



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:58 PM UTC

PDB ID : 6T4H / pdb_00006t4h
Title : Crystal structure of the accessory translocation ATPase, SecA2, from *Clostridium difficile*, in complex with adenosine-5'-(gamma-thio)-triphosphate
Authors : Lindic, N.; Loboda, J.; Usenik, A.; Turk, D.
Deposited on : 2019-10-14
Resolution : 2.90 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

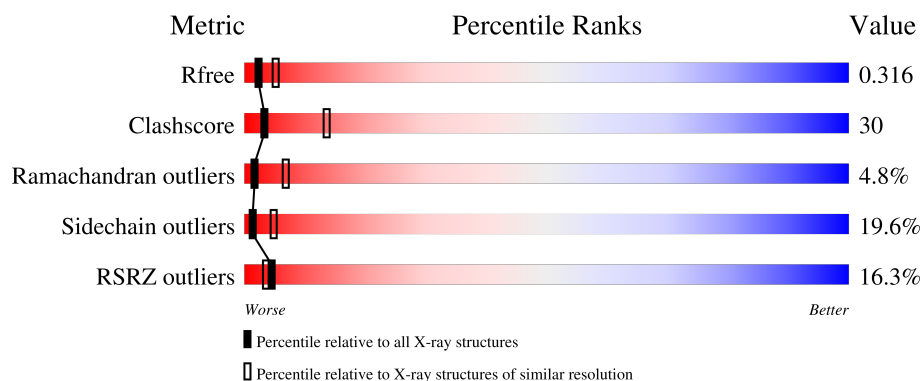
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	781	16% 41% 43% 13% ..

2 Entry composition [i](#)

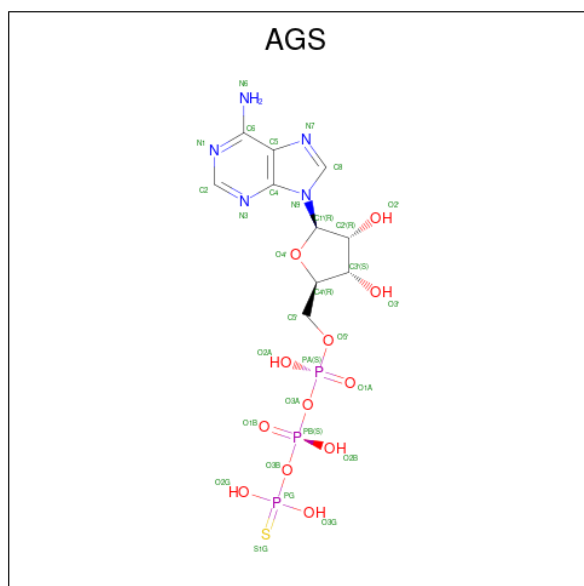
There are 3 unique types of molecules in this entry. The entry contains 7720 atoms, of which 1488 are hydrogens and 0 are deuteriums.

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 Protein translocase subunit SecA 2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	771	Total	C	H	N	O	S		1652	0	0
			7635	3901	1448	1055	1209	22				

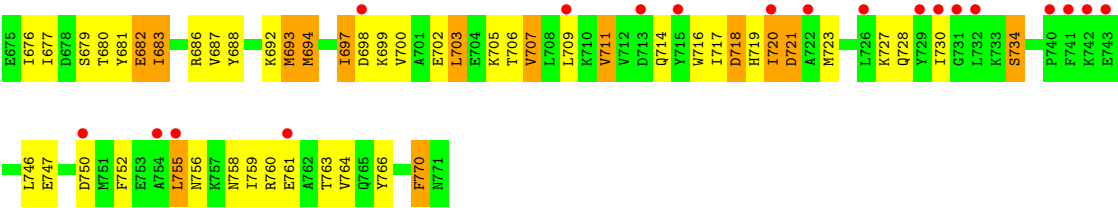
- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	12	0
			43	10	12	5	12	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	H	O	
			42	28	14	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.94Å 96.84Å 114.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.90 49.34 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.34-2.90) 99.7 (49.34-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.61Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.335 , 0.380 0.316 , 0.316	Depositor DCC
R_{free} test set	1502 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.954	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7720	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: AGS

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	0.86	3/6271 (0.0%)	1.33	41/8423 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	638	TYR	CA-C	-6.05	1.44	1.52
1	A	103	PRO	C-N	5.54	1.41	1.33
1	A	359	MET	SD-CE	5.24	1.92	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	LEU	N-CA-C	-9.26	100.10	111.40
1	A	419	GLN	CA-C-N	-8.20	111.72	120.66
1	A	419	GLN	C-N-CA	-8.20	111.72	120.66
1	A	205	ASP	N-CA-C	7.80	119.69	111.03
1	A	271	LYS	N-CA-C	-7.44	98.66	109.59
1	A	654	TYR	N-CA-C	-7.27	103.44	111.36
1	A	70	ARG	N-CA-C	-7.22	101.53	110.41
1	A	465	LYS	N-CA-C	7.06	120.97	110.52
1	A	26	LEU	N-CA-C	6.92	120.27	110.23
1	A	310	GLY	N-CA-C	-6.86	106.00	114.92
1	A	294	ASP	N-CA-C	-6.74	98.25	109.24
1	A	763	THR	N-CA-C	-6.31	104.32	111.14
1	A	192	ASN	N-CA-C	6.13	119.15	111.24
1	A	610	ARG	N-CA-C	-5.88	106.75	114.04
1	A	405	SER	N-CA-C	-5.82	105.01	111.36
1	A	623	ILE	N-CA-CB	5.79	117.32	110.55
1	A	319	THR	N-CA-C	5.74	117.47	110.41
1	A	157	GLN	N-CA-C	5.71	117.18	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	LYS	N-CA-C	5.64	118.87	110.52
1	A	322	LEU	N-CA-C	5.62	117.86	111.11
1	A	241	LEU	N-CA-C	5.61	116.48	108.74
1	A	187	VAL	N-CA-C	5.58	118.54	112.96
1	A	351	ARG	N-CA-C	-5.46	105.43	111.71
1	A	412	ILE	N-CA-C	-5.39	105.12	110.62
1	A	385	ARG	CA-C-N	-5.29	114.47	119.76
1	A	385	ARG	C-N-CA	-5.29	114.47	119.76
1	A	320	ASP	N-CA-C	5.28	122.04	110.80
1	A	616	ASP	N-CA-C	5.25	118.44	111.30
1	A	711	VAL	N-CA-CB	5.25	118.45	110.58
1	A	100	GLU	N-CA-C	5.24	118.13	111.69
1	A	527	ASP	CA-C-N	-5.24	115.18	120.21
1	A	527	ASP	C-N-CA	-5.24	115.18	120.21
1	A	627	VAL	N-CA-C	-5.21	105.42	110.42
1	A	212	ILE	N-CA-C	5.19	115.51	107.78
1	A	764	VAL	N-CA-C	5.17	115.79	110.36
1	A	209	THR	CA-C-N	-5.13	115.31	120.85
1	A	209	THR	C-N-CA	-5.13	115.31	120.85
1	A	668	VAL	N-CA-C	5.08	119.91	109.34
1	A	346	TYR	N-CA-C	-5.06	107.06	113.18
1	A	683	ILE	N-CA-C	-5.05	105.46	110.62
1	A	62	VAL	N-CA-C	-5.00	105.67	110.72

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	6187	1448	6268	367	10
2	A	31	12	12	3	0
3	A	14	28	0	1	0
All	All	6232	1488	6280	367	10

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 30.

All (367) 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:13:VAL:HA	1:A:16:ILE:HD12	1.29	1.10
1:A:34:MET:HA	1:A:37:ILE:HG13	1.45	0.99
1:A:421:ILE:HD11	1:A:469:ILE:HG12	1.47	0.97
1:A:87:ILE:HD11	1:A:376:LEU:HD13	1.49	0.94
1:A:424:GLY:HA3	1:A:518:LEU:HD21	1.53	0.91
1:A:60:ARG:HA	1:A:71:GLN:NE2	1.86	0.90
1:A:483:SER:HA	1:A:524:ARG:HH22	1.40	0.87
1:A:97:THR:HG22	1:A:131:MET:HE3	1.57	0.87
1:A:512:ARG:HG3	1:A:512:ARG:HH11	1.42	0.85
1:A:98:LEU:HD12	1:A:131:MET:SD	2.18	0.83
1:A:9:LEU:HD22	1:A:77:ILE:HG23	1.60	0.83
1:A:483:SER:HA	1:A:524:ARG:NH2	1.94	0.83
1:A:48:LEU:HD22	1:A:106:LEU:HG	1.60	0.83
1:A:421:ILE:HG22	1:A:502:TYR:HB3	1.58	0.83
1:A:60:ARG:HA	1:A:71:GLN:HE22	1.42	0.81
1:A:623:ILE:HG13	1:A:626:MET:HE2	1.63	0.80
1:A:425:THR:HG22	1:A:426:VAL:H	1.46	0.78
1:A:153:ILE:HG22	1:A:157:GLN:HE21	1.49	0.78
1:A:613:VAL:HG13	1:A:705:LYS:HB3	1.63	0.77
1:A:231:VAL:HG11	1:A:283:LEU:HA	1.66	0.77
1:A:96:LYS:HA	1:A:99:VAL:HG23	1.66	0.76
1:A:653:LEU:HD23	1:A:653:LEU:N	2.01	0.75
1:A:77:ILE:HB	1:A:381:ILE:HD11	1.69	0.74
1:A:102:ALA:HB3	1:A:103:PRO:HD3	1.69	0.74
1:A:88:ALA:HB3	1:A:359:MET:HG2	1.70	0.74
1:A:396:VAL:HG11	1:A:570:LEU:HD21	1.70	0.73
1:A:168:SER:O	1:A:172:PHE:HB2	1.89	0.73
1:A:727:LYS:O	1:A:730:ILE:HG12	1.88	0.72
1:A:403:LYS:O	1:A:407:VAL:HG23	1.90	0.71
1:A:56:PHE:O	1:A:59:VAL:HG12	1.90	0.70
1:A:180:VAL:HG21	1:A:185:HIS:HB2	1.73	0.70
1:A:422:LEU:HD21	1:A:521:ARG:HD2	1.73	0.70
1:A:13:VAL:HG13	1:A:76:LEU:HD12	1.74	0.70
1:A:656:THR:HG22	1:A:657:PHE:HD2	1.56	0.69
1:A:56:PHE:CD1	1:A:102:ALA:HB1	2.28	0.69
1:A:118:THR:HG21	1:A:123:LEU:HB3	1.73	0.68
1:A:624:GLN:O	1:A:628:LYS:HG3	1.93	0.68
1:A:609:GLU:HA	1:A:612:LYS:HE2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:HD11	1:A:283:LEU:HD22	1.75	0.68
1:A:87:ILE:HD12	1:A:199:VAL:HG11	1.74	0.67
1:A:193:PHE:HD1	1:A:355:LYS:HB2	1.60	0.67
1:A:120:ASN:HA	1:A:166:THR:HG23	1.77	0.67
1:A:699:LYS:O	1:A:703:LEU:HB2	1.95	0.67
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.10	0.66
1:A:97:THR:CG2	1:A:131:MET:HE3	2.25	0.66
1:A:524:ARG:HG2	1:A:524:ARG:HH11	1.61	0.66
1:A:100:GLU:O	1:A:103:PRO:HD2	1.95	0.66
1:A:693:MET:HE3	1:A:694:MET:HG3	1.78	0.66
1:A:697:ILE:HG23	1:A:698:ASP:N	2.10	0.66
1:A:114:VAL:HG13	1:A:193:PHE:HD2	1.62	0.65
1:A:154:ARG:HH12	1:A:169:GLU:HB3	1.60	0.65
1:A:175:LEU:HD13	1:A:342:ALA:HB1	1.79	0.65
1:A:501:LEU:HD23	1:A:522:SER:HB2	1.78	0.65
1:A:90:MET:HG2	1:A:381:ILE:HG21	1.78	0.65
1:A:61:GLU:HA	1:A:64:LYS:HB3	1.79	0.64
1:A:137:SER:O	1:A:138:LEU:HD23	1.96	0.64
1:A:96:LYS:HD2	2:A:801:AGS:O2B	1.98	0.63
1:A:613:VAL:HG11	1:A:709:LEU:HB2	1.80	0.63
1:A:90:MET:HB2	1:A:96:LYS:HE3	1.80	0.63
1:A:524:ARG:HG2	1:A:524:ARG:NH1	2.13	0.63
1:A:9:LEU:CD2	1:A:77:ILE:HA	2.29	0.63
1:A:61:GLU:HG2	1:A:64:LYS:HD3	1.80	0.63
1:A:424:GLY:HA3	1:A:518:LEU:CD2	2.24	0.63
1:A:448:LEU:HD21	1:A:459:ILE:HG21	1.81	0.62
1:A:420:PRO:HG3	1:A:466:LEU:O	1.99	0.62
1:A:413:ARG:HA	1:A:416:LYS:HE2	1.79	0.62
1:A:137:SER:C	1:A:138:LEU:HD23	2.24	0.62
1:A:104:VAL:HG22	1:A:114:VAL:HG11	1.82	0.62
1:A:273:ILE:HD11	1:A:711:VAL:HG12	1.80	0.62
1:A:207:ALA:HB1	1:A:347:GLN:NE2	2.15	0.61
1:A:271:LYS:O	1:A:271:LYS:HG2	1.98	0.61
1:A:59:VAL:HG11	1:A:102:ALA:HB2	1.83	0.61
1:A:203:LEU:O	1:A:207:ALA:HB2	2.01	0.60
1:A:407:VAL:O	1:A:411:ILE:HG13	2.02	0.60
1:A:463:ALA:HB2	1:A:470:THR:HG21	1.81	0.60
1:A:500:GLY:HA3	1:A:528:PRO:O	2.02	0.60
1:A:472:ALA:HB1	1:A:476:ALA:HB3	1.84	0.60
1:A:385:ARG:HD3	1:A:526:GLY:HA3	1.84	0.59
1:A:755:LEU:HA	3:A:908:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:O	1:A:465:LYS:HG2	2.02	0.59
1:A:623:ILE:O	1:A:627:VAL:HG23	2.03	0.59
1:A:250:LEU:HD11	1:A:254:GLY:HA3	1.85	0.58
1:A:128:LYS:HG3	1:A:129:GLU:N	2.18	0.58
1:A:347:GLN:O	1:A:351:ARG:HG3	2.03	0.58
1:A:104:VAL:HG12	1:A:105:TYR:N	2.18	0.58
1:A:448:LEU:HD21	1:A:459:ILE:CG2	2.34	0.58
1:A:418:ARG:O	1:A:498:LEU:HD13	2.03	0.58
1:A:639:LEU:HD22	1:A:649:TYR:HE2	1.69	0.58
1:A:679:SER:O	1:A:683:ILE:HD13	2.04	0.58
1:A:126:ARG:O	1:A:130:LEU:HG	2.03	0.58
1:A:90:MET:HE2	1:A:381:ILE:HD13	1.85	0.57
1:A:448:LEU:HD22	1:A:456:GLU:HB2	1.86	0.57
1:A:425:THR:HG22	1:A:426:VAL:N	2.16	0.57
1:A:683:ILE:O	1:A:687:VAL:HG23	2.04	0.57
1:A:550:ILE:HG22	1:A:554:MET:HE2	1.87	0.57
1:A:199:VAL:HG12	1:A:360:THR:HB	1.87	0.57
1:A:231:VAL:CG1	1:A:283:LEU:HA	2.34	0.57
1:A:89:GLU:HA	1:A:360:THR:O	2.05	0.57
1:A:408:VAL:HG21	1:A:437:MET:HB2	1.86	0.57
1:A:360:THR:HG21	1:A:363:ALA:HB2	1.86	0.57
1:A:4:GLN:HA	1:A:7:LYS:HB2	1.87	0.56
1:A:114:VAL:HG13	1:A:193:PHE:CD2	2.40	0.56
1:A:118:THR:CG2	1:A:123:LEU:HB3	2.35	0.56
1:A:646:TYR:CZ	1:A:668:VAL:HG13	2.41	0.56
1:A:152:ASN:ND2	1:A:153:ILE:HG12	2.20	0.56
1:A:396:VAL:HA	1:A:535:VAL:HG22	1.87	0.56
1:A:623:ILE:HG13	1:A:626:MET:CE	2.36	0.56
1:A:422:LEU:HD23	1:A:503:VAL:HG22	1.88	0.56
1:A:210:PRO:HG3	1:A:345:THR:HG22	1.87	0.56
1:A:606:ILE:O	1:A:610:ARG:HB2	2.05	0.56
1:A:639:LEU:HD22	1:A:649:TYR:CE2	2.41	0.56
1:A:13:VAL:CG1	1:A:76:LEU:HD12	2.36	0.55
1:A:372:SER:O	1:A:373:ILE:HG13	2.07	0.55
1:A:188:GLN:NE2	1:A:191:LEU:HD21	2.21	0.55
1:A:542:ILE:HG21	1:A:574:ILE:HD13	1.87	0.55
1:A:318:TYR:HB3	1:A:322:LEU:HB3	1.87	0.55
1:A:90:MET:SD	1:A:99:VAL:HG21	2.47	0.55
1:A:273:ILE:CD1	1:A:711:VAL:HG12	2.37	0.55
1:A:13:VAL:HG11	1:A:73:ARG:HG3	1.87	0.55
1:A:69:MET:HE3	2:A:801:AGS:H2'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:CG1	1:A:707:VAL:HG12	2.37	0.54
1:A:540:ASP:HA	1:A:543:LYS:HB3	1.89	0.54
1:A:570:LEU:O	1:A:574:ILE:HG12	2.07	0.54
1:A:51:ILE:HG22	1:A:55:ALA:HB2	1.87	0.54
1:A:96:LYS:HA	1:A:99:VAL:CG2	2.37	0.54
1:A:408:VAL:HG21	1:A:437:MET:SD	2.47	0.54
1:A:650:PHE:CD1	1:A:663:LEU:HD13	2.42	0.54
1:A:115:HIS:HD2	1:A:170:PHE:CE1	2.25	0.54
1:A:656:THR:CG2	1:A:657:PHE:HD2	2.21	0.54
1:A:606:ILE:HG13	1:A:716:TRP:CZ3	2.42	0.54
1:A:505:GLY:HA3	1:A:533:PHE:CE2	2.43	0.54
1:A:174:TYR:C	1:A:174:TYR:CD2	2.86	0.54
1:A:80:ILE:HG22	1:A:84:GLN:NE2	2.23	0.53
1:A:656:THR:HG23	1:A:761:GLU:HG2	1.88	0.53
1:A:421:ILE:HD13	1:A:421:ILE:N	2.23	0.53
1:A:550:ILE:HD12	1:A:550:ILE:H	1.73	0.53
1:A:9:LEU:HD21	1:A:77:ILE:HA	1.89	0.53
1:A:56:PHE:CG	1:A:102:ALA:HB1	2.43	0.53
1:A:180:VAL:CG2	1:A:185:HIS:HB2	2.38	0.53
1:A:273:ILE:HG23	1:A:274:GLU:N	2.23	0.53
1:A:600:ASN:O	1:A:604:LYS:HB2	2.08	0.53
1:A:389:ARG:HG2	1:A:390:ALA:N	2.23	0.53
1:A:61:GLU:O	1:A:65:ARG:HG3	2.09	0.53
1:A:153:ILE:HG22	1:A:157:GLN:NE2	2.23	0.53
1:A:547:GLY:O	1:A:551:GLU:HG3	2.09	0.53
1:A:565:ILE:HG22	1:A:566:GLU:N	2.22	0.53
1:A:637:THR:O	1:A:641:GLY:HA3	2.08	0.53
1:A:78:GLY:HA3	1:A:90:MET:CE	2.39	0.53
1:A:203:LEU:HD23	1:A:203:LEU:N	2.24	0.53
1:A:503:VAL:O	1:A:531:SER:HA	2.08	0.52
1:A:347:GLN:HB3	1:A:593:LEU:HD13	1.90	0.52
1:A:89:GLU:O	1:A:381:ILE:HG22	2.09	0.52
1:A:606:ILE:HG13	1:A:716:TRP:CE3	2.44	0.52
1:A:400:GLU:O	1:A:404:TYR:HD2	1.93	0.52
1:A:585:ASN:HA	1:A:588:ILE:HG12	1.92	0.52
1:A:31:LEU:O	1:A:34:MET:HB2	2.10	0.51
1:A:389:ARG:HG2	1:A:390:ALA:H	1.75	0.51
1:A:668:VAL:HG12	1:A:669:ASP:N	2.24	0.51
1:A:630:ILE:HG21	1:A:656:THR:HG21	1.92	0.51
1:A:697:ILE:CG2	1:A:698:ASP:N	2.72	0.51
1:A:59:VAL:HA	1:A:62:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HG11	1:A:434:LEU:HD11	1.92	0.51
1:A:9:LEU:CD1	1:A:81:VAL:HG23	2.41	0.51
1:A:248:ILE:CD1	1:A:283:LEU:HD22	2.41	0.51
1:A:623:ILE:HA	1:A:626:MET:HE2	1.93	0.51
1:A:421:ILE:HD13	1:A:421:ILE:H	1.76	0.50
1:A:524:ARG:HH11	1:A:524:ARG:CG	2.24	0.50
1:A:501:LEU:HD23	1:A:522:SER:CB	2.41	0.50
1:A:182:ASP:OD2	1:A:184:SER:HB2	2.12	0.50
1:A:109:LEU:HD23	1:A:140:MET:CE	2.41	0.50
1:A:658:MET:HE3	1:A:663:LEU:HD23	1.94	0.50
1:A:68:GLY:O	1:A:70:ARG:N	2.44	0.50
1:A:259:GLU:HA	1:A:264:ILE:O	2.12	0.50
1:A:408:VAL:HG21	1:A:437:MET:CB	2.42	0.50
1:A:445:HIS:HB3	1:A:469:ILE:HB	1.93	0.50
1:A:628:LYS:HE2	1:A:681:TYR:CZ	2.47	0.50
1:A:104:VAL:HG22	1:A:114:VAL:CG1	2.41	0.50
1:A:228:ASN:O	1:A:232:LYS:HB2	2.12	0.50
1:A:9:LEU:HD22	1:A:77:ILE:CG2	2.38	0.49
1:A:88:ALA:H	1:A:359:MET:HA	1.76	0.49
1:A:100:GLU:C	1:A:103:PRO:HD2	2.36	0.49
1:A:270:ILE:HG12	1:A:707:VAL:HB	1.93	0.49
1:A:87:ILE:HA	1:A:358:GLY:O	2.12	0.49
1:A:115:HIS:CD2	1:A:170:PHE:CE1	3.01	0.49
1:A:606:ILE:HG21	1:A:716:TRP:CD2	2.47	0.49
1:A:48:LEU:HD11	1:A:107:ASN:HA	1.95	0.49
1:A:97:THR:OG1	2:A:801:AGS:S1G	2.68	0.49
1:A:228:ASN:OD1	1:A:286:HIS:HE1	1.96	0.49
1:A:238:ASP:O	1:A:250:LEU:HD12	2.13	0.49
1:A:644:ARG:NH2	1:A:646:TYR:OH	2.45	0.49
1:A:682:GLU:O	1:A:686:ARG:HG3	2.13	0.49
1:A:667:GLY:O	1:A:669:ASP:N	2.46	0.48
1:A:270:ILE:HG21	1:A:706:THR:CG2	2.43	0.48
1:A:599:ILE:O	1:A:603:ARG:HB2	2.12	0.48
1:A:448:LEU:HD12	1:A:472:ALA:HB2	1.96	0.48
1:A:483:SER:CA	1:A:524:ARG:HH22	2.17	0.48
1:A:463:ALA:HB1	1:A:470:THR:OG1	2.13	0.48
1:A:434:LEU:HD23	1:A:434:LEU:O	2.14	0.48
1:A:59:VAL:HG11	1:A:102:ALA:CB	2.44	0.48
1:A:104:VAL:CG1	1:A:162:ILE:HG12	2.44	0.47
1:A:275:LEU:O	1:A:279:ILE:HG22	2.14	0.47
1:A:318:TYR:HD1	1:A:323:HIS:ND1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PHE:CD2	1:A:650:PHE:N	2.82	0.47
1:A:677:ILE:HA	1:A:680:THR:OG1	2.13	0.47
1:A:12:ILE:HD12	1:A:80:ILE:HG21	1.97	0.47
1:A:13:VAL:HG13	1:A:76:LEU:CD1	2.44	0.47
1:A:48:LEU:HD21	1:A:106:LEU:O	2.14	0.47
1:A:206:GLU:O	1:A:208:ARG:N	2.47	0.47
1:A:552:LYS:O	1:A:556:ARG:HG3	2.15	0.47
1:A:104:VAL:O	1:A:105:TYR:C	2.58	0.47
1:A:549:THR:O	1:A:553:LEU:HG	2.14	0.47
1:A:268:THR:HG23	1:A:770:PHE:CD2	2.49	0.47
1:A:598:THR:O	1:A:602:GLN:HG3	2.13	0.47
1:A:334:ILE:HD12	1:A:334:ILE:H	1.79	0.47
1:A:519:ARG:HH21	1:A:533:PHE:HD1	1.62	0.47
1:A:142:VAL:HG13	1:A:162:ILE:HB	1.96	0.47
1:A:460:ILE:O	1:A:463:ALA:HB3	2.14	0.47
1:A:9:LEU:HD11	1:A:81:VAL:HG23	1.97	0.46
1:A:87:ILE:HG23	1:A:199:VAL:HG11	1.97	0.46
1:A:112:LYS:C	1:A:189:ARG:HH21	2.24	0.46
1:A:67:LEU:HD11	1:A:134:VAL:HG21	1.98	0.46
1:A:81:VAL:HG22	1:A:379:VAL:HG11	1.96	0.46
1:A:87:ILE:HG13	1:A:378:VAL:HG22	1.96	0.46
1:A:271:LYS:O	1:A:272:ASN:HB2	2.15	0.46
1:A:404:TYR:O	1:A:408:VAL:HG23	2.15	0.46
1:A:72:TYR:O	1:A:75:GLN:N	2.46	0.46
1:A:656:THR:HG22	1:A:657:PHE:CD2	2.45	0.46
1:A:4:GLN:O	1:A:8:LYS:HG2	2.15	0.46
1:A:204:ILE:HG12	1:A:370:PHE:CE2	2.50	0.46
1:A:272:ASN:O	1:A:274:GLU:N	2.49	0.46
1:A:239:PHE:HB2	1:A:249:ALA:O	2.16	0.46
1:A:371:GLU:HA	1:A:375:LYS:HA	1.97	0.46
1:A:683:ILE:HG13	1:A:686:ARG:NH1	2.30	0.46
1:A:90:MET:HG2	1:A:381:ILE:CG2	2.45	0.46
1:A:624:GLN:HG3	1:A:681:TYR:OH	2.15	0.46
1:A:720:ILE:HG22	1:A:721:ASP:N	2.31	0.46
1:A:473:THR:HG22	1:A:474:ASN:H	1.81	0.46
1:A:436:LYS:O	1:A:440:LYS:HB2	2.16	0.46
1:A:75:GLN:O	1:A:99:VAL:HG13	2.16	0.46
1:A:503:VAL:HG13	1:A:518:LEU:HG	1.97	0.46
1:A:213:ILE:HB	1:A:342:ALA:HB3	1.97	0.45
1:A:319:THR:HG22	1:A:320:ASP:H	1.81	0.45
1:A:524:ARG:O	1:A:524:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG13	1:A:165:GLY:HA3	1.98	0.45
1:A:453:HIS:HA	1:A:456:GLU:HG2	1.98	0.45
1:A:658:MET:HG3	1:A:659:PRO:HD2	1.97	0.45
1:A:453:HIS:O	1:A:457:ALA:HB2	2.17	0.45
1:A:200:ASP:HA	1:A:370:PHE:HZ	1.81	0.45
1:A:270:ILE:HG21	1:A:706:THR:HG22	1.99	0.45
1:A:128:LYS:O	1:A:132:SER:HB3	2.17	0.45
1:A:194:ALA:HB2	1:A:353:TYR:CE2	2.51	0.45
1:A:756:ASN:O	1:A:759:ILE:HB	2.17	0.45
1:A:152:ASN:O	1:A:156:GLN:NE2	2.50	0.45
1:A:273:ILE:CG2	1:A:274:GLU:N	2.80	0.45
1:A:362:THR:HB	1:A:513:ARG:HG2	1.99	0.45
1:A:425:THR:HG21	1:A:431:SER:N	2.32	0.45
1:A:409:GLU:O	1:A:412:ILE:HG12	2.17	0.45
1:A:96:LYS:CA	1:A:99:VAL:HG23	2.43	0.44
1:A:602:GLN:HB3	1:A:752:PHE:CE1	2.52	0.44
1:A:175:LEU:HD13	1:A:342:ALA:CB	2.46	0.44
1:A:351:ARG:NH1	1:A:373:ILE:O	2.50	0.44
1:A:404:TYR:HB3	1:A:437:MET:HE1	1.99	0.44
1:A:448:LEU:HB3	1:A:476:ALA:HB1	1.99	0.44
1:A:130:LEU:O	1:A:133:PRO:HD2	2.17	0.44
1:A:239:PHE:HA	1:A:251:THR:HG23	1.99	0.44
1:A:396:VAL:HA	1:A:535:VAL:CG2	2.47	0.44
1:A:152:ASN:HD22	1:A:153:ILE:HG12	1.81	0.44
1:A:267:LEU:O	1:A:268:THR:HB	2.17	0.44
1:A:343:THR:O	1:A:344:VAL:HB	2.17	0.44
1:A:188:GLN:HE22	1:A:191:LEU:HD21	1.82	0.44
1:A:650:PHE:N	1:A:650:PHE:HD2	2.16	0.44
1:A:9:LEU:HD22	1:A:77:ILE:HA	1.99	0.44
1:A:188:GLN:HB3	1:A:189:ARG:H	1.67	0.44
1:A:78:GLY:HA3	1:A:90:MET:HE3	1.99	0.43
1:A:230:PHE:HE1	1:A:279:ILE:HD11	1.83	0.43
1:A:291:LYS:HE3	1:A:297:ILE:HG12	1.99	0.43
1:A:608:ASN:C	1:A:610:ARG:H	2.25	0.43
1:A:631:ILE:HG22	1:A:677:ILE:HG23	1.99	0.43
1:A:104:VAL:HG11	1:A:162:ILE:HG12	1.99	0.43
1:A:264:ILE:HG12	1:A:272:ASN:ND2	2.33	0.43
1:A:389:ARG:CG	1:A:390:ALA:H	2.30	0.43
1:A:393:HIS:O	1:A:532:ARG:HG2	2.18	0.43
1:A:408:VAL:HG13	1:A:438:LEU:HD23	2.00	0.43
1:A:652:HIS:C	1:A:653:LEU:HD23	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:CD2	1:A:175:LEU:N	2.86	0.43
1:A:347:GLN:CB	1:A:593:LEU:HD13	2.47	0.43
1:A:640:ILE:HD11	1:A:673:VAL:HG21	2.00	0.43
1:A:651:LYS:O	1:A:655:SER:HB2	2.19	0.43
1:A:717:ILE:HG13	1:A:718:ASP:N	2.34	0.43
1:A:117:ILE:HD12	1:A:117:ILE:N	2.34	0.43
1:A:475:MET:HE2	1:A:475:MET:HB3	1.93	0.43
1:A:688:TYR:O	1:A:692:LYS:HG3	2.17	0.43
1:A:82:ILE:HD11	1:A:359:MET:CG	2.49	0.43
1:A:189:ARG:HG2	1:A:190:GLU:H	1.84	0.43
1:A:341:MET:HE2	1:A:341:MET:HB3	1.92	0.42
1:A:395:LYS:N	1:A:533:PHE:O	2.52	0.42
1:A:466:LEU:HB3	1:A:467:ASP:H	1.58	0.42
1:A:488:ASP:O	1:A:492:GLU:HB2	2.19	0.42
1:A:638:TYR:CE2	1:A:652:HIS:HB2	2.54	0.42
1:A:189:ARG:HG2	1:A:190:GLU:N	2.35	0.42
1:A:524:ARG:O	1:A:526:GLY:N	2.52	0.42
1:A:672:SER:O	1:A:676:ILE:HG13	2.19	0.42
1:A:59:VAL:HG21	1:A:101:VAL:HG12	2.02	0.42
1:A:270:ILE:HG13	1:A:707:VAL:HG12	2.02	0.42
1:A:605:VAL:HG23	1:A:606:ILE:N	2.33	0.42
1:A:334:ILE:HD12	1:A:334:ILE:N	2.34	0.42
1:A:348:ASN:O	1:A:349:PHE:C	2.61	0.42
1:A:81:VAL:CG2	1:A:379:VAL:HG11	2.50	0.42
1:A:101:VAL:HG11	1:A:134:VAL:HG11	2.01	0.42
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.81	0.42
1:A:271:LYS:O	1:A:272:ASN:CB	2.68	0.42
1:A:560:ASN:HB3	1:A:563:THR:HB	2.01	0.42
1:A:609:GLU:HA	1:A:612:LYS:CE	2.46	0.42
1:A:174:TYR:HD2	1:A:175:LEU:N	2.18	0.42
1:A:426:VAL:HG22	1:A:426:VAL:O	2.20	0.42
1:A:272:ASN:O	1:A:273:ILE:C	2.62	0.42
1:A:318:TYR:HB2	1:A:323:HIS:HB2	2.01	0.42
1:A:122:TYR:CD1	1:A:453:HIS:HB2	2.55	0.41
1:A:230:PHE:HE2	1:A:257:LYS:HB3	1.84	0.41
1:A:273:ILE:HA	1:A:766:TYR:OH	2.19	0.41
1:A:60:ARG:HG2	1:A:71:GLN:HE21	1.85	0.41
1:A:146:ILE:HG22	1:A:147:SER:N	2.35	0.41
1:A:238:ASP:HA	1:A:253:SER:HB2	2.02	0.41
1:A:385:ARG:HB3	1:A:525:GLN:C	2.45	0.41
1:A:371:GLU:O	1:A:375:LYS:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:MET:CE	1:A:694:MET:HG3	2.49	0.41
1:A:7:LYS:O	1:A:10:ASN:HB2	2.20	0.41
1:A:145:ILE:HD11	1:A:170:PHE:CG	2.55	0.41
1:A:230:PHE:CE1	1:A:279:ILE:HD11	2.56	0.41
1:A:550:ILE:O	1:A:554:MET:HB2	2.20	0.41
1:A:96:LYS:O	1:A:97:THR:C	2.63	0.41
1:A:348:ASN:O	1:A:351:ARG:N	2.53	0.41
1:A:363:ALA:HB1	1:A:370:PHE:CE1	2.55	0.41
1:A:389:ARG:CG	1:A:390:ALA:N	2.82	0.41
1:A:484:LEU:O	1:A:492:GLU:HA	2.20	0.41
1:A:82:ILE:HD11	1:A:359:MET:SD	2.61	0.41
1:A:366:GLU:OE2	1:A:513:ARG:HD3	2.20	0.41
1:A:101:VAL:HA	1:A:135:TYR:OH	2.20	0.41
1:A:193:PHE:CD1	1:A:355:LYS:HB2	2.47	0.41
1:A:403:LYS:HE2	1:A:536:SER:HB3	2.03	0.41
1:A:541:VAL:O	1:A:577:ALA:HB1	2.20	0.41
1:A:23:MET:HA	1:A:26:LEU:HG	2.02	0.41
1:A:29:GLU:C	1:A:31:LEU:N	2.78	0.41
1:A:230:PHE:CE2	1:A:257:LYS:HB3	2.56	0.41
1:A:271:LYS:HG2	1:A:272:ASN:OD1	2.21	0.41
1:A:415:HIS:HD2	1:A:443:ILE:HD11	1.86	0.41
1:A:502:TYR:CE2	1:A:530:THR:HG21	2.56	0.41
1:A:608:ASN:O	1:A:612:LYS:HG3	2.20	0.41
1:A:628:LYS:HG2	1:A:681:TYR:CE1	2.56	0.41
1:A:654:TYR:CZ	1:A:663:LEU:HD11	2.56	0.41
1:A:9:LEU:O	1:A:9:LEU:HD23	2.20	0.40
1:A:90:MET:HE1	1:A:99:VAL:HG11	2.02	0.40
1:A:230:PHE:O	1:A:233:THR:HG22	2.21	0.40
1:A:489:LYS:HG3	1:A:492:GLU:OE2	2.21	0.40
1:A:492:GLU:O	1:A:496:LYS:HB2	2.20	0.40
1:A:88:ALA:N	1:A:358:GLY:O	2.54	0.40
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.78	0.40
1:A:239:PHE:HA	1:A:251:THR:H	1.86	0.40
1:A:90:MET:CE	1:A:99:VAL:HG11	2.52	0.40
1:A:403:LYS:HB2	1:A:536:SER:HB2	2.02	0.40
1:A:460:ILE:HG12	1:A:482:ILE:HD11	2.02	0.40
1:A:48:LEU:HA	1:A:48:LEU:HD23	1.84	0.40
1:A:111:GLY:O	1:A:189:ARG:NH2	2.54	0.40
1:A:264:ILE:N	1:A:264:ILE:HD12	2.36	0.40
1:A:181:PRO:O	1:A:614:LEU:HD21	2.21	0.40
1:A:585:ASN:O	1:A:588:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PHE:HE1	1:A:663:LEU:O	2.05	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:OE1	1:A:538:GLU:OE1[4_446]	0.90	1.30
1:A:4:GLN:CD	1:A:538:GLU:OE1[4_446]	1.34	0.86
1:A:150:ASP:OD1	1:A:299:ASN:H[3_545]	0.98	0.62
1:A:4:GLN:OE1	1:A:538:GLU:CD[4_446]	1.68	0.52
1:A:150:ASP:OD1	1:A:299:ASN:N[3_545]	1.89	0.31
1:A:307:GLU:OE2	1:A:553:LEU:CD2[2_454]	1.92	0.28
1:A:265:THR:OG1	1:A:621:GLU:OE2[4_545]	2.10	0.10
1:A:4:GLN:OE1	1:A:538:GLU:CB[4_446]	2.11	0.09
1:A:371:GLU:OE2	1:A:440:LYS:CE[4_446]	2.16	0.04
1:A:129:GLU:OE2	1:A:232:LYS:HZ1[3_545]	1.60	0.00

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	769/781 (98%)	644 (84%)	88 (11%)	37 (5%)	2 7

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	69	MET
1	A	207	ALA
1	A	320	ASP
1	A	373	ILE
1	A	393	HIS

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Mol	Chain	Res	Type
1	A	450	ALA
1	A	556	ARG
1	A	567	SER
1	A	643	LYS
1	A	644	ARG
1	A	659	PRO
1	A	668	VAL
1	A	181	PRO
1	A	188	GLN
1	A	267	LEU
1	A	272	ASN
1	A	466	LEU
1	A	525	GLN
1	A	641	GLY
1	A	734	SER
1	A	266	ASN
1	A	273	ILE
1	A	338	SER
1	A	399	THR
1	A	509	HIS
1	A	52	LEU
1	A	352	LEU
1	A	453	HIS
1	A	639	LEU
1	A	2	ASP
1	A	203	LEU
1	A	426	VAL
1	A	295	TYR
1	A	299	ASN
1	A	101	VAL
1	A	344	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
-----	-------	----------	-----------	----------	-------------

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	678/688 (98%)	545 (80%)	133 (20%)	1 5

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	9	LEU
1	A	14	ASP
1	A	21	ASP
1	A	22	SER
1	A	23	MET
1	A	27	SER
1	A	29	GLU
1	A	37	ILE
1	A	52	LEU
1	A	66	LYS
1	A	67	LEU
1	A	69	MET
1	A	71	GLN
1	A	72	TYR
1	A	77	ILE
1	A	81	VAL
1	A	86	LYS
1	A	89	GLU
1	A	94	GLU
1	A	98	LEU
1	A	100	GLU
1	A	104	VAL
1	A	118	THR
1	A	126	ARG
1	A	128	LYS
1	A	132	SER
1	A	136	GLU
1	A	138	LEU
1	A	142	VAL
1	A	152	ASN
1	A	166	THR
1	A	172	PHE
1	A	177	ASP
1	A	200	ASP

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Mol	Chain	Res	Type
1	A	209	THR
1	A	219	GLU
1	A	222	LYS
1	A	229	SER
1	A	234	VAL
1	A	245	ASP
1	A	248	ILE
1	A	253	SER
1	A	256	SER
1	A	270	ILE
1	A	271	LYS
1	A	274	GLU
1	A	275	LEU
1	A	279	ILE
1	A	280	ASN
1	A	283	LEU
1	A	292	ASP
1	A	297	ILE
1	A	298	SER
1	A	303	MET
1	A	313	MET
1	A	314	ASP
1	A	319	THR
1	A	330	GLU
1	A	338	SER
1	A	364	LYS
1	A	377	ASN
1	A	384	ASN
1	A	394	ASP
1	A	403	LYS
1	A	405	SER
1	A	409	GLU
1	A	410	GLU
1	A	421	ILE
1	A	429	GLU
1	A	443	ILE
1	A	449	ASN
1	A	452	GLN
1	A	458	GLU
1	A	460	ILE
1	A	467	ASP
1	A	475	MET

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Mol	Chain	Res	Type
1	A	478	ARG
1	A	489	LYS
1	A	490	GLU
1	A	493	GLN
1	A	501	LEU
1	A	507	GLU
1	A	512	ARG
1	A	518	LEU
1	A	524	ARG
1	A	525	GLN
1	A	535	VAL
1	A	536	SER
1	A	538	GLU
1	A	542	ILE
1	A	544	LEU
1	A	554	MET
1	A	558	SER
1	A	559	SER
1	A	561	GLU
1	A	582	GLU
1	A	584	LYS
1	A	587	GLU
1	A	601	GLU
1	A	610	ARG
1	A	623	ILE
1	A	624	GLN
1	A	651	LYS
1	A	653	LEU
1	A	663	LEU
1	A	668	VAL
1	A	669	ASP
1	A	673	VAL
1	A	674	GLN
1	A	682	GLU
1	A	693	MET
1	A	694	MET
1	A	697	ILE
1	A	700	VAL
1	A	702	GLU
1	A	703	LEU
1	A	707	VAL
1	A	714	GLN

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Mol	Chain	Res	Type
1	A	718	ASP
1	A	719	HIS
1	A	720	ILE
1	A	721	ASP
1	A	723	MET
1	A	728	GLN
1	A	734	SER
1	A	746	LEU
1	A	747	GLU
1	A	750	ASP
1	A	755	LEU
1	A	758	ASN
1	A	760	ARG
1	A	770	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	84	GLN
1	A	107	ASN
1	A	115	HIS
1	A	149	GLN
1	A	152	ASN
1	A	157	GLN
1	A	188	GLN
1	A	272	ASN
1	A	286	HIS
1	A	384	ASN
1	A	415	HIS
1	A	509	HIS
1	A	517	GLN
1	A	560	ASN
1	A	562	ASN
1	A	756	ASN
1	A	758	ASN
1	A	771	ASN

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](#)

1 ligand is 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	$\# Z > 2$
2	AGS	A	801	-	32,33,33	1.03	3 (9%)	45,52,52	1.01	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	801	-	-	0/21/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	AGS	C5-N7	-3.10	1.33	1.39
2	A	801	AGS	C8-N7	2.65	1.36	1.31
2	A	801	AGS	O5'-C5'	-2.28	1.36	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	AGS	C5-C4-N3	-2.14	123.78	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	AGS	O2B-PB-O3B	2.06	112.83	107.27

There are no chirality outliers.

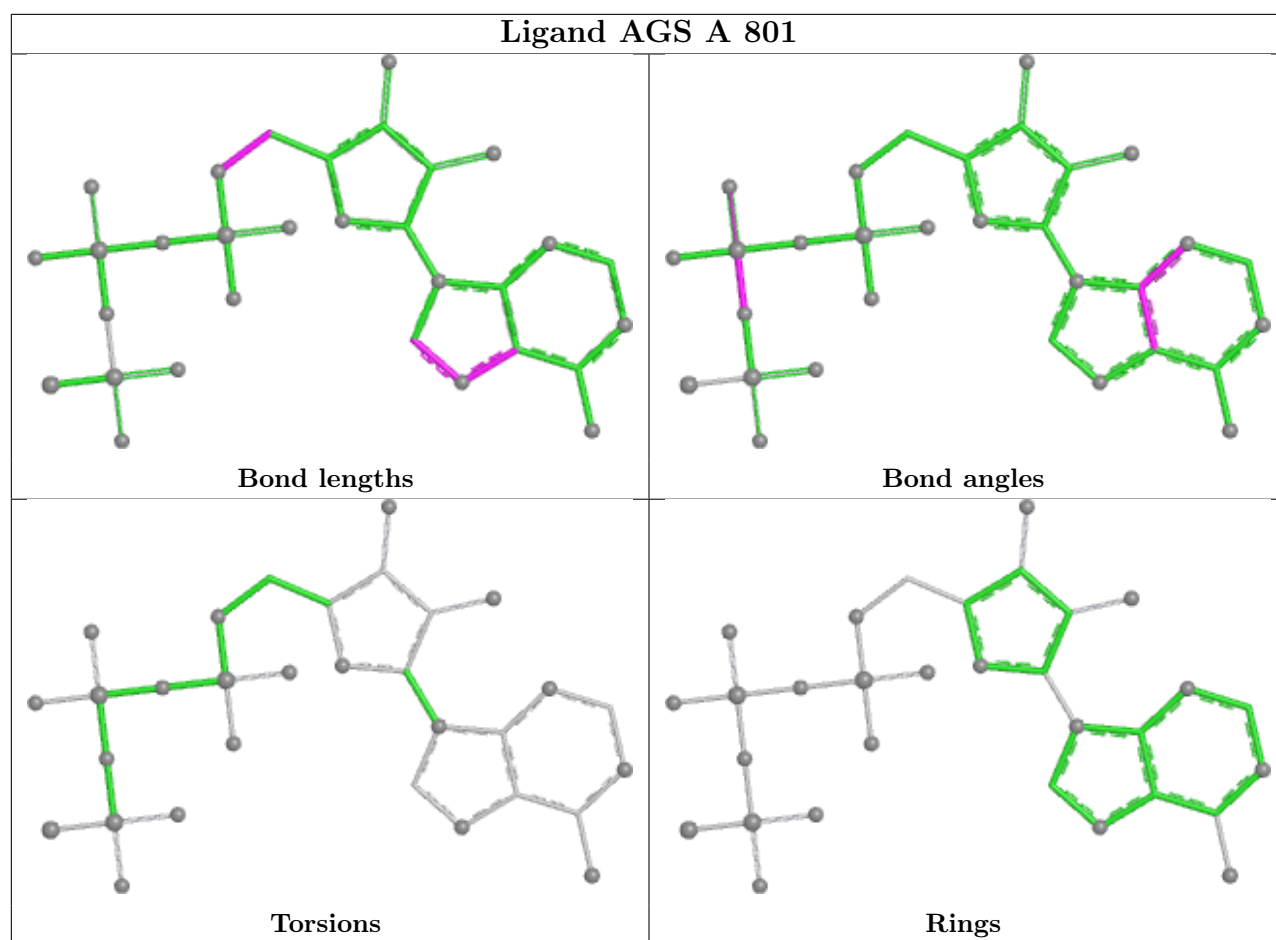
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	AGS	3	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 ⓘ

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(Å ²)	Q<0.9
1	A	760/781 (97%)	1.06	124 (16%) 4 3	8, 34, 83, 139	43 (5%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.0
1	A	544	LEU	4.9
1	A	740	PRO	4.9
1	A	713	ASP	4.9
1	A	288	LEU	4.5
1	A	732	LEU	4.3
1	A	468	ALA	4.0
1	A	665	ILE	4.0
1	A	202	ILE	4.0
1	A	761	GLU	4.0
1	A	731	GLY	3.9
1	A	666	PRO	3.8
1	A	1	ALA	3.8
1	A	318	TYR	3.8
1	A	641	GLY	3.8
1	A	395	LYS	3.7
1	A	171	GLY	3.6
1	A	545	TYR	3.6
1	A	338	SER	3.5
1	A	394	ASP	3.5
1	A	557	THR	3.5
1	A	750	ASP	3.5
1	A	471	ILE	3.4
1	A	466	LEU	3.4
1	A	474	ASN	3.4
1	A	742	LYS	3.4
1	A	569	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLU	3.3
1	A	404	TYR	3.3
1	A	472	ALA	3.3
1	A	294	ASP	3.3
1	A	315	GLY	3.2
1	A	726	LEU	3.2
1	A	335	LYS	3.2
1	A	550	ILE	3.2
1	A	558	SER	3.1
1	A	730	ILE	3.1
1	A	578	GLN	3.0
1	A	362	THR	3.0
1	A	390	ALA	3.0
1	A	573	ALA	3.0
1	A	59	VAL	3.0
1	A	293	VAL	3.0
1	A	475	MET	3.0
1	A	243	ARG	2.9
1	A	385	ARG	2.9
1	A	192	ASN	2.9
1	A	546	GLY	2.9
1	A	354	GLU	2.9
1	A	673	VAL	2.9
1	A	617	GLU	2.8
1	A	142	VAL	2.8
1	A	525	GLN	2.8
1	A	69	MET	2.8
1	A	206	GLU	2.7
1	A	581	VAL	2.7
1	A	236	GLU	2.7
1	A	729	TYR	2.7
1	A	345	THR	2.7
1	A	221	LEU	2.7
1	A	218	ASP	2.7
1	A	52	LEU	2.7
1	A	668	VAL	2.7
1	A	477	GLY	2.6
1	A	526	GLY	2.6
1	A	467	ASP	2.6
1	A	667	GLY	2.6
1	A	118	THR	2.6
1	A	399	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	334	ILE	2.6
1	A	443	ILE	2.6
1	A	226	LEU	2.5
1	A	428	VAL	2.5
1	A	450	ALA	2.5
1	A	662	THR	2.5
1	A	193	PHE	2.5
1	A	381	ILE	2.4
1	A	535	VAL	2.4
1	A	709	LEU	2.4
1	A	51	ILE	2.4
1	A	114	VAL	2.4
1	A	543	LYS	2.4
1	A	556	ARG	2.4
1	A	356	LEU	2.4
1	A	469	ILE	2.4
1	A	521	ARG	2.3
1	A	616	ASP	2.3
1	A	198	GLU	2.3
1	A	476	ALA	2.3
1	A	722	ALA	2.3
1	A	672	SER	2.3
1	A	715	TYR	2.3
1	A	366	GLU	2.3
1	A	755	LEU	2.3
1	A	595	TYR	2.3
1	A	376	LEU	2.2
1	A	353	TYR	2.2
1	A	98	LEU	2.2
1	A	473	THR	2.2
1	A	754	ALA	2.2
1	A	398	LYS	2.2
1	A	330	GLU	2.2
1	A	387	VAL	2.2
1	A	289	MET	2.2
1	A	172	PHE	2.2
1	A	260	SER	2.2
1	A	741	PHE	2.2
1	A	333	GLU	2.1
1	A	195	ILE	2.1
1	A	447	VAL	2.1
1	A	159	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	2.1
1	A	113	GLY	2.1
1	A	264	ILE	2.1
1	A	720	ILE	2.1
1	A	23	MET	2.1
1	A	102	ALA	2.1
1	A	743	GLU	2.1
1	A	548	LYS	2.0
1	A	6	ILE	2.0
1	A	237	GLU	2.0
1	A	314	ASP	2.0
1	A	698	ASP	2.0
1	A	122	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

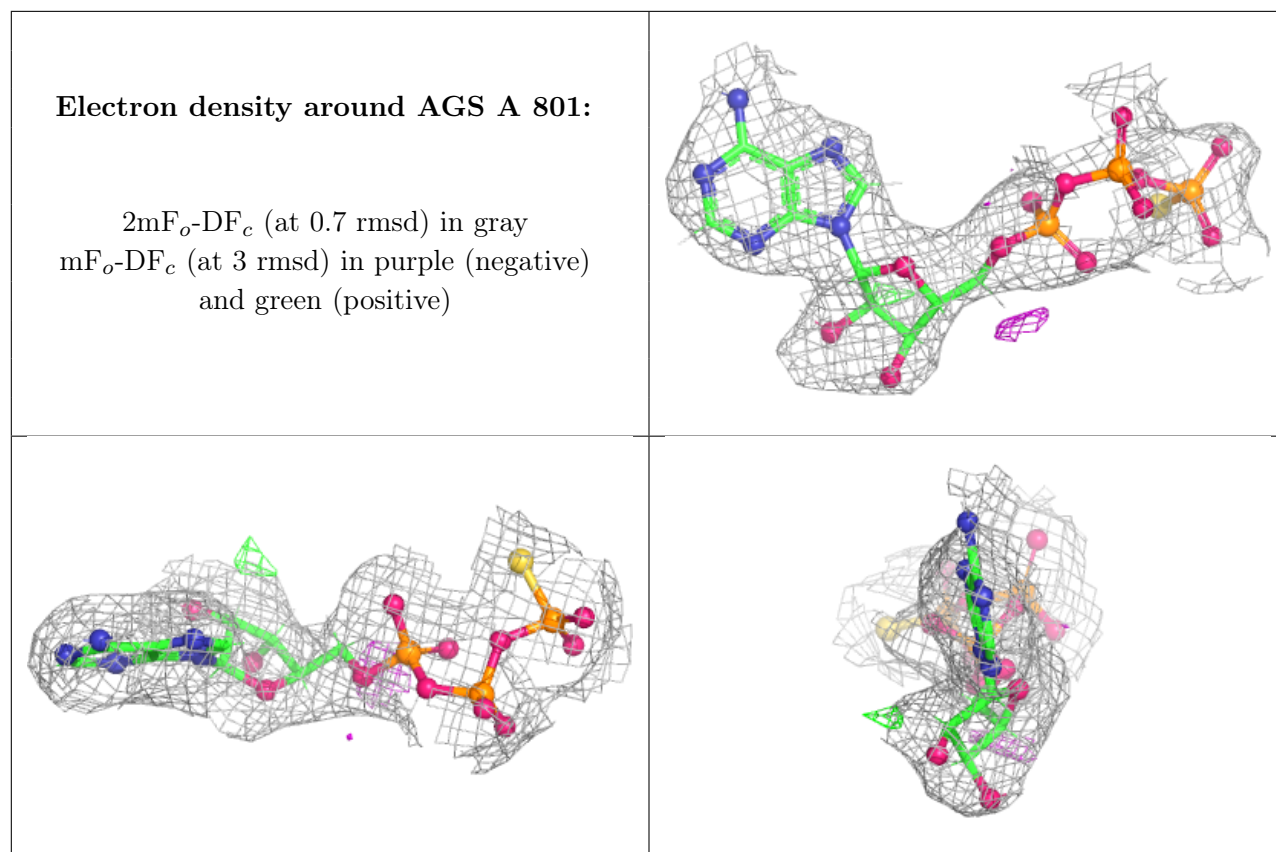
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AGS	A	801	31/31	0.88	0.10	1,18,52,53	12

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.