



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:05 AM UTC

PDB ID : 1KJJ / pdb_00001kjj
Title : Crystal structure of glycylamide ribonucleotide transformylase in complex with Mg-ATP-gamma-S
Authors : Thoden, J.B.; Firestone, S.M.; Benkovic, S.J.; Holden, H.M.
Deposited on : 2001-12-04
Resolution : 1.75 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

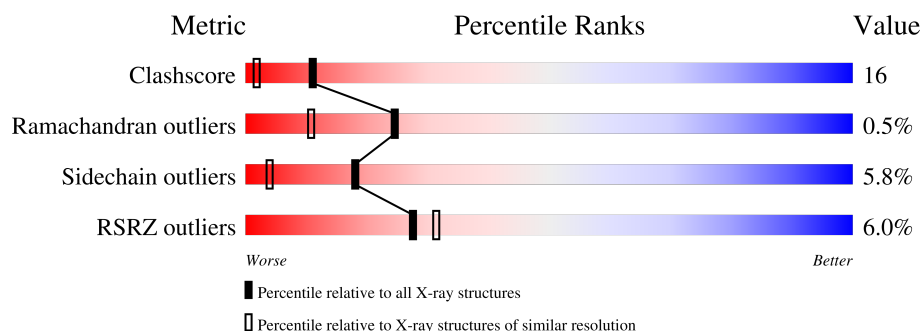
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	391	2% 71% 25% ..
1	B	391	9% 61% 30% 7% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6647 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 phosphoribosylglycinamide formyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	1	0
			2949	1860	522	554	13			
1	B	385	Total	C	N	O	S	0	1	0
			2943	1855	521	553	14			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

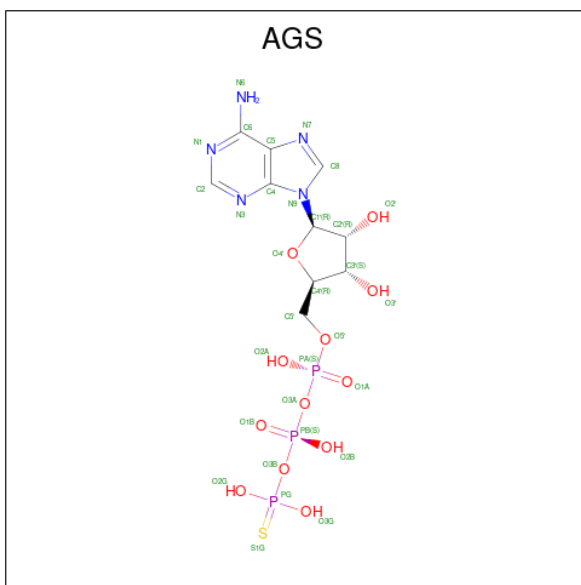
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

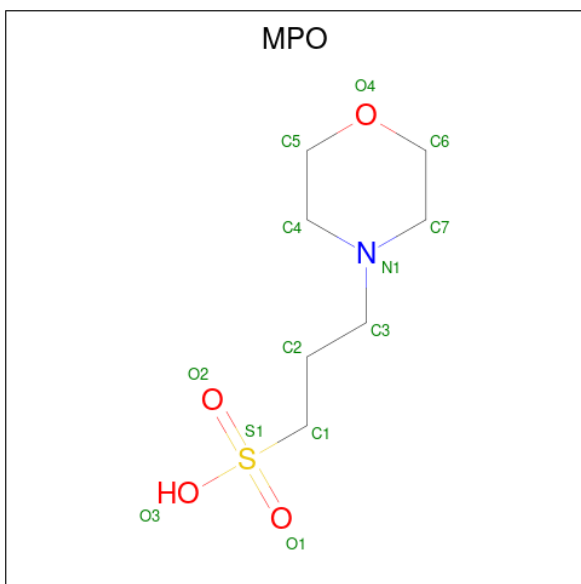
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

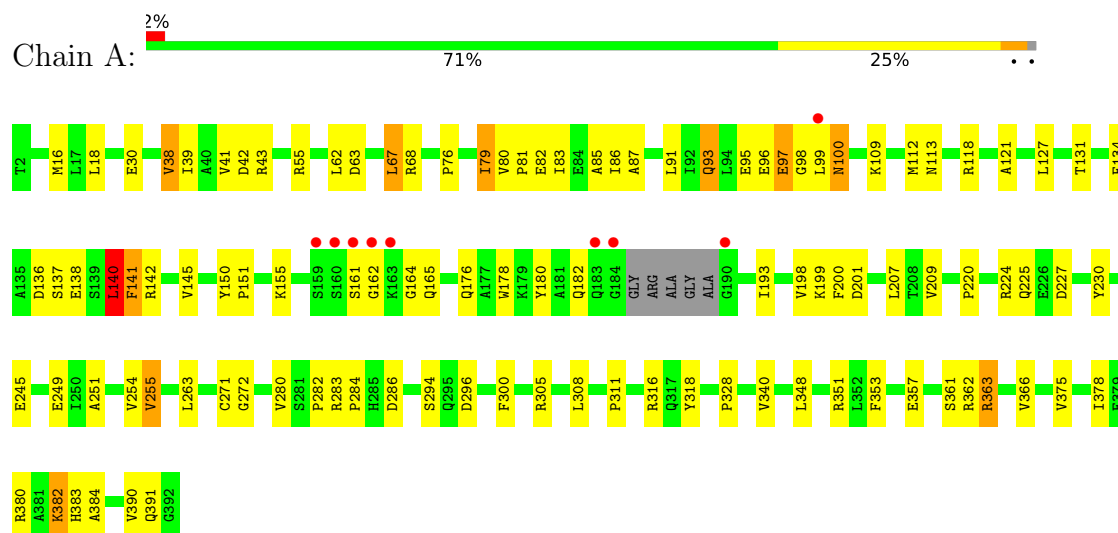
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	396	Total 396	O 396	0	0
7	B	278	Total 278	O 278	0	0

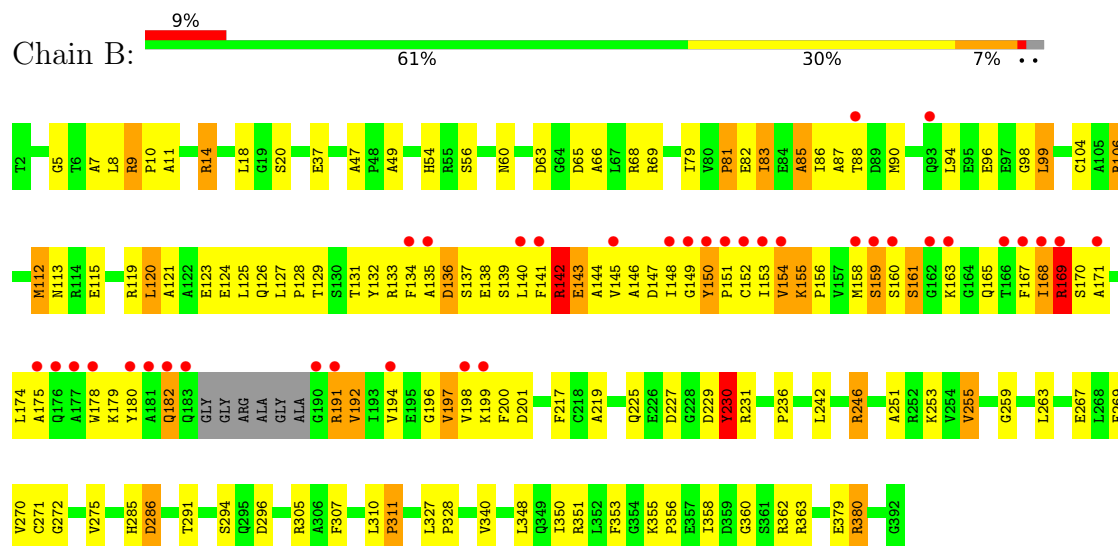
3 Residue-property plots

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

- Molecule 1: phosphoribosylglycinamide formyltransferase 2



- Molecule 1: phosphoribosylglycinamide formyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.90Å 179.30Å 76.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-1.75) 95.8 (30.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.75Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.184 , 0.233 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 98.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: MPO, MG, AGS, CL, NA

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	1.14	2/3002 (0.1%)	1.72	35/4068 (0.9%)
1	B	1.09	1/2996 (0.0%)	1.76	38/4060 (0.9%)
All	All	1.12	3/5998 (0.1%)	1.74	73/8128 (0.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	ASP	CG-OD2	5.19	1.35	1.25
1	B	96	GLU	CD-OE2	5.05	1.34	1.25
1	A	30	GLU	CD-OE2	5.02	1.34	1.25

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	PHE	N-CA-C	11.03	125.84	112.38
1	A	353	PHE	N-CA-C	9.81	124.50	112.54
1	B	168	ILE	N-CA-C	9.65	121.65	107.37
1	B	9	ARG	N-CA-CB	7.78	118.59	109.72
1	A	131	THR	N-CA-C	-7.66	100.21	110.55
1	B	379	GLU	CB-CG-CD	7.61	125.53	112.60
1	A	79	ILE	CB-CA-C	7.35	121.69	110.96
1	B	227	ASP	CA-CB-CG	7.24	119.84	112.60
1	B	380	ARG	CD-NE-CZ	7.06	134.28	124.40
1	B	170	SER	N-CA-C	7.03	121.01	109.06
1	A	300	PHE	CA-CB-CG	-7.02	106.78	113.80
1	B	360	GLY	N-CA-C	-6.95	104.54	111.56
1	A	80	VAL	N-CA-C	6.70	114.78	108.15
1	A	140	LEU	N-CA-CB	-6.69	99.91	110.28
1	A	340	VAL	CA-CB-CG1	-6.69	99.03	110.40
1	A	294	SER	N-CA-C	6.65	121.40	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	VAL	N-CA-C	6.48	117.18	108.11
1	B	285	HIS	N-CA-CB	-6.46	100.29	110.69
1	A	227	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	145	VAL	CB-CA-C	-6.33	103.86	111.97
1	A	134	PHE	CA-CB-CG	-6.07	107.73	113.80
1	B	120	LEU	CA-C-O	6.06	127.74	121.07
1	B	180	TYR	O-C-N	6.06	128.64	122.09
1	A	383	HIS	CA-CB-CG	-6.01	107.79	113.80
1	B	275	VAL	CA-C-O	6.00	126.69	120.39
1	A	85	ALA	N-CA-C	5.96	118.87	109.39
1	A	38	VAL	N-CA-C	5.86	116.30	107.75
1	B	104	CYS	N-CA-CB	5.84	120.53	111.24
1	A	363	ARG	NE-CZ-NH2	-5.84	113.95	119.20
1	B	83	ILE	CB-CA-C	-5.83	102.19	110.82
1	A	284	PRO	CA-C-N	5.82	131.37	122.93
1	A	284	PRO	C-N-CA	5.82	131.37	122.93
1	A	136	ASP	N-CA-CB	5.79	120.54	110.98
1	B	230	TYR	N-CA-C	-5.69	101.86	110.28
1	A	357	GLU	N-CA-C	5.64	116.83	108.60
1	B	112	MET	N-CA-CB	5.63	119.54	110.42
1	A	85	ALA	CB-CA-C	-5.63	102.94	112.00
1	B	192	VAL	N-CA-C	5.63	116.81	108.65
1	A	121	ALA	O-C-N	5.62	127.86	122.07
1	B	128	PRO	N-CA-CB	5.58	107.76	103.30
1	B	142	ARG	CA-C-O	5.57	126.45	120.55
1	B	311	PRO	CB-CA-C	-5.54	103.04	110.85
1	A	318	TYR	N-CA-C	5.53	119.65	113.02
1	A	141	PHE	N-CA-C	-5.51	105.17	111.07
1	B	259	GLY	N-CA-C	5.50	119.81	112.65
1	B	147	ASP	CA-CB-CG	-5.50	107.10	112.60
1	B	217	PHE	CB-CA-C	-5.50	99.31	109.37
1	A	63	ASP	CA-C-O	5.48	126.44	120.58
1	B	98	GLY	CA-C-N	-5.45	112.76	122.07
1	B	98	GLY	C-N-CA	-5.45	112.76	122.07
1	A	67	LEU	CA-C-N	-5.43	113.00	120.28
1	A	67	LEU	C-N-CA	-5.43	113.00	120.28
1	A	198	VAL	CA-C-N	-5.42	114.75	122.77
1	A	198	VAL	C-N-CA	-5.42	114.75	122.77
1	B	286	ASP	N-CA-C	5.40	117.86	111.33
1	B	81	PRO	N-CA-CB	5.35	108.28	103.19
1	B	350	ILE	CA-CB-CG2	5.33	119.57	110.50
1	B	169	ARG	CB-CA-C	5.29	118.27	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ALA	N-CA-C	5.24	116.68	111.07
1	B	56	SER	O-C-N	5.17	129.14	123.25
1	A	118	ARG	N-CA-CB	5.17	117.50	110.01
1	A	280	VAL	N-CA-C	5.15	115.15	108.35
1	B	217	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	220	PRO	N-CA-CB	5.13	107.88	103.31
1	B	246	ARG	CA-C-O	5.13	125.99	120.55
1	B	14	ARG	N-CA-C	5.13	117.32	109.07
1	B	66	ALA	N-CA-C	-5.11	105.60	111.07
1	B	296	ASP	N-CA-C	-5.11	105.79	111.36
1	B	225	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	A	296	ASP	N-CA-C	-5.09	105.73	111.28
1	A	76	PRO	CB-CA-C	-5.01	104.41	110.98
1	A	193	ILE	CA-C-N	-5.01	116.43	123.10
1	A	193	ILE	C-N-CA	-5.01	116.43	123.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2949	0	2974	66	0
1	B	2943	0	2965	128	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	31	0	12	2	0
5	B	31	0	12	2	0
6	A	13	0	15	0	0
7	A	396	0	0	6	0
7	B	278	0	0	10	1
All	All	6647	0	5978	196	2

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 16.

All (196) 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:79:ILE:HD11	1:B:99:LEU:HD22	1.32	1.06
1:B:94:LEU:HB3	1:B:99:LEU:HD13	1.50	0.94
1:B:348:LEU:HB2	1:B:380:ARG:HH11	1.35	0.90
1:B:156:PRO:HG2	1:B:159:SER:HB2	1.52	0.90
1:B:161:SER:HB2	1:B:163:LYS:HE3	1.52	0.89
1:A:93:GLN:HE21	1:A:93:GLN:HA	1.40	0.85
1:B:191:ARG:HG3	1:B:192:VAL:N	1.99	0.78
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.47	0.77
1:B:68:ARG:HB2	1:B:90:MET:HE3	1.68	0.76
1:B:153:ILE:CD1	1:B:197:VAL:HG22	2.14	0.76
1:A:99:LEU:HB2	7:A:625:HOH:O	1.86	0.76
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.20	0.76
1:B:156:PRO:HG2	1:B:159:SER:CB	2.16	0.75
1:A:18:LEU:HG	1:A:79:ILE:HD11	1.69	0.74
1:B:153:ILE:HD11	1:B:197:VAL:HG22	1.71	0.73
1:B:348:LEU:HB2	1:B:380:ARG:NH1	2.01	0.73
1:B:132:TYR:O	1:B:133:ARG:HD2	1.88	0.73
1:A:378:ILE:O	1:A:382:LYS:HG3	1.89	0.72
1:B:143:GLU:O	1:B:146:ALA:HB3	1.88	0.72
1:B:150:TYR:HB3	1:B:151:PRO:HA	1.71	0.70
1:B:171:ALA:HA	1:B:174:LEU:HD13	1.74	0.70
1:B:79:ILE:CD1	1:B:99:LEU:HD22	2.15	0.70
1:A:79:ILE:HB	1:A:99:LEU:HD21	1.71	0.69
1:B:140:LEU:HA	1:B:143:GLU:HB2	1.75	0.69
1:B:174:LEU:HD12	1:B:174:LEU:H	1.58	0.68
1:B:200:PHE:HA	1:B:271[B]:CYS:SG	2.33	0.68
1:B:65:ASP:O	1:B:69:ARG:HG3	1.94	0.68
1:B:113:ASN:HD22	1:B:158:MET:HE2	1.59	0.67
1:B:141:PHE:HE1	1:B:145:VAL:HG21	1.57	0.67
1:B:154:VAL:HG23	1:B:194:VAL:HG22	1.76	0.67
1:A:16:MET:O	1:A:79:ILE:HD12	1.93	0.67
1:B:79:ILE:HD11	1:B:99:LEU:CD2	2.17	0.66
1:B:161:SER:CB	1:B:163:LYS:HE3	2.26	0.66
1:B:174:LEU:HD12	1:B:174:LEU:N	2.10	0.66
1:B:171:ALA:C	1:B:174:LEU:HD13	2.20	0.66
1:B:88:THR:HG21	1:B:112:MET:HG2	1.78	0.66
1:A:16:MET:HB3	1:A:79:ILE:HD13	1.79	0.65
1:A:316:ARG:HD3	7:B:556:HOH:O	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:O	1:B:174:LEU:HD13	1.97	0.65
1:B:178:TRP:O	1:B:182:GLN:NE2	2.28	0.64
1:B:348:LEU:HD22	1:B:380:ARG:NH1	2.12	0.64
1:A:178:TRP:O	1:A:182:GLN:HG2	1.98	0.63
1:A:209:VAL:HG22	1:A:263:LEU:HD12	1.80	0.63
1:B:135:ALA:O	1:B:191:ARG:HD3	1.99	0.63
1:A:164:GLY:HA2	1:A:180:TYR:CE1	2.34	0.62
1:B:169:ARG:HH11	1:B:169:ARG:HG3	1.65	0.62
1:A:380:ARG:HG3	1:A:380:ARG:NH1	2.13	0.62
1:B:81:PRO:HB3	1:B:86:ILE:CD1	2.30	0.61
1:A:82:GLU:HB2	7:A:433:HOH:O	2.00	0.61
1:B:115:GLU:HG3	1:B:134:PHE:CE2	2.36	0.61
1:B:138:GLU:OE2	1:B:142:ARG:NH1	2.33	0.61
1:B:150:TYR:CE2	1:B:168:ILE:HG22	2.35	0.61
1:B:138:GLU:O	1:B:142:ARG:HB2	2.02	0.60
1:B:138:GLU:HA	1:B:141:PHE:HB3	1.84	0.60
1:A:200:PHE:HA	1:A:271:CYS:SG	2.42	0.59
1:B:174:LEU:O	1:B:175:ALA:C	2.44	0.59
1:B:115:GLU:HA	1:B:134:PHE:CZ	2.37	0.59
1:A:127:LEU:HD11	1:A:254:VAL:HG23	1.83	0.59
1:B:9:ARG:HB3	1:B:10:PRO:HD2	1.85	0.59
1:B:136:ASP:OD2	1:B:136:ASP:N	2.35	0.59
1:A:100:ASN:C	1:A:100:ASN:HD22	2.12	0.58
1:A:375:VAL:HG23	7:A:725:HOH:O	2.02	0.58
1:B:20:SER:HB3	1:B:49:ALA:HB3	1.85	0.58
1:B:153:ILE:HD12	1:B:197:VAL:HG22	1.85	0.57
1:A:39[A]:ILE:HD11	1:A:55:ARG:NH2	2.19	0.57
1:B:174:LEU:H	1:B:174:LEU:CD1	2.17	0.57
1:B:106:ARG:HD3	7:B:591:HOH:O	2.04	0.56
1:B:137:SER:O	1:B:141:PHE:N	2.29	0.56
1:B:127:LEU:HD21	1:B:253:LYS:HD2	1.87	0.56
1:B:68:ARG:CB	1:B:90:MET:HE3	2.35	0.56
1:B:68:ARG:HE	1:B:90:MET:HE1	1.71	0.56
1:B:9:ARG:HB3	1:B:10:PRO:CD	2.35	0.56
1:B:115:GLU:O	1:B:119:ARG:HG3	2.06	0.56
1:B:253:LYS:HG3	7:B:616:HOH:O	2.07	0.55
1:B:155:LYS:HG2	1:B:165:GLN:HG3	1.88	0.55
1:B:171:ALA:HA	1:B:174:LEU:CD1	2.37	0.55
1:A:251:ALA:O	1:A:255:VAL:HG13	2.06	0.54
1:B:115:GLU:HG3	1:B:134:PHE:CD2	2.41	0.54
1:B:150:TYR:CB	1:B:151:PRO:HA	2.33	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD21	1:B:246:ARG:NH1	2.23	0.53
1:A:137:SER:OG	1:A:140:LEU:HB2	2.09	0.53
1:B:327:LEU:HD12	1:B:362:ARG:C	2.34	0.53
1:B:348:LEU:HD22	1:B:380:ARG:HH11	1.73	0.52
1:B:219:ALA:HB1	1:B:236:PRO:HB3	1.92	0.52
1:B:198:VAL:HA	7:B:609:HOH:O	2.11	0.51
1:B:199:LYS:O	1:B:199:LYS:HG3	2.10	0.51
1:B:113:ASN:ND2	1:B:158:MET:HE2	2.24	0.51
1:A:138:GLU:O	1:A:142:ARG:HG3	2.11	0.50
1:B:131:THR:OG1	1:B:196:GLY:HA3	2.10	0.50
1:A:16:MET:HG2	1:A:79:ILE:CD1	2.42	0.50
1:A:249:GLU:HB3	7:A:668:HOH:O	2.10	0.50
1:A:348:LEU:HD11	1:A:384:ALA:HB2	1.93	0.50
1:B:132:TYR:N	1:B:132:TYR:CD2	2.80	0.50
1:A:245:GLU:O	1:A:249:GLU:HG3	2.13	0.49
1:A:176:GLN:NE2	1:A:176:GLN:HA	2.27	0.49
1:A:286:ASP:OD2	1:A:363:ARG:NH2	2.43	0.49
1:B:362:ARG:HD2	7:B:577:HOH:O	2.12	0.49
1:A:127:LEU:CD1	1:A:254:VAL:HG23	2.42	0.49
1:B:37:GLU:HA	1:B:54:HIS:CE1	2.47	0.49
1:B:267:GLU:HG2	7:B:562:HOH:O	2.13	0.49
1:A:95:GLU:HA	1:A:99:LEU:O	2.13	0.49
1:A:96:GLU:C	1:A:98:GLY:H	2.21	0.49
1:B:83:ILE:HD12	1:B:85:ALA:HB3	1.94	0.49
1:B:356:PRO:HD2	7:B:628:HOH:O	2.12	0.49
1:A:305:ARG:HD3	1:A:311:PRO:O	2.13	0.48
1:B:20:SER:CB	1:B:49:ALA:HB3	2.43	0.48
1:B:141:PHE:CD2	1:B:178:TRP:HB2	2.48	0.48
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.43	0.48
1:B:171:ALA:CA	1:B:174:LEU:HD13	2.42	0.48
1:B:348:LEU:CB	1:B:380:ARG:HH11	2.16	0.48
1:B:155:LYS:NZ	5:B:395:AGS:N7	2.62	0.48
1:A:328:PRO:HD2	1:A:362:ARG:O	2.14	0.47
1:B:127:LEU:O	1:B:129:THR:HG23	2.13	0.47
1:B:141:PHE:CE1	1:B:145:VAL:CG2	2.94	0.47
1:B:286:ASP:OD2	1:B:363:ARG:NH2	2.45	0.47
1:B:348:LEU:CD2	1:B:380:ARG:NH1	2.76	0.47
1:B:348:LEU:CB	1:B:380:ARG:NH1	2.74	0.47
1:A:390:VAL:C	1:A:391:GLN:HG3	2.39	0.47
1:B:113:ASN:ND2	1:B:158:MET:CE	2.78	0.47
1:B:14:ARG:HG2	1:B:37:GLU:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:HD12	1:B:197:VAL:CG2	2.45	0.47
1:B:18:LEU:HB2	1:B:81:PRO:HA	1.96	0.47
1:B:86:ILE:HG22	1:B:87:ALA:N	2.30	0.47
1:B:242:LEU:CD2	1:B:246:ARG:NH1	2.79	0.46
1:B:137:SER:OG	1:B:140:LEU:HD12	2.14	0.46
1:A:282:PRO:O	1:A:283:ARG:HB3	2.15	0.46
5:A:1:AGS:H8	5:A:1:AGS:O5'	2.14	0.46
1:A:68:ARG:HH12	1:A:97:GLU:CD	2.23	0.46
1:B:120:LEU:HD12	1:B:124:GLU:HB3	1.98	0.46
1:B:291:THR:HA	1:B:294:SER:OG	2.16	0.46
1:A:225:GLN:NE2	7:A:737:HOH:O	2.44	0.46
1:B:362:ARG:NH1	7:B:628:HOH:O	2.48	0.46
1:A:93:GLN:HA	1:A:93:GLN:NE2	2.19	0.45
1:B:305:ARG:HD3	1:B:310:LEU:HB2	1.98	0.45
1:B:5:GLY:HA3	1:B:11:ALA:O	2.16	0.45
1:B:142:ARG:HG3	1:B:174:LEU:HD23	1.97	0.45
1:B:355:LYS:HD3	1:B:362:ARG:HE	1.82	0.45
1:B:60:ASN:O	1:B:63:ASP:HB3	2.16	0.45
1:B:81:PRO:HB3	1:B:86:ILE:HD13	1.96	0.45
1:A:93:GLN:NE2	1:A:96:GLU:OE1	2.49	0.45
1:B:141:PHE:CD1	1:B:141:PHE:C	2.95	0.45
1:B:151:PRO:HB2	1:B:167:PHE:CE1	2.51	0.45
1:A:81:PRO:HB3	1:A:86:ILE:HD12	1.99	0.45
1:A:99:LEU:HG	1:A:100:ASN:N	2.30	0.45
1:A:162:GLY:HA2	1:A:165:GLN:NE2	2.32	0.45
1:B:251:ALA:O	1:B:255:VAL:HG13	2.16	0.45
1:B:149:GLY:O	1:B:152:CYS:HB3	2.16	0.45
1:B:150:TYR:CD2	1:B:169:ARG:C	2.95	0.44
1:A:79:ILE:CB	1:A:99:LEU:HD21	2.42	0.44
1:A:42:ASP:OD2	1:A:43:ARG:N	2.44	0.44
1:B:150:TYR:CE2	1:B:168:ILE:CG2	3.01	0.44
1:B:174:LEU:N	1:B:174:LEU:CD1	2.78	0.44
1:A:43:ARG:O	1:A:43:ARG:HG3	2.18	0.44
1:B:340:VAL:O	1:B:340:VAL:HG12	2.16	0.44
1:A:150:TYR:HA	1:A:151:PRO:C	2.43	0.44
1:A:164:GLY:CA	1:A:180:TYR:CE1	3.01	0.44
1:A:16:MET:CB	1:A:79:ILE:HD13	2.47	0.43
1:A:161:SER:N	5:A:1:AGS:S1G	2.89	0.43
1:B:155:LYS:HE2	1:B:165:GLN:OE1	2.18	0.43
1:B:305:ARG:HD3	1:B:310:LEU:CB	2.48	0.43
1:B:119:ARG:O	1:B:123:GLU:HB2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD23	1:A:41:VAL:HB	2.01	0.43
1:A:79:ILE:HD12	1:A:79:ILE:HA	1.55	0.43
1:B:358:ILE:HD12	1:B:362:ARG:HB3	2.01	0.43
5:B:395:AGS:H8	5:B:395:AGS:O5'	2.18	0.43
1:A:141:PHE:CE2	1:A:178:TRP:HB2	2.54	0.42
1:B:200:PHE:HA	1:B:271[B]:CYS:HG	1.84	0.42
1:A:138:GLU:O	1:A:141:PHE:HB3	2.18	0.42
1:A:391:GLN:NE2	7:A:431:HOH:O	2.51	0.42
1:B:20:SER:HB2	1:B:47:ALA:HB3	2.01	0.42
1:B:150:TYR:HA	1:B:151:PRO:C	2.41	0.42
1:B:305:ARG:HD2	1:B:311:PRO:O	2.19	0.42
1:B:328:PRO:HD2	1:B:362:ARG:O	2.20	0.42
1:B:82:GLU:HB2	7:B:453:HOH:O	2.19	0.42
1:B:140:LEU:O	1:B:144:ALA:N	2.41	0.42
1:B:150:TYR:CD2	1:B:168:ILE:HG22	2.55	0.42
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.86	0.41
1:B:230:TYR:C	1:B:231:ARG:HD3	2.44	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.76	0.41
1:B:113:ASN:HD22	1:B:158:MET:CE	2.28	0.41
1:B:200:PHE:CB	1:B:269:PHE:HB3	2.51	0.41
1:A:79:ILE:CG2	1:A:99:LEU:CD2	2.98	0.41
1:A:67:LEU:HA	1:A:67:LEU:HD12	1.81	0.41
1:A:351:ARG:HB2	1:A:366:VAL:HG12	2.01	0.41
1:B:351:ARG:NH2	7:B:665:HOH:O	2.53	0.41
1:A:16:MET:HG2	1:A:79:ILE:HD11	2.01	0.41
1:B:201:ASP:N	1:B:270:VAL:O	2.49	0.41
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.95	0.41
1:B:125:LEU:O	1:B:126:GLN:HB2	2.21	0.41
1:A:81:PRO:HB3	1:A:86:ILE:CD1	2.52	0.40
1:A:38:VAL:C	1:A:39[A]:ILE:HD13	2.46	0.40
1:B:263:LEU:HD23	1:B:263:LEU:C	2.46	0.40
1:A:201:ASP:OD1	1:A:272:GLY:N	2.53	0.40
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.92	0.40
1:B:7:ALA:O	1:B:8:LEU:HB2	2.20	0.40

All (2) 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:B:191:ARG:NH2	1:B:191:ARG:NH2[2_555]	1.72	0.48
7:B:639:HOH:O	7:B:639:HOH:O[2_655]	1.86	0.34

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	383/391 (98%)	372 (97%)	9 (2%)	2 (0%)	24	11
1	B	382/391 (98%)	365 (96%)	15 (4%)	2 (0%)	24	11
All	All	765/782 (98%)	737 (96%)	24 (3%)	4 (0%)	24	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA
1	A	97	GLU
1	B	85	ALA
1	B	197	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	311/311 (100%)	296 (95%)	15 (5%)	23	6
1	B	311/311 (100%)	290 (93%)	21 (7%)	14	3
All	All	622/622 (100%)	586 (94%)	36 (6%)	18	4

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ILE
1	A	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	100	ASN
1	A	109	LYS
1	A	112	MET
1	A	113	ASN
1	A	140	LEU
1	A	155	LYS
1	A	199	LYS
1	A	207	LEU
1	A	224	ARG
1	A	230	TYR
1	A	255	VAL
1	A	361	SER
1	A	382	LYS
1	B	99	LEU
1	B	106	ARG
1	B	136	ASP
1	B	139	SER
1	B	142	ARG
1	B	143	GLU
1	B	148	ILE
1	B	150	TYR
1	B	154	VAL
1	B	155	LYS
1	B	159	SER
1	B	160	SER
1	B	161	SER
1	B	169	ARG
1	B	179	LYS
1	B	182	GLN
1	B	191	ARG
1	B	229	ASP
1	B	230	TYR
1	B	255	VAL
1	B	307	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	100	ASN
1	A	176	GLN
1	A	248	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	342	ASN
1	A	387	GLN
1	B	100	ASN
1	B	126	GLN
1	B	176	GLN
1	B	225	GLN
1	B	238	GLN
1	B	248	GLN
1	B	333	GLN
1	B	387	GLN
1	B	391	GLN

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](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
5	AGS	B	395	2	32,33,33	2.18	6 (18%)	45,52,52	1.44	9 (20%)
5	AGS	A	1	2	32,33,33	2.25	5 (15%)	45,52,52	1.66	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPO	A	397	-	13,13,13	2.21	3 (23%)	17,17,17	2.07	4 (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
5	AGS	B	395	2	-	2/21/38/38	0/3/3/3
5	AGS	A	1	2	-	3/21/38/38	0/3/3/3
6	MPO	A	397	-	-	0/7/15/15	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	AGS	PG-S1G	-10.69	1.67	1.90
5	B	395	AGS	PG-S1G	-10.36	1.68	1.90
6	A	397	MPO	C1-S1	5.22	1.84	1.77
6	A	397	MPO	C3-N1	4.52	1.57	1.47
5	A	1	AGS	C6-N6	-3.24	1.25	1.34
5	A	1	AGS	C8-N7	2.82	1.37	1.31
5	B	395	AGS	C8-N7	2.72	1.36	1.31
5	B	395	AGS	C2-N1	2.66	1.38	1.33
5	A	1	AGS	C2-N1	2.64	1.38	1.33
6	A	397	MPO	O1-S1	2.21	1.51	1.45
5	B	395	AGS	C5-C4	2.20	1.43	1.39
5	A	1	AGS	PG-O3G	2.19	1.61	1.54
5	B	395	AGS	PA-O3A	-2.19	1.57	1.59
5	B	395	AGS	C6-N6	-2.02	1.29	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	AGS	C2-N1-C6	6.24	128.98	118.73
6	A	397	MPO	O3-S1-O1	-6.16	95.99	111.40
5	A	1	AGS	N3-C2-N1	-4.83	121.27	128.58
5	B	395	AGS	C2-N1-C6	4.02	125.33	118.73
5	A	1	AGS	O2A-PA-O3A	3.36	116.36	107.27
5	B	395	AGS	C5-C6-N6	3.11	130.99	123.29
6	A	397	MPO	O3-S1-C1	3.06	111.99	106.00
5	A	1	AGS	C5-C6-N1	-3.02	109.84	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	395	AGS	C5-C6-N1	-2.64	110.80	117.51
6	A	397	MPO	O2-S1-C1	2.62	110.69	106.73
5	B	395	AGS	C6-C5-C4	2.54	120.65	117.18
5	A	1	AGS	C5-C6-N6	2.45	129.34	123.29
5	B	395	AGS	O2B-PB-O3B	2.43	113.83	107.27
5	B	395	AGS	C4-C5-N7	-2.36	107.88	110.58
5	B	395	AGS	O2A-PA-O3A	2.33	113.56	107.27
5	B	395	AGS	N3-C2-N1	-2.31	125.09	128.58
5	A	1	AGS	O3'-C3'-C2'	2.13	118.64	111.82
5	B	395	AGS	C5-C4-N9	2.09	108.09	105.81
6	A	397	MPO	C5-C4-N1	2.09	113.29	110.12
5	A	1	AGS	PB-O3B-PG	-2.04	125.70	133.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	AGS	PB-O3B-PG-O3G
5	A	1	AGS	PG-O3B-PB-O1B
5	A	1	AGS	PG-O3B-PB-O2B
5	B	395	AGS	PG-O3B-PB-O2B
5	B	395	AGS	PB-O3A-PA-O2A

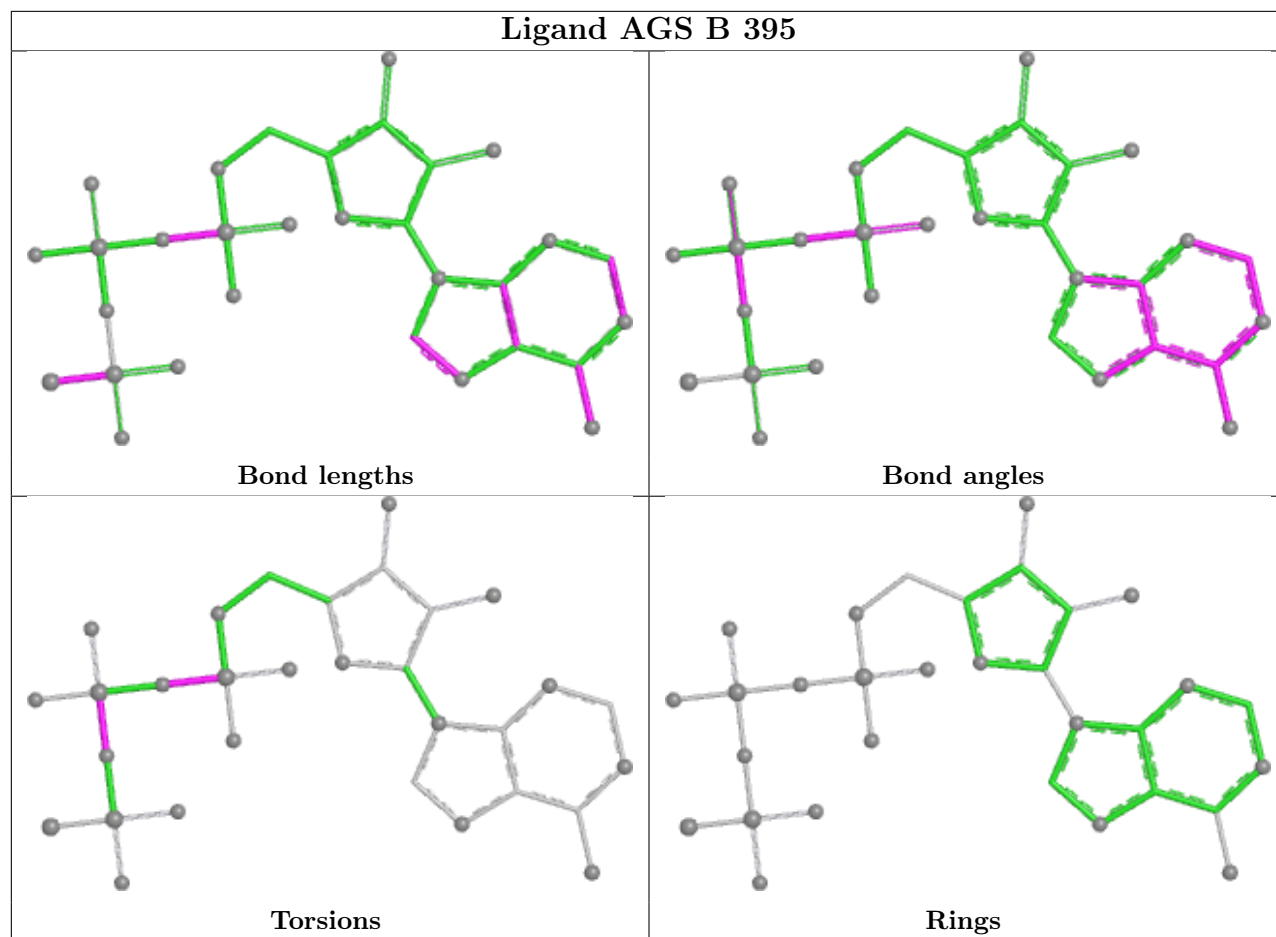
There are no ring outliers.

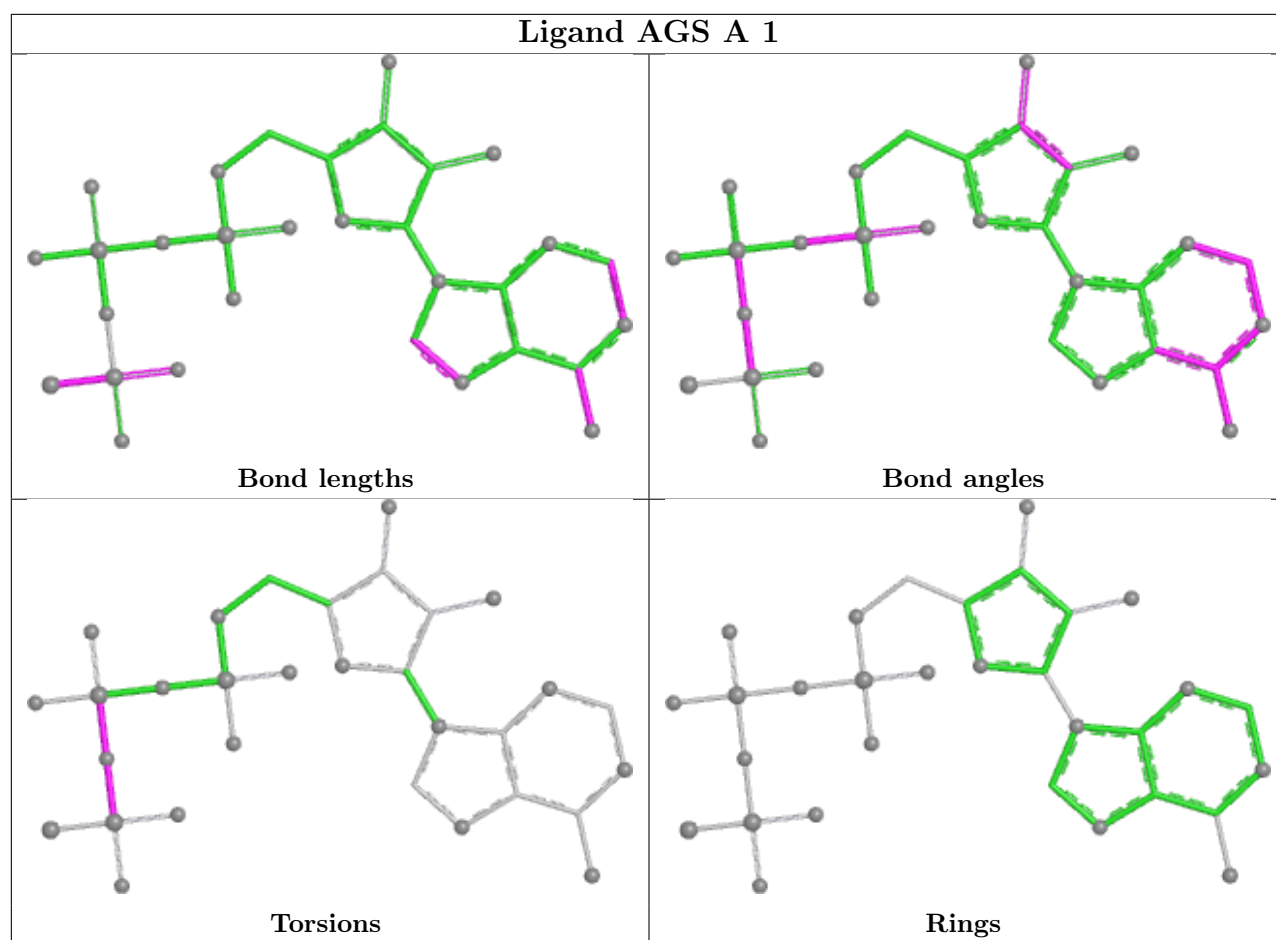
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	395	AGS	2	0
5	A	1	AGS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Ligand AGS B 395





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	386/391 (98%)	-0.24	9 (2%) 61 67	11, 21, 53, 93	1 (0%)
1	B	385/391 (98%)	0.26	37 (9%) 13 16	13, 27, 80, 95	1 (0%)
All	All	771/782 (98%)	0.01	46 (5%) 27 31	11, 23, 71, 95	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	5.7
1	B	162	GLY	4.9
1	A	162	GLY	4.6
1	A	161	SER	4.2
1	B	141	PHE	4.2
1	B	190	GLY	4.2
1	B	181	ALA	4.0
1	B	150	TYR	3.6
1	B	171	ALA	3.6
1	B	154	VAL	3.5
1	B	140	LEU	3.4
1	B	148	ILE	3.4
1	B	149	GLY	3.3
1	B	135	ALA	3.3
1	A	184	GLY	3.2
1	A	163	LYS	3.2
1	B	134	PHE	3.2
1	B	180	TYR	3.2
1	B	178	TRP	3.1
1	B	145	VAL	3.1
1	A	190	GLY	3.1
1	B	168	ILE	3.0
1	B	169	ARG	3.0
1	B	166	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	163	LYS	2.9
1	B	176	GLN	2.8
1	B	151	PRO	2.7
1	B	159	SER	2.7
1	A	99	LEU	2.6
1	B	160	SER	2.5
1	B	198	VAL	2.4
1	B	177	ALA	2.4
1	B	182	GLN	2.4
1	B	153	ILE	2.4
1	B	88	THR	2.3
1	B	158	MET	2.3
1	B	183	GLN	2.3
1	B	199	LYS	2.3
1	B	93	GLN	2.2
1	A	160	SER	2.2
1	A	183	GLN	2.2
1	B	167	PHE	2.2
1	B	194	VAL	2.2
1	A	159	SER	2.2
1	B	152	CYS	2.0
1	B	191	ARG	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
3	NA	A	395	1/1	0.88	0.10	35,35,35,35	0

Continued on next page...

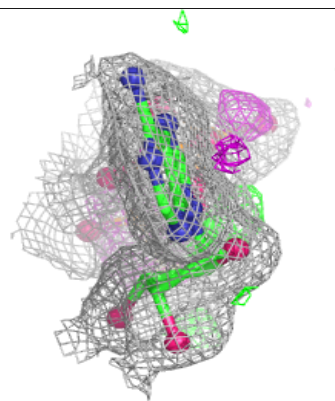
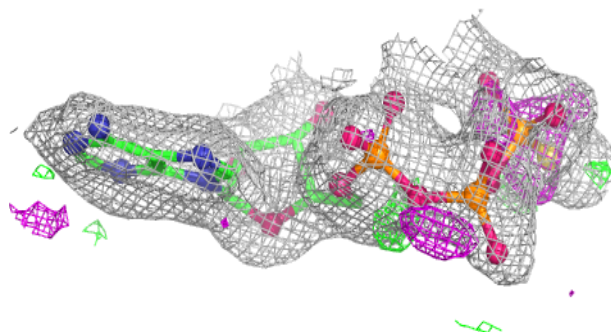
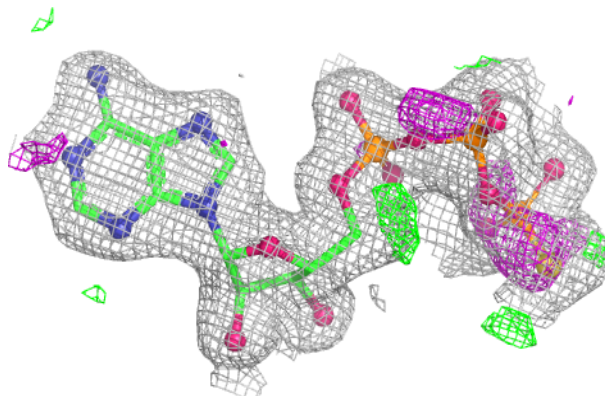
Continued from previous page...

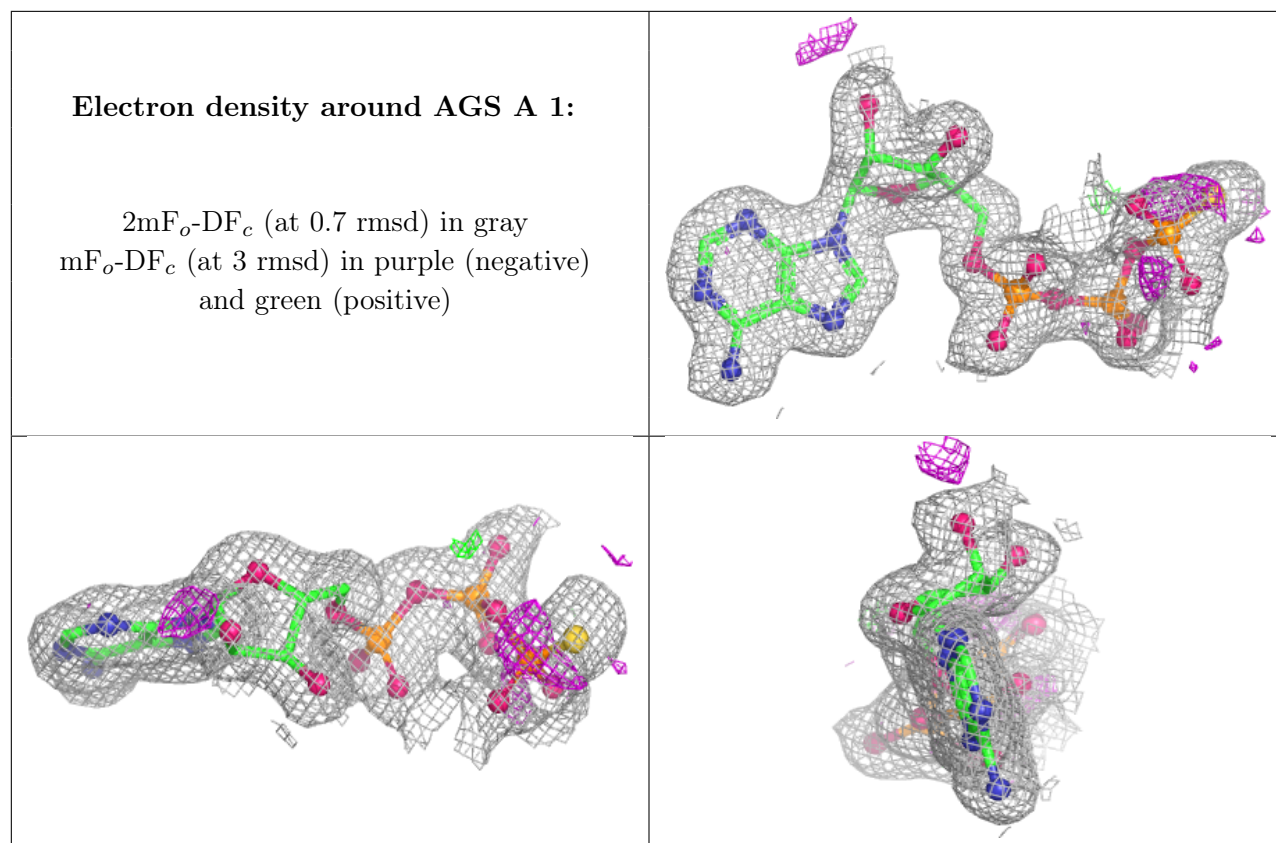
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	AGS	B	395	31/31	0.91	0.09	27,37,60,69	0
2	MG	A	393	1/1	0.95	0.11	46,46,46,46	0
5	AGS	A	1	31/31	0.97	0.07	15,22,64,71	0
2	MG	B	394	1/1	0.97	0.06	39,39,39,39	0
2	MG	B	393	1/1	0.98	0.07	40,40,40,40	0
4	CL	A	396	1/1	0.98	0.05	28,28,28,28	0
6	MPO	A	397	13/13	0.98	0.06	18,23,26,33	0
2	MG	A	394	1/1	0.99	0.10	30,30,30,30	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 AGS B 395:

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.