



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:10 AM UTC

PDB ID : 3NE1 / pdb_00003ne1
Title : Mycobacterium tuberculosis Acyl Carrier Protein Synthase in complex with sulfate ion
Authors : Gokulan, K.
Deposited on : 2010-06-08
Resolution : 2.51 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

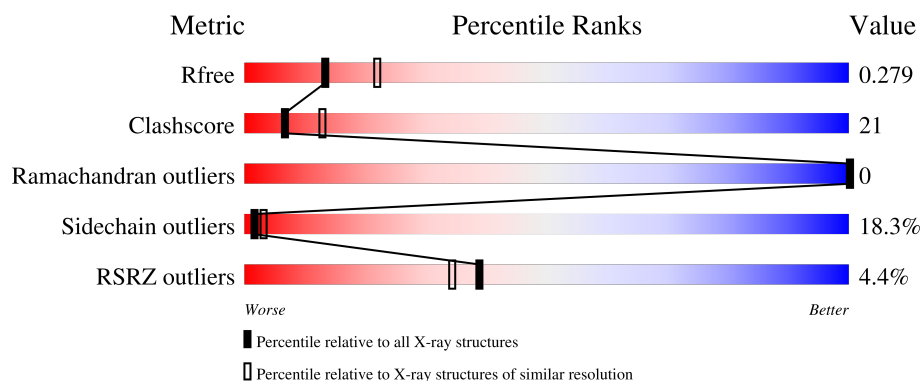
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	130	5% 28% 42% 26% • •
1	B	130	5% 23% 43% 25% 8% •
1	C	130	3% 22% 45% 30% • •

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	SO4	C	131	-	-	X	-

2 Entry composition [i](#)

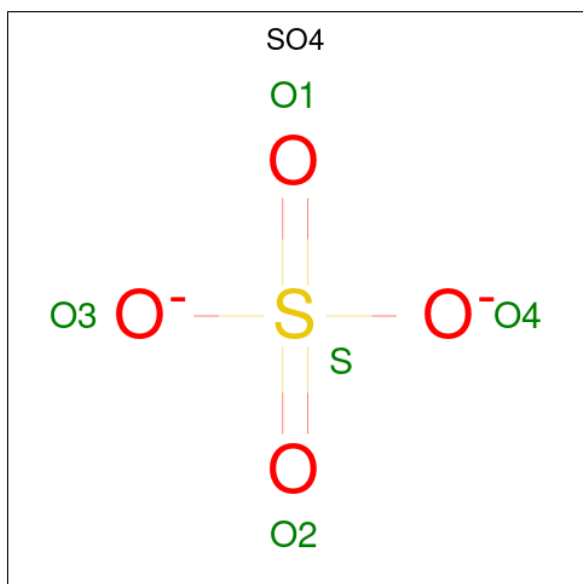
There are 3 unique types of molecules in this entry. The entry contains 2986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Holo-[acyl-carrier-protein] synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			970	606	176	187	1			
1	B	129	Total	C	N	O	S	0	0	0
			970	606	176	187	1			
1	C	129	Total	C	N	O	S	0	0	0
			970	606	176	187	1			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

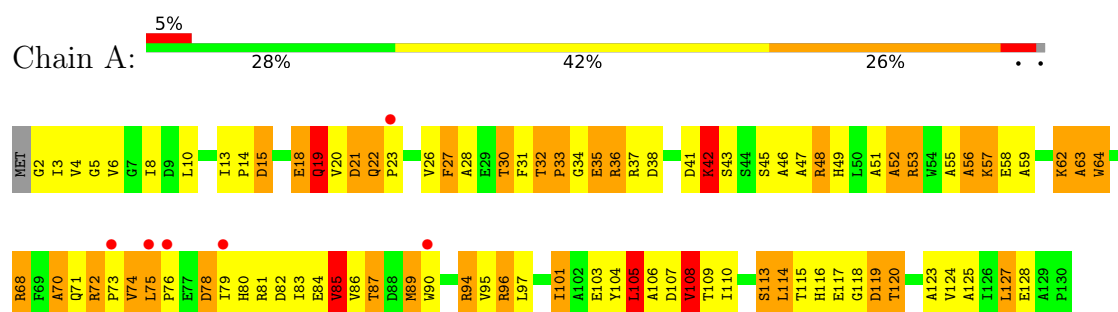
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	25	Total	O	0	0
			25	25		
3	C	12	Total	O	0	0
			12	12		

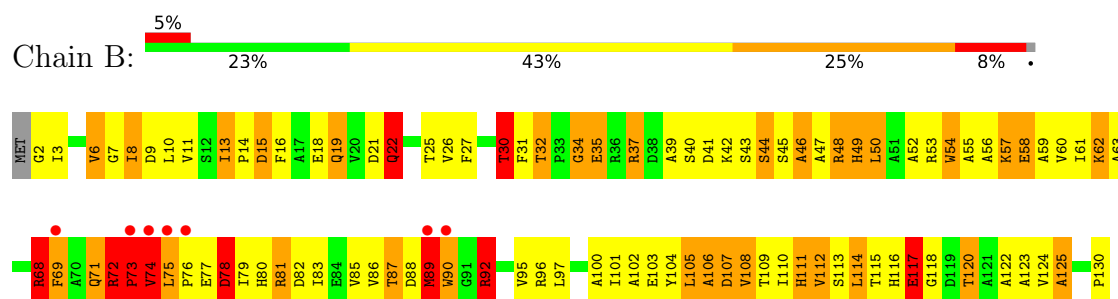
3 Residue-property plots [i](#)

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.

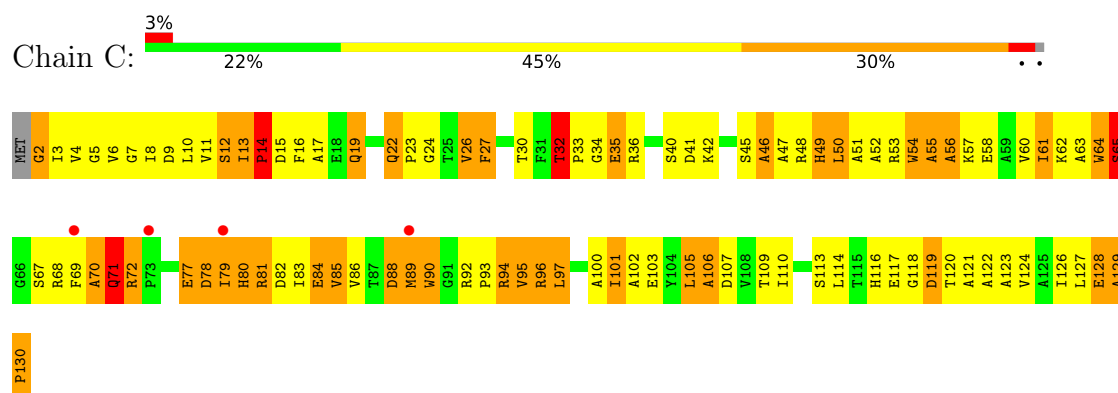
• Molecule 1: Holo-[acyl-carrier-protein] synthase



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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	83.12Å 104.87Å 105.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.07 – 2.51 20.07 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.07-2.51) 93.5 (20.07-2.51)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.228 , 0.301 (Not available) , 0.279	Depositor DCC
R_{free} test set	761 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2986	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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: SO4

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	2.96	85/991 (8.6%)	1.95	22/1354 (1.6%)
1	B	3.23	113/991 (11.4%)	2.18	36/1354 (2.7%)
1	C	3.36	126/991 (12.7%)	2.15	39/1354 (2.9%)
All	All	3.19	324/2973 (10.9%)	2.10	97/4062 (2.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (324) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	MET	SD-CE	17.22	2.22	1.79
1	A	56	ALA	N-CA	13.97	1.63	1.46
1	B	6	VAL	C-O	-13.44	1.10	1.24
1	B	74	VAL	CA-CB	13.12	1.72	1.54
1	C	89	MET	SD-CE	12.59	2.11	1.79
1	C	4	VAL	C-O	-12.09	1.11	1.23
1	C	96	ARG	C-O	12.07	1.37	1.24
1	A	59	ALA	CA-C	-11.80	1.37	1.52
1	C	47	ALA	C-O	-11.73	1.10	1.24
1	C	110	ILE	CA-CB	11.72	1.68	1.54
1	A	83	ILE	CA-CB	11.71	1.68	1.54
1	C	84	GLU	CA-C	-11.14	1.39	1.52
1	C	71	GLN	CA-C	11.06	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	MET	SD-CE	11.03	2.07	1.79
1	A	62	LYS	C-O	-10.95	1.11	1.24
1	C	58	GLU	CA-C	10.71	1.67	1.52
1	B	63	ALA	CA-CB	-10.49	1.35	1.53
1	B	112	VAL	C-O	-10.42	1.12	1.23
1	C	83	ILE	CA-CB	10.37	1.67	1.53
1	B	52	ALA	N-CA	-10.23	1.33	1.46
1	B	21	ASP	C-O	-10.22	1.10	1.24
1	A	125	ALA	C-O	-10.18	1.11	1.23
1	B	85	VAL	CA-CB	-10.08	1.42	1.54
1	C	94	ARG	NE-CZ	10.06	1.44	1.33
1	B	115	THR	N-CA	-9.97	1.32	1.46
1	C	101	ILE	CA-C	-9.93	1.40	1.52
1	C	117	GLU	C-O	9.92	1.35	1.24
1	B	125	ALA	CA-CB	-9.91	1.34	1.53
1	C	54	TRP	CA-C	9.90	1.65	1.52
1	A	94	ARG	NE-CZ	9.66	1.43	1.33
1	B	85	VAL	C-O	-9.54	1.13	1.24
1	C	51	ALA	CA-C	9.50	1.65	1.52
1	B	59	ALA	CA-CB	-9.50	1.38	1.53
1	C	65	SER	CA-C	-9.43	1.40	1.52
1	C	81	ARG	NE-CZ	9.38	1.43	1.33
1	C	13	ILE	C-O	-9.34	1.13	1.24
1	A	108	VAL	C-O	-9.33	1.14	1.24
1	C	7	GLY	CA-C	-9.32	1.38	1.51
1	B	39	ALA	CA-CB	-9.29	1.37	1.53
1	C	121	ALA	CA-CB	9.28	1.71	1.53
1	B	48	ARG	NE-CZ	9.19	1.43	1.33
1	C	16	PHE	C-O	-9.03	1.12	1.24
1	C	55	ALA	N-CA	-9.01	1.35	1.46
1	C	53	ARG	NE-CZ	8.96	1.43	1.33
1	B	59	ALA	N-CA	-8.95	1.35	1.46
1	A	113	SER	C-O	-8.91	1.14	1.23
1	C	100	ALA	CA-C	8.83	1.64	1.52
1	A	35	GLU	CA-C	8.76	1.64	1.52
1	A	56	ALA	CA-CB	-8.60	1.40	1.53
1	C	85	VAL	CA-CB	8.54	1.66	1.54
1	B	116	HIS	C-O	-8.54	1.13	1.24
1	B	57	LYS	N-CA	-8.48	1.36	1.46
1	C	26	VAL	CB-CG1	8.45	1.80	1.52
1	C	61	ILE	CA-C	8.43	1.63	1.52
1	A	47	ALA	CA-CB	8.37	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	THR	CA-CB	-8.34	1.40	1.53
1	C	9	ASP	N-CA	8.32	1.55	1.46
1	B	95	VAL	C-O	-8.29	1.14	1.24
1	B	113	SER	N-CA	-8.23	1.35	1.45
1	C	72	ARG	N-CA	8.18	1.57	1.46
1	B	42	LYS	C-O	8.14	1.34	1.24
1	C	9	ASP	CA-C	-8.14	1.42	1.52
1	B	62	LYS	CA-C	-8.12	1.41	1.52
1	C	113	SER	CA-C	8.11	1.62	1.52
1	C	93	PRO	C-O	-8.08	1.14	1.23
1	A	119	ASP	N-CA	8.06	1.56	1.46
1	B	101	ILE	C-O	-8.06	1.14	1.24
1	A	113	SER	N-CA	8.04	1.56	1.46
1	C	49	HIS	C-O	8.02	1.34	1.24
1	A	124	VAL	CA-C	-8.01	1.43	1.52
1	C	82	ASP	CA-C	-7.98	1.41	1.52
1	C	113	SER	C-O	-7.98	1.13	1.23
1	C	95	VAL	CA-C	-7.96	1.42	1.52
1	A	8	ILE	N-CA	7.95	1.55	1.46
1	A	59	ALA	N-CA	-7.91	1.36	1.46
1	C	103	GLU	C-O	-7.90	1.15	1.24
1	A	51	ALA	CA-CB	-7.83	1.41	1.53
1	C	83	ILE	C-O	7.83	1.32	1.24
1	B	39	ALA	CA-C	-7.82	1.41	1.52
1	B	48	ARG	C-N	-7.81	1.23	1.33
1	C	68	ARG	CA-C	7.80	1.63	1.52
1	B	44	SER	N-CA	-7.77	1.36	1.46
1	B	114	LEU	CA-C	7.77	1.62	1.52
1	A	18	GLU	C-O	-7.74	1.14	1.24
1	B	95	VAL	CA-C	-7.73	1.43	1.52
1	B	88	ASP	CA-C	7.72	1.63	1.52
1	B	30	THR	C-O	-7.68	1.14	1.24
1	A	127	LEU	C-O	-7.66	1.15	1.24
1	C	19	GLN	CG-CD	7.64	1.71	1.52
1	B	60	VAL	CA-C	7.63	1.63	1.52
1	A	96	ARG	CG-CD	7.61	1.75	1.52
1	A	125	ALA	CA-C	-7.51	1.43	1.52
1	B	41	ASP	C-O	-7.49	1.14	1.24
1	B	72	ARG	CA-C	7.47	1.62	1.52
1	B	118	GLY	C-O	-7.47	1.13	1.23
1	B	61	ILE	CA-CB	7.46	1.63	1.54
1	C	30	THR	CA-CB	7.42	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLN	C-O	7.39	1.33	1.24
1	C	58	GLU	CA-CB	-7.38	1.41	1.53
1	C	129	ALA	CA-C	7.36	1.62	1.53
1	A	96	ARG	NE-CZ	-7.35	1.25	1.33
1	C	8	ILE	C-O	-7.35	1.16	1.23
1	B	102	ALA	CA-C	-7.33	1.43	1.52
1	A	97	LEU	C-O	7.30	1.32	1.24
1	C	71	GLN	N-CA	7.30	1.55	1.46
1	C	117	GLU	CA-C	7.29	1.61	1.52
1	C	89	MET	N-CA	7.29	1.55	1.46
1	C	57	LYS	CA-C	-7.27	1.43	1.52
1	B	31	PHE	CG-CD2	7.26	1.54	1.38
1	A	45	SER	N-CA	-7.25	1.36	1.46
1	B	9	ASP	C-O	7.25	1.32	1.23
1	C	88	ASP	C-O	7.23	1.33	1.23
1	B	96	ARG	C-O	7.21	1.32	1.24
1	C	10	LEU	CB-CG	7.17	1.67	1.53
1	C	79	ILE	C-O	7.16	1.32	1.24
1	A	46	ALA	C-O	7.16	1.32	1.24
1	C	56	ALA	CA-CB	-7.08	1.42	1.53
1	B	120	THR	C-O	-7.08	1.16	1.23
1	B	100	ALA	CA-CB	7.07	1.64	1.53
1	B	56	ALA	CA-CB	-7.07	1.42	1.53
1	B	63	ALA	C-O	-7.04	1.15	1.24
1	C	48	ARG	C-O	-7.04	1.15	1.24
1	A	5	GLY	C-O	7.03	1.31	1.24
1	B	43	SER	C-O	-7.02	1.13	1.23
1	B	56	ALA	CA-C	7.00	1.62	1.52
1	B	87	THR	C-O	-7.00	1.14	1.23
1	C	128	GLU	CA-C	6.97	1.61	1.52
1	A	3	ILE	CA-CB	6.96	1.61	1.53
1	C	116	HIS	C-O	-6.95	1.15	1.23
1	A	57	LYS	CD-CE	6.95	1.73	1.52
1	B	107	ASP	CB-CG	6.93	1.69	1.52
1	C	127	LEU	C-O	-6.89	1.15	1.24
1	C	69	PHE	N-CA	6.89	1.53	1.46
1	A	15	ASP	C-O	-6.87	1.15	1.24
1	A	118	GLY	C-O	6.86	1.33	1.23
1	C	114	LEU	N-CA	-6.85	1.37	1.45
1	A	27	PHE	CD1-CE1	6.83	1.59	1.38
1	A	115	THR	C-O	-6.80	1.15	1.23
1	C	124	VAL	N-CA	-6.79	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ILE	CA-CB	6.75	1.62	1.54
1	A	30	THR	CA-CB	6.75	1.64	1.53
1	A	33	PRO	C-O	-6.74	1.15	1.24
1	C	34	GLY	C-O	6.74	1.31	1.23
1	C	122	ALA	CA-CB	-6.73	1.42	1.53
1	C	15	ASP	CG-OD1	6.70	1.38	1.25
1	A	47	ALA	N-CA	-6.63	1.38	1.46
1	B	85	VAL	CA-C	-6.63	1.44	1.52
1	A	105	LEU	CA-C	-6.62	1.44	1.52
1	C	94	ARG	CZ-NH1	6.62	1.42	1.32
1	B	122	ALA	N-CA	6.61	1.54	1.46
1	B	106	ALA	CA-C	-6.59	1.44	1.52
1	C	11	VAL	CA-C	-6.58	1.44	1.52
1	B	110	ILE	CA-CB	-6.58	1.46	1.54
1	C	78	ASP	CA-C	6.57	1.62	1.52
1	C	117	GLU	N-CA	-6.55	1.38	1.46
1	A	36	ARG	CG-CD	-6.54	1.32	1.52
1	C	123	ALA	N-CA	-6.50	1.38	1.46
1	B	11	VAL	CA-C	6.50	1.60	1.52
1	B	89	MET	CG-SD	6.48	1.97	1.80
1	B	90	TRP	C-O	6.47	1.32	1.24
1	C	2	GLY	N-CA	6.46	1.55	1.45
1	A	115	THR	CA-C	-6.45	1.44	1.52
1	B	75	LEU	CA-C	6.43	1.60	1.53
1	B	49	HIS	CA-CB	6.42	1.63	1.53
1	A	43	SER	N-CA	6.41	1.54	1.46
1	A	120	THR	CA-C	6.39	1.60	1.52
1	A	116	HIS	N-CA	6.39	1.53	1.46
1	A	119	ASP	CA-C	-6.38	1.44	1.52
1	B	62	LYS	CE-NZ	6.37	1.68	1.49
1	B	10	LEU	CA-C	-6.33	1.45	1.52
1	B	109	THR	CA-CB	-6.32	1.44	1.53
1	C	5	GLY	C-O	-6.29	1.17	1.24
1	B	13	ILE	CA-C	6.28	1.57	1.52
1	C	10	LEU	C-O	6.27	1.31	1.24
1	B	22	GLN	CD-NE2	6.26	1.46	1.33
1	C	95	VAL	C-O	-6.26	1.16	1.24
1	C	110	ILE	N-CA	-6.26	1.38	1.46
1	B	58	GLU	CA-CB	-6.23	1.43	1.53
1	C	36	ARG	NE-CZ	6.21	1.39	1.33
1	A	85	VAL	C-O	6.19	1.30	1.24
1	C	129	ALA	C-O	6.18	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	MET	CG-SD	6.17	1.96	1.80
1	C	52	ALA	N-CA	-6.16	1.38	1.46
1	C	119	ASP	N-CA	6.15	1.53	1.46
1	A	107	ASP	CB-CG	6.13	1.67	1.52
1	C	96	ARG	CG-CD	6.12	1.70	1.52
1	C	114	LEU	CA-C	-6.09	1.45	1.52
1	B	35	GLU	CA-CB	-6.09	1.44	1.53
1	B	26	VAL	CA-CB	6.07	1.63	1.54
1	B	117	GLU	N-CA	-6.07	1.39	1.46
1	C	14	PRO	C-N	-6.06	1.25	1.33
1	A	38	ASP	C-O	-6.05	1.16	1.24
1	C	65	SER	N-CA	-6.01	1.39	1.46
1	C	48	ARG	CZ-NH1	6.01	1.41	1.32
1	C	81	ARG	CZ-NH1	5.99	1.41	1.32
1	C	23	PRO	C-O	5.96	1.30	1.23
1	A	36	ARG	C-O	-5.94	1.16	1.24
1	C	106	ALA	CA-CB	5.94	1.63	1.53
1	A	41	ASP	C-O	-5.92	1.16	1.24
1	A	110	ILE	C-O	5.92	1.30	1.24
1	A	47	ALA	C-O	-5.92	1.17	1.24
1	C	49	HIS	N-CA	-5.91	1.38	1.46
1	C	62	LYS	CD-CE	-5.89	1.34	1.52
1	A	52	ALA	CA-CB	-5.88	1.44	1.53
1	B	53	ARG	NE-CZ	5.87	1.39	1.33
1	A	6	VAL	CA-CB	5.87	1.65	1.55
1	B	111	HIS	CA-C	5.86	1.59	1.52
1	C	33	PRO	CG-CD	5.86	1.70	1.50
1	C	56	ALA	CA-C	-5.86	1.44	1.52
1	B	82	ASP	CA-C	5.83	1.60	1.52
1	C	90	TRP	CB-CG	5.83	1.68	1.50
1	A	58	GLU	CA-C	5.82	1.60	1.52
1	C	40	SER	C-O	5.82	1.31	1.24
1	C	19	GLN	CB-CG	5.80	1.69	1.52
1	C	51	ALA	C-O	-5.80	1.17	1.24
1	C	100	ALA	C-O	-5.78	1.17	1.24
1	B	60	VAL	C-O	-5.75	1.17	1.24
1	A	42	LYS	CE-NZ	5.75	1.66	1.49
1	B	53	ARG	CZ-NH2	5.75	1.41	1.33
1	C	122	ALA	CA-C	-5.75	1.45	1.52
1	B	89	MET	C-O	5.74	1.31	1.24
1	C	126	ILE	N-CA	5.74	1.53	1.46
1	C	101	ILE	C-O	-5.73	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	48	ARG	CA-C	5.72	1.60	1.52
1	A	87	THR	CA-CB	-5.70	1.44	1.53
1	A	125	ALA	C-N	-5.70	1.25	1.33
1	A	49	HIS	CA-CB	5.69	1.62	1.53
1	A	109	THR	C-O	-5.69	1.17	1.24
1	B	49	HIS	C-O	-5.69	1.17	1.24
1	B	50	LEU	C-O	5.68	1.30	1.24
1	B	42	LYS	CD-CE	5.67	1.69	1.52
1	C	35	GLU	CD-OE2	-5.66	1.14	1.25
1	B	11	VAL	N-CA	-5.63	1.39	1.46
1	A	8	ILE	CA-CB	-5.62	1.47	1.54
1	C	130	PRO	CB-CG	5.61	1.77	1.49
1	C	46	ALA	CA-CB	5.61	1.62	1.53
1	B	8	ILE	N-CA	-5.61	1.39	1.46
1	B	73	PRO	CB-CG	5.61	1.77	1.49
1	A	10	LEU	CG-CD2	5.59	1.71	1.52
1	A	8	ILE	CA-C	-5.58	1.45	1.52
1	A	4	VAL	C-O	-5.58	1.17	1.24
1	A	70	ALA	CA-CB	-5.58	1.46	1.52
1	B	60	VAL	CB-CG2	5.57	1.71	1.52
1	B	106	ALA	CA-CB	5.57	1.62	1.53
1	C	64	TRP	CG-CD1	-5.57	1.23	1.36
1	C	48	ARG	N-CA	-5.56	1.39	1.46
1	B	9	ASP	CG-OD2	-5.56	1.14	1.25
1	B	88	ASP	C-O	5.54	1.30	1.24
1	A	10	LEU	CA-C	-5.54	1.46	1.52
1	C	53	ARG	CZ-NH1	5.51	1.40	1.32
1	C	41	ASP	CA-C	5.48	1.60	1.52
1	C	93	PRO	CB-CG	-5.48	1.22	1.49
1	B	79	ILE	C-O	-5.46	1.17	1.24
1	B	37	ARG	CG-CD	5.45	1.68	1.52
1	C	17	ALA	N-CA	-5.44	1.38	1.46
1	B	116	HIS	N-CA	5.43	1.53	1.46
1	C	89	MET	CA-CB	5.43	1.62	1.53
1	B	116	HIS	CA-C	5.42	1.60	1.52
1	A	123	ALA	CA-CB	5.39	1.62	1.53
1	B	86	VAL	C-O	-5.39	1.17	1.24
1	C	106	ALA	CA-C	-5.39	1.45	1.52
1	A	31	PHE	CA-CB	-5.39	1.44	1.53
1	A	63	ALA	CA-CB	5.38	1.61	1.53
1	B	16	PHE	CB-CG	5.38	1.63	1.50
1	B	125	ALA	C-O	-5.38	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	VAL	C-O	5.38	1.29	1.23
1	B	123	ALA	CA-CB	-5.38	1.44	1.53
1	C	116	HIS	N-CA	5.38	1.52	1.46
1	B	90	TRP	CB-CG	5.37	1.66	1.50
1	A	48	ARG	NE-CZ	-5.34	1.27	1.33
1	A	55	ALA	CA-C	5.34	1.59	1.52
1	B	7	GLY	CA-C	5.33	1.57	1.51
1	B	81	ARG	NE-CZ	5.32	1.39	1.33
1	B	34	GLY	CA-C	-5.32	1.44	1.51
1	C	12	SER	C-N	-5.31	1.26	1.34
1	A	21	ASP	CB-CG	5.30	1.65	1.52
1	B	123	ALA	C-N	-5.28	1.27	1.33
1	A	49	HIS	C-O	-5.28	1.17	1.24
1	A	109	THR	CA-CB	-5.27	1.45	1.53
1	A	114	LEU	CB-CG	-5.27	1.43	1.53
1	B	46	ALA	C-O	5.25	1.30	1.24
1	C	48	ARG	C-N	-5.25	1.27	1.34
1	B	48	ARG	N-CA	-5.24	1.40	1.46
1	B	19	GLN	C-O	-5.24	1.17	1.24
1	B	101	ILE	CA-CB	-5.23	1.47	1.54
1	C	42	LYS	C-O	5.23	1.30	1.24
1	B	53	ARG	CZ-NH1	5.22	1.40	1.32
1	C	126	ILE	CA-C	-5.21	1.46	1.52
1	A	36	ARG	CA-C	-5.21	1.45	1.52
1	C	120	THR	CB-OG1	-5.21	1.35	1.43
1	C	109	THR	CA-CB	-5.21	1.46	1.53
1	C	27	PHE	CA-C	5.20	1.59	1.52
1	A	41	ASP	CA-C	-5.19	1.46	1.52
1	B	27	PHE	C-O	-5.18	1.17	1.24
1	B	19	GLN	CB-CG	-5.18	1.36	1.52
1	B	89	MET	CA-CB	5.17	1.62	1.53
1	A	89	MET	CG-SD	5.17	1.93	1.80
1	C	113	SER	CB-OG	5.17	1.52	1.42
1	C	19	GLN	CD-NE2	5.16	1.44	1.33
1	B	18	GLU	CD-OE2	5.16	1.35	1.25
1	A	56	ALA	C-O	-5.14	1.18	1.24
1	A	62	LYS	CE-NZ	-5.14	1.33	1.49
1	B	15	ASP	C-O	-5.12	1.17	1.24
1	B	32	THR	CA-C	-5.12	1.47	1.53
1	C	82	ASP	C-O	-5.12	1.17	1.24
1	B	13	ILE	CA-CB	5.11	1.57	1.53
1	B	55	ALA	CA-CB	5.11	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ARG	CA-C	5.11	1.59	1.53
1	B	117	GLU	CA-CB	-5.10	1.44	1.53
1	C	32	THR	CA-C	-5.09	1.46	1.52
1	B	83	ILE	C-O	-5.08	1.18	1.24
1	B	105	LEU	CA-CB	-5.07	1.46	1.52
1	A	35	GLU	C-O	5.07	1.29	1.24
1	C	103	GLU	N-CA	5.07	1.52	1.46
1	C	121	ALA	N-CA	-5.04	1.39	1.45
1	C	80	HIS	C-O	-5.04	1.17	1.24
1	C	11	VAL	CA-CB	5.03	1.61	1.54
1	C	97	LEU	N-CA	5.03	1.52	1.46
1	B	54	TRP	CB-CG	5.02	1.65	1.50
1	A	53	ARG	CG-CD	5.02	1.67	1.52
1	A	52	ALA	C-O	5.01	1.29	1.24
1	C	124	VAL	CA-CB	5.01	1.63	1.55
1	B	52	ALA	C-N	-5.01	1.27	1.34
1	A	19	GLN	CG-CD	5.01	1.64	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASP	N-CA-C	-10.71	98.33	111.40
1	C	32	THR	N-CA-C	-9.45	98.11	110.39
1	B	61	ILE	N-CA-C	-8.65	102.40	110.53
1	B	96	ARG	CA-C-N	-8.34	111.48	123.00
1	B	96	ARG	C-N-CA	-8.34	111.48	123.00
1	A	78	ASP	N-CA-C	-8.20	93.75	109.24
1	B	73	PRO	CA-C-N	8.06	136.47	121.97
1	B	73	PRO	C-N-CA	8.06	136.47	121.97
1	B	30	THR	OG1-CB-CG2	-7.50	94.31	109.30
1	A	48	ARG	CG-CD-NE	-7.35	95.84	112.00
1	B	48	ARG	CA-C-O	7.34	128.21	120.42
1	C	114	LEU	N-CA-C	7.05	120.99	109.85
1	A	62	LYS	O-C-N	-6.80	115.01	122.09
1	A	30	THR	OG1-CB-CG2	-6.66	95.99	109.30
1	C	60	VAL	CB-CA-C	-6.64	103.06	112.22
1	A	37	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	C	48	ARG	N-CA-C	6.59	124.84	110.80
1	A	58	GLU	N-CA-C	6.58	118.45	111.28
1	C	54	TRP	O-C-N	-6.51	115.06	122.09
1	C	61	ILE	CA-CB-CG1	6.50	121.45	110.40
1	B	25	THR	N-CA-C	6.47	119.28	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	GLY	CA-C-N	6.45	130.49	120.75
1	C	24	GLY	C-N-CA	6.45	130.49	120.75
1	B	79	ILE	CB-CA-C	-6.35	102.77	112.05
1	A	22	GLN	CA-C-N	6.30	127.72	119.84
1	A	22	GLN	C-N-CA	6.30	127.72	119.84
1	C	61	ILE	N-CA-CB	6.27	117.89	110.55
1	B	77	GLU	N-CA-C	-6.10	103.84	111.90
1	B	112	VAL	CA-CB-CG1	-6.05	100.11	110.40
1	A	110	ILE	CA-C-O	6.04	127.00	120.53
1	C	90	TRP	N-CA-C	-5.99	106.32	113.21
1	B	6	VAL	CA-C-N	5.98	127.14	121.46
1	B	6	VAL	C-N-CA	5.98	127.14	121.46
1	C	63	ALA	N-CA-C	-5.97	104.85	111.36
1	C	118	GLY	N-CA-C	-5.97	99.04	113.18
1	C	15	ASP	N-CA-C	5.90	119.58	112.38
1	B	72	ARG	CB-CA-C	5.90	121.79	110.17
1	C	97	LEU	N-CA-C	5.87	119.39	109.76
1	C	16	PHE	N-CA-C	-5.85	104.32	112.45
1	A	79	ILE	N-CA-C	-5.84	107.59	113.20
1	B	68	ARG	N-CA-C	5.84	117.64	111.28
1	B	41	ASP	CA-C-N	5.83	132.67	121.54
1	B	41	ASP	C-N-CA	5.83	132.67	121.54
1	A	3	ILE	CA-CB-CG1	5.82	120.29	110.40
1	B	62	LYS	CD-CE-NZ	5.80	130.47	111.90
1	B	31	PHE	CA-C-N	5.74	128.64	120.49
1	B	31	PHE	C-N-CA	5.74	128.64	120.49
1	A	119	ASP	CA-C-O	5.74	126.25	119.48
1	B	40	SER	N-CA-C	5.73	118.47	111.82
1	C	101	ILE	CB-CA-C	-5.71	104.43	112.14
1	A	22	GLN	O-C-N	5.71	127.89	121.32
1	A	2	GLY	N-CA-C	-5.64	96.95	113.30
1	B	68	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	C	88	ASP	CA-C-N	5.62	132.28	121.54
1	C	88	ASP	C-N-CA	5.62	132.28	121.54
1	C	50	LEU	CA-CB-CG	5.62	135.96	116.30
1	B	47	ALA	N-CA-C	5.61	117.40	111.28
1	A	83	ILE	N-CA-C	-5.58	100.39	108.36
1	A	31	PHE	N-CA-C	5.51	118.71	109.95
1	A	37	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	A	4	VAL	CB-CA-C	-5.50	103.35	112.26
1	B	59	ALA	N-CA-C	-5.49	104.94	111.69
1	B	87	THR	OG1-CB-CG2	-5.49	98.32	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ALA	N-CA-C	5.49	117.70	111.11
1	B	112	VAL	CG1-CB-CG2	-5.49	98.73	110.80
1	C	70	ALA	O-C-N	5.48	128.83	122.25
1	C	50	LEU	N-CA-C	-5.46	106.75	113.41
1	B	73	PRO	O-C-N	5.44	129.98	122.64
1	C	92	ARG	CA-C-N	5.41	125.35	119.78
1	C	92	ARG	C-N-CA	5.41	125.35	119.78
1	C	56	ALA	N-CA-C	5.40	120.27	111.37
1	C	88	ASP	O-C-N	5.37	131.03	122.81
1	C	61	ILE	CB-CA-C	-5.36	105.12	111.97
1	C	110	ILE	O-C-N	-5.33	117.58	123.18
1	C	105	LEU	N-CA-C	-5.33	106.65	112.72
1	B	89	MET	N-CA-C	-5.32	99.47	110.80
1	C	83	ILE	CA-C-N	-5.30	115.25	122.93
1	C	83	ILE	C-N-CA	-5.30	115.25	122.93
1	B	39	ALA	N-CA-C	-5.30	106.79	113.20
1	B	73	PRO	CB-CA-C	5.26	120.24	111.56
1	B	123	ALA	N-CA-C	5.25	116.26	108.60
1	C	88	ASP	CB-CA-C	-5.23	104.61	112.09
1	B	11	VAL	CA-C-O	5.23	126.81	121.63
1	B	92	ARG	CB-CA-C	5.21	116.92	109.26
1	C	101	ILE	N-CA-C	-5.20	105.31	110.62
1	A	109	THR	N-CA-CB	-5.17	101.62	110.16
1	A	70	ALA	CA-C-O	-5.17	115.54	120.92
1	C	64	TRP	N-CA-C	-5.13	105.14	111.40
1	A	64	TRP	N-CA-C	5.12	116.55	111.07
1	B	10	LEU	CD1-CG-CD2	-5.12	99.54	110.80
1	C	7	GLY	O-C-N	5.08	129.30	122.70
1	C	79	ILE	CA-C-O	5.03	127.07	120.78
1	C	13	ILE	CB-CA-C	-5.01	109.03	114.35
1	C	70	ALA	CA-C-N	5.01	131.11	121.54
1	C	70	ALA	C-N-CA	5.01	131.11	121.54
1	B	85	VAL	N-CA-C	5.01	115.30	107.99
1	A	74	VAL	CB-CA-C	-5.00	103.08	111.29

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	71	GLN	Peptide
1	B	72	ARG	Peptide
1	C	71	GLN	Peptide

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	970	0	918	46	0
1	B	970	0	918	44	1
1	C	970	0	918	38	0
2	A	5	0	0	1	0
2	B	10	0	0	0	0
2	C	5	0	0	3	0
3	A	19	0	0	0	0
3	B	25	0	0	3	1
3	C	12	0	0	2	0
All	All	2986	0	2754	122	2

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 21.

All (122) 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:A:96:ARG:CD	1:A:96:ARG:CG	1.75	1.61
1:C:26:VAL:CG1	1:C:26:VAL:CB	1.80	1.56
1:B:73:PRO:CB	1:B:73:PRO:CG	1.77	1.53
1:B:62:LYS:CE	1:B:62:LYS:NZ	1.68	1.53
1:C:130:PRO:CB	1:C:130:PRO:CG	1.77	1.52
1:A:89:MET:SD	1:A:89:MET:CE	2.07	1.43
1:C:89:MET:CE	1:C:89:MET:SD	2.11	1.37
1:B:89:MET:CE	1:B:89:MET:SD	2.22	1.26
1:A:101:ILE:HG22	1:A:105:LEU:HD23	1.67	0.76
1:B:32:THR:HG21	3:B:138:HOH:O	1.86	0.75
1:A:104:TYR:C	1:A:106:ALA:H	1.95	0.73
1:A:57:LYS:HD3	1:A:80:HIS:O	1.88	0.72
1:A:64:TRP:O	1:A:70:ALA:HB2	1.91	0.70
1:C:32:THR:HG21	3:C:144:HOH:O	1.90	0.70
1:A:15:ASP:O	1:A:19:GLN:HG2	1.91	0.69
1:A:71:GLN:O	1:A:74:VAL:HG13	1.93	0.69
1:C:32:THR:HG22	1:C:35:GLU:H	1.57	0.68
1:C:107:ASP:O	1:C:130:PRO:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ILE:HB	1:C:14:PRO:HD3	1.75	0.68
1:A:56:ALA:HB2	1:A:114:LEU:HD21	1.77	0.66
1:A:108:VAL:HB	1:A:128:GLU:O	1.95	0.66
1:C:70:ALA:O	1:C:71:GLN:HG3	1.94	0.66
1:B:71:GLN:O	1:B:72:ARG:C	2.39	0.66
1:B:81:ARG:NH2	3:B:163:HOH:O	2.29	0.65
1:A:103:GLU:O	1:A:106:ALA:HB2	1.97	0.65
1:C:70:ALA:C	1:C:71:GLN:HG3	2.22	0.64
1:B:45:SER:HA	1:B:48:ARG:NH1	2.12	0.64
1:B:44:SER:O	1:B:46:ALA:N	2.32	0.63
1:C:22:GLN:HE21	1:C:22:GLN:N	1.97	0.63
1:C:84:GLU:HB2	1:C:96:ARG:HB3	1.80	0.63
1:C:79:ILE:O	1:C:80:HIS:HB2	2.00	0.61
1:B:105:LEU:HB3	1:B:108:VAL:HG22	1.82	0.61
1:A:32:THR:HG22	1:A:34:GLY:H	1.66	0.61
1:C:79:ILE:HG23	1:C:80:HIS:ND1	2.17	0.60
1:B:32:THR:HG22	1:B:34:GLY:H	1.68	0.59
1:B:30:THR:HB	1:B:57:LYS:HZ2	1.69	0.58
1:A:104:TYR:C	1:A:106:ALA:N	2.62	0.57
1:A:96:ARG:CD	1:A:96:ARG:CB	2.77	0.57
1:B:2:GLY:O	1:B:3:ILE:C	2.49	0.56
1:B:15:ASP:O	1:B:19:GLN:HG2	2.04	0.56
1:C:26:VAL:CG1	1:C:26:VAL:CA	2.78	0.55
1:A:101:ILE:CG2	1:A:105:LEU:HD23	2.36	0.55
1:B:35:GLU:HB3	1:B:50:LEU:HD11	1.89	0.55
1:B:92:ARG:NH1	1:C:67:SER:O	2.40	0.54
1:C:102:ALA:O	1:C:106:ALA:HA	2.07	0.54
1:A:70:ALA:HB1	1:A:74:VAL:HG11	1.89	0.54
1:C:27:PHE:HE1	1:C:54:TRP:CE2	2.26	0.53
1:B:62:LYS:NZ	3:B:147:HOH:O	2.41	0.53
1:B:72:ARG:HD3	1:B:74:VAL:HG12	1.91	0.53
1:A:32:THR:HG22	1:A:35:GLU:H	1.74	0.52
1:A:56:ALA:HB2	1:A:114:LEU:CD2	2.40	0.52
1:C:101:ILE:HG22	1:C:105:LEU:HD12	1.92	0.52
1:A:20:VAL:HA	1:A:27:PHE:CD2	2.45	0.52
1:B:111:HIS:O	1:B:125:ALA:HA	2.09	0.52
1:B:6:VAL:O	1:B:6:VAL:HG13	2.09	0.51
1:A:28:ALA:HA	1:A:36:ARG:NH1	2.27	0.50
1:A:96:ARG:CG	1:A:96:ARG:NE	2.64	0.50
1:B:37:ARG:HD3	1:B:37:ARG:O	2.12	0.50
1:C:49:HIS:HE1	2:C:131:SO4:S	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:O	1:A:85:VAL:HG11	2.12	0.50
1:A:26:VAL:O	1:A:30:THR:HG22	2.11	0.49
1:A:72:ARG:HG3	1:C:90:TRP:CZ3	2.47	0.49
1:B:2:GLY:O	1:B:3:ILE:O	2.31	0.49
1:B:117:GLU:CD	1:B:117:GLU:O	2.55	0.49
1:B:13:ILE:N	1:B:14:PRO:CD	2.76	0.49
1:B:92:ARG:HH22	1:C:72:ARG:NH1	2.10	0.49
1:A:89:MET:HE2	1:A:90:TRP:CZ2	2.47	0.48
1:C:49:HIS:CE1	2:C:131:SO4:O1	2.67	0.48
1:B:76:PRO:HB2	1:B:78:ASP:HB2	1.96	0.48
1:C:22:GLN:N	1:C:22:GLN:NE2	2.60	0.48
1:A:52:ALA:O	1:A:114:LEU:HD22	2.14	0.48
1:B:92:ARG:HH22	1:C:72:ARG:HH12	1.61	0.48
1:A:14:PRO:CG	1:A:119:ASP:HB3	2.44	0.47
1:A:72:ARG:N	1:A:73:PRO:CD	2.77	0.47
1:A:13:ILE:N	1:A:14:PRO:CD	2.77	0.47
1:C:77:GLU:O	1:C:78:ASP:HB2	2.14	0.47
1:A:14:PRO:CD	1:A:119:ASP:HB3	2.44	0.47
1:C:2:GLY:O	1:C:3:ILE:C	2.53	0.47
1:B:45:SER:CA	1:B:48:ARG:NH1	2.78	0.46
1:A:113:SER:HB3	1:B:8:ILE:HG22	1.98	0.46
1:A:86:VAL:HG22	1:A:87:THR:N	2.30	0.46
1:B:72:ARG:C	1:B:74:VAL:N	2.73	0.46
1:A:105:LEU:HD12	1:A:108:VAL:HG21	1.98	0.46
1:B:6:VAL:O	1:B:6:VAL:CG1	2.63	0.45
1:B:68:ARG:HG3	1:B:69:PHE:N	2.29	0.45
1:B:30:THR:CB	1:B:57:LYS:HZ2	2.28	0.45
1:A:81:ARG:NH1	1:A:84:GLU:HG3	2.32	0.45
1:B:76:PRO:C	1:B:78:ASP:H	2.24	0.45
1:B:54:TRP:O	1:B:58:GLU:HG2	2.17	0.44
1:C:79:ILE:O	1:C:81:ARG:N	2.44	0.44
1:C:49:HIS:HE1	2:C:131:SO4:O1	2.00	0.44
1:A:68:ARG:C	1:A:70:ALA:N	2.73	0.44
1:B:30:THR:HG21	1:B:54:TRP:HZ3	1.82	0.44
1:A:32:THR:HG22	1:A:34:GLY:N	2.30	0.44
1:C:45:SER:O	1:C:46:ALA:C	2.59	0.44
1:A:14:PRO:HD3	1:A:119:ASP:HB3	2.00	0.43
1:C:95:VAL:HG12	1:C:96:ARG:N	2.33	0.43
1:B:117:GLU:HG3	1:C:12:SER:N	2.34	0.43
1:C:61:ILE:O	1:C:65:SER:HB2	2.18	0.43
1:B:103:GLU:O	1:B:106:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PRO:CB	1:B:104:TYR:OH	2.67	0.43
1:B:73:PRO:O	1:B:76:PRO:HD3	2.19	0.42
1:B:45:SER:O	1:B:49:HIS:ND1	2.53	0.42
1:C:56:ALA:HB3	1:C:85:VAL:HG21	2.02	0.42
1:A:62:LYS:O	1:A:63:ALA:C	2.58	0.42
1:A:14:PRO:HB3	1:A:42:LYS:HE2	2.02	0.42
1:A:30:THR:OG1	1:A:57:LYS:HE3	2.20	0.42
1:A:75:LEU:O	1:A:76:PRO:O	2.38	0.42
1:A:82:ASP:N	1:A:82:ASP:OD1	2.53	0.42
1:A:48:ARG:NH1	2:A:131:SO4:O1	2.48	0.42
1:B:117:GLU:CD	1:B:117:GLU:C	2.87	0.41
1:C:26:VAL:HG12	3:C:136:HOH:O	2.21	0.41
1:B:57:LYS:NZ	1:B:80:HIS:O	2.43	0.41
1:C:129:ALA:O	1:C:130:PRO:C	2.62	0.41
1:A:21:ASP:O	1:A:22:GLN:CG	2.69	0.41
1:C:64:TRP:HD1	1:C:105:LEU:HD21	1.85	0.41
1:C:105:LEU:HD23	1:C:105:LEU:HA	1.93	0.41
1:A:63:ALA:HB1	1:A:127:LEU:HD13	2.03	0.40
1:A:68:ARG:C	1:A:70:ALA:H	2.30	0.40
1:B:107:ASP:O	1:B:130:PRO:HD3	2.21	0.40
1:B:71:GLN:O	1:B:71:GLN:HG3	2.20	0.40
1:C:54:TRP:O	1:C:55:ALA:C	2.60	0.40

All (2) 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)
3:B:139:HOH:O	3:B:139:HOH:O[2_565]	2.08	0.12
1:B:22:GLN:NE2	1:B:22:GLN:NE2[2_565]	2.14	0.06

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	C	30/130 (23%)	25 (83%)	5 (17%)	0	100	100

There are no Ramachandran outliers to report.

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	91/101 (90%)	74 (81%)	17 (19%)	1	3
1	B	91/101 (90%)	73 (80%)	18 (20%)	1	2
1	C	91/101 (90%)	76 (84%)	15 (16%)	2	4
All	All	273/303 (90%)	223 (82%)	50 (18%)	2	3

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	19	GLN
1	A	23	PRO
1	A	32	THR
1	A	33	PRO
1	A	42	LYS
1	A	68	ARG
1	A	72	ARG
1	A	75	LEU
1	A	78	ASP
1	A	85	VAL
1	A	94	ARG
1	A	95	VAL
1	A	105	LEU
1	A	108	VAL
1	A	117	GLU
1	A	120	THR
1	B	22	GLN
1	B	30	THR

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Mol	Chain	Res	Type
1	B	68	ARG
1	B	69	PHE
1	B	73	PRO
1	B	74	VAL
1	B	75	LEU
1	B	78	ASP
1	B	87	THR
1	B	89	MET
1	B	90	TRP
1	B	92	ARG
1	B	97	LEU
1	B	108	VAL
1	B	112	VAL
1	B	114	LEU
1	B	117	GLU
1	B	120	THR
1	C	6	VAL
1	C	14	PRO
1	C	19	GLN
1	C	22	GLN
1	C	32	THR
1	C	50	LEU
1	C	65	SER
1	C	71	GLN
1	C	77	GLU
1	C	86	VAL
1	C	88	ASP
1	C	94	ARG
1	C	97	LEU
1	C	119	ASP
1	C	128	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	80	HIS
1	B	71	GLN
1	B	80	HIS
1	B	111	HIS
1	C	22	GLN
1	C	49	HIS

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Mol	Chain	Res	Type
1	C	111	HIS

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 oligosaccharides 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	SO4	A	131	-	4,4,4	0.37	0	6,6,6	1.22	1 (16%)
2	SO4	C	131	-	4,4,4	0.23	0	6,6,6	1.71	2 (33%)
2	SO4	B	131	-	4,4,4	0.63	0	6,6,6	2.48	2 (33%)
2	SO4	B	132	-	4,4,4	0.53	0	6,6,6	1.10	1 (16%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	SO4	O3-S-O1	-4.24	87.37	109.56
2	B	131	SO4	O4-S-O3	3.22	126.32	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	131	SO4	O3-S-O2	2.34	121.80	109.56
2	C	131	SO4	O4-S-O3	2.33	121.39	108.54
2	B	132	SO4	O3-S-O2	-2.23	97.91	109.56
2	C	131	SO4	O3-S-O1	-2.01	99.07	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	131	SO4	1	0
2	C	131	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	129/130 (99%)	0.20	6 (4%)	36 32	43, 73, 137, 154	0
1	B	129/130 (99%)	0.21	7 (5%)	31 27	41, 69, 131, 153	0
1	C	129/130 (99%)	0.30	4 (3%)	51 47	38, 71, 117, 143	0
All	All	387/390 (99%)	0.24	17 (4%)	39 34	38, 71, 131, 154	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	VAL	4.0
1	A	23	PRO	3.6
1	C	73	PRO	3.6
1	A	90	TRP	3.2
1	A	75	LEU	3.2
1	A	73	PRO	2.9
1	B	73	PRO	2.8
1	B	69	PHE	2.7
1	A	76	PRO	2.6
1	B	89	MET	2.6
1	B	75	LEU	2.6
1	B	90	TRP	2.6
1	C	69	PHE	2.5
1	C	79	ILE	2.2
1	C	89	MET	2.1
1	A	79	ILE	2.1
1	B	76	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	131	5/5	0.85	0.10	98,103,109,113	0
2	SO4	B	131	5/5	0.93	0.06	78,79,81,83	0
2	SO4	B	132	5/5	0.94	0.09	99,102,103,105	0
2	SO4	A	131	5/5	0.97	0.06	67,77,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.