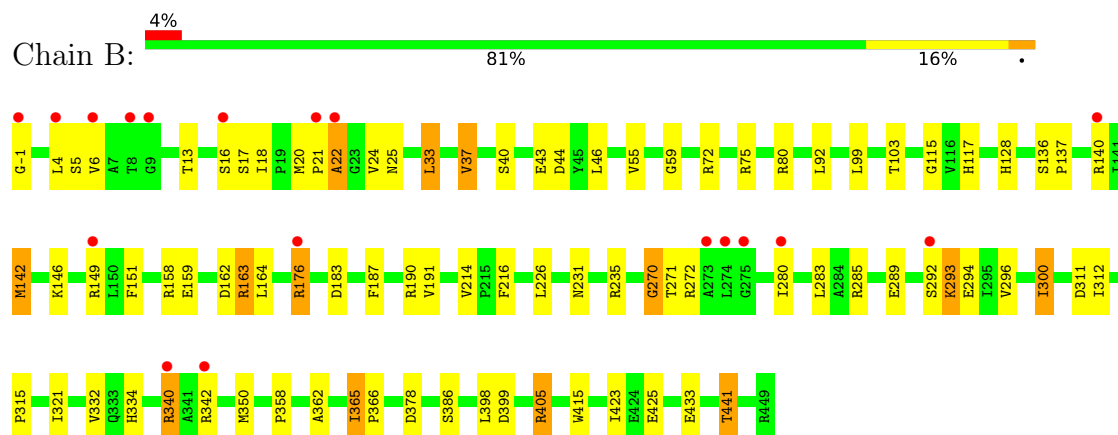
3 Residue-property plots [i](#)

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.

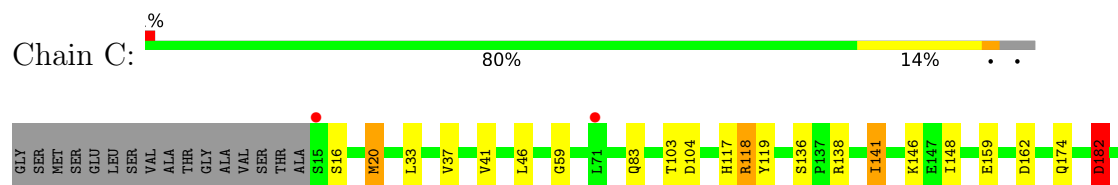
- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

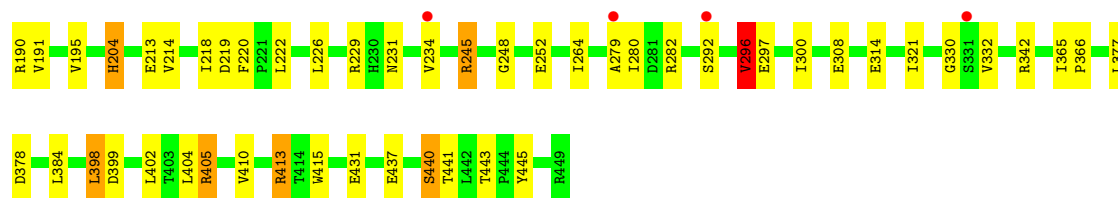


- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

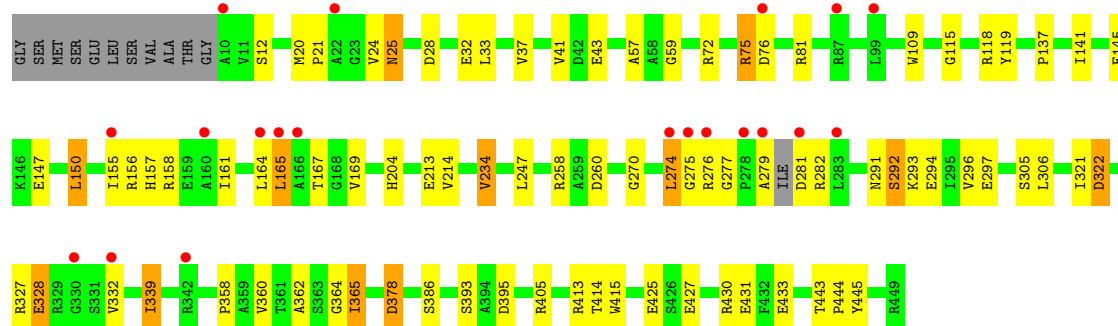
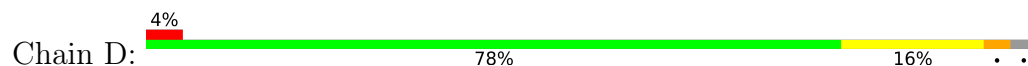


- Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI





- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.236 0.174 , 0.236	Depositor DCC
R_{free} test set	6410 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, OGA, K, SCN, GOL

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	1.39	11/3397 (0.3%)	1.27	13/4613 (0.3%)
1	B	1.39	9/3505 (0.3%)	1.34	15/4759 (0.3%)
1	C	1.41	11/3425 (0.3%)	1.31	15/4646 (0.3%)
1	D	1.32	7/3410 (0.2%)	1.25	10/4631 (0.2%)
All	All	1.38	38/13737 (0.3%)	1.29	53/18649 (0.3%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	HIS	CG-CD2	8.47	1.45	1.35
1	B	117	HIS	CE1-NE2	8.43	1.41	1.32
1	C	248	GLY	N-CA	7.09	1.53	1.45
1	A	117	HIS	CG-CD2	7.02	1.43	1.35
1	C	117	HIS	ND1-CE1	6.87	1.39	1.32
1	C	405	ARG	C-O	6.53	1.32	1.23
1	A	419	GLY	N-CA	6.31	1.51	1.45
1	D	414	THR	C-O	6.19	1.31	1.24
1	C	220	PHE	N-CA	6.15	1.52	1.46
1	A	117	HIS	CE1-NE2	6.15	1.38	1.32
1	D	364	GLY	N-CA	6.06	1.50	1.45
1	B	334	HIS	ND1-CE1	6.04	1.38	1.32
1	C	117	HIS	CE1-NE2	6.03	1.38	1.32
1	C	195	VAL	N-CA	6.03	1.53	1.46
1	C	204	HIS	CG-CD2	5.90	1.42	1.35
1	C	222	LEU	N-CA	5.76	1.53	1.46
1	B	423	ILE	C-O	5.64	1.30	1.23
1	A	106	ALA	N-CA	5.62	1.53	1.45
1	D	415	TRP	CD2-CE2	5.58	1.50	1.41
1	B	43	GLU	N-CA	5.55	1.52	1.46
1	D	25	ASN	CA-C	5.54	1.58	1.52
1	D	378	ASP	N-CA	5.54	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLY	C-O	5.49	1.29	1.23
1	A	109	TRP	CD2-CE2	5.47	1.50	1.41
1	C	402	LEU	N-CA	5.45	1.53	1.46
1	A	298	HIS	CG-CD2	5.43	1.41	1.35
1	B	334	HIS	CG-CD2	5.34	1.41	1.35
1	B	415	TRP	CD2-CE2	5.34	1.50	1.41
1	D	109	TRP	CD2-CE2	5.31	1.50	1.41
1	C	191	VAL	CA-C	5.25	1.59	1.52
1	B	190	ARG	CZ-NH1	5.23	1.40	1.32
1	A	370	GLY	N-CA	5.22	1.52	1.45
1	D	339	ILE	C-O	5.20	1.29	1.24
1	A	43	GLU	CA-C	5.11	1.58	1.52
1	B	21	PRO	C-O	5.09	1.30	1.24
1	B	128	HIS	CG-CD2	5.06	1.41	1.35
1	A	251	PRO	N-CA	5.03	1.53	1.47
1	A	54	TRP	CA-C	-5.01	1.46	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	PHE	CA-C-N	-7.47	111.06	119.28
1	A	220	PHE	C-N-CA	-7.47	111.06	119.28
1	D	234	VAL	CB-CA-C	-7.21	100.41	112.16
1	D	214	VAL	CA-C-N	-7.19	113.49	120.83
1	D	214	VAL	C-N-CA	-7.19	113.49	120.83
1	B	214	VAL	N-CA-C	-6.98	100.64	107.55
1	B	226	LEU	N-CA-C	-6.83	103.91	111.36
1	A	266	GLU	CB-CA-C	-6.73	101.38	111.27
1	D	328	GLU	N-CA-C	6.58	119.26	109.59
1	C	59	GLY	N-CA-C	-6.47	104.65	112.48
1	B	44	ASP	N-CA-C	-6.46	102.20	110.53
1	B	43	GLU	N-CA-C	6.41	119.91	109.59
1	C	296	VAL	CB-CA-C	-6.37	103.43	112.22
1	A	22	ALA	N-CA-C	6.34	118.07	111.03
1	A	124	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	C	182	ASP	N-CA-C	6.12	119.14	110.50
1	B	183	ASP	CA-C-N	6.09	125.98	119.28
1	B	183	ASP	C-N-CA	6.09	125.98	119.28
1	C	37	VAL	N-CA-C	6.05	116.79	110.62
1	C	234	VAL	N-CA-C	-6.02	103.38	111.44
1	D	147	GLU	N-CA-C	5.98	117.33	108.60
1	A	443	THR	CA-C-N	-5.82	113.99	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	THR	C-N-CA	-5.82	113.99	120.45
1	C	440	SER	CB-CA-C	-5.77	99.96	110.63
1	D	12	SER	N-CA-C	5.75	117.71	109.14
1	C	413	ARG	CB-CG-CD	5.71	124.45	111.30
1	A	98	ARG	N-CA-C	5.67	117.46	111.28
1	B	405	ARG	CB-CG-CD	-5.67	98.26	111.30
1	C	443	THR	CA-C-N	-5.65	114.18	120.45
1	C	443	THR	C-N-CA	-5.65	114.18	120.45
1	C	404	LEU	N-CA-C	-5.52	100.92	109.14
1	B	25	ASN	CA-C-N	5.40	125.05	119.05
1	B	25	ASN	C-N-CA	5.40	125.05	119.05
1	C	308	GLU	CA-CB-CG	-5.40	103.30	114.10
1	D	415	TRP	N-CA-C	5.40	117.28	109.07
1	A	180	VAL	N-CA-C	-5.35	107.08	112.17
1	A	396	GLY	CA-C-N	5.32	125.15	120.10
1	A	396	GLY	C-N-CA	5.32	125.15	120.10
1	B	6	VAL	N-CA-C	5.32	118.57	111.44
1	C	159	GLU	N-CA-C	5.32	117.76	111.33
1	D	443	THR	CA-C-N	-5.20	114.68	120.45
1	D	443	THR	C-N-CA	-5.20	114.68	120.45
1	B	22	ALA	O-C-N	-5.18	116.54	122.08
1	C	104	ASP	N-CA-C	5.16	117.80	111.82
1	C	141	ILE	CB-CG1-CD1	-5.15	102.99	113.80
1	B	13	THR	N-CA-C	5.13	117.93	109.72
1	D	321	ILE	N-CA-C	-5.12	107.85	113.43
1	A	214	VAL	N-CA-C	-5.11	101.91	107.73
1	C	245	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	24	VAL	N-CA-C	5.08	115.41	107.99
1	B	270	GLY	N-CA-C	-5.07	101.16	113.18
1	B	235	ARG	CA-C-N	-5.04	113.60	121.87
1	B	235	ARG	C-N-CA	-5.04	113.60	121.87

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	41	0
1	B	3438	0	3440	56	1
1	C	3350	0	3373	54	0
1	D	3347	0	3335	51	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
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	204	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 (204) 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
1:C:20:MET:HA	1:C:20:MET:HE2	1.56	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:20:MET:HE1	1:C:148:ILE:CG1	2.20	0.71
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: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:HG3	1:C:118:ARG:NH2	2.00	0.68
1:B:20:MET:HE3	1:B:24:VAL:CB	2.24	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
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:A:20:MET:HE1	1:A:143:VAL:HG13	1.79	0.64
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:B:17:SER:C	1:B:18:ILE:HG13	2.23	0.61
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:D:322:ASP:C	1:D:322:ASP:OD1	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:213:GLU:CD	1:C:413:ARG:HH11	2.11	0.58
1:B:176:ARG:HG2	1:B:216:PHE:CZ	2.39	0.57
1:A:20:MET:HE2	1:A:148:ILE:HG13	1.86	0.57
1:A:405:ARG:HG2	1:A:441:THR:HG21	1.86	0.57
1:C:245:ARG:HD3	7:C:784:HOH:O	2.02	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:437:GLU:O	1:C:440:SER:HB2	2.05	0.56
1:D:293:LYS:HZ3	1:D:425:GLU:HG3	1.71	0.55
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
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:D:362:ALA:HB1	1:D:386:SER:HB2	1.91	0.53
1:D:275:GLY:C	1:D:277:GLY:H	2.17	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: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:D:213:GLU:CD	1:D:413:ARG:HH11	2.18	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:46:LEU:C	1:B:46:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:213:GLU:CD	1:D:413:ARG:NH1	2.70	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:20:MET:CE	1:A:148:ILE:HG13	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:158:ARG:NH1	1:B:162:ASP:CG	2.69	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
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:O	1:D:164:LEU:HD12	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: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:B:365:ILE:HA	1:B:366:PRO:C	2.39	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ILE:HD12	1:A:431:GLU:HG3	1.97	0.46
1:B:92:LEU:HD23	1:B:350:MET:HE1	1.98	0.46
1:B:312:ILE:C	1:B:312:ILE:HD12	2.41	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: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:C:46:LEU:C	1:C:46:LEU:HD23	2.42	0.45
1:C:20:MET:HE2	1:C:148:ILE:HD11	1.99	0.45
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:D:25:ASN:OD1	1:D:25:ASN:C	2.60	0.44
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:B:293:LYS:HZ3	1:B:425:GLU:HG3	1.82	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: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: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:HD3	1:A:272:ARG:HA	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:A:239:LEU:C	1:A:239:LEU:HD12	2.44	0.42
1:B:59:GLY:O	1:B:137:PRO:HA	2.20	0.42
1:B:340:ARG:HD2	7:B:770:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:247:LEU:HD12	1:D:247:LEU:C	2.44	0.42
1:C:20:MET:HE1	1:C:148:ILE:HG13	1.88	0.41
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:A:138:ARG:HG2	1:A:138:ARG:HH11	1.86	0.41
1:B:55:VAL:HG23	7:B:878:HOH:O	2.20	0.41
1:B:332:VAL:HG12	1:B:405:ARG:NH2	2.36	0.41
1:C:204:HIS:NE2	1:C:297:GLU:OE2	2.42	0.41
1:C:365:ILE:HA	1:C:366:PRO:C	2.45	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:A:380:CYS:HA	1:A:381:PRO:C	2.46	0.41
1:D:20:MET:HE3	1:D:24:VAL:O	2.21	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
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: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

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%)	43	42
1	B	452/451 (100%)	442 (98%)	10 (2%)	0	100	100
1	C	437/451 (97%)	426 (98%)	10 (2%)	1 (0%)	43	42
1	D	437/451 (97%)	427 (98%)	9 (2%)	1 (0%)	43	42
All	All	1761/1804 (98%)	1719 (98%)	39 (2%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	276	ARG
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%)	330 (95%)	18 (5%)	21	18
1	B	359/358 (100%)	338 (94%)	21 (6%)	18	15
1	C	350/358 (98%)	336 (96%)	14 (4%)	28	27
1	D	348/358 (97%)	332 (95%)	16 (5%)	24	22
All	All	1405/1432 (98%)	1336 (95%)	69 (5%)	22	20

All (69) 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

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	165	LEU
1	A	167	THR
1	A	174	GLN
1	A	182	ASP
1	A	234[A]	VAL
1	A	234[B]	VAL
1	A	254	VAL
1	A	282	ARG
1	A	283	LEU
1	A	342	ARG
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
1	B	40	SER
1	B	75	ARG
1	B	99	LEU
1	B	142	MET
1	B	146	LYS
1	B	159	GLU
1	B	163	ARG
1	B	176	ARG
1	B	283	LEU
1	B	293	LYS
1	B	300	ILE
1	B	311	ASP
1	B	340	ARG
1	B	365	ILE
1	B	378	ASP
1	B	433	GLU
1	B	441	THR
1	C	20	MET
1	C	41	VAL
1	C	83	GLN
1	C	118	ARG
1	C	146	LYS
1	C	162	ASP

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Mol	Chain	Res	Type
1	C	174	GLN
1	C	182	ASP
1	C	264	ILE
1	C	282	ARG
1	C	296	VAL
1	C	321	ILE
1	C	378	ASP
1	C	398	LEU
1	D	41	VAL
1	D	75	ARG
1	D	145	GLU
1	D	150	LEU
1	D	155	ILE
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	365	ILE
1	D	378	ASP
1	D	427	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	230	HIS
1	B	291	ASN
1	C	25	ASN
1	C	83	GLN
1	C	231	ASN
1	C	334	HIS
1	D	53	GLN
1	D	83	GLN
1	D	204	HIS
1	D	230	HIS
1	D	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	GOL	C	504	-	5,5,5	0.65	0	5,5,5	1.63	1 (20%)
6	PEG	C	505	-	6,6,6	1.13	0	5,5,5	1.71	1 (20%)
4	GOL	C	506	-	5,5,5	0.62	0	5,5,5	0.51	0
2	0GA	C	501	-	17,17,17	1.97	4 (23%)	21,23,23	1.91	6 (28%)
4	GOL	A	503	-	5,5,5	0.34	0	5,5,5	0.72	0
2	0GA	A	501	-	17,17,17	1.92	5 (29%)	21,23,23	1.89	6 (28%)
3	SCN	B	502	-	1,2,2	0.17	0	0,1,1	-	-
2	0GA	D	501	-	17,17,17	2.02	4 (23%)	21,23,23	1.38	2 (9%)
2	0GA	B	501	-	17,17,17	1.94	4 (23%)	21,23,23	2.31	9 (42%)
4	GOL	B	503	-	5,5,5	0.51	0	5,5,5	0.41	0
3	SCN	A	502	-	1,2,2	0.38	0	0,1,1	-	-
6	PEG	C	503	-	6,6,6	0.68	0	5,5,5	1.31	0
3	SCN	C	502	-	1,2,2	0.11	0	0,1,1	-	-

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	0GA	CAQ-CAO	5.01	1.49	1.41
2	D	501	0GA	CAP-CAO	4.98	1.47	1.40
2	A	501	0GA	CAP-CAO	4.20	1.46	1.40
2	B	501	0GA	CAQ-CAO	4.19	1.48	1.41
2	D	501	0GA	CAQ-CAO	4.15	1.48	1.41
2	B	501	0GA	CAP-CAO	3.70	1.45	1.40
2	A	501	0GA	OAK-CAN	3.63	1.46	1.38
2	C	501	0GA	CAP-CAO	3.55	1.45	1.40
2	B	501	0GA	OAK-CAN	3.49	1.46	1.38
2	A	501	0GA	CAQ-CAO	3.33	1.46	1.41
2	A	501	0GA	CAH-CAJ	3.13	1.44	1.38
2	C	501	0GA	OAK-CAN	2.90	1.45	1.38
2	D	501	0GA	OAC-CAM	-2.78	1.22	1.30
2	B	501	0GA	CAH-CAJ	2.53	1.43	1.38
2	D	501	0GA	OAK-CAN	2.41	1.44	1.38
2	C	501	0GA	OAB-CAL	-2.36	1.24	1.30
2	A	501	0GA	OAB-CAL	-2.20	1.24	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0GA	CAO-CAQ-CAM	-5.42	113.80	119.86
2	C	501	0GA	CAQ-CAO-CAP	-5.11	115.38	119.56
2	A	501	0GA	CAA-CAG-CAN	-4.34	117.11	125.20
2	B	501	0GA	CAQ-CAO-CAP	-4.28	116.05	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	0GA	CAQ-CAO-CAP	-3.46	116.73	119.56
2	B	501	0GA	OAE-CAM-CAQ	-3.45	113.72	121.97
2	C	501	0GA	CAO-CAQ-CAM	-3.42	116.03	119.86
2	B	501	0GA	CAJ-CAQ-CAO	3.22	121.88	118.76
2	A	501	0GA	CAO-CAQ-CAM	-3.10	116.38	119.86
2	A	501	0GA	OAK-CAP-CAI	2.96	126.02	118.89
2	D	501	0GA	CAP-OAK-CAN	2.89	123.24	118.49
2	A	501	0GA	OAE-CAM-CAQ	-2.76	115.38	121.97
2	A	501	0GA	OAB-CAL-CAN	2.68	120.12	114.06
2	A	501	0GA	CAJ-CAQ-CAM	2.60	124.60	118.64
6	C	505	PEG	O2-C3-C4	2.53	121.26	110.11
2	C	501	0GA	CAJ-CAQ-CAM	2.48	124.33	118.64
2	B	501	0GA	CAJ-CAQ-CAM	2.47	124.32	118.64
2	C	501	0GA	CAI-CAP-CAO	2.46	122.26	119.98
2	C	501	0GA	CAA-CAG-CAN	-2.41	120.70	125.20
2	B	501	0GA	CAP-OAK-CAN	2.40	122.44	118.49
4	C	504	GOL	O1-C1-C2	-2.32	99.94	110.38
2	B	501	0GA	OAC-CAM-CAQ	2.31	121.85	115.28
2	B	501	0GA	OAF-CAO-CAP	2.11	123.75	119.21
2	C	501	0GA	OAK-CAP-CAI	2.05	123.84	118.89
2	B	501	0GA	OAB-CAL-CAN	2.02	118.64	114.06

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	GOL	O1-C1-C2-C3
4	C	504	GOL	O1-C1-C2-O2
4	C	504	GOL	O1-C1-C2-C3
4	C	506	GOL	O2-C2-C3-O3
6	C	505	PEG	C4-C3-O2-C2
6	C	505	PEG	O1-C1-C2-O2
4	A	503	GOL	C1-C2-C3-O3
4	B	503	GOL	C1-C2-C3-O3
4	C	506	GOL	C1-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3
4	B	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
6	C	505	PEG	O2-C3-C4-O4
4	C	506	GOL	O1-C1-C2-O2
6	C	503	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	GOL	1	0
6	C	505	PEG	3	0
3	A	502	SCN	1	0
6	C	503	PEG	6	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	435/451 (96%)	-0.15	10 (2%) 61 60	9, 27, 50, 73	9 (2%)
1	B	451/451 (100%)	-0.20	18 (3%) 42 41	8, 25, 53, 76	11 (2%)
1	C	435/451 (96%)	-0.37	6 (1%) 73 73	8, 24, 44, 68	12 (2%)
1	D	439/451 (97%)	-0.13	20 (4%) 37 36	10, 28, 59, 83	8 (1%)
All	All	1760/1804 (97%)	-0.21	54 (3%) 51 50	8, 26, 53, 83	40 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	4.3
1	A	176	ARG	4.2
1	A	280	ILE	4.1
1	B	6	VAL	3.3
1	A	279	ALA	3.2
1	D	160	ALA	3.2
1	B	176	ARG	3.2
1	A	284	ALA	3.1
1	B	16	SER	3.1
1	B	273	ALA	3.1
1	D	164	LEU	3.1
1	D	278	PRO	3.1
1	D	155	ILE	2.9
1	D	279	ALA	2.8
1	D	99	LEU	2.8
1	D	166	ALA	2.7
1	C	331	SER	2.6
1	D	10	ALA	2.6
1	B	274	LEU	2.6
1	D	332	VAL	2.5
1	B	149	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	76	ASP	2.5
1	B	22	ALA	2.5
1	B	340	ARG	2.5
1	D	281	ASP	2.5
1	B	21	PRO	2.5
1	D	165	LEU	2.5
1	D	276	ARG	2.5
1	D	22	ALA	2.4
1	B	4	LEU	2.4
1	A	342	ARG	2.4
1	B	292	SER	2.4
1	B	8	THR	2.4
1	A	174	GLN	2.4
1	C	71	LEU	2.3
1	D	274	LEU	2.3
1	C	292	SER	2.3
1	B	-1	GLY	2.3
1	B	140	ARG	2.3
1	A	22	ALA	2.3
1	D	275	GLY	2.3
1	C	15	SER	2.2
1	D	87	ARG	2.2
1	C	279	ALA	2.2
1	A	283	LEU	2.2
1	D	330	GLY	2.2
1	D	342	ARG	2.2
1	A	292	SER	2.1
1	D	283	LEU	2.1
1	A	23	GLY	2.1
1	B	342	ARG	2.0
1	B	9	GLY	2.0
1	C	234	VAL	2.0
1	B	275	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

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
4	GOL	C	506	6/6	0.82	0.16	50,53,56,56	0
4	GOL	B	503	6/6	0.85	0.16	46,52,58,63	0
6	PEG	C	503	7/7	0.86	0.13	29,38,46,47	0
6	PEG	C	505	7/7	0.87	0.14	25,39,42,43	0
4	GOL	C	504	6/6	0.91	0.10	32,39,42,46	0
4	GOL	A	503	6/6	0.92	0.08	40,47,53,56	0
2	0GA	C	501	17/17	0.95	0.06	19,22,28,28	0
2	0GA	B	501	17/17	0.96	0.06	21,27,32,34	0
5	K	B	504	1/1	0.96	0.24	50,50,50,50	0
2	0GA	A	501	17/17	0.96	0.06	19,22,33,35	0
3	SCN	B	502	3/3	0.96	0.10	28,28,31,35	0
2	0GA	D	501	17/17	0.97	0.05	23,28,44,46	0
5	K	D	502	1/1	0.97	0.19	56,56,56,56	0
3	SCN	A	502	3/3	0.98	0.08	27,27,29,39	0
3	SCN	C	502	3/3	0.99	0.05	27,27,27,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.