Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 08:23 pm GMT

PDB ID	:	4A6G
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 (i) 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 (i)) were used in the production of this report:

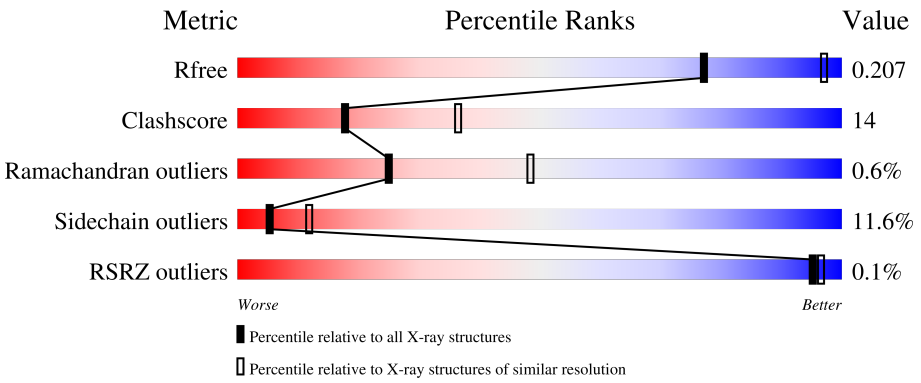
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 <=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	76% 19% 5%
1	B	368	74% 21% •
1	C	368	73% 23% •
1	D	368	73% 22% 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 (i)

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.

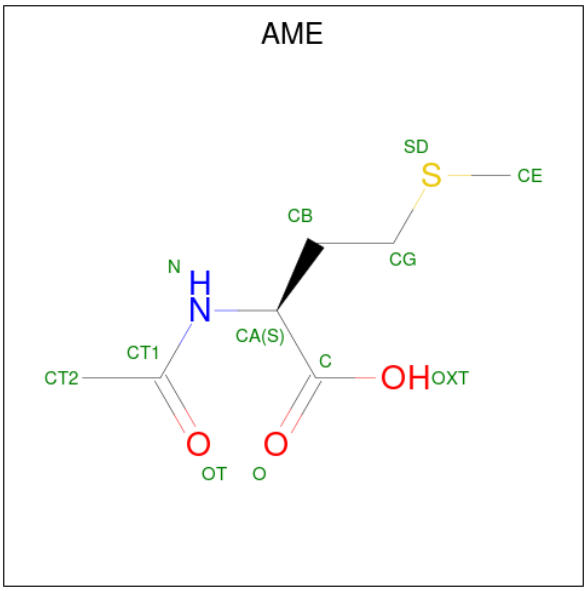
- Molecule 1 is a protein called N-ACYLAMINO ACID RACEMASE.

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

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 (three-letter code: AME) (formula: $C_7H_{13}NO_3S$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

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

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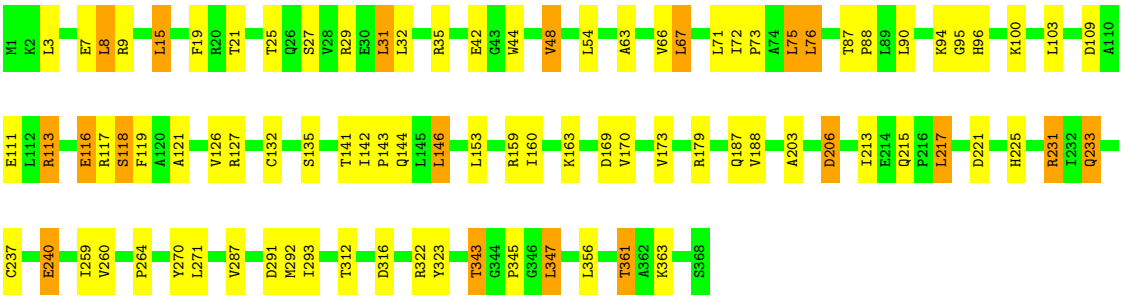
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	69	69	69	0	0
			Total	O		
4	C	48	48	48	0	0
			Total	O		
4	D	54	54	54	0	0

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.

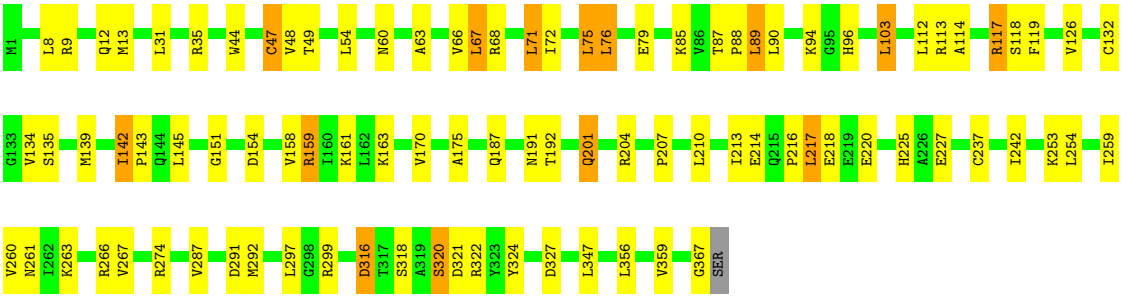
• Molecule 1: N-ACYLAMINO ACID RACEMASE

Chain A:



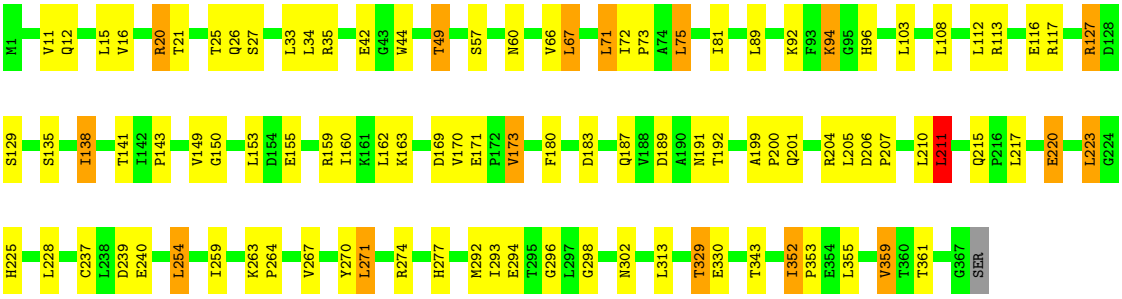
• Molecule 1: N-ACYLAMINO ACID RACEMASE

Chain B:



• Molecule 1: N-ACYLAMINO ACID RACEMASE

Chain C:



• Molecule 1: N-ACYLAMINO ACID RACEMASE

Chain D: 73% 22% 5%

M1 G5 L8 V11 Q12 M13 R20 T21 S22 F23 S27 L31 L32 L33 L34 R35 E42 G45 E46 C47 M50 Y55 S56 L67 L71 L75 L76 E79 A83 K92 R97 A102 L103 A106 V107 L108 D109 A110 E111 L112 R113

A114 H115 E116 R117 S118 F119 A120 A121 V126 R127 S135 I138 M139 I142 P143 L146 L153 V158 R159 I160 K161 L162 K163 W168 A175 V176 R177 V184 N191 T192 A199 P200 R204 L210 L211 L212 Q215 L223 G224 H225 I232 L238

D239 E240 K263 P264 V267 Y270 D291 M292 T295 G296 L297 N302 L305 L313 D316 T317 S318 A319 R322 I328 G336 G337 T343 G344 P345 G346 L347 P351 L355 I366 G367 SER

4 Data and refinement statistics (i)

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 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.31-2.71) 100.0 (88.31-2.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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	0.97	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.99	1/2801 (0.0%)	1.07	9/3821 (0.2%)
1	B	0.94	1/2775 (0.0%)	1.00	5/3786 (0.1%)
1	C	0.89	0/2768	0.97	5/3778 (0.1%)
1	D	0.93	0/2777	1.00	4/3790 (0.1%)
All	All	0.94	2/11121 (0.0%)	1.01	23/15175 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	CYS	CB-SG	5.87	1.92	1.82
1	A	132	CYS	CB-SG	-5.28	1.73	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	D	113	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	B	118	SER	N-CA-CB	-7.11	99.83	110.50
1	C	211	LEU	CA-CB-CG	6.87	131.09	115.30
1	A	8	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	D	204	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	118	SER	CB-CA-C	-6.28	98.17	110.10
1	D	239	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	32	LEU	CB-CG-CD1	-6.17	100.50	111.00
1	A	113	ARG	CG-CD-NE	-5.68	99.88	111.80
1	C	33	LEU	CB-CG-CD1	-5.65	101.40	111.00
1	B	113	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	8	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	31	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	A	231	ARG	NE-CZ-NH2	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	204	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	113	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	239	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	316	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	254	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	343	THR	C-N-CA	-5.01	111.78	122.30
1	C	113	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2766	67	0
1	B	2719	0	2737	77	0
1	C	2712	0	2722	73	0
1	D	2721	0	2739	87	0
2	A	12	0	13	11	0
2	B	12	0	13	13	0
2	C	12	0	13	7	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	298	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 (298) 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:B:163:LYS:HZ1	2:B:1368:AME:HT23	1.11	1.13
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: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: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
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: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: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:32:LEU:C	1:D:32:LEU:HD23	2.00	0.82
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	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ2	1:B:191:ASN:HD21	1.36	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
1:B:163:LYS:HZ1	2:B:1368:AME:CT2	2.00	0.70
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:263:LYS:HZ1	2:B:1368:AME:C	2.07	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:32:LEU:HD23	1:D:33:LEU:N	2.09	0.67
1:D:138:ILE:HG23	1:D:168:TRP:CD1	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:HZ1	2:B:1368:AME:HT22	1.64	0.62
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: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: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: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:C:163:LYS:HZ2	1:C:191:ASN:HD21	1.52	0.57
1:D:32:LEU:C	1:D:32:LEU:CD2	2.71	0.56
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:D:163:LYS:HZ2	1:D:191:ASN:HD21	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:163:LYS:HE3	2:B:1368:AME:HT23	1.88	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:D:212:LEU:C	1:D:212:LEU:HD12	2.30	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: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:291:ASP:HB2	1:B:316:ASP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:35:ARG:HD2	1:B:44:TRP:CH2	2.48	0.49
1:B:367:GLY:C	4:B:2001:HOH:O	2.51	0.49
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:HZ3	1:D:191:ASN:HD21	1.61	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:B:163:LYS:NZ	2:B:1368:AME:CT2	2.68	0.46
1:D:163:LYS:HE3	2:D:1368:AME:CT2	2.35	0.46
1:C:189:ASP:C	1:C:189:ASP:OD1	2.54	0.46
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:263:LYS:NZ	2:B:1368:AME:C	2.78	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: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:8:LEU:HD23	1:A:8:LEU:C	2.38	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: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:72:ILE:O	1:C:73:PRO:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:260:VAL:HB	1:B:287:VAL:HG12	2.01	0.42
1:D:31:LEU:CD1	1:D:33:LEU:CD1	2.97	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: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:C:163:LYS:HZ2	1:C:191:ASN:ND2	2.17	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:135:SER:HG	2:A:1369:AME:CT2	2.32	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: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: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:B:85:LYS:O	1:B:89:LEU:HD22	2.20	0.41
1:D:135:SER:HG	2:D:1368:AME:HT21	1.77	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: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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/368 (100%)	352 (96%)	14 (4%)	0	100	100
1	B	365/368 (99%)	334 (92%)	29 (8%)	2 (0%)	29	53
1	C	365/368 (99%)	340 (93%)	23 (6%)	2 (0%)	29	53
1	D	365/368 (99%)	344 (94%)	16 (4%)	5 (1%)	11	26
All	All	1461/1472 (99%)	1370 (94%)	82 (6%)	9 (1%)	25	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	GLU
1	C	16	VAL
1	C	92	LYS
1	D	192	THR

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	284/292 (97%)	256 (90%)	28 (10%)	8 17
1	B	277/292 (95%)	250 (90%)	27 (10%)	8 18
1	C	276/292 (94%)	238 (86%)	38 (14%)	3 7
1	D	277/292 (95%)	241 (87%)	36 (13%)	4 9
All	All	1114/1168 (95%)	985 (88%)	129 (12%)	5 12

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	15	LEU
1	A	25	THR
1	A	48	VAL
1	A	54	LEU
1	A	66	VAL
1	A	67	LEU
1	A	71	LEU
1	A	75	LEU
1	A	76	LEU
1	A	116	GLU
1	A	126	VAL
1	A	127	ARG
1	A	146	LEU
1	A	153	LEU
1	A	173	VAL

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Mol	Chain	Res	Type
1	A	206	ASP
1	A	217	LEU
1	A	231	ARG
1	A	233	GLN
1	A	240	GLU
1	A	271	LEU
1	A	312	THR
1	A	322	ARG
1	A	343	THR
1	A	347	LEU
1	A	356	LEU
1	A	361	THR
1	B	13	MET
1	B	31	LEU
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	103	LEU
1	B	112	LEU
1	B	117	ARG
1	B	119	PHE
1	B	126	VAL
1	B	142	ILE
1	B	159	ARG
1	B	201	GLN
1	B	210	LEU
1	B	213	ILE
1	B	217	LEU
1	B	227	GLU
1	B	267	VAL
1	B	274	ARG
1	B	297	LEU
1	B	320	SER
1	B	347	LEU
1	C	15	LEU
1	C	20	ARG
1	C	27	SER

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Mol	Chain	Res	Type
1	C	34	LEU
1	C	49	THR
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	183	ASP
1	C	210	LEU
1	C	211	LEU
1	C	220	GLU
1	C	223	LEU
1	C	228	LEU
1	C	254	LEU
1	C	267	VAL
1	C	271	LEU
1	C	313	LEU
1	C	329	THR
1	C	343	THR
1	C	352	ILE
1	C	359	VAL
1	C	361	THR
1	D	8	LEU
1	D	13	MET
1	D	27	SER
1	D	32	LEU
1	D	34	LEU
1	D	42	GLU
1	D	50	MET

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	96	HIS

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Mol	Chain	Res	Type
1	C	191	ASN
1	C	225	HIS
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 (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 monosaccharides 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	A	1369	3	11,11,11	3.58	4 (36%)	13,13,13	4.41	7 (53%)
2	AME	D	1368	3	11,11,11	3.99	4 (36%)	13,13,13	3.65	7 (53%)
2	AME	B	1368	3	11,11,11	4.02	4 (36%)	13,13,13	4.33	9 (69%)

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	3.84	4 (36%)	13,13,13	4.69	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	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	-
2	AME	C	1368	3	-	7/12/12/12	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1368	AME	OT-CT1	9.23	1.44	1.23
2	C	1368	AME	OT-CT1	9.11	1.43	1.23
2	B	1368	AME	OT-CT1	8.96	1.43	1.23
2	A	1369	AME	OT-CT1	8.51	1.42	1.23
2	D	1368	AME	O-C	7.54	1.45	1.22
2	B	1368	AME	O-C	7.53	1.45	1.22
2	C	1368	AME	O-C	7.36	1.44	1.22
2	A	1369	AME	O-C	6.73	1.42	1.22
2	B	1368	AME	OXT-C	4.33	1.44	1.30
2	D	1368	AME	OXT-C	4.23	1.44	1.30
2	C	1368	AME	OXT-C	4.08	1.43	1.30
2	B	1368	AME	CT1-N	3.93	1.47	1.34
2	A	1369	AME	OXT-C	3.65	1.42	1.30
2	D	1368	AME	CT1-N	3.60	1.46	1.34
2	A	1369	AME	CT1-N	2.66	1.43	1.34
2	C	1368	AME	CT1-N	2.51	1.43	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1368	AME	CT2-CT1-N	-10.40	98.50	116.10
2	B	1368	AME	OT-CT1-N	-8.60	106.14	121.95
2	A	1369	AME	CT2-CT1-N	-8.53	101.66	116.10
2	B	1368	AME	OT-CT1-CT2	-8.45	106.37	122.06
2	A	1369	AME	OXT-C-O	-7.75	106.49	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1368	AME	OXT-C-O	-7.65	106.71	124.09
2	A	1369	AME	OT-CT1-CT2	-7.60	107.95	122.06
2	D	1368	AME	OT-CT1-CT2	-6.66	109.69	122.06
2	D	1368	AME	CT2-CT1-N	-6.49	105.10	116.10
2	D	1368	AME	OXT-C-O	-6.22	109.98	124.09
2	C	1368	AME	OT-CT1-CT2	-6.18	110.58	122.06
2	B	1368	AME	C-CA-N	5.13	122.69	110.55
2	A	1369	AME	OT-CT1-N	-5.09	112.59	121.95
2	C	1368	AME	OT-CT1-N	-5.02	112.72	121.95
2	B	1368	AME	CA-N-CT1	4.63	135.25	121.48
2	D	1368	AME	CE-SD-CG	4.55	116.03	100.40
2	B	1368	AME	OXT-C-O	-4.49	113.90	124.09
2	C	1368	AME	O-C-CA	-4.16	108.61	122.26
2	C	1368	AME	CB-CA-C	4.10	120.24	110.35
2	A	1369	AME	CE-SD-CG	3.64	112.92	100.40
2	B	1368	AME	CB-CG-SD	-3.20	96.27	113.48
2	D	1368	AME	CA-N-CT1	3.04	130.53	121.48
2	A	1369	AME	O-C-CA	-3.01	112.39	122.26
2	B	1368	AME	CT2-CT1-N	2.98	121.14	116.10
2	C	1368	AME	CE-SD-CG	2.89	110.31	100.40
2	D	1368	AME	O-C-CA	-2.70	113.40	122.26
2	C	1368	AME	CG-CB-CA	2.63	120.38	112.91
2	C	1368	AME	C-CA-N	-2.49	104.65	110.55
2	D	1368	AME	CB-CA-N	-2.49	105.85	110.88
2	A	1369	AME	CB-CG-SD	-2.38	100.66	113.48
2	B	1368	AME	CG-CB-CA	-2.36	106.20	112.91
2	B	1368	AME	O-C-CA	-2.06	115.48	122.26

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	CA-CB-CG-SD
2	B	1368	AME	C-CA-CB-CG
2	C	1368	AME	CA-CB-CG-SD
2	C	1368	AME	C-CA-CB-CG
2	D	1368	AME	CT2-CT1-N-CA
2	D	1368	AME	CA-CB-CG-SD
2	A	1369	AME	OT-CT1-N-CA
2	C	1368	AME	OT-CT1-N-CA
2	B	1368	AME	CT2-CT1-N-CA

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

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1369	AME	11	0
2	D	1368	AME	14	0
2	B	1368	AME	13	0
2	C	1368	AME	7	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%)	-0.47	0	100	100	24, 39, 60, 81	0
1	B	367/368 (99%)	-0.48	0	100	100	28, 45, 66, 95	0
1	C	367/368 (99%)	-0.39	0	100	100	30, 51, 74, 91	0
1	D	367/368 (99%)	-0.32	1 (0%)	94	95	30, 49, 71, 90	0
All	All	1469/1472 (99%)	-0.42	1 (0%)	95	96	24, 47, 70, 95	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	355	LEU	2.1

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 monosaccharides 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
3	MG	A	1370	1/1	0.92	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	1369	1/1	0.95	0.08	63,63,63,63	0
3	MG	C	1369	1/1	0.95	0.04	55,55,55,55	0
2	AME	D	1368	12/12	0.97	0.28	49,64,80,83	0
2	AME	B	1368	12/12	0.97	0.20	38,58,72,78	0
2	AME	A	1369	12/12	0.98	0.20	50,61,71,77	0
2	AME	C	1368	12/12	0.98	0.17	56,67,76,79	0
3	MG	D	1369	1/1	0.99	0.21	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.