



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:31 PM EDT

PDB ID : 2ZZG / pdb_00002zzg
Title : Crystal structure of alanyl-tRNA synthetase in complex with 5''-O-(N-(L-alanyl)-sulfamoyl) 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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

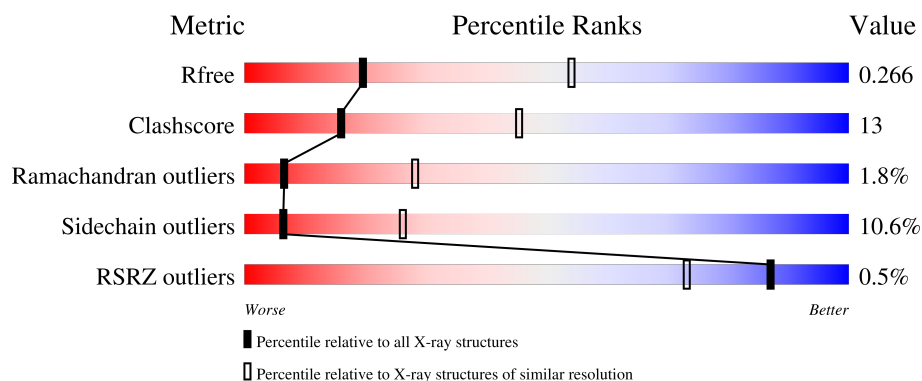
1 Overall quality at a glance i

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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	752	% 65% 29% ..
1	B	752	60% 34% ...

2 Entry composition [i](#)

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.

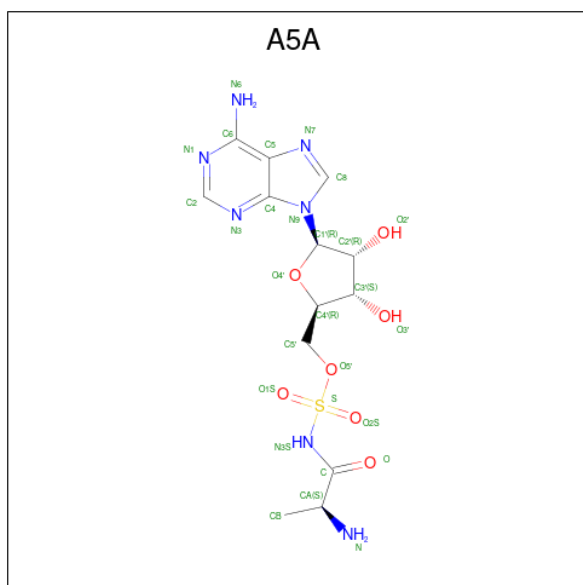
- Molecule 1 is a protein called Alanyl-tRNA synthetase.

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 (CCD ID: 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 (CCD ID: A5A) (formula: C₁₃H₁₉N₇O₇S).



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		

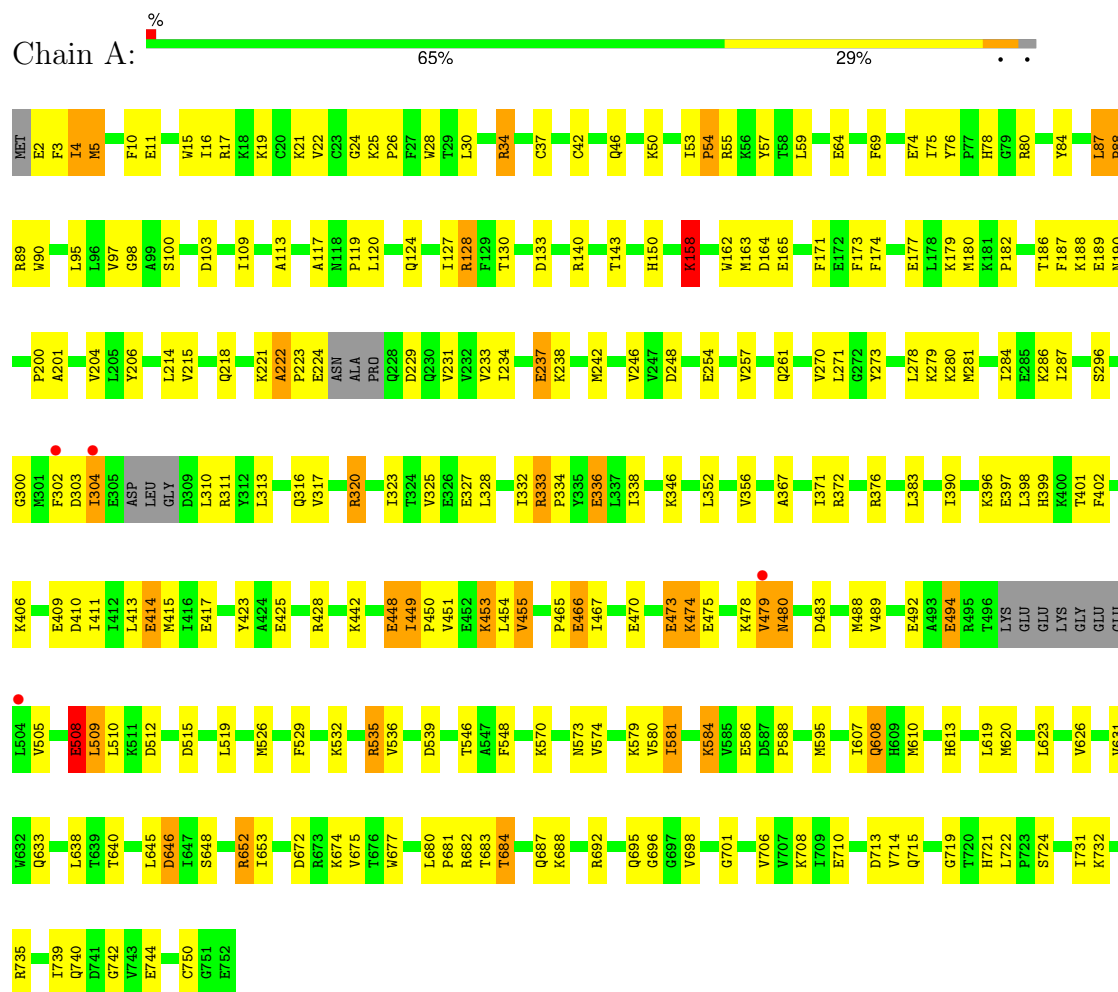
- Molecule 4 is water.

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

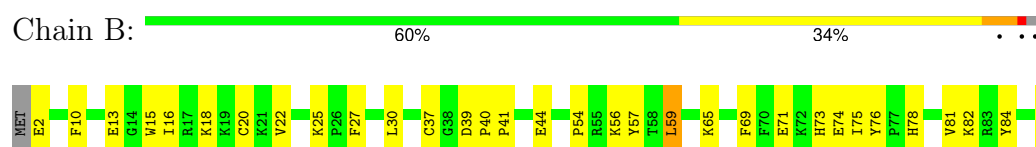
3 Residue-property plots [i](#)

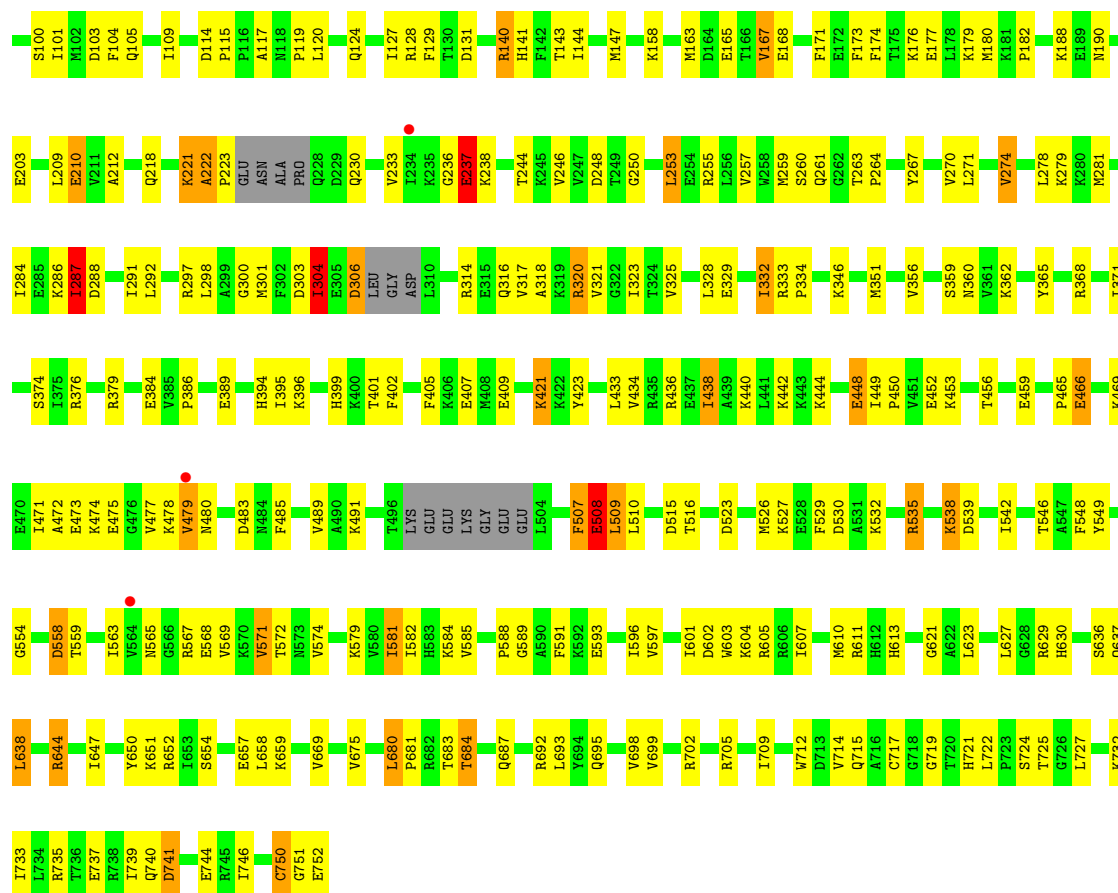
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alanyl-tRNA synthetase



• Molecule 1: Alanyl-tRNA synthetase





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 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-3.10) 96.4 (50.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.80%)	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 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A5A

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	0.70	1/6143 (0.0%)	0.97	10/8290 (0.1%)
1	B	0.70	0/6127	0.99	9/8269 (0.1%)
All	All	0.70	1/12270 (0.0%)	0.98	19/16559 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	VAL	CA-CB	5.08	1.61	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	LYS	N-CA-C	6.82	121.15	110.17
1	A	595	MET	N-CA-C	6.80	119.83	110.24
1	A	53	ILE	CA-C-N	6.66	128.17	119.84
1	A	53	ILE	C-N-CA	6.66	128.17	119.84
1	B	237	GLU	N-CA-C	6.36	124.34	110.80
1	B	478	LYS	N-CA-C	6.29	120.07	109.76
1	B	230	GLN	N-CA-C	-5.98	106.63	112.97
1	A	505	VAL	N-CA-C	5.87	121.55	109.34
1	B	304	ILE	N-CA-C	5.59	116.85	107.18
1	A	494	GLU	N-CA-C	5.51	117.46	108.76
1	B	737	GLU	N-CA-C	5.48	117.30	108.32
1	B	287	ILE	N-CA-C	5.29	120.35	109.34
1	B	246	VAL	N-CA-C	5.29	115.52	108.11
1	A	409	GLU	N-CA-C	5.23	117.65	111.33
1	A	190	ASN	CA-C-N	-5.14	115.27	120.31
1	A	190	ASN	C-N-CA	-5.14	115.27	120.31
1	B	190	ASN	CA-C-N	5.13	125.12	119.89
1	B	190	ASN	C-N-CA	5.13	125.12	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	GLY	N-CA-C	5.03	117.92	112.29

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	155	0
1	B	5989	0	6060	167	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	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	12055	0	12170	320	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 (320) 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:B:174:PHE:HB3	1:B:180:MET:HE2	1.53	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:MET:HE2	1:B:722:LEU:HD23	1.60	0.81
1:A:222:ALA:HB1	1:A:223:PRO:CA	2.11	0.81
1:B:526:MET:HE2	1:B:529:PHE:HB3	1.64	0.79
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:B:298:LEU:HB3	1:B:301:MET:HE2	1.65	0.76
1:A:411:ILE:HG22	1:A:415:MET:HE2	1.69	0.75
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
1:A:221:LYS:HZ1	1:A:237:GLU:HB3	1.59	0.66
1:B:147:MET:HE2	3:B:999:A5A:H5'1	1.78	0.66
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:303:ASP:C	1:B:304:ILE:HG13	2.21	0.65
1:B:222:ALA:HB1	1:B:223:PRO:CA	2.19	0.65
1:B:278:LEU:HA	1:B:281:MET:HE3	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:117:ALA:HB3	1:A:120:LEU:HB3	1.82	0.60
1:B:209:LEU:HD11	1:B:255:ARG:HD3	1.82	0.59
1:A:473:GLU:C	1:A:475:GLU:H	2.11	0.59
1:A:278:LEU:HA	1:A:281:MET:HE3	1.84	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:411:ILE:HG22	1:A:415:MET:CE	2.31	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:A:411:ILE:CG2	1:A:415:MET:HE2	2.32	0.58
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:B:209:LEU:HD23	1:B:259:MET:HE2	1.86	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:610:MET:HE2	1:A:722:LEU:CD2	2.35	0.56
1:A:218:GLN:C	1:A:242:MET:HG2	2.31	0.56
1:A:254:GLU:H	1:A:254:GLU:CD	2.13	0.56
1:A:474:LYS:O	1:A:474:LYS:HG2	2.04	0.56
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:376:ARG:HD3	1:A:467:ILE:HD11	1.87	0.55
1:A:221:LYS:NZ	1:A:237:GLU:HB3	2.21	0.55
1:A:610:MET:HE2	1:A:722:LEU:HD23	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ARG:HB2	1:B:535:ARG:HH21	1.72	0.55
1:A:570:LYS:HB2	1:A:586:GLU:CD	2.31	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: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:A:303:ASP:C	1:A:304:ILE:HG13	2.32	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:A:672:ASP:OD1	1:A:724:SER:OG	2.26	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:B:473:GLU:C	1:B:475:GLU:H	2.16	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: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: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:B:448:GLU:H	1:B:448:GLU:CD	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:129:PHE:C	1:B:131:ASP:H	2.19	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: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:162:TRP:CG	1:A:163:MET:H	2.30	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: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:473:GLU:C	1:A:475:GLU:N	2.70	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:174:PHE:HB3	1:A:180:MET:HE2	1.93	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HA	1:A:402:PHE:O	2.14	0.48
1:A:448:GLU:N	1:A:448:GLU:CD	2.72	0.48
1:A:508:GLU:C	1:A:510:LEU:H	2.21	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: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:613:HIS:HE1	1:A:719:GLY:HA3	1.78	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:713:ASP:OD2	1:A:715:GLN:NE2	2.48	0.47
1:A:620:MET:HE1	1:A:631:VAL:HG12	1.97	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:731:ILE:HG12	1:A:750:CYS:SG	2.55	0.46
1:B:69:PHE:CD2	1:B:69:PHE:C	2.93	0.46
1:B:613:HIS:CD2	1:B:721:HIS:NE2	2.84	0.46
1:A:21:LYS:O	1:B:659:LYS:NZ	2.35	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
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: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:A:646:ASP:OD1	1:A:646:ASP:N	2.48	0.45
1:B:74:GLU:HB2	1:B:75:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:101:ILE:HD11	1:B:109:ILE:HD11	1.99	0.45
1:B:174:PHE:CB	1:B:180:MET:HE2	2.35	0.45
1:A:69:PHE:CD2	1:A:69:PHE:C	2.95	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:B:508:GLU:C	1:B:510:LEU:H	2.26	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:A:448:GLU:CD	1:A:448:GLU:H	2.25	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:B:253:LEU:O	1:B:257:VAL:HG23	2.18	0.43
1:B:421:LYS:C	1:B:423:TYR:H	2.26	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:351:MET:HE2	1:B:356:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:129:PHE:C	1:B:131:ASP:N	2.76	0.42
1:B:173:PHE:HA	1:B:177:GLU:HG2	2.01	0.42
1:B:448:GLU:CD	1:B:448:GLU:N	2.77	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:B:559:THR:C	1:B:602:ASP:HB2	2.45	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: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: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:589:GLY:C	1:B:591:PHE:H	2.28	0.41
1:B:636:SER:O	1:B:637:GLN:HB2	2.20	0.41
1:B:509:LEU:H	1:B:509:LEU:HD12	1.85	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
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:147:MET:HE2	3:B:999:A5A:C5'	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HB2	1:A:682:ARG:HD2	2.03	0.41
1:B:603:TRP:C	1:B:605:ARG:N	2.78	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:147:MET:HE1	3:B:999:A5A:O	2.21	0.41
1:B:386:PRO:HG2	1:B:389:GLU:CG	2.45	0.41
1:B:473:GLU:C	1:B:475:GLU:N	2.78	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:A:519:LEU:HD13	1:A:526:MET:HE1	2.03	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%)	7	30
1	B	729/752 (97%)	641 (88%)	74 (10%)	14 (2%)	6	27
All	All	1459/1504 (97%)	1298 (89%)	135 (9%)	26 (2%)	6	28

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 ⓘ

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%)	582 (90%)	62 (10%)	8	30
1	B	642/655 (98%)	568 (88%)	74 (12%)	5	23
All	All	1286/1310 (98%)	1150 (89%)	136 (11%)	6	26

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	5	MET
1	A	11	GLU
1	A	16	ILE
1	A	46	GLN
1	A	50	LYS
1	A	59	LEU
1	A	87	LEU
1	A	95	LEU
1	A	97	VAL
1	A	128	ARG
1	A	130	THR
1	A	133	ASP
1	A	158	LYS
1	A	186	THR
1	A	214	LEU
1	A	224	GLU
1	A	234	ILE
1	A	237	GLU
1	A	261	GLN
1	A	280	LYS
1	A	286	LYS
1	A	296	SER
1	A	304	ILE
1	A	310	LEU
1	A	311	ARG
1	A	320	ARG
1	A	325	VAL
1	A	333	ARG
1	A	336	GLU
1	A	396	LYS
1	A	401	THR
1	A	406	LYS
1	A	414	GLU
1	A	442	LYS
1	A	448	GLU
1	A	453	LYS
1	A	455	VAL
1	A	466	GLU
1	A	473	GLU
1	A	474	LYS
1	A	479	VAL

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Mol	Chain	Res	Type
1	A	480	ASN
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	584	LYS
1	A	608	GLN
1	A	626	VAL
1	A	638	LEU
1	A	646	ASP
1	A	652	ARG
1	A	684	THR
1	A	688	LYS
1	A	692	ARG
1	A	710	GLU
1	A	732	LYS
1	A	735	ARG
1	B	2	GLU
1	B	13	GLU
1	B	16	ILE
1	B	44	GLU
1	B	82	LYS
1	B	87	LEU
1	B	95	LEU
1	B	140	ARG
1	B	158	LYS
1	B	167	VAL
1	B	168	GLU
1	B	210	GLU
1	B	218	GLN
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	274	VAL
1	B	286	LYS
1	B	292	LEU

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Mol	Chain	Res	Type
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	384	GLU
1	B	396	LYS
1	B	401	THR
1	B	407	GLU
1	B	409	GLU
1	B	421	LYS
1	B	433	LEU
1	B	438	ILE
1	B	442	LYS
1	B	448	GLU
1	B	452	GLU
1	B	456	THR
1	B	459	GLU
1	B	466	GLU
1	B	471	ILE
1	B	479	VAL
1	B	480	ASN
1	B	491	LYS
1	B	507	PHE
1	B	508	GLU
1	B	515	ASP
1	B	527	LYS
1	B	535	ARG
1	B	538	LYS
1	B	558	ASP
1	B	568	GLU
1	B	571	VAL
1	B	572	THR
1	B	579	LYS
1	B	581	ILE
1	B	584	LYS
1	B	601	ILE
1	B	638	LEU
1	B	644	ARG
1	B	658	LEU
1	B	680	LEU

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Mol	Chain	Res	Type
1	B	684	THR
1	B	699	VAL
1	B	717	CYS
1	B	724	SER
1	B	732	LYS
1	B	733	ILE
1	B	735	ARG
1	B	741	ASP
1	B	746	ILE
1	B	752	GLU

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	124	GLN
1	A	134	ASN
1	A	218	GLN
1	A	316	GLN
1	A	377	HIS
1	A	480	ASN
1	A	608	GLN
1	A	633	GLN
1	A	695	GLN
1	A	715	GLN
1	B	124	GLN
1	B	228	GLN
1	B	230	GLN
1	B	399	HIS
1	B	461	HIS
1	B	480	ASN
1	B	608	GLN
1	B	612	HIS
1	B	637	GLN
1	B	715	GLN
1	B	740	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	999	-	29,30,30	2.08	4 (13%)	42,45,45	2.38	13 (30%)
3	A5A	B	999	-	29,30,30	2.17	5 (17%)	42,45,45	2.24	10 (23%)

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	A	999	-	-	1/18/35/35	0/3/3/3
3	A5A	B	999	-	-	1/18/35/35	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	6.65	1.48	1.42
3	B	999	A5A	O2S-S	6.57	1.48	1.42
3	A	999	A5A	O1S-S	6.49	1.48	1.42
3	A	999	A5A	O2S-S	5.17	1.47	1.42
3	A	999	A5A	S-N3S	-4.96	1.51	1.59
3	B	999	A5A	S-N3S	-3.99	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	A5A	C-N3S	-2.62	1.32	1.37
3	B	999	A5A	C8-N7	2.09	1.35	1.31
3	B	999	A5A	C-N3S	-2.02	1.34	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	A5A	O2S-S-O1S	-8.71	107.81	120.85
3	B	999	A5A	O2S-S-O1S	-7.70	109.32	120.85
3	B	999	A5A	N3-C2-N1	-4.76	121.38	128.58
3	A	999	A5A	N3-C2-N1	-4.75	121.39	128.58
3	A	999	A5A	C5-C4-N3	-4.47	120.56	126.72
3	B	999	A5A	C5-C4-N3	-4.46	120.57	126.72
3	B	999	A5A	N9-C8-N7	-4.44	107.64	113.94
3	A	999	A5A	N9-C8-N7	-4.08	108.15	113.94
3	A	999	A5A	O5'-S-O1S	3.76	116.85	105.48
3	B	999	A5A	C4-N9-C8	3.57	109.49	105.74
3	A	999	A5A	C4-N9-C8	3.47	109.38	105.74
3	B	999	A5A	C5-N7-C8	3.38	108.76	103.45
3	B	999	A5A	C4-C5-N7	-3.33	106.77	110.58
3	A	999	A5A	C2-N3-C4	3.25	119.76	111.83
3	B	999	A5A	C2-N3-C4	3.18	119.60	111.83
3	A	999	A5A	N3-C4-N9	3.10	132.44	127.17
3	A	999	A5A	C2'-C1'-N9	-2.92	106.05	113.30
3	B	999	A5A	N3-C4-N9	2.90	132.10	127.17
3	A	999	A5A	C5-N7-C8	2.88	107.98	103.45
3	A	999	A5A	C4-C5-N7	-2.71	107.48	110.58
3	B	999	A5A	O5'-S-O1S	2.71	113.67	105.48
3	A	999	A5A	O4'-C1'-N9	2.64	113.17	108.09
3	A	999	A5A	O5'-C5'-C4'	2.62	112.23	107.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

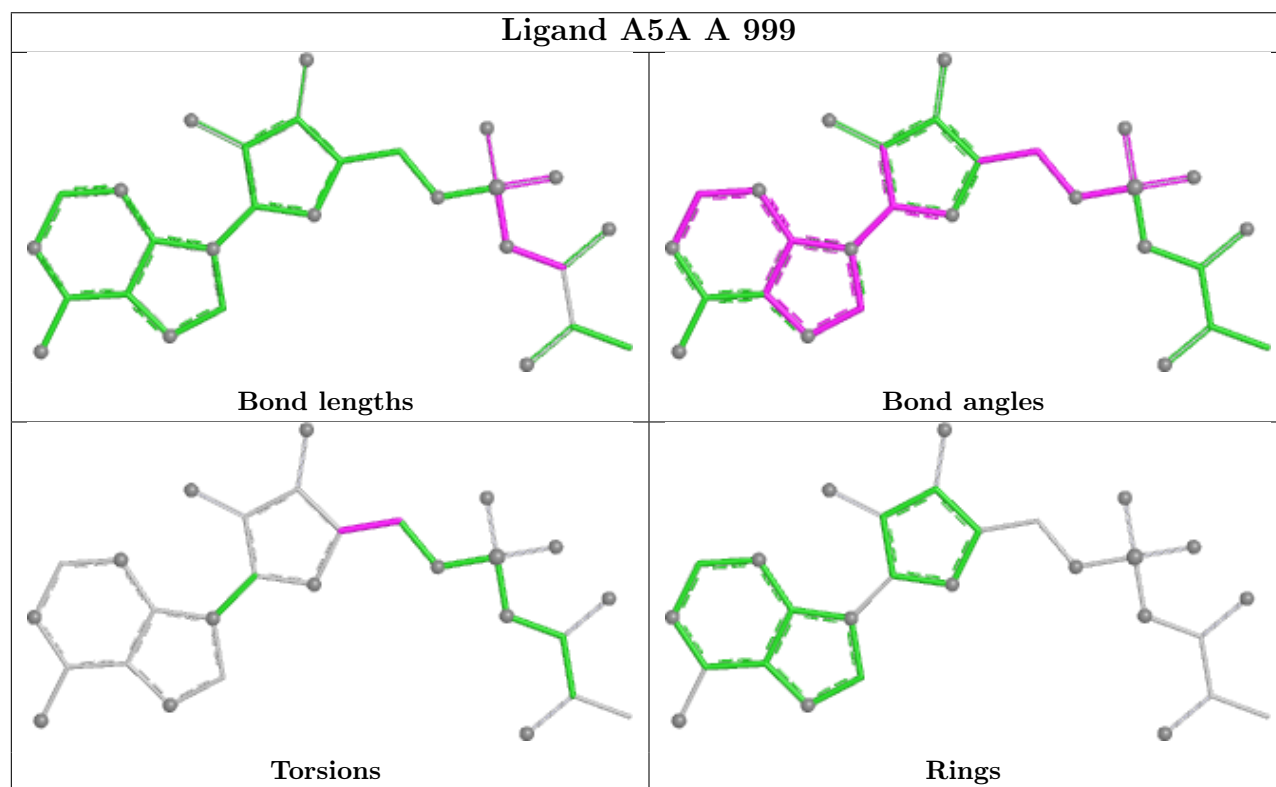
Mol	Chain	Res	Type	Atoms
3	B	999	A5A	C5'-O5'-S-N3S
3	A	999	A5A	C3'-C4'-C5'-O5'

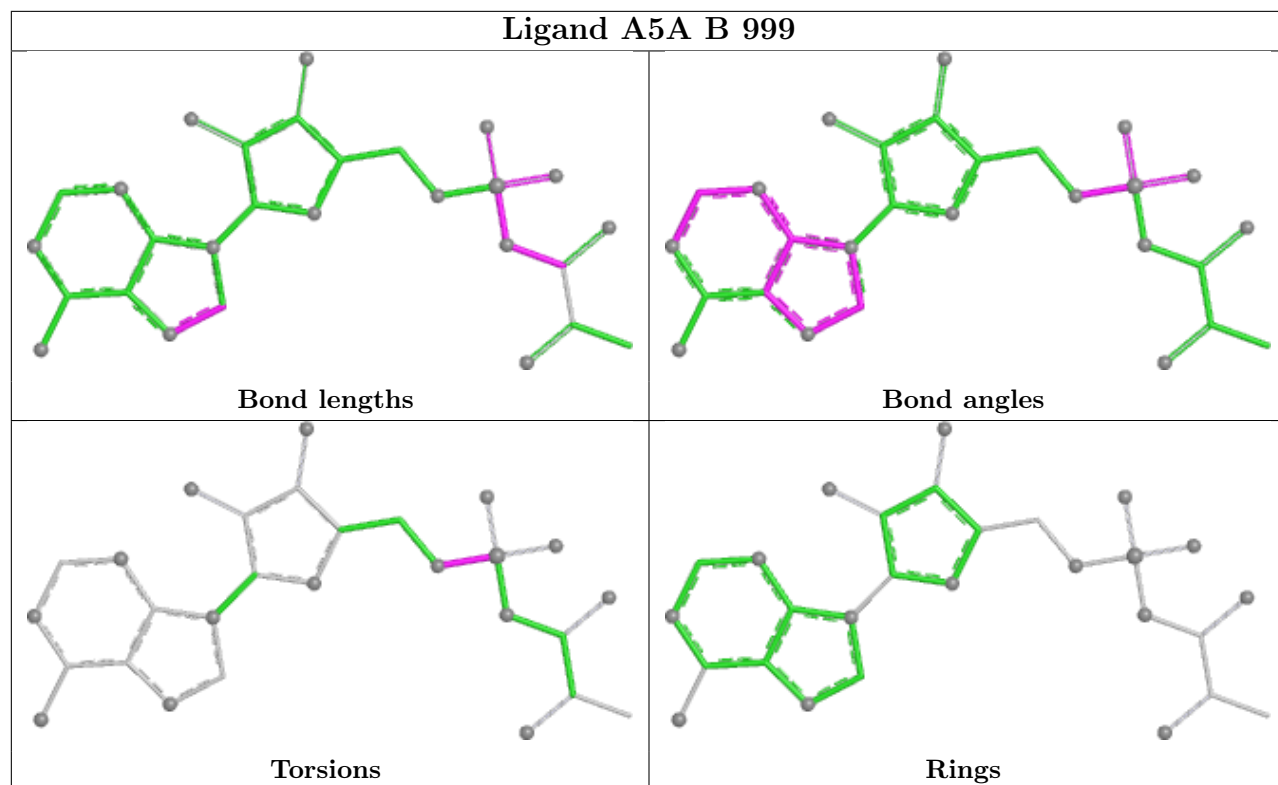
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	A5A	1	0
3	B	999	A5A	5	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 than 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.





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	738/752 (98%)	-0.37	4 (0%)	87 73	53, 72, 104, 118	0
1	B	737/752 (98%)	-0.31	3 (0%)	88 76	47, 74, 113, 127	0
All	All	1475/1504 (98%)	-0.34	7 (0%)	87 73	47, 73, 110, 127	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	VAL	3.1
1	B	479	VAL	2.8
1	B	234	ILE	2.5
1	A	504	LEU	2.4
1	A	304	ILE	2.2
1	A	302	PHE	2.1
1	B	564	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

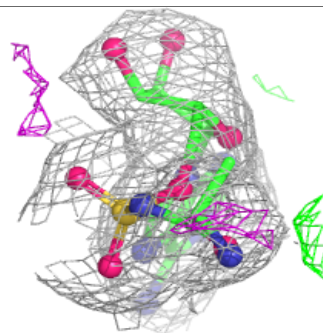
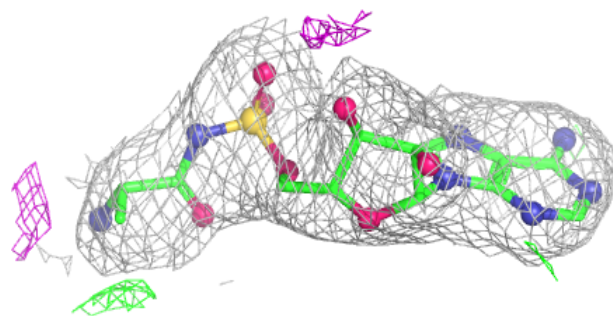
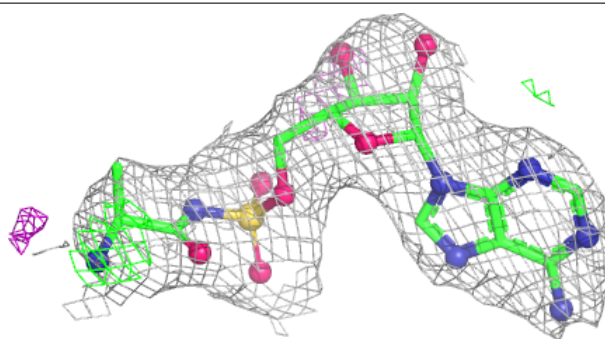
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A5A	A	999	28/28	0.97	0.06	52,60,64,64	0
3	A5A	B	999	28/28	0.97	0.06	51,55,56,57	0
2	ZN	A	901	1/1	0.98	0.06	106,106,106,106	0
2	ZN	B	901	1/1	0.98	0.03	96,96,96,96	0
2	ZN	B	900	1/1	1.00	0.01	69,69,69,69	0
2	ZN	A	900	1/1	1.00	0.01	65,65,65,65	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.

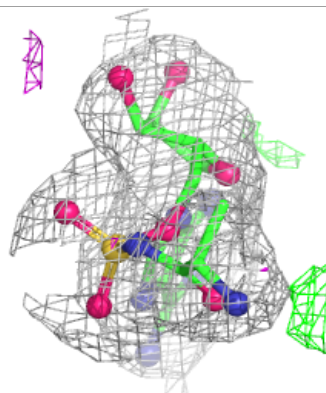
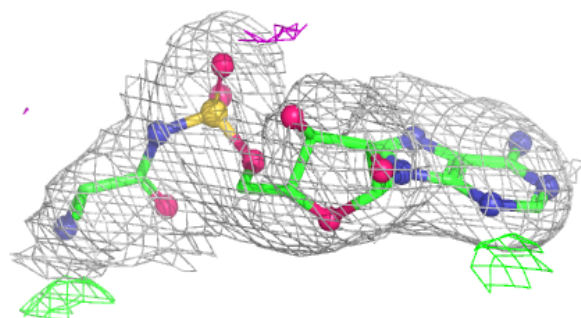
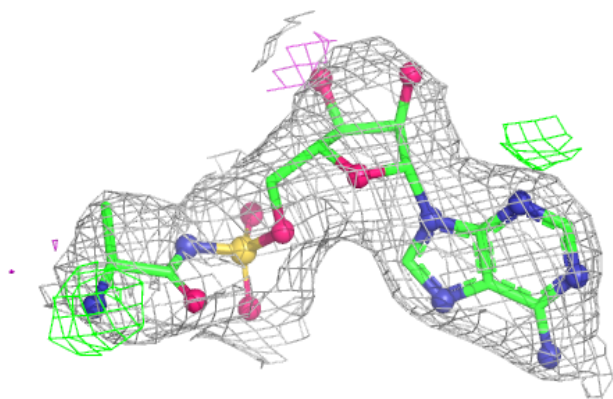
Electron density around A5A A 999:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-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 [i](#)

There are no such residues in this entry.