



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 10:41 AM EST

PDB ID : 3KAL  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

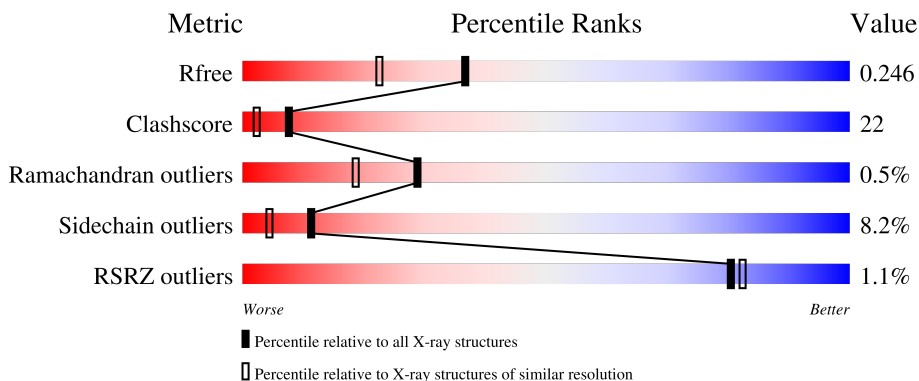
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


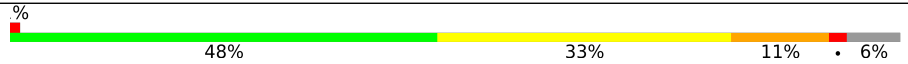
The reported resolution of this entry is 1.90 Å.

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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](#)

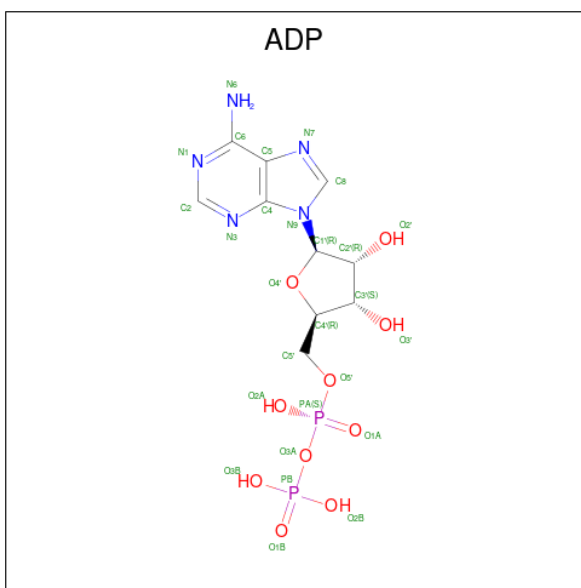
There are 6 unique types of molecules in this entry. The entry contains 8571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 homogluthathione synthetase.

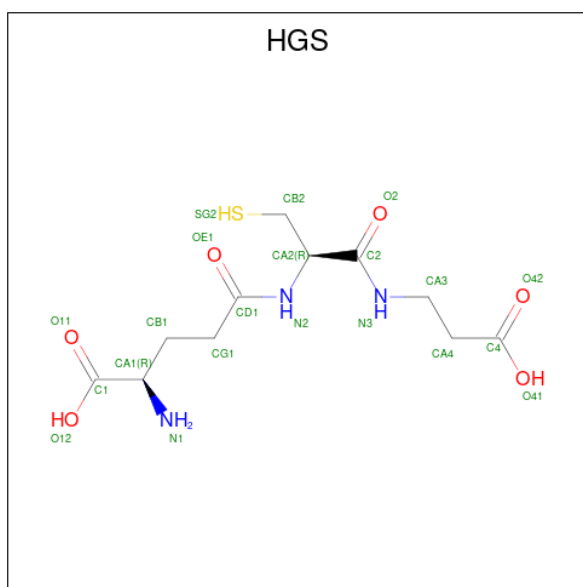
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	470	Total	C	N	O	S	0	14	0
			3828	2423	667	720	18			
1	B	468	Total	C	N	O	S	0	19	0
			3855	2434	676	728	17			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 (three-letter code: HGS) (formula:  $C_{11}H_{19}N_3O_6S$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

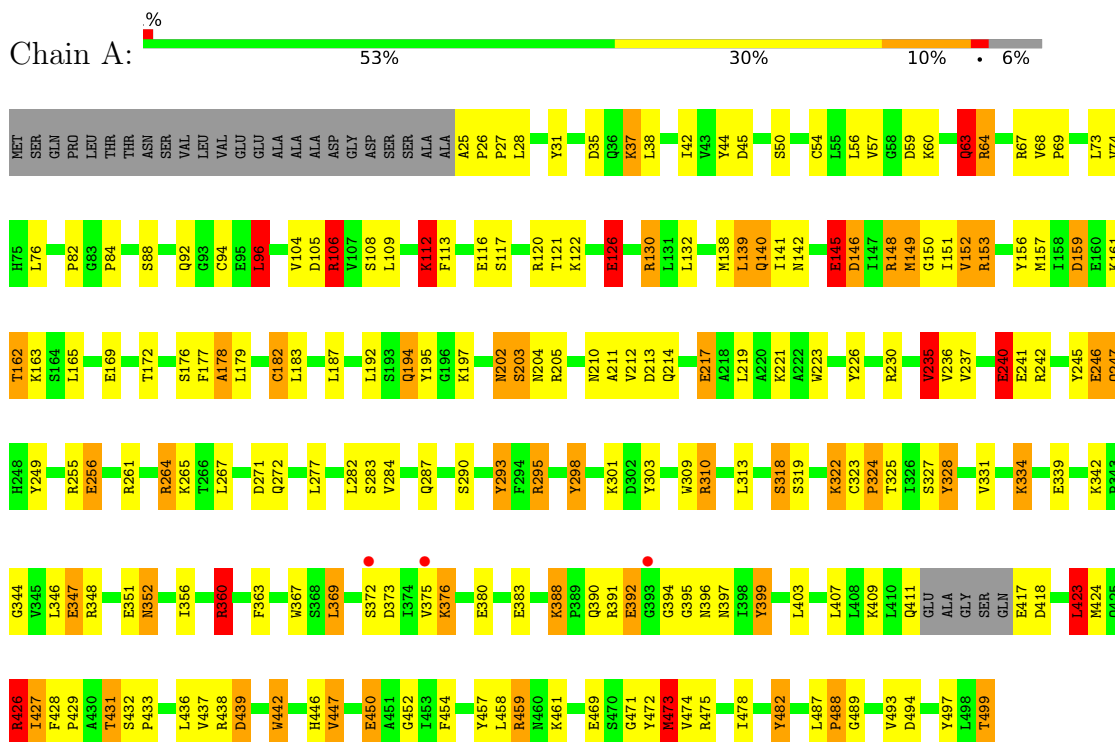
- Molecule 6 is water.

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

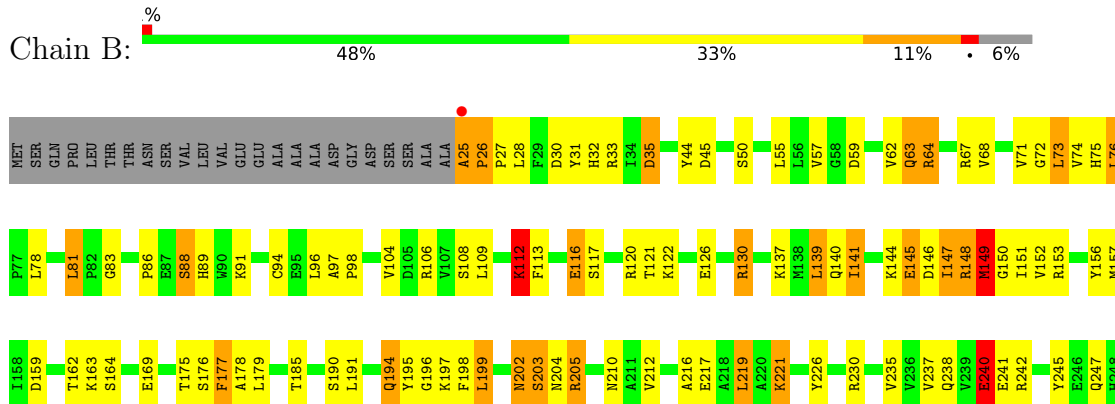
### 3 Residue-property plots

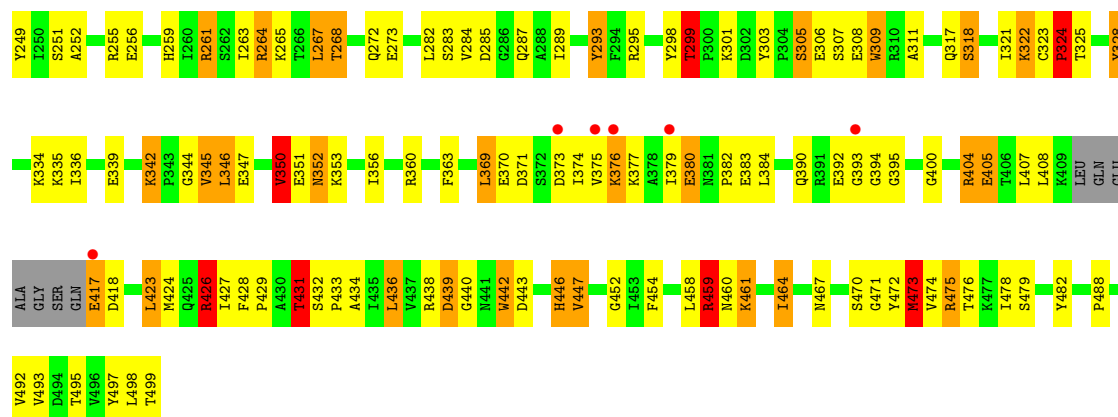
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: homogluthatione synthetase







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.70Å 115.70Å 101.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.26 – 1.90 28.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.26-1.90) 99.8 (28.09-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.250 0.198 , 0.246	Depositor DCC
$R_{free}$ test set	5992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, SO4, HGS, 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	2.09	125/3901 (3.2%)	1.72	74/5269 (1.4%)
1	B	2.08	109/3927 (2.8%)	1.71	75/5303 (1.4%)
All	All	2.09	234/7828 (3.0%)	1.72	149/10572 (1.4%)

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	A	1	3
1	B	0	5
All	All	1	8

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	GLU	CB-CG	12.81	1.76	1.52
1	A	240	GLU	CB-CG	11.81	1.74	1.52
1	B	245	TYR	CG-CD2	11.19	1.53	1.39
1	B	226	TYR	CG-CD1	10.67	1.53	1.39
1	A	126	GLU	CG-CD	10.20	1.67	1.51
1	B	252	ALA	CA-CB	10.09	1.73	1.52
1	A	264	ARG	CG-CD	10.01	1.76	1.51
1	A	256	GLU	CG-CD	-9.50	1.37	1.51
1	A	489	GLY	N-CA	9.44	1.60	1.46
1	A	126	GLU	CB-CG	9.30	1.69	1.52
1	B	44	TYR	CD2-CE2	9.28	1.53	1.39
1	B	74	VAL	CB-CG2	9.20	1.72	1.52
1	B	57	VAL	CB-CG2	9.19	1.72	1.52
1	A	156	TYR	CE1-CZ	9.08	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	ASP	CB-CG	8.97	1.70	1.51
1	B	31	TYR	CD2-CE2	8.92	1.52	1.39
1	A	74	VAL	CB-CG2	8.91	1.71	1.52
1	B	475	ARG	CG-CD	8.90	1.74	1.51
1	A	245	TYR	CG-CD2	8.81	1.50	1.39
1	A	235	VAL	CB-CG1	-8.79	1.34	1.52
1	A	240	GLU	CG-CD	-8.76	1.38	1.51
1	A	264	ARG	CB-CG	-8.60	1.29	1.52
1	A	351	GLU	CB-CG	8.52	1.68	1.52
1	B	442	TRP	CE3-CZ3	8.24	1.52	1.38
1	B	178	ALA	CA-CB	8.22	1.69	1.52
1	A	31	TYR	CD2-CE2	8.11	1.51	1.39
1	A	126	GLU	CD-OE1	8.06	1.34	1.25
1	B	88	SER	CA-CB	8.03	1.65	1.52
1	A	475	ARG	CG-CD	8.02	1.72	1.51
1	B	264	ARG	CB-CG	-7.97	1.31	1.52
1	B	108	SER	CA-CB	7.89	1.64	1.52
1	A	178	ALA	CA-CB	7.88	1.69	1.52
1	B	350	VAL	CA-CB	7.74	1.71	1.54
1	A	442	TRP	CE3-CZ3	7.73	1.51	1.38
1	A	447	VAL	CA-CB	7.65	1.70	1.54
1	B	156	TYR	CE1-CZ	7.61	1.48	1.38
1	A	88	SER	CA-CB	7.59	1.64	1.52
1	B	454	PHE	CE2-CZ	7.57	1.51	1.37
1	B	471	GLY	C-O	7.39	1.35	1.23
1	B	303	TYR	CE2-CZ	7.37	1.48	1.38
1	B	405	GLU	CG-CD	7.34	1.62	1.51
1	B	240	GLU	CG-CD	-7.32	1.41	1.51
1	B	210	ASN	CB-CG	7.29	1.67	1.51
1	B	264	ARG	CG-CD	7.28	1.70	1.51
1	A	482	TYR	CD1-CE1	7.23	1.50	1.39
1	A	363	PHE	CE1-CZ	7.21	1.51	1.37
1	A	113	PHE	CE2-CZ	7.17	1.50	1.37
1	A	145	GLU	CG-CD	7.17	1.62	1.51
1	A	195	TYR	CG-CD1	7.12	1.48	1.39
1	A	177	PHE	CD1-CE1	7.02	1.53	1.39
1	B	488	PRO	N-CD	7.00	1.57	1.47
1	A	454	PHE	CE2-CZ	6.96	1.50	1.37
1	A	245	TYR	CD1-CE1	6.93	1.49	1.39
1	B	226	TYR	CD2-CE2	6.93	1.49	1.39
1	A	247[A]	GLN	CD-OE1	6.91	1.39	1.24
1	A	247[B]	GLN	CD-OE1	6.91	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	VAL	CB-CG2	-6.84	1.38	1.52
1	B	461	LYS	N-CA	6.81	1.59	1.46
1	A	380	GLU	CG-CD	6.79	1.62	1.51
1	B	169	GLU	CG-CD	-6.77	1.41	1.51
1	A	235	VAL	CB-CG2	6.75	1.67	1.52
1	B	237	VAL	C-O	6.74	1.36	1.23
1	B	478	ILE	N-CA	6.73	1.59	1.46
1	B	237	VAL	CB-CG2	6.71	1.67	1.52
1	B	256	GLU	CG-CD	6.71	1.62	1.51
1	B	261	ARG	CG-CD	6.70	1.68	1.51
1	A	150	GLY	N-CA	6.67	1.56	1.46
1	A	44	TYR	CB-CG	6.66	1.61	1.51
1	A	497	TYR	CG-CD2	6.62	1.47	1.39
1	A	57	VAL	CB-CG2	6.60	1.66	1.52
1	B	482	TYR	CD1-CE1	6.60	1.49	1.39
1	B	311	ALA	CA-CB	6.57	1.66	1.52
1	A	247[A]	GLN	CB-CG	-6.56	1.34	1.52
1	A	247[B]	GLN	CB-CG	-6.56	1.34	1.52
1	A	82	PRO	CA-C	6.55	1.66	1.52
1	B	25	ALA	CA-CB	6.55	1.66	1.52
1	A	195	TYR	CE2-CZ	6.54	1.47	1.38
1	B	235	VAL	N-CA	6.53	1.59	1.46
1	B	432	SER	CA-CB	6.51	1.62	1.52
1	A	246	GLU	C-O	6.46	1.35	1.23
1	B	195	TYR	CG-CD1	6.44	1.47	1.39
1	B	283	SER	CA-CB	6.44	1.62	1.52
1	B	433	PRO	CA-C	6.43	1.65	1.52
1	A	272	GLN	CG-CD	6.42	1.65	1.51
1	B	251	SER	CA-CB	6.41	1.62	1.52
1	A	226	TYR	CE1-CZ	6.41	1.46	1.38
1	A	347	GLU	CB-CG	6.40	1.64	1.52
1	A	255	ARG	CD-NE	6.38	1.57	1.46
1	A	108	SER	CA-CB	6.34	1.62	1.52
1	B	272	GLN	CG-CD	6.29	1.65	1.51
1	B	50	SER	CB-OG	-6.28	1.34	1.42
1	A	471	GLY	C-O	6.25	1.33	1.23
1	A	283	SER	CA-CB	6.25	1.62	1.52
1	B	493	VAL	CB-CG1	6.25	1.66	1.52
1	B	177	PHE	CD2-CE2	6.19	1.51	1.39
1	A	44	TYR	CD2-CE2	6.19	1.48	1.39
1	A	96	LEU	CG-CD1	6.17	1.74	1.51
1	A	284	VAL	CB-CG2	6.14	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	ARG	CG-CD	6.14	1.67	1.51
1	A	63	GLN	N-CA	6.12	1.58	1.46
1	B	324	PRO	CG-CD	6.09	1.70	1.50
1	A	482	TYR	CD2-CE2	6.07	1.48	1.39
1	A	76	LEU	CG-CD2	6.07	1.74	1.51
1	B	497	TYR	CG-CD2	6.03	1.47	1.39
1	A	210	ASN	CB-CG	6.01	1.64	1.51
1	B	273	GLU	CG-CD	5.99	1.60	1.51
1	B	91	LYS	CD-CE	5.97	1.66	1.51
1	B	256	GLU	CD-OE2	5.97	1.32	1.25
1	B	363	PHE	CE1-CZ	5.96	1.48	1.37
1	B	432	SER	CB-OG	5.96	1.50	1.42
1	A	303	TYR	CG-CD1	5.96	1.46	1.39
1	A	454	PHE	CD1-CE1	5.96	1.51	1.39
1	A	223	TRP	CD2-CE2	5.94	1.48	1.41
1	A	383	GLU	CB-CG	5.94	1.63	1.52
1	B	309	TRP	CD1-NE1	5.92	1.48	1.38
1	A	432	SER	CB-OG	5.91	1.50	1.42
1	A	226	TYR	CG-CD1	5.91	1.46	1.39
1	B	264	ARG	CZ-NH1	5.90	1.40	1.33
1	A	50	SER	CB-OG	-5.90	1.34	1.42
1	B	104	VAL	CB-CG2	5.89	1.65	1.52
1	A	104	VAL	CB-CG2	5.88	1.65	1.52
1	B	241	GLU	CG-CD	5.86	1.60	1.51
1	A	303	TYR	CD1-CE1	5.86	1.48	1.39
1	A	488	PRO	CB-CG	5.83	1.79	1.50
1	A	236	VAL	CB-CG2	5.80	1.65	1.52
1	B	446	HIS	N-CA	-5.80	1.34	1.46
1	B	230	ARG	CG-CD	5.79	1.66	1.51
1	B	447	VAL	CA-CB	5.76	1.66	1.54
1	A	392	GLU	CG-CD	5.75	1.60	1.51
1	A	241	GLU	CG-CD	5.74	1.60	1.51
1	A	203	SER	N-CA	5.73	1.57	1.46
1	A	109	LEU	N-CA	5.73	1.57	1.46
1	B	242	ARG	CZ-NH2	5.72	1.40	1.33
1	A	142	ASN	CB-CG	5.71	1.64	1.51
1	A	145	GLU	CB-CG	5.71	1.63	1.52
1	A	427	ILE	CA-CB	5.71	1.68	1.54
1	B	150	GLY	N-CA	5.71	1.54	1.46
1	B	334	LYS	CB-CG	5.69	1.68	1.52
1	A	112	LYS	CD-CE	5.69	1.65	1.51
1	A	433	PRO	CA-C	5.69	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	SER	N-CA	5.69	1.57	1.46
1	A	319	SER	CB-OG	5.68	1.49	1.42
1	A	217	GLU	CB-CG	-5.64	1.41	1.52
1	B	245	TYR	CG-CD1	5.64	1.46	1.39
1	B	303	TYR	CG-CD1	5.64	1.46	1.39
1	A	146	ASP	CB-CG	5.64	1.63	1.51
1	A	237	VAL	CB-CG2	5.62	1.64	1.52
1	A	120	ARG	CG-CD	5.62	1.66	1.51
1	A	478	ILE	N-CA	5.59	1.57	1.46
1	B	322	LYS	CD-CE	5.58	1.65	1.51
1	A	68	VAL	CB-CG2	5.56	1.64	1.52
1	A	472	TYR	CD2-CE2	5.55	1.47	1.39
1	B	96	LEU	CG-CD2	5.55	1.72	1.51
1	A	454	PHE	CE1-CZ	5.54	1.47	1.37
1	A	249	TYR	CG-CD1	5.54	1.46	1.39
1	B	76	LEU	CG-CD2	5.53	1.72	1.51
1	B	256	GLU	CD-OE1	5.52	1.31	1.25
1	B	33	ARG	CG-CD	5.51	1.65	1.51
1	B	380	GLU	CG-CD	5.50	1.60	1.51
1	B	405	GLU	CD-OE2	5.50	1.31	1.25
1	B	83	GLY	C-O	5.50	1.32	1.23
1	B	265	LYS	CD-CE	5.49	1.65	1.51
1	A	177	PHE	CG-CD2	5.48	1.47	1.38
1	A	242	ARG	CZ-NH2	5.48	1.40	1.33
1	B	394	GLY	C-O	5.47	1.32	1.23
1	B	68	VAL	CB-CG2	5.45	1.64	1.52
1	A	493	VAL	CB-CG1	5.45	1.64	1.52
1	B	216	ALA	N-CA	5.44	1.57	1.46
1	B	393	GLY	N-CA	5.43	1.54	1.46
1	A	255	ARG	CZ-NH2	5.42	1.40	1.33
1	B	342	LYS	CD-CE	5.41	1.64	1.51
1	A	265	LYS	CD-CE	5.40	1.64	1.51
1	B	472	TYR	CA-CB	5.39	1.65	1.53
1	B	461	LYS	CB-CG	5.38	1.67	1.52
1	A	290	SER	CA-CB	-5.38	1.44	1.52
1	B	190	SER	CA-CB	5.38	1.61	1.52
1	A	328	TYR	CG-CD1	5.37	1.46	1.39
1	B	195	TYR	CE2-CZ	5.37	1.45	1.38
1	A	325	THR	CB-CG2	5.36	1.70	1.52
1	A	298	TYR	CE1-CZ	5.35	1.45	1.38
1	B	442	TRP	CB-CG	5.35	1.59	1.50
1	A	245	TYR	CG-CD1	5.35	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	LYS	CE-NZ	5.35	1.62	1.49
1	B	328	TYR	CG-CD1	5.33	1.46	1.39
1	A	249	TYR	CG-CD2	5.33	1.46	1.39
1	A	383	GLU	CG-CD	5.32	1.59	1.51
1	A	214	GLN	CG-CD	5.32	1.63	1.51
1	A	437	VAL	CB-CG1	5.31	1.64	1.52
1	A	309	TRP	CB-CG	5.29	1.59	1.50
1	A	334	LYS	CB-CG	5.29	1.66	1.52
1	A	301	LYS	CD-CE	5.28	1.64	1.51
1	A	367	TRP	CA-CB	5.28	1.65	1.53
1	A	494	ASP	C-O	5.27	1.33	1.23
1	B	112	LYS	CD-CE	5.26	1.64	1.51
1	A	309	TRP	CZ3-CH2	5.26	1.48	1.40
1	A	478	ILE	CB-CG2	5.26	1.69	1.52
1	B	370	GLU	CG-CD	5.25	1.59	1.51
1	A	152	VAL	CB-CG1	5.25	1.63	1.52
1	A	334	LYS	CD-CE	5.25	1.64	1.51
1	A	106	ARG	CG-CD	5.25	1.65	1.51
1	B	113	PHE	CE1-CZ	5.23	1.47	1.37
1	A	458	LEU	N-CA	5.22	1.56	1.46
1	A	293	TYR	CG-CD2	5.21	1.46	1.39
1	B	303	TYR	CD1-CE1	5.20	1.47	1.39
1	B	71	VAL	CA-CB	5.19	1.65	1.54
1	B	417	GLU	CG-CD	5.18	1.59	1.51
1	A	54	CYS	CB-SG	-5.17	1.73	1.81
1	B	59	ASP	N-CA	5.17	1.56	1.46
1	B	471	GLY	N-CA	5.17	1.53	1.46
1	A	284	VAL	CA-CB	5.16	1.65	1.54
1	B	479	SER	CB-OG	5.16	1.49	1.42
1	A	169	GLU	CB-CG	5.16	1.61	1.52
1	A	116	GLU	N-CA	5.15	1.56	1.46
1	A	211	ALA	CA-CB	5.14	1.63	1.52
1	A	457	TYR	CD2-CE2	5.14	1.47	1.39
1	B	492	VAL	CB-CG1	5.11	1.63	1.52
1	B	482	TYR	CE2-CZ	5.10	1.45	1.38
1	A	264	ARG	NE-CZ	-5.10	1.26	1.33
1	A	367	TRP	CD2-CE2	5.10	1.47	1.41
1	B	351	GLU	CD-OE1	5.09	1.31	1.25
1	A	249	TYR	CE1-CZ	5.08	1.45	1.38
1	A	472	TYR	CA-CB	5.07	1.65	1.53
1	B	116[A]	GLU	CG-CD	5.06	1.59	1.51
1	B	116[B]	GLU	CG-CD	5.06	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	TYR	CG-CD1	5.05	1.45	1.39
1	B	152	VAL	CA-CB	5.05	1.65	1.54
1	A	342	LYS	CE-NZ	5.05	1.61	1.49
1	B	284	VAL	CA-CB	5.05	1.65	1.54
1	B	461	LYS	C-N	-5.04	1.22	1.34
1	B	104	VAL	CA-CB	5.04	1.65	1.54
1	B	443	ASP	CG-OD1	5.03	1.36	1.25
1	B	447	VAL	CB-CG1	5.03	1.63	1.52
1	B	336	ILE	CA-CB	5.01	1.66	1.54
1	A	446	HIS	CA-CB	5.01	1.65	1.53

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	-29.96	105.32	120.30
1	B	264	ARG	NE-CZ-NH1	-20.81	109.89	120.30
1	A	264	ARG	NE-CZ-NH2	17.19	128.90	120.30
1	B	130	ARG	NE-CZ-NH2	-16.69	111.95	120.30
1	A	475	ARG	NE-CZ-NH2	-15.43	112.58	120.30
1	B	459[A]	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	B	459[B]	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	A	310	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	B	242	ARG	NE-CZ-NH2	13.82	127.21	120.30
1	A	310	ARG	NE-CZ-NH2	-13.55	113.52	120.30
1	A	205	ARG	NE-CZ-NH1	13.10	126.85	120.30
1	B	475	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	B	460	ASN	C-N-CA	-11.39	93.21	121.70
1	A	242	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	A	488	PRO	C-N-CA	-10.71	99.81	122.30
1	B	242	ARG	NE-CZ-NH1	-10.45	115.08	120.30
1	B	264	ARG	NE-CZ-NH2	10.41	125.50	120.30
1	B	426	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	153	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	B	473	MET	CG-SD-CE	-10.15	83.95	100.20
1	A	205	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	475	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	B	426	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	B	443	ASP	CB-CG-OD2	-9.02	110.18	118.30
1	B	81	LEU	CB-CG-CD1	8.98	126.26	111.00
1	A	96	LEU	CB-CG-CD1	8.96	126.23	111.00
1	A	153	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	264	ARG	CD-NE-CZ	-8.93	111.10	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	459	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	473	MET	CA-CB-CG	8.71	128.10	113.30
1	B	459[A]	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	459[B]	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	130	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	B	346	LEU	CB-CG-CD1	-8.52	96.53	111.00
1	A	240	GLU	CG-CD-OE1	-8.42	101.45	118.30
1	A	159	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	B	424	MET	CG-SD-CE	-8.41	86.74	100.20
1	A	348	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	235	VAL	CG1-CB-CG2	8.37	124.29	110.90
1	B	261	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	145	GLU	C-N-CA	-8.10	101.46	121.70
1	B	30	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	264	ARG	CG-CD-NE	7.88	128.34	111.80
1	A	120	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	B	267	LEU	CB-CG-CD1	7.78	124.23	111.00
1	A	59	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	A	431	THR	OG1-CB-CG2	7.60	127.49	110.00
1	B	299	THR	CB-CA-C	-7.56	91.19	111.60
1	A	473	MET	CG-SD-CE	-7.42	88.33	100.20
1	A	45	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	458	LEU	CB-CG-CD2	-7.33	98.53	111.00
1	B	35	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	439	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	426	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	240	GLU	CG-CD-OE1	-7.13	104.05	118.30
1	B	44	TYR	CB-CG-CD1	-7.08	116.75	121.00
1	B	147	ILE	C-N-CA	-7.04	104.09	121.70
1	B	78	LEU	CB-CG-CD1	-7.01	99.09	111.00
1	A	310	ARG	CD-NE-CZ	6.91	133.28	123.60
1	B	458	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	B	55	LEU	CB-CG-CD2	-6.80	99.44	111.00
1	B	460	ASN	O-C-N	-6.77	111.86	122.70
1	A	249	TYR	CD1-CE1-CZ	-6.57	113.89	119.80
1	A	277	LEU	CB-CG-CD1	-6.57	99.83	111.00
1	B	26	PRO	C-N-CD	6.50	142.06	128.40
1	A	130	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	B	267	LEU	CA-CB-CG	6.36	129.93	115.30
1	A	488	PRO	CA-C-N	6.35	128.90	116.20
1	A	256	GLU	OE1-CD-OE2	6.33	130.90	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ARG	CG-CD-NE	-6.32	98.52	111.80
1	A	423	LEU	CB-CG-CD1	6.24	121.60	111.00
1	A	426	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	240	GLU	CB-CG-CD	-6.21	97.44	114.20
1	B	240	GLU	CB-CG-CD	-6.18	97.52	114.20
1	B	149[A]	MET	CA-CB-CG	6.17	123.80	113.30
1	B	149[B]	MET	CA-CB-CG	6.17	123.80	113.30
1	B	106	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	130	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	109	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	A	488	PRO	O-C-N	-6.05	112.91	123.20
1	B	199	LEU	CA-C-N	5.96	128.12	116.20
1	A	139	LEU	CB-CG-CD1	5.92	121.07	111.00
1	A	187	LEU	CB-CG-CD1	-5.89	100.99	111.00
1	B	139	LEU	CB-CG-CD1	5.85	120.95	111.00
1	A	249	TYR	CE1-CZ-CE2	5.83	129.12	119.80
1	A	245	TYR	CD1-CE1-CZ	-5.83	114.56	119.80
1	A	322	LYS	CD-CE-NZ	-5.83	98.30	111.70
1	A	295	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	B	475	ARG	CD-NE-CZ	5.81	131.73	123.60
1	B	199	LEU	C-N-CA	-5.79	110.15	122.30
1	B	249	TYR	CD1-CE1-CZ	-5.72	114.65	119.80
1	B	221	LYS	CD-CE-NZ	-5.70	98.59	111.70
1	B	426	ARG	CB-CG-CD	5.69	126.39	111.60
1	A	267	LEU	CB-CG-CD2	5.68	120.66	111.00
1	B	289	ILE	CG1-CB-CG2	5.64	123.81	111.40
1	B	31	TYR	CZ-CE2-CD2	-5.64	114.73	119.80
1	B	219	LEU	CB-CG-CD2	5.64	120.58	111.00
1	B	226	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	106	ARG	CB-CG-CD	5.60	126.15	111.60
1	A	360	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	498	LEU	CB-CG-CD2	5.58	120.48	111.00
1	B	191	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	B	285	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	149[A]	MET	CG-SD-CE	5.55	109.07	100.20
1	A	149[B]	MET	CG-SD-CE	5.55	109.07	100.20
1	A	499	THR	CB-CA-C	-5.55	96.63	111.60
1	A	213	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	475	ARG	CD-NE-CZ	5.51	131.31	123.60
1	A	35	ASP	CB-CA-C	-5.50	99.40	110.40
1	B	28	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	A	369	LEU	CA-CB-CG	5.49	127.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	CA-CB-CG	5.47	125.44	113.40
1	A	403	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	45	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	73	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	A	56	LEU	CB-CG-CD2	-5.40	101.81	111.00
1	A	277	LEU	CB-CG-CD2	5.39	120.17	111.00
1	B	106	ARG	CD-NE-CZ	-5.39	116.05	123.60
1	B	263	ILE	CG1-CB-CG2	-5.38	99.56	111.40
1	A	162	THR	C-N-CA	-5.36	108.29	121.70
1	A	423	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	424	MET	CG-SD-CE	-5.30	91.72	100.20
1	A	240	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	A	264	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	B	392	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	450	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	213	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	130	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	460	ASN	N-CA-CB	5.20	119.95	110.60
1	A	76	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	A	183	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	B	470	SER	N-CA-CB	-5.15	102.77	110.50
1	A	205	ARG	CD-NE-CZ	5.14	130.79	123.60
1	B	461	LYS	CA-C-N	-5.13	105.91	117.20
1	B	431	THR	OG1-CB-CG2	5.13	121.79	110.00
1	B	268	THR	N-CA-CB	5.09	119.97	110.30
1	B	436	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	A	230	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	245	TYR	CE1-CZ-CE2	5.07	127.92	119.80
1	B	431	THR	N-CA-CB	-5.07	100.66	110.30
1	A	459	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	149[A]	MET	CG-SD-CE	5.04	108.26	100.20
1	B	149[B]	MET	CG-SD-CE	5.04	108.26	100.20
1	B	443	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	126	GLU	CA-CB-CG	5.01	124.42	113.40
1	A	313	LEU	CB-CG-CD2	-5.00	102.50	111.00
1	A	346	LEU	CB-CG-CD1	-5.00	102.50	111.00
1	B	78	LEU	CB-CG-CD2	-5.00	102.50	111.00

All (1) chirality outliers are listed below:

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	149	0
1	B	3855	0	3864	178	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	42	0	33	18	0
3	B	42	0	30	28	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	30	0
All	All	8571	0	7801	346	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 (346) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:B:506:HGS:HB1	3:B:506:HGS:HA2	1.30	1.06
1:A:240:GLU:CB	1:A:240:GLU:OE1	1.95	1.04
1:B:149[A]:MET:HE3	1:B:323:CYS:HB2	1.37	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
3:B:506:HGS:SG2	3:B:506:HGS:O2	2.19	1.00
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:149[B]:MET:HE3	1:A:323:CYS:HB2	1.44	0.97
1:B:369:LEU:HD22	1:B:423:LEU:HD22	1.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:506:HGS:HA2	3:B:506:HGS:CB1	1.99	0.93
1:B:176[B]:SER:HG	3:B:501:HGS:HA3	1.30	0.93
1:B:63:GLN:NE2	1:B:67[B]:ARG:HH22	1.67	0.92
1:B:347:GLU:OE1	1:B:360[B]:ARG:NH2	2.01	0.92
1:A:240:GLU:CB	1:A:240:GLU:CD	2.36	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:240:GLU:CB	1:B:240:GLU:CD	2.39	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: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: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:A:395:GLY:C	6:A:721:HOH:O	2.21	0.78
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
1:B:347:GLU:OE2	1:B:360[B]:ARG:NH1	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
3:A:506:HGS:SG2	3:A:506:HGS:O2	2.48	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:A:352:ASN:HD22	1:A:352:ASN:C	1.95	0.69
1:A:246:GLU:C	1:A:247[B]:GLN:CA	2.61	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
1:A:439:ASP:CG	6:A:875:HOH:O	2.32	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:369:LEU:CD2	1:A:423:LEU:HD22	2.25	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149[B]:MET:HE1	1:A:323:CYS:HB2	1.73	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:347:GLU:CD	1:B:360[B]:ARG:HH22	1.99	0.64
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: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:A:63:GLN:H	1:A:63:GLN:CD	2.04	0.61
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:A:161:LYS:O	1:A:161:LYS:HG2	2.01	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:63:GLN:CD	1:A:63:GLN:N	2.56	0.59
1:A:247[B]:GLN:NE2	1:A:264:ARG:HH11	1.78	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
3:B:506:HGS:CB1	3:B:506:HGS:CA2	2.79	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: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:B:148:ARG:CD	1:B:325:THR:HG21	2.35	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:506:HGS:HG1	3:A:506:HGS:O12	2.04	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: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:149[A]:MET:HE2	1:B:323:CYS:HB2	1.83	0.55
1:B:148:ARG:HD3	1:B:325:THR:HG23	1.88	0.55
1:B:352:ASN:C	1:B:352:ASN:HD22	2.09	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: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:B:438[B]:ARG:O	1:B:439[B]:ASP:C	2.46	0.53
1:A:176[A]:SER:HG	3:A:501:HGS:HA3	1.72	0.53
1:B:26:PRO:O	1:B:27:PRO:C	2.45	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:A:149[B]:MET:HE3	1:A:323:CYS:CB	2.29	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
3:B:506:HGS:O11	3:B:506:HGS:HB2	2.11	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:A:182:CYS:CB	3:A:506:HGS:HSG2	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLU:OE1	2:A:500:ADP:O3'	2.20	0.50
1:B:141:ILE:HD12	1:B:141:ILE:O	2.11	0.50
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:130:ARG:HH22	1:B:306:GLU:CD	2.16	0.48
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:438[B]:ARG:NE	6:A:805:HOH:O	1.79	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:146:ASP:O	1:B:146:ASP:CG	2.47	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:A:347:GLU:CD	1:A:360:ARG:HH12	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:352:ASN:C	1:A:352:ASN:ND2	2.66	0.46
1:B:305:SER:HB2	1:B:308:GLU:OE1	2.15	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: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: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: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: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:A:394:GLY:HA2	6:A:650:HOH:O	2.16	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:MET:HE3	1:B:473:MET:C	2.38	0.43
1:B:293:TYR:CZ	1:B:295:ARG:HD3	2.53	0.43
1:B:345:VAL:O	1:B:346:LEU:C	2.55	0.43
1:B:146:ASP:OD1	1:B:146:ASP:C	2.51	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:A:388:LYS:HD3	1:A:397:ASN:ND2	2.34	0.42
1:B:473:MET:HE3	1:B:473:MET:O	2.18	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: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
3:B:506:HGS:HA2	3:B:506:HGS:CA1	2.49	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:153:ARG:NE	1:A:473:MET:HE2	2.35	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
3:B:506:HGS:CB2	3:B:506:HGS:HA1	2.50	0.41
1:A:63:GLN:HG3	6:A:644:HOH:O	2.21	0.41
1:A:126:GLU:H	1:A:126:GLU:CD	2.23	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: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:473:MET:HB3	1:B:473:MET:HE2	1.67	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:B:112:LYS:HG2	1:B:116[B]:GLU:CD	2.42	0.40
1:A:121:THR:HG21	1:A:390:GLN:HG3	2.04	0.40
1:A:140:GLN:O	1:A:141:ILE:C	2.60	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%)	47	38
1	B	483/499 (97%)	448 (93%)	28 (6%)	7 (1%)	11	3
All	All	963/998 (96%)	906 (94%)	49 (5%)	8 (1%)	29	9

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

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Mol	Chain	Res	Type
1	B	318[B]	SER
1	A	344	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	424/431 (98%)	391 (92%)	33 (8%)	12 5
1	B	427/431 (99%)	388 (91%)	39 (9%)	9 3
All	All	851/862 (99%)	779 (92%)	72 (8%)	11 4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	60	LYS
1	A	63	GLN
1	A	64[A]	ARG
1	A	64[B]	ARG
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	318[A]	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	318[B]	SER
1	A	324	PRO
1	A	352	ASN
1	A	360	ARG
1	A	376	LYS
1	A	388	LYS
1	A	399	TYR
1	A	409	LYS
1	A	411	GLN
1	A	423	LEU
1	A	426	ARG
1	A	473	MET
1	B	35	ASP
1	B	63	GLN
1	B	64[A]	ARG
1	B	64[B]	ARG
1	B	81	LEU
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	194	GLN
1	B	202	ASN
1	B	205	ARG
1	B	240	GLU
1	B	267	LEU
1	B	268	THR
1	B	299	THR
1	B	305	SER
1	B	322	LYS
1	B	324	PRO
1	B	345	VAL
1	B	350	VAL
1	B	352	ASN
1	B	376	LYS
1	B	377	LYS
1	B	404	ARG
1	B	405	GLU

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Mol	Chain	Res	Type
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	194	GLN
1	A	202	ASN
1	A	204	ASN
1	A	238	GLN
1	A	287	GLN
1	A	352	ASN
1	A	396	ASN
1	A	411	GLN
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	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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	A	505	4	4,4,4	1.67	1 (25%)	6,6,6	1.28	0
3	HGS	A	501	-	19,20,20	4.27	11 (57%)	24,25,25	6.75	16 (66%)
2	ADP	A	500	4	24,29,29	2.00	7 (29%)	29,45,45	1.65	6 (20%)
3	HGS	B	501	-	19,20,20	3.46	7 (36%)	24,25,25	6.33	17 (70%)
3	HGS	A	506	-	19,20,20	2.95	7 (36%)	24,25,25	3.36	12 (50%)
3	HGS	B	506	-	19,20,20	2.19	5 (26%)	24,25,25	3.00	11 (45%)
5	SO4	B	505	4	4,4,4	1.49	1 (25%)	6,6,6	1.54	1 (16%)
2	ADP	B	500	4	24,29,29	1.68	7 (29%)	29,45,45	1.50	5 (17%)

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	HGS	A	501	-	-	12/25/25/25	-
2	ADP	A	500	4	-	2/12/32/32	0/3/3/3
3	HGS	B	501	-	-	12/25/25/25	-
3	HGS	A	506	-	-	10/25/25/25	-

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

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HGS	CB2-CA2	9.86	1.63	1.53
3	B	501	HGS	CB2-CA2	8.28	1.62	1.53
3	A	501	HGS	CA4-C4	8.01	1.69	1.50
3	A	506	HGS	O2-C2	7.82	1.38	1.23
3	A	501	HGS	CA3-N3	6.65	1.61	1.46
3	B	501	HGS	CA3-N3	6.09	1.60	1.46
3	B	501	HGS	OE1-CD1	6.07	1.35	1.23
3	A	501	HGS	OE1-CD1	6.03	1.35	1.23
3	B	501	HGS	CA4-C4	5.93	1.64	1.50
3	A	506	HGS	OE1-CD1	5.89	1.35	1.23
3	B	506	HGS	OE1-CD1	5.57	1.34	1.23
2	A	500	ADP	C2-N3	5.22	1.40	1.32
3	B	506	HGS	O2-C2	5.21	1.33	1.23
3	A	501	HGS	C2-N3	4.83	1.44	1.33
3	A	501	HGS	O42-C4	4.47	1.37	1.22
3	A	506	HGS	CD1-N2	-4.32	1.24	1.34
3	B	501	HGS	CD1-N2	-3.97	1.25	1.34
3	A	501	HGS	CA3-CA4	3.91	1.63	1.51
3	A	501	HGS	CD1-N2	-3.61	1.26	1.34
2	A	500	ADP	C2-N1	3.35	1.40	1.33
2	B	500	ADP	C2-N1	3.32	1.40	1.33
2	A	500	ADP	C5-C4	3.29	1.49	1.40
3	A	501	HGS	O41-C4	3.27	1.41	1.30
2	B	500	ADP	C2-N3	3.26	1.37	1.32
2	B	500	ADP	C5-C4	3.15	1.49	1.40
2	A	500	ADP	PB-O2B	-3.12	1.42	1.54
3	B	501	HGS	CA3-CA4	3.04	1.61	1.51
3	A	506	HGS	CB1-CA1	2.99	1.59	1.53
3	B	501	HGS	C2-N3	2.90	1.40	1.33
3	A	501	HGS	O2-C2	2.83	1.29	1.23
5	A	505	SO4	O2-S	2.74	1.60	1.46
5	B	505	SO4	O2-S	2.72	1.60	1.46
3	B	506	HGS	CD1-N2	-2.68	1.28	1.34
2	B	500	ADP	PB-O2B	-2.64	1.44	1.54
3	B	506	HGS	C2-N3	-2.58	1.28	1.33
3	A	506	HGS	CB1-CG1	2.56	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	HGS	C2-N3	-2.55	1.28	1.33
2	A	500	ADP	C6-C5	2.52	1.52	1.43
3	A	501	HGS	CA2-C2	2.43	1.59	1.52
2	A	500	ADP	C4-N3	2.42	1.39	1.35
3	A	506	HGS	O12-C1	-2.40	1.22	1.30
2	B	500	ADP	O4'-C1'	2.36	1.44	1.41
2	B	500	ADP	C5'-C4'	2.35	1.58	1.51
2	B	500	ADP	C2'-C1'	-2.28	1.50	1.53
2	A	500	ADP	C8-N7	2.17	1.38	1.34
3	B	506	HGS	CA2-C2	-2.01	1.47	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HGS	CA3-N3-C2	18.29	155.21	122.59
3	B	501	HGS	CA3-N3-C2	18.07	154.82	122.59
3	A	501	HGS	CA2-CB2-SG2	-16.08	96.12	114.19
3	B	501	HGS	CA2-CB2-SG2	-13.00	99.58	114.19
3	B	501	HGS	CA2-C2-N3	9.86	136.43	116.54
3	A	501	HGS	CA2-C2-N3	9.66	136.01	116.54
3	A	501	HGS	CA3-CA4-C4	9.61	129.94	113.51
3	A	501	HGS	CA4-CA3-N3	8.47	129.00	111.90
3	A	506	HGS	CA2-CB2-SG2	-8.30	104.87	114.19
3	A	506	HGS	OE1-CD1-N2	-8.04	109.38	122.95
3	B	506	HGS	CA4-CA3-N3	-7.86	96.03	111.90
3	A	501	HGS	O2-C2-CA2	-7.38	104.92	120.45
3	B	501	HGS	CA4-CA3-N3	6.63	125.28	111.90
3	B	501	HGS	CB1-CA1-C1	-6.60	94.59	110.30
3	B	501	HGS	CG1-CD1-N2	-6.56	104.45	115.83
3	B	501	HGS	O2-C2-CA2	-6.46	106.87	120.45
3	A	501	HGS	CG1-CB1-CA1	-6.32	99.09	113.84
3	B	501	HGS	CA2-N2-CD1	5.82	136.62	121.65
3	B	506	HGS	CA3-N3-C2	5.69	132.74	122.59
3	B	501	HGS	OE1-CD1-N2	5.21	131.74	122.95
3	B	506	HGS	CB2-CA2-N2	-5.21	103.86	111.28
3	B	501	HGS	O41-C4-O42	-5.17	110.42	123.30
3	A	501	HGS	OE1-CD1-N2	5.06	131.50	122.95
3	B	506	HGS	CG1-CD1-N2	5.06	124.60	115.83
3	B	501	HGS	CA3-CA4-C4	5.00	122.05	113.51
3	A	501	HGS	O41-C4-O42	4.77	135.18	123.30
3	A	501	HGS	O11-C1-CA1	-4.58	105.98	122.14
3	A	506	HGS	OE1-CD1-CG1	4.45	130.15	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	HGS	CA3-N3-C2	4.35	130.34	122.59
2	A	500	ADP	N3-C2-N1	-4.32	121.93	128.68
3	B	501	HGS	O12-C1-CA1	4.20	127.69	113.38
3	A	501	HGS	O12-C1-CA1	4.07	127.25	113.38
2	A	500	ADP	C4-C5-N7	-3.99	105.24	109.40
2	B	500	ADP	N3-C2-N1	-3.99	122.45	128.68
3	A	501	HGS	CG1-CD1-N2	-3.92	109.04	115.83
3	A	506	HGS	CB1-CG1-CD1	3.78	121.48	113.04
3	B	501	HGS	O41-C4-CA4	3.76	126.10	114.03
3	A	506	HGS	CA3-CA4-C4	3.76	119.93	113.51
3	B	501	HGS	O11-C1-CA1	-3.74	108.92	122.14
3	A	501	HGS	O42-C4-CA4	-3.74	111.07	123.08
3	B	506	HGS	CA2-CB2-SG2	-3.57	110.18	114.19
3	A	506	HGS	CB2-CA2-N2	-3.56	106.20	111.28
3	B	501	HGS	CG1-CB1-CA1	-3.49	105.69	113.84
3	A	501	HGS	CB2-CA2-C2	3.47	116.91	109.76
3	A	506	HGS	CB1-CA1-N1	3.28	118.77	110.17
3	B	506	HGS	CB1-CG1-CD1	3.10	119.96	113.04
3	B	501	HGS	O2-C2-N3	-3.00	116.55	122.99
3	A	506	HGS	C2-CA2-N2	2.86	118.96	111.16
3	B	506	HGS	CA2-C2-N3	2.83	122.26	116.54
3	A	506	HGS	CA4-CA3-N3	-2.81	106.22	111.90
3	B	506	HGS	OE1-CD1-CG1	-2.80	116.89	122.02
2	B	500	ADP	C5'-C4'-C3'	2.79	125.65	115.18
5	B	505	SO4	O4-S-O3	-2.79	97.16	109.06
3	B	501	HGS	CB2-CA2-N2	-2.78	107.32	111.28
3	B	506	HGS	OE1-CD1-N2	-2.64	118.49	122.95
3	A	506	HGS	CG1-CD1-N2	2.64	120.41	115.83
2	B	500	ADP	O4'-C4'-C3'	-2.50	100.17	105.11
2	A	500	ADP	O4'-C1'-C2'	2.48	110.55	106.93
2	B	500	ADP	C4-C5-N7	-2.47	106.83	109.40
2	B	500	ADP	O3B-PB-O3A	2.43	112.79	104.64
2	A	500	ADP	C1'-N9-C4	-2.36	122.49	126.64
3	A	501	HGS	CB1-CG1-CD1	2.33	118.25	113.04
3	B	506	HGS	CB2-CA2-C2	-2.32	104.99	109.76
3	A	501	HGS	CB1-CA1-N1	2.27	116.11	110.17
2	A	500	ADP	O3B-PB-O3A	2.23	112.11	104.64
2	A	500	ADP	C3'-C2'-C1'	-2.19	97.68	100.98
3	B	506	HGS	O2-C2-CA2	-2.17	115.89	120.45
3	A	506	HGS	CA2-N2-CD1	-2.17	116.07	121.65

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

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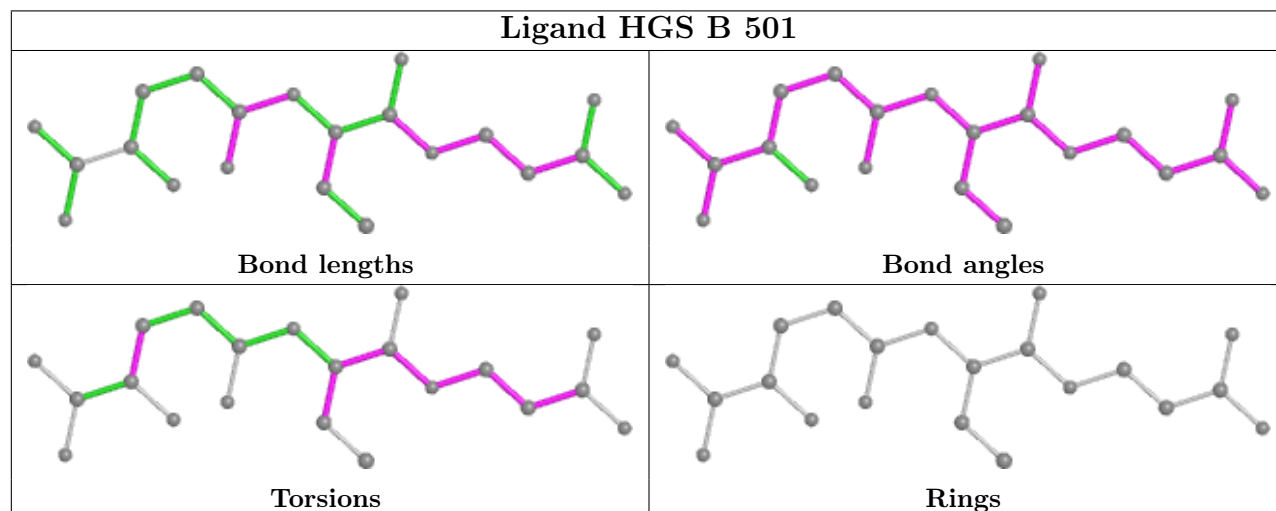
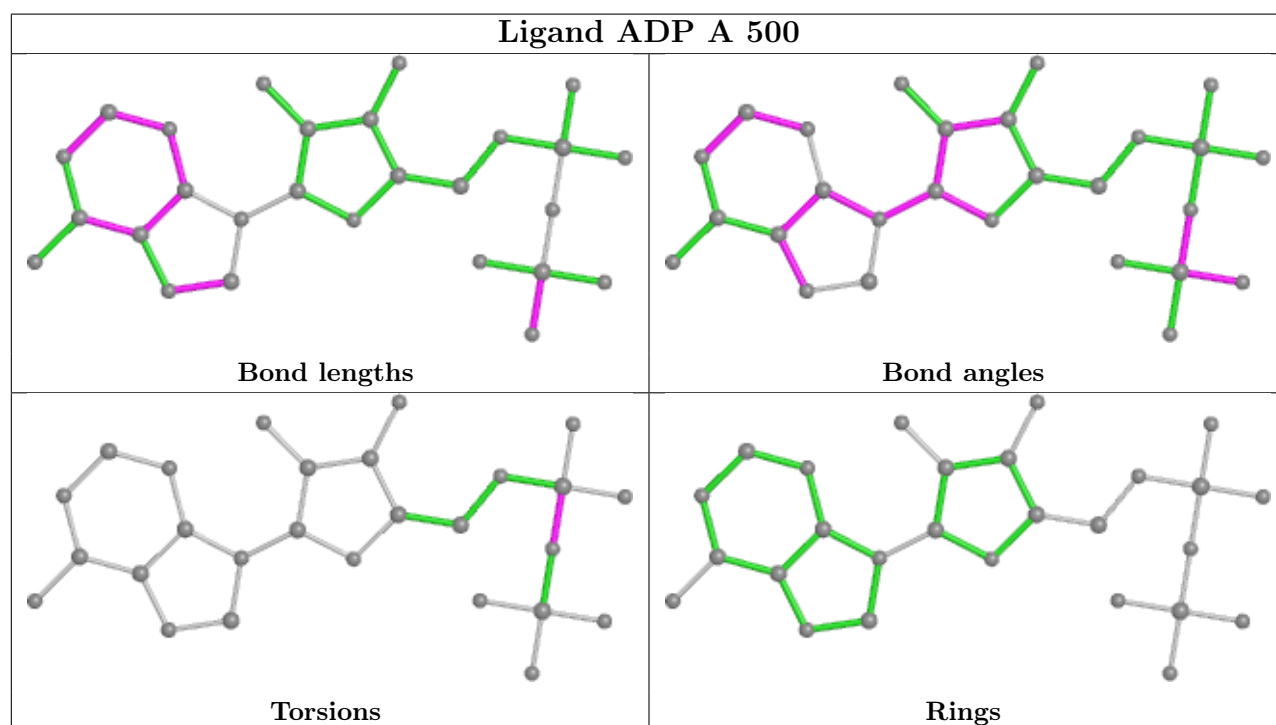
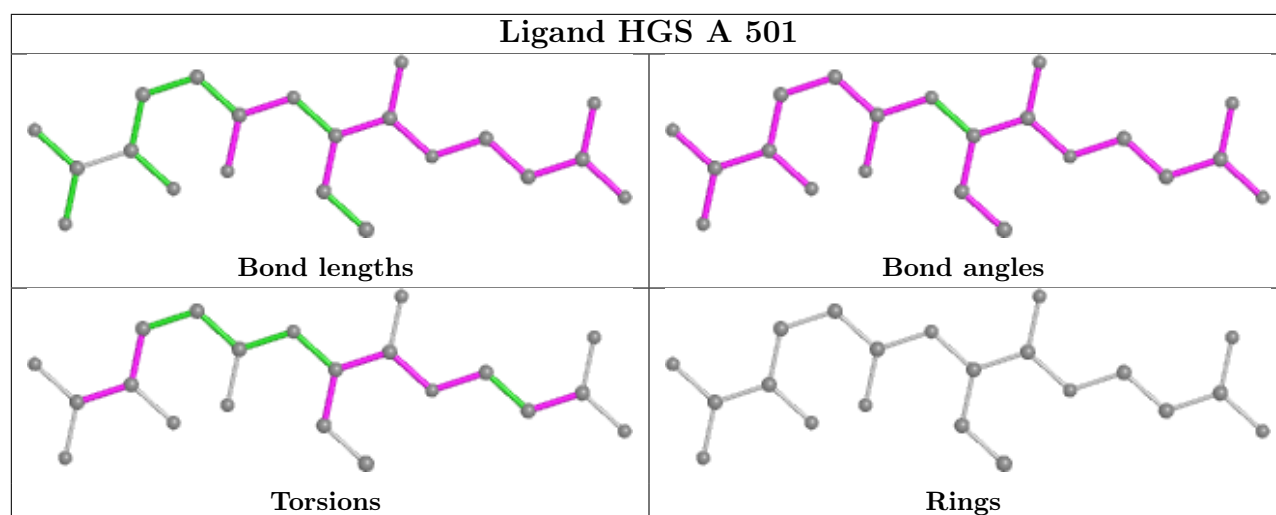
Mol	Chain	Res	Type	Atoms
2	A	500	ADP	PB-O3A-PA-O1A
3	A	506	HGS	O2-C2-CA2-N2
3	B	501	HGS	O41-C4-CA4-CA3
3	B	501	HGS	C2-CA2-CB2-SG2
3	B	506	HGS	O11-C1-CA1-N1
3	B	501	HGS	O42-C4-CA4-CA3
3	A	506	HGS	N3-C2-CA2-N2
3	B	506	HGS	O12-C1-CA1-N1
2	B	500	ADP	PB-O3A-PA-O2A
3	A	501	HGS	O41-C4-CA4-CA3
3	A	501	HGS	O42-C4-CA4-CA3

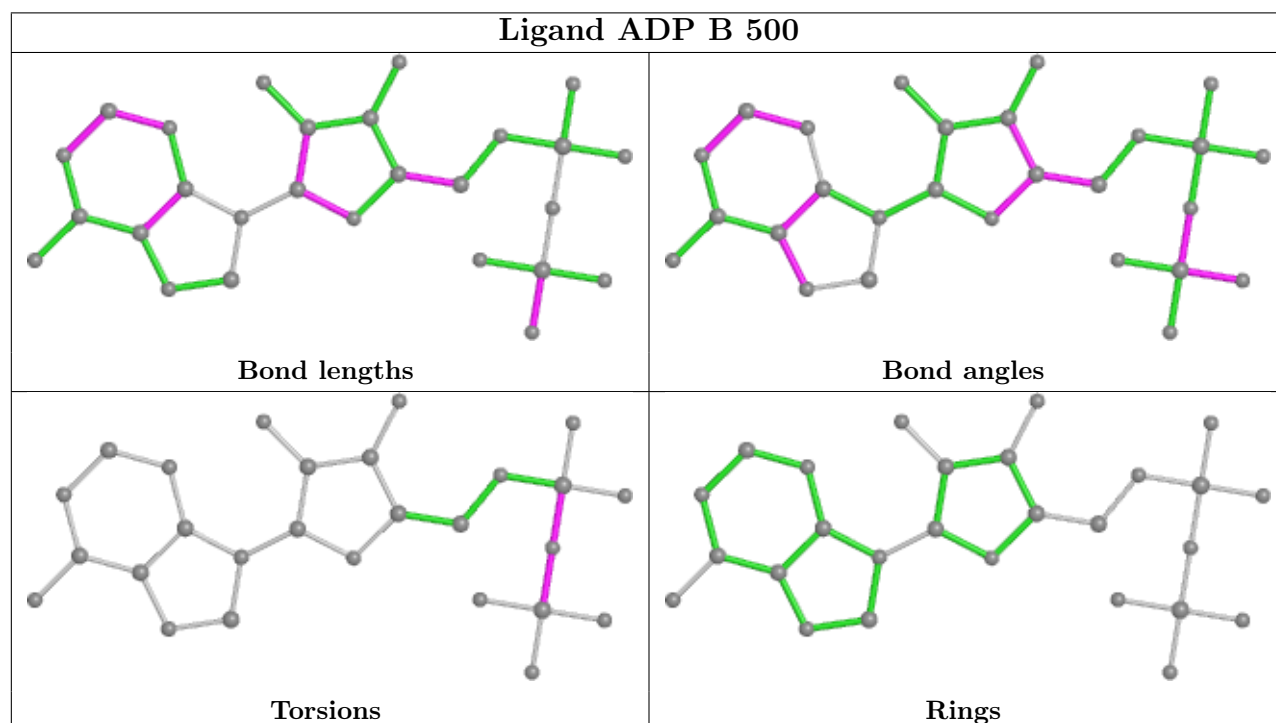
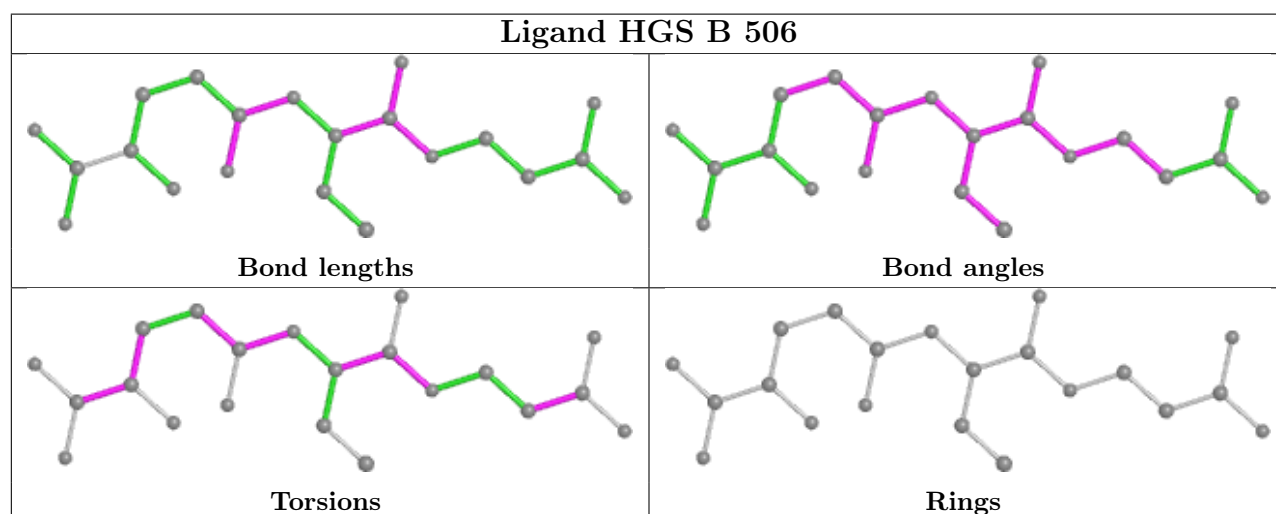
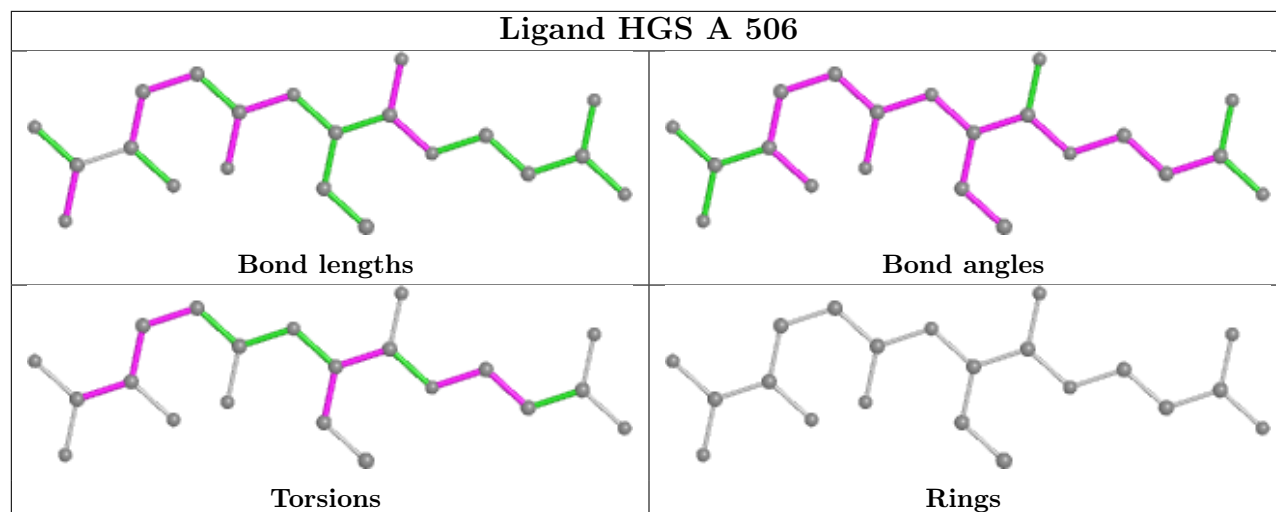
There are no ring outliers.

7 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	SO4	4	0
3	A	501	HGS	12	0
2	A	500	ADP	1	0
3	B	501	HGS	21	0
3	A	506	HGS	6	0
3	B	506	HGS	7	0
5	B	505	SO4	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.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	470/499 (94%)	-0.19	3 (0%) 89 90	18, 31, 64, 84	0
1	B	468/499 (93%)	-0.14	7 (1%) 73 76	20, 31, 65, 89	0
All	All	938/998 (93%)	-0.17	10 (1%) 80 82	18, 31, 66, 89	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	ILE	3.2
1	B	25	ALA	3.1
1	B	393	GLY	2.8
1	A	372	SER	2.7
1	B	376	LYS	2.6
1	A	375	VAL	2.6
1	B	417	GLU	2.5
1	B	375	VAL	2.4
1	A	393	GLY	2.3
1	B	373	ASP	2.2

### 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 monosaccharides in this entry.

## 6.4 Ligands

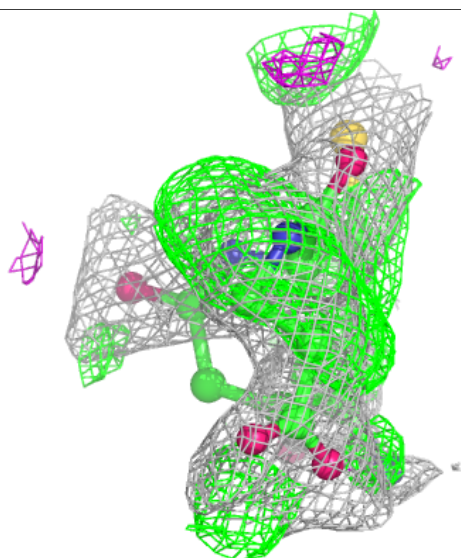
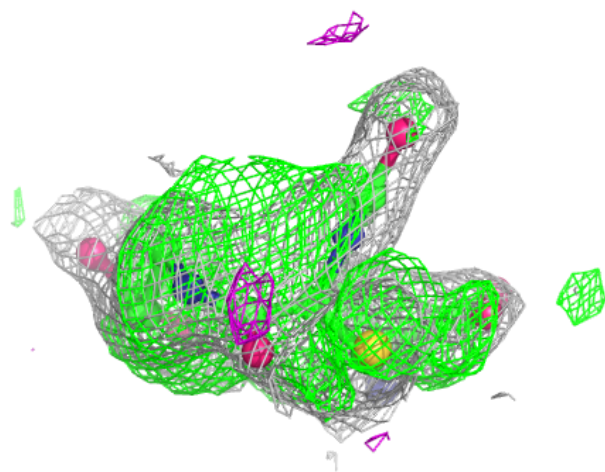
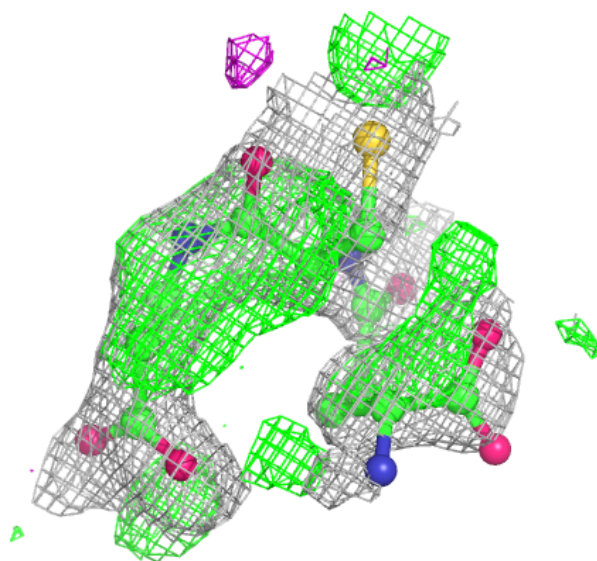
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HGS	B	506	21/21	0.76	0.26	34,42,50,52	21
3	HGS	A	501	21/21	0.87	0.18	25,51,57,61	0
3	HGS	B	501	21/21	0.89	0.17	27,52,57,64	0
3	HGS	A	506	21/21	0.90	0.23	14,27,56,59	21
4	MG	B	504	1/1	0.97	0.06	36,36,36,36	0
5	SO4	A	505	5/5	0.97	0.08	29,37,46,49	0
4	MG	A	504	1/1	0.98	0.07	36,36,36,36	0
4	MG	A	502	1/1	0.98	0.07	39,39,39,39	0
4	MG	A	503	1/1	0.98	0.07	27,27,27,27	0
5	SO4	B	505	5/5	0.98	0.10	31,35,42,45	0
4	MG	B	503	1/1	0.99	0.06	29,29,29,29	0
2	ADP	B	500	27/27	0.99	0.09	27,33,37,39	0
2	ADP	A	500	27/27	0.99	0.08	24,31,37,37	0
4	MG	B	502	1/1	0.99	0.07	34,34,34,34	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.

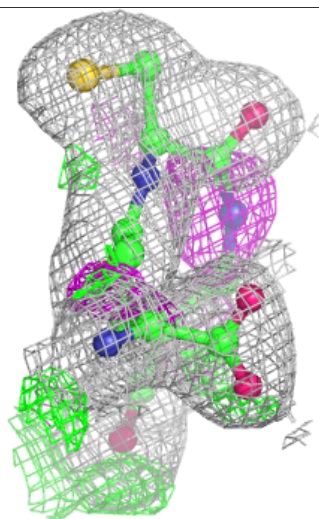
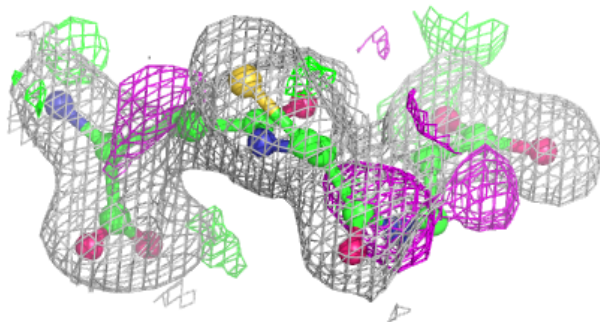
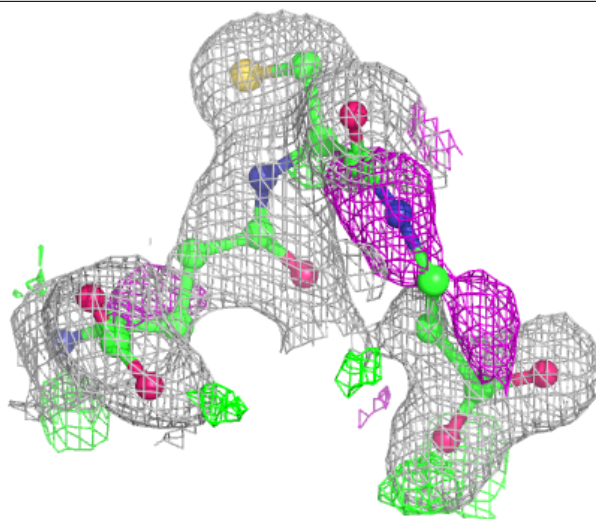
**Electron density around HGS B 506:**

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



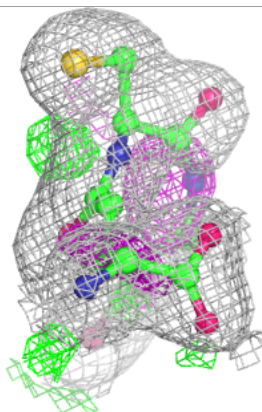
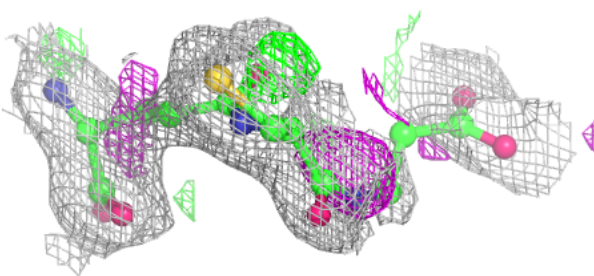
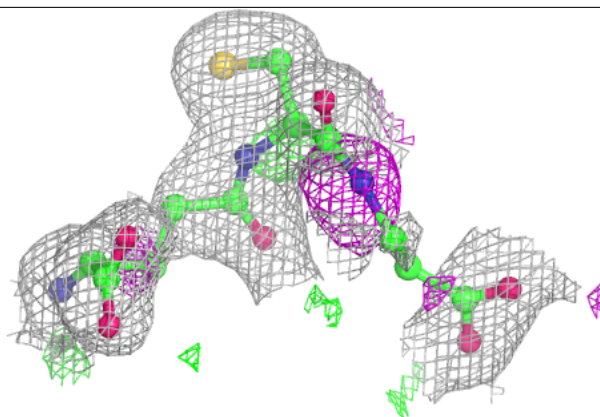
**Electron density around HGS A 501:**

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

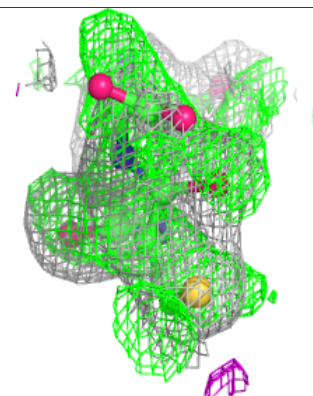
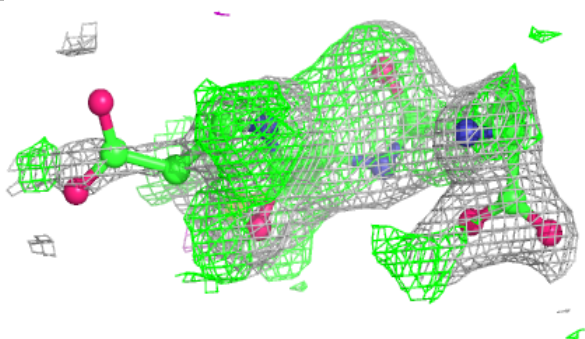
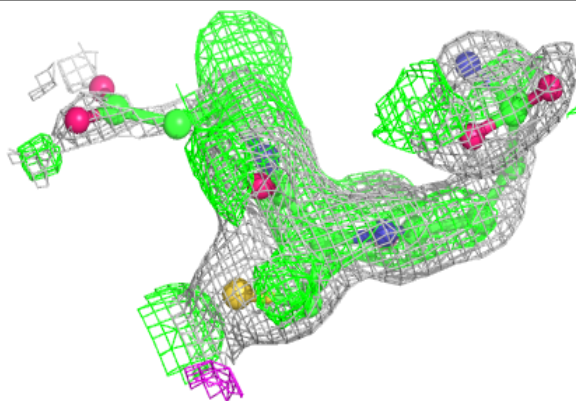


**Electron density around HGS B 501:**

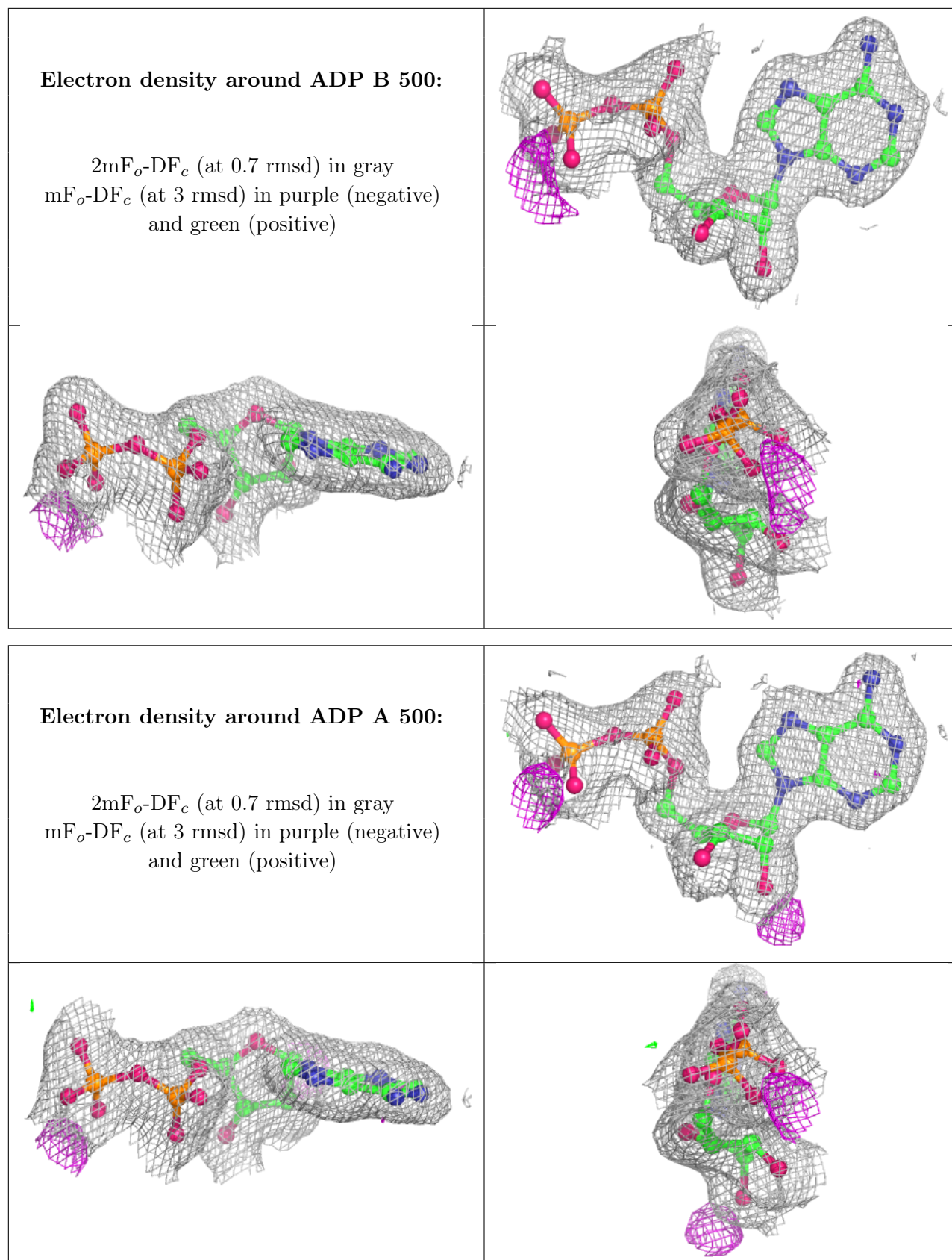
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.