Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 10:40 AM EDT

PDB ID	:	2ZZG
Title	:	Crystal structure of alanyl-tRNA synthetase in complex with 5''-O-(N-(L-alanyl)-sulfamyoxyl) adenine without oligomerization domain
Authors	:	Sokabe, M.; Ose, T.; Tokunaga, K.; Nakamura, A.; Nureki, O.; Yao, M.; Tanaka, I.
Deposited on	:	2009-02-10
Resolution	:	3.10 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 3.10 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.

Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution
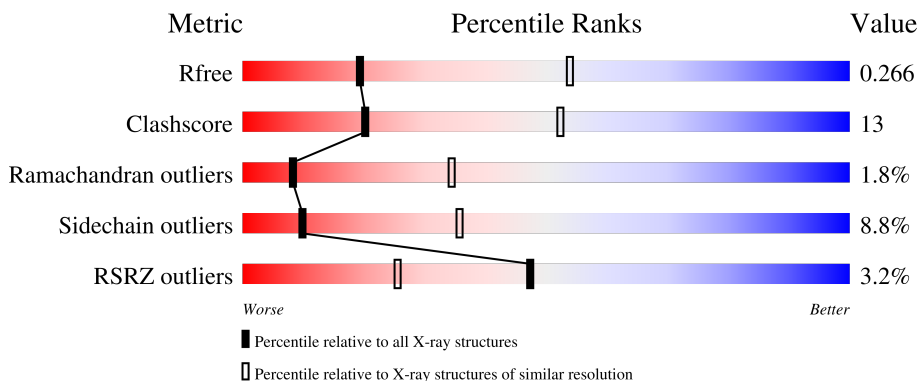
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	752	3% / 68% / 27% / • •
1	B	752	4% / 63% / 31% / • •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12055 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 Alanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			6004	3871	1024	1079	30			
1	B	737	Total	C	N	O	S	0	0	0
			5989	3860	1023	1076	30			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is '5'-O-(N-(L-ALANYL)-SULFAMOYL)ADENOSINE (three-letter code: A5A) (formula: $C_{13}H_{19}N_7O_7S$).
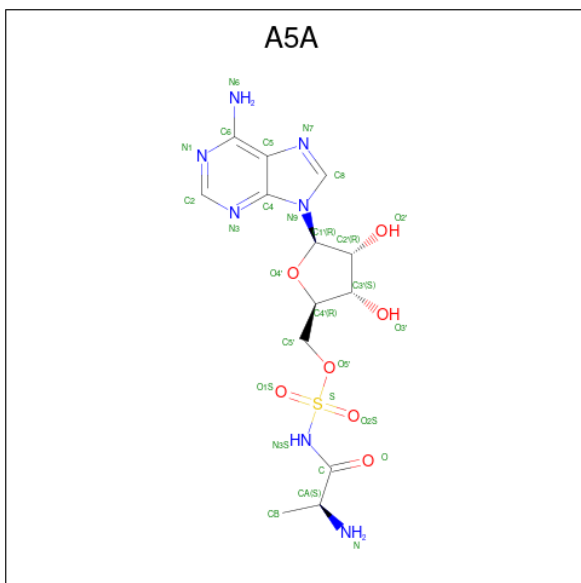
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	13	7	7	1		
3	B	1	Total	C	N	O	S	0	0
			28	13	7	7	1		

• Molecule 4 is water.

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

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: Alanyl-tRNA synthetase

Chain A:

• Molecule 1: Alanyl-tRNA synthetase

Chain B:
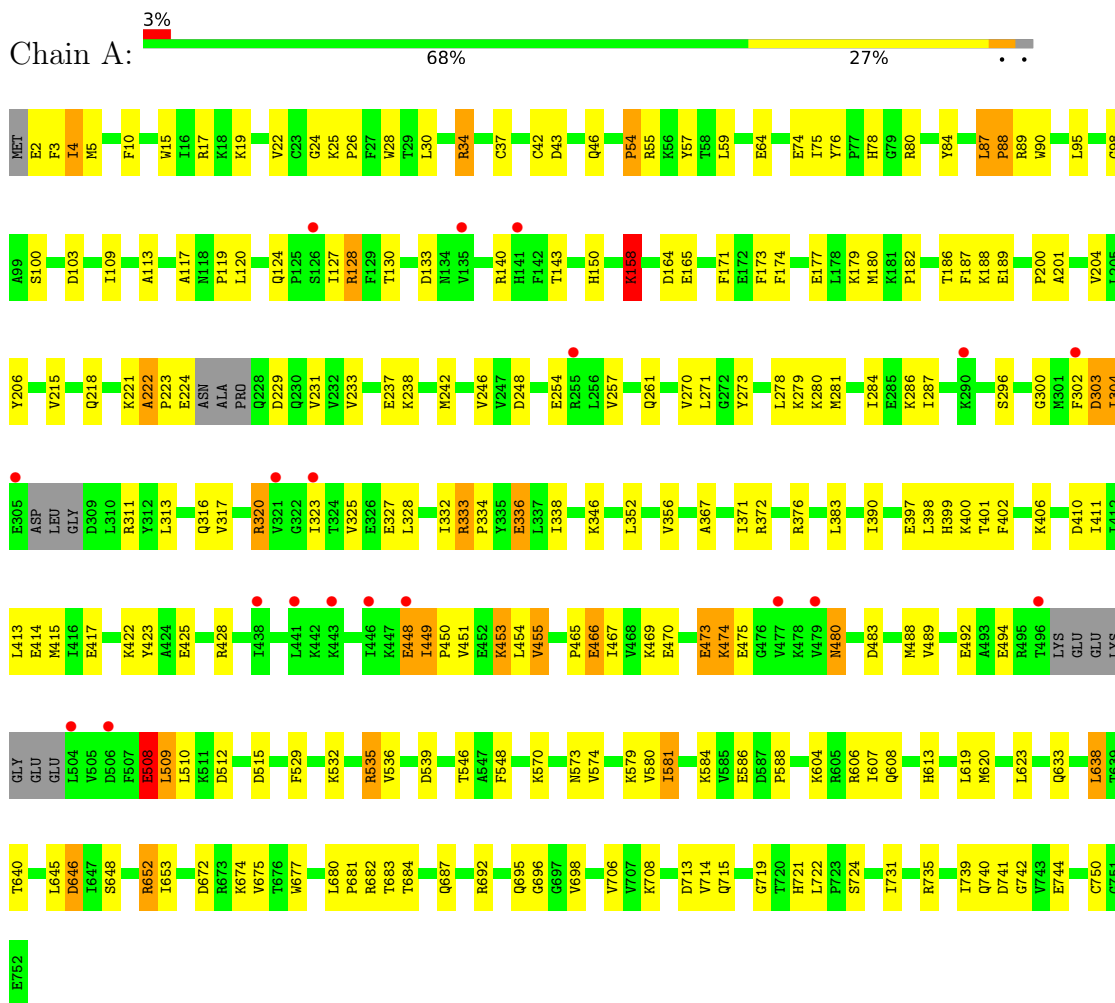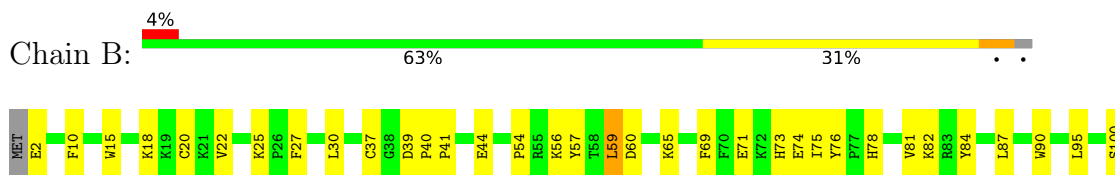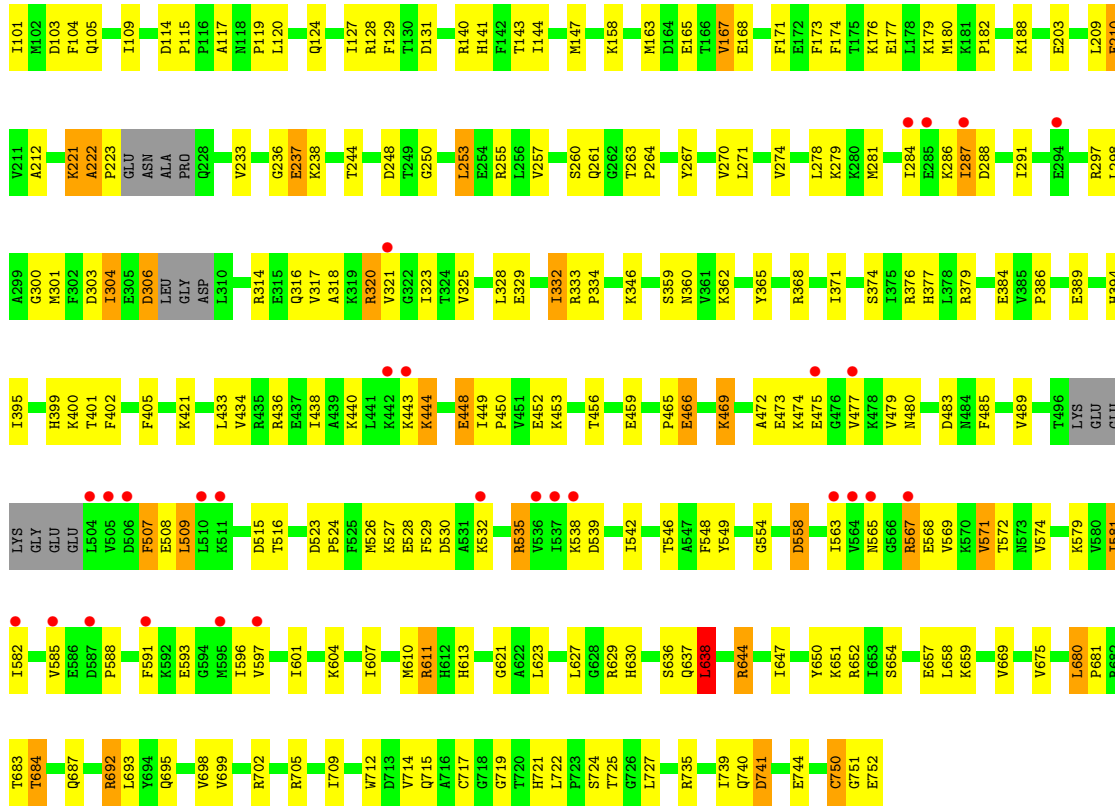
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.87Å 89.20Å 94.91Å 117.31° 90.40° 107.36°	Depositor
Resolution (Å)	50.00 – 3.10 38.59 – 3.07	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-3.10) 96.0 (38.59-3.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0039	Depositor
R, R_{free}	0.199 , 0.272 0.192 , 0.266	Depositor DCC
R_{free} test set	1736 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	70.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12055	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: A5A, ZN

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	0.57	0/6143	0.68	1/8290 (0.0%)
1	B	0.56	0/6127	0.68	1/8269 (0.0%)
All	All	0.57	0/12270	0.68	2/16559 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	638	LEU	CA-CB-CG	5.24	127.35	115.30

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	6004	0	6072	146	0
1	B	5989	0	6060	158	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	28	0	19	1	0
3	B	28	0	19	3	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
All	All	12055	0	12170	303	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 13.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:GLN:HE21	1:A:640:THR:HB	1.08	1.14
1:A:683:THR:O	1:A:687:GLN:HG2	1.55	1.07
1:B:222:ALA:HB1	1:B:223:PRO:HA	1.35	1.04
1:B:222:ALA:CB	1:B:223:PRO:HA	1.97	0.93
1:A:608:GLN:NE2	1:A:640:THR:HB	1.83	0.93
1:A:222:ALA:HB1	1:A:223:PRO:HA	1.50	0.92
1:A:222:ALA:CB	1:A:223:PRO:HA	2.05	0.86
1:A:54:PRO:HG2	1:A:179:LYS:HB2	1.58	0.85
1:B:654:SER:OG	1:B:657:GLU:HG3	1.76	0.85
1:A:4:ILE:HG23	1:A:5:MET:H	1.44	0.81
1:A:222:ALA:HB1	1:A:223:PRO:CA	2.11	0.81
1:B:25:LYS:HD2	1:B:188:LYS:HE2	1.66	0.78
1:B:669:VAL:HG13	1:B:725:THR:O	1.85	0.77
1:A:173:PHE:O	1:A:177:GLU:HB2	1.88	0.74
1:A:4:ILE:CG2	1:A:5:MET:H	2.01	0.74
1:B:237:GLU:O	1:B:238:LYS:HB2	1.88	0.73
1:B:304:ILE:HG21	1:B:483:ASP:HB2	1.70	0.73
1:A:279:LYS:HG2	1:A:284:ILE:HD11	1.71	0.72
1:A:4:ILE:HG23	1:A:5:MET:N	2.04	0.72
1:A:652:ARG:HH11	1:A:744:GLU:HB3	1.54	0.71
1:B:222:ALA:CB	1:B:223:PRO:CA	2.68	0.71
1:B:604:LYS:HA	1:B:607:ILE:HG22	1.72	0.71
1:B:386:PRO:HG2	1:B:389:GLU:HG3	1.72	0.70
1:A:128:ARG:NH2	3:A:999:A5A:O1S	2.26	0.69
1:A:470:GLU:HA	1:A:473:GLU:OE1	1.91	0.69
1:A:84:TYR:H	1:A:124:GLN:HE22	1.41	0.69
1:A:270:VAL:HG23	1:A:271:LEU:HG	1.75	0.69
1:B:613:HIS:CD2	1:B:721:HIS:CE1	2.82	0.68
1:B:549:TYR:H	1:B:558:ASP:HB2	1.57	0.68
1:A:78:HIS:CD2	1:A:119:PRO:HB2	2.29	0.68
1:B:329:GLU:O	1:B:333:ARG:HB2	1.94	0.67
1:A:10:PHE:HA	1:A:15:TRP:CD1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:HIS:CD2	1:B:119:PRO:HB2	2.30	0.66
1:A:448:GLU:OE2	1:A:449:ILE:N	2.28	0.66
1:B:222:ALA:HB1	1:B:223:PRO:CA	2.19	0.65
1:B:440:LYS:O	1:B:444:LYS:HE3	1.97	0.65
1:B:306:ASP:OD1	1:B:306:ASP:N	2.30	0.64
1:A:708:LYS:HB2	1:A:714:VAL:HG23	1.79	0.64
1:B:563:ILE:HA	1:B:567:ARG:O	1.97	0.64
1:A:215:VAL:HB	1:A:248:ASP:HB3	1.80	0.64
1:B:695:GLN:HG3	1:B:715:GLN:HG3	1.81	0.63
1:B:333:ARG:HB3	1:B:334:PRO:HD3	1.80	0.63
1:B:546:THR:HG21	1:B:581:ILE:CD1	2.30	0.62
1:A:739:ILE:HG22	1:A:740:GLN:HG2	1.82	0.62
1:A:222:ALA:CB	1:A:223:PRO:CA	2.71	0.62
1:A:34:ARG:HH11	1:A:34:ARG:HG3	1.64	0.62
1:B:165:GLU:N	1:B:165:GLU:OE1	2.33	0.62
1:B:535:ARG:NH2	1:B:535:ARG:HB2	2.15	0.61
1:B:683:THR:O	1:B:687:GLN:HG2	2.00	0.61
1:B:613:HIS:HD2	1:B:721:HIS:CE1	2.18	0.61
1:B:675:VAL:HG22	1:B:709:ILE:HG12	1.82	0.61
1:B:611:ARG:HA	1:B:722:LEU:HD11	1.82	0.61
1:B:303:ASP:C	1:B:304:ILE:HG13	2.21	0.61
1:A:117:ALA:HB3	1:A:120:LEU:HB3	1.82	0.60
1:B:278:LEU:HA	1:B:281:MET:HE3	1.83	0.60
1:B:209:LEU:HD11	1:B:255:ARG:HD3	1.82	0.59
1:A:411:ILE:HG22	1:A:415:MET:CE	2.31	0.59
1:B:10:PHE:HA	1:B:15:TRP:CD1	2.37	0.59
1:B:279:LYS:HG2	1:B:284:ILE:HD11	1.82	0.59
1:A:454:LEU:HD22	1:A:465:PRO:HB3	1.84	0.59
1:A:376:ARG:HB3	1:A:466:GLU:OE2	2.02	0.59
1:B:542:ILE:HG12	1:B:582:ILE:HG22	1.84	0.58
1:B:680:LEU:HD23	1:B:681:PRO:HD2	1.86	0.58
1:B:15:TRP:CE2	1:B:30:LEU:HD13	2.38	0.58
1:B:15:TRP:CD2	1:B:30:LEU:HD13	2.39	0.57
1:A:26:PRO:HB2	1:A:189:GLU:HB2	1.86	0.57
1:A:546:THR:HG21	1:A:581:ILE:CD1	2.34	0.57
1:B:472:ALA:HB1	1:B:477:VAL:HB	1.86	0.57
1:A:539:ASP:HA	1:A:588:PRO:HB3	1.87	0.57
1:A:103:ASP:OD2	1:A:124:GLN:NE2	2.37	0.57
1:B:176:LYS:HB3	1:B:177:GLU:OE2	2.04	0.57
1:A:474:LYS:O	1:A:474:LYS:HG2	2.04	0.56
1:B:147:MET:HE1	3:B:999:A5A:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:LEU:HD13	1:B:647:ILE:HG21	1.86	0.56
1:A:174:PHE:HE2	1:A:204:VAL:HG11	1.70	0.56
1:A:221:LYS:NZ	1:A:237:GLU:HB3	2.21	0.56
1:A:376:ARG:HD3	1:A:467:ILE:HD11	1.87	0.55
1:A:229:ASP:HA	1:A:231:VAL:HG13	1.88	0.55
1:A:17:ARG:NH1	1:A:19:LYS:HE2	2.21	0.55
1:B:535:ARG:HB2	1:B:535:ARG:HH21	1.72	0.55
1:A:87:LEU:HG	1:A:356:VAL:HG22	1.88	0.55
1:A:410:ASP:O	1:A:414:GLU:HB2	2.07	0.55
1:A:473:GLU:C	1:A:475:GLU:H	2.11	0.55
1:B:117:ALA:HB3	1:B:120:LEU:HB3	1.88	0.54
1:B:270:VAL:HG23	1:B:271:LEU:HG	1.89	0.54
1:A:278:LEU:HD21	1:A:390:ILE:HD11	1.90	0.54
1:B:638:LEU:O	1:B:638:LEU:HD22	2.08	0.54
1:A:573:ASN:HB3	1:A:584:LYS:HB3	1.90	0.54
1:B:549:TYR:N	1:B:558:ASP:HB2	2.23	0.54
1:A:451:VAL:O	1:A:455:VAL:HG23	2.08	0.54
1:A:273:TYR:CZ	1:A:397:GLU:HG2	2.43	0.54
1:A:3:PHE:CD2	1:A:200:PRO:HB3	2.42	0.53
1:A:34:ARG:HG3	1:A:34:ARG:NH1	2.23	0.53
1:B:128:ARG:NH2	3:B:999:A5A:O1S	2.41	0.53
1:A:411:ILE:HG22	1:A:415:MET:HE3	1.90	0.53
1:B:59:LEU:HD22	1:B:253:LEU:HG	1.89	0.53
1:A:411:ILE:O	1:A:415:MET:HG3	2.08	0.53
1:A:174:PHE:CE2	1:A:204:VAL:HG11	2.44	0.53
1:A:620:MET:HA	1:A:623:LEU:HD12	1.91	0.53
1:A:15:TRP:CD2	1:A:30:LEU:HD13	2.44	0.52
1:A:352:LEU:HD23	1:A:356:VAL:O	2.09	0.52
1:B:54:PRO:HG3	1:B:179:LYS:HB2	1.91	0.52
1:B:84:TYR:H	1:B:124:GLN:HE22	1.56	0.52
1:B:288:ASP:HB3	1:B:291:ILE:HD12	1.90	0.52
1:B:469:LYS:HB2	1:B:479:VAL:HB	1.92	0.52
1:A:218:GLN:C	1:A:242:MET:HG2	2.31	0.52
1:A:254:GLU:H	1:A:254:GLU:CD	2.13	0.52
1:B:465:PRO:HD3	1:B:485:PHE:CE2	2.45	0.52
1:A:281:MET:HB3	1:A:383:LEU:HD21	1.92	0.52
1:B:90:TRP:O	1:B:698:VAL:HG11	2.10	0.52
1:B:368:ARG:HA	1:B:371:ILE:HD12	1.92	0.52
1:A:509:LEU:HD12	1:A:509:LEU:H	1.75	0.52
1:B:629:ARG:O	1:B:692:ARG:NH2	2.43	0.51
1:A:76:TYR:OH	1:A:165:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:CD2	1:B:253:LEU:HG	2.41	0.51
1:A:613:HIS:CE1	1:A:719:GLY:HA3	2.45	0.51
1:A:681:PRO:HG2	1:A:684:THR:OG1	2.11	0.51
1:A:536:VAL:HG12	1:A:536:VAL:O	2.11	0.51
1:B:163:MET:O	1:B:167:VAL:HG13	2.10	0.51
1:B:681:PRO:HG2	1:B:684:THR:OG1	2.10	0.51
1:B:81:VAL:HG21	1:B:120:LEU:HD22	1.93	0.51
1:B:171:PHE:HZ	1:B:182:PRO:HB3	1.75	0.50
1:A:680:LEU:HD23	1:A:681:PRO:HD2	1.93	0.50
1:B:314:ARG:O	1:B:325:VAL:HG12	2.12	0.50
1:B:18:LYS:HB2	1:B:27:PHE:CE2	2.47	0.50
1:B:591:PHE:CE1	1:B:597:VAL:HG11	2.47	0.50
1:A:304:ILE:HG21	1:A:483:ASP:HB2	1.93	0.50
1:A:570:LYS:HB2	1:A:586:GLU:CD	2.31	0.50
1:B:255:ARG:NH1	3:B:999:A5A:H2'	2.26	0.50
1:B:650:TYR:CE2	1:B:651:LYS:HD3	2.46	0.50
1:A:174:PHE:O	1:A:180:MET:HG3	2.11	0.50
1:A:367:ALA:O	1:A:371:ILE:HG13	2.12	0.50
1:B:523:ASP:OD2	1:B:526:MET:HB2	2.11	0.50
1:B:174:PHE:HB3	1:B:180:MET:HE2	1.94	0.50
1:B:376:ARG:HH22	1:B:379:ARG:HH11	1.58	0.50
1:A:127:ILE:HA	1:A:143:THR:O	2.12	0.49
1:A:372:ARG:HG2	1:A:423:TYR:CE2	2.47	0.49
1:A:425:GLU:HG3	1:A:428:ARG:HH12	1.77	0.49
1:A:675:VAL:HB	1:A:722:LEU:O	2.12	0.49
1:A:57:TYR:O	1:A:257:VAL:HG13	2.12	0.49
1:B:739:ILE:HG22	1:B:740:GLN:HG2	1.94	0.49
1:A:334:PRO:O	1:A:338:ILE:HG13	2.12	0.49
1:B:359:SER:HB2	1:B:741:ASP:O	2.12	0.49
1:A:221:LYS:HZ1	1:A:237:GLU:HB3	1.77	0.49
1:A:332:ILE:HD12	1:A:333:ARG:N	2.28	0.49
1:A:515:ASP:OD1	1:A:579:LYS:CD	2.61	0.49
1:B:237:GLU:O	1:B:238:LYS:CB	2.59	0.49
1:B:473:GLU:C	1:B:475:GLU:H	2.16	0.49
1:A:317:VAL:HG13	1:A:328:LEU:HD21	1.94	0.49
1:B:702:ARG:HB3	1:B:702:ARG:HH11	1.78	0.49
1:A:37:CYS:SG	1:A:188:LYS:HE2	2.53	0.49
1:A:548:PHE:HB3	1:A:574:VAL:HG21	1.94	0.49
1:B:73:HIS:HB3	1:B:76:TYR:O	2.13	0.49
1:A:608:GLN:HE21	1:A:640:THR:CB	2.01	0.48
1:A:221:LYS:HD3	1:A:238:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:LEU:HD23	1:A:645:LEU:HD23	1.95	0.48
1:A:25:LYS:HD2	1:A:188:LYS:HD3	1.94	0.48
1:A:413:LEU:O	1:A:417:GLU:HG2	2.13	0.48
1:B:546:THR:HG21	1:B:581:ILE:HD11	1.94	0.48
1:A:90:TRP:O	1:A:698:VAL:HG11	2.14	0.48
1:A:399:HIS:HA	1:A:402:PHE:O	2.14	0.48
1:B:516:THR:HB	1:B:581:ILE:HG23	1.96	0.48
1:A:512:ASP:OD2	1:A:535:ARG:NH1	2.47	0.48
1:A:87:LEU:HD13	1:A:89:ARG:CZ	2.43	0.47
1:B:298:LEU:HB3	1:B:301:MET:CE	2.44	0.47
1:B:434:VAL:O	1:B:438:ILE:N	2.45	0.47
1:B:574:VAL:CG1	1:B:581:ILE:HD12	2.44	0.47
1:A:515:ASP:OD1	1:A:579:LYS:HD2	2.15	0.47
1:A:646:ASP:OD1	1:A:646:ASP:N	2.48	0.47
1:A:613:HIS:HE1	1:A:719:GLY:HA3	1.78	0.47
1:A:174:PHE:HB3	1:A:180:MET:HE2	1.95	0.47
1:A:323:ILE:HB	1:A:327:GLU:HG2	1.97	0.47
1:B:56:LYS:HA	1:B:260:SER:O	2.14	0.47
1:B:318:ALA:HB1	1:B:323:ILE:O	2.15	0.47
1:A:411:ILE:HG22	1:A:415:MET:HE2	1.96	0.47
1:B:524:PRO:HB2	1:B:610:MET:HE3	1.96	0.47
1:A:713:ASP:OD2	1:A:715:GLN:NE2	2.48	0.47
1:B:448:GLU:H	1:B:448:GLU:CD	2.17	0.47
1:A:303:ASP:C	1:A:304:ILE:HG13	2.32	0.47
1:A:529:PHE:CE2	1:A:546:THR:HA	2.50	0.47
1:B:221:LYS:HZ1	1:B:237:GLU:HG2	1.80	0.47
1:B:287:ILE:HD11	1:B:291:ILE:HG22	1.96	0.47
1:B:613:HIS:HD2	1:B:721:HIS:NE2	2.13	0.47
1:B:263:THR:HB	1:B:264:PRO:HD2	1.97	0.46
1:B:317:VAL:O	1:B:321:VAL:HG23	2.15	0.46
1:A:180:MET:HB3	1:A:206:TYR:CZ	2.50	0.46
1:A:165:GLU:OE1	1:A:165:GLU:N	2.39	0.46
1:A:346:LYS:HE3	1:A:398:LEU:HD11	1.97	0.46
1:A:672:ASP:OD1	1:A:724:SER:OG	2.26	0.46
1:A:731:ILE:HG12	1:A:750:CYS:SG	2.55	0.46
1:B:613:HIS:CD2	1:B:721:HIS:NE2	2.84	0.46
1:A:120:LEU:O	1:A:150:HIS:HA	2.15	0.46
1:A:17:ARG:HH12	1:A:19:LYS:HE2	1.80	0.46
1:B:103:ASP:OD2	1:B:124:GLN:NE2	2.43	0.46
1:A:22:VAL:HB	1:A:42:CYS:SG	2.55	0.46
1:B:203:GLU:HB3	1:B:210:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:LEU:HD23	1:A:580:VAL:HB	1.98	0.46
1:B:39:ASP:HA	1:B:40:PRO:HD2	1.86	0.46
1:B:129:PHE:C	1:B:131:ASP:H	2.19	0.46
1:A:201:ALA:HB2	1:A:215:VAL:HG13	1.98	0.46
1:A:316:GLN:O	1:A:320:ARG:HB2	2.16	0.45
1:A:74:GLU:HB2	1:A:75:ILE:HD12	1.98	0.45
1:B:144:ILE:HG23	1:B:144:ILE:O	2.15	0.45
1:B:74:GLU:HB2	1:B:75:ILE:HD12	1.98	0.45
1:A:109:ILE:HG12	1:A:246:VAL:HG21	1.99	0.45
1:A:24:GLY:HA3	1:B:659:LYS:HG3	1.98	0.45
1:B:654:SER:HG	1:B:657:GLU:HG3	1.77	0.45
1:B:376:ARG:HB3	1:B:466:GLU:OE2	2.16	0.45
1:B:548:PHE:CZ	1:B:571:VAL:HG21	2.52	0.45
1:A:15:TRP:CE2	1:A:30:LEU:HD13	2.52	0.45
1:A:473:GLU:C	1:A:475:GLU:N	2.70	0.45
1:B:101:ILE:HD11	1:B:109:ILE:HD11	1.99	0.45
1:A:100:SER:HA	1:A:124:GLN:HG2	1.99	0.45
1:B:298:LEU:HD12	1:B:317:VAL:HG23	1.99	0.45
1:B:405:PHE:N	1:B:405:PHE:CD1	2.85	0.45
1:A:508:GLU:C	1:A:510:LEU:H	2.21	0.44
1:B:105:GLN:HG3	1:B:109:ILE:HD12	1.98	0.44
1:B:722:LEU:HD13	1:B:727:LEU:O	2.18	0.44
1:B:621:GLY:HA3	1:B:712:TRP:NE1	2.33	0.44
1:A:140:ARG:NH2	1:A:300:GLY:O	2.50	0.44
1:B:274:VAL:HG21	1:B:394:HIS:CE1	2.52	0.44
1:A:677:TRP:HA	1:A:706:VAL:O	2.18	0.44
1:B:750:CYS:HB2	1:B:751:GLY:H	1.63	0.44
1:A:100:SER:HB3	1:A:124:GLN:HB3	2.00	0.44
1:A:200:PRO:HD2	1:A:218:GLN:HE21	1.82	0.44
1:B:507:PHE:N	1:B:507:PHE:CD2	2.85	0.44
1:B:37:CYS:SG	1:B:188:LYS:HE3	2.58	0.44
1:A:4:ILE:CG2	1:A:5:MET:N	2.66	0.44
1:A:613:HIS:CD2	1:A:721:HIS:CE1	3.06	0.44
1:B:114:ASP:HA	1:B:115:PRO:HD3	1.87	0.44
1:B:332:ILE:H	1:B:332:ILE:HG13	1.58	0.43
1:B:359:SER:OG	1:B:360:ASN:N	2.49	0.43
1:B:532:LYS:HG2	1:B:596:ILE:HG13	2.00	0.43
1:A:333:ARG:HA	1:A:336:GLU:HG3	2.00	0.43
1:A:158:LYS:HB2	1:A:158:LYS:HE3	1.73	0.43
1:A:448:GLU:N	1:A:448:GLU:CD	2.72	0.43
1:B:253:LEU:O	1:B:257:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HB3	1:B:301:MET:HE1	1.99	0.43
1:A:171:PHE:HZ	1:A:182:PRO:HB3	1.84	0.43
1:B:539:ASP:HA	1:B:588:PRO:HB3	2.00	0.43
1:A:652:ARG:CZ	1:A:653:ILE:H	2.31	0.43
1:B:316:GLN:O	1:B:320:ARG:HB2	2.19	0.43
1:B:317:VAL:HA	1:B:320:ARG:HB2	2.00	0.43
1:B:650:TYR:O	1:B:651:LYS:HB3	2.19	0.43
1:A:304:ILE:HG21	1:A:483:ASP:CB	2.49	0.43
1:B:40:PRO:HA	1:B:41:PRO:HA	1.87	0.43
1:B:212:ALA:HA	1:B:250:GLY:O	2.18	0.43
1:B:637:GLN:HB3	1:B:644:ARG:HG2	2.00	0.43
1:A:98:GLY:O	1:A:128:ARG:NH1	2.48	0.42
1:B:141:HIS:O	1:B:267:TYR:HE1	2.01	0.42
1:B:236:GLY:O	1:B:238:LYS:N	2.52	0.42
1:B:399:HIS:HA	1:B:402:PHE:O	2.19	0.42
1:B:705:ARG:NH1	1:B:719:GLY:O	2.39	0.42
1:B:526:MET:CE	1:B:529:PHE:HB3	2.49	0.42
1:B:395:ILE:HG23	1:B:405:PHE:HB3	2.01	0.42
1:B:530:ASP:HA	1:B:597:VAL:O	2.19	0.42
1:A:333:ARG:NH1	1:A:336:GLU:OE1	2.52	0.42
1:B:554:GLY:O	1:B:638:LEU:HD13	2.19	0.42
1:B:173:PHE:HA	1:B:177:GLU:HG2	2.01	0.42
1:A:633:GLN:NE2	1:A:696:GLY:HA3	2.35	0.42
1:B:485:PHE:CE2	1:B:489:VAL:HG21	2.54	0.42
1:A:55:ARG:HG3	1:A:57:TYR:CE2	2.54	0.42
1:B:59:LEU:HA	1:B:257:VAL:HG21	2.02	0.42
1:B:526:MET:HE2	1:B:528:GLU:O	2.20	0.42
1:B:627:LEU:O	1:B:630:HIS:HE1	2.03	0.42
1:A:233:VAL:HA	1:A:237:GLU:O	2.20	0.42
1:B:127:ILE:HA	1:B:143:THR:O	2.20	0.42
1:B:636:SER:O	1:B:637:GLN:HB2	2.20	0.42
1:A:317:VAL:HG13	1:A:328:LEU:CD2	2.49	0.41
1:A:535:ARG:HG3	1:A:536:VAL:N	2.35	0.41
1:A:648:SER:HA	1:A:742:GLY:O	2.20	0.41
1:B:69:PHE:CD2	1:B:69:PHE:C	2.93	0.41
1:B:174:PHE:HB3	1:B:180:MET:CE	2.49	0.41
1:B:509:LEU:H	1:B:509:LEU:HD12	1.85	0.41
1:B:610:MET:CE	1:B:722:LEU:HD23	2.51	0.41
1:A:64:GLU:OE2	1:A:80:ARG:NH2	2.53	0.41
1:B:57:TYR:HE1	1:B:65:LYS:HD2	1.85	0.41
1:B:652:ARG:HH11	1:B:744:GLU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:TRP:HB2	1:A:187:PHE:HB2	2.02	0.41
1:B:346:LYS:HB2	1:B:394:HIS:CE1	2.55	0.41
1:A:164:ASP:HB2	1:A:165:GLU:OE1	2.21	0.41
1:B:450:PRO:HG2	1:B:453:LYS:HB2	2.01	0.41
1:B:526:MET:HE2	1:B:529:PHE:HB3	2.03	0.41
1:B:507:PHE:N	1:B:507:PHE:HD2	2.18	0.41
1:B:569:VAL:HG12	1:B:585:VAL:HB	2.03	0.41
1:A:113:ALA:HB2	1:A:682:ARG:HD2	2.03	0.41
1:A:448:GLU:O	1:A:449:ILE:HB	2.21	0.41
1:B:100:SER:HA	1:B:124:GLN:HG2	2.02	0.41
1:B:328:LEU:O	1:B:332:ILE:HG13	2.21	0.41
1:A:87:LEU:HA	1:A:88:PRO:HD2	1.88	0.41
1:A:674:LYS:HD3	1:A:674:LYS:HA	1.89	0.41
1:B:386:PRO:HG2	1:B:389:GLU:CG	2.45	0.41
1:A:302:PHE:CG	1:A:313:LEU:HB2	2.56	0.40
1:A:450:PRO:HG2	1:A:453:LYS:HB2	2.02	0.40
1:B:140:ARG:HH21	1:B:300:GLY:HA2	1.86	0.40
1:A:480:ASN:HD22	1:A:480:ASN:HA	1.58	0.40
1:A:607:ILE:HD12	1:A:607:ILE:HA	1.92	0.40
1:B:104:PHE:O	1:B:109:ILE:HG13	2.22	0.40
1:B:405:PHE:N	1:B:405:PHE:HD1	2.20	0.40
1:B:20:CYS:HB2	1:B:37:CYS:HB3	2.03	0.40
1:B:71:GLU:HA	1:B:78:HIS:O	2.22	0.40
1:B:362:LYS:O	1:B:365:TYR:HB3	2.22	0.40
1:B:693:LEU:HD23	1:B:714:VAL:HG13	2.04	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	730/752 (97%)	657 (90%)	61 (8%)	12 (2%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	729/752 (97%)	641 (88%)	74 (10%)	14 (2%)	8	33
All	All	1459/1504 (97%)	1298 (89%)	135 (9%)	26 (2%)	8	34

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ALA
1	B	222	ALA
1	B	237	GLU
1	B	287	ILE
1	B	593	GLU
1	A	508	GLU
1	B	59	LEU
1	B	474	LYS
1	B	508	GLU
1	B	538	LYS
1	A	449	ILE
1	A	509	LEU
1	B	449	ILE
1	B	509	LEU
1	B	750	CYS
1	A	34	ARG
1	A	54	PRO
1	A	695	GLN
1	B	436	ARG
1	A	88	PRO
1	A	492	GLU
1	B	565	ASN
1	A	158	LYS
1	A	4	ILE
1	A	287	ILE
1	B	22	VAL

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	644/655 (98%)	594 (92%)	50 (8%)	12	40
1	B	642/655 (98%)	579 (90%)	63 (10%)	8	29
All	All	1286/1310 (98%)	1173 (91%)	113 (9%)	10	36

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	43	ASP
1	A	46	GLN
1	A	59	LEU
1	A	87	LEU
1	A	95	LEU
1	A	128	ARG
1	A	130	THR
1	A	133	ASP
1	A	158	LYS
1	A	186	THR
1	A	224	GLU
1	A	261	GLN
1	A	280	LYS
1	A	286	LYS
1	A	296	SER
1	A	303	ASP
1	A	304	ILE
1	A	311	ARG
1	A	320	ARG
1	A	325	VAL
1	A	333	ARG
1	A	336	GLU
1	A	400	LYS
1	A	401	THR
1	A	406	LYS
1	A	422	LYS
1	A	448	GLU
1	A	453	LYS
1	A	455	VAL
1	A	466	GLU
1	A	469	LYS
1	A	473	GLU
1	A	474	LYS
1	A	480	ASN

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Mol	Chain	Res	Type
1	A	488	MET
1	A	489	VAL
1	A	494	GLU
1	A	508	GLU
1	A	532	LYS
1	A	535	ARG
1	A	581	ILE
1	A	604	LYS
1	A	606	ARG
1	A	638	LEU
1	A	646	ASP
1	A	652	ARG
1	A	692	ARG
1	A	735	ARG
1	A	741	ASP
1	B	2	GLU
1	B	44	GLU
1	B	60	ASP
1	B	82	LYS
1	B	87	LEU
1	B	95	LEU
1	B	158	LYS
1	B	167	VAL
1	B	168	GLU
1	B	210	GLU
1	B	221	LYS
1	B	233	VAL
1	B	244	THR
1	B	248	ASP
1	B	253	LEU
1	B	261	GLN
1	B	286	LYS
1	B	297	ARG
1	B	304	ILE
1	B	306	ASP
1	B	320	ARG
1	B	332	ILE
1	B	374	SER
1	B	377	HIS
1	B	384	GLU
1	B	400	LYS
1	B	401	THR

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Mol	Chain	Res	Type
1	B	421	LYS
1	B	433	LEU
1	B	443	LYS
1	B	444	LYS
1	B	448	GLU
1	B	452	GLU
1	B	456	THR
1	B	459	GLU
1	B	466	GLU
1	B	469	LYS
1	B	480	ASN
1	B	507	PHE
1	B	515	ASP
1	B	527	LYS
1	B	535	ARG
1	B	558	ASP
1	B	567	ARG
1	B	568	GLU
1	B	571	VAL
1	B	572	THR
1	B	579	LYS
1	B	581	ILE
1	B	601	ILE
1	B	611	ARG
1	B	638	LEU
1	B	644	ARG
1	B	658	LEU
1	B	680	LEU
1	B	684	THR
1	B	692	ARG
1	B	699	VAL
1	B	717	CYS
1	B	724	SER
1	B	735	ARG
1	B	741	ASP
1	B	752	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	316	GLN
1	A	480	ASN
1	A	608	GLN
1	A	633	GLN
1	A	715	GLN
1	B	124	GLN
1	B	134	ASN
1	B	228	GLN
1	B	480	ASN
1	B	608	GLN
1	B	715	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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	#$|Z| > 2$
3	A5A	B	999	-	26,30,30	2.28	4 (15%)	30,45,45	1.95	5 (16%)
3	A5A	A	999	-	26,30,30	2.15	5 (19%)	30,45,45	2.15	5 (16%)

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
3	A5A	B	999	-	-	1/14/35/35	0/3/3/3
3	A5A	A	999	-	-	1/14/35/35	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	A5A	O1S-S	6.85	1.48	1.42
3	B	999	A5A	O2S-S	6.77	1.48	1.42
3	A	999	A5A	O1S-S	6.69	1.48	1.42
3	A	999	A5A	O2S-S	5.32	1.47	1.42
3	A	999	A5A	S-N3S	-4.77	1.51	1.59
3	B	999	A5A	S-N3S	-3.86	1.53	1.59
3	B	999	A5A	O4'-C1'	2.54	1.44	1.41
3	A	999	A5A	C-N3S	-2.43	1.32	1.37
3	A	999	A5A	O4'-C1'	2.12	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	A5A	O2S-S-O1S	-8.31	107.81	120.76
3	B	999	A5A	O2S-S-O1S	-7.34	109.32	120.76
3	B	999	A5A	N3-C2-N1	-4.67	121.38	128.68
3	A	999	A5A	N3-C2-N1	-4.66	121.39	128.68
3	A	999	A5A	O5'-S-O1S	3.68	116.85	105.59
3	A	999	A5A	CB-CA-C	-2.65	105.11	110.14
3	B	999	A5A	O5'-S-O1S	2.64	113.67	105.59
3	B	999	A5A	C4-C5-N7	-2.52	106.77	109.40
3	A	999	A5A	O5'-C5'-C4'	2.47	112.23	107.62
3	B	999	A5A	C1'-N9-C4	-2.39	122.44	126.64

There are no chirality outliers.
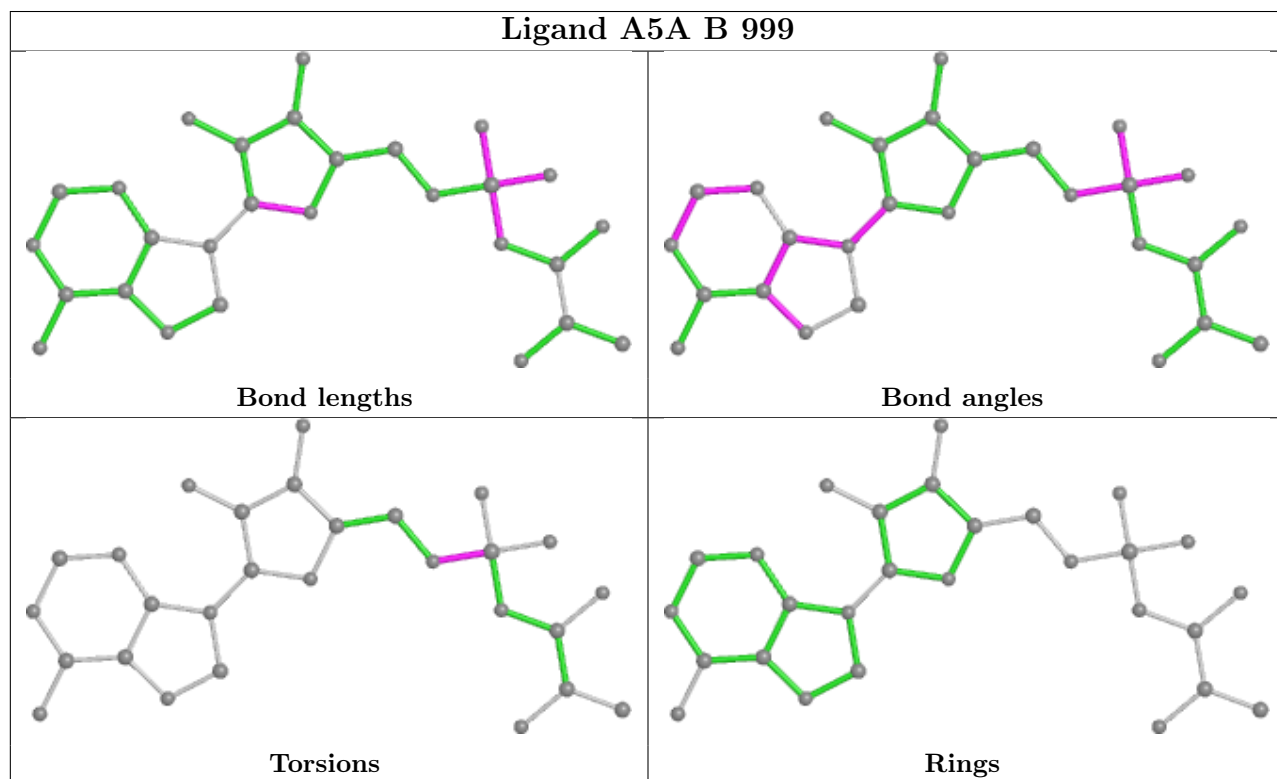
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	999	A5A	C5'-O5'-S-N3S
3	A	999	A5A	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	A5A	3	0
3	A	999	A5A	1	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 A5A B 999

Bond lengths

Bond angles

Torsions

Rings

Ligand A5A A 999

Bond lengths

Bond angles

Torsions

Rings
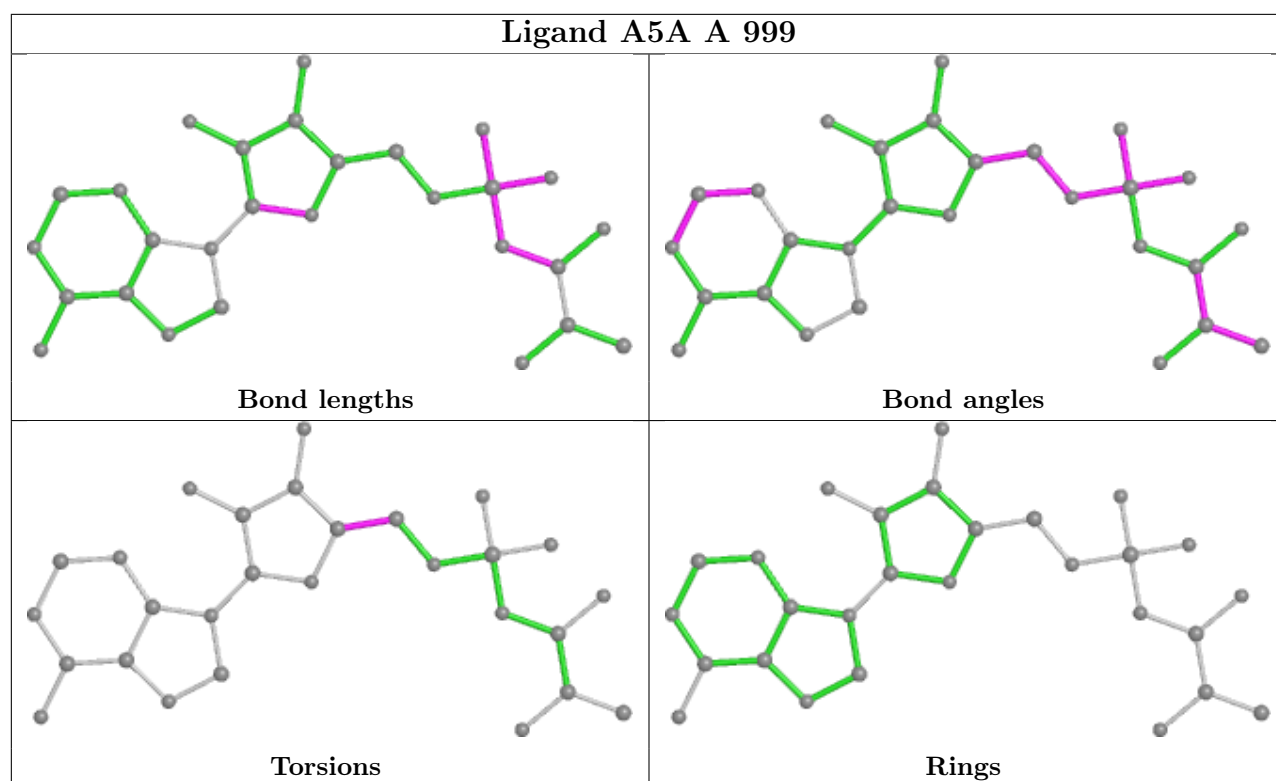
5.7 Other polymers ⓘ

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	738/752 (98%)	-0.01	19 (2%)	56	33	53, 72, 104, 118	0
1	B	737/752 (98%)	0.09	28 (3%)	40	20	47, 74, 113, 127	0
All	All	1475/1504 (98%)	0.04	47 (3%)	47	25	47, 73, 110, 127	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	VAL	4.0
1	A	446	ILE	3.8
1	B	565	ASN	3.6
1	B	506	ASP	3.6
1	B	567	ARG	3.4
1	A	443	LYS	3.4
1	B	587	ASP	3.3
1	A	479	VAL	3.2
1	B	595	MET	3.1
1	B	591	PHE	3.1
1	A	506	ASP	3.0
1	A	496	THR	3.0
1	B	511	LYS	3.0
1	B	536	VAL	2.9
1	A	323	ILE	2.9
1	B	585	VAL	2.9
1	B	510	LEU	2.8
1	A	305	GLU	2.8
1	B	597	VAL	2.8
1	B	532	LYS	2.8
1	B	321	VAL	2.8
1	B	285	GLU	2.7
1	B	563	ILE	2.7
1	B	443	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	438	ILE	2.5
1	B	294	GLU	2.5
1	B	538	LYS	2.5
1	A	126	SER	2.5
1	B	504	LEU	2.5
1	A	448	GLU	2.4
1	B	284	ILE	2.4
1	B	505	VAL	2.4
1	A	441	LEU	2.4
1	A	477	VAL	2.3
1	B	287	ILE	2.3
1	B	442	LYS	2.3
1	B	582	ILE	2.3
1	B	475	GLU	2.2
1	A	255	ARG	2.2
1	B	537	ILE	2.2
1	A	504	LEU	2.1
1	A	135	VAL	2.1
1	A	290	LYS	2.1
1	A	302	PHE	2.1
1	A	321	VAL	2.1
1	A	141	HIS	2.1
1	B	477	VAL	2.0

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

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

6.3   Carbohydrates ⓘ

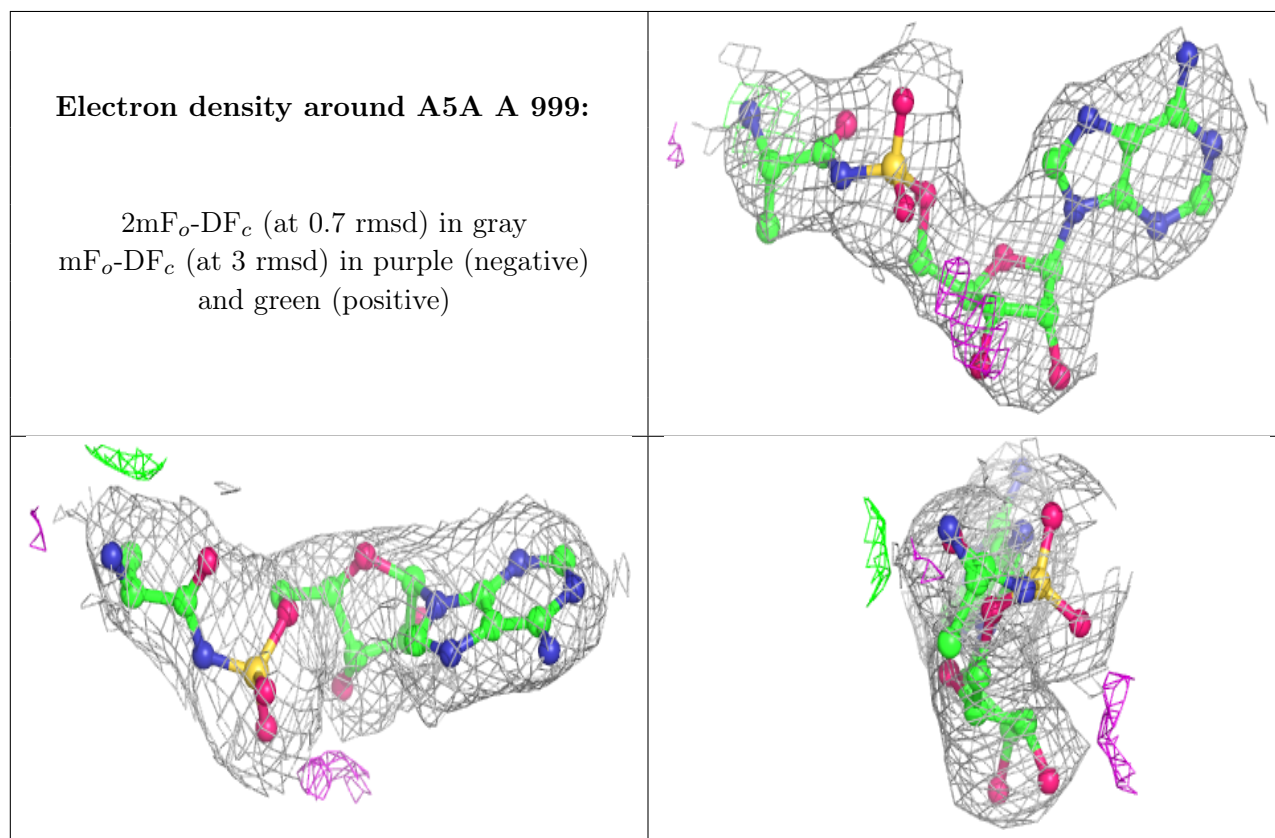There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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.
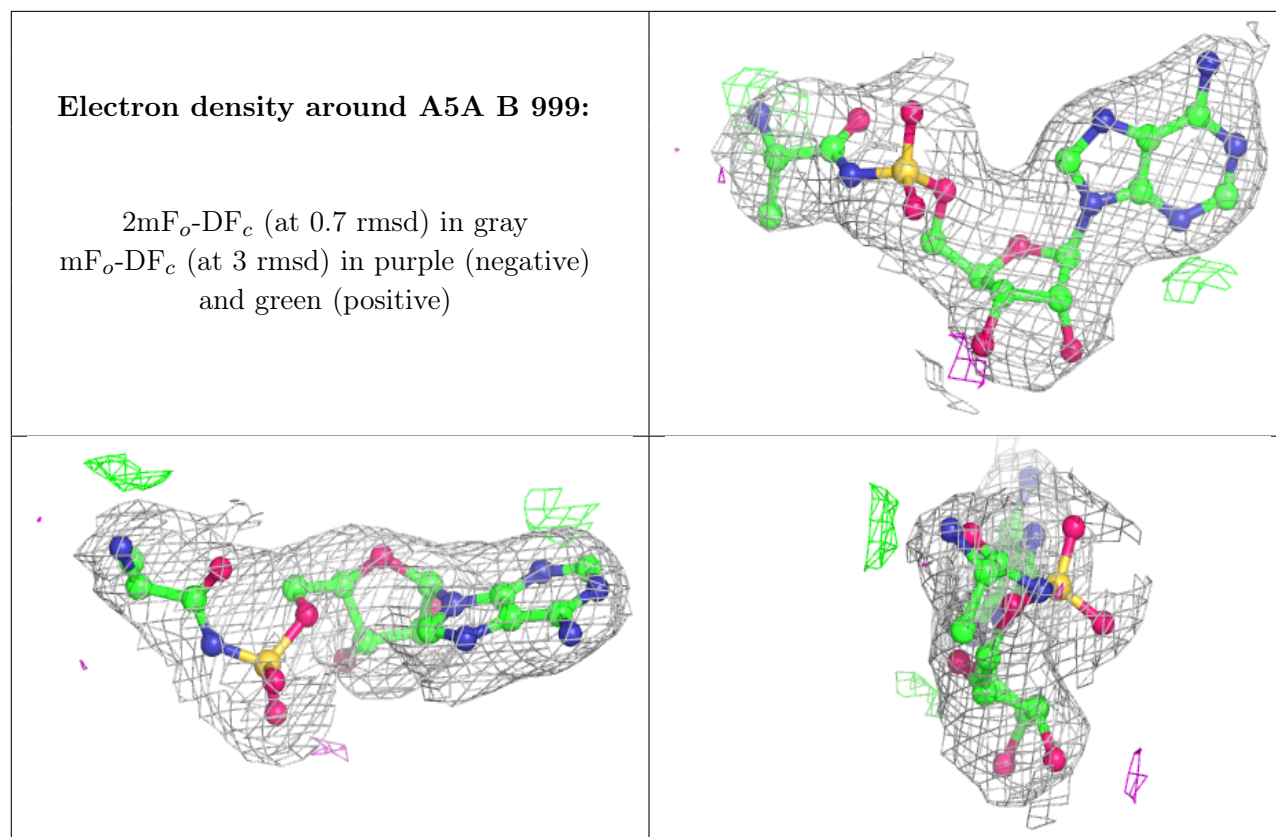
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	901	1/1	0.97	0.19	106,106,106,106	0
2	ZN	B	901	1/1	0.97	0.15	96,96,96,96	0
3	A5A	A	999	28/28	0.97	0.39	52,60,64,64	0
2	ZN	A	900	1/1	0.98	0.18	65,65,65,65	0
3	A5A	B	999	28/28	0.98	0.31	51,55,56,57	0
2	ZN	B	900	1/1	0.99	0.18	69,69,69,69	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 A5A A 999:

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

Electron density around A5A B 999:

$2mF_o$-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.