



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:32 AM UTC

PDB ID : 3QUS / pdb_00003qus
Title : Crystal Structure of N10-Formyltetrahydrofolate Synthetase with ATPgS
Authors : Celeste, L.R.; Chai, G.; Bielak, M.; Lovelace, L.L.; Lebioda, L.
Deposited on : 2011-02-24
Resolution : 2.84 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

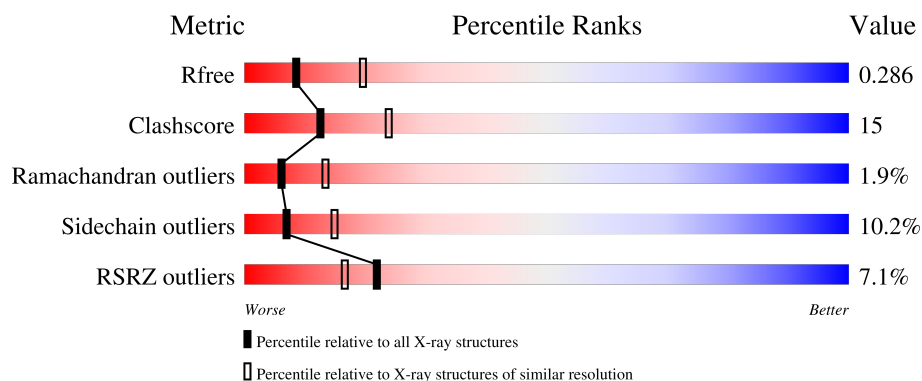
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	557	4% 67% 28% • •
1	B	557	10% 70% 24% 5% •

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8438 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 Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4100	2596	706	777	21			
1	B	549	Total	C	N	O	S	0	0	0
			3966	2507	680	758	21			

There are 4 discrepancies between the modelled and reference sequences:

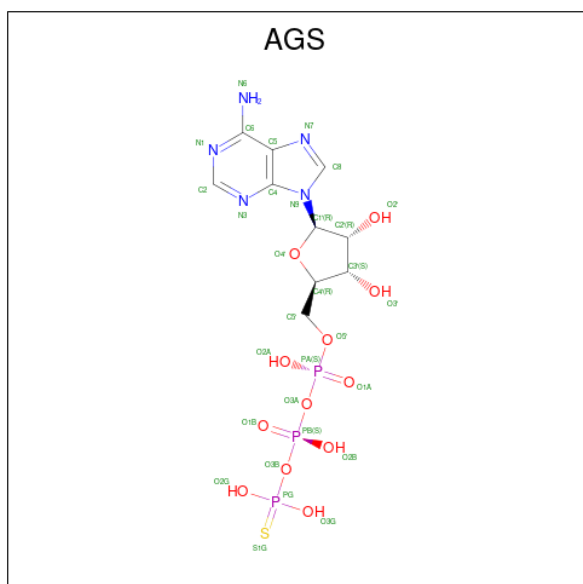
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



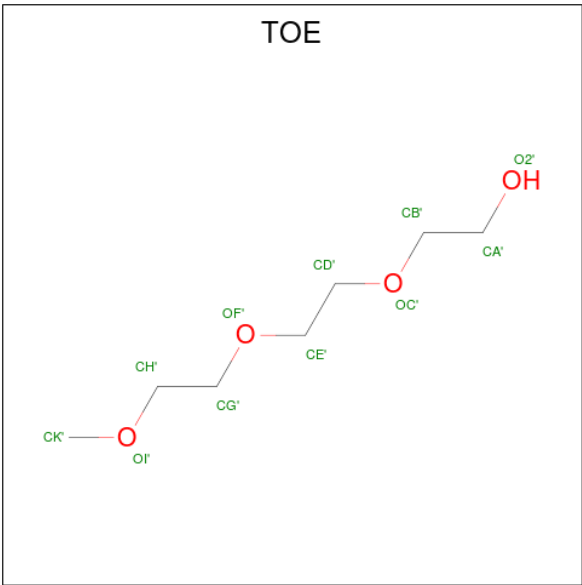
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



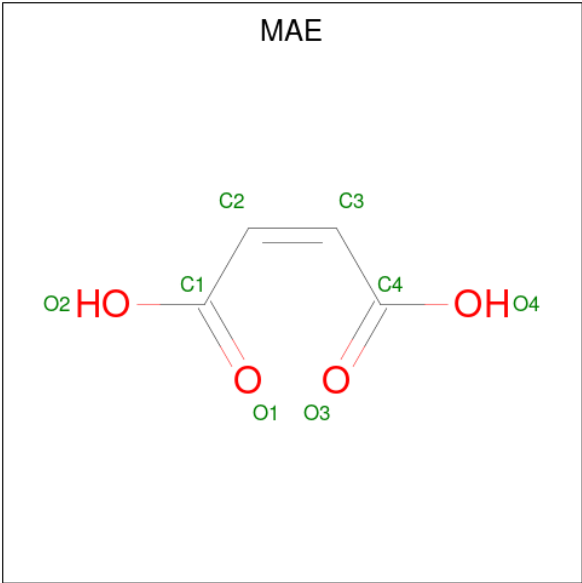
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: C₇H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	7	4		
4	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 5 is MALEIC ACID (CCD ID: MAE) (formula: C₄H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

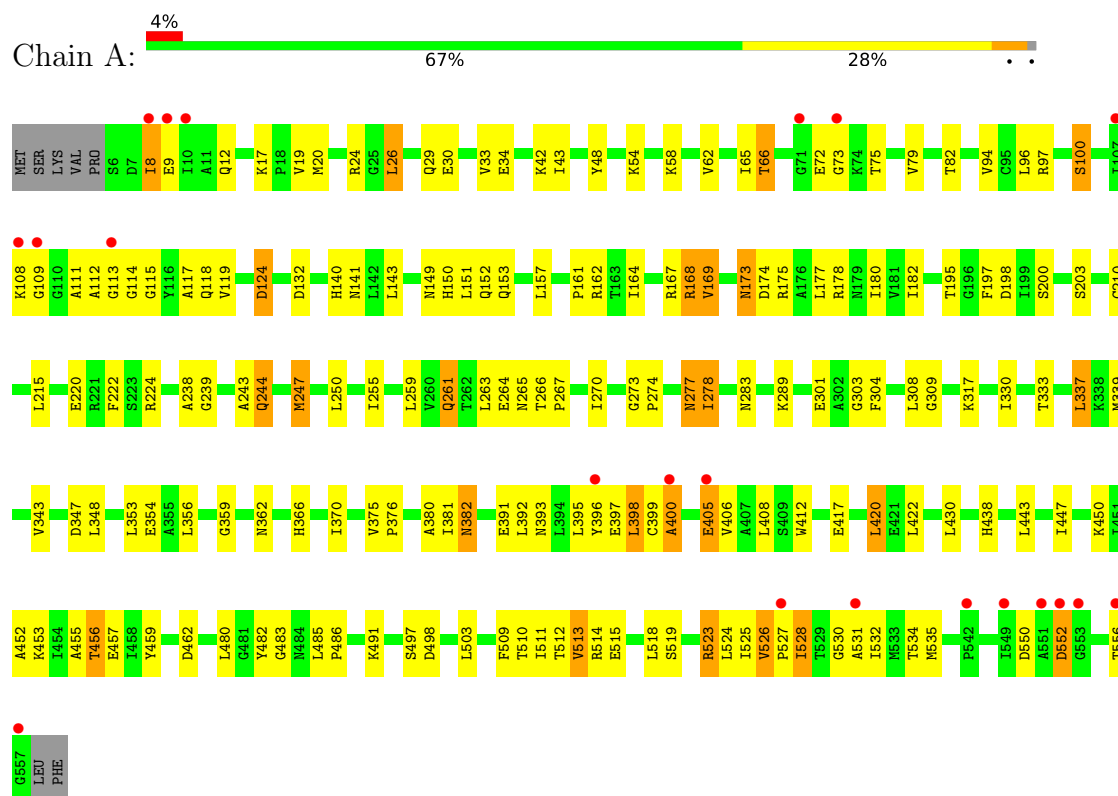
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total 173	O 173	0	0
6	B	69	Total 69	O 69	0	0

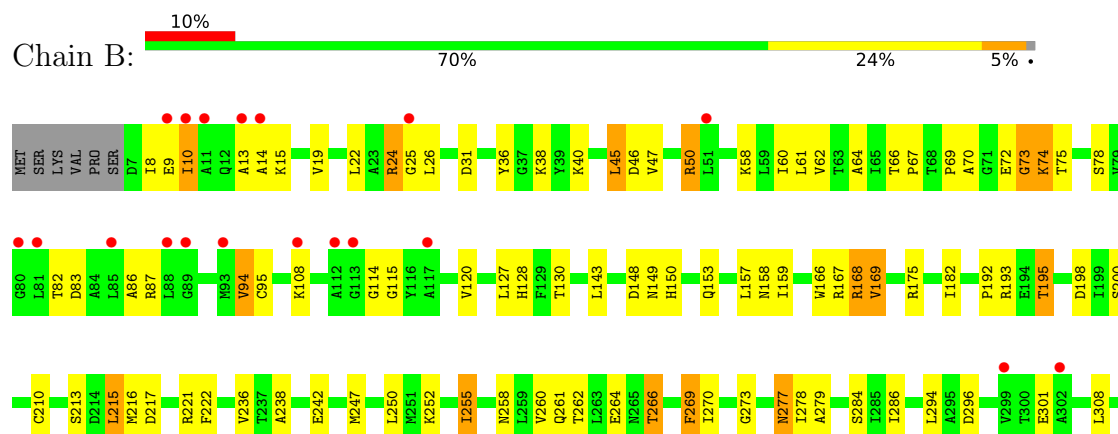
3 Residue-property plots [i](#)

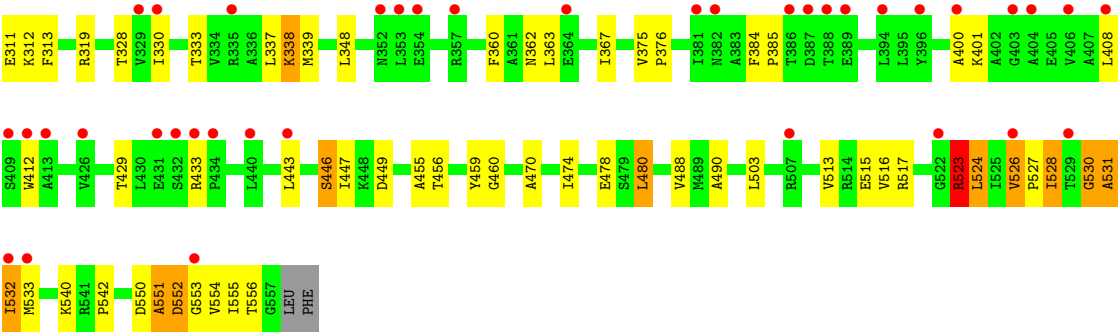
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Formate--tetrahydrofolate ligase



• Molecule 1: Formate--tetrahydrofolate ligase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	160.84Å 160.84Å 256.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.40 – 2.84 122.40 – 2.84	Depositor EDS
% Data completeness (in resolution range)	97.0 (122.40-2.84) 97.0 (122.40-2.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.289 0.216 , 0.286	Depositor DCC
R_{free} test set	1489 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	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	0.86	EDS
Total number of atoms	8438	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: SO4, AGS, TOE, MAE

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	0.93	3/4168 (0.1%)	1.17	18/5652 (0.3%)
1	B	0.82	4/4034 (0.1%)	1.12	20/5493 (0.4%)
All	All	0.88	7/8202 (0.1%)	1.14	38/11145 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	LEU	C-N	10.15	1.46	1.33
1	B	14	ALA	C-N	8.82	1.46	1.33
1	A	550	ASP	CA-C	8.39	1.56	1.52
1	B	412	TRP	C-N	-7.39	1.20	1.33
1	A	408	LEU	C-N	-6.76	1.24	1.34
1	A	526	VAL	CA-C	5.46	1.58	1.52
1	B	10	ILE	CA-CB	5.37	1.60	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	VAL	CB-CA-C	9.20	119.82	111.08
1	B	127	LEU	N-CA-C	9.17	116.30	108.78
1	B	531	ALA	N-CA-C	-9.03	101.97	113.16
1	A	526	VAL	N-CA-CB	-8.95	102.14	111.36
1	A	109	GLY	N-CA-C	-8.49	102.16	115.67
1	B	128	HIS	N-CA-C	-7.87	97.25	109.76
1	B	523	ARG	N-CA-C	7.29	117.59	108.19
1	A	513	VAL	CB-CA-C	6.94	119.52	110.91
1	B	556	THR	N-CA-C	6.70	120.75	112.58
1	A	531	ALA	N-CA-C	-6.60	104.26	113.37
1	A	162	ARG	N-CA-C	-6.26	105.65	113.28
1	B	554	VAL	N-CA-C	6.17	117.47	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	VAL	CA-C-N	6.04	127.39	119.84
1	B	375	VAL	C-N-CA	6.04	127.39	119.84
1	A	343	VAL	N-CA-C	5.91	113.72	108.63
1	A	526	VAL	CA-C-N	5.88	125.79	119.85
1	A	526	VAL	C-N-CA	5.88	125.79	119.85
1	A	247	MET	N-CA-C	-5.87	104.80	111.14
1	A	24	ARG	N-CA-C	-5.83	105.27	112.38
1	A	151	LEU	N-CA-C	-5.79	104.17	111.11
1	B	15	LYS	N-CA-C	5.77	123.10	110.80
1	B	408	LEU	CA-C-N	5.67	129.33	120.82
1	B	408	LEU	C-N-CA	5.67	129.33	120.82
1	B	130	THR	N-CA-C	-5.57	106.37	112.72
1	B	14	ALA	CA-C-N	5.47	131.99	121.54
1	B	14	ALA	C-N-CA	5.47	131.99	121.54
1	A	266	THR	CA-C-N	-5.39	114.22	119.78
1	A	266	THR	C-N-CA	-5.39	114.22	119.78
1	A	100	SER	N-CA-C	-5.32	102.61	110.48
1	B	269	PHE	CA-C-N	-5.27	116.23	123.14
1	B	269	PHE	C-N-CA	-5.27	116.23	123.14
1	B	261	GLN	N-CA-C	5.22	116.91	109.14
1	B	480	LEU	N-CA-C	-5.21	106.92	113.28
1	A	261	GLN	N-CA-C	5.15	116.90	109.07
1	B	114	GLY	N-CA-C	5.13	118.06	110.63
1	B	553	GLY	N-CA-C	5.07	118.98	111.18
1	A	66	THR	CA-C-N	5.04	125.32	119.92
1	A	66	THR	C-N-CA	5.04	125.32	119.92

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	4100	0	4128	137	0
1	B	3966	0	3854	122	0
2	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	1	0
3	A	31	0	12	4	0
3	B	31	0	12	4	0
4	A	22	0	32	0	0
5	B	16	0	4	0	0
6	A	173	0	0	12	0
6	B	69	0	0	4	0
All	All	8438	0	8042	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:HA2	3:B:700:AGS:S1G	1.52	1.48
1:B:73:GLY:CA	3:B:700:AGS:S1G	2.41	1.07
1:B:523:ARG:HG2	1:B:523:ARG:HH11	0.93	1.07
1:B:262:THR:HG22	1:B:264:GLU:H	1.20	1.01
1:B:277:ASN:ND2	1:B:278:ILE:H	1.56	1.01
1:B:277:ASN:HD22	1:B:278:ILE:N	1.60	0.99
1:A:278:ILE:HG12	1:A:525:ILE:HG21	1.44	0.97
1:A:277:ASN:HD22	1:A:278:ILE:N	1.64	0.95
1:B:523:ARG:HG2	1:B:523:ARG:NH1	1.73	0.94
1:B:75:THR:HB	3:B:700:AGS:O3G	1.67	0.94
1:A:380:ALA:HA	1:A:405:GLU:OE1	1.69	0.93
1:B:523:ARG:HH11	1:B:523:ARG:CG	1.83	0.92
1:B:515:GLU:O	1:B:527:PRO:HD2	1.69	0.90
1:A:277:ASN:ND2	1:A:278:ILE:H	1.70	0.88
1:A:149:ASN:HD21	1:A:153:GLN:HE21	1.21	0.86
1:A:405:GLU:C	1:A:405:GLU:CD	2.43	0.84
1:A:149:ASN:HD22	1:B:175:ARG:NH2	1.76	0.84
1:B:47:VAL:HG11	1:B:294:LEU:HD21	1.60	0.83
1:A:277:ASN:HD22	1:A:278:ILE:H	0.89	0.83
1:B:149:ASN:HD21	1:B:153:GLN:HE21	1.27	0.82
1:A:149:ASN:ND2	1:A:153:GLN:HE21	1.78	0.81
1:A:17:LYS:H	1:A:261:GLN:HE22	1.28	0.81
1:A:530:GLY:C	1:A:532:ILE:H	1.88	0.80
1:B:516:VAL:HG22	1:B:526:VAL:HG12	1.64	0.79
1:B:9:GLU:HG2	1:B:115:GLY:H	1.49	0.78
1:A:175:ARG:HH12	1:B:149:ASN:HD22	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HG22	1:B:200:SER:HA	1.64	0.77
1:B:150:HIS:HE1	1:B:157:LEU:H	1.35	0.74
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.89	0.73
1:A:405:GLU:CD	1:A:405:GLU:O	2.32	0.71
1:B:45:LEU:HD21	1:B:255:ILE:HG23	1.71	0.71
1:B:169:VAL:CG2	1:B:200:SER:HA	2.21	0.70
1:A:523:ARG:HD3	1:A:523:ARG:N	2.06	0.69
1:A:244:GLN:H	1:A:244:GLN:NE2	1.90	0.69
1:A:452:ALA:O	1:A:456:THR:HB	1.93	0.69
1:A:72:GLU:OE1	3:A:700:AGS:S1G	2.51	0.69
1:B:337:LEU:HD23	1:B:360:PHE:HA	1.76	0.68
1:B:470:ALA:O	1:B:474:ILE:HG12	1.92	0.68
1:A:168:ARG:HG2	1:A:197:PHE:CZ	2.29	0.68
1:A:58:LYS:HE2	6:A:809:HOH:O	1.94	0.67
1:A:173:ASN:N	1:A:173:ASN:HD22	1.91	0.67
1:A:244:GLN:H	1:A:244:GLN:HE21	1.43	0.67
1:B:149:ASN:ND2	1:B:153:GLN:HE21	1.93	0.67
1:B:455:ALA:HA	1:B:459:TYR:CD2	2.30	0.66
1:B:474:ILE:HD11	1:B:516:VAL:HG21	1.77	0.66
1:A:491:LYS:HB3	1:A:528:ILE:HG13	1.77	0.66
1:B:82:THR:HG21	1:B:94:VAL:HG22	1.77	0.66
1:A:530:GLY:C	1:A:532:ILE:N	2.53	0.66
1:A:54:LYS:HB3	6:A:692:HOH:O	1.97	0.65
1:A:140:HIS:HD2	1:A:203:SER:OG	1.80	0.65
1:B:82:THR:OG1	1:B:94:VAL:HG13	1.97	0.64
1:A:149:ASN:HD22	1:B:175:ARG:HH22	1.46	0.64
1:A:380:ALA:HA	1:A:405:GLU:CD	2.22	0.64
1:B:338:LYS:HZ3	1:B:348:LEU:HA	1.63	0.64
1:B:474:ILE:CD1	1:B:516:VAL:HG21	2.28	0.63
1:A:9:GLU:O	1:A:12:GLN:HG2	1.99	0.63
1:A:17:LYS:H	1:A:261:GLN:NE2	1.95	0.62
1:A:43:ILE:CD1	1:A:259:LEU:HB2	2.29	0.62
1:A:43:ILE:HD11	1:A:259:LEU:HB2	1.81	0.62
1:A:17:LYS:N	1:A:261:GLN:HE22	1.97	0.62
1:B:175:ARG:HD3	2:B:602:SO4:O3	2.00	0.62
1:A:149:ASN:HD21	1:A:153:GLN:NE2	1.97	0.61
1:A:167:ARG:NH2	1:A:178:ARG:O	2.34	0.61
1:A:447:ILE:HD11	1:A:483:GLY:HA2	1.82	0.61
1:B:277:ASN:HD22	1:B:278:ILE:H	0.77	0.61
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.36	0.61
1:A:54:LYS:CB	6:A:692:HOH:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:HA2	3:A:700:AGS:O2B	2.01	0.61
1:B:74:LYS:HB3	1:B:301:GLU:OE1	2.00	0.60
1:A:528:ILE:HB	6:A:667:HOH:O	2.01	0.60
1:A:512:THR:O	1:A:528:ILE:HG23	2.02	0.59
1:A:405:GLU:OE1	1:A:405:GLU:O	2.20	0.59
1:A:97:ARG:NH1	6:A:784:HOH:O	2.35	0.59
1:A:515:GLU:O	1:A:527:PRO:HD2	2.02	0.59
1:A:112:ALA:HB1	1:A:119:VAL:O	2.03	0.58
1:A:141:ASN:OD1	1:A:168:ARG:HG3	2.04	0.58
1:B:319:ARG:NE	1:B:443:LEU:HD13	2.18	0.58
1:B:62:VAL:HG11	1:B:78:SER:OG	2.04	0.57
1:A:150:HIS:CE1	1:A:157:LEU:H	2.22	0.57
1:A:169:VAL:HG22	1:A:200:SER:HA	1.85	0.57
1:A:412:TRP:HB3	6:A:621:HOH:O	2.04	0.57
1:B:552:ASP:OD2	1:B:552:ASP:N	2.37	0.57
1:A:150:HIS:HE1	1:A:157:LEU:H	1.51	0.57
1:B:262:THR:HB	1:B:266:THR:H	1.70	0.57
1:B:447:ILE:HD12	1:B:524:LEU:HD22	1.85	0.57
1:B:447:ILE:HG21	1:B:474:ILE:HD12	1.87	0.57
1:A:486:PRO:O	1:A:523:ARG:HB2	2.05	0.56
1:A:337:LEU:O	1:A:359:GLY:HA3	2.05	0.56
1:A:405:GLU:HG3	1:A:422:LEU:HB2	1.87	0.56
1:B:47:VAL:CG1	1:B:294:LEU:HD21	2.35	0.56
1:B:515:GLU:C	1:B:527:PRO:HD2	2.30	0.56
1:B:64:ALA:HB2	1:B:74:LYS:HG3	1.87	0.55
1:B:222:PHE:CD1	1:B:247:MET:HB3	2.40	0.55
1:B:550:ASP:C	1:B:552:ASP:H	2.13	0.55
1:B:182:ILE:O	1:B:192:PRO:HA	2.05	0.55
1:B:74:LYS:HB2	3:B:700:AGS:O1B	2.07	0.55
1:A:150:HIS:CE1	1:A:157:LEU:HB2	2.41	0.55
1:A:491:LYS:HB3	1:A:528:ILE:CG1	2.37	0.55
1:B:216:MET:HE2	1:B:216:MET:HA	1.88	0.55
1:B:312:LYS:HE2	1:B:488:VAL:HG13	1.89	0.55
1:A:42:LYS:NZ	1:A:132:ASP:OD2	2.40	0.54
1:A:149:ASN:ND2	1:B:175:ARG:HH22	2.06	0.54
1:B:148:ASP:OD2	1:B:168:ARG:NH2	2.30	0.54
1:B:58:LYS:N	1:B:296:ASP:O	2.37	0.54
1:B:83:ASP:O	1:B:86:ALA:HB3	2.08	0.54
1:A:239:GLY:HA2	1:A:244:GLN:NE2	2.23	0.53
1:A:9:GLU:OE2	1:A:9:GLU:HA	2.07	0.53
1:B:159:ILE:HG12	1:B:236:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:VAL:HG22	1:B:526:VAL:CG1	2.37	0.53
1:B:523:ARG:NH1	1:B:523:ARG:CG	2.51	0.53
1:A:381:ILE:HD12	1:A:395:LEU:HD23	1.90	0.52
1:A:174:ASP:OD2	1:B:168:ARG:NH1	2.42	0.52
1:B:150:HIS:CE1	1:B:157:LEU:H	2.21	0.52
1:B:488:VAL:HG23	1:B:523:ARG:HG3	1.91	0.52
1:B:95:CYS:HA	1:B:269:PHE:O	2.08	0.52
1:A:264:GLU:O	1:A:265:ASN:HB2	2.10	0.52
1:B:446:SER:O	1:B:447:ILE:C	2.51	0.52
1:A:82:THR:OG1	1:A:94:VAL:HB	2.10	0.51
1:B:62:VAL:HG13	1:B:301:GLU:HB3	1.92	0.51
1:B:531:ALA:C	1:B:533:MET:H	2.18	0.51
1:A:523:ARG:HE	1:A:525:ILE:HD11	1.75	0.51
1:B:429:THR:HA	1:B:433:ARG:HE	1.75	0.51
1:B:550:ASP:O	1:B:552:ASP:N	2.44	0.51
1:B:530:GLY:C	1:B:532:ILE:H	2.16	0.51
1:A:75:THR:N	3:A:700:AGS:O1B	2.25	0.51
1:B:308:LEU:O	1:B:312:LYS:HG3	2.11	0.51
1:A:398:LEU:C	1:A:400:ALA:H	2.19	0.51
1:B:24:ARG:C	1:B:26:LEU:H	2.19	0.50
1:A:277:ASN:ND2	1:A:278:ILE:N	2.43	0.50
1:A:26:LEU:HD11	1:A:267:PRO:HG2	1.94	0.50
1:A:8:ILE:HD11	1:A:114:GLY:HA2	1.94	0.50
1:A:124:ASP:OD1	1:A:124:ASP:N	2.45	0.50
1:A:417:GLU:HA	1:A:420:LEU:HD22	1.92	0.49
1:A:152:GLN:HG2	1:B:175:ARG:NE	2.28	0.49
1:A:330:ILE:HD11	1:A:366:HIS:HB3	1.94	0.49
1:B:13:ALA:HB3	6:B:677:HOH:O	2.12	0.49
1:A:118:GLN:HB2	1:A:263:LEU:HG	1.95	0.49
1:B:456:THR:O	1:B:460:GLY:HA2	2.13	0.49
1:B:531:ALA:C	1:B:533:MET:N	2.71	0.48
1:B:31:ASP:HB2	6:B:664:HOH:O	2.12	0.48
1:A:485:LEU:HD13	1:A:523:ARG:HA	1.96	0.48
1:A:73:GLY:CA	3:A:700:AGS:O2B	2.61	0.48
1:A:8:ILE:CD1	1:A:115:GLY:H	2.27	0.48
1:A:124:ASP:HB3	6:A:703:HOH:O	2.14	0.48
1:A:180:ILE:HG22	1:B:182:ILE:HA	1.95	0.48
1:B:66:THR:H	1:B:362:ASN:HD21	1.61	0.48
1:A:149:ASN:ND2	1:B:175:ARG:NH2	2.56	0.48
1:B:384:PHE:CD1	1:B:385:PRO:HD2	2.49	0.48
1:A:48:TYR:CZ	1:A:289:LYS:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:THR:HA	1:B:433:ARG:NE	2.29	0.48
1:A:239:GLY:HA2	1:A:244:GLN:HE22	1.79	0.47
1:B:488:VAL:CG2	1:B:523:ARG:HG3	2.43	0.47
1:A:66:THR:H	1:A:362:ASN:HD21	1.62	0.47
1:A:330:ILE:HD11	1:A:366:HIS:CB	2.44	0.47
1:B:36:TYR:HB2	1:B:40:LYS:HB2	1.95	0.47
1:B:193:ARG:NH2	1:B:195:THR:CG2	2.77	0.47
1:A:304:PHE:N	2:A:601:SO4:O3	2.46	0.47
1:A:381:ILE:HD12	1:A:395:LEU:CD2	2.45	0.47
1:A:20:MET:HE1	1:A:33:VAL:HG21	1.96	0.47
1:A:339:MET:CG	1:A:348:LEU:HD11	2.44	0.47
1:A:149:ASN:HD22	1:B:175:ARG:HH21	1.60	0.47
1:A:405:GLU:HG3	1:A:422:LEU:CB	2.44	0.46
1:B:447:ILE:HG12	1:B:478:GLU:OE2	2.15	0.46
1:A:317:LYS:HD2	6:A:611:HOH:O	2.14	0.46
1:A:175:ARG:HH12	1:B:149:ASN:ND2	2.06	0.46
1:A:198:ASP:OD1	1:A:534:THR:OG1	2.29	0.46
1:A:177:LEU:HB3	1:A:197:PHE:HB2	1.98	0.46
1:B:46:ASP:O	1:B:50:ARG:HG2	2.16	0.46
1:B:490:ALA:HB3	1:B:527:PRO:HA	1.98	0.46
1:A:482:TYR:O	1:A:524:LEU:HD11	2.16	0.46
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.77	0.46
1:A:396:TYR:O	1:A:397:GLU:C	2.58	0.45
1:A:149:ASN:O	1:A:153:GLN:HG2	2.17	0.45
1:B:279:ALA:HA	1:B:523:ARG:NH2	2.31	0.45
1:A:12:GLN:OE1	1:A:12:GLN:HA	2.16	0.45
6:A:568:HOH:O	1:B:168:ARG:HD3	2.16	0.45
1:B:9:GLU:CG	1:B:115:GLY:H	2.25	0.45
1:A:140:HIS:CD2	1:A:203:SER:OG	2.66	0.45
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.75	0.45
1:B:83:ASP:O	1:B:87:ARG:HG2	2.16	0.45
1:B:222:PHE:CE1	1:B:247:MET:HB3	2.52	0.45
1:B:337:LEU:CD2	1:B:360:PHE:HA	2.46	0.45
1:A:161:PRO:HA	1:A:164:ILE:HD12	1.98	0.45
1:A:308:LEU:HD21	1:A:491:LYS:HG3	1.99	0.45
1:A:498:ASP:CG	1:A:528:ILE:HG21	2.42	0.45
1:B:446:SER:H	1:B:449:ASP:HB2	1.80	0.45
1:A:58:LYS:CE	6:A:809:HOH:O	2.57	0.45
1:A:498:ASP:OD2	1:A:511:ILE:HA	2.17	0.45
1:A:75:THR:HA	1:A:301:GLU:OE2	2.17	0.45
1:B:70:ALA:HB2	1:B:339:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ASP:OD2	1:A:552:ASP:N	2.50	0.44
1:A:222:PHE:O	1:A:238:ALA:HB3	2.18	0.44
1:B:19:VAL:HG22	1:B:38:LYS:O	2.16	0.44
1:B:167:ARG:NH1	1:B:198:ASP:OD2	2.50	0.44
1:B:550:ASP:C	1:B:552:ASP:N	2.75	0.44
1:A:210:CYS:SG	1:A:274:PRO:HD3	2.57	0.44
1:B:528:ILE:HD12	1:B:528:ILE:HA	1.79	0.44
1:A:333:THR:HG22	1:A:382:ASN:HB3	1.99	0.44
1:B:67:PRO:HA	1:B:72:GLU:OE1	2.18	0.44
1:A:405:GLU:OE1	1:A:405:GLU:N	2.51	0.43
1:A:450:LYS:O	1:A:453:LYS:HB2	2.18	0.43
1:A:198:ASP:C	1:A:535:MET:HE2	2.43	0.43
1:B:217:ASP:O	1:B:221:ARG:HG3	2.18	0.43
1:A:111:ALA:O	1:A:112:ALA:C	2.62	0.43
1:B:60:ILE:O	1:B:60:ILE:HG22	2.18	0.43
1:B:143:LEU:HD23	1:B:166:TRP:CZ2	2.53	0.43
1:B:286:ILE:HG12	6:B:578:HOH:O	2.19	0.43
1:B:210:CYS:HA	1:B:284:SER:HB2	2.00	0.42
1:B:61:LEU:HD13	1:B:313:PHE:CD1	2.54	0.42
1:B:555:ILE:HG12	6:B:647:HOH:O	2.18	0.42
1:A:96:LEU:O	1:A:270:ILE:HA	2.19	0.42
1:B:222:PHE:O	1:B:238:ALA:HB3	2.18	0.42
1:A:54:LYS:HB2	6:A:692:HOH:O	2.15	0.42
1:A:456:THR:HG22	1:A:457:GLU:N	2.34	0.42
1:B:215:LEU:O	1:B:215:LEU:HD22	2.20	0.42
1:B:193:ARG:NH2	1:B:195:THR:HG23	2.33	0.42
1:B:384:PHE:CG	1:B:385:PRO:HD2	2.54	0.42
1:A:376:PRO:HA	6:A:619:HOH:O	2.20	0.42
1:A:447:ILE:CD1	1:A:524:LEU:HD13	2.49	0.42
1:A:447:ILE:HD12	1:A:524:LEU:HD13	2.02	0.42
1:B:193:ARG:HH21	1:B:195:THR:HG23	1.85	0.42
1:A:114:GLY:H	1:A:118:GLN:HG2	1.85	0.41
1:A:303:GLY:O	1:A:309:GLY:HA3	2.20	0.41
1:B:551:ALA:C	1:B:552:ASP:OD2	2.62	0.41
1:A:366:HIS:O	1:A:370:ILE:HD12	2.20	0.41
1:A:152:GLN:HG2	1:B:175:ARG:HE	1.84	0.41
1:A:514:ARG:HG3	1:A:528:ILE:O	2.19	0.41
1:B:363:LEU:O	1:B:367:ILE:HG13	2.20	0.41
1:A:43:ILE:HD11	1:A:259:LEU:CB	2.50	0.41
1:A:497:SER:HA	1:A:509:PHE:CE1	2.55	0.41
1:A:523:ARG:HH11	1:A:523:ARG:HD2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLN:O	1:A:33:VAL:HG23	2.21	0.41
1:A:255:ILE:O	1:A:255:ILE:HG13	2.20	0.41
1:A:391:GLU:O	1:A:392:LEU:C	2.62	0.41
1:A:455:ALA:HA	1:A:459:TYR:CD2	2.56	0.41
1:A:519:SER:O	1:A:523:ARG:N	2.49	0.41
1:A:161:PRO:HA	1:A:164:ILE:CD1	2.51	0.41
1:B:61:LEU:O	1:B:328:THR:HA	2.21	0.41
1:B:167:ARG:NH1	1:B:198:ASP:CG	2.79	0.41
1:B:540:LYS:O	1:B:542:PRO:HD3	2.21	0.41
1:B:429:THR:HG23	1:B:433:ARG:HD2	2.03	0.40
1:A:79:VAL:HB	1:A:117:ALA:HB1	2.03	0.40
1:A:169:VAL:CG2	1:A:200:SER:HA	2.50	0.40
1:A:173:ASN:N	1:A:173:ASN:ND2	2.62	0.40
1:B:515:GLU:HG2	1:B:516:VAL:H	1.86	0.40
1:B:531:ALA:O	1:B:533:MET:N	2.54	0.40
1:A:65:ILE:CD1	1:A:337:LEU:HD13	2.51	0.40
1:A:243:ALA:O	1:A:247:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	548/557 (98%)	494 (90%)	46 (8%)	8 (2%)	8	17
1	B	547/557 (98%)	489 (89%)	45 (8%)	13 (2%)	4	10
All	All	1095/1114 (98%)	983 (90%)	91 (8%)	21 (2%)	6	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ALA

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Mol	Chain	Res	Type
1	B	551	ALA
1	A	399	CYS
1	B	108	LYS
1	B	401	LYS
1	B	532	ILE
1	A	8	ILE
1	B	74	LYS
1	B	400	ALA
1	A	556	THR
1	B	73	GLY
1	B	376	PRO
1	A	552	ASP
1	B	25	GLY
1	A	108	LYS
1	A	113	GLY
1	B	69	PRO
1	B	530	GLY
1	B	273	GLY
1	A	273	GLY
1	B	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/440 (95%)	373 (89%)	46 (11%)	6	12
1	B	387/440 (88%)	351 (91%)	36 (9%)	8	19
All	All	806/880 (92%)	724 (90%)	82 (10%)	7	15

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	LEU
1	A	30	GLU

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Mol	Chain	Res	Type
1	A	34	GLU
1	A	62	VAL
1	A	100	SER
1	A	124	ASP
1	A	143	LEU
1	A	168	ARG
1	A	169	VAL
1	A	173	ASN
1	A	182	ILE
1	A	195	THR
1	A	215	LEU
1	A	220	GLU
1	A	224	ARG
1	A	244	GLN
1	A	250	LEU
1	A	277	ASN
1	A	278	ILE
1	A	283	ASN
1	A	337	LEU
1	A	347	ASP
1	A	353	LEU
1	A	354	GLU
1	A	356	LEU
1	A	375	VAL
1	A	382	ASN
1	A	393	ASN
1	A	398	LEU
1	A	405	GLU
1	A	406	VAL
1	A	420	LEU
1	A	430	LEU
1	A	438	HIS
1	A	443	LEU
1	A	456	THR
1	A	462	ASP
1	A	480	LEU
1	A	503	LEU
1	A	510	THR
1	A	513	VAL
1	A	518	LEU
1	A	523	ARG
1	A	526	VAL

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Mol	Chain	Res	Type
1	A	528	ILE
1	B	10	ILE
1	B	22	LEU
1	B	24	ARG
1	B	45	LEU
1	B	50	ARG
1	B	94	VAL
1	B	120	VAL
1	B	158	ASN
1	B	168	ARG
1	B	169	VAL
1	B	195	THR
1	B	213	SER
1	B	215	LEU
1	B	242	GLU
1	B	250	LEU
1	B	252	LYS
1	B	255	ILE
1	B	258	ASN
1	B	260	VAL
1	B	266	THR
1	B	270	ILE
1	B	277	ASN
1	B	311	GLU
1	B	330	ILE
1	B	333	THR
1	B	338	LYS
1	B	446	SER
1	B	480	LEU
1	B	503	LEU
1	B	513	VAL
1	B	517	ARG
1	B	523	ARG
1	B	524	LEU
1	B	526	VAL
1	B	528	ILE
1	B	552	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS

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Mol	Chain	Res	Type
1	A	149	ASN
1	A	150	HIS
1	A	173	ASN
1	A	189	ASN
1	A	244	GLN
1	A	261	GLN
1	A	265	ASN
1	A	277	ASN
1	A	283	ASN
1	A	362	ASN
1	A	465	ASN
1	B	12	GLN
1	B	29	GLN
1	B	149	ASN
1	B	150	HIS
1	B	158	ASN
1	B	265	ASN
1	B	277	ASN
1	B	283	ASN
1	B	362	ASN
1	B	428	GLN
1	B	465	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	B	700	-	32,33,33	1.48	6 (18%)	45,52,52	1.82	8 (17%)
2	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.31	0
4	TOE	A	702	-	10,10,10	0.58	0	9,9,9	0.32	0
3	AGS	A	700	-	32,33,33	1.63	8 (25%)	45,52,52	2.03	9 (20%)
4	TOE	A	701	-	10,10,10	0.60	0	9,9,9	0.22	0
2	SO4	A	604	-	4,4,4	0.25	0	6,6,6	0.26	0
2	SO4	B	602	-	4,4,4	0.36	0	6,6,6	0.46	0
2	SO4	A	603	-	4,4,4	0.29	0	6,6,6	0.24	0
5	MAE	B	702	-	7,7,7	1.14	1 (14%)	8,8,8	1.26	1 (12%)
2	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.42	0
2	SO4	A	605	-	4,4,4	0.25	0	6,6,6	0.36	0
5	MAE	B	703	-	7,7,7	1.24	1 (14%)	8,8,8	1.88	2 (25%)

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	AGS	B	700	-	-	6/21/38/38	0/3/3/3
4	TOE	A	702	-	-	4/8/8/8	-
4	TOE	A	701	-	-	3/8/8/8	-
3	AGS	A	700	-	-	10/21/38/38	0/3/3/3
5	MAE	B	702	-	-	4/5/5/5	-
5	MAE	B	703	-	-	2/5/5/5	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	AGS	C5-C4	5.27	1.48	1.39
3	B	700	AGS	C5-C4	4.43	1.47	1.39
3	A	700	AGS	C5-C6	3.29	1.50	1.41
3	B	700	AGS	C5-N7	-2.59	1.34	1.39
3	A	700	AGS	C8-N7	2.43	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	AGS	C5-C6	2.39	1.47	1.41
3	A	700	AGS	PB-O3B	2.37	1.62	1.59
3	B	700	AGS	PG-S1G	2.32	1.95	1.90
3	A	700	AGS	PG-S1G	2.28	1.95	1.90
3	A	700	AGS	C5-N7	-2.16	1.35	1.39
5	B	703	MAE	O2-C1	-2.14	1.25	1.30
5	B	702	MAE	O4-C4	-2.13	1.25	1.30
3	A	700	AGS	PG-O2G	2.11	1.61	1.54
3	A	700	AGS	PG-O3G	2.04	1.61	1.54
3	B	700	AGS	PG-O2G	2.04	1.61	1.54
3	B	700	AGS	C4-N9	-2.01	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	AGS	C5-C4-N3	-6.52	117.73	126.72
3	B	700	AGS	C5-C4-N3	-5.79	118.74	126.72
3	A	700	AGS	N3-C4-N9	5.05	135.75	127.17
3	B	700	AGS	N3-C4-N9	4.92	135.53	127.17
3	A	700	AGS	C2-N3-C4	4.16	121.98	111.83
5	B	703	MAE	O2-C1-O1	-3.80	114.96	122.70
3	A	700	AGS	PB-O3B-PG	-3.67	119.74	133.17
3	B	700	AGS	PB-O3B-PG	-3.55	120.18	133.17
3	B	700	AGS	C2-N3-C4	3.51	120.41	111.83
3	A	700	AGS	C4-C5-N7	-3.49	106.60	110.58
3	A	700	AGS	N3-C2-N1	-3.40	123.43	128.58
3	A	700	AGS	O4'-C1'-N9	3.33	114.48	108.09
5	B	703	MAE	O4-C4-O3	-2.85	116.90	122.70
3	B	700	AGS	N3-C2-N1	-2.84	124.28	128.58
3	B	700	AGS	C4-C5-N7	-2.62	107.59	110.58
3	B	700	AGS	C3'-C2'-C1'	2.53	106.25	101.46
3	B	700	AGS	C4-N9-C8	2.53	108.39	105.74
3	A	700	AGS	C5-N7-C8	2.43	107.26	103.45
5	B	702	MAE	O4-C4-O3	-2.23	118.16	122.70
3	A	700	AGS	C6-C5-N7	2.22	136.36	132.09

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	AGS	PB-O3B-PG-O2G
3	A	700	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	A	700	AGS	C5'-O5'-PA-O3A
3	B	700	AGS	PB-O3B-PG-O2G
3	B	700	AGS	PB-O3B-PG-O3G
3	B	700	AGS	O4'-C4'-C5'-O5'
3	B	700	AGS	C3'-C4'-C5'-O5'
5	B	703	MAE	O1-C1-C2-C3
5	B	702	MAE	O1-C1-C2-C3
5	B	703	MAE	O2-C1-C2-C3
5	B	702	MAE	O2-C1-C2-C3
5	B	702	MAE	C2-C3-C4-O4
3	A	700	AGS	O4'-C4'-C5'-O5'
5	B	702	MAE	C2-C3-C4-O3
4	A	701	TOE	O2'-CA'-CB'-OC'
3	A	700	AGS	C3'-C4'-C5'-O5'
4	A	702	TOE	OC'-CD'-CE'-OF'
3	A	700	AGS	PB-O3A-PA-O1A
3	B	700	AGS	PA-O3A-PB-O1B
4	A	702	TOE	OF'-CG'-CH'-OI'
4	A	702	TOE	CG'-CH'-OI'-CK'
3	A	700	AGS	C5'-O5'-PA-O1A
4	A	702	TOE	O2'-CA'-CB'-OC'
3	A	700	AGS	PB-O3A-PA-O2A
3	B	700	AGS	PA-O3A-PB-O2B
3	A	700	AGS	C2'-C1'-N9-C8
3	A	700	AGS	C2'-C1'-N9-C4
4	A	701	TOE	CD'-CE'-OF'-CG'
4	A	701	TOE	OF'-CG'-CH'-OI'

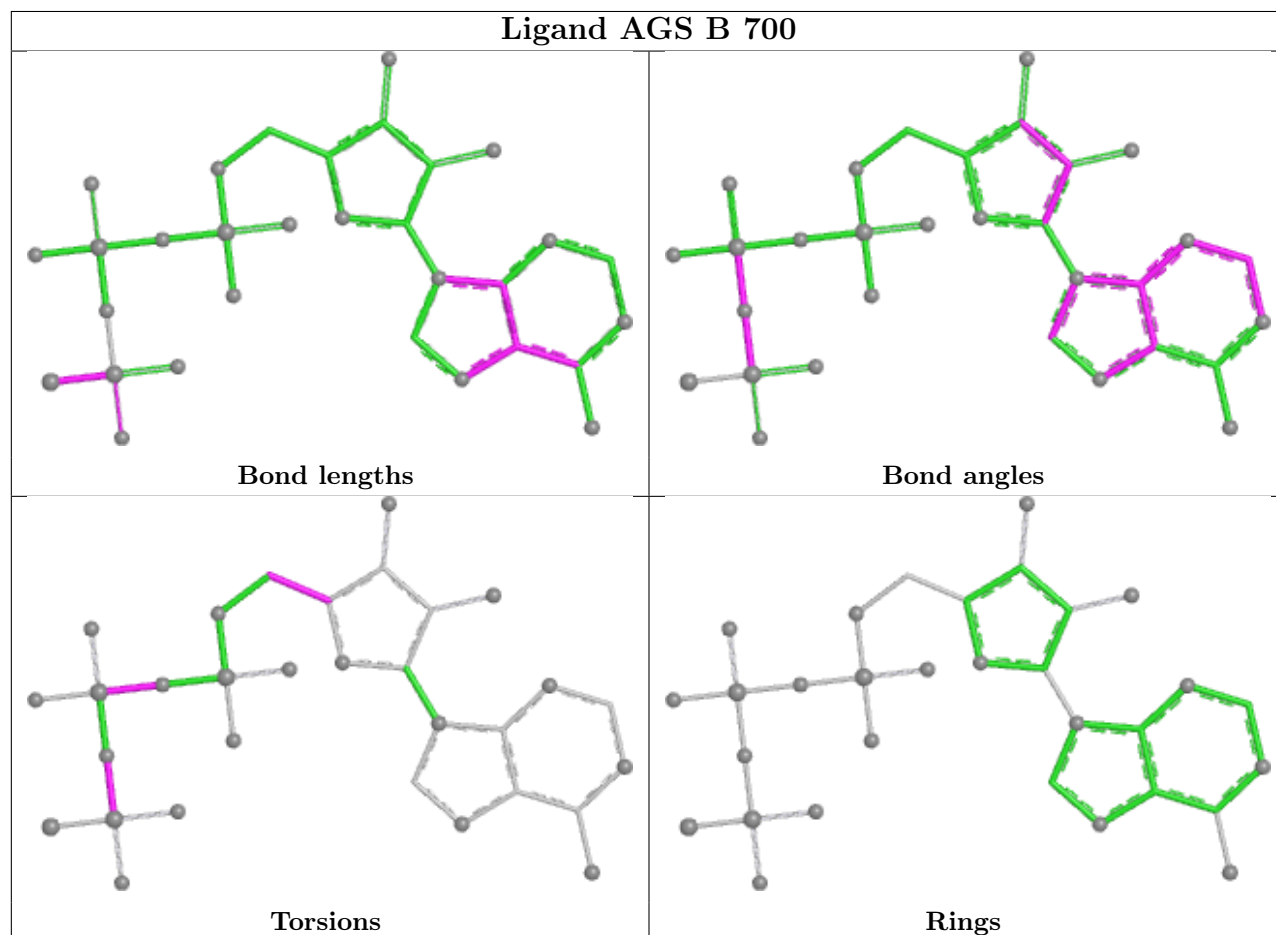
There are no ring outliers.

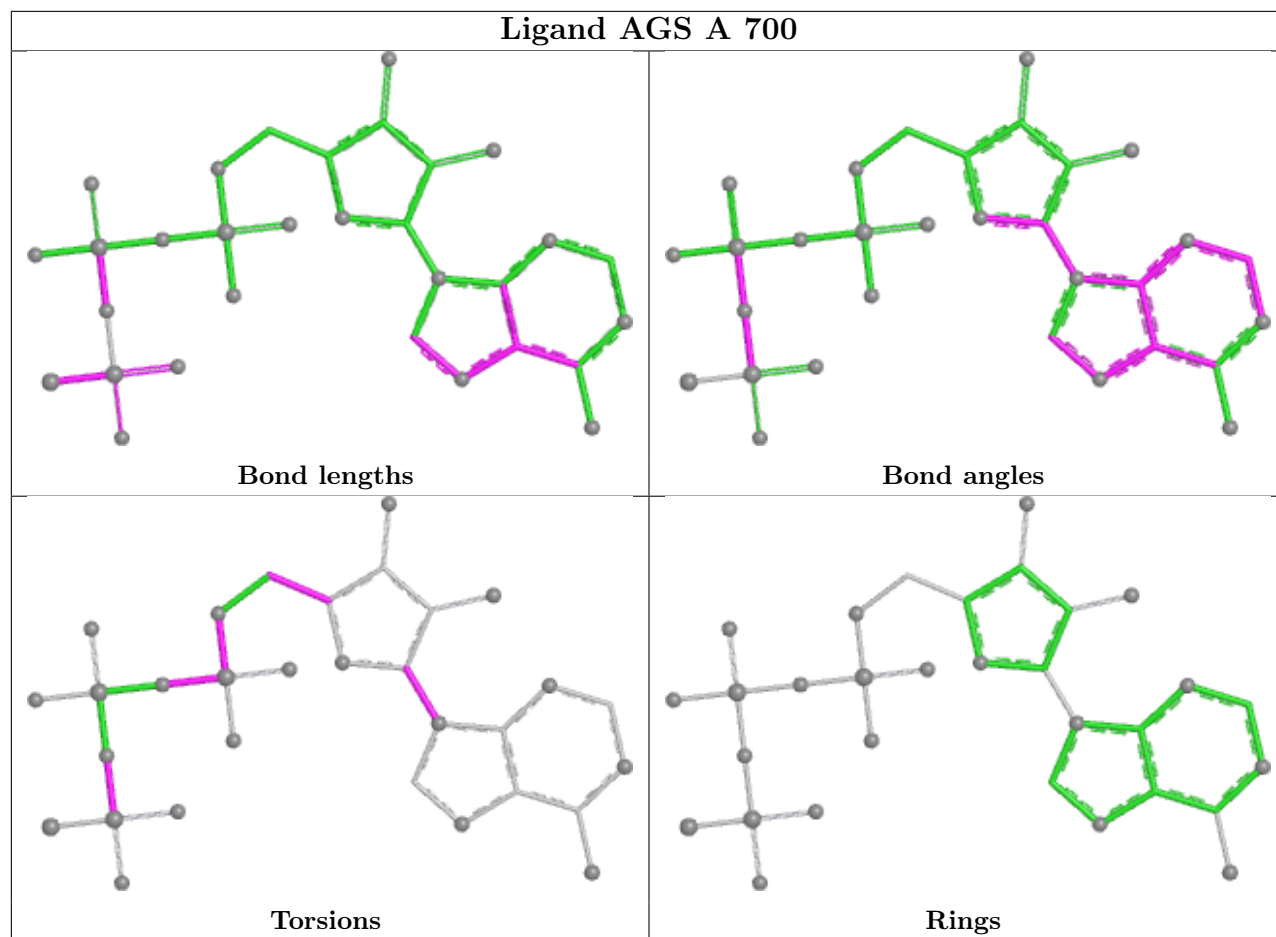
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	AGS	4	0
3	A	700	AGS	4	0
2	B	602	SO4	1	0
2	A	601	SO4	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 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	550/557 (98%)	0.08	21 (3%) 44 35	9, 14, 43, 58	0
1	B	549/557 (98%)	0.87	57 (10%) 11 9	9, 38, 67, 92	0
All	All	1099/1114 (98%)	0.48	78 (7%) 22 16	9, 22, 58, 92	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	SER	4.6
1	A	551	ALA	4.6
1	B	412	TRP	4.2
1	A	400	ALA	4.2
1	B	400	ALA	3.9
1	A	109	GLY	3.6
1	B	387	ASP	3.6
1	A	8	ILE	3.5
1	B	108	LYS	3.5
1	B	432	SER	3.3
1	B	396	TYR	3.1
1	A	71	GLY	3.1
1	A	556	THR	3.1
1	A	527	PRO	3.0
1	A	531	ALA	3.0
1	B	80	GLY	2.9
1	B	532	ILE	2.9
1	B	302	ALA	2.9
1	A	542	PRO	2.8
1	B	117	ALA	2.8
1	B	81	LEU	2.8
1	B	11	ALA	2.7
1	B	381	ILE	2.7
1	A	552	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	299	VAL	2.7
1	B	406	VAL	2.7
1	B	88	LEU	2.7
1	B	112	ALA	2.6
1	A	557	GLY	2.6
1	A	405	GLU	2.6
1	B	364	GLU	2.6
1	B	507	ARG	2.6
1	B	10	ILE	2.6
1	B	335	ARG	2.5
1	B	353	LEU	2.5
1	B	329	VAL	2.5
1	A	107	ILE	2.5
1	A	113	GLY	2.5
1	B	431	GLU	2.5
1	B	352	ASN	2.5
1	B	426	VAL	2.4
1	B	389	GLU	2.4
1	A	396	TYR	2.4
1	B	14	ALA	2.4
1	A	553	GLY	2.4
1	B	403	GLY	2.4
1	B	13	ALA	2.4
1	B	51	LEU	2.4
1	B	113	GLY	2.4
1	A	549	ILE	2.4
1	B	443	LEU	2.3
1	B	526	VAL	2.3
1	A	9	GLU	2.3
1	B	413	ALA	2.3
1	B	85	LEU	2.3
1	B	394	LEU	2.3
1	A	10	ILE	2.3
1	B	522	GLY	2.3
1	B	553	GLY	2.2
1	B	93	MET	2.2
1	B	533	MET	2.2
1	B	434	PRO	2.2
1	B	388	THR	2.2
1	B	330	ILE	2.1
1	B	357	ARG	2.1
1	B	25	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLY	2.1
1	B	89	GLY	2.1
1	B	408	LEU	2.1
1	B	440	LEU	2.1
1	B	354	GLU	2.1
1	B	382	ASN	2.1
1	B	433	ARG	2.1
1	A	108	LYS	2.0
1	B	386	THR	2.0
1	B	529	THR	2.0
1	B	404	ALA	2.0
1	B	9	GLU	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.

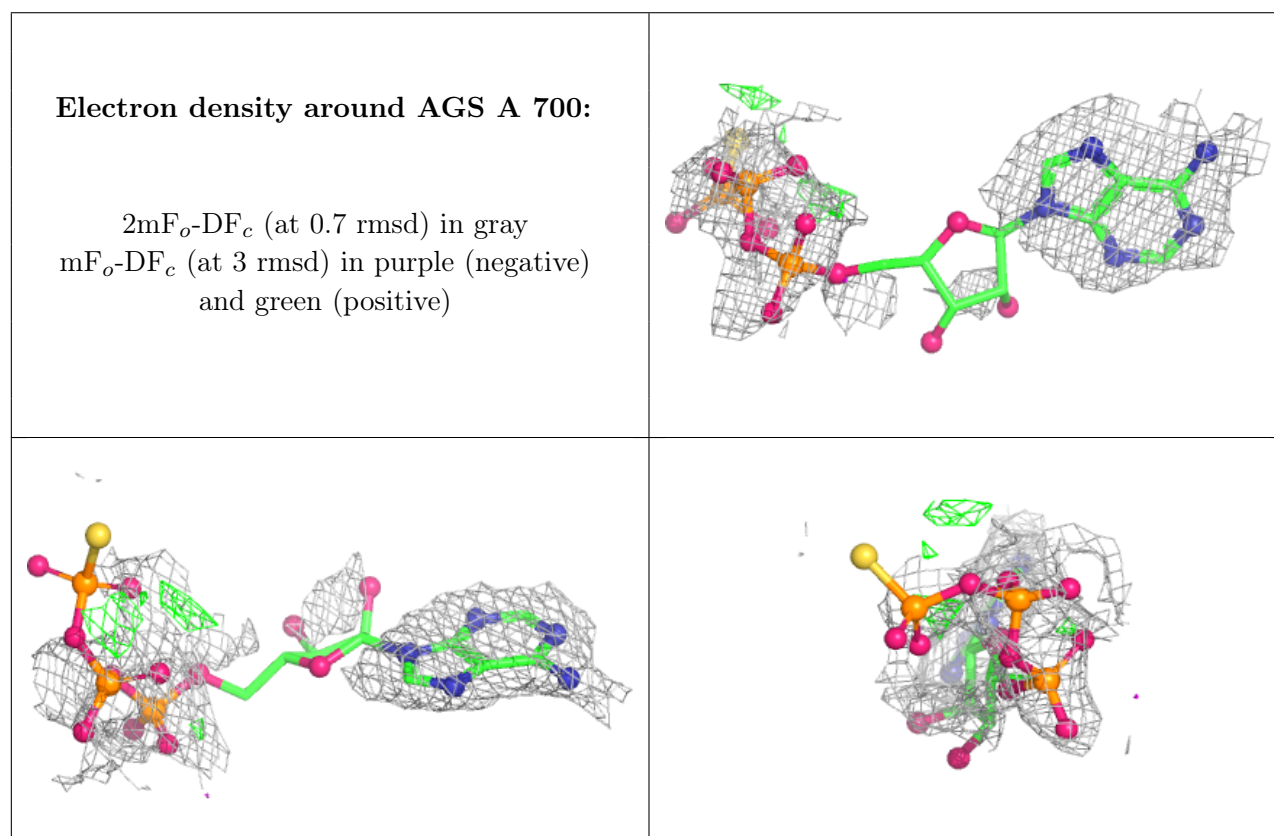
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAE	B	702	8/8	0.65	0.21	59,60,62,63	0
3	AGS	A	700	31/31	0.67	0.24	46,49,49,50	21
3	AGS	B	700	31/31	0.73	0.24	33,38,41,43	31
2	SO4	A	603	5/5	0.76	0.17	66,66,67,68	0
2	SO4	A	604	5/5	0.80	0.14	47,47,49,49	0
4	TOE	A	701	11/11	0.81	0.17	14,22,32,32	0
5	MAE	B	703	8/8	0.82	0.17	37,40,42,43	0
4	TOE	A	702	11/11	0.84	0.14	34,35,49,49	0
2	SO4	A	605	5/5	0.86	0.17	55,56,57,59	0
2	SO4	B	602	5/5	0.86	0.11	44,44,45,46	0
2	SO4	B	601	5/5	0.94	0.08	48,49,50,50	0

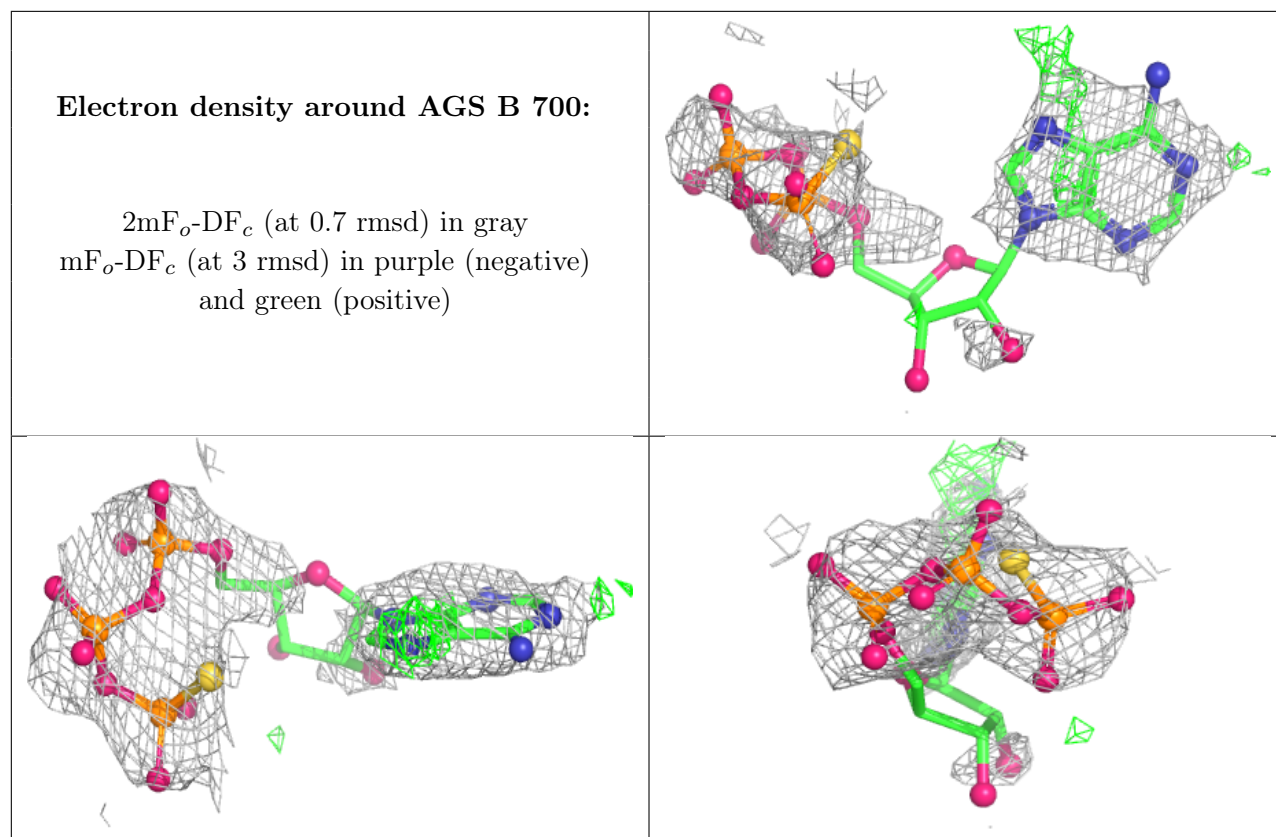
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	601	5/5	0.98	0.06	21,22,23,23	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.