



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:50 PM UTC

PDB ID : 3KAL / pdb_00003kal
Title : Structure of homoglutathione synthetase from Glycine max in closed conformation with homoglutathione, ADP, a sulfate ion, and three magnesium ions bound
Authors : Galant, A.; Arkus, K.A.J.; Zubieta, C.; Cahoon, R.E.; Jez, J.M.
Deposited on : 2009-10-19
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

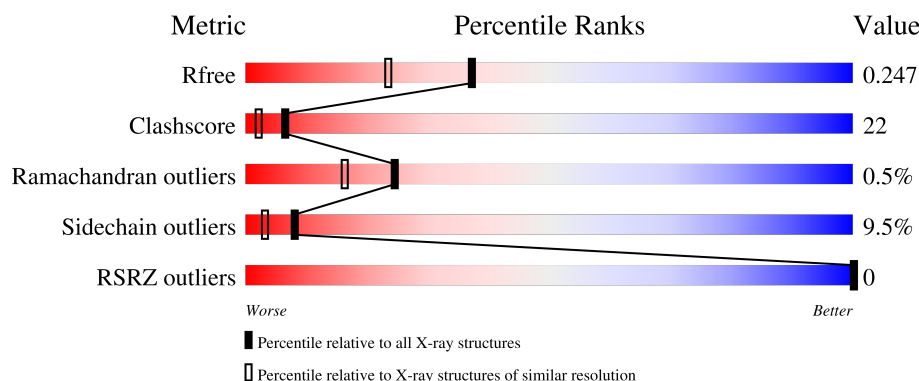
1 Overall quality at a glance

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	499	
1	B	499	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HGS	A	501	-	X	X	-
3	HGS	A	506	-	X	-	-
3	HGS	B	501	-	X	X	-
3	HGS	B	506	-	X	-	-
5	SO4	A	505	-	-	X	-
5	SO4	B	505	-	-	X	-

2 Entry composition [i](#)

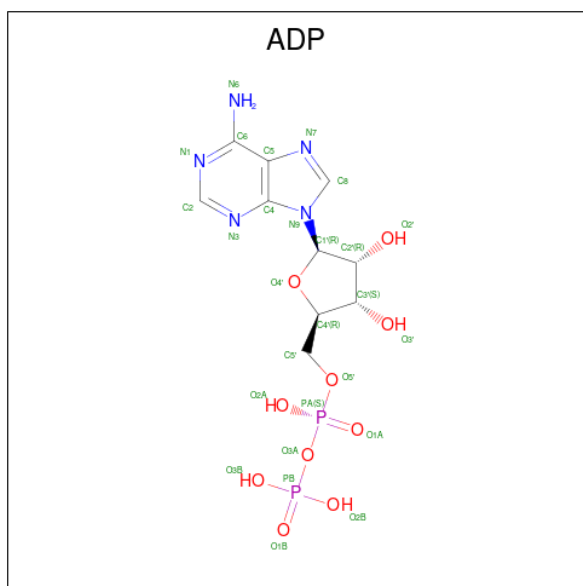
There are 6 unique types of molecules in this entry. The entry contains 8571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 homoglutathione synthetase.

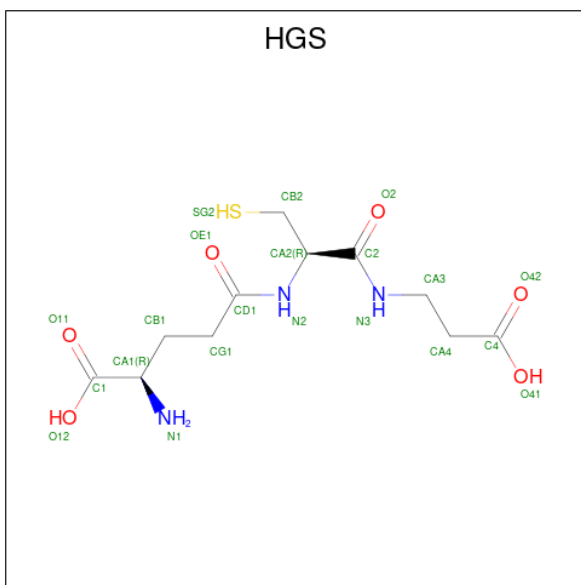
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	14	0
			3828	2423	667	720	18			
1	B	468	Total	C	N	O	S	0	19	0
			3855	2434	676	728	17			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is D-gamma-glutamyl-L-cysteinyl-beta-alanine (CCD ID: HGS) (formula: $C_{11}H_{19}N_3O_6S$).

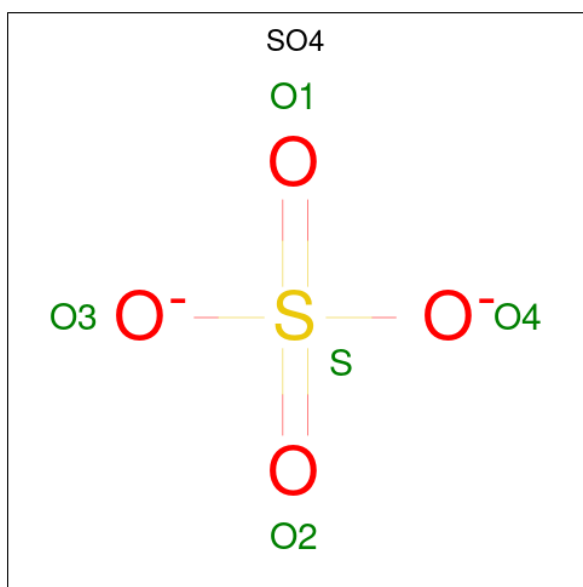


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 21	C 11	N 3	O 6	S 1	0	0
3	A	1	Total 21	C 11	N 3	O 6	S 1	0	0
3	B	1	Total 21	C 11	N 3	O 6	S 1	0	0
3	B	1	Total 21	C 11	N 3	O 6	S 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

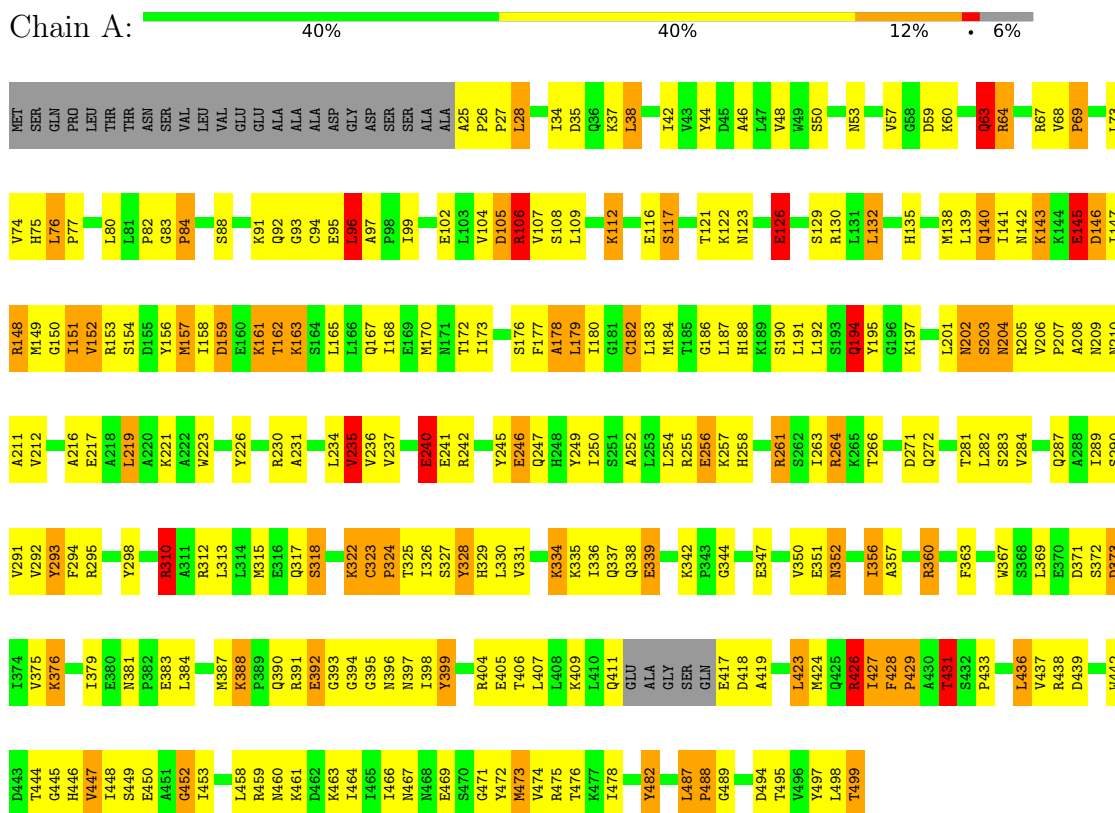
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	371	Total	O	0	0
			371	371		
6	B	363	Total	O	0	0
			363	363		

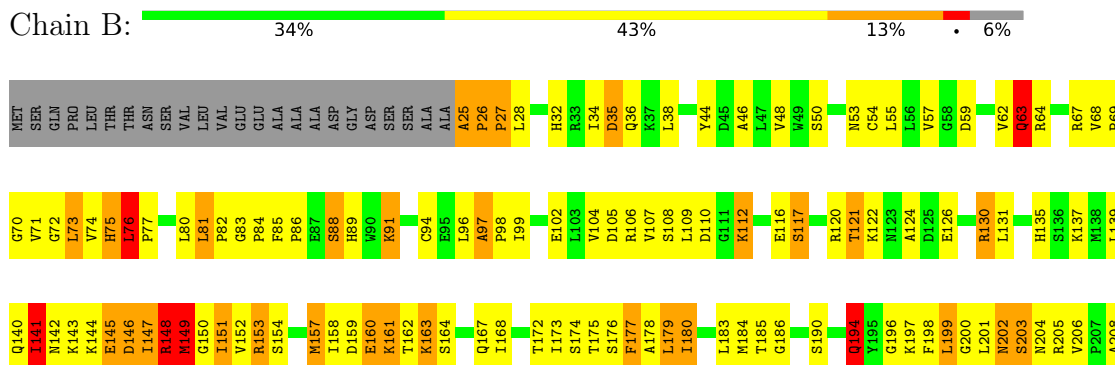
3 Residue-property plots

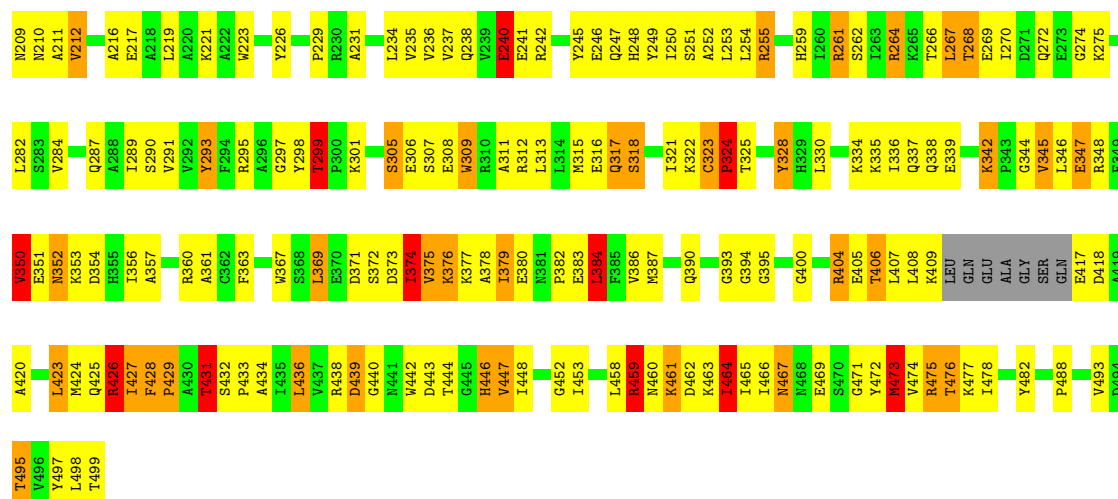
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: homogluthathione synthetase



• Molecule 1: homogluthathione synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	115.70Å 115.70Å 101.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.26 – 1.90 29.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.26-1.90) 99.8 (29.26-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.250 0.198 , 0.247	Depositor DCC
R_{free} test set	5992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l 0.488 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8571	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: HGS, SO4, MG, ADP

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	2.47	214/3901 (5.5%)	1.90	93/5269 (1.8%)
1	B	2.50	212/3927 (5.4%)	1.95	117/5303 (2.2%)
All	All	2.48	426/7828 (5.4%)	1.93	210/10572 (2.0%)

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	A	1	3
1	B	0	5
All	All	1	8

All (426) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	ALA	CA-CB	13.04	1.73	1.53
1	B	350	VAL	CA-CB	11.67	1.71	1.54
1	B	478	ILE	N-CA	10.90	1.59	1.46
1	B	461	LYS	N-CA	10.69	1.59	1.46
1	A	447	VAL	CA-CB	10.67	1.70	1.54
1	A	427	ILE	CA-CB	10.56	1.68	1.54
1	B	178	ALA	CA-CB	10.52	1.69	1.53
1	A	82	PRO	CA-C	10.34	1.66	1.52
1	B	235	VAL	N-CA	10.29	1.59	1.46
1	A	489	GLY	N-CA	10.23	1.60	1.45
1	A	178	ALA	CA-CB	10.06	1.69	1.53
1	A	246	GLU	C-O	10.02	1.35	1.24
1	B	424	MET	SD-CE	-10.01	1.54	1.79
1	A	34	ILE	CA-CB	9.97	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	PRO	CA-C	9.95	1.65	1.52
1	A	63	GLN	N-CA	9.94	1.58	1.46
1	B	237	VAL	C-O	9.76	1.36	1.23
1	B	446	HIS	N-CA	-9.65	1.34	1.46
1	B	336	ILE	CA-CB	9.53	1.66	1.54
1	B	209	ASN	CA-C	9.51	1.63	1.52
1	A	209	ASN	CA-C	9.25	1.63	1.52
1	A	203	SER	N-CA	9.20	1.57	1.46
1	A	478	ILE	N-CA	9.08	1.57	1.46
1	B	216	ALA	N-CA	8.98	1.57	1.46
1	A	109	LEU	N-CA	8.91	1.57	1.46
1	B	203	SER	N-CA	8.85	1.57	1.46
1	A	433	PRO	CA-C	8.84	1.64	1.52
1	B	473	MET	CA-C	8.82	1.63	1.52
1	A	494	ASP	C-O	8.74	1.33	1.23
1	B	141	ILE	CA-CB	8.70	1.65	1.54
1	B	104	VAL	CA-CB	8.69	1.65	1.54
1	A	284	VAL	CA-CB	8.60	1.65	1.54
1	A	116	GLU	N-CA	8.57	1.56	1.46
1	B	183	LEU	CA-C	8.57	1.64	1.52
1	A	458	LEU	N-CA	8.51	1.56	1.46
1	B	34	ILE	CA-CB	8.49	1.63	1.54
1	B	59	ASP	N-CA	8.46	1.56	1.46
1	B	379	ILE	CA-CB	8.41	1.65	1.54
1	B	284	VAL	CA-CB	8.40	1.65	1.54
1	A	424	MET	SD-CE	-8.39	1.58	1.79
1	B	458	LEU	N-CA	8.39	1.56	1.46
1	A	158	ILE	CA-CB	-8.30	1.44	1.53
1	B	323	CYS	CA-C	8.25	1.61	1.52
1	B	357	ALA	CA-C	8.22	1.63	1.52
1	B	311	ALA	CA-CB	8.22	1.66	1.53
1	A	264	ARG	CG-CD	8.17	1.76	1.52
1	B	97	ALA	N-CA	8.16	1.52	1.46
1	B	447	VAL	CA-CB	8.05	1.66	1.54
1	B	291	VAL	N-CA	8.01	1.55	1.46
1	B	240	GLU	CB-CG	8.01	1.76	1.52
1	A	255	ARG	CD-NE	7.89	1.57	1.46
1	B	429	PRO	CA-C	7.87	1.61	1.52
1	B	226	TYR	CA-C	7.86	1.63	1.52
1	A	292	VAL	CA-CB	7.80	1.64	1.54
1	B	461	LYS	C-N	-7.78	1.22	1.33
1	A	264	ARG	CB-CG	-7.71	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	ASP	CA-C	7.68	1.63	1.52
1	A	263	ILE	CA-C	7.67	1.61	1.52
1	B	177	PHE	CA-CB	7.65	1.64	1.53
1	B	117	SER	N-CA	7.62	1.55	1.46
1	B	289	ILE	C-O	7.62	1.32	1.24
1	B	71	VAL	CA-CB	7.60	1.65	1.54
1	B	361	ALA	N-CA	7.59	1.55	1.46
1	A	135	HIS	CA-C	7.59	1.62	1.52
1	B	105	ASP	CA-C	7.53	1.62	1.52
1	B	109	LEU	N-CA	7.52	1.56	1.46
1	A	84	PRO	CA-C	7.52	1.62	1.52
1	B	427	ILE	CA-CB	7.52	1.64	1.54
1	B	88	SER	CA-CB	7.51	1.65	1.53
1	B	99	ILE	CA-CB	7.48	1.63	1.54
1	A	473	MET	CA-C	7.42	1.61	1.52
1	B	35	ASP	CB-CG	7.42	1.70	1.52
1	A	216	ALA	N-CA	7.41	1.55	1.46
1	B	194	GLN	CA-C	7.40	1.62	1.52
1	A	208	ALA	N-CA	7.39	1.55	1.46
1	A	240	GLU	CB-CG	7.38	1.74	1.52
1	A	150	GLY	N-CA	7.37	1.56	1.45
1	A	290	SER	CA-C	7.34	1.62	1.52
1	B	444	THR	CA-CB	7.33	1.65	1.53
1	A	338	GLN	N-CA	7.32	1.55	1.46
1	A	154	SER	CA-C	7.30	1.61	1.52
1	B	154	SER	CA-C	7.29	1.61	1.52
1	B	473	MET	SD-CE	-7.28	1.61	1.79
1	B	475	ARG	CG-CD	7.25	1.74	1.52
1	B	444	THR	C-O	7.24	1.32	1.23
1	B	472	TYR	CA-CB	7.22	1.65	1.53
1	B	211	ALA	C-O	7.21	1.32	1.24
1	B	172	THR	CA-CB	7.19	1.66	1.53
1	A	163	LYS	CA-C	7.18	1.61	1.53
1	B	290	SER	CA-C	7.16	1.62	1.52
1	B	153	ARG	N-CA	7.15	1.55	1.46
1	B	264	ARG	CB-CG	-7.14	1.31	1.52
1	A	471	GLY	C-O	7.13	1.33	1.24
1	B	180	ILE	N-CA	7.10	1.54	1.46
1	A	335	LYS	N-CA	7.09	1.54	1.46
1	B	253	LEU	CA-CB	7.08	1.64	1.53
1	B	324	PRO	CG-CD	7.08	1.70	1.51
1	B	488	PRO	N-CD	7.08	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	SER	CA-CB	7.08	1.64	1.53
1	B	152	VAL	CA-CB	7.07	1.65	1.54
1	B	460	ASN	N-CA	7.03	1.55	1.46
1	B	151	ILE	CB-CG1	7.02	1.67	1.53
1	A	96	LEU	N-CA	-7.02	1.36	1.46
1	B	363	PHE	C-O	7.01	1.32	1.24
1	A	180	ILE	N-CA	7.00	1.54	1.46
1	B	108	SER	CA-CB	6.99	1.64	1.53
1	B	69	PRO	CA-C	6.97	1.61	1.52
1	B	63	GLN	N-CA	6.96	1.54	1.46
1	A	498	LEU	CA-C	6.96	1.61	1.52
1	A	194	GLN	CA-C	6.89	1.61	1.52
1	A	363	PHE	C-O	6.89	1.32	1.24
1	B	374	ILE	CA-CB	6.86	1.63	1.54
1	B	462	ASP	N-CA	-6.86	1.36	1.46
1	A	406	THR	CA-CB	6.86	1.64	1.53
1	A	367	TRP	CA-CB	6.85	1.65	1.53
1	B	466	ILE	N-CA	6.85	1.54	1.46
1	A	95	GLU	CA-C	-6.85	1.43	1.52
1	B	245	TYR	CG-CD2	6.83	1.53	1.39
1	B	124	ALA	CA-C	6.79	1.62	1.52
1	A	472	TYR	CA-CB	6.79	1.65	1.53
1	B	206	VAL	N-CA	6.78	1.51	1.46
1	B	55	LEU	N-CA	-6.78	1.38	1.46
1	A	497	TYR	CA-CB	6.78	1.63	1.53
1	B	74	VAL	C-O	6.78	1.31	1.23
1	A	460	ASN	CA-C	6.75	1.60	1.52
1	A	186	GLY	CA-C	6.74	1.59	1.52
1	A	241	GLU	CA-CB	6.73	1.61	1.52
1	A	266	THR	CA-C	6.71	1.62	1.53
1	A	156	TYR	C-O	6.71	1.32	1.23
1	B	406	THR	CA-CB	6.71	1.64	1.53
1	A	96	LEU	CG-CD1	6.70	1.74	1.52
1	A	323	CYS	CA-C	6.70	1.59	1.52
1	A	223	TRP	CA-C	6.68	1.61	1.52
1	B	135	HIS	CA-C	6.67	1.61	1.52
1	A	152	VAL	CA-CB	6.67	1.63	1.54
1	A	453	ILE	CA-C	6.61	1.61	1.52
1	B	75	HIS	C-O	6.60	1.32	1.23
1	B	84	PRO	CA-C	6.59	1.61	1.52
1	A	76	LEU	CG-CD2	6.59	1.74	1.52
1	A	235	VAL	N-CA	6.59	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	SER	N-CA	6.58	1.54	1.46
1	B	471	GLY	C-O	6.58	1.35	1.24
1	A	83	GLY	C-N	6.58	1.42	1.33
1	A	495	THR	CA-C	6.57	1.61	1.52
1	A	428	PHE	CA-C	-6.56	1.45	1.52
1	A	237	VAL	C-O	6.55	1.31	1.23
1	A	494	ASP	CA-CB	6.54	1.62	1.53
1	A	475	ARG	CG-CD	6.52	1.72	1.52
1	A	177	PHE	C-N	6.52	1.42	1.33
1	B	428	PHE	C-N	6.51	1.41	1.33
1	B	226	TYR	CG-CD1	6.51	1.53	1.39
1	A	252	ALA	C-O	6.48	1.31	1.24
1	B	328	TYR	N-CA	6.46	1.54	1.46
1	B	246	GLU	C-O	6.46	1.31	1.24
1	B	84	PRO	N-CA	-6.45	1.39	1.47
1	A	339	GLU	N-CA	6.45	1.54	1.46
1	B	212	VAL	CA-C	6.44	1.60	1.52
1	A	429	PRO	CA-C	6.44	1.60	1.52
1	B	234	LEU	CA-C	6.44	1.60	1.52
1	A	107	VAL	CA-CB	6.43	1.63	1.54
1	A	447	VAL	C-O	6.43	1.31	1.23
1	A	342	LYS	N-CA	6.43	1.53	1.45
1	B	469	GLU	CA-C	6.42	1.61	1.52
1	A	210	ASN	CA-CB	6.42	1.62	1.53
1	A	99	ILE	CA-CB	6.41	1.61	1.54
1	B	177	PHE	C-N	6.40	1.42	1.33
1	B	27	PRO	CA-C	6.37	1.61	1.52
1	B	150	GLY	N-CA	6.37	1.54	1.45
1	A	488	PRO	N-CA	6.37	1.54	1.47
1	B	255	ARG	C-O	6.36	1.31	1.24
1	B	131	LEU	C-O	6.35	1.31	1.24
1	A	223	TRP	N-CA	6.34	1.54	1.46
1	A	57	VAL	CA-CB	6.33	1.64	1.54
1	B	172	THR	C-O	6.32	1.32	1.23
1	B	269	GLU	C-O	-6.32	1.16	1.24
1	A	170	MET	C-O	6.32	1.31	1.24
1	A	250	ILE	CB-CG1	6.32	1.66	1.53
1	B	493	VAL	CA-CB	6.30	1.63	1.54
1	B	210	ASN	CB-CG	6.30	1.67	1.52
1	B	223	TRP	CA-C	6.30	1.61	1.52
1	A	249	TYR	CA-CB	6.29	1.63	1.53
1	B	495	THR	CA-C	6.29	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLY	C-O	6.28	1.32	1.24
1	A	151	ILE	CA-C	6.28	1.59	1.52
1	B	448	ILE	CA-C	6.28	1.60	1.52
1	A	211	ALA	CA-CB	6.28	1.63	1.53
1	A	211	ALA	CA-C	6.27	1.60	1.52
1	A	428	PHE	C-N	6.27	1.41	1.33
1	A	44	TYR	CA-C	6.26	1.60	1.52
1	B	210	ASN	CA-CB	6.26	1.62	1.53
1	B	322	LYS	N-CA	6.26	1.53	1.45
1	B	63	GLN	CA-C	6.26	1.60	1.52
1	B	337	GLN	CA-C	6.25	1.60	1.52
1	B	201	LEU	N-CA	6.24	1.53	1.46
1	B	53	ASN	CA-C	-6.24	1.44	1.52
1	A	157	MET	N-CA	6.23	1.53	1.45
1	A	463	LYS	C-N	-6.23	1.26	1.33
1	A	387	MET	N-CA	-6.21	1.38	1.46
1	A	84	PRO	CA-CB	6.21	1.62	1.53
1	B	110	ASP	CA-C	-6.21	1.46	1.53
1	B	262	SER	CA-C	-6.17	1.45	1.52
1	B	375	VAL	N-CA	6.17	1.53	1.46
1	A	444	THR	CA-CB	6.16	1.62	1.53
1	B	309	TRP	C-O	-6.16	1.16	1.24
1	A	50	SER	CA-C	6.15	1.61	1.52
1	A	180	ILE	CG1-CD1	-6.15	1.27	1.51
1	B	267	LEU	CA-CB	-6.12	1.43	1.53
1	A	226	TYR	CA-C	6.11	1.60	1.52
1	A	180	ILE	C-O	6.11	1.31	1.24
1	B	394	GLY	C-O	6.11	1.32	1.23
1	A	206	VAL	CA-CB	6.10	1.60	1.53
1	B	174	SER	C-O	6.10	1.30	1.23
1	B	249	TYR	CA-CB	6.10	1.62	1.53
1	B	443	ASP	CG-OD1	6.09	1.36	1.25
1	B	393	GLY	N-CA	6.09	1.54	1.45
1	A	126	GLU	CG-CD	6.08	1.67	1.52
1	A	291	VAL	N-CA	6.08	1.53	1.46
1	B	142	ASN	N-CA	6.07	1.54	1.46
1	A	105	ASP	CA-C	6.03	1.60	1.52
1	A	264	ARG	NE-CZ	-6.03	1.26	1.33
1	B	186	GLY	CA-C	6.02	1.58	1.52
1	B	96	LEU	CG-CD2	6.01	1.72	1.52
1	B	464	ILE	CA-CB	6.00	1.61	1.54
1	A	428	PHE	N-CA	6.00	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	CB-CG1	6.00	1.65	1.53
1	A	330	LEU	C-O	-6.00	1.17	1.24
1	B	312	ARG	CA-C	5.99	1.60	1.52
1	B	76	LEU	CG-CD2	5.99	1.72	1.52
1	B	158	ILE	CA-C	5.98	1.60	1.52
1	B	236	VAL	C-O	-5.97	1.17	1.24
1	B	267	LEU	N-CA	-5.97	1.39	1.46
1	A	173	ILE	C-O	5.97	1.30	1.24
1	B	467	ASN	CA-CB	5.96	1.60	1.52
1	B	74	VAL	CB-CG2	5.95	1.72	1.52
1	B	57	VAL	CB-CG2	5.94	1.72	1.52
1	B	251	SER	CA-CB	5.94	1.62	1.53
1	B	54	CYS	N-CA	5.94	1.55	1.46
1	A	250	ILE	CA-C	5.94	1.60	1.52
1	A	59	ASP	N-CA	5.93	1.53	1.46
1	A	317	GLN	N-CA	5.93	1.53	1.46
1	A	104	VAL	CA-CB	5.93	1.62	1.54
1	A	63	GLN	CA-CB	5.92	1.62	1.53
1	A	143	LYS	N-CA	5.92	1.53	1.46
1	B	476	THR	C-N	5.92	1.40	1.33
1	B	477	LYS	CA-C	5.92	1.59	1.52
1	A	336	ILE	CA-CB	5.91	1.61	1.54
1	A	446	HIS	CA-CB	5.90	1.65	1.53
1	B	264	ARG	CG-CD	5.90	1.70	1.52
1	A	326	ILE	N-CA	-5.90	1.39	1.46
1	A	488	PRO	CB-CG	5.89	1.79	1.49
1	A	151	ILE	C-O	-5.89	1.17	1.24
1	A	146	ASP	CA-C	5.89	1.60	1.52
1	A	177	PHE	CA-CB	5.88	1.62	1.53
1	A	329	HIS	CA-C	5.88	1.60	1.52
1	B	107	VAL	CA-CB	5.88	1.62	1.54
1	A	437	VAL	N-CA	5.88	1.53	1.46
1	B	38	LEU	C-O	5.87	1.30	1.24
1	A	231	ALA	CA-C	5.87	1.60	1.52
1	A	445	GLY	C-O	-5.87	1.18	1.23
1	A	448	ILE	CA-C	5.86	1.60	1.52
1	A	252	ALA	CA-CB	5.85	1.62	1.53
1	B	432	SER	CA-CB	5.85	1.62	1.54
1	B	208	ALA	N-CA	5.82	1.53	1.46
1	B	152	VAL	N-CA	5.81	1.52	1.46
1	A	77	PRO	N-CA	5.81	1.54	1.47
1	A	159	ASP	CA-C	5.80	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	SER	CA-C	5.80	1.60	1.52
1	A	126	GLU	CB-CG	5.79	1.69	1.52
1	A	162	THR	N-CA	5.79	1.53	1.46
1	B	478	ILE	CB-CG1	5.79	1.65	1.53
1	A	466	ILE	C-O	-5.79	1.18	1.24
1	B	274	GLY	CA-C	5.78	1.57	1.52
1	A	419	ALA	N-CA	5.77	1.53	1.46
1	A	74	VAL	CB-CG2	5.76	1.71	1.52
1	B	425	GLN	CA-C	5.75	1.60	1.52
1	A	256	GLU	CG-CD	-5.74	1.37	1.52
1	A	482	TYR	CA-C	5.74	1.60	1.52
1	B	384	LEU	CA-C	5.74	1.61	1.52
1	B	73	LEU	CA-C	5.73	1.60	1.52
1	A	68	VAL	CA-C	5.73	1.58	1.53
1	B	173	ILE	C-O	5.72	1.29	1.24
1	A	328	TYR	N-CA	5.72	1.53	1.46
1	B	250	ILE	CA-C	5.71	1.60	1.52
1	B	448	ILE	N-CA	-5.70	1.39	1.46
1	B	264	ARG	CZ-NH1	5.70	1.40	1.32
1	B	50	SER	CA-C	5.68	1.60	1.52
1	B	143	LYS	N-CA	5.66	1.53	1.45
1	A	312	ARG	CA-CB	5.65	1.62	1.53
1	B	147	ILE	C-N	-5.65	1.25	1.33
1	A	290	SER	CA-CB	-5.65	1.44	1.53
1	B	367	TRP	CA-CB	5.64	1.63	1.53
1	A	428	PHE	CA-CB	5.64	1.61	1.53
1	A	452	GLY	N-CA	5.63	1.52	1.44
1	A	464	ILE	CA-CB	5.63	1.60	1.53
1	B	168	ILE	CA-CB	5.62	1.60	1.54
1	A	322	LYS	CG-CD	5.62	1.69	1.52
1	B	151	ILE	C-O	-5.62	1.17	1.24
1	A	474	VAL	C-O	5.61	1.29	1.24
1	A	97	ALA	N-CA	5.60	1.51	1.46
1	A	168	ILE	CA-CB	5.60	1.61	1.54
1	B	46	ALA	CA-CB	5.60	1.62	1.53
1	A	446	HIS	N-CA	-5.59	1.39	1.46
1	A	313	LEU	CA-C	5.58	1.60	1.52
1	A	350	VAL	CA-CB	5.58	1.64	1.55
1	A	38	LEU	CA-C	5.57	1.60	1.52
1	A	35	ASP	CA-C	-5.56	1.46	1.52
1	A	313	LEU	N-CA	5.56	1.53	1.46
1	B	184	MET	N-CA	5.56	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	PRO	CA-C	5.55	1.59	1.52
1	A	315	MET	N-CA	-5.55	1.39	1.46
1	B	432	SER	C-O	5.54	1.30	1.24
1	A	254	LEU	CA-C	5.53	1.60	1.52
1	A	379	ILE	CA-CB	5.53	1.61	1.54
1	A	108	SER	CA-CB	5.53	1.62	1.53
1	A	187	LEU	C-O	-5.51	1.17	1.24
1	A	272	GLN	CG-CD	5.51	1.65	1.52
1	A	235	VAL	CB-CG1	-5.50	1.34	1.52
1	B	83	GLY	C-N	5.49	1.40	1.33
1	A	91	LYS	C-O	5.48	1.30	1.24
1	B	312	ARG	CA-CB	5.48	1.61	1.53
1	B	472	TYR	CA-C	-5.47	1.46	1.52
1	A	236	VAL	C-O	-5.47	1.18	1.24
1	A	337	GLN	CA-C	5.46	1.59	1.52
1	A	371	ASP	CA-C	5.44	1.60	1.52
1	B	35	ASP	CG-OD1	5.44	1.35	1.25
1	A	294	PHE	C-O	5.44	1.30	1.24
1	B	460	ASN	C-N	-5.44	1.26	1.33
1	B	420	ALA	CA-C	5.43	1.60	1.52
1	A	75	HIS	C-O	5.43	1.31	1.23
1	A	476	THR	C-N	5.42	1.40	1.33
1	A	219	LEU	CA-C	5.42	1.59	1.52
1	B	70	GLY	CA-C	-5.42	1.44	1.51
1	B	475	ARG	CA-C	5.42	1.59	1.52
1	B	242	ARG	CZ-NH2	5.41	1.40	1.33
1	B	261	ARG	CG-CD	5.41	1.68	1.52
1	B	262	SER	N-CA	5.41	1.52	1.45
1	B	148	ARG	CA-CB	5.40	1.62	1.53
1	A	93	GLY	N-CA	5.40	1.52	1.45
1	B	393	GLY	C-O	5.39	1.31	1.23
1	B	272	GLN	CG-CD	5.39	1.65	1.52
1	A	449[A]	SER	N-CA	5.39	1.52	1.45
1	A	449[B]	SER	N-CA	5.39	1.52	1.45
1	B	264	ARG	NE-CZ	-5.38	1.27	1.33
1	A	467	ASN	C-O	5.38	1.29	1.23
1	A	326	ILE	CA-CB	5.38	1.61	1.54
1	B	465	ILE	CA-C	5.38	1.60	1.53
1	B	498	LEU	C-O	-5.37	1.17	1.24
1	B	338	GLN	C-O	5.37	1.30	1.24
1	A	241	GLU	CA-C	-5.37	1.47	1.53
1	A	474	VAL	CA-CB	5.36	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	PRO	C-O	5.36	1.29	1.23
1	B	293	TYR	CA-C	5.36	1.59	1.52
1	A	245	TYR	CG-CD2	5.36	1.50	1.39
1	B	77	PRO	N-CA	5.36	1.53	1.47
1	B	386	VAL	CA-C	5.36	1.58	1.52
1	A	38	LEU	C-O	5.35	1.30	1.24
1	A	258	HIS	CA-C	5.34	1.59	1.52
1	B	173	ILE	CB-CG1	5.34	1.64	1.53
1	A	264	ARG	CD-NE	5.33	1.53	1.46
1	B	270	ILE	CA-CB	-5.32	1.47	1.54
1	B	153	ARG	CA-C	5.32	1.58	1.52
1	A	173	ILE	CA-CB	5.32	1.62	1.54
1	A	183	LEU	CB-CG	5.30	1.64	1.53
1	B	208	ALA	CA-CB	5.30	1.62	1.53
1	A	325	THR	CB-CG2	5.30	1.70	1.52
1	A	351	GLU	CB-CG	5.30	1.68	1.52
1	A	184	MET	CA-CB	5.29	1.61	1.53
1	A	240	GLU	CG-CD	-5.29	1.38	1.52
1	A	201	LEU	N-CA	5.28	1.52	1.46
1	B	347	GLU	C-O	-5.28	1.17	1.24
1	A	371	ASP	C-N	5.27	1.39	1.33
1	A	293	TYR	CA-C	5.27	1.59	1.52
1	A	129	SER	CA-C	5.27	1.59	1.52
1	B	91	LYS	C-O	5.27	1.30	1.24
1	B	48	VAL	C-O	5.26	1.30	1.24
1	B	342	LYS	C-N	5.26	1.39	1.33
1	B	497	TYR	CA-CB	5.26	1.61	1.53
1	A	195	TYR	C-O	5.26	1.30	1.24
1	A	48	VAL	CA-C	5.26	1.59	1.52
1	B	394	GLY	N-CA	5.25	1.50	1.45
1	B	35	ASP	CG-OD2	5.25	1.35	1.25
1	B	488	PRO	N-CA	5.24	1.54	1.47
1	A	357	ALA	CA-C	5.24	1.59	1.52
1	B	297	GLY	N-CA	5.23	1.52	1.45
1	B	121	THR	C-O	5.23	1.30	1.24
1	B	248	HIS	CA-CB	-5.22	1.45	1.53
1	B	179	LEU	CA-C	5.22	1.59	1.52
1	A	475	ARG	CA-C	5.18	1.58	1.52
1	B	316	GLU	CA-CB	5.17	1.61	1.53
1	A	219	LEU	CA-CB	5.17	1.61	1.53
1	A	242	ARG	CZ-NH2	5.17	1.40	1.33
1	A	383	GLU	CA-C	5.17	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	LYS	CB-CG	5.16	1.68	1.52
1	A	437	VAL	C-O	-5.14	1.18	1.24
1	B	266	THR	CA-C	5.14	1.60	1.53
1	A	190	SER	CA-C	5.13	1.59	1.52
1	A	210	ASN	CB-CG	5.13	1.64	1.52
1	A	53	ASN	CA-C	-5.13	1.46	1.52
1	A	255	ARG	CZ-NH2	5.11	1.40	1.33
1	A	188	HIS	N-CA	5.11	1.52	1.46
1	A	255	ARG	NE-CZ	5.10	1.38	1.33
1	B	57	VAL	CA-CB	5.08	1.62	1.54
1	A	334	LYS	C-O	-5.08	1.17	1.24
1	B	216	ALA	CA-CB	-5.08	1.45	1.53
1	B	38	LEU	CA-C	5.07	1.59	1.52
1	B	44	TYR	CA-C	5.07	1.59	1.52
1	A	208	ALA	CA-CB	5.07	1.61	1.53
1	A	203	SER	CA-C	-5.07	1.45	1.52
1	A	326	ILE	C-O	-5.06	1.18	1.24
1	B	471	GLY	N-CA	5.05	1.53	1.45
1	A	46	ALA	CA-C	5.05	1.59	1.52
1	A	69	PRO	CB-CG	5.05	1.74	1.49
1	A	142	ASN	N-CA	5.04	1.52	1.46
1	A	156	TYR	CE1-CZ	5.04	1.50	1.38
1	A	322	LYS	N-CA	5.04	1.52	1.46
1	A	84	PRO	N-CA	-5.04	1.41	1.47
1	B	372	SER	N-CA	5.04	1.52	1.46
1	A	478	ILE	CB-CG2	5.03	1.69	1.52
1	B	97	ALA	CA-C	5.03	1.58	1.52
1	B	211	ALA	CA-CB	5.02	1.61	1.53
1	B	241	GLU	CA-C	-5.02	1.48	1.53
1	A	145	GLU	N-CA	5.02	1.52	1.46
1	B	231	ALA	CA-C	5.02	1.59	1.53
1	B	261	ARG	NE-CZ	5.02	1.38	1.33
1	A	283	SER	CA-C	-5.00	1.46	1.52
1	B	157	MET	N-CA	5.00	1.52	1.45

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	-16.18	105.32	121.50
1	B	460	ASN	CA-C-N	-14.83	93.21	121.54
1	B	460	ASN	C-N-CA	-14.83	93.21	121.54
1	B	145	GLU	CA-C-N	-13.99	101.46	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	GLU	C-N-CA	-13.99	101.46	122.86
1	B	26	PRO	CA-C-N	-12.01	104.83	119.84
1	B	26	PRO	C-N-CA	-12.01	104.83	119.84
1	B	264	ARG	NE-CZ-NH1	-11.61	109.89	121.50
1	B	299	THR	CB-CA-C	-11.23	91.19	109.15
1	A	488	PRO	CA-C-N	-11.02	99.81	121.41
1	A	488	PRO	C-N-CA	-11.02	99.81	121.41
1	A	264	ARG	NE-CZ-NH2	10.77	128.90	119.20
1	B	336	ILE	N-CA-C	10.63	121.47	110.62
1	B	36	GLN	OE1-CD-NE2	-10.19	112.41	122.60
1	B	317	GLN	OE1-CD-NE2	-9.90	112.70	122.60
1	A	487	LEU	CA-C-N	9.83	129.88	119.76
1	A	487	LEU	C-N-CA	9.83	129.88	119.76
1	A	264	ARG	CD-NE-CZ	-9.50	111.10	124.40
1	B	146	ASP	CA-C-N	-9.28	111.05	123.12
1	B	146	ASP	C-N-CA	-9.28	111.05	123.12
1	A	162	THR	CA-C-N	-9.24	108.29	122.16
1	A	162	THR	C-N-CA	-9.24	108.29	122.16
1	B	147	ILE	CA-C-N	-9.21	104.09	121.68
1	B	147	ILE	C-N-CA	-9.21	104.09	121.68
1	A	431	THR	OG1-CB-CG2	9.09	127.49	109.30
1	A	240	GLU	CB-CG-CD	-8.92	97.44	112.60
1	B	242	ARG	NE-CZ-NH2	8.90	127.21	119.20
1	B	462	ASP	N-CA-C	-8.89	101.97	113.17
1	B	240	GLU	CB-CG-CD	-8.87	97.52	112.60
1	A	167	GLN	OE1-CD-NE2	-8.70	113.90	122.60
1	A	488	PRO	O-C-N	-8.36	112.91	123.03
1	B	460	ASN	O-C-N	-8.07	111.86	122.59
1	B	130	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	A	143	LYS	CA-C-N	-7.74	112.47	122.77
1	A	143	LYS	C-N-CA	-7.74	112.47	122.77
1	B	473	MET	CG-SD-CE	-7.70	83.95	100.90
1	A	246	GLU	CA-C-O	-7.64	112.80	120.82
1	B	463	LYS	CA-C-N	-7.52	113.27	122.90
1	B	463	LYS	C-N-CA	-7.52	113.27	122.90
1	B	183	LEU	N-CA-C	-7.49	102.79	112.23
1	A	264	ARG	CG-CD-NE	7.43	128.34	112.00
1	A	240	GLU	CG-CD-OE1	-7.37	101.45	118.40
1	A	475	ARG	NE-CZ-NH2	-7.35	112.58	119.20
1	A	95	GLU	N-CA-C	7.31	119.00	111.04
1	A	226	TYR	N-CA-C	-7.27	103.35	111.28
1	A	223	TRP	O-C-N	7.26	129.81	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	GLN	CG-CD-NE2	7.24	127.25	116.40
1	A	242	ARG	NE-CZ-NH2	7.17	125.66	119.20
1	A	83	GLY	CA-C-N	7.09	127.01	119.85
1	A	83	GLY	C-N-CA	7.09	127.01	119.85
1	B	36	GLN	CG-CD-NE2	7.09	127.04	116.40
1	B	264	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	B	473	MET	CA-CB-CG	7.00	128.10	114.10
1	A	235	VAL	CB-CA-C	6.95	120.29	110.84
1	A	373	ASP	N-CA-C	-6.86	102.16	112.04
1	A	392	GLU	CA-C-N	-6.84	112.99	122.63
1	A	392	GLU	C-N-CA	-6.84	112.99	122.63
1	B	68	VAL	O-C-N	6.80	125.66	121.37
1	A	351	GLU	N-CA-C	-6.77	104.89	113.43
1	A	161	LYS	N-CA-C	-6.74	99.44	109.15
1	B	268	THR	N-CA-CB	6.68	119.97	109.82
1	A	381	ASN	CA-C-N	6.67	126.62	119.28
1	A	381	ASN	C-N-CA	6.67	126.62	119.28
1	B	226	TYR	N-CA-C	-6.61	103.18	111.11
1	B	426	ARG	CB-CG-CD	6.56	126.39	111.30
1	B	160	GLU	N-CA-C	6.54	118.07	111.07
1	B	476	THR	CA-C-O	6.54	128.18	120.66
1	B	488	PRO	N-CA-C	6.47	122.26	113.84
1	A	132	LEU	N-CA-C	6.46	118.32	111.28
1	A	106	ARG	CB-CG-CD	6.46	126.15	111.30
1	A	167	GLN	CG-CD-NE2	6.45	126.08	116.40
1	B	436	LEU	CD1-CG-CD2	-6.45	96.60	110.80
1	B	431	THR	N-CA-CB	-6.44	100.66	110.45
1	B	424	MET	CG-SD-CE	-6.43	86.74	100.90
1	B	242	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	A	336	ILE	N-CA-C	6.37	117.11	110.62
1	B	28	LEU	N-CA-C	-6.34	101.98	110.55
1	A	310	ARG	CD-NE-CZ	6.34	133.28	124.40
1	B	102	GLU	N-CA-C	6.34	118.19	111.28
1	B	234	LEU	CA-C-N	-6.32	114.96	122.93
1	B	234	LEU	C-N-CA	-6.32	114.96	122.93
1	A	310	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	234	LEU	CA-C-N	-6.29	115.01	122.93
1	A	234	LEU	C-N-CA	-6.29	115.01	122.93
1	B	493	VAL	N-CA-C	6.25	116.86	110.05
1	B	431	THR	OG1-CB-CG2	6.25	121.79	109.30
1	B	240	GLU	CG-CD-OE1	-6.24	104.05	118.40
1	A	235	VAL	CG1-CB-CG2	6.13	124.29	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	CG-CD-NE	-6.13	98.52	112.00
1	B	464	ILE	N-CA-CB	6.08	118.33	111.21
1	B	149[A]	MET	N-CA-C	6.08	119.07	110.14
1	B	149[B]	MET	N-CA-C	6.08	119.07	110.14
1	B	426	ARG	N-CA-CB	6.00	118.99	109.51
1	A	444	THR	CA-CB-OG1	-5.96	100.65	109.60
1	B	106	ARG	CD-NE-CZ	-5.96	116.05	124.40
1	A	326	ILE	CA-C-O	-5.96	114.75	120.95
1	B	223	TRP	CA-C-N	5.96	128.27	120.28
1	B	223	TRP	C-N-CA	5.96	128.27	120.28
1	B	35	ASP	CB-CA-C	5.95	119.01	109.61
1	B	453	ILE	N-CA-C	-5.93	98.59	107.37
1	B	458	LEU	CA-C-N	-5.85	113.11	122.53
1	B	458	LEU	C-N-CA	-5.85	113.11	122.53
1	A	170	MET	CA-C-N	-5.79	114.88	123.11
1	A	170	MET	C-N-CA	-5.79	114.88	123.11
1	A	35	ASP	CB-CA-C	-5.79	99.40	109.64
1	B	68	VAL	CA-C-O	-5.77	114.86	119.25
1	A	334	LYS	N-CA-C	-5.76	104.97	112.23
1	B	145	GLU	O-C-N	-5.76	116.54	122.64
1	B	199	LEU	CA-C-N	-5.75	110.15	121.41
1	B	199	LEU	C-N-CA	-5.75	110.15	121.41
1	A	183	LEU	N-CA-C	-5.74	105.16	111.82
1	B	99	ILE	N-CA-C	5.73	115.92	110.53
1	A	310	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	473	MET	CG-SD-CE	-5.72	88.33	100.90
1	B	323	CYS	C-N-CD	5.71	133.16	120.60
1	B	378	ALA	N-CA-C	5.71	118.71	111.69
1	B	394	GLY	O-C-N	5.70	128.59	122.60
1	B	167	GLN	N-CA-C	5.70	117.97	109.59
1	A	194	GLN	CB-CA-C	-5.68	101.25	110.79
1	B	199	LEU	N-CA-C	-5.68	101.79	110.14
1	A	28	LEU	N-CA-C	-5.67	102.89	110.55
1	A	499	THR	CB-CA-C	-5.67	96.63	109.10
1	A	148	ARG	CA-CB-CG	5.67	125.44	114.10
1	A	261	ARG	N-CA-C	5.66	118.66	110.28
1	A	431	THR	N-CA-CB	-5.66	101.85	110.45
1	B	313	LEU	O-C-N	5.65	127.97	122.09
1	B	461	LYS	CA-C-N	5.65	131.86	122.54
1	B	461	LYS	C-N-CA	5.65	131.86	122.54
1	B	80	LEU	N-CA-C	5.62	118.13	111.33
1	B	473	MET	N-CA-C	-5.61	100.77	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	460	ASN	N-CA-CB	5.60	119.95	110.49
1	B	199	LEU	O-C-N	-5.59	115.19	122.97
1	B	348	ARG	N-CA-C	-5.59	105.28	111.71
1	A	257	LYS	N-CA-C	-5.58	106.14	113.12
1	A	123	ASN	N-CA-C	5.58	117.44	111.36
1	A	180	ILE	CB-CG1-CD1	-5.56	102.13	113.80
1	B	375	VAL	N-CA-C	5.55	115.75	110.42
1	A	289	ILE	CA-C-N	-5.55	112.32	121.92
1	A	289	ILE	C-N-CA	-5.55	112.32	121.92
1	B	482	TYR	N-CA-C	-5.52	104.01	111.13
1	A	426	ARG	CB-CG-CD	5.51	123.97	111.30
1	B	168	ILE	CB-CG1-CD1	-5.51	102.23	113.80
1	A	406	THR	N-CA-C	-5.50	104.93	111.69
1	A	281	THR	N-CA-C	5.48	117.64	109.25
1	B	431	THR	CA-CB-OG1	5.47	117.81	109.60
1	B	464	ILE	CA-CB-CG2	5.46	119.79	110.50
1	B	97	ALA	O-C-N	5.45	124.69	120.38
1	A	177	PHE	N-CA-C	5.44	119.95	113.31
1	A	204	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	431	THR	CA-CB-OG1	5.42	117.74	109.60
1	A	223	TRP	CA-C-N	5.42	127.54	120.28
1	A	223	TRP	C-N-CA	5.42	127.54	120.28
1	B	141	ILE	N-CA-C	-5.42	107.08	113.42
1	A	80	LEU	N-CA-C	5.39	117.91	111.71
1	B	498	LEU	O-C-N	5.38	129.34	123.04
1	B	444	THR	CA-CB-OG1	-5.38	101.53	109.60
1	B	472	TYR	N-CA-C	5.38	116.45	108.60
1	A	205	ARG	NE-CZ-NH1	5.35	126.85	121.50
1	B	223	TRP	O-C-N	5.35	127.79	122.12
1	B	330	LEU	CA-C-O	-5.35	114.88	120.55
1	B	433	PRO	N-CA-C	-5.34	102.81	111.19
1	B	254	LEU	N-CA-C	-5.32	105.38	111.07
1	B	151	ILE	CA-C-N	-5.26	115.46	122.77
1	B	151	ILE	C-N-CA	-5.26	115.46	122.77
1	B	477	LYS	CG-CD-CE	-5.26	99.21	111.30
1	A	335	LYS	N-CA-C	5.25	117.41	111.11
1	A	482	TYR	N-CA-C	-5.24	104.87	111.27
1	A	206	VAL	CA-C-N	-5.24	114.37	119.76
1	A	206	VAL	C-N-CA	-5.24	114.37	119.76
1	B	229	PRO	CA-C-O	5.23	126.08	118.86
1	B	475	ARG	CD-NE-CZ	5.23	131.73	124.40
1	B	461	LYS	O-C-N	5.23	129.55	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	CA-CB-CG	-5.23	103.64	114.10
1	A	191	LEU	N-CA-C	-5.22	105.67	111.36
1	A	179	LEU	N-CA-C	-5.21	105.04	111.40
1	A	325	THR	N-CA-C	5.19	117.38	110.53
1	B	374	ILE	CB-CA-C	5.19	120.61	112.16
1	B	81	LEU	CB-CG-CD1	5.19	126.26	110.70
1	A	96	LEU	CB-CG-CD1	5.18	126.23	110.70
1	B	342	LYS	CA-C-N	5.17	125.47	119.93
1	B	342	LYS	C-N-CA	5.17	125.47	119.93
1	A	147	ILE	N-CA-CB	5.17	118.18	111.67
1	A	126	GLU	CA-CB-CG	5.16	124.42	114.10
1	B	76	LEU	CA-C-N	-5.16	114.26	119.83
1	B	76	LEU	C-N-CA	-5.16	114.26	119.83
1	B	25	ALA	CA-C-N	5.16	125.69	120.38
1	B	25	ALA	C-N-CA	5.16	125.69	120.38
1	B	245	TYR	CA-CB-CG	-5.15	104.63	113.90
1	A	163	LYS	N-CA-C	-5.14	99.61	108.56
1	A	428	PHE	CA-C-N	-5.13	114.95	120.03
1	A	428	PHE	C-N-CA	-5.13	114.95	120.03
1	B	315	MET	N-CA-C	5.12	116.86	111.28
1	B	201	LEU	N-CA-C	5.12	117.79	109.24
1	B	85	PHE	CA-C-N	-5.10	114.70	119.85
1	B	85	PHE	C-N-CA	-5.10	114.70	119.85
1	B	253	LEU	N-CA-C	5.10	117.23	111.11
1	A	102	GLU	N-CA-C	5.08	116.51	111.07
1	A	393	GLY	N-CA-C	-5.08	108.00	114.85
1	A	467	ASN	CB-CA-C	-5.08	105.05	111.70
1	B	59	ASP	CA-C-N	5.07	127.78	120.38
1	B	59	ASP	C-N-CA	5.07	127.78	120.38
1	B	299	THR	CA-CB-CG2	5.05	119.08	110.50
1	B	200	GLY	CA-C-N	-5.04	114.57	122.73
1	B	200	GLY	C-N-CA	-5.04	114.57	122.73
1	A	475	ARG	O-C-N	5.02	129.22	123.29
1	A	223	TRP	CA-C-O	-5.02	115.23	120.55
1	B	469	GLU	N-CA-C	-5.01	102.44	109.96
1	A	310	ARG	CA-CB-CG	5.01	124.12	114.10
1	A	436	LEU	CD1-CG-CD2	-5.01	99.79	110.80
1	B	151	ILE	N-CA-CB	5.00	118.20	112.15

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	A	431	THR	CB

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	372	SER	Peptide
1	A	392	GLU	Peptide
1	A	417	GLU	Peptide
1	B	148	ARG	Mainchain,Peptide
1	B	317	GLN	Mainchain
1	B	395	GLY	Peptide
1	B	459[A]	ARG	Sidechain

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	3828	0	3850	151	0
1	B	3855	0	3865	181	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	42	0	33	15	0
3	B	42	0	30	21	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	5	0	0	4	0
5	B	5	0	0	5	0
6	A	371	0	0	35	0
6	B	363	0	0	31	0
All	All	8571	0	7802	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LEU:CD1	1:A:96:LEU:CG	1.74	1.62
1:B:459[B]:ARG:CB	1:B:459[B]:ARG:CG	1.81	1.59
1:B:240:GLU:CG	1:B:240:GLU:CB	1.76	1.58
1:A:240:GLU:CG	1:A:240:GLU:CB	1.74	1.57
1:A:264:ARG:CD	1:A:264:ARG:CG	1.77	1.56
1:B:459[B]:ARG:CG	1:B:459[B]:ARG:CD	1.85	1.49
1:A:488:PRO:CB	1:A:488:PRO:CG	1.79	1.49
1:A:69:PRO:CB	1:A:69:PRO:CG	1.74	1.44
1:A:161:LYS:O	1:A:162:THR:HG22	1.15	1.27
1:B:247[A]:GLN:OE1	1:B:264:ARG:NH1	1.69	1.26
1:A:204:ASN:HB2	6:A:737:HOH:O	1.20	1.26
1:B:126:GLU:HG3	6:B:584:HOH:O	1.35	1.24
1:A:247[B]:GLN:NE2	1:A:264:ARG:NH1	1.87	1.21
1:A:240:GLU:HB2	1:A:240:GLU:OE1	1.39	1.20
1:B:204:ASN:HB2	6:B:789:HOH:O	1.46	1.15
1:B:240:GLU:OE1	1:B:240:GLU:HB2	1.48	1.12
1:B:176[B]:SER:OG	3:B:501:HGS:HA3	1.46	1.11
1:A:197:LYS:HG2	6:A:811:HOH:O	1.46	1.11
1:A:106:ARG:HG2	1:A:106:ARG:HH11	0.97	1.11
1:B:438[B]:ARG:NH1	6:B:779:HOH:O	1.83	1.10
1:A:63:GLN:OE1	1:A:64[A]:ARG:HG3	1.52	1.08
1:B:149[A]:MET:HE3	1:B:323:CYS:HB2	1.13	1.08
1:A:247[B]:GLN:NE2	1:A:264:ARG:HH12	1.47	1.07
1:A:161:LYS:O	1:A:162:THR:CG2	2.00	1.07
1:A:149[B]:MET:HE3	1:A:323:CYS:HB2	1.07	1.06
1:A:240:GLU:CB	1:A:240:GLU:OE1	1.95	1.04
1:A:96:LEU:CD1	1:A:96:LEU:HG	1.86	1.03
1:A:106:ARG:HH11	1:A:106:ARG:CG	1.71	1.03
1:B:162:THR:HG23	1:B:164:SER:OG	1.56	1.03
1:A:27:PRO:HB3	6:A:694:HOH:O	1.55	1.03
1:B:240:GLU:CB	1:B:240:GLU:OE1	2.04	1.02
1:A:182:CYS:HB2	3:A:506:HGS:SG2	2.01	1.01
1:A:431:THR:HG23	6:A:527:HOH:O	1.59	0.99
3:A:501:HGS:C2	5:A:505:SO4:O4	2.10	0.99
1:A:149[B]:MET:CE	1:A:323:CYS:HB2	1.93	0.98
1:A:240:GLU:CB	1:A:240:GLU:CD	2.36	0.97
1:B:369:LEU:HD22	1:B:423:LEU:HD22	1.48	0.96
1:A:149[B]:MET:HE3	1:A:323:CYS:CB	1.95	0.96
1:B:459[B]:ARG:NH2	6:B:693:HOH:O	1.99	0.96
1:B:149[A]:MET:CE	1:B:323:CYS:HB2	1.94	0.96
1:B:431:THR:HG23	6:B:524:HOH:O	1.64	0.95
1:B:240:GLU:CB	1:B:240:GLU:CD	2.39	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLN:HE22	1:B:67[B]:ARG:HH22	0.98	0.95
1:B:146:ASP:OD1	1:B:146:ASP:O	1.85	0.94
1:A:247[B]:GLN:HE22	1:A:264:ARG:NH1	1.54	0.94
1:B:475:ARG:NH1	3:B:501:HGS:O41	2.00	0.93
1:A:106:ARG:HG2	1:A:106:ARG:NH1	1.77	0.93
3:B:501:HGS:C2	5:B:505:SO4:O4	2.15	0.93
1:B:63:GLN:NE2	1:B:67[B]:ARG:HH22	1.67	0.92
1:B:149[A]:MET:HE3	1:B:323:CYS:CB	1.99	0.92
1:B:347:GLU:OE1	1:B:360[B]:ARG:NH2	2.01	0.92
1:A:247[B]:GLN:HE21	1:A:264:ARG:HH12	1.12	0.91
1:B:162:THR:CG2	1:B:164:SER:OG	2.19	0.91
1:B:475:ARG:HD3	3:B:501:HGS:O41	1.67	0.91
1:B:148:ARG:HD2	6:B:756:HOH:O	1.72	0.89
3:B:501:HGS:HA2	5:B:505:SO4:O4	1.73	0.89
1:B:63:GLN:HE22	1:B:67[B]:ARG:NH2	1.69	0.89
1:B:147:ILE:O	1:B:148:ARG:CG	2.22	0.88
1:A:264:ARG:CD	1:A:264:ARG:CB	2.52	0.88
1:B:475:ARG:HH11	3:B:501:HGS:C4	1.87	0.88
1:B:176[B]:SER:OG	3:B:501:HGS:CA3	2.22	0.86
1:A:247[B]:GLN:HE22	1:A:264:ARG:HH11	1.16	0.86
1:A:499:THR:OXT	1:A:499:THR:OG1	1.76	0.85
1:B:94[A]:CYS:SG	6:B:658:HOH:O	2.35	0.84
1:A:145:GLU:HB2	6:A:666:HOH:O	1.76	0.83
1:A:395:GLY:C	6:A:721:HOH:O	2.21	0.82
1:B:25:ALA:N	1:B:26:PRO:CD	2.42	0.82
1:B:299:THR:HG23	6:B:835:HOH:O	1.79	0.82
1:A:369:LEU:HD22	1:A:423:LEU:HD22	1.60	0.82
1:A:178:ALA:O	1:A:182:CYS:SG	2.38	0.81
1:B:89:HIS:HE1	1:B:163:LYS:O	1.63	0.81
1:B:146:ASP:CB	1:B:461:LYS:NZ	2.44	0.81
1:A:140:GLN:HB3	6:A:585:HOH:O	1.81	0.80
1:A:202:ASN:HD22	1:A:204:ASN:H	1.29	0.80
1:B:67[B]:ARG:NE	1:B:240:GLU:OE2	2.12	0.80
1:A:194:GLN:HG3	6:A:838:HOH:O	1.80	0.80
1:B:146:ASP:HB2	1:B:461:LYS:NZ	1.97	0.79
1:B:176[B]:SER:HG	3:B:501:HGS:HA3	1.47	0.79
1:B:148:ARG:HD3	1:B:325:THR:CG2	2.12	0.79
1:A:145:GLU:O	1:A:145:GLU:HG2	1.81	0.79
1:B:194:GLN:HG3	6:B:751:HOH:O	1.82	0.78
1:B:147:ILE:O	1:B:148:ARG:HG3	1.83	0.78
1:A:176[A]:SER:OG	3:A:501:HGS:HA3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:OE2	1:B:360[B]:ARG:NH1	2.16	0.77
1:B:369:LEU:CD2	1:B:423:LEU:HD22	2.14	0.77
1:B:147:ILE:O	1:B:148:ARG:CB	2.26	0.77
1:B:146:ASP:HB2	1:B:461:LYS:HZ2	1.51	0.76
3:B:501:HGS:CA2	5:B:505:SO4:O4	2.33	0.76
3:A:501:HGS:HA2	5:A:505:SO4:O4	1.86	0.75
1:A:352:ASN:HD22	1:A:352:ASN:C	1.95	0.75
1:A:105:ASP:OD1	1:A:148:ARG:HD2	1.87	0.74
1:A:148:ARG:NH1	1:A:459:ARG:HD3	2.03	0.74
1:A:159:ASP:HB2	1:A:427:ILE:HG23	1.69	0.74
1:A:246:GLU:C	1:A:247[B]:GLN:CA	2.61	0.74
1:A:388:LYS:HE3	6:A:568:HOH:O	1.87	0.73
1:B:299:THR:HG22	1:B:301:LYS:H	1.54	0.73
1:A:439:ASP:CG	6:A:875:HOH:O	2.32	0.73
1:A:235:VAL:HG21	1:A:247[B]:GLN:HG2	1.70	0.72
1:A:182:CYS:CB	3:A:506:HGS:SG2	2.76	0.72
1:A:396:ASN:N	6:A:721:HOH:O	2.23	0.72
3:A:501:HGS:CA2	5:A:505:SO4:O4	2.38	0.71
1:B:146:ASP:CB	1:B:461:LYS:HZ3	2.01	0.71
1:A:27:PRO:CB	6:A:694:HOH:O	2.24	0.71
1:A:438[A]:ARG:NE	6:A:719:HOH:O	2.23	0.71
1:B:204:ASN:CB	6:B:789:HOH:O	2.18	0.71
6:A:511:HOH:O	1:B:194:GLN:CG	2.37	0.71
1:A:126:GLU:HB3	6:A:881:HOH:O	1.91	0.71
1:A:63:GLN:H	1:A:63:GLN:NE2	1.88	0.71
1:B:202:ASN:HD22	1:B:204:ASN:H	1.40	0.70
1:B:383:GLU:HG2	1:B:384:LEU:HD13	1.71	0.70
3:B:501:HGS:HB1	6:B:545:HOH:O	1.90	0.70
1:A:63:GLN:OE1	1:A:64[A]:ARG:CG	2.35	0.70
1:A:145:GLU:O	1:A:145:GLU:CG	2.40	0.69
1:B:347:GLU:CD	1:B:360[B]:ARG:HH22	1.99	0.69
1:A:159:ASP:O	1:A:162:THR:O	2.10	0.69
1:B:130:ARG:NH2	1:B:306:GLU:OE1	2.25	0.69
1:A:106:ARG:CG	1:A:106:ARG:NH1	2.43	0.69
1:A:176[A]:SER:OG	3:A:501:HGS:CA3	2.40	0.68
6:A:511:HOH:O	1:B:194:GLN:HG3	1.94	0.68
1:B:137:LYS:O	1:B:141:ILE:HG23	1.93	0.67
1:B:298:TYR:CZ	3:B:501:HGS:HG1A	2.30	0.67
1:B:26:PRO:O	1:B:27:PRO:O	2.13	0.67
1:A:63:GLN:H	1:A:63:GLN:CD	2.04	0.66
1:A:369:LEU:CD2	1:A:423:LEU:HD22	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:N	1:B:26:PRO:HD3	2.10	0.66
1:B:148:ARG:CD	1:B:325:THR:CG2	2.73	0.66
1:A:240:GLU:CG	1:A:240:GLU:CA	2.71	0.66
1:B:146:ASP:HB3	1:B:461:LYS:NZ	2.09	0.66
1:A:176[A]:SER:OG	3:A:501:HGS:N3	2.29	0.66
1:B:117:SER:HB3	1:B:339:GLU:HG3	1.78	0.65
1:B:86:PRO:HA	1:B:499:THR:OG1	1.96	0.65
1:B:240:GLU:CG	1:B:240:GLU:CA	2.74	0.64
1:A:94[A]:CYS:SG	6:A:671:HOH:O	2.22	0.64
1:A:63:GLN:CD	1:A:63:GLN:N	2.56	0.63
1:B:144:LYS:HD3	1:B:461:LYS:HZ1	1.63	0.63
3:A:501:HGS:HA4	6:A:835:HOH:O	1.98	0.63
1:B:350:VAL:HG22	1:B:356:ILE:HG12	1.81	0.62
1:A:73:LEU:HB2	1:B:73:LEU:HB2	1.81	0.62
1:A:162:THR:O	1:A:162:THR:HG23	1.98	0.62
1:B:148:ARG:HD2	1:B:325:THR:HG21	1.82	0.61
1:A:67[B]:ARG:HD3	1:A:240:GLU:OE2	2.00	0.61
3:B:501:HGS:N3	5:B:505:SO4:O4	2.33	0.61
1:B:353:LYS:HD2	6:B:858:HOH:O	2.01	0.61
1:A:122:LYS:HD2	1:A:132:LEU:HD13	1.83	0.60
1:B:352:ASN:C	1:B:352:ASN:HD22	2.09	0.60
1:B:382:PRO:HB2	1:B:400:GLY:O	2.01	0.59
1:A:298:TYR:OH	3:A:501:HGS:HG1A	2.02	0.59
1:A:369:LEU:HD12	1:A:418:ASP:HB2	1.83	0.59
1:A:487:LEU:N	1:A:488:PRO:HD2	2.16	0.59
1:A:247[B]:GLN:NE2	1:A:264:ARG:HH11	1.78	0.59
1:A:161:LYS:O	1:A:161:LYS:HG2	2.01	0.59
1:B:369:LEU:HD12	1:B:418:ASP:HB2	1.85	0.59
1:A:106:ARG:NH1	6:A:813:HOH:O	2.27	0.58
1:B:25:ALA:N	1:B:26:PRO:HD2	2.19	0.58
1:B:177:PHE:HB2	1:B:473:MET:HG3	1.85	0.58
1:A:298:TYR:CZ	3:A:501:HGS:HG1A	2.37	0.58
1:B:438[B]:ARG:O	1:B:439[B]:ASP:C	2.46	0.58
1:B:26:PRO:O	1:B:27:PRO:C	2.45	0.58
1:A:487:LEU:HB2	1:A:488:PRO:HD3	1.84	0.58
1:A:399:TYR:HB3	6:A:627:HOH:O	2.03	0.57
1:B:475:ARG:CD	3:B:501:HGS:O41	2.48	0.57
1:A:271:ASP:OD1	1:A:310:ARG:HD2	2.03	0.57
3:A:501:HGS:N3	5:A:505:SO4:O4	2.37	0.57
1:A:153:ARG:CZ	1:A:473:MET:HE2	2.35	0.56
1:B:148:ARG:CD	1:B:325:THR:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:CB	1:B:473:MET:HG3	2.35	0.56
1:A:426:ARG:HD2	1:A:428:PHE:CE2	2.40	0.56
1:B:75:HIS:HD2	1:B:76:LEU:O	1.89	0.56
1:A:347:GLU:OE2	1:A:360:ARG:NH1	2.39	0.56
1:A:217:GLU:OE1	1:A:221:LYS:HE3	2.06	0.56
1:B:64[B]:ARG:HG2	6:B:815:HOH:O	2.04	0.56
1:B:473:MET:HE3	1:B:473:MET:C	2.31	0.56
1:A:426:ARG:HD2	1:A:428:PHE:CZ	2.41	0.55
1:A:204:ASN:ND2	6:A:737:HOH:O	2.40	0.55
1:B:148:ARG:HD3	1:B:325:THR:HG23	1.88	0.55
1:A:194:GLN:CG	6:B:521:HOH:O	2.55	0.54
1:B:282:LEU:HB2	1:B:318[B]:SER:HB2	1.89	0.54
1:A:396:ASN:HB2	6:A:734:HOH:O	2.07	0.54
1:A:450:GLU:OE1	2:A:500:ADP:O3'	2.20	0.54
1:B:176[B]:SER:OG	3:B:501:HGS:N3	2.41	0.54
1:A:194:GLN:HG3	6:B:521:HOH:O	2.07	0.54
1:B:146:ASP:HB3	1:B:461:LYS:HZ3	1.69	0.53
1:B:371:ASP:OD1	1:B:374:ILE:HG12	2.08	0.53
1:A:176[A]:SER:HG	3:A:501:HGS:HA3	1.72	0.53
1:B:130:ARG:HH22	1:B:306:GLU:CD	2.16	0.53
1:A:347:GLU:CD	1:A:360:ARG:HH12	2.17	0.53
1:B:148:ARG:NH2	6:B:645:HOH:O	2.40	0.53
1:B:375:VAL:HG13	1:B:407:LEU:HD13	1.90	0.53
1:B:89:HIS:CE1	1:B:163:LYS:O	2.53	0.53
1:B:196:GLY:O	1:B:199:LEU:O	2.27	0.53
1:B:185:THR:HA	1:B:495:THR:HG21	1.90	0.52
1:B:146:ASP:O	1:B:146:ASP:CG	2.47	0.52
1:B:436:LEU:HD12	1:B:438[A]:ARG:HH21	1.74	0.52
1:B:261:ARG:HH11	1:B:287:GLN:HE21	1.59	0.51
1:A:152:VAL:HG12	1:A:172:THR:HA	1.92	0.51
1:A:426:ARG:HH22	1:A:482:TYR:HE1	1.57	0.51
1:B:162:THR:HG21	1:B:164:SER:OG	2.09	0.51
1:B:426:ARG:HD2	1:B:428:PHE:CE2	2.45	0.51
1:B:148:ARG:HB3	6:B:647:HOH:O	2.10	0.51
1:B:426:ARG:HD2	1:B:428:PHE:CZ	2.46	0.51
1:A:64[A]:ARG:NH2	1:B:439[A]:ASP:O	2.31	0.51
1:B:197:LYS:HE3	1:B:198:PHE:CZ	2.45	0.51
6:A:511:HOH:O	1:B:194:GLN:HG2	2.08	0.51
1:A:106:ARG:HG3	6:A:607:HOH:O	2.11	0.50
1:B:446:HIS:CD2	6:B:524:HOH:O	2.63	0.50
1:B:141:ILE:HD12	1:B:141:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:HD13	1:B:467:ASN:HB2	1.93	0.50
1:B:88:SER:OG	1:B:89:HIS:HD2	1.94	0.50
1:A:94[A]:CYS:SG	1:A:469:GLU:HG3	2.51	0.50
1:B:176[A]:SER:HB2	3:B:501:HGS:N3	2.26	0.50
1:B:202:ASN:HD22	1:B:203:SER:N	2.09	0.50
1:B:347:GLU:HG3	1:B:356:ILE:HD13	1.93	0.50
1:A:38:LEU:O	1:A:42:ILE:HG13	2.12	0.49
1:B:438[B]:ARG:NH2	6:B:657:HOH:O	2.23	0.49
1:B:217:GLU:OE2	1:B:221:LYS:HE3	2.12	0.49
1:B:146:ASP:HB3	1:B:461:LYS:CE	2.42	0.49
1:A:487:LEU:N	1:A:488:PRO:CD	2.74	0.49
1:B:202:ASN:ND2	1:B:204:ASN:H	2.09	0.49
1:B:299:THR:CG2	1:B:301:LYS:H	2.24	0.49
1:B:376:LYS:HA	1:B:379:ILE:HG12	1.94	0.49
1:B:305:SER:HB3	1:B:307[A]:SER:H	1.78	0.48
1:A:202:ASN:ND2	1:A:204:ASN:H	2.07	0.48
1:A:334:LYS:NZ	1:A:391:ARG:O	2.46	0.48
1:B:148:ARG:HG2	1:B:321:ILE:HG23	1.94	0.48
1:B:157:MET:HB3	1:B:429:PRO:HG3	1.94	0.48
1:B:163:LYS:CG	6:B:701:HOH:O	2.61	0.48
1:A:92[B]:GLN:O	1:A:96:LEU:HB2	2.14	0.48
1:A:352:ASN:C	1:A:352:ASN:ND2	2.66	0.48
1:B:345:VAL:O	1:B:346:LEU:C	2.55	0.48
1:A:438[B]:ARG:NE	6:A:805:HOH:O	1.79	0.48
1:B:146:ASP:OD1	1:B:146:ASP:C	2.51	0.48
1:B:324:PRO:HB2	1:B:328:TYR:HB2	1.95	0.48
1:B:148:ARG:HB2	6:B:693:HOH:O	2.12	0.47
1:B:344:GLY:HA2	1:B:347:GLU:OE1	2.15	0.47
1:B:369:LEU:HD22	1:B:423:LEU:CD2	2.32	0.47
1:A:293:TYR:CZ	1:A:295:ARG:HD3	2.49	0.47
1:A:37:LYS:HE3	6:A:611:HOH:O	2.14	0.47
1:B:75:HIS:CD2	1:B:76:LEU:O	2.66	0.47
1:B:179:LEU:HA	1:B:212:VAL:HB	1.95	0.47
1:A:324:PRO:HB2	1:A:328:TYR:HB2	1.96	0.47
1:A:373:ASP:O	1:A:376:LYS:HG2	2.14	0.46
1:A:182:CYS:SG	3:A:506:HGS:SG2	3.04	0.46
1:B:238:GLN:NE2	6:B:540:HOH:O	2.48	0.46
1:A:28:LEU:HD22	1:A:84:PRO:HD3	1.96	0.46
1:B:176[A]:SER:HB2	3:B:501:HGS:HA3	1.98	0.46
1:A:138[B]:MET:HB3	6:A:876:HOH:O	2.15	0.46
1:A:327:SER:O	1:A:331:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:SER:HB2	1:B:308:GLU:OE1	2.15	0.46
1:A:126:GLU:H	1:A:126:GLU:CD	2.23	0.46
1:A:37:LYS:HD2	6:A:700:HOH:O	2.15	0.46
1:B:299:THR:HG21	1:B:301:LYS:HD2	1.96	0.46
1:B:431:THR:HA	1:B:447:VAL:O	2.15	0.46
1:B:438[B]:ARG:NH1	6:B:657:HOH:O	2.46	0.46
1:B:122:LYS:O	6:B:695:HOH:O	2.20	0.46
1:A:138[A]:MET:HE1	1:A:143:LYS:HE3	1.98	0.45
1:B:97:ALA:HB3	1:B:98:PRO:HD3	1.97	0.45
1:B:121:THR:HG21	1:B:390:GLN:HG3	1.98	0.45
1:A:240:GLU:HG2	6:A:779:HOH:O	2.16	0.45
1:B:373:ASP:HB3	1:B:374:ILE:HD13	1.99	0.45
1:A:161:LYS:O	1:A:161:LYS:CG	2.64	0.45
1:A:179:LEU:HA	1:A:182:CYS:SG	2.56	0.45
1:A:247[B]:GLN:HE22	1:A:264:ARG:HD2	1.74	0.45
1:B:112:LYS:HG2	1:B:116[B]:GLU:CD	2.42	0.45
1:B:352:ASN:O	1:B:356:ILE:HG13	2.15	0.45
1:A:162:THR:CG2	1:A:162:THR:O	2.64	0.45
1:B:205:ARG:HA	1:B:205:ARG:HD2	1.67	0.45
1:B:379:ILE:O	1:B:404:ARG:HG3	2.17	0.45
1:B:148:ARG:CB	6:B:647:HOH:O	2.64	0.45
1:A:140:GLN:O	1:A:141:ILE:C	2.60	0.45
1:A:352:ASN:O	1:A:356:ILE:HG13	2.17	0.45
1:A:64[A]:ARG:HG3	1:A:64[A]:ARG:H	1.53	0.45
1:B:75:HIS:HE1	1:B:440:GLY:N	2.11	0.45
1:A:151:ILE:HD11	1:A:219:LEU:HG	1.98	0.45
1:A:153:ARG:NE	1:A:473:MET:HE2	2.32	0.45
1:A:148:ARG:HH11	1:A:459:ARG:HD3	1.80	0.44
1:B:342:LYS:O	1:B:345:VAL:HG13	2.17	0.44
1:B:255:ARG:O	1:B:259:HIS:HA	2.17	0.44
1:B:447:VAL:HB	1:B:476:THR:HG23	2.00	0.44
1:A:197:LYS:CG	6:A:811:HOH:O	2.28	0.44
1:B:446:HIS:HD2	6:B:524:HOH:O	1.98	0.44
1:A:261:ARG:HH12	1:A:287:GLN:NE2	2.15	0.44
1:A:176[B]:SER:HB2	3:A:501:HGS:N3	2.32	0.44
1:A:375:VAL:HG13	1:A:407:LEU:HD13	1.98	0.44
1:B:305:SER:HB3	1:B:307[B]:SER:H	1.82	0.44
1:B:475:ARG:CZ	3:B:501:HGS:O41	2.62	0.44
1:A:436:LEU:O	1:A:442:TRP:HA	2.17	0.44
1:B:160:GLU:O	1:B:161:LYS:C	2.60	0.44
1:A:394:GLY:HA2	6:A:650:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:N	1:A:399:TYR:CD1	2.86	0.44
1:B:112:LYS:HG2	1:B:116[B]:GLU:OE2	2.17	0.44
1:B:130:ARG:HD2	6:B:672:HOH:O	2.16	0.44
1:A:431:THR:HA	1:A:447:VAL:O	2.18	0.44
1:B:64[B]:ARG:HG2	1:B:64[B]:ARG:H	1.29	0.44
1:B:323:CYS:HA	1:B:324:PRO:HA	1.79	0.44
1:A:192:LEU:HD12	1:A:203:SER:HA	1.99	0.43
1:A:25:ALA:HA	1:A:26:PRO:HD2	1.81	0.43
1:A:112:LYS:HE2	6:A:541:HOH:O	2.18	0.43
1:B:293:TYR:CZ	1:B:295:ARG:HD3	2.53	0.43
1:B:438[B]:ARG:C	1:B:440:GLY:N	2.76	0.43
1:B:324:PRO:HB2	1:B:328:TYR:CB	2.48	0.43
1:B:436:LEU:O	1:B:442:TRP:HA	2.18	0.43
3:B:501:HGS:O11	3:B:501:HGS:HG1	2.18	0.43
1:A:179:LEU:HA	1:A:212:VAL:HB	2.01	0.42
1:A:426:ARG:NH2	1:A:482:TYR:HE1	2.16	0.42
1:B:153:ARG:HD2	1:B:452:GLY:HA3	2.01	0.42
1:B:464:ILE:C	1:B:464:ILE:HD12	2.44	0.42
1:A:388:LYS:HD3	1:A:397:ASN:ND2	2.34	0.42
1:B:163:LYS:CB	6:B:701:HOH:O	2.67	0.42
3:B:501:HGS:HA2	5:B:505:SO4:S	2.59	0.42
1:B:32:HIS:HE1	1:B:434:ALA:O	2.03	0.42
1:B:282:LEU:HB2	1:B:318[B]:SER:CB	2.50	0.42
1:A:438[B]:ARG:O	1:A:439:ASP:C	2.63	0.42
1:A:439:ASP:OD1	6:A:875:HOH:O	2.22	0.42
1:B:62:VAL:HG11	1:B:72:GLY:HA3	2.01	0.42
1:B:32:HIS:CD2	6:B:515:HOH:O	2.72	0.42
1:A:146:ASP:HB3	1:A:461:LYS:HG2	2.02	0.41
1:A:153:ARG:HD2	1:A:452:GLY:HA3	2.01	0.41
1:B:130:ARG:HB3	1:B:309:TRP:CH2	2.56	0.41
1:A:92[B]:GLN:HG2	1:A:165:LEU:HD23	2.02	0.41
1:A:157:MET:HB3	1:A:429:PRO:HG3	2.02	0.41
1:B:151:ILE:HD11	1:B:219:LEU:HG	2.02	0.41
1:B:217:GLU:OE2	1:B:221:LYS:CE	2.67	0.41
1:B:159:ASP:HB2	1:B:427:ILE:HG23	2.01	0.41
1:A:63:GLN:HG3	6:A:644:HOH:O	2.21	0.41
1:A:261:ARG:HH12	1:A:287:GLN:HE21	1.68	0.41
1:A:117:SER:HB3	1:A:339:GLU:HG3	2.01	0.41
1:B:275:LYS:NZ	6:B:749:HOH:O	2.44	0.41
1:B:387:MET:HE1	1:B:406:THR:HG22	2.03	0.41
1:B:404:ARG:O	1:B:408:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:CB	6:B:693:HOH:O	2.68	0.41
1:B:335:LYS:HD2	1:B:335:LYS:O	2.21	0.41
1:B:347:GLU:HG3	1:B:356:ILE:CD1	2.50	0.41
1:B:376:LYS:O	1:B:380:GLU:HB3	2.21	0.41
1:B:175:THR:HA	3:B:501:HGS:O2	2.20	0.40
1:B:238:GLN:NE2	3:B:501:HGS:HN1A	2.19	0.40
1:A:322:LYS:HE2	6:A:640:HOH:O	2.21	0.40
1:A:121:THR:HG21	1:A:390:GLN:HG3	2.04	0.40
1:A:397:ASN:C	1:A:398:ILE:HG13	2.46	0.40
1:A:282:LEU:HB2	1:A:318[B]:SER:CB	2.52	0.40

There are no symmetry-related clashes.

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	480/499 (96%)	458 (95%)	21 (4%)	1 (0%)	43	36
1	B	483/499 (97%)	448 (93%)	28 (6%)	7 (1%)	9	3
All	All	963/998 (96%)	906 (94%)	49 (5%)	8 (1%)	24	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149[A]	MET
1	B	149[B]	MET
1	B	439[A]	ASP
1	B	439[B]	ASP
1	B	369	LEU
1	B	318[A]	SER
1	B	318[B]	SER
1	A	344	GLY

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	424/431 (98%)	386 (91%)	38 (9%)	9	3
1	B	427/431 (99%)	383 (90%)	44 (10%)	7	2
All	All	851/862 (99%)	769 (90%)	82 (10%)	8	3

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

Mol	Chain	Res	Type
1	A	60	LYS
1	A	63	GLN
1	A	64[A]	ARG
1	A	64[B]	ARG
1	A	76	LEU
1	A	96	LEU
1	A	106	ARG
1	A	112	LYS
1	A	126	GLU
1	A	130	ARG
1	A	139	LEU
1	A	140	GLN
1	A	145	GLU
1	A	163	LYS
1	A	182	CYS
1	A	194	GLN
1	A	202	ASN
1	A	235	VAL
1	A	240	GLU
1	A	256	GLU
1	A	310	ARG
1	A	318[A]	SER
1	A	318[B]	SER
1	A	324	PRO
1	A	352	ASN
1	A	356	ILE
1	A	360	ARG

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Mol	Chain	Res	Type
1	A	376	LYS
1	A	384	LEU
1	A	388	LYS
1	A	399	TYR
1	A	404	ARG
1	A	405	GLU
1	A	409	LYS
1	A	411	GLN
1	A	423	LEU
1	A	426	ARG
1	A	431	THR
1	B	35	ASP
1	B	63	GLN
1	B	76	LEU
1	B	81	LEU
1	B	91	LYS
1	B	112	LYS
1	B	120	ARG
1	B	139	LEU
1	B	140	GLN
1	B	141	ILE
1	B	145	GLU
1	B	149[A]	MET
1	B	149[B]	MET
1	B	161	LYS
1	B	163	LYS
1	B	180	ILE
1	B	194	GLN
1	B	202	ASN
1	B	240	GLU
1	B	267	LEU
1	B	268	THR
1	B	299	THR
1	B	305	SER
1	B	324	PRO
1	B	345	VAL
1	B	350	VAL
1	B	351	GLU
1	B	352	ASN
1	B	374	ILE
1	B	376	LYS
1	B	377	LYS

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Mol	Chain	Res	Type
1	B	384	LEU
1	B	404	ARG
1	B	405	GLU
1	B	409	LYS
1	B	417	GLU
1	B	423	LEU
1	B	426	ARG
1	B	431	THR
1	B	459[A]	ARG
1	B	459[B]	ARG
1	B	464	ILE
1	B	473	MET
1	B	474	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	194	GLN
1	A	202	ASN
1	A	238	GLN
1	A	272	GLN
1	A	287	GLN
1	A	352	ASN
1	A	468	ASN
1	B	32	HIS
1	B	40	GLN
1	B	63	GLN
1	B	75	HIS
1	B	89	HIS
1	B	194	GLN
1	B	202	ASN
1	B	238	GLN
1	B	287	GLN
1	B	352	ASN
1	B	355	HIS
1	B	446	HIS
1	B	468	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are 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$
5	SO4	B	505	4	4,4,4	1.48	1 (25%)	6,6,6	1.37	1 (16%)
2	ADP	B	500	4	28,29,29	1.98	8 (28%)	43,45,45	1.88	13 (30%)
3	HGS	A	506	-	19,20,20	3.01	7 (36%)	22,25,25	3.45	12 (54%)
3	HGS	B	501	-	19,20,20	3.50	7 (36%)	22,25,25	6.37	15 (68%)
2	ADP	A	500	4	28,29,29	2.31	9 (32%)	43,45,45	2.15	12 (27%)
5	SO4	A	505	4	4,4,4	1.66	1 (25%)	6,6,6	1.25	0
3	HGS	B	506	-	19,20,20	2.23	5 (26%)	22,25,25	3.04	11 (50%)
3	HGS	A	501	-	19,20,20	4.30	11 (57%)	22,25,25	6.75	14 (63%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	500	4	-	3/16/32/32	0/3/3/3
3	HGS	A	506	-	-	10/25/25/25	-
3	HGS	B	501	-	-	12/25/25/25	-
2	ADP	A	500	4	-	2/16/32/32	0/3/3/3
3	HGS	B	506	-	-	14/25/25/25	-
3	HGS	A	501	-	-	12/25/25/25	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HGS	CB2-CA2	10.01	1.63	1.53
3	B	501	HGS	CB2-CA2	8.40	1.62	1.53
3	A	506	HGS	O2-C2	8.10	1.38	1.23
3	A	501	HGS	CA4-C4	8.05	1.69	1.50
3	A	501	HGS	CA3-N3	6.76	1.61	1.46
3	B	501	HGS	OE1-CD1	6.23	1.35	1.23
3	B	501	HGS	CA3-N3	6.19	1.60	1.46
3	A	501	HGS	OE1-CD1	6.19	1.35	1.23
3	A	506	HGS	OE1-CD1	6.04	1.35	1.23
3	B	501	HGS	CA4-C4	5.96	1.64	1.50
2	A	500	ADP	C5-C4	5.91	1.49	1.39
3	B	506	HGS	OE1-CD1	5.72	1.34	1.23
2	B	500	ADP	C5-C4	5.71	1.49	1.39
3	B	506	HGS	O2-C2	5.39	1.33	1.23
3	A	501	HGS	O42-C4	4.55	1.37	1.22
3	A	501	HGS	C2-N3	4.49	1.44	1.33
3	A	506	HGS	CD1-N2	-4.34	1.24	1.34
2	A	500	ADP	C5-C6	4.18	1.52	1.41
3	B	501	HGS	CD1-N2	-4.00	1.25	1.34
3	A	501	HGS	CA3-CA4	3.77	1.63	1.51
2	A	500	ADP	PA-O3A	-3.71	1.55	1.59
2	A	500	ADP	C2-N3	3.70	1.40	1.33
3	A	501	HGS	CD1-N2	-3.63	1.26	1.34
2	A	500	ADP	C8-N7	3.58	1.38	1.31
2	A	500	ADP	C2-N1	3.50	1.40	1.33
2	B	500	ADP	C2-N1	3.46	1.40	1.33
2	B	500	ADP	PA-O3A	-3.37	1.55	1.59
3	A	501	HGS	O41-C4	3.30	1.41	1.30
2	A	500	ADP	PB-O2B	-3.23	1.42	1.54
3	A	506	HGS	CB1-CA1	2.95	1.59	1.53
3	B	501	HGS	CA3-CA4	2.93	1.61	1.51
3	A	501	HGS	O2-C2	2.93	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	ADP	PB-O2B	-2.73	1.44	1.54
2	B	500	ADP	C5-C6	2.72	1.48	1.41
3	B	506	HGS	CD1-N2	-2.70	1.28	1.34
3	B	501	HGS	C2-N3	2.69	1.40	1.33
5	A	505	SO4	O2-S	2.69	1.60	1.44
5	B	505	SO4	O2-S	2.68	1.60	1.44
3	A	506	HGS	CB1-CG1	2.64	1.60	1.52
3	A	506	HGS	O12-C1	-2.50	1.22	1.30
3	A	501	HGS	CA2-C2	2.49	1.59	1.52
2	B	500	ADP	C5'-C4'	2.45	1.58	1.51
2	A	500	ADP	C4-N3	2.45	1.39	1.34
3	B	506	HGS	C2-N3	-2.42	1.28	1.33
3	A	506	HGS	C2-N3	-2.39	1.28	1.33
2	A	500	ADP	C8-N9	-2.30	1.33	1.37
2	B	500	ADP	C8-N7	2.26	1.36	1.31
2	B	500	ADP	C5-N7	-2.25	1.35	1.39
3	B	506	HGS	CA2-C2	-2.08	1.47	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HGS	CA3-N3-C2	18.18	155.21	122.55
3	B	501	HGS	CA3-N3-C2	17.96	154.82	122.55
3	A	501	HGS	CA2-CB2-SG2	-16.00	96.12	114.16
3	B	501	HGS	CA2-CB2-SG2	-12.93	99.58	114.16
3	B	501	HGS	CA2-C2-N3	9.26	136.43	116.54
3	A	501	HGS	CA2-C2-N3	9.07	136.01	116.54
3	A	506	HGS	CA2-CB2-SG2	-8.24	104.87	114.16
3	A	506	HGS	OE1-CD1-N2	-8.02	109.38	122.95
3	A	501	HGS	CA4-CA3-N3	7.99	129.00	112.00
3	A	501	HGS	CA3-CA4-C4	7.83	129.94	112.98
3	B	506	HGS	CA4-CA3-N3	-7.50	96.03	112.00
3	A	501	HGS	O2-C2-CA2	-7.43	104.92	120.48
3	B	501	HGS	O2-C2-CA2	-6.50	106.87	120.48
3	B	501	HGS	CG1-CD1-N2	-6.48	104.45	115.86
3	A	501	HGS	CG1-CB1-CA1	-6.44	99.09	113.86
3	B	501	HGS	CA4-CA3-N3	6.24	125.28	112.00
2	A	500	ADP	C5-C4-N3	-5.99	118.47	126.72
3	B	501	HGS	CB1-CA1-C1	-5.98	94.59	110.45
3	B	501	HGS	CA2-N2-CD1	5.96	136.62	121.68
3	B	506	HGS	CA3-N3-C2	5.68	132.74	122.55
3	B	506	HGS	CB2-CA2-N2	-5.21	103.86	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	HGS	OE1-CD1-N2	5.19	131.74	122.95
3	A	501	HGS	OE1-CD1-N2	5.05	131.50	122.95
3	B	501	HGS	O41-C4-O42	-5.02	110.42	123.33
3	B	506	HGS	CG1-CD1-N2	4.96	124.60	115.86
2	B	500	ADP	O2A-PA-O3A	4.80	120.25	107.27
2	A	500	ADP	C4-C5-N7	-4.67	105.24	110.58
3	A	501	HGS	O41-C4-O42	4.61	135.18	123.33
3	A	506	HGS	OE1-CD1-CG1	4.49	130.15	122.02
2	A	500	ADP	N3-C4-N9	4.43	134.69	127.17
2	A	500	ADP	N3-C2-N1	-4.40	121.93	128.58
3	A	506	HGS	CA3-N3-C2	4.34	130.34	122.55
3	B	501	HGS	CA3-CA4-C4	4.19	122.05	112.98
2	B	500	ADP	N3-C2-N1	-4.05	122.45	128.58
2	A	500	ADP	C2-N3-C4	3.94	121.44	111.83
3	A	501	HGS	CG1-CD1-N2	-3.87	109.04	115.86
3	B	501	HGS	O41-C4-CA4	3.83	126.10	114.00
3	A	501	HGS	O42-C4-CA4	-3.79	111.07	123.09
3	A	506	HGS	CB1-CG1-CD1	3.78	121.48	113.06
2	B	500	ADP	C5-C4-N3	-3.58	121.79	126.72
3	A	506	HGS	CB2-CA2-N2	-3.56	106.20	111.28
3	B	501	HGS	CG1-CB1-CA1	-3.56	105.69	113.86
3	B	506	HGS	CA2-CB2-SG2	-3.53	110.18	114.16
3	A	501	HGS	CB2-CA2-C2	3.41	116.91	109.50
3	A	506	HGS	CB1-CA1-N1	3.32	118.77	110.12
2	A	500	ADP	O2A-PA-O3A	3.30	116.20	107.27
2	B	500	ADP	C4-C5-N7	-3.29	106.83	110.58
3	A	506	HGS	CA3-CA4-C4	3.21	119.93	112.98
2	B	500	ADP	N3-C4-N9	3.18	132.57	127.17
2	A	500	ADP	C5-N7-C8	3.11	108.34	103.45
3	B	506	HGS	CB1-CG1-CD1	3.09	119.96	113.06
3	B	501	HGS	O2-C2-N3	-3.04	116.55	122.98
3	A	506	HGS	C2-CA2-N2	2.90	118.96	111.11
2	B	500	ADP	C5'-C4'-C3'	2.90	125.65	115.21
2	B	500	ADP	C2-N3-C4	2.88	118.87	111.83
3	B	506	HGS	OE1-CD1-CG1	-2.83	116.89	122.02
3	B	501	HGS	CB2-CA2-N2	-2.78	107.32	111.28
2	A	500	ADP	C2'-C1'-N9	-2.75	106.48	113.30
3	A	506	HGS	CA4-CA3-N3	-2.72	106.22	112.00
3	B	506	HGS	CA2-C2-N3	2.66	122.26	116.54
3	B	506	HGS	OE1-CD1-N2	-2.63	118.49	122.95
3	A	506	HGS	CG1-CD1-N2	2.58	120.41	115.86
2	A	500	ADP	C4-N9-C8	2.57	108.44	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ADP	O4'-C4'-C3'	-2.51	100.17	105.15
2	B	500	ADP	C6-C5-N7	2.47	136.86	132.09
2	B	500	ADP	O3B-PB-O3A	2.43	112.79	104.64
3	A	501	HGS	CB1-CG1-CD1	2.32	118.25	113.06
2	B	500	ADP	C4-N9-C8	2.31	108.17	105.74
2	A	500	ADP	C6-C5-N7	2.30	136.52	132.09
3	A	501	HGS	CB1-CA1-N1	2.30	116.11	110.12
3	A	506	HGS	CA2-N2-CD1	-2.24	116.07	121.68
2	A	500	ADP	O3B-PB-O3A	2.23	112.11	104.64
3	B	506	HGS	O2-C2-CA2	-2.19	115.89	120.48
3	B	506	HGS	CB2-CA2-C2	-2.08	104.99	109.50
5	B	505	SO4	O4-S-O3	-2.06	97.16	108.54
2	B	500	ADP	C5-N7-C8	2.02	106.63	103.45
2	B	500	ADP	C2-N1-C6	2.02	122.04	118.73
2	A	500	ADP	C3'-C2'-C1'	-2.00	97.68	101.46

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HGS	O11-C1-CA1-N1
3	A	501	HGS	N1-CA1-CB1-CG1
3	A	501	HGS	N2-CA2-CB2-SG2
3	A	506	HGS	O11-C1-CA1-N1
3	A	506	HGS	C1-CA1-CB1-CG1
3	A	506	HGS	C2-CA2-CB2-SG2
3	A	506	HGS	N2-CA2-CB2-SG2
3	B	501	HGS	N1-CA1-CB1-CG1
3	B	501	HGS	N2-CA2-CB2-SG2
3	B	506	HGS	C1-CA1-CB1-CG1
3	B	506	HGS	N1-CA1-CB1-CG1
3	A	501	HGS	CA4-CA3-N3-C2
3	A	506	HGS	CA4-CA3-N3-C2
3	B	501	HGS	CA4-CA3-N3-C2
3	B	506	HGS	CG1-CD1-N2-CA2
3	A	501	HGS	O2-C2-N3-CA3
3	B	501	HGS	O2-C2-N3-CA3
3	B	506	HGS	O2-C2-N3-CA3
3	B	506	HGS	OE1-CD1-N2-CA2
3	A	501	HGS	CA2-C2-N3-CA3
3	B	501	HGS	CA2-C2-N3-CA3
3	B	506	HGS	CA2-C2-N3-CA3

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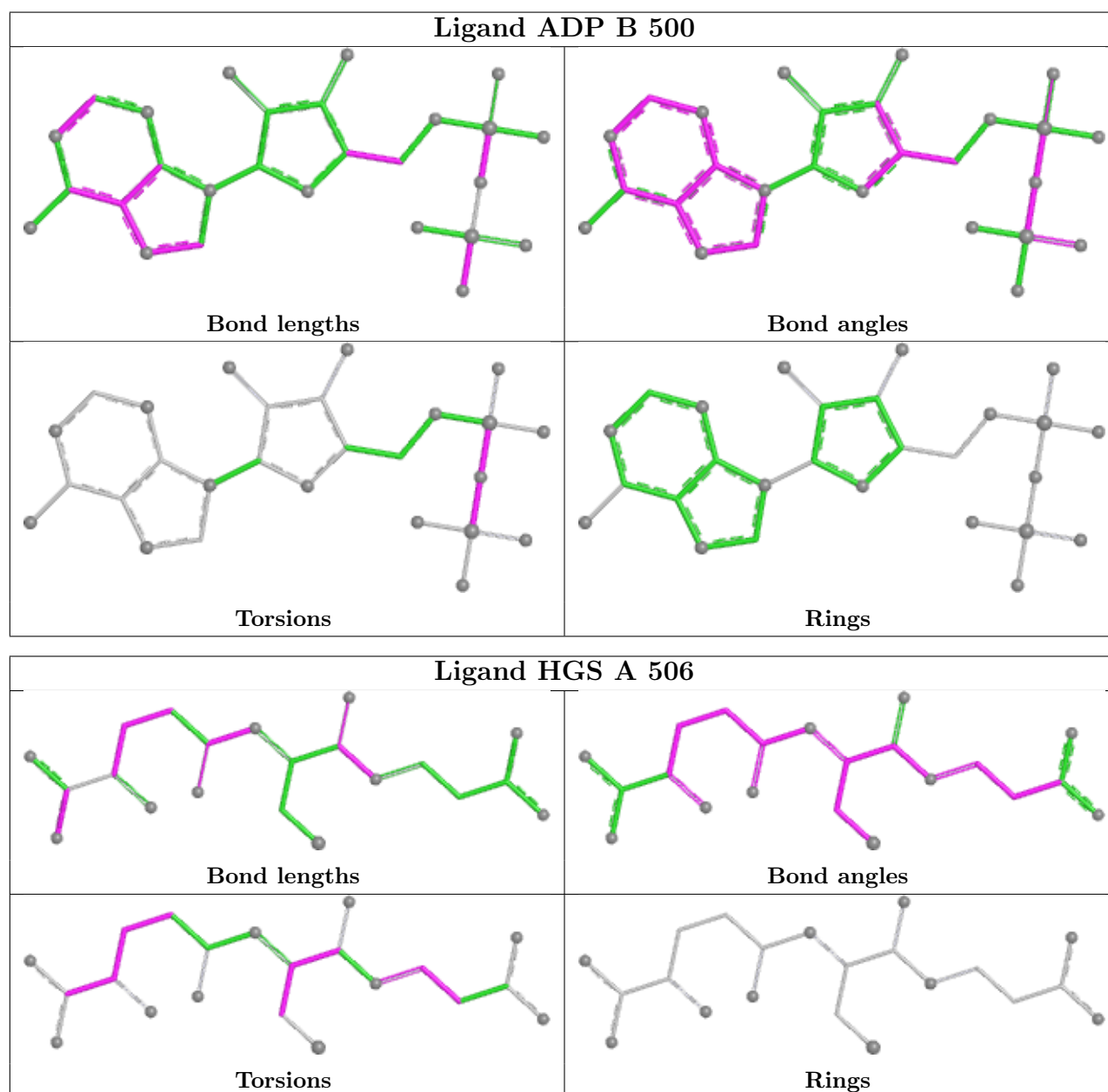
Mol	Chain	Res	Type	Atoms
3	A	506	HGS	O12-C1-CA1-N1
3	A	506	HGS	N3-CA3-CA4-C4
3	B	501	HGS	N3-CA3-CA4-C4
3	A	501	HGS	O12-C1-CA1-N1
3	B	506	HGS	N2-CD1-CG1-CB1
3	B	506	HGS	OE1-CD1-CG1-CB1
2	B	500	ADP	PB-O3A-PA-O1A
3	B	506	HGS	O2-C2-CA2-N2
3	A	501	HGS	N3-C2-CA2-N2
3	B	506	HGS	N3-C2-CA2-N2
3	B	501	HGS	N3-C2-CA2-N2
3	A	506	HGS	CA1-CB1-CG1-CD1
2	B	500	ADP	PA-O3A-PB-O2B
3	A	501	HGS	O2-C2-CA2-N2
3	B	501	HGS	O2-C2-CA2-N2
3	A	501	HGS	C1-CA1-CB1-CG1
3	B	501	HGS	C1-CA1-CB1-CG1
2	A	500	ADP	PB-O3A-PA-O2A
3	B	506	HGS	O41-C4-CA4-CA3
3	B	506	HGS	O42-C4-CA4-CA3
2	A	500	ADP	PB-O3A-PA-O1A
3	A	506	HGS	O2-C2-CA2-N2
3	B	506	HGS	O11-C1-CA1-N1
3	B	501	HGS	O41-C4-CA4-CA3
3	B	501	HGS	O42-C4-CA4-CA3
3	B	506	HGS	O12-C1-CA1-N1
3	B	501	HGS	C2-CA2-CB2-SG2
2	B	500	ADP	PB-O3A-PA-O2A
3	A	501	HGS	O41-C4-CA4-CA3
3	A	501	HGS	O42-C4-CA4-CA3
3	A	506	HGS	N3-C2-CA2-N2

There are no ring outliers.

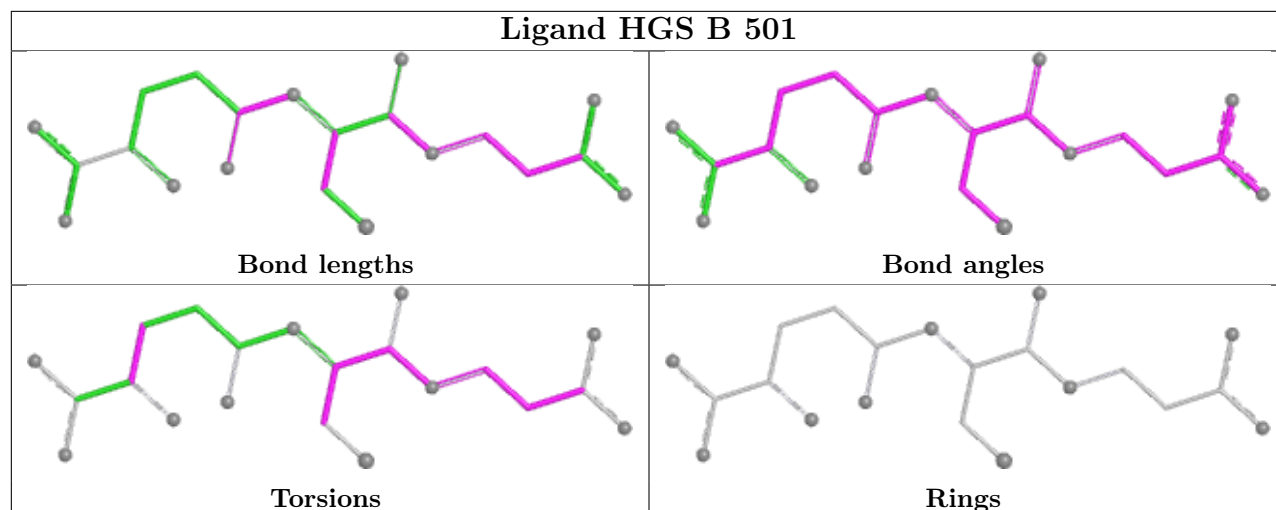
6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	SO4	5	0
3	A	506	HGS	3	0
3	B	501	HGS	21	0
2	A	500	ADP	1	0
5	A	505	SO4	4	0
3	A	501	HGS	12	0

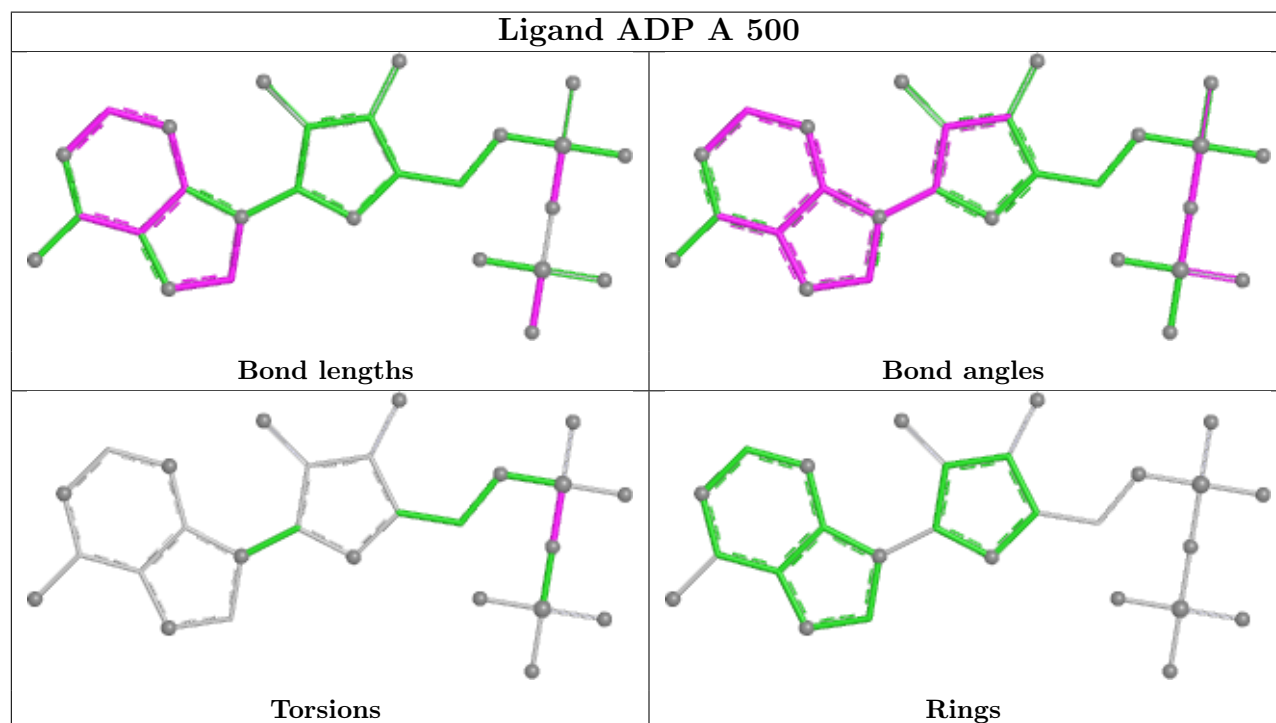
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



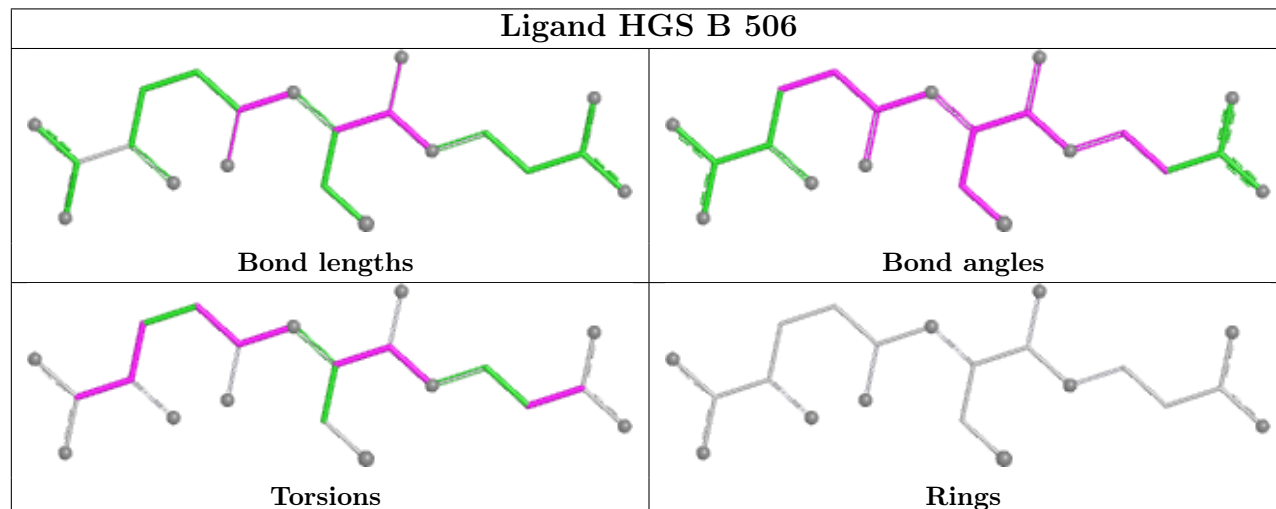
Ligand HGS B 501

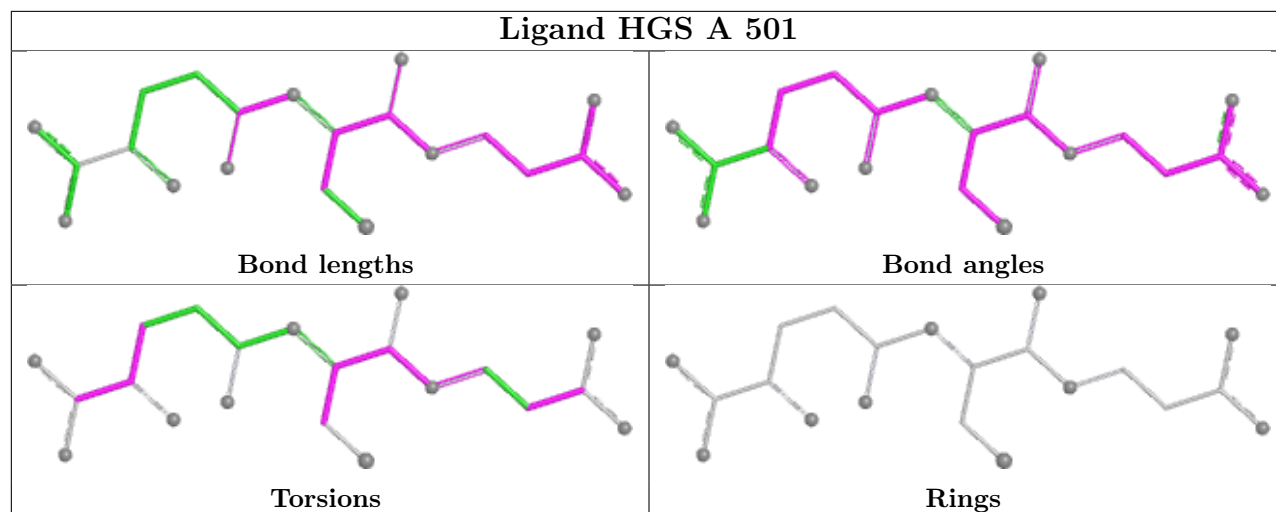


Ligand ADP A 500



Ligand HGS B 506





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	470/499 (94%)	-1.26	0 100 100	9, 31, 64, 84	14 (2%)
1	B	468/499 (93%)	-1.24	0 100 100	10, 31, 65, 89	19 (4%)
All	All	938/998 (93%)	-1.25	0 100 100	9, 31, 66, 89	33 (3%)

There are no RSRZ outliers to report.

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	HGS	B	506	21/21	0.97	0.08	34,42,50,52	21
3	HGS	A	506	21/21	0.98	0.07	14,27,56,59	21
3	HGS	B	501	21/21	0.99	0.04	27,52,57,64	0
3	HGS	A	501	21/21	0.99	0.05	25,51,57,61	0
4	MG	B	502	1/1	0.99	0.03	34,34,34,34	0
4	MG	B	504	1/1	0.99	0.03	36,36,36,36	0
5	SO4	A	505	5/5	0.99	0.06	29,37,46,49	0

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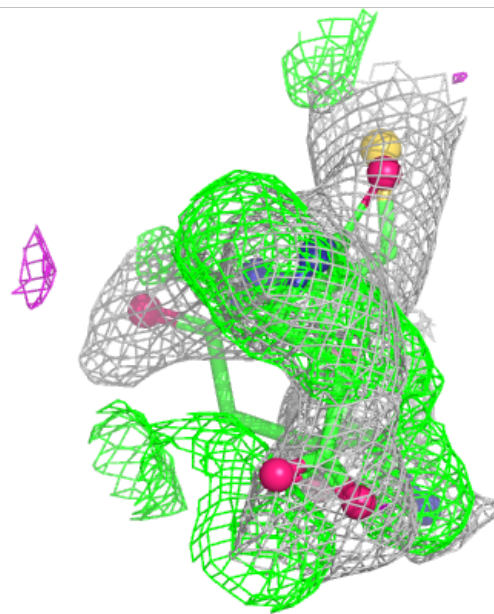
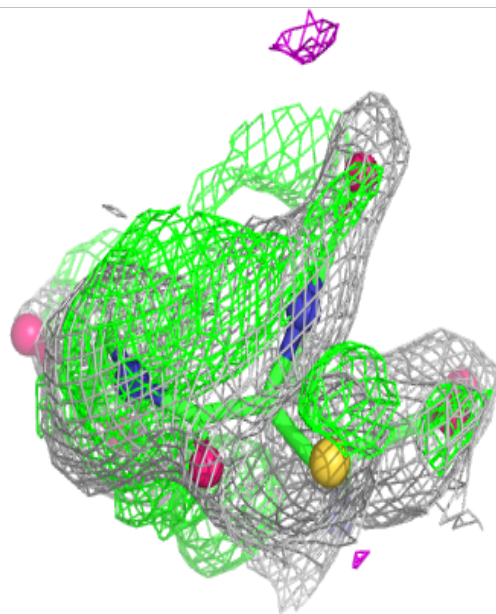
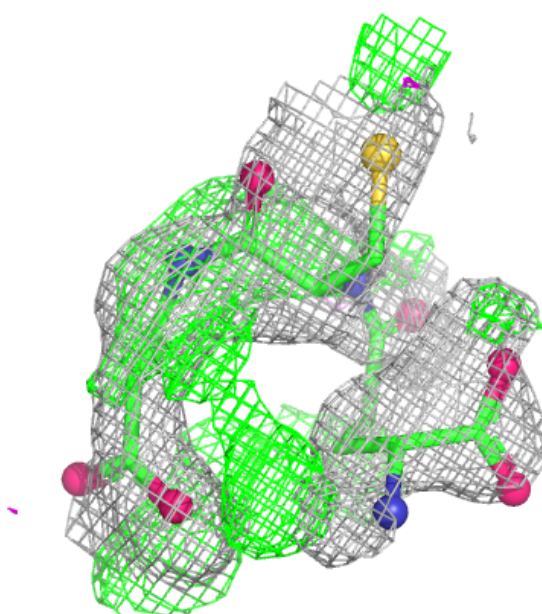
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	505	5/5	0.99	0.07	31,35,42,45	0
4	MG	A	504	1/1	1.00	0.02	36,36,36,36	0
2	ADP	A	500	27/27	1.00	0.02	24,31,37,37	0
4	MG	B	503	1/1	1.00	0.02	29,29,29,29	0
2	ADP	B	500	27/27	1.00	0.02	27,33,37,39	0
4	MG	A	502	1/1	1.00	0.03	39,39,39,39	0
4	MG	A	503	1/1	1.00	0.02	27,27,27,27	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.

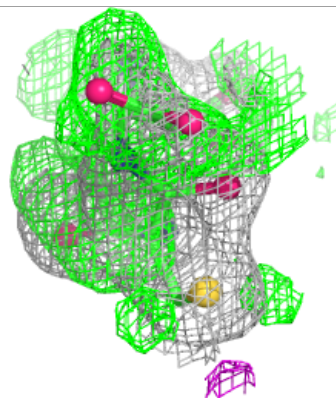
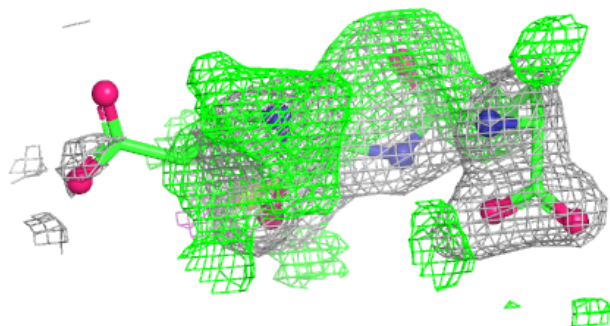
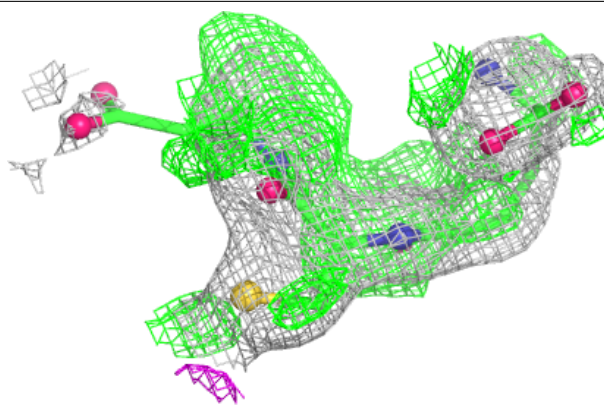
Electron density around HGS B 506:

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

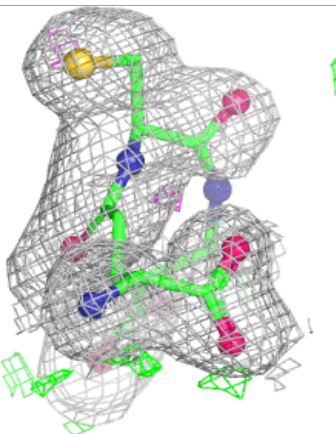
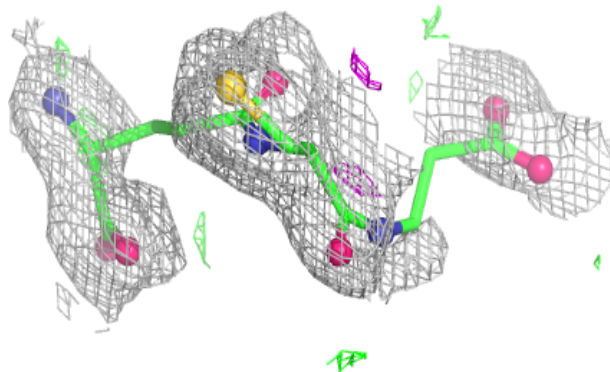
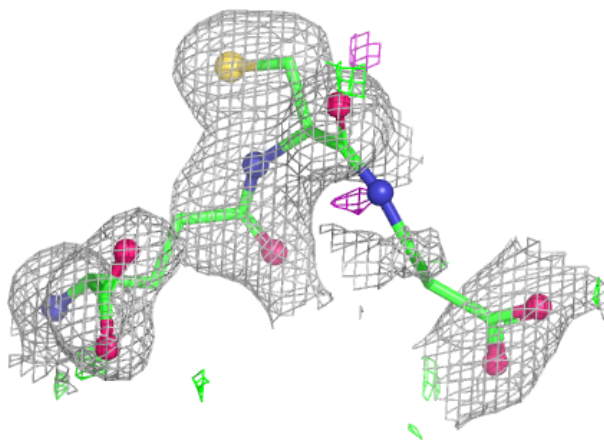


Electron density around HGS A 506:

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

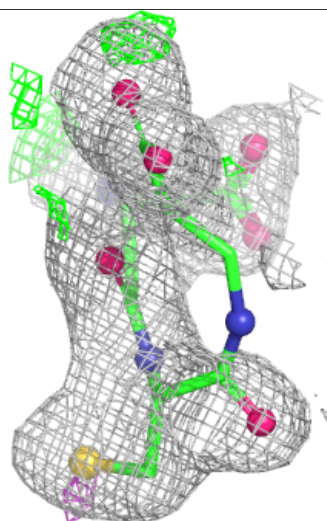
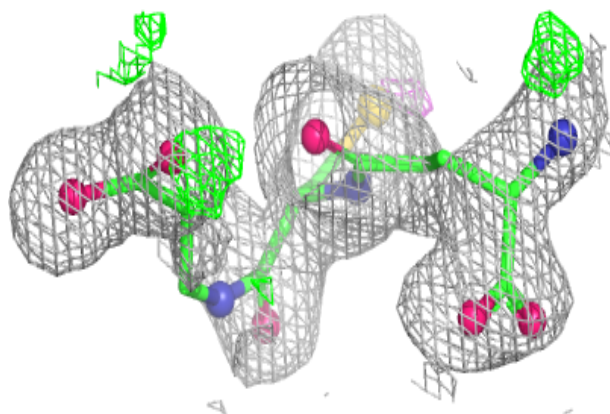
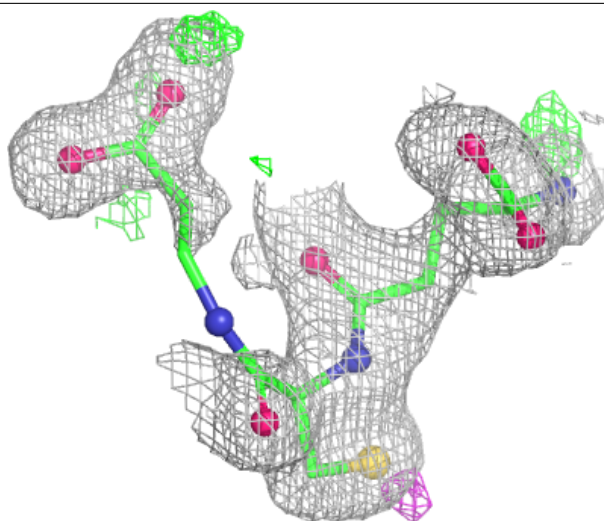
**Electron density around HGS B 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



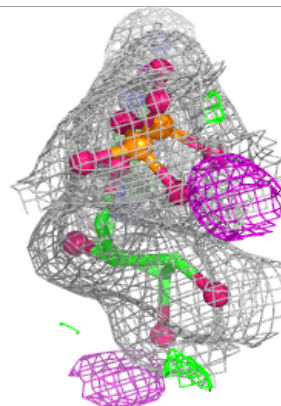
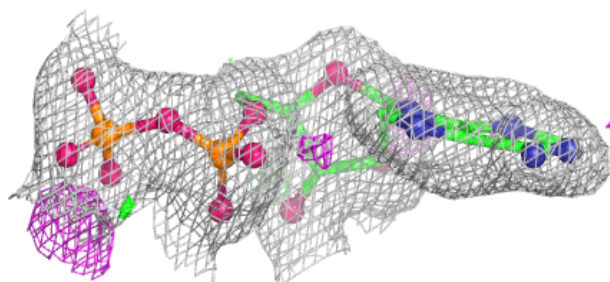
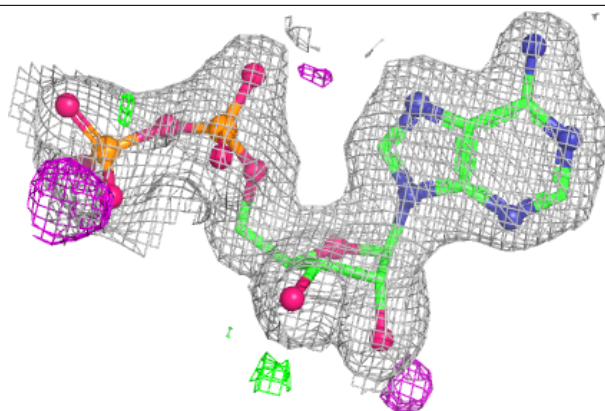
Electron density around HGS A 501:

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and green (positive)

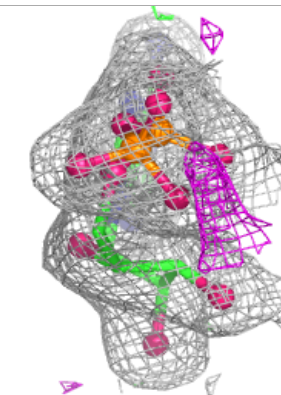
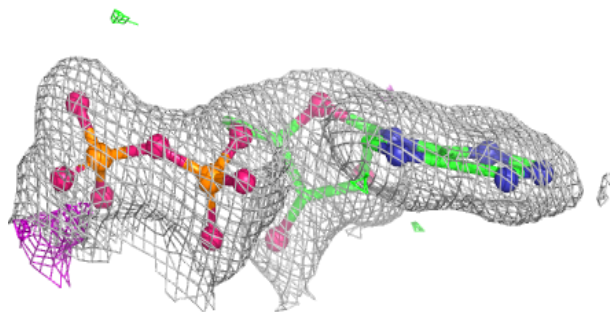
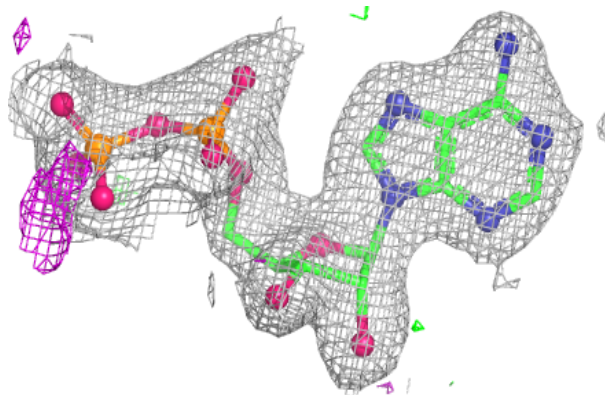


Electron density around ADP A 500:

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

**Electron density around ADP B 500:**

$2mF_o-DF_c$ (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.