



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 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 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

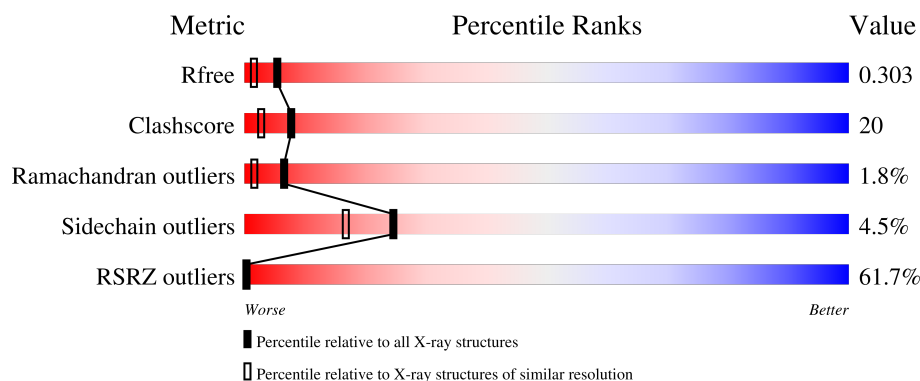
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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](#)

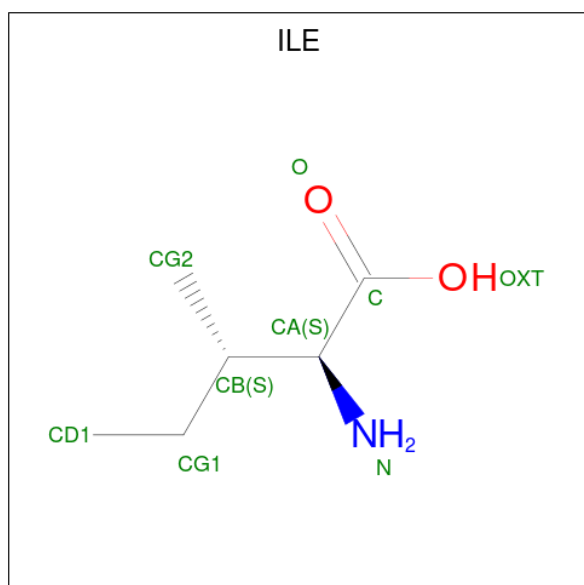
There are 6 unique types of molecules in this entry. The entry contains 9718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).



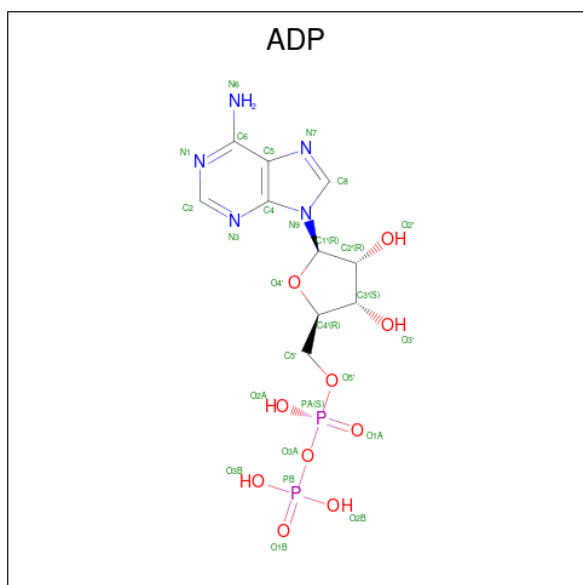
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		

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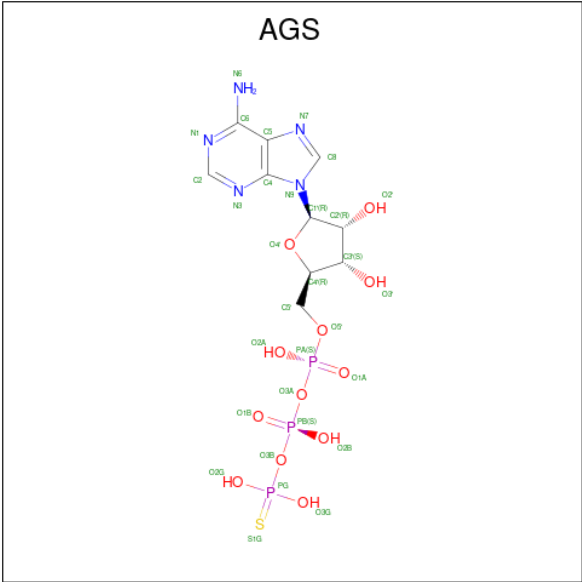
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			9	6	1	2		
2	D	1	Total	C	N	O	0	0
			9	6	1	2		

- 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	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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

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

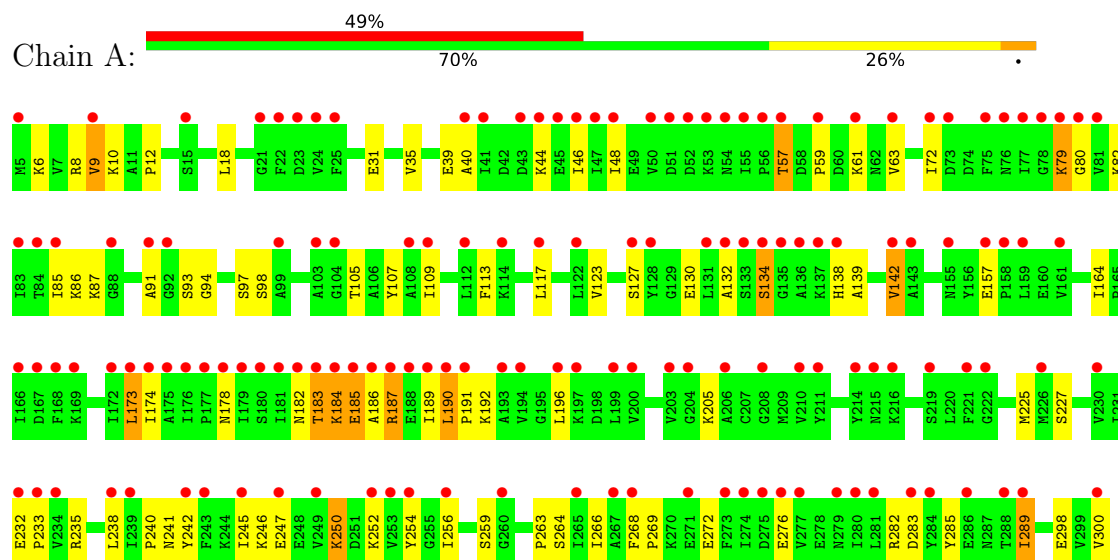
- Molecule 6 is water.

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

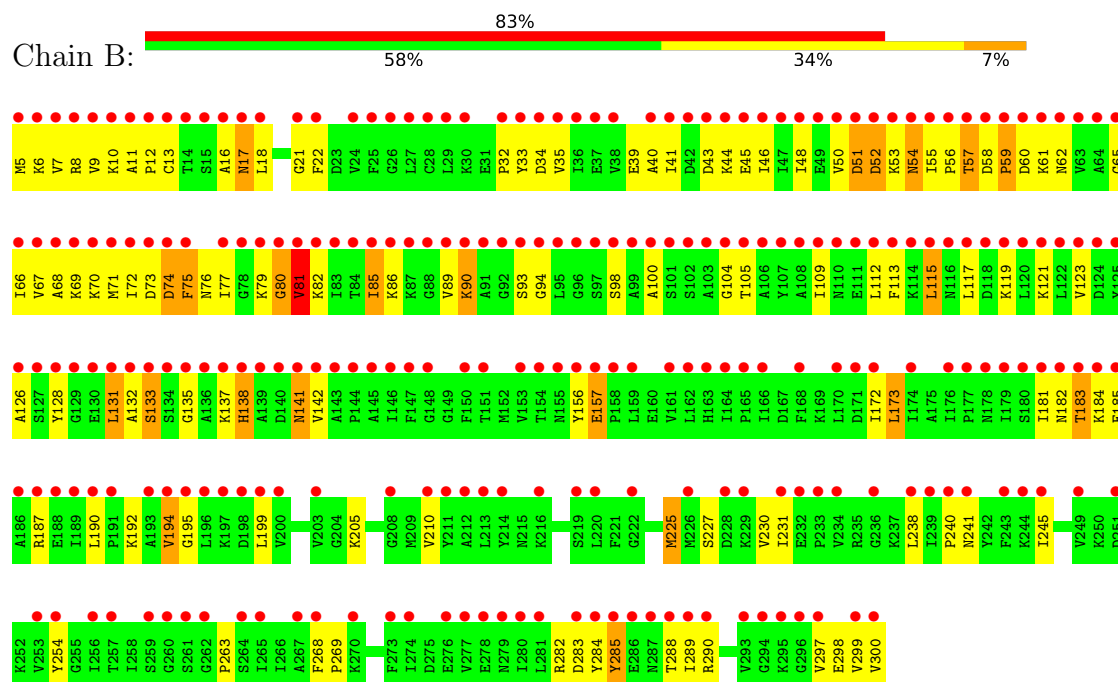
3 Residue-property plots

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.

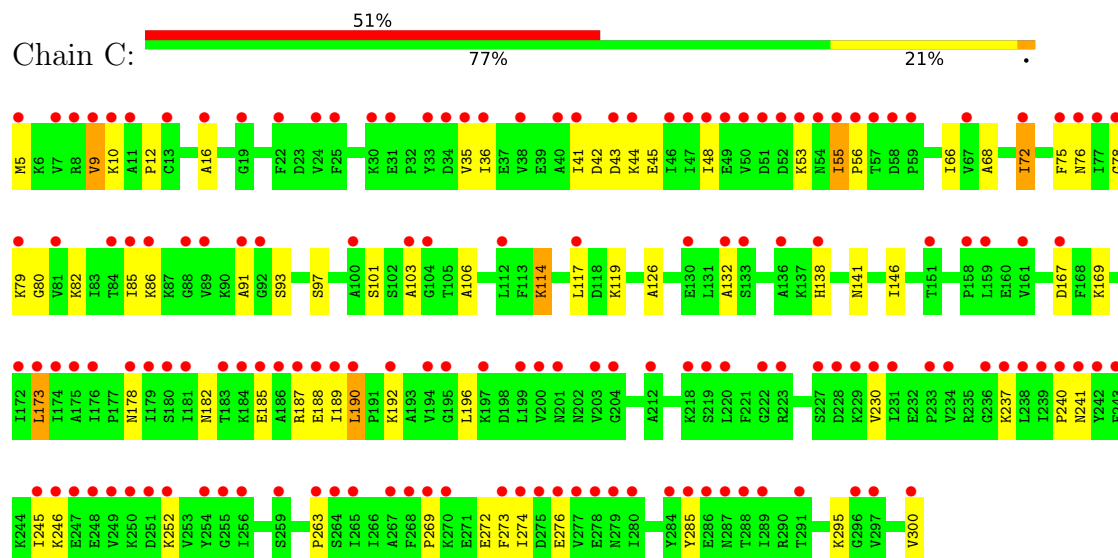
• Molecule 1: HOMOSERINE KINASE



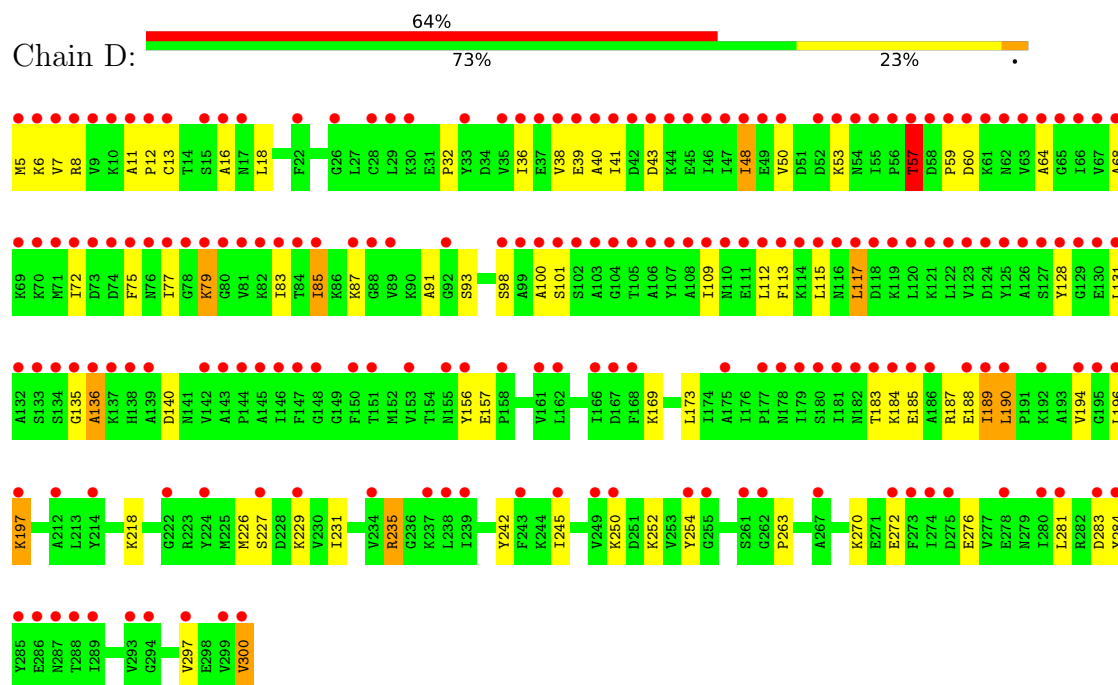
• Molecule 1: HOMOSERINE KINASE



• Molecule 1: HOMOSERINE KINASE



• Molecule 1: HOMOSERINE KINASE



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 [i](#)

5.1 Standard geometry [i](#)

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

All (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
1	B	199	LEU	N-CA-C	-6.55	104.22	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	ASP	N-CA-C	6.50	120.47	112.54
1	C	12	PRO	N-CA-C	6.42	122.40	111.68
1	B	285	TYR	N-CA-C	-6.42	99.99	109.81
1	D	12	PRO	N-CA-C	6.39	121.53	111.38
1	B	85	ILE	N-CA-C	6.38	117.06	107.75
1	A	184	LYS	N-CA-C	-6.37	105.16	113.12
1	D	85	ILE	N-CA-C	6.36	117.02	107.80
1	B	81	VAL	N-CA-C	6.35	117.50	108.42
1	B	254	TYR	N-CA-C	-6.35	104.45	111.82
1	C	192	LYS	N-CA-C	-6.31	105.72	113.41
1	A	254	TYR	N-CA-C	-6.11	104.53	112.23
1	B	12	PRO	N-CA-C	6.07	121.03	111.38
1	C	230	VAL	N-CA-C	6.04	117.06	111.45
1	C	48	ILE	N-CA-C	5.96	116.69	108.12
1	B	34	ASP	N-CA-C	-5.94	102.53	110.55
1	C	82	LYS	N-CA-C	-5.94	99.51	109.07
1	A	12	PRO	N-CA-C	5.74	120.30	111.57
1	C	85	ILE	N-CA-C	5.74	116.15	108.11
1	A	164	ILE	CA-C-N	-5.60	114.19	119.85
1	A	164	ILE	C-N-CA	-5.60	114.19	119.85
1	A	85	ILE	N-CA-C	5.56	115.89	108.11
1	C	274	ILE	N-CA-C	5.51	116.15	110.36
1	D	57	THR	N-CA-C	-5.50	106.56	113.72
1	C	55	ILE	CA-C-N	5.49	125.49	119.89
1	C	55	ILE	C-N-CA	5.49	125.49	119.89
1	C	9	VAL	N-CA-CB	-5.43	102.55	111.45
1	C	78	GLY	N-CA-C	5.42	119.70	112.77
1	D	79	LYS	N-CA-C	5.34	118.33	109.94
1	A	72	ILE	N-CA-C	-5.24	105.27	110.62
1	B	210	VAL	N-CA-C	-5.24	105.61	110.53
1	D	48	ILE	N-CA-C	5.24	115.44	108.11
1	D	87	LYS	N-CA-C	5.18	117.95	110.28
1	C	35	VAL	N-CA-C	-5.10	100.30	107.75
1	B	141	ASN	N-CA-C	-5.10	107.13	113.55
1	C	42	ASP	N-CA-C	5.08	116.82	111.28
1	B	80	GLY	N-CA-C	-5.07	103.56	111.12
1	D	254	TYR	N-CA-C	-5.06	105.85	112.23
1	D	270	LYS	N-CA-C	-5.06	103.36	110.50
1	A	61	LYS	N-CA-C	-5.03	107.21	113.55

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.

All (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
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
1:C:106:ALA:HB3	6:C:2049:HOH:O	1.57	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ILE:HG23	6:C:2104:HOH:O	1.61	1.00
1:B:50:VAL:HG22	1:B:85:ILE:HB	1.45	0.99
1:D:245:ILE:HD11	1:D:281:LEU:HD23	1.42	0.97
1:B:173:LEU:HD13	6:B:2028:HOH:O	1.66	0.95
1:C:119:LYS:HE2	6:C:2066:HOH:O	1.66	0.95
1:D:189:ILE:HB	6:D:2059:HOH:O	1.67	0.95
1:B:13:CYS:HA	6:B:2014:HOH:O	1.63	0.94
1:D:109:ILE:HG13	6:D:2015:HOH:O	1.66	0.94
1:A:182:ASN:HB2	6:A:2067:HOH:O	1.66	0.94
1:A:174:ILE:HB	6:A:2097:HOH:O	1.69	0.93
1:D:72:ILE:HG23	1:D:77:ILE:HB	1.51	0.92
1:D:64:ALA:HB1	6:D:2014:HOH:O	1.69	0.92
1:C:103:ALA:HA	6:C:2049:HOH:O	1.70	0.91
1:C:141:ASN:HD21	2:C:500:ILE:HD11	1.34	0.91
1:B:79:LYS:HB3	6:B:2008:HOH:O	1.72	0.88
1:B:141:ASN:ND2	2:B:500:ILE:HD13	1.88	0.87
1:A:138:HIS:HB3	6:A:2041:HOH:O	1.74	0.87
1:A:184:LYS:HG3	6:A:2067:HOH:O	1.75	0.86
1:D:5:MET:HE3	1:D:5:MET:HA	1.58	0.84
1:B:141:ASN:HD21	2:B:500:ILE:CD1	1.90	0.83
1:D:187:ARG:HB2	6:D:2058:HOH:O	1.77	0.82
1:B:181:ILE:HG12	6:B:2052:HOH:O	1.78	0.82
1:D:50:VAL:HB	6:D:2011:HOH:O	1.80	0.82
1:D:250:LYS:HB3	6:D:2084:HOH:O	1.76	0.82
1:B:77:ILE:HD13	1:B:113:PHE:HD1	1.44	0.82
1:D:183:THR:HG21	6:D:2035:HOH:O	1.79	0.82
1:C:167:ASP:HB2	6:C:2114:HOH:O	1.81	0.81
1:C:141:ASN:HD21	2:C:500:ILE:CD1	1.94	0.80
1:C:182:ASN:HB3	1:C:185:GLU:CG	2.13	0.78
1:D:245:ILE:CD1	1:D:281:LEU:HD23	2.13	0.78
1:B:185:GLU:HA	6:B:2030:HOH:O	1.84	0.78
1:B:117:LEU:HD22	1:B:121:LYS:HG2	1.66	0.78
1:B:98:SER:HB2	6:B:2074:HOH:O	1.82	0.78
1:B:182:ASN:ND2	1:B:185:GLU:HG3	1.99	0.78
1:D:68:ALA:HA	6:D:2015:HOH:O	1.85	0.77
1:A:10:LYS:HG3	1:A:300:VAL:HG11	1.65	0.76
1:D:169:LYS:O	6:D:2053:HOH:O	2.03	0.76
1:B:9:VAL:HG23	1:B:298:GLU:C	2.10	0.76
1:C:53:LYS:HG2	6:C:2034:HOH:O	1.84	0.76
1:A:282:ARG:HA	1:A:285:TYR:O	1.83	0.76
1:D:235:ARG:HD3	6:D:2090:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:GLU:HB2	6:C:2104:HOH:O	1.85	0.76
1:A:252:LYS:HE2	1:A:276:GLU:OE1	1.86	0.76
1:D:187:ARG:HD2	6:D:2057:HOH:O	1.86	0.75
1:B:77:ILE:HD13	1:B:113:PHE:CD1	2.20	0.75
1:A:35:VAL:HB	1:A:86:LYS:HE3	1.66	0.74
1:D:72:ILE:HA	1:D:77:ILE:HD12	1.70	0.74
1:D:83:ILE:HD13	6:D:2014:HOH:O	1.86	0.74
1:A:18:LEU:HD22	1:A:225:MET:CE	2.17	0.74
1:B:6:LYS:HA	1:B:112:LEU:HD11	1.70	0.73
1:C:44:LYS:HE2	6:C:2040:HOH:O	1.87	0.73
1:B:94:GLY:HA2	4:B:400:AGS:S1G	2.29	0.73
1:A:238:LEU:HD23	6:A:2082:HOH:O	1.88	0.73
1:A:82:LYS:HG2	6:A:2023:HOH:O	1.89	0.73
1:A:246:LYS:HE3	6:A:2086:HOH:O	1.88	0.73
1:B:8:ARG:HH11	1:B:300:VAL:HG11	1.54	0.72
1:A:289:ILE:HG12	6:A:2097:HOH:O	1.90	0.72
1:B:6:LYS:HD3	1:B:39:GLU:HG2	1.72	0.71
1:B:35:VAL:HB	1:B:86:LYS:HB2	1.71	0.71
1:A:289:ILE:HG23	6:A:2097:HOH:O	1.91	0.71
1:A:187:ARG:HB2	6:A:2068:HOH:O	1.91	0.71
1:A:94:GLY:C	6:A:2026:HOH:O	2.33	0.71
1:C:187:ARG:HA	1:C:190:LEU:HD22	1.73	0.70
1:D:38:VAL:HB	6:D:2026:HOH:O	1.91	0.70
1:C:187:ARG:O	1:C:190:LEU:HB2	1.91	0.70
1:C:182:ASN:HB3	1:C:185:GLU:HG2	1.74	0.70
1:A:8:ARG:HD3	6:A:2013:HOH:O	1.90	0.70
1:B:56:PRO:O	1:B:62:ASN:HB2	1.92	0.70
1:A:183:THR:HG21	2:A:500:ILE:HD11	1.73	0.70
2:D:500:ILE:HG22	6:D:2040:HOH:O	1.90	0.70
1:A:94:GLY:O	6:A:2026:HOH:O	2.10	0.69
1:A:187:ARG:O	1:A:190:LEU:HB2	1.93	0.69
1:D:18:LEU:HD23	6:D:2089:HOH:O	1.91	0.69
1:B:282:ARG:O	1:B:285:TYR:O	2.10	0.69
1:C:91:ALA:HB1	3:C:400:ADP:H5'1	1.72	0.69
1:D:218:LYS:HD3	6:D:2053:HOH:O	1.93	0.69
1:B:9:VAL:HG23	1:B:298:GLU:O	1.92	0.68
1:C:178:ASN:HB2	6:C:2102:HOH:O	1.92	0.68
1:B:18:LEU:HD22	1:B:225:MET:CE	2.24	0.68
1:B:112:LEU:HD22	1:B:113:PHE:CD2	2.28	0.68
1:B:18:LEU:HD23	6:B:2004:HOH:O	1.93	0.68
1:B:187:ARG:O	1:B:190:LEU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLU:HG3	1:C:273:PHE:CD1	2.29	0.67
1:B:60:ASP:HA	1:B:69:LYS:NZ	2.10	0.67
1:B:225:MET:HE1	1:B:268:PHE:HE1	1.59	0.67
1:B:48:ILE:HD12	1:B:59:PRO:HA	1.77	0.67
1:B:60:ASP:HA	1:B:69:LYS:HZ2	1.59	0.67
4:B:400:AGS:S1G	6:B:2060:HOH:O	2.51	0.67
1:C:272:GLU:HG3	1:C:273:PHE:CE1	2.30	0.66
1:B:18:LEU:HD22	1:B:225:MET:HE2	1.77	0.66
1:B:41:ILE:HG21	1:B:82:LYS:HG3	1.78	0.65
1:D:252:LYS:HE2	1:D:276:GLU:OE1	1.96	0.65
1:D:112:LEU:HD22	6:D:2026:HOH:O	1.96	0.65
1:C:246:LYS:HD2	6:C:2129:HOH:O	1.96	0.65
1:C:68:ALA:O	1:C:72:ILE:HG12	1.98	0.63
1:B:184:LYS:O	1:B:187:ARG:HB2	1.99	0.63
1:B:238:LEU:HB3	6:B:2052:HOH:O	1.98	0.63
1:B:9:VAL:HG21	1:B:297:VAL:HG12	1.80	0.63
1:C:246:LYS:CD	6:C:2129:HOH:O	2.47	0.63
1:D:7:VAL:HG12	6:D:2026:HOH:O	1.98	0.63
1:A:79:LYS:HD2	1:A:113:PHE:HE2	1.63	0.63
1:C:10:LYS:HE3	1:C:300:VAL:HG21	1.81	0.62
1:B:39:GLU:HB2	1:B:82:LYS:HB2	1.81	0.62
1:B:98:SER:N	6:B:2074:HOH:O	2.31	0.62
1:B:185:GLU:C	1:B:187:ARG:H	2.07	0.62
1:B:187:ARG:NH2	2:B:500:ILE:HA	2.13	0.62
1:C:189:ILE:N	6:C:2104:HOH:O	2.32	0.62
1:D:91:ALA:HB1	4:D:400:AGS:H5'1	1.81	0.62
1:D:64:ALA:C	6:D:2014:HOH:O	2.44	0.61
1:B:7:VAL:HG23	6:B:2002:HOH:O	1.99	0.61
1:C:295:LYS:HE2	6:C:2095:HOH:O	2.00	0.61
1:B:72:ILE:HA	1:B:77:ILE:HD12	1.82	0.60
1:C:146:ILE:HD11	6:C:2049:HOH:O	2.00	0.60
1:C:246:LYS:HD3	6:C:2133:HOH:O	2.00	0.60
1:A:252:LYS:HE2	1:A:276:GLU:CD	2.27	0.60
1:D:250:LYS:HD3	6:D:2084:HOH:O	2.00	0.60
1:A:238:LEU:HA	6:A:2082:HOH:O	2.00	0.60
1:D:6:LYS:HD3	1:D:39:GLU:OE1	2.01	0.60
1:B:131:LEU:HD22	1:B:135:GLY:O	2.01	0.60
1:B:194:VAL:HG11	1:B:230:VAL:HG22	1.82	0.60
1:A:18:LEU:HD22	1:A:225:MET:HE1	1.83	0.60
1:A:91:ALA:HB1	3:A:400:ADP:H5'1	1.83	0.59
1:B:112:LEU:HD22	1:B:113:PHE:CE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:HD12	1:B:285:TYR:CE1	2.37	0.59
1:B:172:ILE:C	6:B:2028:HOH:O	2.45	0.59
1:B:7:VAL:HA	6:B:2002:HOH:O	2.03	0.59
1:B:59:PRO:HB3	6:B:2009:HOH:O	2.01	0.59
1:C:182:ASN:HB3	1:C:185:GLU:CD	2.28	0.59
1:B:299:VAL:HA	6:B:2072:HOH:O	2.03	0.58
1:D:112:LEU:HB2	6:D:2026:HOH:O	2.04	0.58
1:D:75:PHE:HZ	1:D:117:LEU:HD11	1.67	0.58
1:D:75:PHE:CZ	1:D:117:LEU:HD11	2.38	0.57
1:D:188:GLU:N	6:D:2058:HOH:O	2.37	0.57
1:A:18:LEU:HB3	1:A:225:MET:HE3	1.85	0.57
1:A:6:LYS:HB3	1:A:39:GLU:HG3	1.86	0.57
1:D:226:MET:HE1	6:D:2085:HOH:O	2.04	0.57
1:B:8:ARG:HB3	1:B:300:VAL:HG12	1.87	0.56
1:C:66:ILE:HD13	1:C:132:ALA:CB	2.34	0.56
1:C:252:LYS:HE2	1:C:276:GLU:OE1	2.04	0.56
1:A:187:ARG:HA	1:A:190:LEU:HD22	1.88	0.56
1:B:46:ILE:HG21	6:B:2009:HOH:O	2.05	0.56
1:D:284:TYR:HB3	6:D:2097:HOH:O	2.06	0.56
1:A:272:GLU:HG2	6:A:2093:HOH:O	2.06	0.56
1:B:89:VAL:HG22	1:B:90:LYS:HG2	1.87	0.56
1:A:182:ASN:CB	6:A:2067:HOH:O	2.40	0.56
1:A:264:SER:HB2	6:A:2026:HOH:O	2.05	0.55
1:A:40:ALA:HB1	1:A:79:LYS:HD3	1.87	0.55
1:D:284:TYR:CB	6:D:2097:HOH:O	2.55	0.55
1:B:6:LYS:HD3	1:B:39:GLU:CG	2.37	0.55
1:C:173:LEU:HD22	1:C:269:PRO:HG3	1.89	0.55
1:C:93:SER:HA	1:C:263:PRO:HD2	1.89	0.55
1:B:52:ASP:OD2	1:B:54:ASN:HB2	2.08	0.54
1:B:66:ILE:O	1:B:69:LYS:HG2	2.07	0.54
1:B:113:PHE:O	1:B:115:LEU:HD12	2.07	0.54
1:D:72:ILE:HA	1:D:77:ILE:CD1	2.37	0.54
1:D:50:VAL:HG22	1:D:85:ILE:HD12	1.89	0.54
1:B:52:ASP:C	1:B:54:ASN:H	2.15	0.54
1:A:259[A]:SER:OG	1:A:266:ILE:HB	2.07	0.54
1:B:48:ILE:HD11	1:B:65:GLY:HA3	1.90	0.54
1:B:123:VAL:HG13	1:B:142:VAL:HG12	1.90	0.54
1:C:272:GLU:HG2	6:C:2140:HOH:O	2.08	0.53
1:D:185:GLU:O	1:D:189:ILE:HG13	2.08	0.53
1:B:173:LEU:HD22	1:B:269:PRO:HG3	1.90	0.53
1:B:8:ARG:NH1	1:B:300:VAL:HG21	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLU:HG2	6:B:2030:HOH:O	2.08	0.53
1:D:187:ARG:O	1:D:190:LEU:HB2	2.08	0.53
1:B:69:LYS:HG3	1:B:70:LYS:H	1.74	0.53
1:B:112:LEU:HD22	1:B:113:PHE:HD2	1.74	0.53
1:D:252:LYS:HE2	1:D:276:GLU:CD	2.33	0.53
1:D:75:PHE:CD2	1:D:115:LEU:HD22	2.43	0.53
1:C:114:LYS:HD2	1:C:114:LYS:N	2.24	0.52
1:A:205:LYS:HG3	1:A:227[B]:SER:OG	2.08	0.52
1:B:69:LYS:HG3	1:B:70:LYS:N	2.24	0.52
1:B:81:VAL:N	6:B:2011:HOH:O	2.12	0.52
1:A:10:LYS:CG	1:A:300:VAL:HG11	2.38	0.52
1:C:86:LYS:HE2	6:C:2042:HOH:O	2.09	0.52
1:B:5:MET:HE3	1:B:40:ALA:HB3	1.92	0.52
1:B:55:ILE:HD12	1:B:55:ILE:N	2.25	0.52
1:C:41:ILE:O	1:C:79:LYS:HB3	2.09	0.52
1:C:97:SER:HB3	3:C:400:ADP:O1B	2.10	0.52
1:A:105:THR:O	1:A:109:ILE:HG12	2.10	0.52
1:B:16:ALA:O	1:B:17:ASN:HB2	2.10	0.51
1:A:40:ALA:HB1	1:A:79:LYS:CD	2.40	0.51
1:B:41:ILE:CG2	1:B:82:LYS:HG3	2.40	0.51
1:B:8:ARG:HB3	1:B:300:VAL:CG1	2.40	0.51
1:B:57:THR:O	1:B:59:PRO:HD3	2.09	0.51
1:B:282:ARG:HG3	6:B:2067:HOH:O	2.09	0.51
1:B:126:ALA:HB3	1:B:142:VAL:HG11	1.92	0.51
1:D:5:MET:HA	1:D:5:MET:CE	2.36	0.51
1:A:178:ASN:O	1:A:178:ASN:ND2	2.43	0.51
1:D:197:LYS:HB2	1:D:197:LYS:NZ	2.25	0.51
1:B:131:LEU:C	1:B:131:LEU:HD13	2.36	0.50
1:A:173:LEU:HD22	1:A:269:PRO:HG3	1.92	0.50
1:B:75:PHE:HZ	1:B:117:LEU:HD21	1.75	0.50
1:B:77:ILE:O	1:B:79:LYS:HG3	2.11	0.50
1:B:32:PRO:HG3	1:B:289:ILE:HD13	1.92	0.50
1:B:181:ILE:CG1	6:B:2052:HOH:O	2.49	0.50
1:A:242:TYR:CZ	1:A:246:LYS:HD2	2.47	0.50
1:B:48:ILE:CD1	1:B:59:PRO:HA	2.40	0.50
1:A:241:ASN:O	1:A:245:ILE:HG13	2.12	0.50
1:B:9:VAL:CG2	1:B:297:VAL:HG12	2.42	0.50
1:A:189:ILE:HD11	1:A:235:ARG:HG2	1.94	0.50
1:A:79:LYS:HD2	1:A:113:PHE:CE2	2.45	0.50
1:A:97:SER:HB3	3:A:400:ADP:O1B	2.11	0.49
1:A:192:LYS:HD2	6:A:2069:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:HG2	1:A:256:ILE:HG23	1.94	0.49
1:C:138:HIS:HB3	6:C:2006:HOH:O	2.10	0.49
1:B:93:SER:HA	1:B:263:PRO:HD2	1.94	0.49
1:D:235:ARG:CD	6:D:2090:HOH:O	2.52	0.49
1:A:35:VAL:CB	1:A:86:LYS:HE3	2.38	0.49
1:B:72:ILE:HA	1:B:77:ILE:CD1	2.43	0.49
1:D:109:ILE:HG21	6:D:2015:HOH:O	2.13	0.49
1:A:18:LEU:HB3	1:A:225:MET:CE	2.43	0.49
1:C:119:LYS:NZ	6:C:2065:HOH:O	2.45	0.49
1:C:246:LYS:HE2	6:C:2048:HOH:O	2.12	0.49
1:B:46:ILE:HD13	6:B:2009:HOH:O	2.12	0.49
1:B:137:LYS:O	1:B:138:HIS:C	2.54	0.49
1:C:252:LYS:HE2	1:C:276:GLU:CD	2.38	0.49
1:D:188:GLU:HG2	6:D:2058:HOH:O	2.12	0.49
1:D:7:VAL:CG1	6:D:2026:HOH:O	2.58	0.49
1:D:36:ILE:HD11	1:D:101:SER:HA	1.94	0.49
1:D:187:ARG:NH1	2:D:500:ILE:HA	2.28	0.49
1:B:11:ALA:HB2	1:B:104:GLY:HA3	1.94	0.49
1:D:284:TYR:CA	6:D:2097:HOH:O	2.60	0.49
1:B:48:ILE:HD13	1:B:62:ASN:HB3	1.94	0.48
1:B:71:MET:O	1:B:72:ILE:C	2.56	0.48
1:B:299:VAL:HG22	6:B:2072:HOH:O	2.12	0.48
1:A:130:GLU:O	1:A:134:SER:HB2	2.13	0.48
1:D:184:LYS:O	6:D:2058:HOH:O	2.20	0.48
1:D:48:ILE:O	1:D:57:THR:HG22	2.13	0.48
1:B:185:GLU:C	1:B:187:ARG:N	2.71	0.48
1:D:5:MET:O	1:D:39:GLU:HG3	2.13	0.48
1:B:6:LYS:HB3	1:B:39:GLU:HG2	1.96	0.48
1:B:119:LYS:O	1:B:123:VAL:HG23	2.14	0.48
1:D:187:ARG:HH12	2:D:500:ILE:HA	1.79	0.48
1:B:89:VAL:HG22	1:B:90:LYS:N	2.28	0.48
1:D:8:ARG:HB3	1:D:300:VAL:HG13	1.95	0.48
1:B:137:LYS:O	1:B:138:HIS:O	2.32	0.48
1:C:141:ASN:ND2	2:C:500:ILE:HD11	2.16	0.48
1:D:11:ALA:HB1	1:D:100:ALA:O	2.14	0.48
1:B:51:ASP:OD2	1:B:86:LYS:HA	2.14	0.47
1:B:183:THR:CG2	6:B:2073:HOH:O	2.61	0.47
1:D:16:ALA:HB3	6:D:2040:HOH:O	2.13	0.47
1:D:183:THR:CG2	6:D:2035:HOH:O	2.52	0.47
1:B:56:PRO:HB2	1:B:61:LYS:HB3	1.95	0.47
1:B:245:ILE:HD11	1:B:284:TYR:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:MET:HE1	1:B:268:PHE:CE1	2.45	0.47
1:B:245:ILE:HD11	1:B:284:TYR:CB	2.45	0.47
1:A:182:ASN:OD1	1:A:185:GLU:HG3	2.14	0.47
1:B:46:ILE:O	1:B:59:PRO:CG	2.63	0.47
1:C:10:LYS:HE2	6:C:2003:HOH:O	2.15	0.47
1:D:190:LEU:HG	1:D:231:ILE:HD12	1.97	0.47
1:B:74:ASP:C	1:B:76:ASN:H	2.23	0.47
1:D:242:TYR:O	1:D:245:ILE:HG22	2.15	0.47
1:D:40:ALA:HB1	1:D:79:LYS:CD	2.45	0.46
1:B:33:TYR:CD1	1:B:33:TYR:O	2.67	0.46
1:B:43:ASP:O	1:B:45:GLU:N	2.48	0.46
1:B:138:HIS:CE1	1:B:187:ARG:NH2	2.83	0.46
1:B:156:TYR:O	1:B:157:GLU:C	2.58	0.46
1:B:5:MET:HE3	1:B:40:ALA:CB	2.45	0.46
1:D:187:ARG:HA	1:D:190:LEU:HD22	1.97	0.46
1:B:52:ASP:O	1:B:54:ASN:N	2.48	0.46
1:B:68:ALA:O	1:B:72:ILE:HG13	2.16	0.46
1:B:282:ARG:CG	6:B:2067:HOH:O	2.62	0.46
1:C:182:ASN:CB	1:C:185:GLU:HG2	2.44	0.46
1:B:105:THR:O	1:B:109:ILE:HG12	2.15	0.46
1:D:40:ALA:HB1	1:D:79:LYS:HD2	1.97	0.46
1:B:33:TYR:O	1:B:33:TYR:HD1	1.99	0.46
1:D:64:ALA:CA	6:D:2014:HOH:O	2.64	0.45
1:A:182:ASN:C	1:A:184:LYS:H	2.25	0.45
1:B:32:PRO:CG	1:B:289:ILE:HD13	2.47	0.45
1:B:69:LYS:CG	1:B:70:LYS:H	2.28	0.45
1:B:245:ILE:CD1	1:B:285:TYR:CE1	2.99	0.45
1:C:241:ASN:O	1:C:245:ILE:HG13	2.16	0.45
1:A:183:THR:O	1:A:183:THR:HG22	2.16	0.45
1:B:77:ILE:HG21	1:B:113:PHE:CD1	2.52	0.45
1:D:6:LYS:HB3	1:D:39:GLU:HG3	1.98	0.45
1:D:135:GLY:O	1:D:136:ALA:HB2	2.17	0.45
1:B:181:ILE:CD1	6:B:2052:HOH:O	2.64	0.45
1:B:288:THR:HG22	1:B:289:ILE:N	2.32	0.45
1:C:36:ILE:HD11	1:C:101:SER:HA	1.98	0.45
1:D:41:ILE:HG13	1:D:43:ASP:O	2.16	0.45
1:D:227:SER:O	1:D:229:LYS:HE2	2.16	0.45
1:B:113:PHE:CD2	1:B:113:PHE:N	2.83	0.45
1:B:132:ALA:O	1:B:133:SER:HB2	2.16	0.45
1:A:187:ARG:NH1	2:A:500:ILE:OXT	2.50	0.44
1:D:284:TYR:C	6:D:2097:HOH:O	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG13	1:A:142:VAL:HG23	1.99	0.44
1:D:93:SER:HA	1:D:263:PRO:HD2	1.98	0.44
1:D:50:VAL:HG22	1:D:85:ILE:HB	1.99	0.44
1:B:58:ASP:O	1:B:60:ASP:N	2.50	0.44
1:B:67:VAL:O	1:B:71:MET:HB2	2.18	0.44
1:B:182:ASN:O	1:B:183:THR:C	2.61	0.44
1:B:173:LEU:HD12	1:B:290:ARG:HA	1.98	0.44
1:A:46:ILE:O	1:A:59:PRO:HG3	2.18	0.44
1:B:6:LYS:HA	1:B:112:LEU:CD1	2.45	0.44
1:A:183:THR:HA	1:A:186:ALA:CB	2.48	0.44
1:A:9:VAL:HG21	1:A:107:TYR:CD2	2.53	0.44
1:B:41:ILE:N	6:B:2008:HOH:O	2.51	0.44
1:B:46:ILE:HB	1:B:59:PRO:HB3	2.00	0.43
1:B:194:VAL:HG12	1:B:195:GLY:H	1.83	0.43
1:B:128:TYR:CE1	1:B:137:LYS:HE2	2.53	0.43
1:C:178:ASN:CB	6:C:2102:HOH:O	2.61	0.43
1:D:77:ILE:HD13	1:D:113:PHE:CD1	2.53	0.43
1:B:245:ILE:HD12	1:B:285:TYR:HE1	1.80	0.43
1:A:225:MET:HE1	1:A:268:PHE:HE1	1.84	0.43
1:B:51:ASP:O	1:B:52:ASP:C	2.62	0.43
1:D:131:LEU:O	1:D:135:GLY:N	2.51	0.43
1:D:156:TYR:C	1:D:157:GLU:HG2	2.43	0.43
1:D:229:LYS:HA	1:D:229:LYS:HD3	1.72	0.43
1:B:69:LYS:CG	1:B:70:LYS:N	2.81	0.43
2:D:500:ILE:HG21	4:D:400:AGS:S1G	2.59	0.43
1:C:75:PHE:O	1:C:76:ASN:C	2.62	0.43
1:A:98:SER:HB3	3:A:400:ADP:O2B	2.17	0.43
1:A:190:LEU:HD11	1:A:235:ARG:NH2	2.33	0.43
1:B:48:ILE:HD11	1:B:65:GLY:CA	2.49	0.43
1:B:52:ASP:C	1:B:54:ASN:N	2.76	0.43
1:D:64:ALA:CB	6:D:2014:HOH:O	2.44	0.43
1:C:43:ASP:O	1:C:45:GLU:N	2.52	0.42
1:D:98:SER:OG	4:D:400:AGS:O2B	2.28	0.42
1:C:103:ALA:CA	6:C:2049:HOH:O	2.46	0.42
1:D:250:LYS:CD	6:D:2084:HOH:O	2.63	0.42
1:B:115:LEU:HD12	1:B:115:LEU:H	1.84	0.42
1:A:93:SER:HA	1:A:263:PRO:HD2	2.00	0.42
1:B:8:ARG:HH12	1:B:300:VAL:HG21	1.82	0.42
1:C:240:PRO:O	1:C:285:TYR:OH	2.28	0.42
1:D:11:ALA:HA	1:D:297:VAL:HG22	2.02	0.42
1:A:48:ILE:O	1:A:57:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ALA:HA	1:A:142:VAL:HG22	2.02	0.42
1:B:100:ALA:HB2	6:B:2014:HOH:O	2.20	0.42
1:C:141:ASN:ND2	2:C:500:ILE:CD1	2.73	0.42
1:B:183:THR:HG23	6:B:2073:HOH:O	2.19	0.42
1:B:46:ILE:O	1:B:59:PRO:HG3	2.20	0.41
1:B:58:ASP:O	1:B:61:LYS:N	2.51	0.41
1:D:13:CYS:SG	1:D:32:PRO:HG2	2.60	0.41
1:A:79:LYS:H	1:A:79:LYS:HG3	1.60	0.41
1:A:247:GLU:O	1:A:250:LYS:HB2	2.19	0.41
1:B:33:TYR:CD1	1:B:33:TYR:C	2.98	0.41
1:B:75:PHE:CE2	1:B:115:LEU:HG	2.55	0.41
1:A:242:TYR:OH	1:A:246:LYS:HD2	2.20	0.41
1:B:50:VAL:C	1:B:51:ASP:O	2.64	0.41
1:B:80:GLY:O	1:B:81:VAL:HG13	2.21	0.41
1:B:190:LEU:HG	1:B:231:ILE:CD1	2.49	0.41
1:D:187:ARG:CD	6:D:2057:HOH:O	2.56	0.41
1:B:18:LEU:HD22	1:B:225:MET:HE1	2.01	0.41
1:B:205:LYS:HG3	1:B:227[A]:SER:OG	2.21	0.41
4:B:400:AGS:PB	6:B:2074:HOH:O	2.79	0.41
1:C:16:ALA:HB3	2:C:500:ILE:HD11	2.03	0.41
1:B:58:ASP:C	1:B:60:ASP:H	2.29	0.41
2:D:500:ILE:CG2	6:D:2040:HOH:O	2.59	0.41
1:B:9:VAL:HG22	1:B:10:LYS:N	2.36	0.41
1:B:51:ASP:O	1:B:52:ASP:O	2.39	0.41
1:B:21:GLY:O	1:B:22:PHE:C	2.63	0.41
1:A:240:PRO:O	1:A:241:ASN:HB2	2.21	0.41
1:B:11:ALA:HB1	1:B:100:ALA:O	2.21	0.41
1:B:194:VAL:HG12	1:B:195:GLY:N	2.36	0.41
1:C:55:ILE:HA	1:C:56:PRO:HD3	1.90	0.41
1:D:18:LEU:HD23	1:D:18:LEU:HA	1.86	0.41
1:A:190:LEU:HA	1:A:191:PRO:HD3	1.93	0.41
1:C:246:LYS:CB	6:C:2129:HOH:O	2.40	0.41
1:B:75:PHE:O	1:B:76:ASN:C	2.64	0.40
1:D:197:LYS:HB2	1:D:197:LYS:HZ2	1.86	0.40
1:B:157:GLU:O	1:B:157:GLU:OE1	2.40	0.40
1:B:240:PRO:O	1:B:241:ASN:HB2	2.21	0.40
1:B:113:PHE:O	1:B:115:LEU:CD1	2.69	0.40
1:A:8:ARG:HB2	6:A:2013:HOH:O	2.22	0.40
1:A:9:VAL:HG22	1:A:298:GLU:O	2.22	0.40
1:B:66:ILE:HA	1:B:69:LYS:HG2	2.02	0.40
1:D:173:LEU:HD23	1:D:173:LEU:HA	1.95	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)
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

All (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
1	B	51	ASP
1	B	53	LYS
1	B	90	LYS
1	A	79	LYS
1	B	74	ASP
1	B	75	PHE
1	B	183	THR
1	D	136	ALA
1	A	134	SER

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Mol	Chain	Res	Type
1	A	250	LYS
1	B	52	ASP
1	A	44	LYS
1	A	132	ALA
1	B	59	PRO
1	B	17	ASN
1	D	59	PRO

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	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

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	31	GLU
1	A	57	THR
1	A	63	VAL
1	A	117	LEU
1	A	127[A]	SER
1	A	127[B]	SER
1	A	157	GLU
1	A	173	LEU
1	A	187	ARG
1	A	190	LEU
1	A	196	LEU
1	A	232	GLU
1	A	233	PRO

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Mol	Chain	Res	Type
1	A	283	ASP
1	A	289	ILE
1	B	54	ASN
1	B	57	THR
1	B	73	ASP
1	B	81	VAL
1	B	131	LEU
1	B	157	GLU
1	B	173	LEU
1	B	192	LYS
1	B	194	VAL
1	C	5	MET
1	C	9	VAL
1	C	114	LYS
1	C	117	LEU
1	C	173	LEU
1	C	190	LEU
1	C	196	LEU
1	D	53	LYS
1	D	57	THR
1	D	60	ASP
1	D	117	LEU
1	D	189	ILE
1	D	190	LEU
1	D	194	VAL
1	D	196	LEU
1	D	197	LYS
1	D	235	ARG
1	D	272	GLU
1	D	283	ASP
1	D	300	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	B	138	HIS
1	B	141	ASN
1	B	163	HIS
1	C	54	ASN
1	C	141	ASN
1	D	138	HIS

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Mol	Chain	Res	Type
1	D	287	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	-

All (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
4	B	400	AGS	PG-S1G	3.03	1.97	1.90
3	A	400	ADP	C5-N7	-2.96	1.33	1.39
4	D	400	AGS	C5-C4	2.78	1.44	1.39
4	D	400	AGS	PA-O3A	2.57	1.62	1.59
3	A	400	ADP	C2-N1	2.56	1.38	1.33
4	D	400	AGS	PB-O3B	-2.49	1.56	1.59
4	D	400	AGS	C4-N3	2.45	1.39	1.34
4	D	400	AGS	C2-N1	2.38	1.38	1.33
3	A	400	ADP	C2-N3	2.30	1.38	1.33
3	A	400	ADP	C5-C4	2.23	1.43	1.39
4	B	400	AGS	C2-N3	2.16	1.37	1.33
4	B	400	AGS	C5-C4	2.14	1.42	1.39
4	B	400	AGS	C1'-N9	2.11	1.52	1.46
3	C	400	ADP	C6-N1	2.01	1.41	1.35

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	400	ADP	C4-N9-C1'	3.37	134.52	126.63
3	C	400	ADP	C1'-N9-C8	-3.31	119.75	127.09
3	C	400	ADP	O4'-C1'-N9	3.17	114.17	108.09
4	D	400	AGS	C1'-N9-C8	-3.08	120.26	127.09
4	B	400	AGS	C1'-N9-C8	-3.07	120.29	127.09
4	B	400	AGS	O2G-PG-O3B	2.55	113.14	104.64
3	A	400	ADP	O2'-C2'-C3'	2.48	119.76	111.82
3	C	400	ADP	O2B-PB-O1B	2.28	119.70	110.83
3	C	400	ADP	N3-C2-N1	-2.25	125.18	128.58
3	A	400	ADP	O2B-PB-O1B	2.21	119.46	110.83
4	D	400	AGS	O2G-PG-O3B	2.19	111.96	104.64
3	C	400	ADP	O5'-PA-O1A	2.04	117.03	108.94

There are no chirality outliers.

All (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
3	C	400	ADP	PA-O3A-PB-O2B
3	A	400	ADP	C3'-C4'-C5'-O5'
3	C	400	ADP	C3'-C4'-C5'-O5'
4	D	400	AGS	C3'-C4'-C5'-O5'
2	C	500	ILE	CA-CB-CG1-CD1
4	D	400	AGS	O4'-C4'-C5'-O5'
4	B	400	AGS	PG-O3B-PB-O1B
3	A	400	ADP	O4'-C4'-C5'-O5'
3	C	400	ADP	O4'-C4'-C5'-O5'
2	C	500	ILE	CG2-CB-CG1-CD1
4	B	400	AGS	C3'-C4'-C5'-O5'
2	C	500	ILE	OXT-C-CA-N
3	A	400	ADP	PA-O3A-PB-O1B
4	B	400	AGS	C4'-C5'-O5'-PA
4	B	400	AGS	PG-O3B-PB-O2B
3	C	400	ADP	C4'-C5'-O5'-PA
4	D	400	AGS	C4'-C5'-O5'-PA
3	C	400	ADP	PA-O3A-PB-O1B
4	D	400	AGS	O4'-C1'-N9-C8
3	C	400	ADP	O4'-C1'-N9-C8

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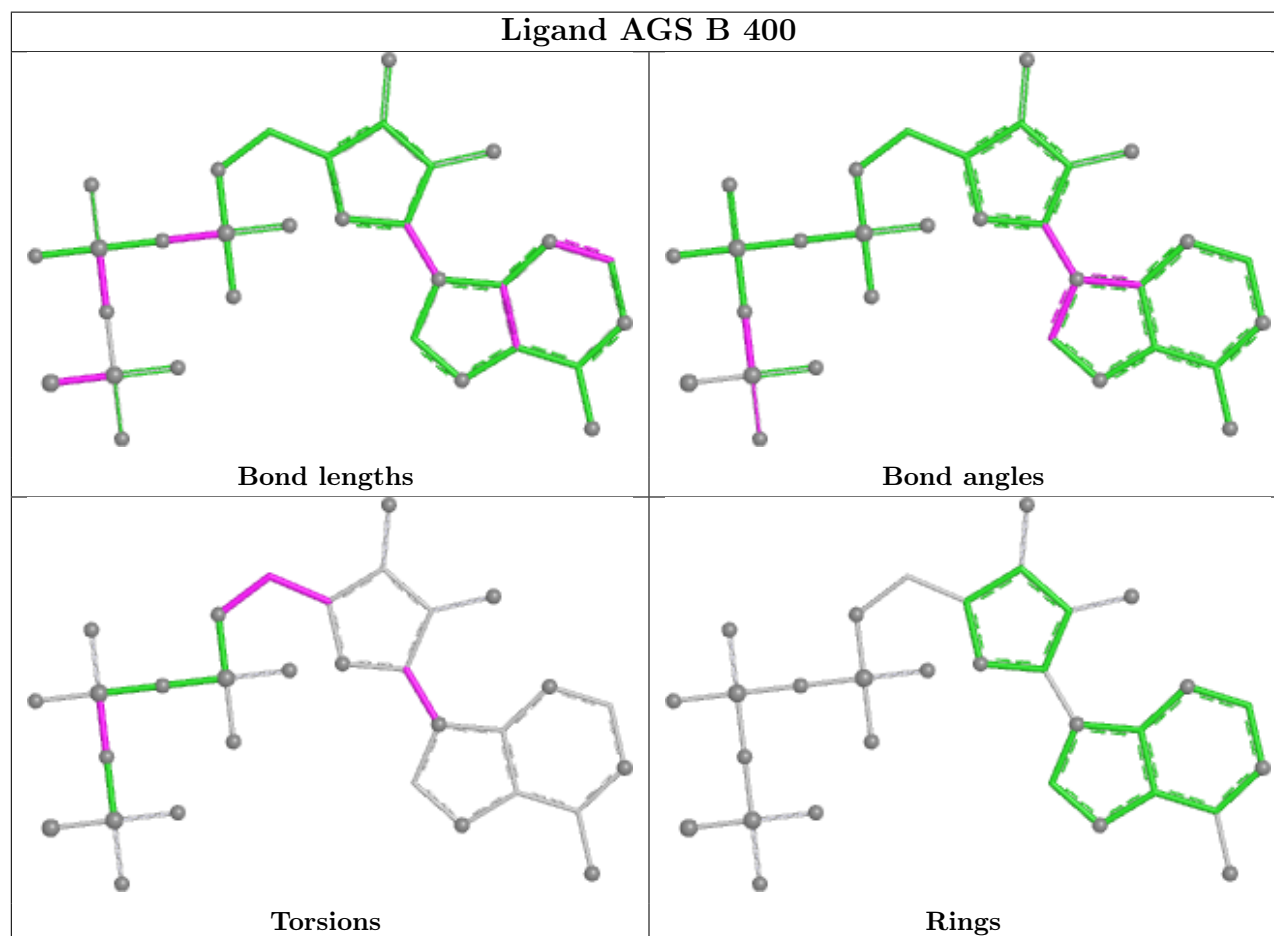
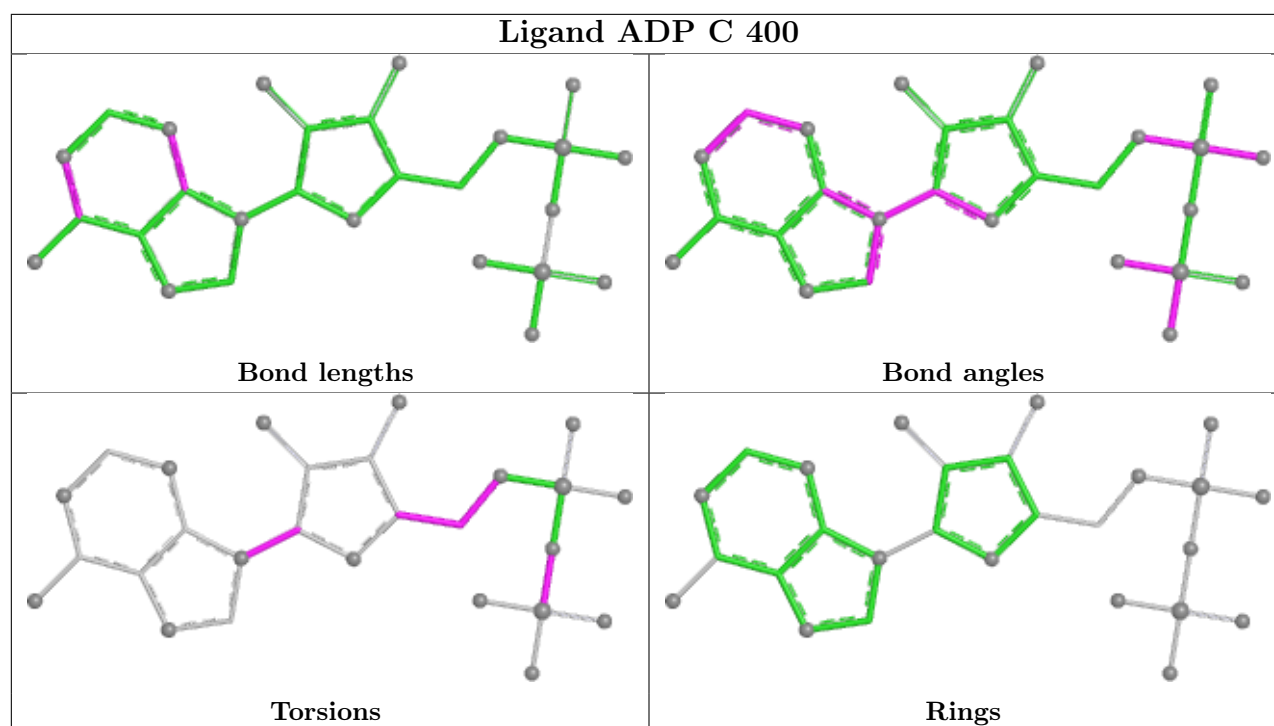
Mol	Chain	Res	Type	Atoms
4	B	400	AGS	O4'-C1'-N9-C8
3	A	400	ADP	O4'-C1'-N9-C8

There are no ring outliers.

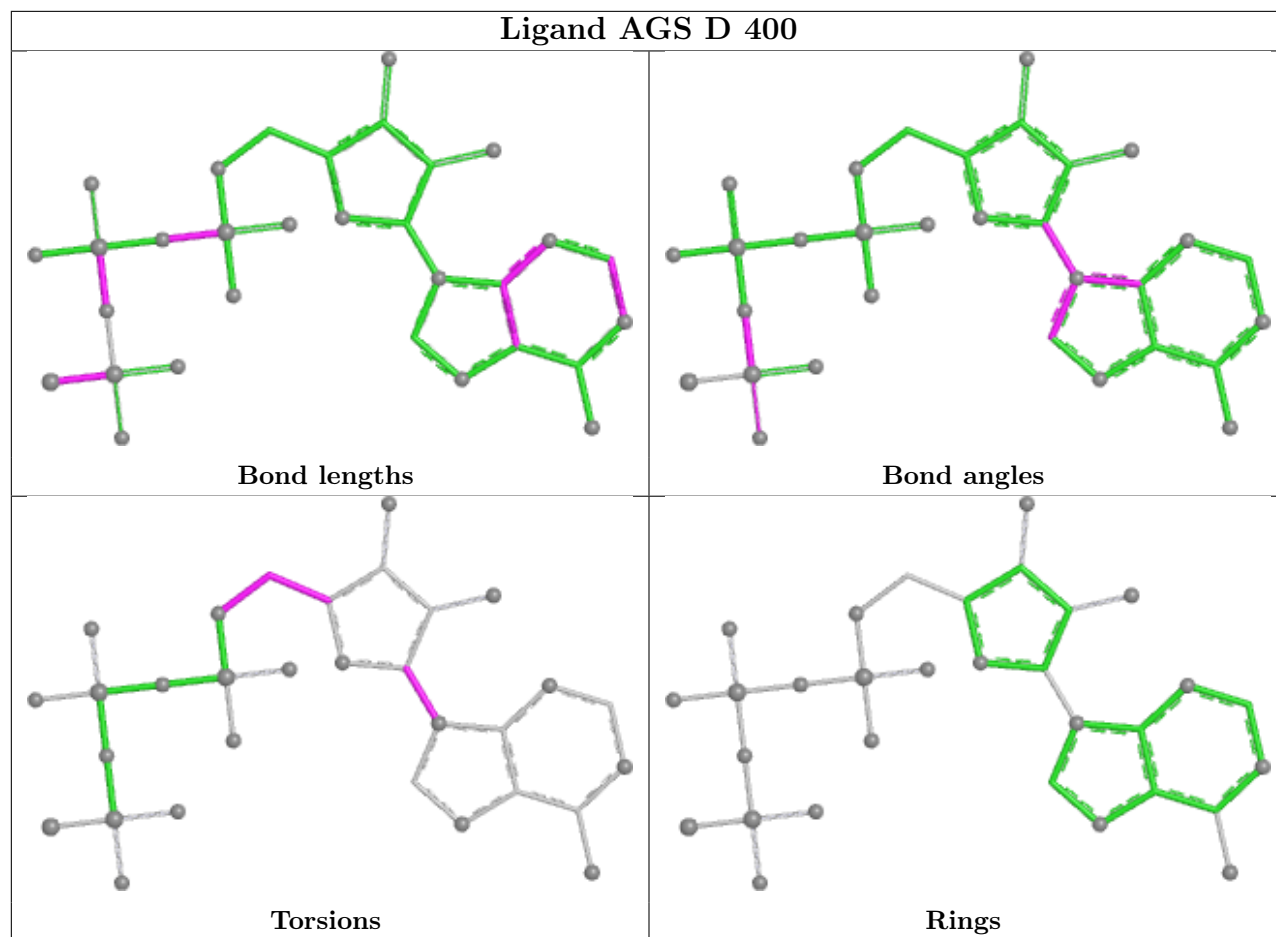
8 monomers are involved in 26 short contacts:

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

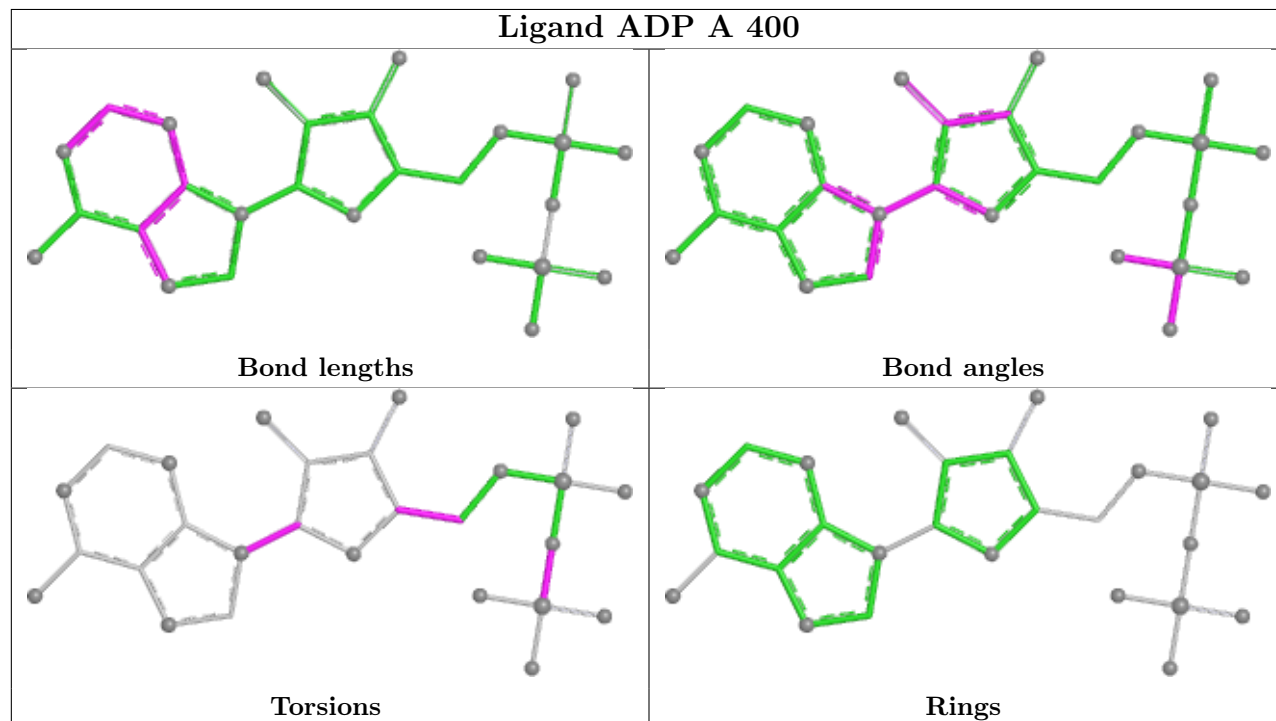
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	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%)

All (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
1	B	189	ILE	8.2
1	B	134	SER	7.3
1	B	77	ILE	7.2
1	B	107	TYR	7.2
1	D	133	SER	7.1
1	B	106	ALA	7.0
1	C	189	ILE	6.9
1	B	81	VAL	6.8
1	B	56	PRO	6.7
1	B	48	ILE	6.7
1	B	131	LEU	6.7
1	B	109	ILE	6.7
1	D	7	VAL	6.6
1	D	78	GLY	6.6
1	B	80	GLY	6.5
1	D	40	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	11	ALA	6.5
1	B	128	TYR	6.5
1	D	134	SER	6.4
1	B	88	GLY	6.4
1	B	41	ILE	6.3
1	C	186	ALA	6.3
1	B	66	ILE	6.2
1	D	50	VAL	6.2
1	B	75	PHE	6.2
1	B	136	ALA	6.0
1	B	50	VAL	6.0
1	B	63	VAL	6.0
1	C	78	GLY	5.9
1	D	81	VAL	5.8
1	B	55	ILE	5.8
1	B	115	LEU	5.8
1	D	113	PHE	5.7
1	B	129	GLY	5.6
1	B	38	VAL	5.6
1	B	40	ALA	5.6
1	D	72	ILE	5.6
1	D	59	PRO	5.6
1	B	166	ILE	5.5
1	B	138	HIS	5.5
1	B	98	SER	5.4
1	B	142	VAL	5.4
1	D	136	ALA	5.4
1	D	109	ILE	5.4
1	C	190	LEU	5.4
1	B	84	THR	5.3
1	B	123	VAL	5.3
1	C	41	ILE	5.3
1	B	68	ALA	5.3
1	A	41	ILE	5.3
1	B	46	ILE	5.3
1	D	66	ILE	5.3
1	B	120	LEU	5.3
1	D	131	LEU	5.3
1	D	46	ILE	5.2
1	C	88	GLY	5.2
1	B	144	PRO	5.2
1	B	119	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	245	ILE	5.2
1	C	245	ILE	5.2
1	D	48	ILE	5.2
1	B	183	THR	5.1
1	D	299	VAL	5.1
1	A	189	ILE	5.1
1	B	83	ILE	5.1
1	B	117	LEU	5.1
1	D	57	THR	5.1
1	B	135	GLY	5.1
1	D	300	VAL	5.1
1	B	36	ILE	5.0
1	A	135	GLY	5.0
1	B	100	ALA	5.0
1	D	80	GLY	5.0
1	B	284	TYR	5.0
1	B	35	VAL	5.0
1	B	89	VAL	5.0
1	A	183	THR	5.0
1	A	277	VAL	5.0
1	D	5	MET	4.9
1	C	249	VAL	4.9
1	B	176	ILE	4.9
1	B	97	SER	4.8
1	B	122	LEU	4.8
1	D	107	TYR	4.8
1	B	7	VAL	4.8
1	D	143	ALA	4.8
1	D	115	LEU	4.8
1	D	120	LEU	4.8
1	B	61	LYS	4.7
1	C	280	ILE	4.7
1	B	37	GLU	4.7
1	D	189	ILE	4.7
1	B	190	LEU	4.7
1	B	113	PHE	4.7
1	C	284	TYR	4.6
1	A	46	ILE	4.6
1	A	190	LEU	4.6
1	B	44	LYS	4.6
1	B	53	LYS	4.6
1	C	77	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	4.6
1	B	101	SER	4.5
1	D	43	ASP	4.5
1	B	57	THR	4.5
1	B	108	ALA	4.5
1	D	64	ALA	4.5
1	A	5	MET	4.5
1	B	73	ASP	4.5
1	C	251	ASP	4.5
1	B	121	LYS	4.5
1	B	65	GLY	4.4
1	B	29	LEU	4.4
1	B	240	PRO	4.4
1	C	56	PRO	4.4
1	C	241	ASN	4.4
1	B	102	SER	4.3
1	D	89	VAL	4.3
1	B	285	TYR	4.3
1	D	47	ILE	4.3
1	D	183	THR	4.3
1	A	91	ALA	4.3
1	D	135	GLY	4.3
1	B	187	ARG	4.3
1	B	158	PRO	4.3
1	A	57	THR	4.3
1	D	102	SER	4.3
1	D	138	HIS	4.3
1	D	9	VAL	4.2
1	B	86	LYS	4.2
1	C	44	LYS	4.2
1	D	250	LYS	4.2
1	A	40	ALA	4.2
1	B	78	GLY	4.2
1	A	99	ALA	4.2
1	D	186	ALA	4.2
1	D	110	ASN	4.2
1	B	5	MET	4.2
1	D	38	VAL	4.2
1	A	55	ILE	4.2
1	B	96	GLY	4.2
1	B	260	GLY	4.2
1	D	284	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	GLY	4.1
1	C	273	PHE	4.1
1	D	274	ILE	4.1
1	A	44	LYS	4.1
1	B	12	PRO	4.1
1	A	187	ARG	4.1
1	A	178	ASN	4.1
1	B	82	LYS	4.1
1	B	9	VAL	4.1
1	D	73	ASP	4.1
1	B	157	GLU	4.1
1	A	77	ILE	4.1
1	B	181	ILE	4.1
1	B	105	THR	4.1
1	B	79	LYS	4.1
1	D	75	PHE	4.0
1	B	286	GLU	4.0
1	D	112	LEU	4.0
1	C	50	VAL	4.0
1	C	274	ILE	4.0
1	B	238	LEU	4.0
1	A	138	HIS	4.0
1	C	43	ASP	4.0
1	B	6	LYS	4.0
1	B	243	PHE	4.0
1	B	180	SER	4.0
1	B	148	GLY	4.0
1	B	156	TYR	4.0
1	B	112	LEU	4.0
1	B	143	ALA	4.0
1	B	300	VAL	4.0
1	D	129	GLY	3.9
1	C	53	LYS	3.9
1	B	178	ASN	3.9
1	B	126	ALA	3.9
1	D	68	ALA	3.9
1	C	184	LYS	3.9
1	D	60	ASP	3.9
1	D	76	ASN	3.9
1	B	139	ALA	3.9
1	B	296	GLY	3.9
1	D	83	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	280	ILE	3.9
1	B	147	PHE	3.9
1	A	206	ALA	3.9
1	B	151	THR	3.9
1	D	11	ALA	3.9
1	D	245	ILE	3.9
1	A	196	LEU	3.8
1	C	183	THR	3.8
1	A	136	ALA	3.8
1	A	186	ALA	3.8
1	D	65	GLY	3.8
1	B	67	VAL	3.8
1	A	182	ASN	3.8
1	D	158	PRO	3.8
1	D	84	THR	3.8
1	D	105	THR	3.8
1	B	155	ASN	3.8
1	C	54	ASN	3.8
1	A	286	GLU	3.8
1	D	185	GLU	3.8
1	C	288	THR	3.8
1	B	16	ALA	3.8
1	C	267	ALA	3.8
1	A	289	ILE	3.8
1	A	134	SER	3.8
1	B	222	GLY	3.7
1	B	59	PRO	3.7
1	B	267	ALA	3.7
1	A	137	LYS	3.7
1	B	137	LYS	3.7
1	A	274	ILE	3.7
1	C	48	ILE	3.7
1	B	198	ASP	3.7
1	B	145	ALA	3.7
1	D	106	ALA	3.7
1	D	13	CYS	3.7
1	B	118	ASP	3.7
1	B	104	GLY	3.7
1	B	70	LYS	3.7
1	C	59	PRO	3.7
1	B	95	LEU	3.6
1	C	219	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	52	ASP	3.6
1	D	123	VAL	3.6
1	A	188	GLU	3.6
1	C	188	GLU	3.6
1	C	132	ALA	3.6
1	D	132	ALA	3.6
1	D	128	TYR	3.6
1	D	55	ILE	3.6
1	C	247	GLU	3.6
1	A	85	ILE	3.6
1	C	265	ILE	3.6
1	A	203	VAL	3.6
1	B	249	VAL	3.6
1	B	294	GLY	3.5
1	B	28	CYS	3.5
1	C	5	MET	3.5
1	B	174	ILE	3.5
1	D	85	ILE	3.5
1	B	30	LYS	3.5
1	C	30	LYS	3.5
1	A	243	PHE	3.5
1	B	33	TYR	3.5
1	A	52	ASP	3.5
1	B	34	ASP	3.5
1	D	53	LYS	3.5
1	A	48	ILE	3.5
1	D	63	VAL	3.5
1	C	243	PHE	3.5
1	B	162	LEU	3.5
1	C	227	SER	3.5
1	D	6	LYS	3.5
1	D	127	SER	3.5
1	D	17	ASN	3.5
1	B	274	ILE	3.5
1	B	210	VAL	3.5
1	B	71	MET	3.5
1	C	16	ALA	3.5
1	B	21	GLY	3.5
1	B	188	GLU	3.4
1	B	146	ILE	3.4
1	B	299	VAL	3.4
1	A	193	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	168	PHE	3.4
1	C	40	ALA	3.4
1	C	270	LYS	3.4
1	B	159	LEU	3.4
1	B	182	ASN	3.4
1	A	214	TYR	3.4
1	B	179	ILE	3.4
1	B	114	LYS	3.4
1	C	237	LYS	3.4
1	D	114	LYS	3.4
1	D	142	VAL	3.4
1	A	132	ALA	3.4
1	A	131	LEU	3.4
1	D	101	SER	3.4
1	B	125	TYR	3.4
1	A	179	ILE	3.4
1	B	85	ILE	3.4
1	D	77	ILE	3.4
1	B	194	VAL	3.4
1	A	267	ALA	3.4
1	A	199	LEU	3.4
1	A	59	PRO	3.4
1	B	231	ILE	3.3
1	C	55	ILE	3.3
1	C	179	ILE	3.3
1	A	127[A]	SER	3.3
1	B	15[A]	SER	3.3
1	C	180	SER	3.3
1	B	234	VAL	3.3
1	D	297	VAL	3.3
1	B	150	PHE	3.3
1	B	185	GLU	3.3
1	D	82	LYS	3.3
1	A	73	ASP	3.3
1	C	289	ILE	3.3
1	C	22	PHE	3.3
1	B	54	ASN	3.3
1	B	287	ASN	3.3
1	D	285	TYR	3.3
1	C	136	ALA	3.3
1	C	240	PRO	3.3
1	A	168	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	3.3
1	D	10	LYS	3.2
1	A	47	ILE	3.2
1	C	176	ILE	3.2
1	C	277	VAL	3.2
1	C	238	LEU	3.2
1	A	273	PHE	3.2
1	B	241	ASN	3.2
1	D	98	SER	3.2
1	D	229	LYS	3.2
1	A	72	ILE	3.2
1	D	42	ASP	3.2
1	B	193	ALA	3.2
1	B	14	THR	3.2
1	B	257	THR	3.2
1	B	229	LYS	3.2
1	D	167	ASP	3.2
1	A	176	ILE	3.2
1	D	130	GLU	3.2
1	B	253	VAL	3.2
1	C	35	VAL	3.2
1	B	93	SER	3.2
1	C	236	GLY	3.2
1	D	147	PHE	3.2
1	B	51	ASP	3.2
1	C	286	GLU	3.2
1	A	83	ILE	3.1
1	C	197	LYS	3.1
1	D	126	ALA	3.1
1	D	289	ILE	3.1
1	A	9	VAL	3.1
1	A	300	VAL	3.1
1	B	27	LEU	3.1
1	B	133	SER	3.1
1	B	297	VAL	3.1
1	C	9	VAL	3.1
1	C	173	LEU	3.1
1	C	300	VAL	3.1
1	D	58	ASP	3.1
1	D	12	PRO	3.1
1	A	180	SER	3.1
1	C	187	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	156	TYR	3.1
1	B	273	PHE	3.1
1	C	250	LYS	3.1
1	B	141	ASN	3.1
1	A	204	GLY	3.1
1	C	104	GLY	3.1
1	C	234	VAL	3.1
1	D	124	ASP	3.1
1	B	268	PHE	3.1
1	C	76	ASN	3.1
1	D	15[A]	SER	3.1
1	A	271	GLU	3.1
1	A	92	GLY	3.1
1	A	104	GLY	3.1
1	B	60	ASP	3.0
1	B	265	ILE	3.0
1	D	166	ILE	3.0
1	D	196	LEU	3.0
1	A	50	VAL	3.0
1	B	153	VAL	3.0
1	C	81	VAL	3.0
1	B	22	PHE	3.0
1	D	168	PHE	3.0
1	D	79	LYS	3.0
1	B	281	LEU	3.0
1	B	62	ASN	3.0
1	D	54	ASN	3.0
1	A	24	VAL	3.0
1	B	293	VAL	3.0
1	D	273	PHE	3.0
1	C	57	THR	3.0
1	A	51	ASP	3.0
1	C	275	ASP	3.0
1	A	197	LYS	3.0
1	B	69	LYS	3.0
1	D	121	LYS	3.0
1	D	71	MET	3.0
1	C	178	ASN	3.0
1	C	181	ILE	3.0
1	A	249	VAL	3.0
1	B	91	ALA	3.0
1	B	163	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	161	VAL	2.9
1	A	114	LYS	2.9
1	B	283	ASP	2.9
1	D	137	LYS	2.9
1	A	84	THR	2.9
1	B	236	GLY	2.9
1	B	165	PRO	2.9
1	A	185	GLU	2.9
1	D	37	GLU	2.9
1	A	175	ALA	2.9
1	C	175	ALA	2.9
1	B	290	ARG	2.9
1	C	92	GLY	2.9
1	D	243	PHE	2.9
1	B	184	LYS	2.9
1	A	43	ASP	2.9
1	A	245	ILE	2.9
1	A	280	ILE	2.9
1	B	58	ASP	2.9
1	B	239	ILE	2.9
1	C	264	SER	2.9
1	A	284	TYR	2.9
1	C	84	THR	2.9
1	C	285	TYR	2.9
1	D	103	ALA	2.9
1	B	10	LYS	2.9
1	D	8	ARG	2.9
1	D	70	LYS	2.9
1	B	74	ASP	2.9
1	A	159	LEU	2.9
1	D	179	ILE	2.9
1	D	281	LEU	2.9
1	B	92	GLY	2.9
1	C	195	GLY	2.9
1	D	92	GLY	2.9
1	A	54	ASN	2.8
1	B	87	LYS	2.8
1	C	248	GLU	2.8
1	D	283	ASP	2.8
1	D	117	LEU	2.8
1	D	238	LEU	2.8
1	A	79	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	233	PRO	2.8
1	C	230	VAL	2.8
1	C	254	TYR	2.8
1	A	167	ASP	2.8
1	B	124	ASP	2.8
1	B	103	ALA	2.8
1	B	127	SER	2.8
1	B	219	SER	2.8
1	A	117	LEU	2.8
1	C	47	ILE	2.8
1	C	117	LEU	2.8
1	D	239	ILE	2.8
1	B	295	LYS	2.8
1	A	56	PRO	2.8
1	B	191	PRO	2.8
1	C	185	GLU	2.8
1	C	263	PRO	2.8
1	D	286	GLU	2.8
1	B	24	VAL	2.8
1	B	43	ASP	2.8
1	C	52	ASP	2.8
1	A	128	TYR	2.8
1	B	99	ALA	2.8
1	D	139	ALA	2.8
1	B	110	ASN	2.8
1	C	276	GLU	2.8
1	C	46	ILE	2.8
1	C	256	ILE	2.8
1	D	56	PRO	2.8
1	B	228	ASP	2.8
1	C	167	ASP	2.8
1	A	230	VAL	2.8
1	C	7	VAL	2.8
1	A	211	TYR	2.7
1	B	8	ARG	2.7
1	C	75	PHE	2.7
1	D	69	LYS	2.7
1	B	45	GLU	2.7
1	B	94	GLY	2.7
1	C	296	GLY	2.7
1	C	36	ILE	2.7
1	D	118	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	264	SER	2.7
1	C	223	ARG	2.7
1	D	194	VAL	2.7
1	D	108	ALA	2.7
1	A	80	GLY	2.7
1	A	222	GLY	2.7
1	C	204	GLY	2.7
1	D	122	LEU	2.7
1	C	79	LYS	2.7
1	D	44	LYS	2.7
1	B	200	VAL	2.7
1	A	143	ALA	2.7
1	D	100	ALA	2.7
1	C	228	ASP	2.7
1	D	275	ASP	2.7
1	B	154	THR	2.7
1	D	49	GLU	2.7
1	D	182	ASN	2.7
1	A	234	VAL	2.7
1	D	35	VAL	2.7
1	C	19	GLY	2.6
1	D	99	ALA	2.6
1	B	140	ASP	2.6
1	C	33	TYR	2.6
1	B	170	LEU	2.6
1	D	29	LEU	2.6
1	D	36	ILE	2.6
1	A	253	VAL	2.6
1	C	242	TYR	2.6
1	B	244	LYS	2.6
1	C	259	SER	2.6
1	B	196	LEU	2.6
1	C	112	LEU	2.6
1	A	276	GLU	2.6
1	B	276	GLU	2.6
1	D	188	GLU	2.6
1	A	184	LYS	2.6
1	B	90	LYS	2.6
1	B	197	LYS	2.6
1	A	288	THR	2.6
1	C	138	HIS	2.6
1	A	109	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	174	ILE	2.6
1	A	88	GLY	2.6
1	A	252	LYS	2.6
1	D	192	LYS	2.6
1	C	89	VAL	2.6
1	C	158	PRO	2.5
1	D	45	GLU	2.5
1	B	164	ILE	2.5
1	B	216	LYS	2.5
1	D	195	GLY	2.5
1	A	76	ASN	2.5
1	A	157	GLU	2.5
1	D	177	PRO	2.5
1	C	51	ASP	2.5
1	B	26	GLY	2.5
1	C	287	ASN	2.5
1	D	62	ASN	2.5
1	B	259	SER	2.5
1	B	261	SER	2.5
1	B	288	THR	2.5
1	C	297	VAL	2.5
1	D	234	VAL	2.5
1	D	74	ASP	2.5
1	D	119	LYS	2.5
1	D	33	TYR	2.5
1	D	214	TYR	2.5
1	D	254	TYR	2.5
1	A	260	GLY	2.5
1	B	199	LEU	2.5
1	D	88	GLY	2.5
1	A	133	SER	2.5
1	A	166	ILE	2.5
1	C	72	ILE	2.5
1	B	278	GLU	2.5
1	B	226	MET	2.5
1	D	212	ALA	2.5
1	A	210	VAL	2.5
1	A	275	ASP	2.5
1	C	86	LYS	2.5
1	D	178	ASN	2.4
1	A	22	PHE	2.4
1	A	281	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	278	GLU	2.4
1	D	272	GLU	2.4
1	B	289	ILE	2.4
1	C	246	LYS	2.4
1	D	184	LYS	2.4
1	A	142	VAL	2.4
1	D	155	ASN	2.4
1	D	28	CYS	2.4
1	A	242	TYR	2.4
1	D	125	TYR	2.4
1	C	218	LYS	2.4
1	C	172	ILE	2.4
1	B	212	ALA	2.4
1	C	11	ALA	2.4
1	A	78	GLY	2.4
1	A	169	LYS	2.4
1	D	190	LEU	2.4
1	B	52	ASP	2.4
1	A	172	ILE	2.4
1	D	181	ILE	2.4
1	C	103	ALA	2.4
1	D	145	ALA	2.4
1	C	31	GLU	2.4
1	D	39	GLU	2.4
1	D	111	GLU	2.4
1	A	177	PRO	2.4
1	A	233	PRO	2.4
1	D	287	ASN	2.4
1	B	195	GLY	2.4
1	C	38	VAL	2.4
1	D	222	GLY	2.4
1	D	293	VAL	2.4
1	D	87	LYS	2.4
1	D	197	LYS	2.4
1	B	213	LEU	2.3
1	A	181	ILE	2.3
1	A	265	ILE	2.3
1	C	239	ILE	2.3
1	D	267	ALA	2.3
1	B	17	ASN	2.3
1	D	255	GLY	2.3
1	B	130	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	220	LEU	2.3
1	D	151	THR	2.3
1	A	155	ASN	2.3
1	B	177	PRO	2.3
1	C	233	PRO	2.3
1	D	144	PRO	2.3
1	A	61	LYS	2.3
1	C	229	LYS	2.3
1	C	255	GLY	2.3
1	D	61	LYS	2.3
1	D	67	VAL	2.3
1	B	254	TYR	2.3
1	C	212	ALA	2.3
1	A	21	GLY	2.3
1	A	219	SER	2.3
1	B	49	GLU	2.3
1	C	67	VAL	2.3
1	D	249	VAL	2.3
1	A	112	LEU	2.3
1	A	173	LEU	2.3
1	C	159	LEU	2.3
1	D	162	LEU	2.3
1	B	64	ALA	2.2
1	B	232	GLU	2.2
1	D	261	SER	2.2
1	C	231	ILE	2.2
1	C	161	VAL	2.2
1	A	279	ASN	2.2
1	D	116	ASN	2.2
1	A	216	LYS	2.2
1	C	151	THR	2.2
1	A	45	GLU	2.2
1	A	232	GLU	2.2
1	A	238	LEU	2.2
1	B	262	GLY	2.2
1	D	148	GLY	2.2
1	D	180	SER	2.2
1	C	100	ALA	2.2
1	D	175	ALA	2.2
1	D	22	PHE	2.2
1	D	146	ILE	2.2
1	C	279	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	8	ARG	2.2
1	A	63	VAL	2.2
1	C	49	GLU	2.2
1	C	199	LEU	2.2
1	B	251	ASP	2.2
1	C	58	ASP	2.2
1	D	104	GLY	2.2
1	A	158	PRO	2.2
1	A	268	PHE	2.2
1	B	25	PHE	2.2
1	D	150	PHE	2.2
1	C	24	VAL	2.2
1	C	269	PRO	2.2
1	C	91	ALA	2.2
1	A	226	MET	2.1
1	A	75	PHE	2.1
1	A	221	PHE	2.1
1	A	254	TYR	2.1
1	B	111	GLU	2.1
1	C	25	PHE	2.1
1	B	214	TYR	2.1
1	C	130	GLU	2.1
1	B	42	ASP	2.1
1	A	200	VAL	2.1
1	B	203	VAL	2.1
1	C	291	THR	2.1
1	D	153	VAL	2.1
1	D	262	GLY	2.1
1	B	13	CYS	2.1
1	A	191	PRO	2.1
1	C	10	LYS	2.1
1	C	192	LYS	2.1
1	A	247	GLU	2.1
1	A	103	ALA	2.1
1	C	268	PHE	2.1
1	A	23	ASP	2.1
1	B	171	ASP	2.1
1	D	294	GLY	2.1
1	D	237	LYS	2.1
1	A	215	ASN	2.1
1	B	18	LEU	2.1
1	B	220	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	108	ALA	2.1
1	D	16	ALA	2.1
1	A	239	ILE	2.1
1	C	174	ILE	2.1
1	D	224	TYR	2.1
1	B	270	LYS	2.1
1	C	252	LYS	2.1
1	D	30	LYS	2.1
1	D	288	THR	2.1
1	B	208	GLY	2.1
1	C	222	GLY	2.1
1	A	194	VAL	2.1
1	B	277	VAL	2.1
1	B	279	ASN	2.1
1	C	194	VAL	2.1
1	C	201	ASN	2.1
1	B	32	PRO	2.1
1	A	122	LEU	2.1
1	C	13	CYS	2.1
1	C	34	ASP	2.1
1	A	15[A]	SER	2.0
1	B	172	ILE	2.0
1	C	85	ILE	2.0
1	B	211	TYR	2.0
1	A	81	VAL	2.0
1	B	161	VAL	2.0
1	C	200	VAL	2.0
1	A	283	ASP	2.0
1	D	278	GLU	2.0
1	A	53	LYS	2.0
1	C	133	SER	2.0
1	D	227	SER	2.0
1	A	25	PHE	2.0
1	A	256	ILE	2.0
1	B	256	ILE	2.0
1	B	116	ASN	2.0
1	A	161	VAL	2.0
1	C	203	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

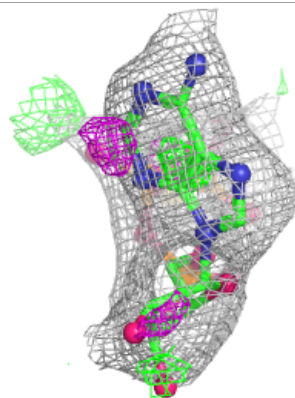
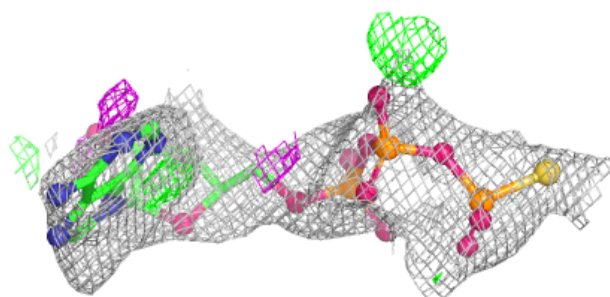
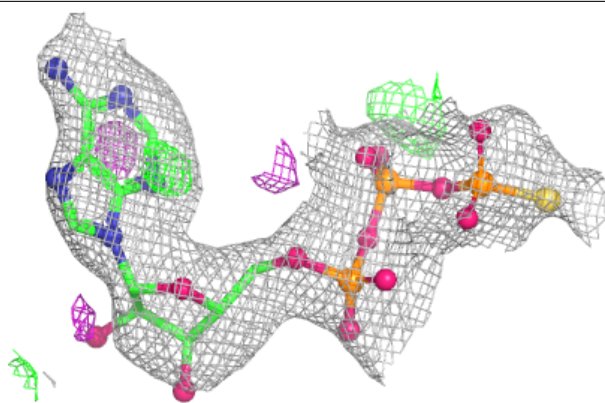
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

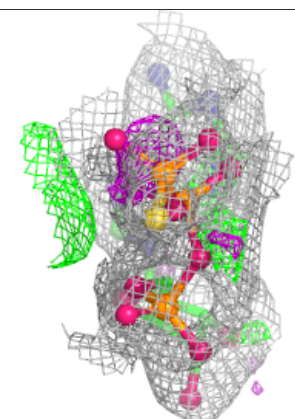
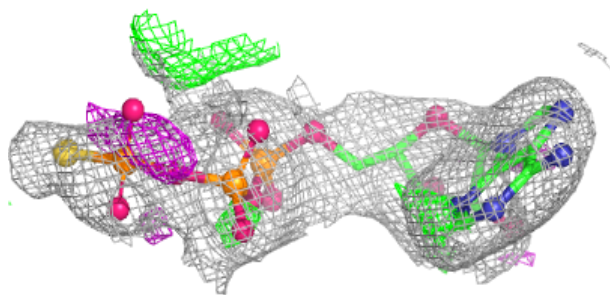
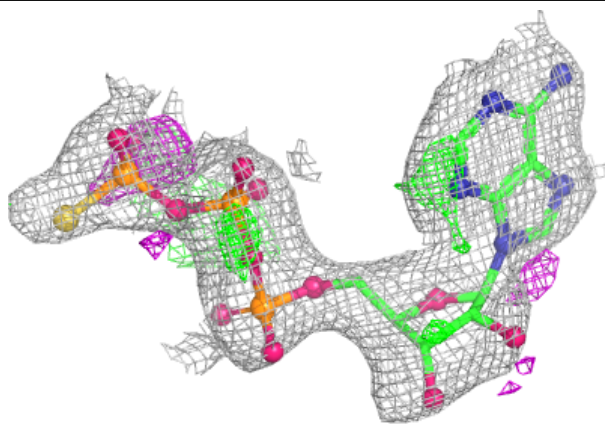
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS B 400:

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

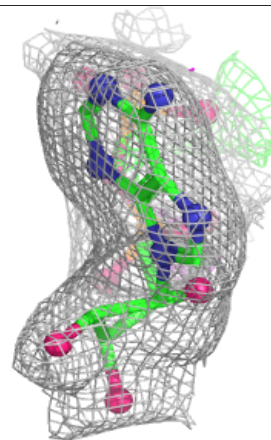
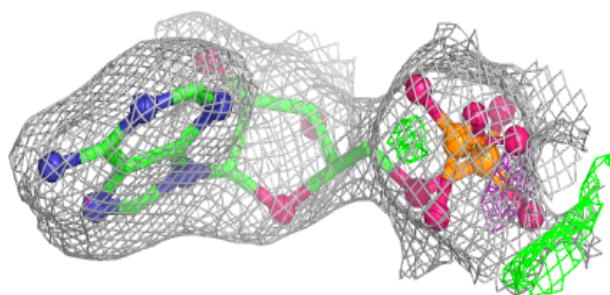
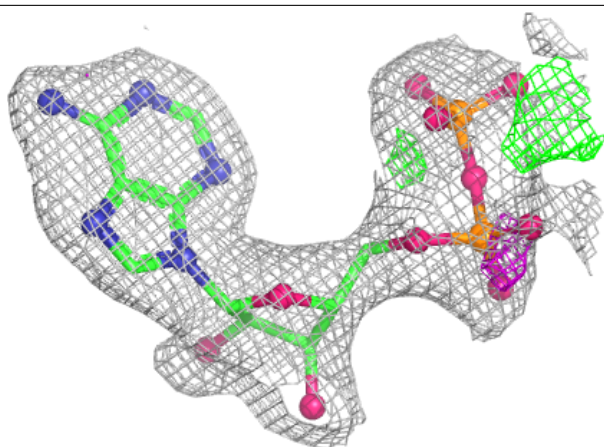
**Electron density around AGS D 400:**

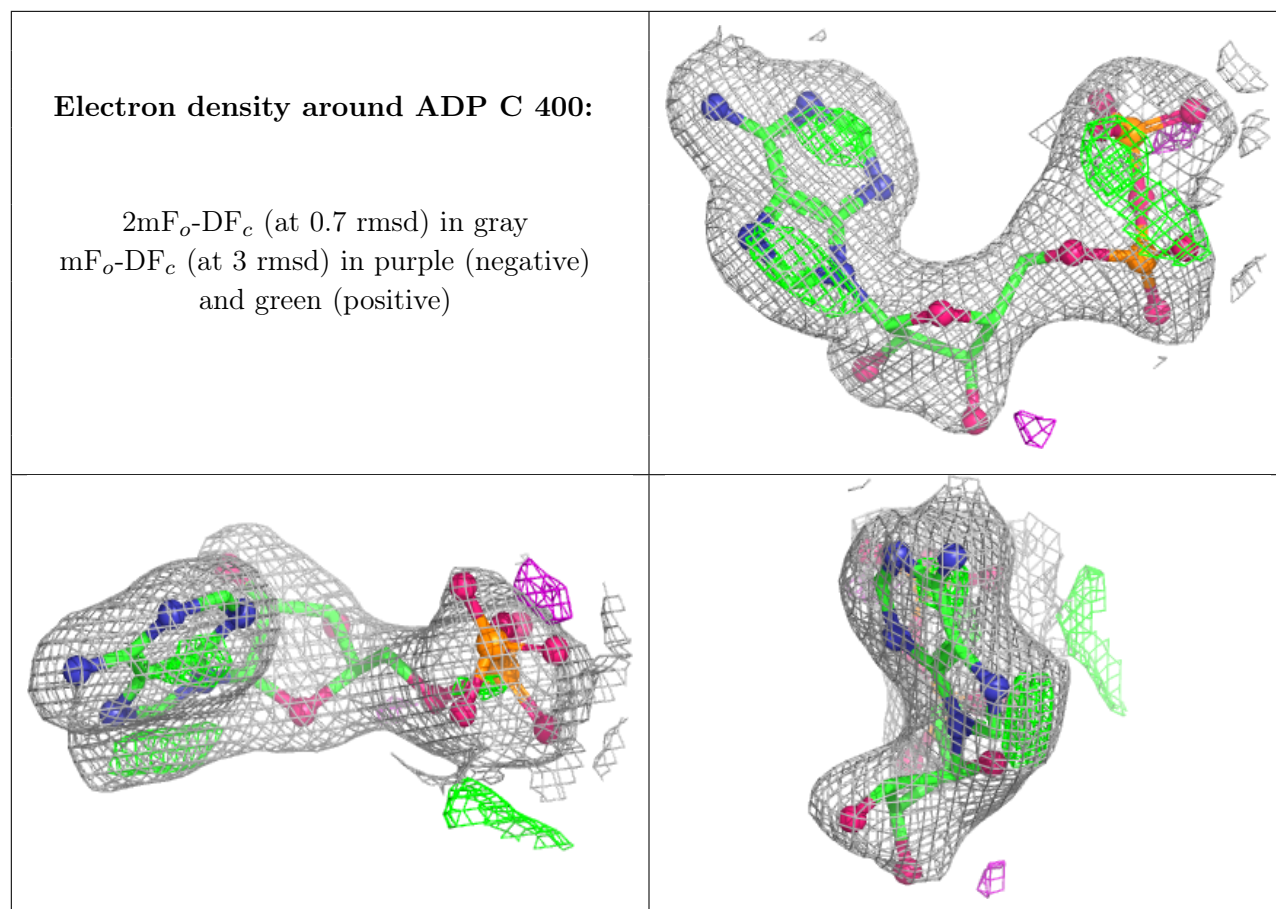
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.