Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 04:38 PM EST

PDB ID	:	2QRE
Title	:	Crystal structure of the adenylate sensor from AMP-activated protein kinase in complex with 5-aminoimidazole-4-carboxamide 1-beta-D-ribofuranotide (ZMP)
Authors	:	Jin, X.; Townley, R.; Shapiro, L.
Deposited on	:	2007-07-28
Resolution	:	3.01 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

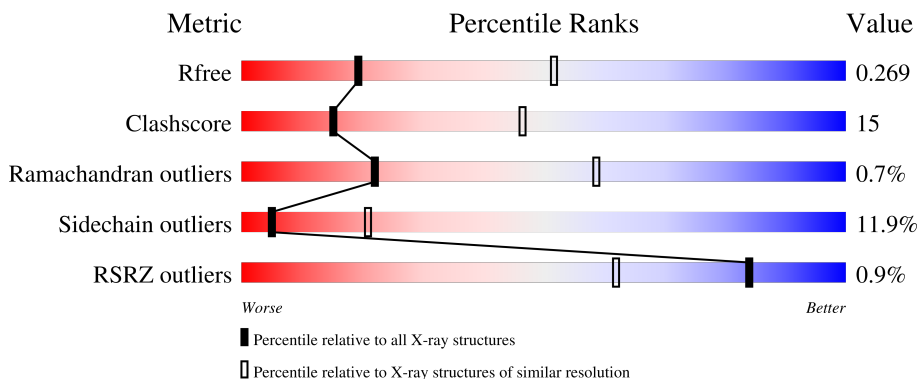|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.
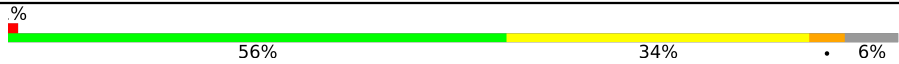
Metric	Percentile Ranks	Value
Rfree		0.269
Clashscore		15
Ramachandran outliers		0.7%
Sidechain outliers		11.9%
RSRZ outliers		0.9%

Worse *Better*

▌ Percentile relative to all X-ray structures

⫿ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	137	47% 28% · · 20%
1	C	137	.% 55% 23% · 18%
2	B	97	2% 55% 27% 6% 12%
2	D	97	2% 57% 32% 5% 6%

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Mol	Chain	Length	Quality of chain
3	E	334	56% 34% 6%
3	G	334	63% 25% 6% 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8201 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total 882	C 572	N 148	O 153	S 9	0	0	0
1	C	113	Total 903	C 583	N 155	O 156	S 9	0	0	0

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	85	Total 668	C 428	N 115	O 123	S 2	0	0	0
2	D	91	Total 718	C 459	N 123	O 134	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	expression tag	UNP P78789
D	202	MET	-	expression tag	UNP P78789

- Molecule 3 is a protein called Protein C1556.08c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	315	Total 2478	C 1585	N 414	O 464	S 15	0	0	0
3	E	315	Total 2489	C 1591	N 417	O 466	S 15	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP Q10343
G	2	MET	-	expression tag	UNP Q10343

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	expression tag	UNP Q10343
E	2	MET	-	expression tag	UNP Q10343

- Molecule 4 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (three-letter code: AMZ) (formula: $C_9H_{15}N_4O_8P$).
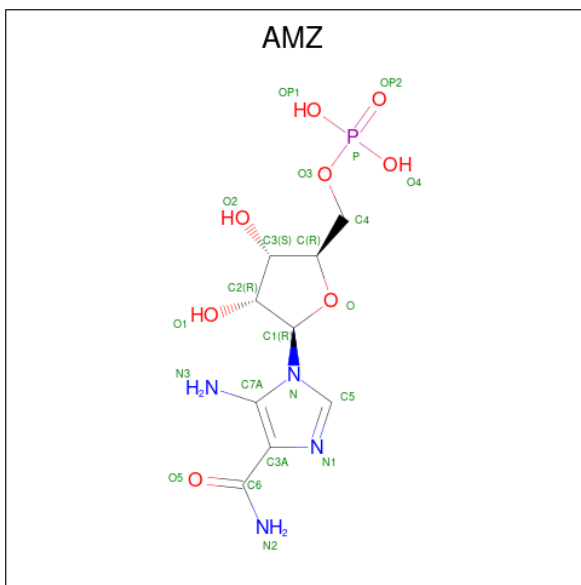
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total 22	C 9	N 4	O 8	P 1	0	0
4	E	1	Total 22	C 9	N 4	O 8	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	G	9	Total 9	O 9	0	0
5	C	2	Total 2	O 2	0	0
5	D	2	Total 2	O 2	0	0
5	E	4	Total 4	O 4	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: SNF1-like protein kinase ssp2
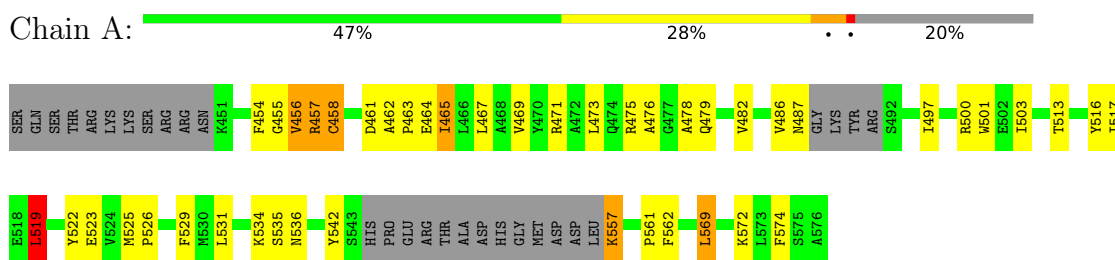
- Molecule 1: SNF1-like protein kinase ssp2
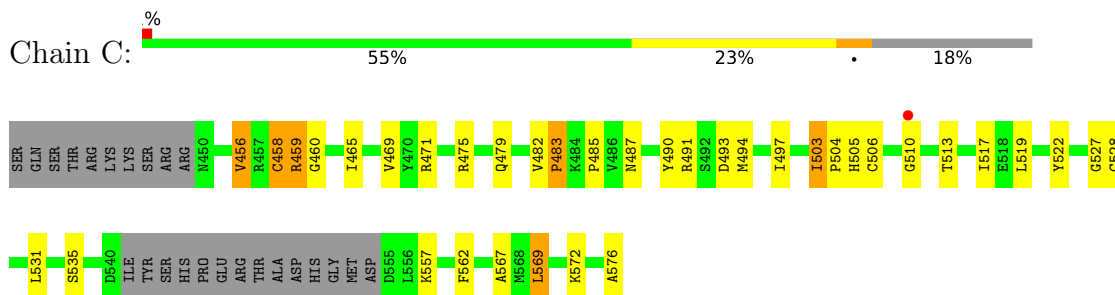
- Molecule 2: SPCC1919.03c protein

- Molecule 2: SPCC1919.03c protein

D297 VAL

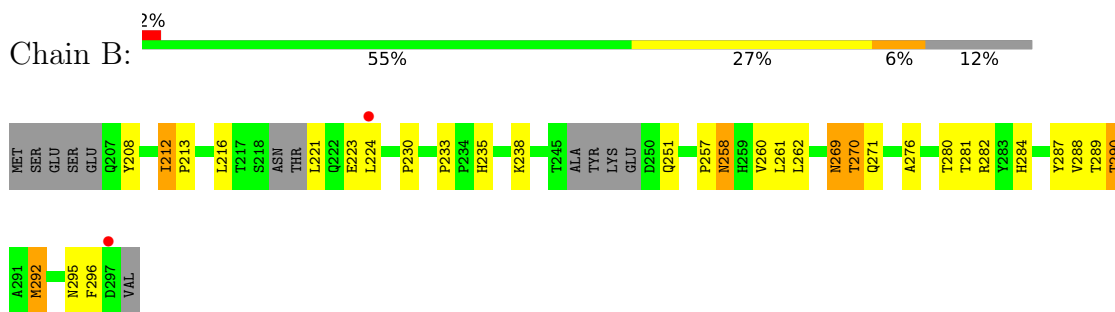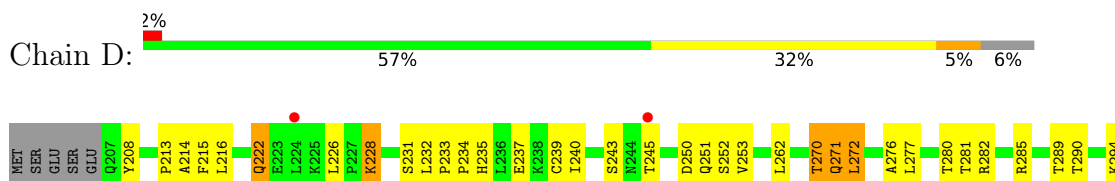• Molecule 3: Protein C1556.08c

Chain G: 63%   25%   6%   6%

ALA M2 Q5 E6 T7 A11 L12 I15 Q16 L28 P29 T30 S31 F37 D38 V39 T40 L41 L47 L50 T51 N54 S57 L60 A69 F77 I81 F90 P91 E92 E96 I97 D98 K99 F100 R101 L102 L103 G104 L105 R106 E107 V108 E109 R110

K111 I112 V122 H123 P124 M125 H126 C132 M135 R139 I143 P144 L145 I146 S154 V158 L161 S171 M179 L180 R181 V182 P183 L184 I189 W192 L195 A196 T197 A198 Y205 D206 V207 I208 K209 M210 L211 K214 S217 I221 T227 L228

L229 N230 D236 L240 I241 Q242 N248 V253 L257 R260 P261 R271 A272 T273 D274 R275 L276 D277 G278 I279 F280 I283 R287 V288 N297 I303 L304 S305 D308 I309 L310 N311 Y312 I313 I314 Y315 D316 LYS THR THR PRO GLY VAL PRO GLU GLN THR

ASP ASN PHE GLU SER ALA VAL

• Molecule 3: Protein C1556.08c

Chain E: %   56%   34%   •   6%

ALA M2 D3 V4 Q5 E6 K9 F18 I19 R20 T30 R33 L34 I35 V36 F37 D38 V39 T40 L41 T45 S48 N54 I55 A69 G70 L71 L72 T73 M74 A75 D76 F77 V78 I81 K82 Y83 S89 F90 P91 E92 A93 I94 A95 E96 I97 D98 K99 F100 R101

L102 E107 V108 E109 R110 K111 I112 I115 P116 P117 E118 T119 V122 H123 H126 S127 L128 M129 D130 A131 R139 R142 I143 P144 L145 I146 D147 V148 T152 E155 M156 I157 V158 S159 V160 L161 T162 R165 I166 L167 I170 S171 C174 K175 E176 T177 L180

L184 N185 T188 I189 L195 A196 T197 A198 T202 K203 V204 Y205 D206 V207 I208 K209 M210 L211 K214 N215 I216 P220 I221 V222 N223 T227 L228 L229 N230 V231 H239 L240 I241 Q242 D243 L249 S252 E255 A256 L257 R260 P261 D265 G266 V267 A272

R275 L276 D277 G278 I279 F280 I283 R287 V288 H289 F292 E296 G302 I303 L304 S305 D308 I309 L310 N311 Y312 I313 D316 LYS THR THR PRO GLY VAL PRO GLU GLN THR ASP ASN PHE GLU SER ALA VAL

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.47Å 78.15Å 108.51Å 90.00° 124.04° 90.00°	Depositor
Resolution (Å)	41.34 – 3.01 41.34 – 3.01	Depositor EDS
% Data completeness (in resolution range)	89.2 (41.34-3.01) 89.2 (41.34-3.01)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.297 0.247 , 0.269	Depositor DCC
R_{free} test set	1074 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	84.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8201	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.58	0/904	0.70	2/1215 (0.2%)
1	C	0.55	0/926	0.63	0/1246
2	B	0.49	0/683	0.85	4/931 (0.4%)
2	D	0.49	0/736	0.75	1/1006 (0.1%)
3	E	0.53	0/2534	0.68	0/3433
3	G	0.52	0/2520	0.69	2/3415 (0.1%)
All	All	0.53	0/8303	0.70	9/11246 (0.1%)

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
3	E	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	258	ASN	CB-CA-C	6.89	124.17	110.40
2	B	224	LEU	N-CA-C	-6.25	94.13	111.00
2	B	223	GLU	N-CA-C	6.10	127.48	111.00
1	A	519	LEU	CA-CB-CG	5.86	128.79	115.30
2	B	223	GLU	CB-CA-C	-5.77	98.86	110.40
2	D	297	ASP	N-CA-CB	5.60	120.69	110.60
3	G	228	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	569	LEU	CA-CB-CG	5.17	127.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	96	GLU	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	2	MET	Peptide
3	G	209	LYS	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	882	0	880	33	0
1	C	903	0	889	23	0
2	B	668	0	676	23	0
2	D	718	0	724	22	0
3	E	2489	0	2545	90	0
3	G	2478	0	2530	81	0
4	E	22	0	13	1	0
4	G	22	0	13	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	0	0
5	G	9	0	0	0	0
All	All	8201	0	8270	246	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 15.

All (246) 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)
3:G:81:ILE:HD11	3:G:208:ILE:CD1	1.41	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:81:ILE:CD1	3:G:208:ILE:CD1	2.22	1.18
3:G:81:ILE:CD1	3:G:208:ILE:HD11	1.72	1.16
3:E:3:ASP:O	3:E:4:VAL:HG12	1.57	1.03
3:G:208:ILE:HA	3:G:211:LEU:HD12	1.41	1.02
3:G:81:ILE:HD11	3:G:208:ILE:HD12	1.42	0.98
1:C:456:VAL:HG13	1:C:531:LEU:HB3	1.49	0.94
3:G:81:ILE:HD11	3:G:208:ILE:HD11	0.93	0.91
3:G:81:ILE:CD1	3:G:208:ILE:HD12	1.97	0.89
3:E:239:HIS:HA	3:E:242:GLN:HE21	1.38	0.86
3:E:4:VAL:HG13	3:E:5:GLN:N	1.94	0.83
3:E:4:VAL:CG1	3:E:5:GLN:H	1.93	0.82
3:G:144:PRO:HB2	3:G:146:ILE:CD1	2.09	0.82
3:G:123:HIS:HB3	3:G:126:HIS:CD2	2.15	0.81
3:G:122:VAL:HG22	3:G:143:ILE:HD13	1.63	0.80
3:E:4:VAL:CG1	3:E:5:GLN:N	2.44	0.79
3:E:296:GLU:CD	3:E:296:GLU:H	1.86	0.79
3:G:181:ARG:HA	3:G:275:ARG:HG3	1.64	0.79
3:E:265:ASP:CG	3:E:289:HIS:HE2	1.86	0.78
3:G:207:VAL:O	3:G:210:MET:HB2	1.83	0.78
3:E:83:TYR:CD1	3:E:112:ILE:HD13	2.18	0.77
3:E:123:HIS:HE1	3:E:147:ASP:OD1	1.66	0.77
3:G:81:ILE:CG1	3:G:208:ILE:HD12	2.15	0.77
3:E:123:HIS:CE1	3:E:147:ASP:OD1	2.38	0.76
1:A:462:ALA:HB3	1:A:463:PRO:HD3	1.68	0.74
3:G:283:ILE:HG22	3:G:288:VAL:HB	1.68	0.74
3:E:265:ASP:HB3	3:E:287:ARG:NH2	2.03	0.73
3:G:279:ILE:HD11	3:G:309:ILE:HD13	1.70	0.71
2:D:222:GLN:HE21	2:D:222:GLN:HA	1.56	0.70
1:A:534:LYS:HE3	1:A:536:ASN:HD21	1.58	0.69
3:E:208:ILE:HA	3:E:211:LEU:HD12	1.73	0.69
3:E:37:PHE:HB3	3:E:41:LEU:HD12	1.74	0.68
3:G:123:HIS:HD2	3:G:125:MET:H	1.41	0.68
3:G:304:LEU:HD11	3:G:309:ILE:HG22	1.76	0.68
3:E:205:TYR:HA	3:E:208:ILE:HG12	1.74	0.68
3:G:96:GLU:O	3:G:96:GLU:HG2	1.93	0.67
1:A:465:ILE:HG23	3:E:89:SER:HB3	1.77	0.66
1:A:482:VAL:HG22	2:B:213:PRO:HG3	1.78	0.66
2:D:234:PRO:O	2:D:237:GLU:HB2	1.95	0.66
1:A:557:LYS:O	2:B:281:THR:OG1	2.14	0.66
1:C:485:PRO:HG3	1:C:490:TYR:CE2	2.31	0.65
1:C:503:ILE:HD11	1:C:505:HIS:ND1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:VAL:HG12	3:E:5:GLN:H	1.62	0.65
3:G:106:ARG:HH21	3:G:110:ARG:NH1	1.95	0.65
3:E:265:ASP:HB3	3:E:287:ARG:CZ	2.28	0.64
1:C:479:GLN:HB3	2:D:208:TYR:HB3	1.80	0.64
3:G:97:ILE:HG12	3:G:97:ILE:O	1.97	0.64
3:E:122:VAL:HG21	3:E:131:ALA:HB2	1.81	0.63
3:G:81:ILE:HG12	3:G:208:ILE:HD12	1.81	0.62
3:G:221:ILE:HD11	3:G:253:VAL:HG11	1.81	0.62
1:C:503:ILE:HD12	1:C:506:CYS:SG	2.39	0.62
3:G:305:SER:O	3:G:308:ASP:HB2	1.99	0.62
3:G:144:PRO:HB2	3:G:146:ILE:HD13	1.80	0.61
1:C:459:ARG:HD2	1:C:528:CYS:SG	2.40	0.61
3:E:252:SER:OG	3:E:255:GLU:HG3	2.00	0.61
3:G:108:VAL:O	3:G:112:ILE:HG12	2.00	0.61
3:G:196:ALA:HB2	3:G:214:LYS:HD2	1.82	0.60
1:A:475:ARG:HB3	1:A:572:LYS:HE2	1.83	0.60
3:G:210:MET:O	3:G:214:LYS:HB2	2.01	0.60
3:E:167:LEU:HB3	3:E:283:ILE:CD1	2.32	0.60
3:G:16:GLN:HG2	3:G:313:ILE:O	2.03	0.59
2:B:280:THR:HA	2:B:289:THR:HA	1.84	0.59
3:E:77:PHE:O	3:E:81:ILE:HG13	2.03	0.59
1:C:503:ILE:HG22	1:C:513:THR:O	2.03	0.59
1:A:534:LYS:HE3	1:A:536:ASN:ND2	2.18	0.58
3:E:292:PHE:HD2	3:E:303:ILE:HG12	1.68	0.58
3:G:77:PHE:O	3:G:81:ILE:HG23	2.04	0.58
3:G:311:ASN:HA	3:G:314:ILE:HG12	1.84	0.58
2:B:233:PRO:HB2	2:B:235:HIS:CD2	2.39	0.58
3:E:204:VAL:HG11	3:E:240:LEU:HD21	1.85	0.58
2:D:280:THR:OG1	2:D:289:THR:HG23	2.04	0.58
3:G:37:PHE:HB3	3:G:41:LEU:HD12	1.86	0.57
1:C:465:ILE:O	1:C:469:VAL:HG23	2.05	0.57
3:E:305:SER:O	3:E:308:ASP:HB2	2.05	0.56
1:A:458:CYS:HB3	3:E:90:PHE:CD2	2.40	0.56
3:G:38:ASP:OD1	3:G:40:THR:OG1	2.17	0.56
3:G:96:GLU:O	3:G:96:GLU:CG	2.52	0.56
1:A:503:ILE:HD13	1:A:561:PRO:HG3	1.86	0.56
2:B:258:ASN:O	2:B:262:LEU:HD13	2.05	0.56
3:G:39:VAL:HG11	3:G:69:ALA:CB	2.35	0.56
3:G:221:ILE:CD1	3:G:253:VAL:HG11	2.36	0.56
1:C:557:LYS:O	2:D:281:THR:OG1	2.24	0.56
3:E:40:THR:O	3:E:101:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HH11	1:A:457:ARG:HB3	1.71	0.55
2:D:271:GLN:O	2:D:271:GLN:HG3	2.05	0.55
2:B:296:PHE:CD2	3:E:96:GLU:HG2	2.42	0.55
3:E:3:ASP:O	3:E:4:VAL:CG1	2.44	0.55
3:E:39:VAL:HG11	3:E:69:ALA:CB	2.37	0.55
3:G:205:TYR:HA	3:G:208:ILE:CD1	2.37	0.55
3:E:265:ASP:OD1	3:E:289:HIS:NE2	2.26	0.54
1:C:519:LEU:HD11	1:C:569:LEU:HD11	1.89	0.54
1:A:535:SER:HB2	1:A:562:PHE:CD1	2.42	0.54
3:E:142:ARG:HG2	3:E:162:THR:HG22	1.90	0.54
3:E:214:LYS:O	3:E:216:ILE:HG23	2.06	0.54
3:E:292:PHE:CD2	3:E:303:ILE:HG12	2.43	0.54
1:A:501:TRP:CD1	1:A:517:ILE:HD12	2.43	0.53
3:G:139:ARG:O	3:G:139:ARG:HG3	2.08	0.53
3:E:276:LEU:HA	3:E:279:ILE:HG12	1.90	0.53
1:A:456:VAL:HG13	1:A:531:LEU:HB3	1.91	0.53
3:E:276:LEU:HD13	3:E:279:ILE:HG12	1.91	0.53
3:G:310:LEU:HD23	3:G:313:ILE:HD11	1.92	0.52
1:A:523:GLU:HA	1:A:529:PHE:CD2	2.44	0.52
1:A:486:VAL:HG13	1:A:486:VAL:O	2.08	0.52
3:G:209:LYS:HG2	3:G:210:MET:N	2.24	0.52
2:D:250:ASP:HB3	2:D:252:SER:OG	2.09	0.52
3:E:33[B]:ARG:NH2	3:E:35:ILE:HD11	2.25	0.52
3:E:116:PRO:HG2	3:E:118:GLU:O	2.09	0.52
1:C:471:ARG:O	1:C:475:ARG:HG3	2.08	0.52
1:C:491:ARG:O	1:C:494:MET:HB2	2.10	0.52
3:E:180:LEU:O	3:E:277:ASP:HB3	2.09	0.52
3:E:3:ASP:O	3:E:3:ASP:CG	2.48	0.52
3:E:204:VAL:HG11	3:E:240:LEU:CD2	2.40	0.52
1:C:458:CYS:O	1:C:459:ARG:HD3	2.10	0.52
1:A:465:ILE:CG2	3:E:89:SER:HB3	2.40	0.52
3:G:139:ARG:HD3	4:G:1001:AMZ:H7	1.92	0.52
3:G:236:ASP:OD2	3:G:260:ARG:NH1	2.43	0.52
3:E:101:ARG:HG2	3:E:101:ARG:HH11	1.75	0.52
2:D:272:LEU:HD13	3:E:45:THR:HG23	1.92	0.51
1:A:479:GLN:HB3	2:B:208:TYR:HB3	1.92	0.51
3:G:180:LEU:O	3:G:277:ASP:HB3	2.10	0.51
3:E:107:GLU:HG3	3:E:110:ARG:HH21	1.75	0.51
2:D:251:GLN:OE1	3:E:54:ASN:HB3	2.11	0.51
3:E:39:VAL:HG11	3:E:69:ALA:HB1	1.92	0.51
3:E:195:LEU:HD11	3:E:302:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:231:VAL:HG12	3:E:267:VAL:HG22	1.92	0.51
2:B:295:ASN:HD21	3:G:41:LEU:HA	1.76	0.51
3:E:40:THR:O	3:E:101:ARG:HG2	2.11	0.50
1:A:461:ASP:HB3	1:A:464:GLU:HB2	1.93	0.50
3:E:123:HIS:HB3	3:E:126:HIS:ND1	2.26	0.50
3:E:72:LEU:HD22	3:E:102:LEU:HD21	1.93	0.50
3:E:145:LEU:HD11	3:E:161:LEU:HD13	1.92	0.50
3:E:76:ASP:HA	3:E:109:GLU:OE1	2.12	0.50
1:A:497:ILE:HB	1:A:519:LEU:HD23	1.94	0.50
2:B:282:ARG:HG2	2:B:284:HIS:O	2.12	0.49
1:A:478:ALA:HB2	1:A:501:TRP:CD2	2.47	0.49
3:E:223:ASN:OD1	3:E:227:THR:HG23	2.11	0.49
3:G:260:ARG:HG3	3:G:261:PRO:HD2	1.94	0.49
1:A:454:PHE:CZ	2:B:261:LEU:HD13	2.48	0.49
1:A:523:GLU:HG3	1:A:529:PHE:CE2	2.48	0.49
2:D:262:LEU:HD21	2:D:282:ARG:HB2	1.95	0.49
3:E:279:ILE:HG13	3:E:280:PHE:N	2.28	0.49
1:A:500:ARG:HD3	2:B:208:TYR:CE1	2.48	0.48
3:G:7:THR:HG21	3:G:181:ARG:HH21	1.77	0.48
3:G:39:VAL:CG1	3:G:69:ALA:HB3	2.43	0.48
3:G:171:SER:HB2	3:G:280:PHE:HD2	1.77	0.48
3:E:205:TYR:O	3:E:208:ILE:HG13	2.13	0.48
2:B:251:GLN:HE22	3:G:54:ASN:HD22	1.61	0.48
3:E:159:SER:OG	3:E:160:VAL:N	2.46	0.48
1:A:574:PHE:CD1	3:E:93:ALA:HA	2.48	0.48
3:G:240:LEU:HG	3:G:248:ASN:HB3	1.95	0.48
2:B:276:ALA:HA	2:B:292:MET:O	2.14	0.48
3:G:111:LYS:HG2	3:G:112:ILE:HD13	1.96	0.48
3:G:123:HIS:CD2	3:G:125:MET:H	2.28	0.48
3:G:15:ILE:H	3:G:15:ILE:HG12	1.59	0.47
3:E:35:ILE:HD12	3:E:55:ILE:HD13	1.96	0.47
3:G:124:PRO:HG3	3:G:145:LEU:HB3	1.96	0.47
3:E:19:ILE:O	3:E:128:LEU:HB3	2.15	0.47
1:C:517:ILE:HD12	1:C:562:PHE:HD1	1.80	0.47
3:G:39:VAL:HG13	3:G:60:LEU:HB3	1.97	0.46
3:E:166:ILE:H	3:E:166:ILE:HG12	1.59	0.46
3:G:183:PRO:HB3	3:G:273:THR:O	2.16	0.46
3:E:19:ILE:HG22	3:E:128:LEU:HD23	1.96	0.46
3:E:196:ALA:HB2	3:E:214:LYS:HD2	1.97	0.46
3:G:310:LEU:HA	3:G:313:ILE:HD13	1.97	0.46
3:E:101:ARG:NH1	3:E:101:ARG:HG2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:195:LEU:HD22	3:G:303:ILE:HD12	1.98	0.46
1:A:522:TYR:HA	2:B:230:PRO:O	2.15	0.46
1:A:454:PHE:HZ	2:B:261:LEU:HD13	1.81	0.46
2:B:261:LEU:O	2:B:262:LEU:C	2.53	0.46
2:B:288:VAL:HG12	2:B:290:THR:HG22	1.98	0.46
3:E:4:VAL:HG13	3:E:5:GLN:H	1.63	0.46
3:E:170:ILE:O	3:E:174:CYS:HB2	2.16	0.45
3:G:106:ARG:HH21	3:G:110:ARG:HH12	1.62	0.45
3:G:51:THR:HG21	3:G:242:GLN:OE1	2.16	0.45
3:E:123:HIS:HB3	3:E:126:HIS:CE1	2.51	0.45
1:C:460:GLY:O	1:C:527:GLY:HA2	2.17	0.45
3:G:104:GLY:O	3:G:108:VAL:HG23	2.16	0.45
3:G:171:SER:CB	3:G:280:PHE:HD2	2.28	0.45
2:D:270:THR:HG23	2:D:276:ALA:HB2	1.99	0.45
2:B:270:THR:O	2:B:271:GLN:HB2	2.17	0.44
3:E:171:SER:HA	3:E:177:THR:HG21	1.99	0.44
3:E:210:MET:O	3:E:214:LYS:HB2	2.18	0.44
3:E:198:ALA:HB1	3:E:202:THR:OG1	2.17	0.44
3:E:198:ALA:O	3:E:221:ILE:HG23	2.17	0.44
3:G:39:VAL:HG11	3:G:69:ALA:HB1	2.00	0.44
3:E:6:GLU:O	3:E:9:LYS:HB3	2.18	0.44
1:A:467:LEU:HB2	2:B:216:LEU:HD22	2.00	0.44
1:C:572:LYS:O	1:C:576:ALA:HB2	2.17	0.44
3:G:39:VAL:HG11	3:G:69:ALA:HB3	1.99	0.44
2:B:257:PRO:HG2	2:B:287:TYR:CD2	2.53	0.43
3:G:28:LEU:HD21	3:G:145:LEU:HD12	2.00	0.43
3:G:132:CYS:HB3	3:G:314:ILE:HG21	2.01	0.43
3:G:271:ARG:HB3	3:G:273:THR:OG1	2.18	0.43
2:B:287:TYR:HB2	3:G:31:SER:HB2	2.00	0.43
3:G:16:GLN:CG	3:G:313:ILE:O	2.67	0.43
1:A:458:CYS:HA	3:E:91:PRO:HD3	2.00	0.43
3:G:145:LEU:HD11	3:G:161:LEU:HD13	1.99	0.43
3:G:217:SER:N	4:G:1001:AMZ:OP1	2.51	0.43
1:C:503:ILE:HA	1:C:504:PRO:HD3	1.83	0.43
2:D:276:ALA:O	2:D:277:LEU:HD23	2.19	0.43
3:E:139:ARG:HA	3:E:139:ARG:HD2	1.80	0.43
2:D:250:ASP:HB2	2:D:253:VAL:HG23	1.99	0.43
3:E:71:LEU:HD13	3:E:144:PRO:HG3	1.99	0.43
2:B:212:ILE:HA	2:B:213:PRO:HD3	1.90	0.43
2:B:269:ASN:OD1	2:B:269:ASN:N	2.52	0.43
3:E:189:ILE:HG21	3:E:312:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:MET:HB2	1:A:526:PRO:HD2	2.00	0.43
3:G:11:ALA:O	3:G:15:ILE:HG12	2.18	0.43
2:D:214:ALA:C	2:D:216:LEU:H	2.22	0.42
1:C:522:TYR:CD1	2:D:233:PRO:HD3	2.54	0.42
3:E:185:ASN:OD1	3:E:272:ALA:O	2.37	0.42
3:G:97:ILE:HA	3:G:100:PHE:HD1	1.84	0.42
3:E:72:LEU:HD11	3:E:77:PHE:CE1	2.54	0.42
3:E:197:THR:HG22	3:E:220:PRO:HG2	2.00	0.42
3:G:230:ASN:OD1	3:G:260:ARG:NH2	2.53	0.42
2:D:272:LEU:HD22	3:E:48:SER:CB	2.50	0.42
3:G:47:LEU:HD23	3:G:50:LEU:HD12	2.02	0.42
3:G:205:TYR:O	3:G:208:ILE:HG12	2.19	0.42
1:C:483:PRO:HB3	1:C:494:MET:HG3	2.02	0.42
3:E:39:VAL:CG1	3:E:69:ALA:CB	2.97	0.42
3:E:265:ASP:CG	3:E:289:HIS:NE2	2.64	0.42
3:G:198:ALA:O	3:G:221:ILE:HA	2.19	0.42
3:E:189:ILE:CG2	3:E:312:TYR:CD2	3.03	0.42
3:E:74:MET:O	3:E:78:VAL:HG23	2.20	0.41
1:C:483:PRO:O	1:C:485:PRO:HD3	2.20	0.41
2:D:251:GLN:NE2	3:E:54:ASN:OD1	2.47	0.41
3:G:184:LEU:HD13	3:G:274:ASP:O	2.20	0.41
3:E:148:VAL:HG12	3:E:155:GLU:HA	2.02	0.41
3:E:260:ARG:HG3	3:E:261:PRO:HD2	2.01	0.41
1:A:467:LEU:O	1:A:471:ARG:HG3	2.20	0.41
3:E:18:PHE:CE1	3:E:170:ILE:HG22	2.56	0.41
1:C:497:ILE:HB	1:C:519:LEU:HB2	2.03	0.41
3:E:240:LEU:HD23	3:E:249:LEU:HD23	2.02	0.41
3:G:90:PHE:HA	3:G:91:PRO:HD3	1.92	0.41
1:A:476:ALA:HB1	1:A:501:TRP:CZ3	2.56	0.41
1:A:500:ARG:HG3	1:A:516:TYR:CE1	2.56	0.41
3:G:189:ILE:O	3:G:192:TRP:NE1	2.31	0.41
3:G:96:GLU:O	3:G:99:LYS:HG2	2.21	0.41
3:G:124:PRO:HG2	3:G:158:VAL:HG21	2.02	0.41
1:A:469:VAL:O	1:A:473:LEU:HG	2.21	0.40
1:C:482:VAL:HG22	2:D:213:PRO:HG3	2.02	0.40
1:C:567:ALA:HB1	2:D:294:LYS:HE2	2.03	0.40
2:D:228:LYS:HD2	2:D:228:LYS:H	1.85	0.40
2:D:226:LEU:H	2:D:226:LEU:HD12	1.86	0.40
3:E:139:ARG:HH21	4:E:1002:AMZ:P	2.45	0.40
2:D:232:LEU:HA	2:D:233:PRO:HD3	1.90	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	103/137 (75%)	97 (94%)	5 (5%)	1 (1%)	15	50
1	C	109/137 (80%)	102 (94%)	5 (5%)	2 (2%)	8	35
2	B	79/97 (81%)	73 (92%)	6 (8%)	0	100	100
2	D	89/97 (92%)	74 (83%)	13 (15%)	2 (2%)	6	30
3	E	314/334 (94%)	284 (90%)	29 (9%)	1 (0%)	41	75
3	G	313/334 (94%)	291 (93%)	21 (7%)	1 (0%)	41	75
All	All	1007/1136 (89%)	921 (92%)	79 (8%)	7 (1%)	22	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	GLY
1	A	455	GLY
3	G	135	MET
2	D	215	PHE
2	D	243	SER
1	C	483	PRO
3	E	94	ILE

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	95/120 (79%)	85 (90%)	10 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	94/120 (78%)	86 (92%)	8 (8%)	10	36
2	B	77/88 (88%)	69 (90%)	8 (10%)	7	26
2	D	82/88 (93%)	70 (85%)	12 (15%)	3	14
3	E	280/296 (95%)	244 (87%)	36 (13%)	4	18
3	G	278/296 (94%)	244 (88%)	34 (12%)	5	20
All	All	906/1008 (90%)	798 (88%)	108 (12%)	5	21

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	VAL
1	A	457	ARG
1	A	458	CYS
1	A	465	ILE
1	A	487	ASN
1	A	513	THR
1	A	519	LEU
1	A	542	TYR
1	A	557	LYS
1	A	569	LEU
2	B	212	ILE
2	B	221	LEU
2	B	238	LYS
2	B	260	VAL
2	B	269	ASN
2	B	270	THR
2	B	290	THR
2	B	292	MET
3	G	5	GLN
3	G	12	LEU
3	G	15	ILE
3	G	28	LEU
3	G	30	THR
3	G	31	SER
3	G	39	VAL
3	G	57	SER
3	G	81	ILE
3	G	92	GLU
3	G	97	ILE
3	G	102	LEU

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Mol	Chain	Res	Type
3	G	110	ARG
3	G	143	ILE
3	G	154	SER
3	G	171	SER
3	G	179	MET
3	G	197	THR
3	G	206	ASP
3	G	209	LYS
3	G	214	LYS
3	G	227	THR
3	G	230	ASN
3	G	257	LEU
3	G	271	ARG
3	G	275	ARG
3	G	277	ASP
3	G	279	ILE
3	G	283	ILE
3	G	287	ARG
3	G	297	ASN
3	G	305	SER
3	G	310	LEU
3	G	313	ILE
1	C	456	VAL
1	C	458	CYS
1	C	459	ARG
1	C	487	ASN
1	C	493	ASP
1	C	503	ILE
1	C	535	SER
1	C	569	LEU
2	D	222	GLN
2	D	228	LYS
2	D	231	SER
2	D	235	HIS
2	D	239	CYS
2	D	240	ILE
2	D	245	THR
2	D	270	THR
2	D	271	GLN
2	D	272	LEU
2	D	285	ARG
2	D	290	THR

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Mol	Chain	Res	Type
3	E	2	MET
3	E	5	GLN
3	E	20	ARG
3	E	30	THR
3	E	39	VAL
3	E	94	ILE
3	E	96	GLU
3	E	98	ASP
3	E	99	LYS
3	E	101	ARG
3	E	112	ILE
3	E	115	ILE
3	E	119	THR
3	E	129	MET
3	E	130	ASP
3	E	139	ARG
3	E	148	VAL
3	E	157	ILE
3	E	161	LEU
3	E	165	ARG
3	E	166	ILE
3	E	175	LYS
3	E	184	LEU
3	E	185	ASN
3	E	188	THR
3	E	207	VAL
3	E	227	THR
3	E	228	LEU
3	E	243	ASP
3	E	257	LEU
3	E	265	ASP
3	E	275	ARG
3	E	279	ILE
3	E	309	ILE
3	E	310	LEU
3	E	313	ILE

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	487	ASN
1	A	536	ASN

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Mol	Chain	Res	Type
2	B	235	HIS
2	B	284	HIS
2	B	295	ASN
3	G	53	ASN
3	G	54	ASN
3	G	86	GLN
3	G	123	HIS
3	G	126	HIS
3	G	173	ASN
3	G	185	ASN
1	C	536	ASN
2	D	219	ASN
2	D	222	GLN
2	D	263	ASN
2	D	284	HIS
3	E	66	ASN
3	E	123	HIS
3	E	163	GLN
3	E	242	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\#|Z| > 2$
4	AMZ	E	1002	-	18,23,23	0.77	0	22,35,35	1.36	3 (13%)
4	AMZ	G	1001	-	18,23,23	0.81	0	22,35,35	1.17	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMZ	E	1002	-	-	5/6/30/30	0/2/2/2
4	AMZ	G	1001	-	-	0/6/30/30	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1002	AMZ	C5-N1-C3A	2.86	108.44	102.99
4	E	1002	AMZ	C3A-C6-N2	2.65	119.94	115.75
4	G	1001	AMZ	O4-P-OP2	2.14	119.06	110.68
4	G	1001	AMZ	O4-P-O3	-2.04	101.31	106.73
4	E	1002	AMZ	O4-P-OP1	2.03	115.40	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1002	AMZ	C4-O3-P-OP1
4	E	1002	AMZ	C4-O3-P-O4
4	E	1002	AMZ	C4-O3-P-OP2
4	E	1002	AMZ	O-C-C4-O3
4	E	1002	AMZ	C3-C-C4-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1002	AMZ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1001	AMZ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AMZ E 1002

Bond lengths   Bond angles   Torsions   Rings

Ligand AMZ G 1001

Bond lengths   Bond angles   Torsions   Rings
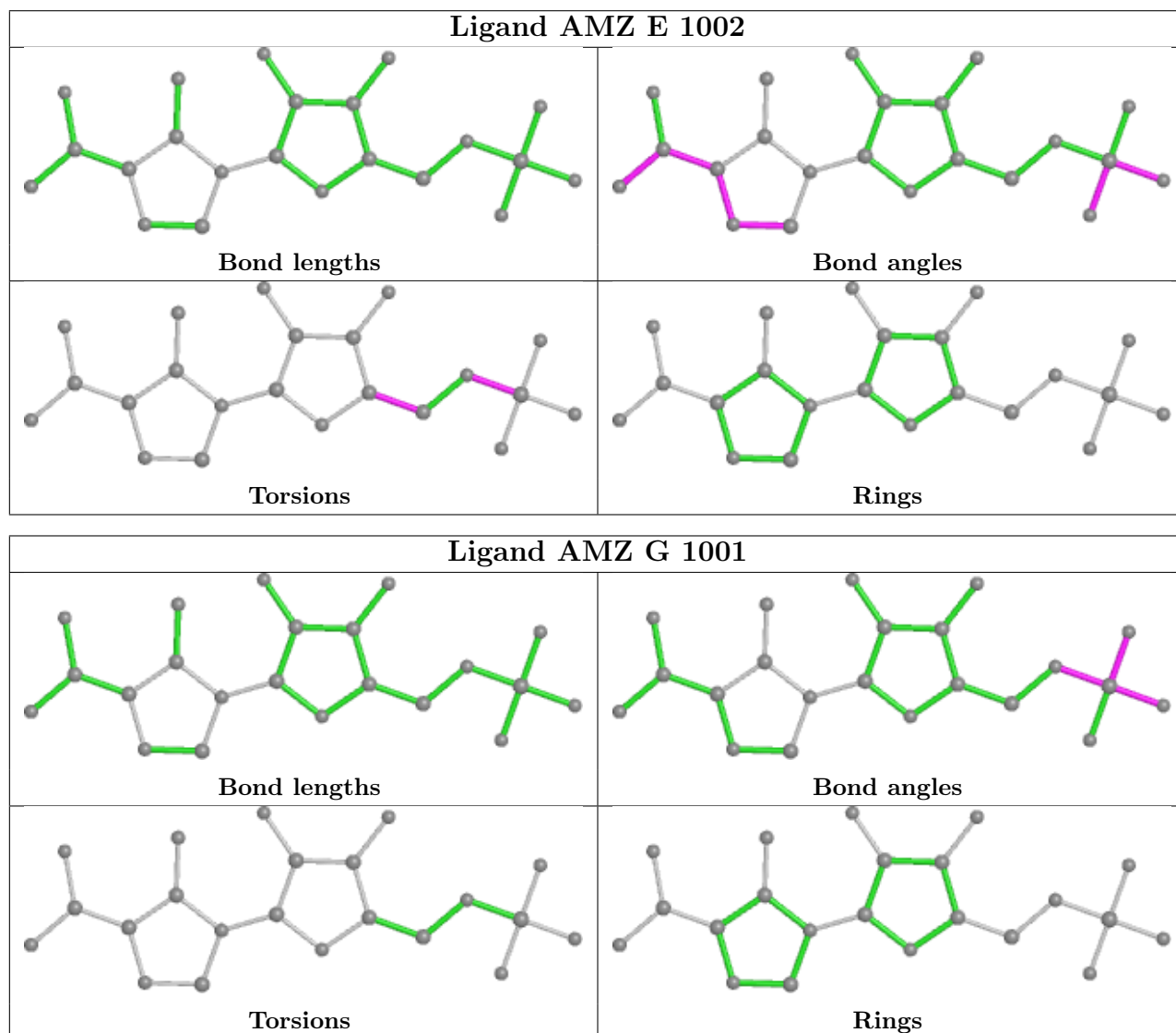
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	109/137 (79%)	-0.25	0	100	100	82, 90, 94, 98	1 (0%)
1	C	113/137 (82%)	-0.15	1 (0%)	84	62	84, 90, 95, 98	0
2	B	85/97 (87%)	-0.20	2 (2%)	59	30	28, 89, 95, 99	0
2	D	91/97 (93%)	0.07	2 (2%)	62	32	28, 90, 94, 96	0
3	E	315/334 (94%)	-0.34	3 (0%)	82	58	32, 90, 97, 104	1 (0%)
3	G	315/334 (94%)	-0.39	1 (0%)	94	83	28, 89, 97, 109	1 (0%)
All	All	1028/1136 (90%)	-0.28	9 (0%)	84	62	28, 90, 96, 109	3 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	224	LEU	3.6
3	E	304	LEU	3.3
2	B	224	LEU	3.3
1	C	510	GLY	3.3
3	E	152	THR	2.6
2	B	297	ASP	2.3
2	D	245	THR	2.3
3	E	230	ASN	2.2
3	G	304	LEU	2.2

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

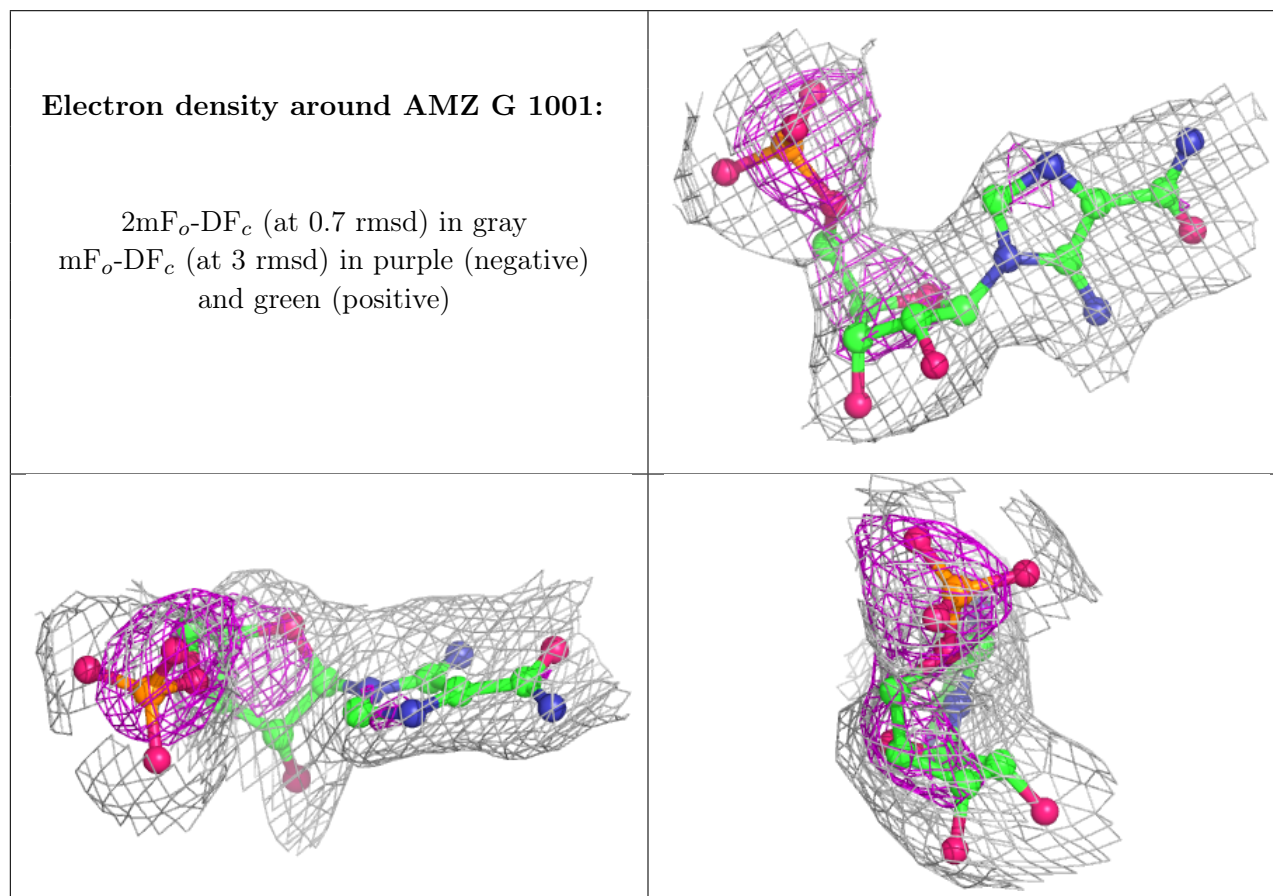There are no non-standard protein/DNA/RNA residues in this entry.

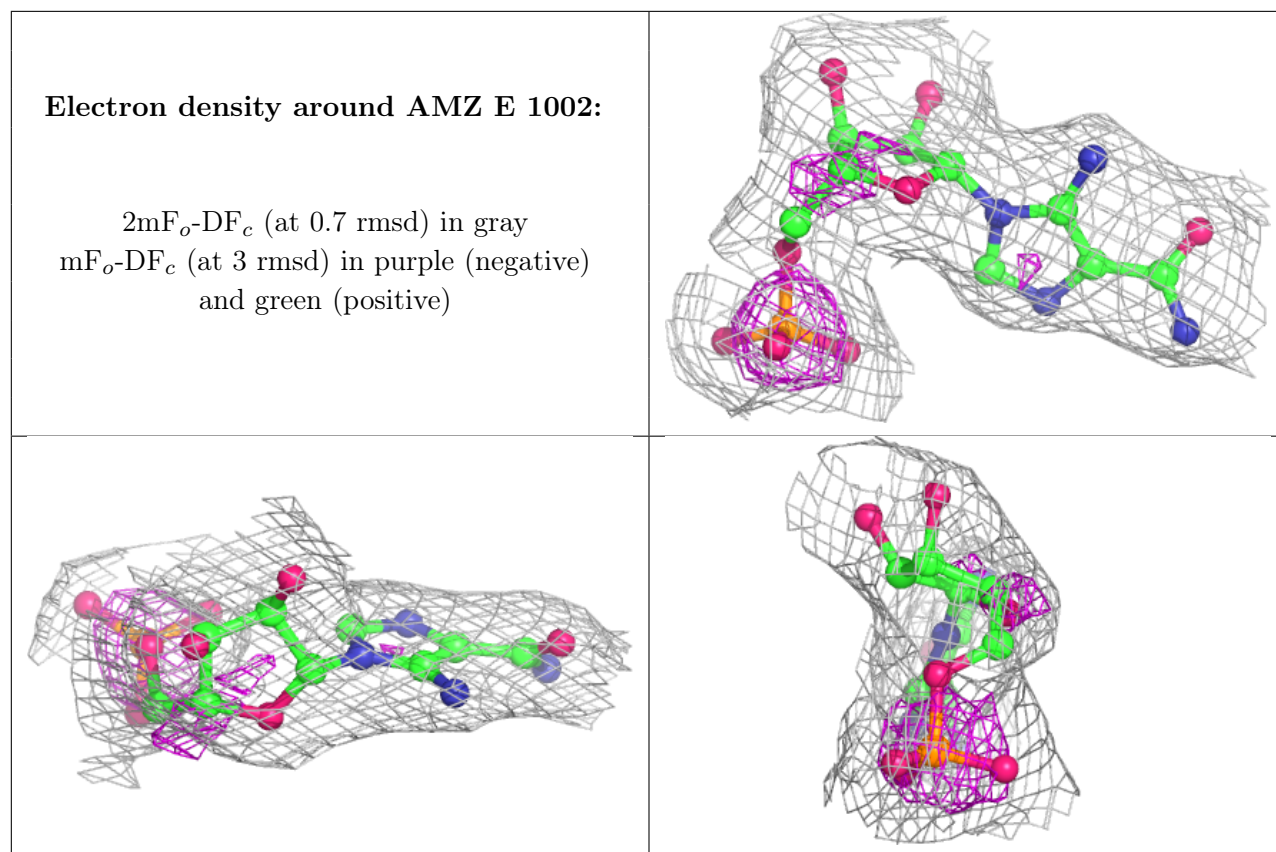## 6.3 Carbohydrates ⓘ

There are no 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($\mathring{A}^2$)	Q<0.9
4	AMZ	G	1001	22/22	0.95	0.15	77,79,80,81	0
4	AMZ	E	1002	22/22	0.96	0.14	82,85,90,90	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMZ G 1001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around AMZ E 1002:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.