



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:10 AM UTC

PDB ID : 4A6G / pdb_00004a6g
Title : N-acyl amino acid racemase from *Amycalotopsis* sp. Ts-1-60: G291D- F323Y mutant in complex with N-acetyl methionine
Authors : Baxter, S.; Royer, S.; Grogan, G.; Holt-Tiffin, K.E.; Taylor, I.N.; Fotheringham, I.G.; Campopiano, D.J.
Deposited on : 2011-11-02
Resolution : 2.71 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

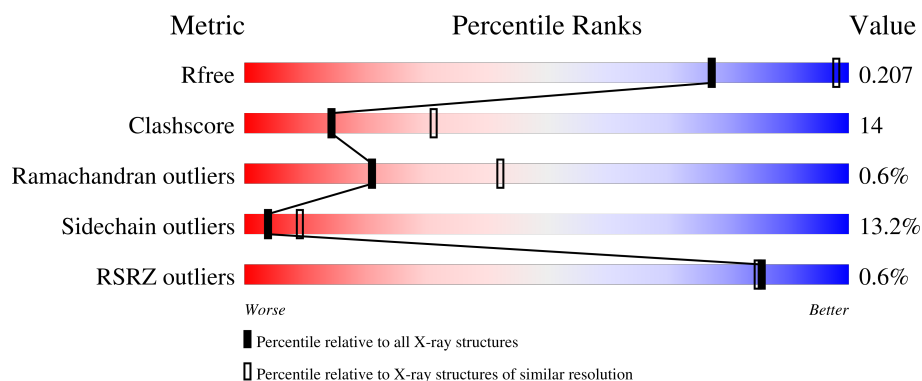
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	368	 72% 22% 6% •
1	B	368	 70% 25% 5% •
1	C	368	 68% 24% 6% •
1	D	368	 68% 26% 5% •

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	AME	A	1369	-	X	X	-
2	AME	B	1368	-	X	X	-
2	AME	C	1368	-	X	X	-
2	AME	D	1368	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11214 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.

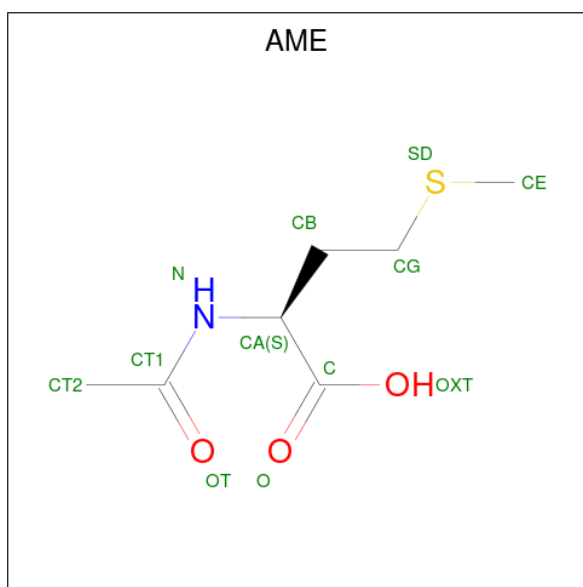
- Molecule 1 is a protein called N-ACYLAMINO ACID RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2745	1747	477	510	11			
1	B	367	Total	C	N	O	S	0	0	0
			2719	1736	472	500	11			
1	C	367	Total	C	N	O	S	0	0	0
			2712	1730	470	501	11			
1	D	367	Total	C	N	O	S	0	0	0
			2721	1736	475	499	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ASP	GLY	engineered mutation	UNP Q44244
A	323	TYR	PHE	engineered mutation	UNP Q44244
B	291	ASP	GLY	engineered mutation	UNP Q44244
B	323	TYR	PHE	engineered mutation	UNP Q44244
C	291	ASP	GLY	engineered mutation	UNP Q44244
C	323	TYR	PHE	engineered mutation	UNP Q44244
D	291	ASP	GLY	engineered mutation	UNP Q44244
D	323	TYR	PHE	engineered mutation	UNP Q44244

- Molecule 2 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	7	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			12	7	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			12	7	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			12	7	1	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		

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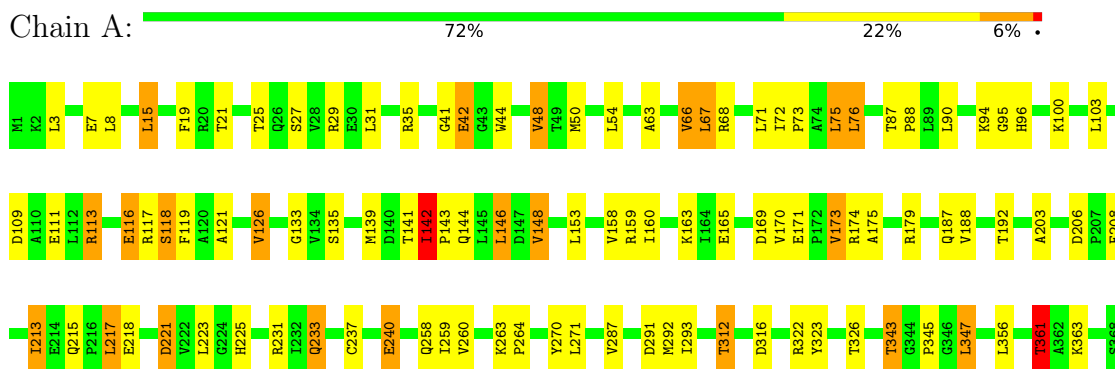
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	69	Total 69	O 69	0	0
4	C	48	Total 48	O 48	0	0
4	D	54	Total 54	O 54	0	0

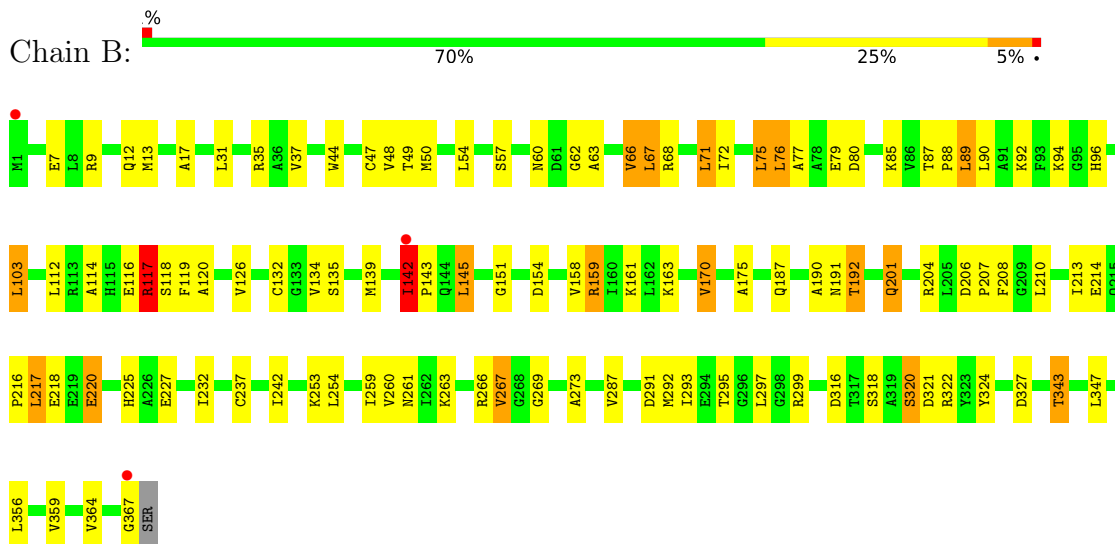
3 Residue-property plots

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.

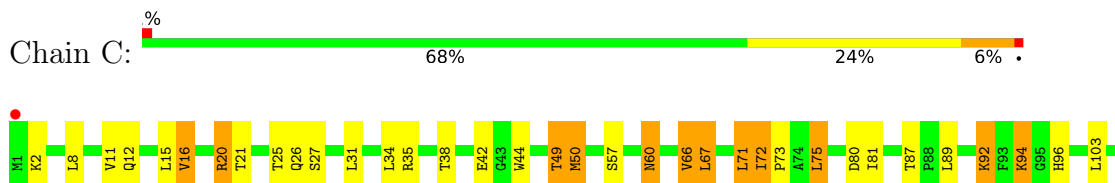
• Molecule 1: N-ACYLAMINO ACID RACEMASE

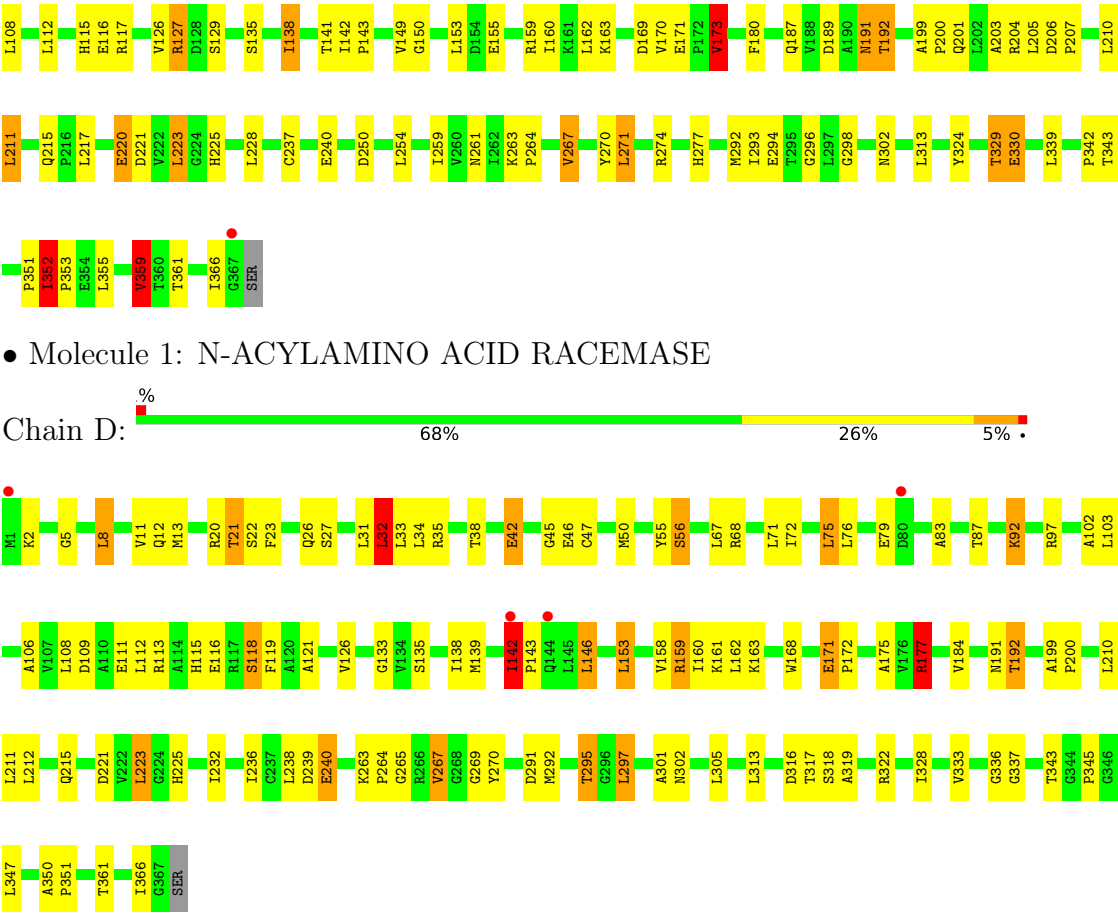


• Molecule 1: N-ACYLAMINO ACID RACEMASE



• Molecule 1: N-ACYLAMINO ACID RACEMASE





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	216.71Å 216.71Å 261.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.31 – 2.71 88.31 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.31-2.71) 100.0 (88.31-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.155 , 0.210 0.153 , 0.207	Depositor DCC
R_{free} test set	3768 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.021 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.016 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AME, MG

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	1.26	6/2801 (0.2%)	1.31	17/3821 (0.4%)
1	B	1.20	3/2775 (0.1%)	1.31	18/3786 (0.5%)
1	C	1.16	4/2768 (0.1%)	1.33	30/3778 (0.8%)
1	D	1.19	5/2777 (0.2%)	1.33	17/3790 (0.4%)
All	All	1.20	18/11121 (0.2%)	1.32	82/15175 (0.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	171	GLU	N-CA	7.33	1.51	1.46
1	C	142	ILE	CA-CB	7.00	1.58	1.54
1	A	173	VAL	CA-CB	6.27	1.62	1.54
1	B	273	ALA	CA-CB	-6.17	1.43	1.53
1	A	326	THR	CA-CB	6.16	1.61	1.52
1	D	72	ILE	CA-CB	5.67	1.56	1.54
1	A	41	GLY	N-CA	5.49	1.50	1.45
1	A	171	GLU	CA-C	5.40	1.58	1.52
1	C	173	VAL	CA-CB	5.36	1.61	1.54
1	C	87	THR	N-CA	-5.35	1.42	1.46
1	B	57	SER	CA-C	5.35	1.60	1.52
1	A	218	GLU	CA-C	5.33	1.59	1.52
1	C	66	VAL	CA-CB	5.30	1.60	1.54
1	D	142	ILE	CA-C	5.26	1.58	1.52
1	B	192	THR	CA-CB	5.17	1.62	1.53
1	A	192	THR	CA-CB	5.12	1.61	1.53
1	D	221	ASP	CA-C	5.08	1.59	1.53
1	D	32	LEU	CA-C	5.06	1.58	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	THR	CA-C-N	-10.30	108.27	119.19
1	D	38	THR	C-N-CA	-10.30	108.27	119.19
1	B	206	ASP	CA-C-N	-9.53	109.96	119.87
1	B	206	ASP	C-N-CA	-9.53	109.96	119.87
1	D	269	GLY	N-CA-C	9.51	123.26	111.85
1	D	87	THR	CA-C-N	-9.13	110.34	119.56
1	D	87	THR	C-N-CA	-9.13	110.34	119.56
1	C	66	VAL	N-CA-CB	8.37	120.34	110.55
1	C	351	PRO	CA-C-N	-8.33	116.59	122.59
1	C	351	PRO	C-N-CA	-8.33	116.59	122.59
1	B	208	PHE	N-CA-C	7.55	122.21	112.92
1	D	68	ARG	N-CA-C	7.35	122.08	113.18
1	C	87	THR	CA-C-N	-6.97	111.61	119.28
1	C	87	THR	C-N-CA	-6.97	111.61	119.28
1	A	118	SER	CB-CA-C	-6.96	98.17	109.72
1	C	192	THR	N-CA-CB	-6.94	107.16	114.10
1	C	221	ASP	N-CA-C	6.92	119.36	110.65
1	A	208	PHE	N-CA-C	6.90	121.36	113.15
1	B	17	ALA	CA-C-N	-6.89	113.56	120.31
1	B	17	ALA	C-N-CA	-6.89	113.56	120.31
1	C	126	VAL	CB-CA-C	-6.76	103.49	110.93
1	C	359	VAL	CB-CA-C	6.76	117.92	110.62
1	A	221	ASP	N-CA-C	6.50	119.36	109.62
1	C	72	ILE	CA-C-N	-6.47	111.95	119.32
1	C	72	ILE	C-N-CA	-6.47	111.95	119.32
1	C	339	LEU	CA-C-N	-6.45	111.54	120.25
1	C	339	LEU	C-N-CA	-6.45	111.54	120.25
1	C	2	LYS	N-CA-C	-6.44	99.14	109.96
1	A	343	THR	CA-C-N	-6.43	111.78	121.87
1	A	343	THR	C-N-CA	-6.43	111.78	121.87
1	C	66	VAL	CB-CA-C	-6.39	103.79	111.97
1	B	77	ALA	N-CA-C	6.34	120.74	113.19
1	C	38	THR	CA-C-N	-6.33	113.10	119.56
1	C	38	THR	C-N-CA	-6.33	113.10	119.56
1	B	142	ILE	CA-C-N	-6.31	113.27	119.64
1	B	142	ILE	C-N-CA	-6.31	113.27	119.64
1	C	80	ASP	N-CA-C	-6.28	100.40	110.14
1	D	333	VAL	N-CA-C	6.21	116.81	107.75
1	B	118	SER	N-CA-CB	-6.20	99.83	109.69
1	D	133	GLY	N-CA-C	-6.12	102.90	112.58
1	D	350	ALA	CA-C-N	-6.09	113.69	120.14
1	D	350	ALA	C-N-CA	-6.09	113.69	120.14
1	C	330	GLU	CA-C-N	-6.07	114.02	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	GLU	C-N-CA	-6.07	114.02	120.03
1	B	343	THR	CA-C-N	-6.02	112.41	121.87
1	B	343	THR	C-N-CA	-6.02	112.41	121.87
1	B	66	VAL	N-CA-CB	6.00	119.58	110.58
1	D	2	LYS	N-CA-C	-5.89	100.69	110.17
1	C	267	VAL	N-CA-C	-5.87	107.27	112.90
1	D	171	GLU	N-CA-CB	5.86	115.96	110.39
1	D	301	ALA	N-CA-C	-5.82	104.30	111.40
1	A	165	GLU	N-CA-C	-5.81	102.90	108.13
1	C	191	ASN	CA-C-N	-5.76	117.81	126.86
1	C	191	ASN	C-N-CA	-5.76	117.81	126.86
1	A	148	VAL	N-CA-C	5.73	116.19	110.23
1	D	26	GLN	N-CA-C	-5.70	99.61	108.90
1	A	263	LYS	CA-C-N	5.51	124.97	119.24
1	A	263	LYS	C-N-CA	5.51	124.97	119.24
1	A	113	ARG	CG-CD-NE	-5.51	99.88	112.00
1	B	117	ARG	CA-C-N	5.50	128.66	120.90
1	B	117	ARG	C-N-CA	5.50	128.66	120.90
1	C	267	VAL	N-CA-CB	-5.50	105.17	112.26
1	A	66	VAL	CB-CA-C	-5.49	103.65	112.16
1	D	236	ILE	CB-CA-C	-5.42	104.11	111.15
1	A	142	ILE	N-CA-CB	5.40	113.90	110.50
1	A	361	THR	N-CA-CB	-5.39	102.60	110.47
1	C	324	TYR	N-CA-C	5.36	117.63	108.90
1	D	177	ARG	N-CA-C	-5.30	105.41	111.14
1	B	267	VAL	N-CA-CB	-5.28	105.45	112.26
1	A	42	GLU	CB-CA-C	-5.26	100.62	109.83
1	D	221	ASP	N-CA-C	5.24	117.71	109.39
1	A	133	GLY	N-CA-C	-5.20	105.64	112.81
1	A	312	THR	N-CA-CB	-5.19	103.03	110.65
1	B	80	ASP	N-CA-C	-5.19	102.18	109.96
1	B	269	GLY	N-CA-C	5.18	117.34	111.85
1	C	60	ASN	N-CA-C	5.17	117.32	111.11
1	B	62	GLY	N-CA-C	-5.17	106.23	112.49
1	C	115	HIS	N-CA-C	-5.13	106.26	112.88
1	C	203	ALA	N-CA-C	-5.11	105.79	111.36
1	C	352	ILE	CB-CA-C	5.07	116.14	110.71
1	A	126	VAL	N-CA-CB	-5.04	102.91	111.23
1	C	92	LYS	N-CA-CB	-5.01	102.02	110.49

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	2745	0	2766	71	0
1	B	2719	0	2737	80	0
1	C	2712	0	2722	77	0
1	D	2721	0	2739	89	0
2	A	12	0	13	10	0
2	B	12	0	13	13	0
2	C	12	0	13	10	0
2	D	12	0	13	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	94	0	0	7	0
4	B	69	0	0	2	0
4	C	48	0	0	4	0
4	D	54	0	0	5	0
All	All	11214	0	11016	310	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (310) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LYS:HB2	1:D:92:LYS:NZ	1.70	1.06
1:C:191:ASN:O	1:C:192:THR:HB	1.53	1.06
1:D:135:SER:OG	2:D:1368:AME:HT21	1.56	1.05
1:D:163:LYS:CE	2:D:1368:AME:HT23	1.87	1.04
1:C:50:MET:HE1	2:C:1368:AME:HE1	1.40	0.99
1:D:295:THR:HG23	1:D:297:LEU:H	1.25	0.99
1:D:92:LYS:HB2	1:D:92:LYS:HZ2	1.23	0.98
1:B:163:LYS:HZ1	2:B:1368:AME:HT23	1.25	0.97
1:D:21:THR:HG22	1:D:23:PHE:H	1.26	0.97
1:D:92:LYS:NZ	1:D:92:LYS:CB	2.29	0.95
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:NZ	2:B:1368:AME:HT23	1.84	0.91
1:A:135:SER:OG	2:A:1369:AME:CT2	2.22	0.88
1:B:163:LYS:HZ3	1:B:191:ASN:HD21	1.22	0.88
1:C:296:GLY:HA3	1:C:329:THR:HG21	1.56	0.88
1:D:163:LYS:HE3	2:D:1368:AME:HT23	1.54	0.88
1:C:75:LEU:HD22	1:C:103:LEU:HD21	1.54	0.87
1:D:32:LEU:C	1:D:32:LEU:HD23	2.00	0.87
1:D:295:THR:CG2	1:D:297:LEU:H	1.88	0.86
1:D:191:ASN:O	1:D:192:THR:HB	1.76	0.84
1:D:92:LYS:CB	1:D:92:LYS:HZ3	1.89	0.84
1:B:72:ILE:HG22	1:B:76:LEU:HD22	1.58	0.84
1:C:12:GLN:O	1:C:359:VAL:HG22	1.79	0.83
1:D:163:LYS:NZ	2:D:1368:AME:HT23	1.93	0.82
1:B:135:SER:OG	2:B:1368:AME:HT21	1.80	0.82
1:C:163:LYS:HE2	2:C:1368:AME:HT23	1.63	0.80
1:A:159:ARG:NH2	1:A:316:ASP:OD1	2.15	0.80
1:D:163:LYS:HZ1	2:D:1368:AME:HT23	1.47	0.80
1:B:216:PRO:HD2	1:B:225:HIS:CE1	2.18	0.79
1:D:8:LEU:HD12	1:D:366:ILE:HD13	1.65	0.78
1:D:75:LEU:HD22	1:D:103:LEU:HD21	1.65	0.78
1:D:295:THR:CG2	1:D:297:LEU:HB2	2.13	0.78
1:C:135:SER:CB	2:C:1368:AME:HT21	2.12	0.78
1:D:46:GLU:OE1	1:D:295:THR:HG22	1.84	0.78
1:A:135:SER:OG	2:A:1369:AME:HT22	1.82	0.78
1:B:163:LYS:NZ	1:B:191:ASN:HD21	1.82	0.77
1:D:118:SER:HB3	1:D:121:ALA:H	1.51	0.76
1:B:48:VAL:HG11	1:B:292:MET:HG3	1.69	0.74
1:A:163:LYS:HE2	2:A:1369:AME:HT23	1.68	0.74
1:D:159:ARG:HG3	1:D:160:ILE:N	2.02	0.74
1:A:3:LEU:HD23	1:A:76:LEU:HD13	1.71	0.73
1:B:320:SER:OG	1:B:327:ASP:OD2	2.08	0.72
1:A:361:THR:CG2	4:A:2003:HOH:O	2.37	0.72
1:B:48:VAL:CG1	1:B:292:MET:CB	2.68	0.72
1:D:92:LYS:HZ3	1:D:92:LYS:HB3	1.53	0.72
1:A:116:GLU:HA	1:A:345:PRO:HB3	1.70	0.71
1:B:163:LYS:HZ1	2:B:1368:AME:CT2	1.99	0.71
1:D:292:MET:SD	2:D:1368:AME:HB2	2.30	0.71
1:C:49:THR:HG23	1:C:60:ASN:OD1	1.89	0.71
1:C:191:ASN:O	1:C:192:THR:CB	2.31	0.70
1:C:135:SER:OG	2:C:1368:AME:HT21	1.91	0.70
1:C:135:SER:OG	2:C:1368:AME:CT2	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:HH11	1:C:127:ARG:CG	2.02	0.69
1:D:163:LYS:NZ	1:D:191:ASN:HD21	1.91	0.69
1:B:142:ILE:HG23	1:B:143:PRO:HD3	1.73	0.69
1:A:135:SER:OG	2:A:1369:AME:HT21	1.92	0.69
1:C:163:LYS:NZ	1:C:191:ASN:HD21	1.90	0.69
1:B:132:CYS:O	1:B:158:VAL:HG12	1.92	0.68
1:B:142:ILE:HD11	1:B:175:ALA:HB2	1.75	0.68
1:B:75:LEU:HD22	1:B:103:LEU:HD13	1.75	0.68
1:B:49:THR:HG23	1:B:60:ASN:OD1	1.94	0.68
1:C:127:ARG:HG3	1:C:127:ARG:NH1	2.05	0.68
1:C:20:ARG:HG2	1:C:138:ILE:HB	1.76	0.68
1:A:118:SER:HB2	1:A:121:ALA:H	1.59	0.67
1:A:135:SER:CB	2:A:1369:AME:HT21	2.24	0.67
1:B:163:LYS:CE	2:B:1368:AME:HT23	2.24	0.67
1:C:352:ILE:HG12	1:C:355:LEU:HD12	1.76	0.67
1:D:21:THR:HG22	1:D:23:PHE:N	2.06	0.67
1:D:138:ILE:HG23	1:D:168:TRP:CD1	2.30	0.67
1:C:50:MET:CE	2:C:1368:AME:HE1	2.21	0.67
1:D:46:GLU:OE1	1:D:295:THR:CG2	2.43	0.67
1:B:134:VAL:HG23	1:B:322:ARG:HD3	1.76	0.67
1:A:109:ASP:OD2	1:A:113:ARG:NH1	2.27	0.66
1:C:352:ILE:CG1	1:C:355:LEU:HD12	2.26	0.66
1:A:159:ARG:HG2	1:A:160:ILE:N	2.11	0.66
1:D:32:LEU:HD23	1:D:33:LEU:N	2.09	0.66
1:B:47:CYS:SG	1:B:49:THR:HG22	2.36	0.65
1:D:21:THR:HG21	1:D:23:PHE:CE2	2.32	0.64
1:C:49:THR:CG2	1:C:60:ASN:OD1	2.45	0.64
1:B:216:PRO:HD2	1:B:225:HIS:HE1	1.59	0.64
1:A:361:THR:HG23	4:A:2003:HOH:O	1.99	0.63
1:D:153:LEU:HD13	1:D:160:ILE:HD11	1.81	0.63
1:B:96:HIS:HD2	4:B:2016:HOH:O	1.81	0.63
1:B:192:THR:HB	1:B:218:GLU:HA	1.80	0.62
1:D:20:ARG:HG2	1:D:138:ILE:HB	1.81	0.62
1:C:96:HIS:HD2	4:C:2008:HOH:O	1.83	0.62
1:D:8:LEU:HD12	1:D:366:ILE:CD1	2.28	0.62
1:A:94:LYS:NZ	1:C:192:THR:HG21	2.15	0.62
1:C:11:VAL:HG13	1:C:359:VAL:HG13	1.82	0.62
1:A:7:GLU:OE2	1:A:363:LYS:HE3	2.00	0.61
1:B:163:LYS:HE3	2:B:1368:AME:CT2	2.30	0.61
1:D:192:THR:CG2	1:D:192:THR:O	2.49	0.61
1:D:32:LEU:C	1:D:32:LEU:CD2	2.71	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:NH1	1:D:42:GLU:OE1	2.33	0.61
1:D:83:ALA:CB	1:D:108:LEU:HD13	2.31	0.61
1:B:159:ARG:HG2	1:B:159:ARG:HH11	1.65	0.61
1:C:296:GLY:HA3	1:C:329:THR:CG2	2.29	0.60
1:D:163:LYS:CE	2:D:1368:AME:CT2	2.72	0.60
1:C:163:LYS:HZ1	1:C:191:ASN:HD21	1.49	0.60
1:A:21:THR:HG22	1:A:163:LYS:HE3	1.84	0.59
1:D:163:LYS:HZ1	2:D:1368:AME:CT2	2.15	0.59
1:C:199:ALA:HB3	1:C:200:PRO:HD3	1.85	0.58
1:C:352:ILE:HD11	1:C:355:LEU:CD1	2.33	0.58
1:D:192:THR:O	1:D:192:THR:HG22	2.04	0.58
1:C:67:LEU:HA	1:C:71:LEU:HB2	1.85	0.58
1:D:161:LYS:NZ	1:D:316:ASP:OD2	2.33	0.58
1:C:21:THR:HG22	1:C:163:LYS:HE3	1.84	0.58
1:D:295:THR:HG22	1:D:297:LEU:HB2	1.86	0.57
1:A:75:LEU:HD13	1:A:90:LEU:HD21	1.86	0.57
1:D:163:LYS:HZ2	1:D:191:ASN:HD21	1.52	0.57
1:D:212:LEU:C	1:D:212:LEU:HD12	2.30	0.57
1:A:135:SER:HB3	2:A:1369:AME:HT21	1.85	0.57
1:B:48:VAL:CG1	1:B:292:MET:HG3	2.33	0.57
1:A:96:HIS:HD2	4:A:2024:HOH:O	1.85	0.57
1:B:75:LEU:HD22	1:B:103:LEU:CD1	2.35	0.57
1:D:118:SER:HB2	4:D:2022:HOH:O	2.03	0.56
1:D:113:ARG:NH2	4:D:2021:HOH:O	2.37	0.56
1:A:75:LEU:HD22	1:A:103:LEU:HD21	1.87	0.56
1:B:163:LYS:CE	2:B:1368:AME:CT2	2.84	0.56
1:B:142:ILE:HD11	1:B:175:ALA:CB	2.35	0.55
1:A:94:LYS:HZ2	1:C:192:THR:HG21	1.71	0.55
1:C:217:LEU:H	1:C:225:HIS:CE1	2.24	0.55
1:C:206:ASP:HB2	1:C:207:PRO:HD3	1.89	0.55
1:D:215:GLN:HG2	1:D:240:GLU:HG2	1.88	0.55
1:C:294:GLU:HG2	1:C:298:GLY:HA3	1.88	0.55
1:C:293:ILE:O	1:C:293:ILE:HG22	2.07	0.55
1:B:87:THR:HB	1:B:88:PRO:HD3	1.89	0.55
1:C:173:VAL:HG11	1:C:205:LEU:HD22	1.88	0.55
1:A:29:ARG:HG2	1:A:31:LEU:HD23	1.89	0.54
1:A:118:SER:CB	1:A:121:ALA:H	2.18	0.54
1:D:191:ASN:O	1:D:192:THR:CB	2.52	0.54
1:C:352:ILE:HD11	1:C:355:LEU:HD12	1.90	0.54
1:D:31:LEU:CD1	1:D:33:LEU:HD13	2.38	0.54
1:B:151:GLY:O	1:B:154:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:HE3	2:B:1368:AME:HT23	1.88	0.54
1:B:367:GLY:C	4:B:2001:HOH:O	2.51	0.54
1:B:217:LEU:HB2	1:B:225:HIS:CE1	2.43	0.54
1:A:87:THR:HB	1:A:88:PRO:CD	2.37	0.53
1:C:352:ILE:CD1	1:C:355:LEU:HD12	2.38	0.53
1:B:254:LEU:HD21	1:D:223:LEU:HD11	1.91	0.53
2:D:1368:AME:HG1	2:D:1368:AME:OXT	2.08	0.53
1:D:295:THR:HG21	1:D:297:LEU:HB2	1.88	0.53
1:A:215:GLN:HG2	1:A:240:GLU:HG2	1.91	0.53
1:B:139:MET:HG3	1:B:145:LEU:HA	1.91	0.53
1:A:179:ARG:NH1	4:A:2054:HOH:O	2.42	0.52
1:B:48:VAL:CG1	1:B:292:MET:HB3	2.36	0.52
1:B:161:LYS:NZ	2:B:1368:AME:HT22	2.25	0.52
1:C:264:PRO:HG2	1:C:270:TYR:CE2	2.44	0.52
1:C:274:ARG:O	1:C:277:HIS:HB3	2.09	0.52
1:D:291:ASP:O	2:D:1368:AME:HA	2.09	0.52
1:B:261:ASN:O	1:B:266:ARG:NH2	2.36	0.52
1:A:3:LEU:HD23	1:A:76:LEU:CD1	2.38	0.52
1:A:48:VAL:HG22	1:A:292:MET:HB2	1.92	0.52
1:C:237:CYS:HA	1:C:259:ILE:O	2.10	0.52
1:A:19:PHE:HZ	2:A:1369:AME:CT2	2.23	0.52
1:D:295:THR:CG2	1:D:297:LEU:N	2.66	0.51
1:B:35:ARG:HD2	1:B:44:TRP:CZ2	2.46	0.51
1:C:215:GLN:HG2	1:C:240:GLU:HG2	1.93	0.51
1:C:169:ASP:O	1:C:173:VAL:HG12	2.10	0.51
1:A:159:ARG:HD2	1:A:187:GLN:OE1	2.11	0.50
1:C:189:ASP:C	1:C:189:ASP:OD1	2.54	0.50
1:D:111:GLU:O	1:D:115:HIS:HD2	1.95	0.50
1:D:21:THR:HG21	1:D:23:PHE:CD2	2.46	0.50
1:C:25:THR:HG22	1:C:26:GLN:N	2.25	0.50
1:D:239:ASP:OD2	1:D:263:LYS:NZ	2.45	0.50
1:B:50:MET:SD	2:B:1368:AME:HE1	2.52	0.50
1:B:291:ASP:HB2	1:B:316:ASP:O	2.12	0.49
1:D:199:ALA:N	1:D:200:PRO:CD	2.75	0.49
1:C:217:LEU:H	1:C:225:HIS:HE1	1.59	0.49
1:D:270:TYR:OH	1:D:302:ASN:ND2	2.45	0.49
1:B:47:CYS:SG	1:B:49:THR:CG2	3.01	0.49
1:C:263:LYS:HZ3	2:C:1368:AME:C	2.26	0.49
1:A:35:ARG:NH1	1:A:42:GLU:OE2	2.44	0.49
1:A:8:LEU:HD23	1:A:8:LEU:C	2.38	0.49
1:B:35:ARG:HD2	1:B:44:TRP:CH2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ILE:HD12	1:D:351:PRO:HB3	1.95	0.49
1:B:48:VAL:CG1	1:B:292:MET:HB2	2.42	0.49
1:B:321:ASP:HA	1:B:324:TYR:O	2.13	0.49
1:C:135:SER:HB3	2:C:1368:AME:HT21	1.91	0.49
1:D:263:LYS:NZ	2:D:1368:AME:C	2.76	0.49
1:A:119:PHE:CE1	1:A:347:LEU:HD13	2.48	0.48
1:D:55:TYR:CD2	1:D:56:SER:HB3	2.48	0.48
1:A:35:ARG:HD2	1:A:42:GLU:OE2	2.13	0.48
1:B:161:LYS:HZ1	2:B:1368:AME:HT22	1.78	0.48
1:C:263:LYS:NZ	2:C:1368:AME:C	2.76	0.48
1:B:159:ARG:HG2	1:B:159:ARG:NH1	2.27	0.48
1:A:217:LEU:H	1:A:225:HIS:CE1	2.32	0.48
1:C:163:LYS:HZ3	2:C:1368:AME:HN1	1.61	0.48
1:C:187:GLN:HB3	1:C:211:LEU:CD2	2.44	0.48
1:A:19:PHE:HZ	2:A:1369:AME:HT23	1.78	0.48
1:B:48:VAL:HG11	1:B:292:MET:CG	2.41	0.48
1:B:12:GLN:O	1:B:359:VAL:HB	2.14	0.48
1:D:45:GLY:N	1:D:106:ALA:HB2	2.28	0.47
1:A:188:VAL:HG23	1:A:213:ILE:HG13	1.96	0.47
1:C:72:ILE:O	1:C:73:PRO:C	2.56	0.47
1:C:170:VAL:HG11	1:C:204:ARG:HB3	1.96	0.47
1:D:21:THR:HG21	1:D:23:PHE:CZ	2.50	0.47
1:C:35:ARG:HD3	1:C:44:TRP:CZ2	2.50	0.47
1:C:141:THR:HB	1:C:143:PRO:HD2	1.97	0.47
1:D:138:ILE:HG23	1:D:168:TRP:CG	2.49	0.47
1:A:111:GLU:OE2	1:B:117:ARG:NH2	2.48	0.47
1:C:201:GLN:O	1:C:204:ARG:HB2	2.14	0.47
1:A:221:ASP:O	1:A:225:HIS:HD2	1.98	0.47
1:B:48:VAL:HG12	1:B:292:MET:HB3	1.96	0.47
1:D:142:ILE:HD12	1:D:175:ALA:HB2	1.97	0.47
1:B:9:ARG:HD2	1:B:356:LEU:HD11	1.97	0.46
1:B:263:LYS:NZ	2:B:1368:AME:C	2.78	0.46
1:A:15:LEU:HB2	1:A:27:SER:O	2.14	0.46
1:A:48:VAL:HG22	1:A:292:MET:CB	2.45	0.46
1:A:63:ALA:O	1:A:67:LEU:HB2	2.15	0.46
1:A:237:CYS:HA	1:A:259:ILE:O	2.16	0.46
1:B:75:LEU:HD13	1:B:90:LEU:HD21	1.98	0.46
1:C:329:THR:HG23	1:C:330:GLU:O	2.15	0.46
1:A:264:PRO:HG2	1:A:270:TYR:CE1	2.51	0.46
1:D:47:CYS:HA	1:D:102:ALA:HB2	1.98	0.46
1:D:163:LYS:HE3	2:D:1368:AME:CT2	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2068:HOH:O	1:C:94:LYS:NZ	2.49	0.46
1:C:159:ARG:CG	1:C:160:ILE:N	2.78	0.46
1:C:352:ILE:HA	1:C:353:PRO:HD3	1.80	0.46
1:B:48:VAL:CG1	1:B:292:MET:CG	2.93	0.45
1:B:253:LYS:HE3	1:D:223:LEU:HD23	1.99	0.45
1:D:177:ARG:HA	1:D:177:ARG:HD3	1.65	0.45
1:A:35:ARG:HD3	1:A:44:TRP:CZ2	2.51	0.45
1:D:11:VAL:HG21	1:D:33:LEU:HD22	1.97	0.45
1:D:21:THR:CG2	1:D:22:SER:N	2.79	0.45
1:B:94:LYS:NZ	1:D:192:THR:HG21	2.31	0.45
1:D:163:LYS:HZ3	1:D:191:ASN:HD21	1.62	0.45
1:A:117:ARG:HA	4:A:2042:HOH:O	2.17	0.45
1:B:139:MET:HG3	1:B:145:LEU:CA	2.47	0.45
1:B:242:ILE:HB	1:B:266:ARG:NH1	2.32	0.45
1:C:35:ARG:NH1	1:C:42:GLU:OE1	2.51	0.44
1:D:225:HIS:CG	1:D:238:LEU:HD21	2.53	0.44
1:B:67:LEU:HA	1:B:71:LEU:HB2	2.00	0.44
1:A:95:GLY:O	1:A:100:LYS:HE3	2.17	0.44
1:A:113:ARG:HA	1:A:345:PRO:HB2	2.00	0.44
1:C:127:ARG:CG	1:C:127:ARG:NH1	2.72	0.44
1:D:75:LEU:CD2	1:D:103:LEU:HD21	2.41	0.44
1:D:97:ARG:HD2	4:D:2020:HOH:O	2.17	0.44
1:B:67:LEU:HD13	1:B:71:LEU:HD23	1.99	0.44
1:A:217:LEU:HB2	1:A:225:HIS:NE2	2.32	0.44
1:A:142:ILE:HG23	1:A:146:LEU:HD22	2.00	0.43
1:D:319:ALA:O	1:D:322:ARG:HB3	2.18	0.43
1:B:216:PRO:HB2	1:B:217:LEU:HD13	1.99	0.43
1:B:299:ARG:HD3	1:B:318:SER:O	2.18	0.43
1:A:203:ALA:HA	1:A:206:ASP:OD1	2.18	0.43
1:A:223:LEU:HD12	1:C:250:ASP:CG	2.43	0.43
1:B:142:ILE:O	1:B:142:ILE:HG13	2.18	0.43
1:D:109:ASP:O	1:D:113:ARG:HG3	2.19	0.43
1:B:161:LYS:HE3	1:B:214:GLU:OE1	2.18	0.43
1:C:159:ARG:NE	4:C:2027:HOH:O	2.52	0.43
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.76	0.43
1:C:270:TYR:OH	1:C:302:ASN:ND2	2.51	0.43
1:A:96:HIS:HE1	1:C:57:SER:O	2.01	0.43
1:A:139:MET:HE3	1:A:148:VAL:HG11	1.99	0.43
1:B:159:ARG:HD2	1:B:187:GLN:OE1	2.19	0.43
1:C:171:GLU:HA	4:C:2030:HOH:O	2.18	0.43
1:D:264:PRO:HG3	1:D:305:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:VAL:HB	1:B:287:VAL:HG12	2.01	0.42
1:B:293:ILE:HD12	2:B:1368:AME:HE3	2.01	0.42
1:D:31:LEU:CD1	1:D:33:LEU:CD1	2.97	0.42
1:D:135:SER:HG	2:D:1368:AME:HT21	1.76	0.42
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.84	0.42
1:A:159:ARG:HD3	4:A:2060:HOH:O	2.19	0.42
1:B:50:MET:HE3	1:B:50:MET:HB2	1.83	0.42
1:B:63:ALA:O	1:B:67:LEU:HB2	2.19	0.42
1:B:217:LEU:H	1:B:225:HIS:HE1	1.67	0.42
1:C:117:ARG:HG3	1:C:117:ARG:HH11	1.84	0.42
1:A:322:ARG:HD3	1:A:322:ARG:C	2.44	0.42
1:D:5:GLY:HA2	1:D:76:LEU:HD21	2.02	0.42
1:D:135:SER:CB	2:D:1368:AME:HT21	2.46	0.42
1:B:48:VAL:HG13	1:B:292:MET:HB2	2.02	0.42
1:D:316:ASP:O	1:D:318:SER:N	2.52	0.42
1:C:271:LEU:HA	1:C:271:LEU:HD12	1.79	0.42
1:A:19:PHE:CZ	2:A:1369:AME:HT23	2.55	0.42
1:A:141:THR:HG23	1:A:144:GLN:OE1	2.20	0.42
1:A:206:ASP:OD2	1:A:233:GLN:HB2	2.20	0.42
1:C:35:ARG:CD	1:C:44:TRP:CZ2	3.03	0.42
1:C:150:GLY:HA2	1:C:180:PHE:CE2	2.54	0.42
1:A:141:THR:OG1	1:A:143:PRO:HG2	2.19	0.42
1:A:174:ARG:O	1:A:175:ALA:C	2.62	0.42
1:C:261:ASN:OD1	1:C:261:ASN:C	2.62	0.42
1:B:190:ALA:O	1:B:191:ASN:C	2.62	0.41
1:A:72:ILE:HB	1:A:73:PRO:HD3	2.02	0.41
1:A:291:ASP:O	2:A:1369:AME:HA	2.20	0.41
1:B:119:PHE:O	1:B:120:ALA:C	2.63	0.41
1:C:220:GLU:HB3	4:C:2035:HOH:O	2.19	0.41
1:B:237:CYS:HA	1:B:259:ILE:O	2.20	0.41
1:C:192:THR:O	1:C:192:THR:CG2	2.67	0.41
1:D:146:LEU:HD12	1:D:146:LEU:HA	1.77	0.41
1:D:171:GLU:O	1:D:172:PRO:C	2.63	0.41
1:B:85:LYS:O	1:B:89:LEU:HD22	2.20	0.41
1:D:295:THR:HG23	1:D:297:LEU:N	2.10	0.41
1:A:87:THR:HB	1:A:88:PRO:HD3	2.02	0.41
1:B:220:GLU:HG3	4:D:2044:HOH:O	2.20	0.41
1:B:204:ARG:O	1:B:207:PRO:CD	2.69	0.41
1:C:35:ARG:HD3	1:C:44:TRP:CH2	2.55	0.41
1:A:72:ILE:O	1:A:73:PRO:C	2.63	0.41
1:A:142:ILE:O	1:A:146:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HG23	1:A:323:TYR:CD1	2.56	0.41
1:C:263:LYS:HD3	1:C:292:MET:HG2	2.03	0.41
1:A:169:ASP:OD1	1:A:170:VAL:HG23	2.21	0.40
1:C:25:THR:CG2	1:C:26:GLN:N	2.84	0.40
1:D:116:GLU:HA	1:D:345:PRO:HB3	2.02	0.40
1:D:142:ILE:HG23	1:D:143:PRO:HD3	2.03	0.40
1:A:260:VAL:HB	1:A:287:VAL:HG12	2.03	0.40
1:B:87:THR:HB	1:B:88:PRO:CD	2.50	0.40
1:B:170:VAL:HG12	1:B:201:GLN:HE22	1.87	0.40
1:D:265:GLY:C	1:D:267:VAL:H	2.30	0.40
1:A:35:ARG:HD3	1:A:44:TRP:CH2	2.56	0.40
1:D:343:THR:HG23	4:D:2053:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	366/368 (100%)	352 (96%)	14 (4%)	0	100	100
1	B	365/368 (99%)	334 (92%)	29 (8%)	2 (0%)	24	46
1	C	365/368 (99%)	340 (93%)	23 (6%)	2 (0%)	24	46
1	D	365/368 (99%)	344 (94%)	16 (4%)	5 (1%)	9	22
All	All	1461/1472 (99%)	1370 (94%)	82 (6%)	9 (1%)	21	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	GLU
1	C	16	VAL
1	C	92	LYS

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Mol	Chain	Res	Type
1	D	192	THR
1	D	317	THR
1	B	114	ALA
1	D	79	GLU
1	D	336	GLY
1	D	337	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	284/292 (97%)	254 (89%)	30 (11%)	6	16
1	B	277/292 (95%)	241 (87%)	36 (13%)	4	10
1	C	276/292 (94%)	233 (84%)	43 (16%)	2	6
1	D	277/292 (95%)	239 (86%)	38 (14%)	3	8
All	All	1114/1168 (95%)	967 (87%)	147 (13%)	4	9

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	25	THR
1	A	48	VAL
1	A	50	MET
1	A	54	LEU
1	A	66	VAL
1	A	67	LEU
1	A	68	ARG
1	A	71	LEU
1	A	75	LEU
1	A	76	LEU
1	A	116	GLU
1	A	126	VAL
1	A	142	ILE
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	153	LEU
1	A	158	VAL
1	A	173	VAL
1	A	213	ILE
1	A	217	LEU
1	A	231	ARG
1	A	233	GLN
1	A	240	GLU
1	A	258	GLN
1	A	271	LEU
1	A	312	THR
1	A	343	THR
1	A	347	LEU
1	A	356	LEU
1	A	361	THR
1	B	7	GLU
1	B	13	MET
1	B	31	LEU
1	B	37	VAL
1	B	54	LEU
1	B	66	VAL
1	B	67	LEU
1	B	68	ARG
1	B	71	LEU
1	B	75	LEU
1	B	76	LEU
1	B	89	LEU
1	B	92	LYS
1	B	103	LEU
1	B	112	LEU
1	B	116	GLU
1	B	117	ARG
1	B	126	VAL
1	B	142	ILE
1	B	145	LEU
1	B	159	ARG
1	B	170	VAL
1	B	201	GLN
1	B	210	LEU
1	B	213	ILE
1	B	217	LEU
1	B	220	GLU

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Mol	Chain	Res	Type
1	B	227	GLU
1	B	232	ILE
1	B	267	VAL
1	B	295	THR
1	B	297	LEU
1	B	320	SER
1	B	343	THR
1	B	347	LEU
1	B	364	VAL
1	C	8	LEU
1	C	15	LEU
1	C	16	VAL
1	C	20	ARG
1	C	27	SER
1	C	31	LEU
1	C	34	LEU
1	C	49	THR
1	C	50	MET
1	C	66	VAL
1	C	67	LEU
1	C	71	LEU
1	C	75	LEU
1	C	81	ILE
1	C	89	LEU
1	C	94	LYS
1	C	108	LEU
1	C	112	LEU
1	C	116	GLU
1	C	127	ARG
1	C	129	SER
1	C	138	ILE
1	C	149	VAL
1	C	153	LEU
1	C	155	GLU
1	C	162	LEU
1	C	173	VAL
1	C	210	LEU
1	C	211	LEU
1	C	220	GLU
1	C	223	LEU
1	C	228	LEU
1	C	254	LEU

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Mol	Chain	Res	Type
1	C	267	VAL
1	C	271	LEU
1	C	313	LEU
1	C	329	THR
1	C	342	PRO
1	C	343	THR
1	C	352	ILE
1	C	359	VAL
1	C	361	THR
1	C	366	ILE
1	D	8	LEU
1	D	12	GLN
1	D	13	MET
1	D	21	THR
1	D	27	SER
1	D	32	LEU
1	D	34	LEU
1	D	42	GLU
1	D	50	MET
1	D	56	SER
1	D	67	LEU
1	D	71	LEU
1	D	75	LEU
1	D	92	LYS
1	D	112	LEU
1	D	118	SER
1	D	119	PHE
1	D	126	VAL
1	D	139	MET
1	D	142	ILE
1	D	146	LEU
1	D	153	LEU
1	D	158	VAL
1	D	159	ARG
1	D	162	LEU
1	D	177	ARG
1	D	184	VAL
1	D	210	LEU
1	D	211	LEU
1	D	223	LEU
1	D	232	ILE
1	D	240	GLU

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Mol	Chain	Res	Type
1	D	267	VAL
1	D	295	THR
1	D	297	LEU
1	D	313	LEU
1	D	347	LEU
1	D	361	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	191	ASN
1	A	225	HIS
1	B	96	HIS
1	B	191	ASN
1	B	201	GLN
1	B	225	HIS
1	B	302	ASN
1	C	69	HIS
1	C	96	HIS
1	C	191	ASN
1	C	225	HIS
1	C	258	GLN
1	C	283	HIS
1	C	302	ASN
1	C	338	HIS
1	D	96	HIS
1	D	115	HIS
1	D	191	ASN
1	D	225	HIS
1	D	302	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	AME	C	1368	3	11,11,11	3.92	4 (36%)	13,13,13	4.74	8 (61%)
2	AME	A	1369	3	11,11,11	3.65	4 (36%)	13,13,13	4.43	7 (53%)
2	AME	D	1368	3	11,11,11	4.08	4 (36%)	13,13,13	3.61	7 (53%)
2	AME	B	1368	3	11,11,11	4.11	4 (36%)	13,13,13	4.43	9 (69%)

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	AME	C	1368	3	-	7/12/12/12	-
2	AME	A	1369	3	-	5/12/12/12	-
2	AME	D	1368	3	-	6/12/12/12	-
2	AME	B	1368	3	-	8/12/12/12	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1368	AME	OT-CT1	9.33	1.44	1.23
2	C	1368	AME	OT-CT1	9.20	1.43	1.23
2	B	1368	AME	OT-CT1	9.05	1.43	1.23
2	A	1369	AME	OT-CT1	8.60	1.42	1.23
2	D	1368	AME	O-C	7.78	1.45	1.22
2	B	1368	AME	O-C	7.77	1.45	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1368	AME	O-C	7.60	1.44	1.22
2	A	1369	AME	O-C	6.95	1.42	1.22
2	B	1368	AME	OXT-C	4.43	1.44	1.30
2	D	1368	AME	OXT-C	4.32	1.44	1.30
2	B	1368	AME	CT1-N	4.19	1.47	1.34
2	C	1368	AME	OXT-C	4.16	1.43	1.30
2	D	1368	AME	CT1-N	3.84	1.46	1.34
2	A	1369	AME	OXT-C	3.73	1.42	1.30
2	A	1369	AME	CT1-N	2.83	1.43	1.34
2	C	1368	AME	CT1-N	2.68	1.43	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1368	AME	CT2-CT1-N	-10.63	98.50	116.12
2	B	1368	AME	OT-CT1-N	-8.97	106.14	121.98
2	B	1368	AME	OT-CT1-CT2	-8.81	106.37	122.05
2	A	1369	AME	CT2-CT1-N	-8.72	101.66	116.12
2	A	1369	AME	OT-CT1-CT2	-7.92	107.95	122.05
2	A	1369	AME	OXT-C-O	-7.75	106.49	124.08
2	C	1368	AME	OXT-C-O	-7.66	106.71	124.08
2	D	1368	AME	OT-CT1-CT2	-6.95	109.69	122.05
2	D	1368	AME	CT2-CT1-N	-6.64	105.10	116.12
2	C	1368	AME	OT-CT1-CT2	-6.44	110.58	122.05
2	D	1368	AME	OXT-C-O	-6.22	109.98	124.08
2	A	1369	AME	OT-CT1-N	-5.31	112.59	121.98
2	C	1368	AME	OT-CT1-N	-5.24	112.72	121.98
2	B	1368	AME	C-CA-N	5.22	122.69	110.57
2	B	1368	AME	CA-N-CT1	4.88	135.25	121.58
2	B	1368	AME	OXT-C-O	-4.49	113.90	124.08
2	C	1368	AME	O-C-CA	-4.23	108.61	122.26
2	C	1368	AME	CB-CA-C	4.16	120.24	110.35
2	D	1368	AME	CA-N-CT1	3.19	130.53	121.58
2	A	1369	AME	O-C-CA	-3.06	112.39	122.26
2	D	1368	AME	CE-SD-CG	3.04	116.03	100.32
2	B	1368	AME	CT2-CT1-N	3.03	121.14	116.12
2	D	1368	AME	O-C-CA	-2.75	113.40	122.26
2	B	1368	AME	CB-CG-SD	-2.66	96.27	113.82
2	D	1368	AME	CB-CA-N	-2.56	105.85	110.91
2	C	1368	AME	C-CA-N	-2.55	104.65	110.57
2	A	1369	AME	CE-SD-CG	2.43	112.92	100.32
2	C	1368	AME	CG-CB-CA	2.42	120.38	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1368	AME	CG-CB-CA	-2.13	106.20	112.83
2	B	1368	AME	O-C-CA	-2.10	115.48	122.26
2	A	1369	AME	CB-CA-C	-2.02	105.55	110.35

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1368	AME	OT-CT1-N-CA
2	B	1368	AME	C-CA-CB-CG
2	C	1368	AME	C-CA-CB-CG
2	D	1368	AME	CT2-CT1-N-CA
2	A	1369	AME	OT-CT1-N-CA
2	B	1368	AME	CA-CB-CG-SD
2	C	1368	AME	CA-CB-CG-SD
2	C	1368	AME	OT-CT1-N-CA
2	D	1368	AME	CA-CB-CG-SD
2	B	1368	AME	CT2-CT1-N-CA
2	B	1368	AME	N-CA-CB-CG
2	C	1368	AME	N-CA-CB-CG
2	A	1369	AME	OXT-C-CA-N
2	C	1368	AME	O-C-CA-N
2	D	1368	AME	CB-CG-SD-CE
2	B	1368	AME	OXT-C-CA-CB
2	C	1368	AME	O-C-CA-CB
2	D	1368	AME	O-C-CA-N
2	C	1368	AME	CT2-CT1-N-CA
2	D	1368	AME	OT-CT1-N-CA
2	A	1369	AME	CB-CG-SD-CE
2	A	1369	AME	O-C-CA-CB
2	D	1368	AME	O-C-CA-CB
2	A	1369	AME	CA-CB-CG-SD
2	B	1368	AME	OXT-C-CA-N
2	B	1368	AME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1368	AME	10	0
2	A	1369	AME	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1368	AME	14	0
2	B	1368	AME	13	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	368/368 (100%)	-0.95	0	100 100	24, 39, 60, 81	0
1	B	367/368 (99%)	-0.72	3 (0%)	82 81	28, 45, 66, 95	0
1	C	367/368 (99%)	-0.65	2 (0%)	87 86	30, 51, 74, 91	0
1	D	367/368 (99%)	-0.60	4 (1%)	78 76	30, 49, 71, 90	0
All	All	1469/1472 (99%)	-0.73	9 (0%)	85 85	24, 47, 70, 95	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	142	ILE	3.5
1	C	1	MET	3.2
1	D	80	ASP	3.1
1	B	1	MET	2.6
1	C	367	GLY	2.3
1	D	144	GLN	2.2
1	D	1	MET	2.1
1	B	142	ILE	2.1
1	B	367	GLY	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	AME	A	1369	12/12	0.97	0.08	50,61,71,77	0
2	AME	B	1368	12/12	0.97	0.07	38,58,72,78	0
2	AME	D	1368	12/12	0.97	0.08	49,64,80,83	0
3	MG	D	1369	1/1	0.97	0.06	62,62,62,62	0
3	MG	B	1369	1/1	0.98	0.04	63,63,63,63	0
2	AME	C	1368	12/12	0.98	0.07	56,67,76,79	0
3	MG	C	1369	1/1	0.99	0.04	55,55,55,55	0
3	MG	A	1370	1/1	0.99	0.03	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.