



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 1H74 / pdb_00001h74
Title : CRYSTAL STRUCTURE OF HOMOSERINE KINASE COMPLEXED WITH ILE
Authors : Krishna, S.S.; Zhou, T.; Daugherty, M.; Osterman, A.L.; Zhang, H.
Deposited on : 2001-07-02
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

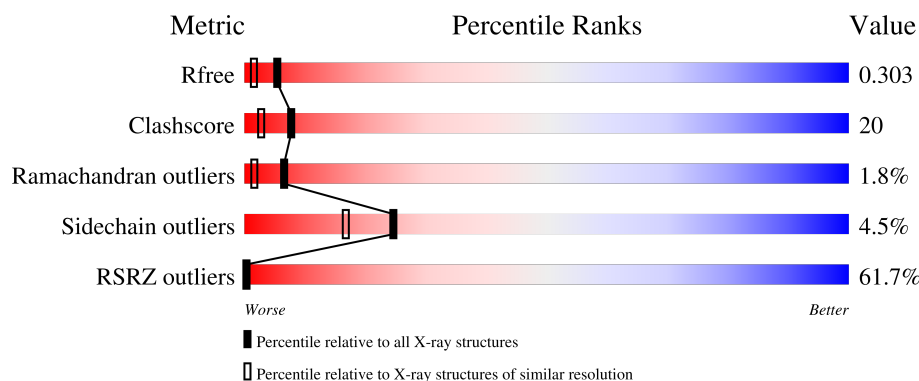
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	296	49% 70% 26% .
1	B	296	83% 58% 34% 7%
1	C	296	51% 77% 21% .
1	D	296	64% 73% 23% .

2 Entry composition [i](#)

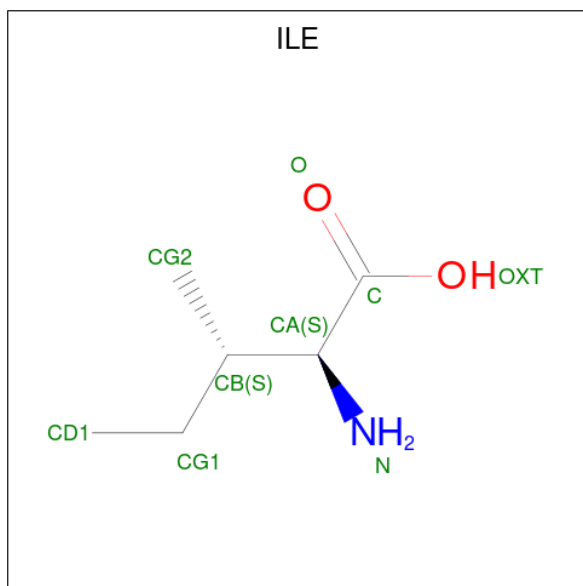
There are 6 unique types of molecules in this entry. The entry contains 9718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HOMOSERINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	4	0
			2293	1472	370	442	9			
1	B	296	Total	C	N	O	S	0	2	0
			2281	1466	368	438	9			
1	C	296	Total	C	N	O	S	0	1	0
			2275	1463	367	436	9			
1	D	296	Total	C	N	O	S	0	1	0
			2275	1463	367	436	9			

- Molecule 2 is ISOLEUCINE (CCD ID: ILE) (formula: C₆H₁₃NO₂).



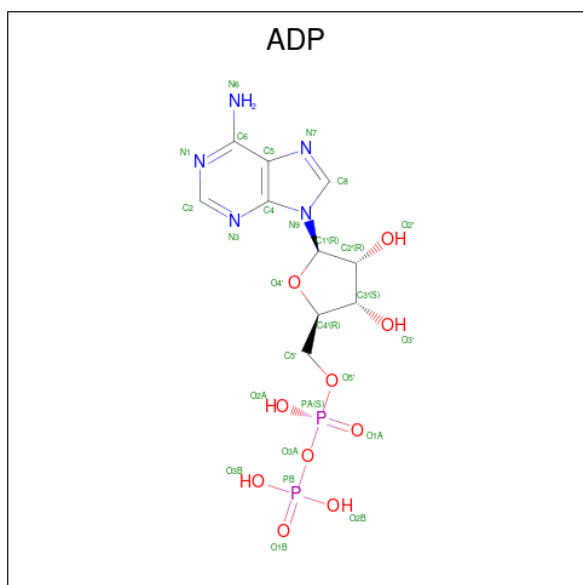
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		

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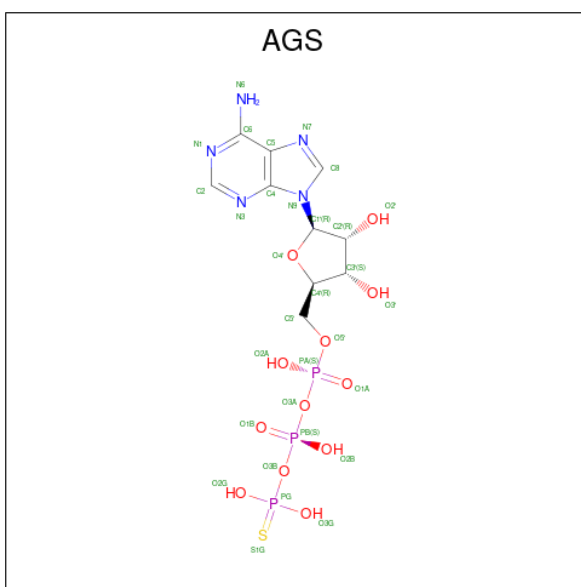
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			9	6	1	2		
2	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

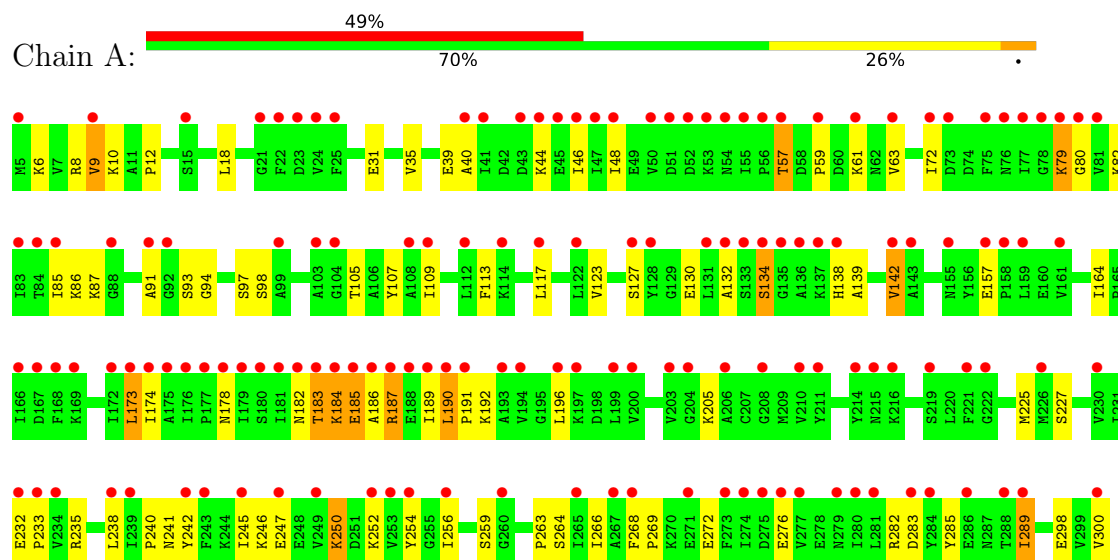
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	105	Total O 105 105	0	0
6	B	73	Total O 73 73	0	0
6	C	157	Total O 157 157	0	0
6	D	106	Total O 106 106	0	0

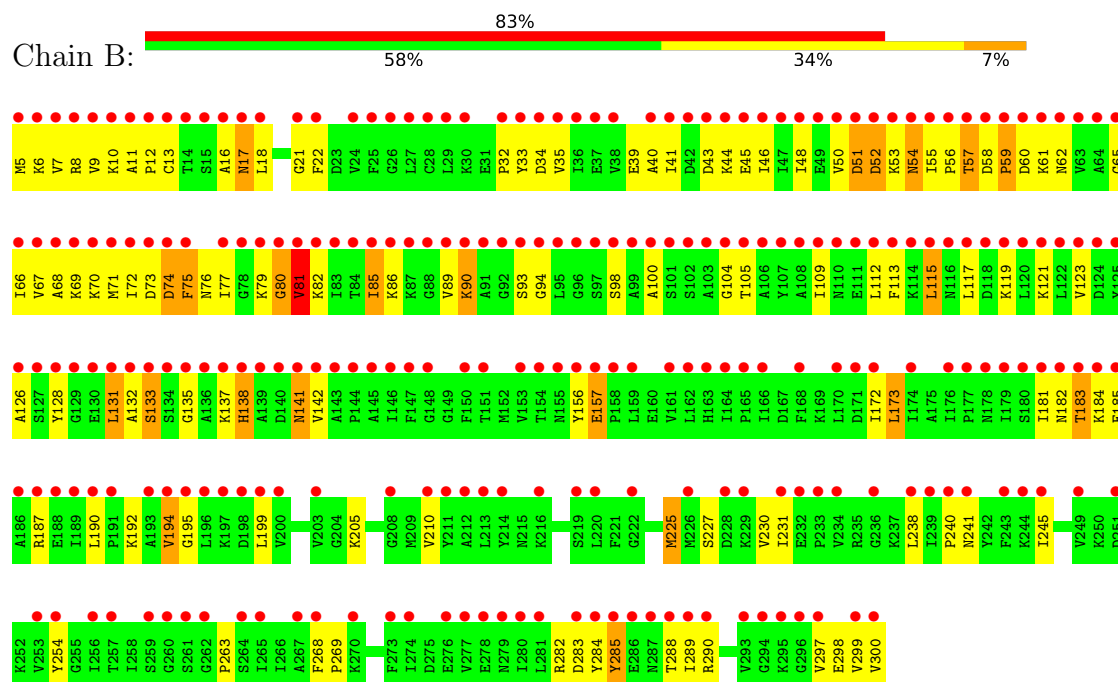
3 Residue-property plots

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: HOMOSERINE KINASE



• Molecule 1: HOMOSERINE KINASE



Chain C:

51% 77% 21%

M5 K79 I172 K244

K6 G80 L173 K245

V7 R81 L174 K246

R8 K82 A175 E247

V9 T83 I176 E248

K10 P177 V249

A11 R85 K250

P12 K86 D251

C13 K87 S180

A16 K88 V253

G19 V89 Y254

F22 K90 A191

D23 G92 A194

V24 S93 A186

F25 S97 R187

K30 A100 E188

E31 S101 I189

P32 S102 A1000

Y33 A103 K192

D34 G104 A1030

V35 T105 A193

I36 A106 V194

E37 L112 G195

V38 F113 K197

E39 K114 D198

A40 L117 E272

I41 D118 K199

D42 K119 V200

D43 K119 V201

K44 A126 N202

E45 I260 E277

I46 L131 L278

I47 L131 V203

I48 A132 G204

E49 S133 K218

V50 S133 K219

I289 G221

D51 G222 K220

D52 A136 K223

K53 A137 S227

N54 H138 D228

I55 N141 K229

P56 N141 V230

T57 I146 I231

D58 T151 E232

P59 T151 P233

I66 P158 K235

A68 L159 G236

A68 E160 K237

I72 V161 K237

F75 D167 L238

N76 F168 L239

T77 K169 K241

C79 K169 K242

V291 V300

Chain D:

64% 73% 23%

Label	Color
M5	Red
K6	Red
M70	Red
V7	Red
R8	Red
V9	Red
K10	Red
P11	Red
P12	Red
C13	Red
T14	Red
S15	Red
A16	Red
N17	Red
L18	Red
F22	Red
G26	Red
L27	Red
C28	Red
L29	Red
K30	Red
F31	Red
P32	Red
Y33	Red
D34	Red
V35	Red
I36	Red
F37	Red
V38	Red
E39	Red
A40	Red
I41	Red
D42	Red
A43	Red
K44	Red
E45	Red
I46	Red
I47	Red
I48	Red
F49	Red
V50	Red
D51	Red
D52	Red
K53	Red
N54	Red
I55	Red
P56	Red
T57	Red
D58	Red
P59	Red
D60	Red
K61	Red
N62	Red
V63	Red
A64	Red
G65	Red
I66	Red
G67	Red
A68	Red
K69	Red
M70	Red
M71	Red
I72	Red
D73	Red
D74	Red
F75	Red
M76	Red
I77	Red
G78	Red
K79	Red
G80	Red
V81	Red
K82	Red
I83	Red
T84	Red
I85	Red
K86	Red
K87	Red
G88	Red
V89	Red
K90	Red
A91	Red
G92	Red
S93	Red
S98	Red
A99	Red
A100	Red
S101	Red
S102	Red
A103	Red
G104	Red
T105	Red
A106	Red
Y107	Red
A108	Red
I109	Red
M110	Red
E111	Red
L112	Red
F113	Red
A114	Red
M116	Red
L117	Red
D118	Red
K119	Red
L120	Red
K121	Red
L122	Red
V123	Red
D124	Red
Y125	Red
A126	Red
S127	Red
Y128	Red
G129	Red
I130	Red
F131	Red
L132	Red
A132	Red
S133	Red
S134	Red
G135	Red
A136	Red
K137	Red
H138	Red
A139	Red
D140	Red
N141	Red
V142	Red
A143	Red
P144	Red
A145	Red
S227	Red
D228	Red
K229	Red
V230	Red
I231	Red
V234	Red
G235	Red
G236	Red
K237	Red
L238	Red
L239	Red
E157	Red
P158	Red
V161	Red
L162	Red
I166	Red
D167	Red
F168	Red
K169	Red
L173	Red
I174	Red
A175	Red
I176	Red
P177	Red
N178	Red
I179	Red
S180	Red
L181	Red
N182	Red
T183	Red
K184	Red
E185	Red
A186	Red
R187	Red
D275	Red
E188	Red
I189	Red
L190	Red
P191	Red
K192	Red
I193	Red
V194	Red
G195	Red
L196	Red
K197	Red
A212	Red
L213	Red
Y214	Red
K218	Red
G222	Red
R223	Red
Y224	Red
M225	Red
M226	Red
S227	Red
D228	Red
K229	Red
V230	Red
I231	Red
V234	Red
G235	Red
G236	Red
K237	Red
L238	Red
L239	Red
Y242	Red
F243	Red
K244	Red
I245	Red
V249	Red
K250	Red
D251	Red
K252	Red
V253	Red
Y254	Red
G255	Red
S261	Red
G262	Red
P263	Red
A267	Red
K270	Red

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.99Å 128.72Å 109.42Å 90.00° 105.57° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.90) 99.5 (50.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.238 0.283 , 0.303	Depositor DCC
R_{free} test set	6521 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9718	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: ADP, AGS, MG

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	0.79	1/2330 (0.0%)	1.12	11/3144 (0.3%)
1	B	0.67	1/2318 (0.0%)	1.04	10/3128 (0.3%)
1	C	0.90	1/2312 (0.0%)	1.11	15/3120 (0.5%)
1	D	0.81	0/2312	1.05	9/3120 (0.3%)
All	All	0.80	3/9272 (0.0%)	1.08	45/12512 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	MET	SD-CE	-10.22	1.54	1.79
1	C	126	ALA	CA-CB	6.44	1.63	1.53
1	A	142	VAL	CA-CB	5.11	1.61	1.54

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	GLU	N-CA-C	-8.47	102.05	111.28
1	C	80	GLY	N-CA-C	-7.53	102.42	112.81
1	C	72	ILE	N-CA-C	-6.95	103.75	110.42
1	A	87	LYS	N-CA-C	6.72	120.04	109.96
1	A	80	GLY	N-CA-C	-6.63	97.46	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	128	TYR	Sidechain

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	2293	0	2355	70	0
1	B	2281	0	2347	161	1
1	C	2275	0	2343	56	1
1	D	2275	0	2343	83	0
2	A	9	0	10	2	0
2	B	9	0	10	4	0
2	C	9	0	10	5	0
2	D	9	0	10	5	0
3	A	27	0	12	3	0
3	C	27	0	12	2	0
4	B	31	0	12	3	0
4	D	31	0	12	3	0
5	B	1	0	0	0	0
6	A	105	0	0	19	0
6	B	73	0	0	31	1
6	C	157	0	0	26	1
6	D	106	0	0	39	0
All	All	9718	0	9476	375	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 20.

The worst 5 of 375 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:46:ILE:HA	6:B:2011:HOH:O	1.48	1.12
1:C:169:LYS:HD2	6:C:2097:HOH:O	1.54	1.06
1:B:288:THR:HB	6:B:2067:HOH:O	1.55	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASN:HD21	2:B:500:ILE:HD13	1.19	1.04
1:C:246:LYS:HB2	6:C:2129:HOH:O	1.58	1.03

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)
6:B:2069:HOH:O	6:C:2127:HOH:O[2_747]	1.90	0.30
1:B:283:ASP:O	1:C:237:LYS:NZ[2_747]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/296 (101%)	283 (95%)	9 (3%)	6 (2%)	6	1
1	B	296/296 (100%)	252 (85%)	31 (10%)	13 (4%)	2	0
1	C	295/296 (100%)	287 (97%)	8 (3%)	0	100	100
1	D	295/296 (100%)	279 (95%)	14 (5%)	2 (1%)	18	10
All	All	1184/1184 (100%)	1101 (93%)	62 (5%)	21 (2%)	6	1

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	LEU
1	B	133	SER
1	B	138	HIS
1	A	183	THR
1	B	44	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/248 (102%)	236 (94%)	16 (6%)	16	8
1	B	250/248 (101%)	241 (96%)	9 (4%)	31	23
1	C	249/248 (100%)	242 (97%)	7 (3%)	38	32
1	D	249/248 (100%)	236 (95%)	13 (5%)	21	13
All	All	1000/992 (101%)	955 (96%)	45 (4%)	24	17

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	117	LEU
1	D	117	LEU
1	C	173	LEU
1	D	53	LYS
1	D	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	287	ASN
1	D	138	HIS
1	C	54	ASN
1	B	163	HIS
1	C	141	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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	400	-	28,29,29	1.23	2 (7%)	43,45,45	1.31	6 (13%)
4	AGS	B	400	5	32,33,33	2.00	6 (18%)	45,52,52	1.13	3 (6%)
2	ILE	B	500	-	8,8,8	0.76	0	9,10,10	0.73	0
2	ILE	D	500	-	8,8,8	0.77	0	9,10,10	0.72	0
2	ILE	A	500	-	8,8,8	0.98	0	9,10,10	0.80	0
4	AGS	D	400	-	32,33,33	1.51	6 (18%)	45,52,52	1.09	3 (6%)
3	ADP	A	400	-	28,29,29	1.42	5 (17%)	43,45,45	1.45	5 (11%)
2	ILE	C	500	-	8,8,8	0.88	0	9,10,10	0.93	0

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	ADP	C	400	-	-	6/16/32/32	0/3/3/3
4	AGS	B	400	5	-	5/21/38/38	0/3/3/3
2	ILE	B	500	-	-	0/10/10/10	-
2	ILE	D	500	-	-	0/10/10/10	-
2	ILE	A	500	-	-	0/10/10/10	-
4	AGS	D	400	-	-	4/21/38/38	0/3/3/3
3	ADP	A	400	-	-	5/16/32/32	0/3/3/3
2	ILE	C	500	-	-	7/10/10/10	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	AGS	PB-O3B	-7.44	1.51	1.59
4	B	400	AGS	PA-O3A	4.78	1.64	1.59
3	C	400	ADP	C4-N3	4.26	1.42	1.34
4	D	400	AGS	PG-S1G	4.13	1.99	1.90
3	A	400	ADP	C4-N3	3.63	1.41	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ADP	C4-N9-C1'	4.29	136.67	126.63
4	B	400	AGS	C4-N9-C1'	3.82	135.56	126.63
3	A	400	ADP	O4'-C1'-N9	3.78	115.35	108.09
3	A	400	ADP	C1'-N9-C8	-3.77	118.73	127.09
4	D	400	AGS	C4-N9-C1'	3.70	135.28	126.63

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	ILE	N-CA-CB-CG1
2	C	500	ILE	N-CA-CB-CG2
2	C	500	ILE	C-CA-CB-CG1
2	C	500	ILE	C-CA-CB-CG2
3	A	400	ADP	PA-O3A-PB-O2B

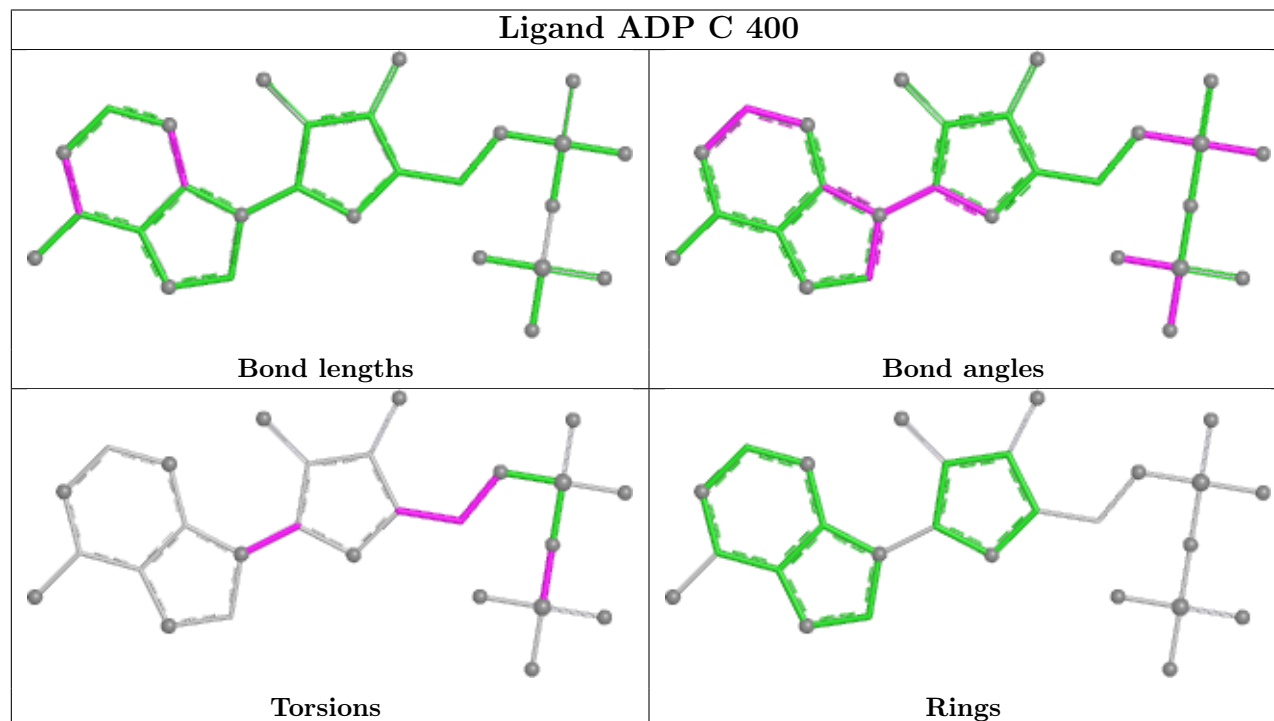
There are no ring outliers.

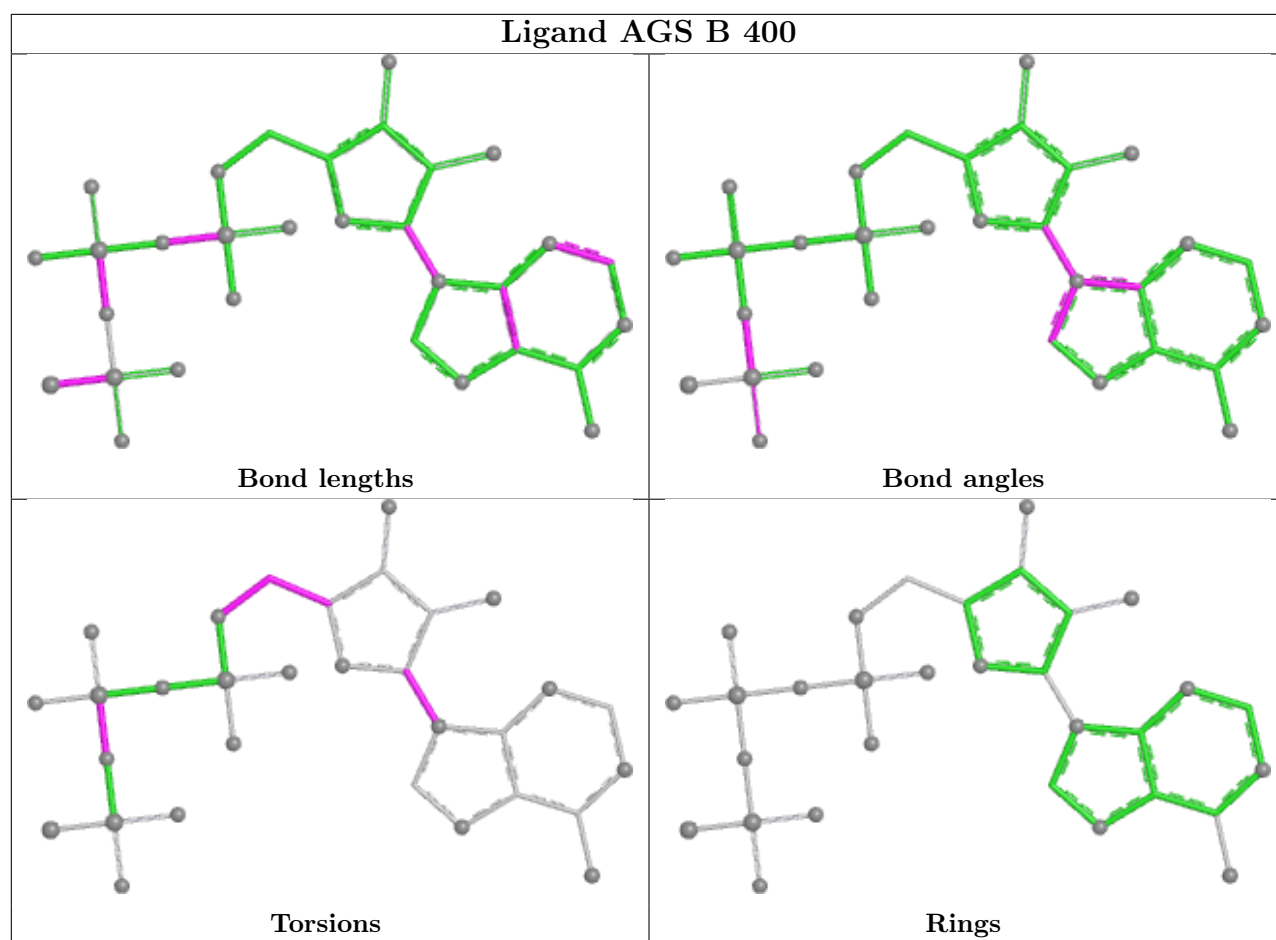
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	400	ADP	2	0
4	B	400	AGS	3	0
2	B	500	ILE	4	0
2	D	500	ILE	5	0
2	A	500	ILE	2	0
4	D	400	AGS	3	0
3	A	400	ADP	3	0
2	C	500	ILE	5	0

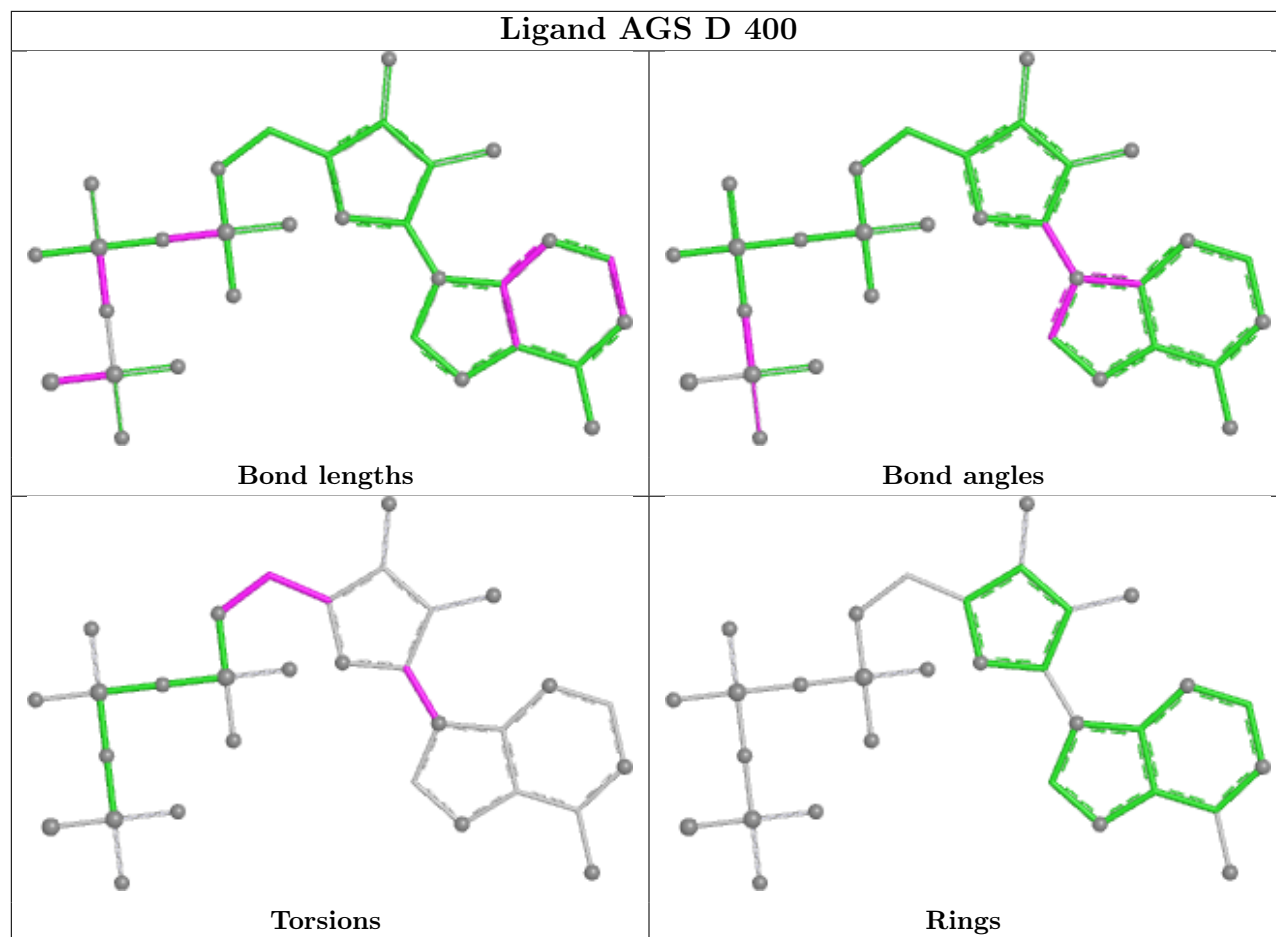
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

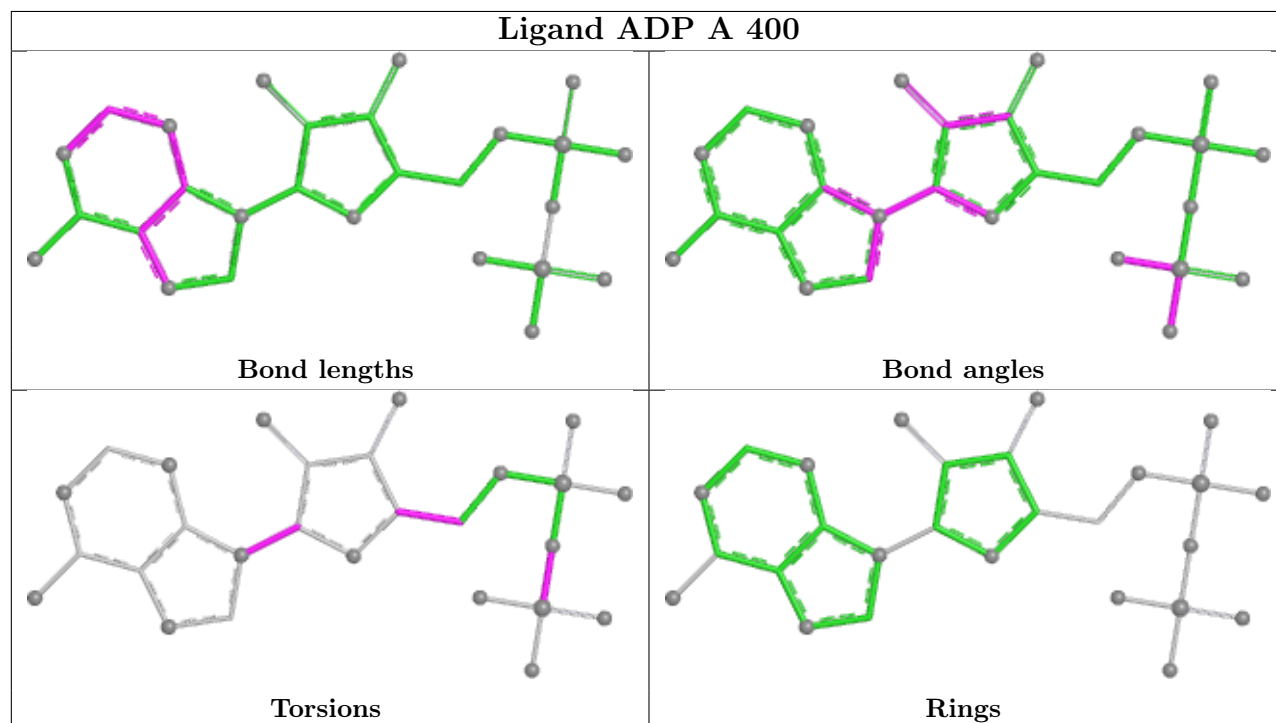




Ligand AGS D 400



Ligand ADP A 400



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/296 (100%)	2.21	145 (48%) 0 0	16, 44, 71, 84	4 (1%)
1	B	296/296 (100%)	3.47	246 (83%) 0 0	20, 56, 109, 115	2 (0%)
1	C	296/296 (100%)	2.25	151 (51%) 0 0	14, 39, 64, 80	1 (0%)
1	D	296/296 (100%)	2.69	189 (63%) 0 0	15, 43, 77, 89	1 (0%)
All	All	1184/1184 (100%)	2.65	731 (61%) 0 0	14, 45, 97, 115	8 (0%)

The worst 5 of 731 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	ALA	12.6
1	B	47	ILE	9.8
1	B	132	ALA	8.7
1	D	41	ILE	8.4
1	B	72	ILE	8.3

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](#)

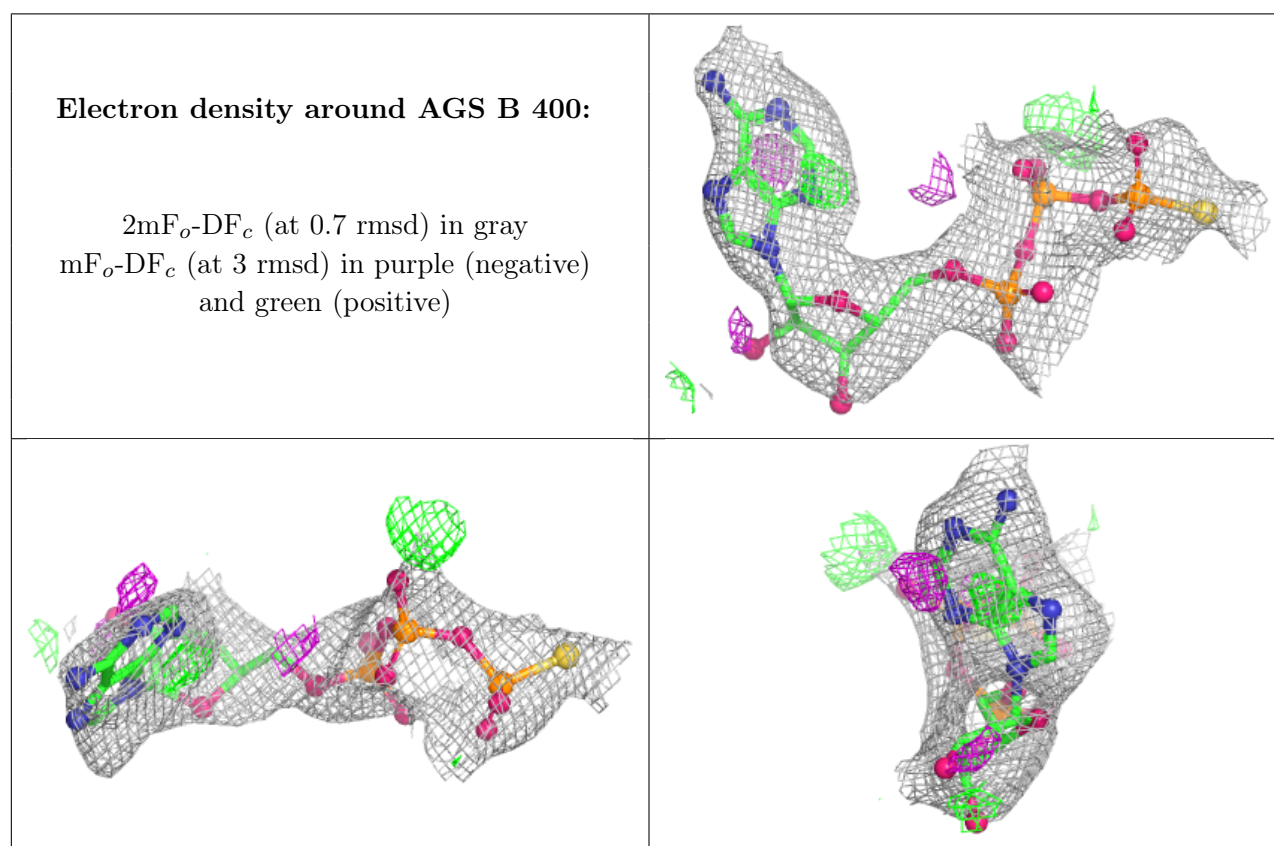
There are no oligosaccharides in this entry.

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.

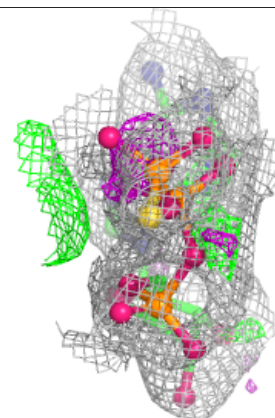
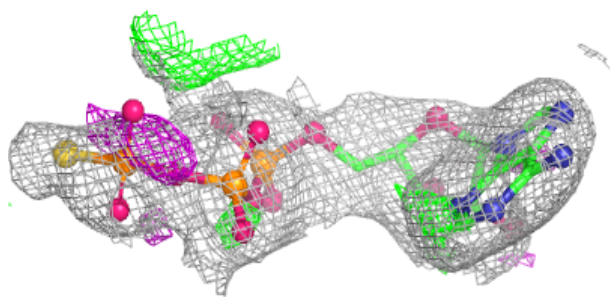
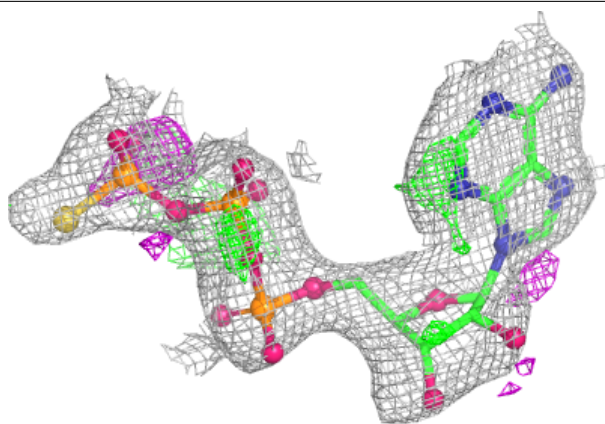
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ILE	B	500	9/9	0.63	0.30	78,80,81,83	0
2	ILE	C	500	9/9	0.63	0.27	56,59,61,61	0
5	MG	B	600	1/1	0.65	0.26	87,87,87,87	0
4	AGS	B	400	31/31	0.68	0.21	72,83,104,105	0
2	ILE	D	500	9/9	0.69	0.23	69,71,71,71	0
2	ILE	A	500	9/9	0.73	0.25	63,65,67,69	0
4	AGS	D	400	31/31	0.74	0.20	55,69,91,92	0
3	ADP	A	400	27/27	0.86	0.15	42,62,76,77	0
3	ADP	C	400	27/27	0.87	0.16	34,49,67,68	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.



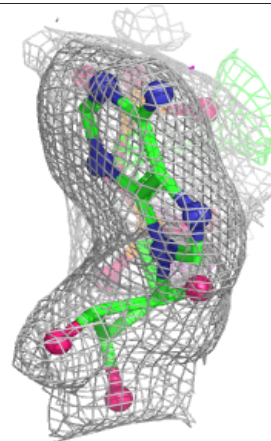
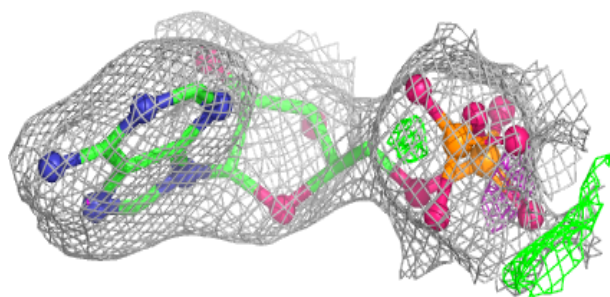
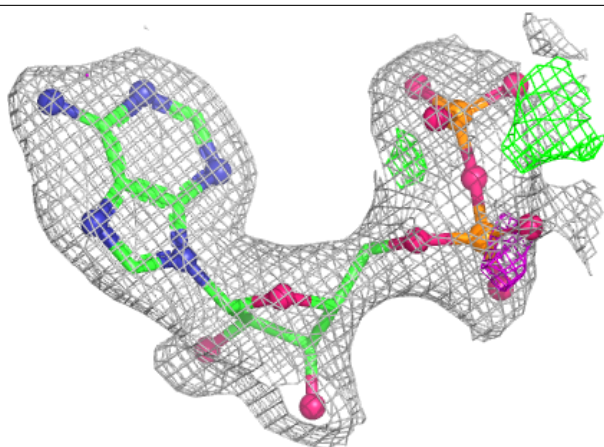
Electron density around AGS D 400:

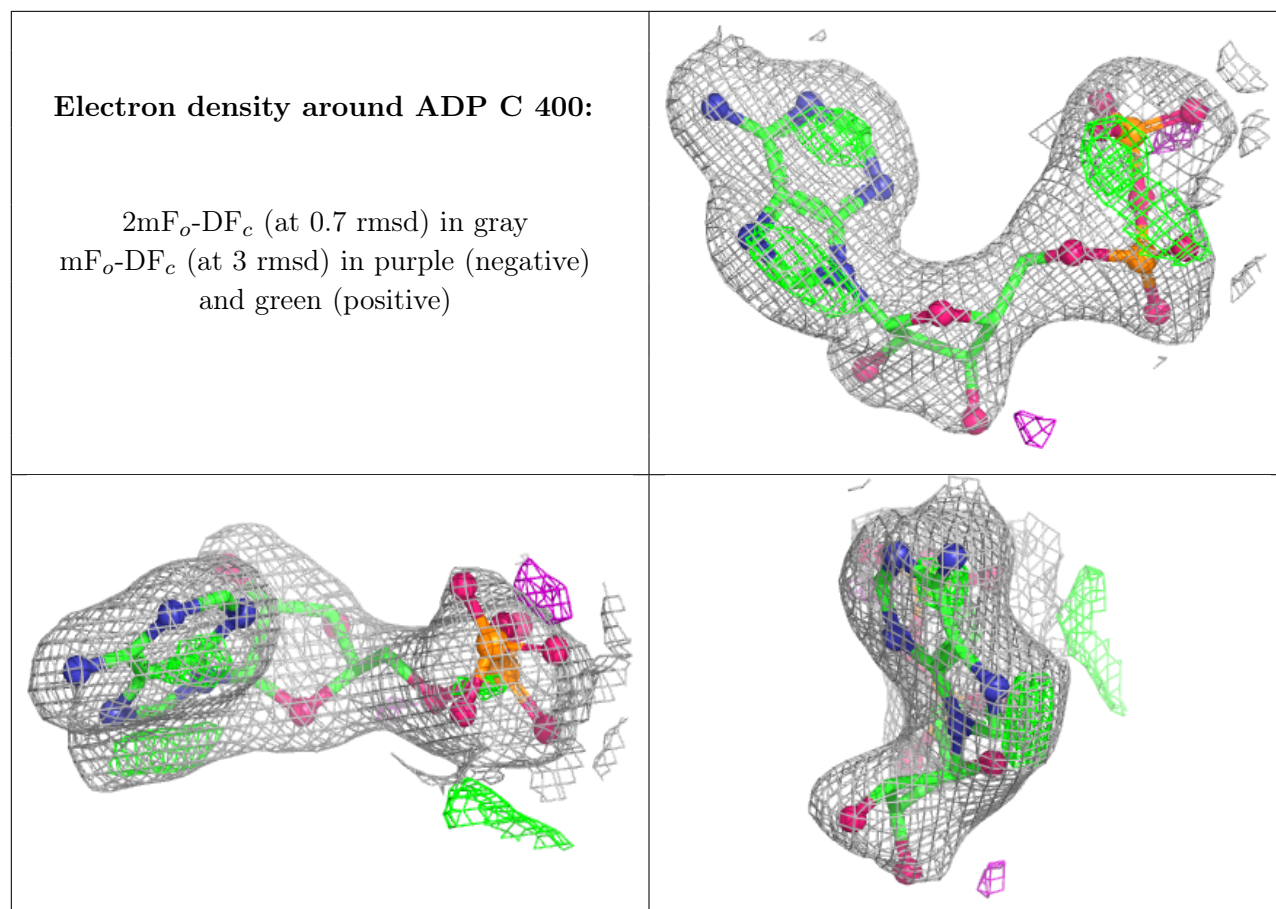
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 400:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.