



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 06:03 AM EDT

PDB ID : 1SXJ  
Title : Crystal Structure of the Eukaryotic Clamp Loader (Replication Factor C, RFC) Bound to the DNA Sliding Clamp (Proliferating Cell Nuclear Antigen, PCNA)  
Authors : Bowman, G.D.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2004-03-30  
Resolution : 2.85 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

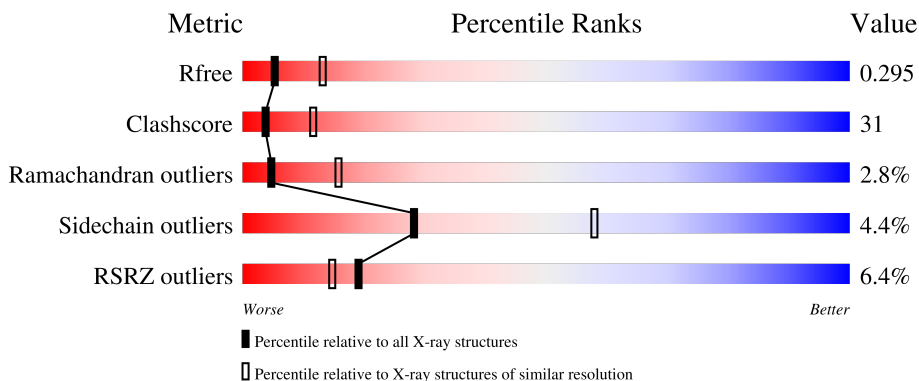
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

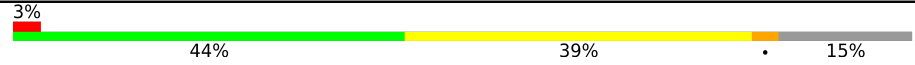


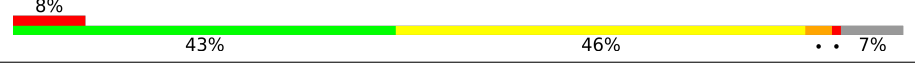
The reported resolution of this entry is 2.85 Å.

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.



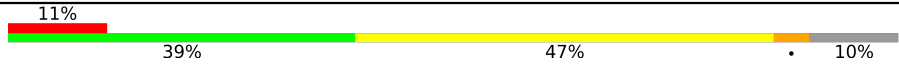

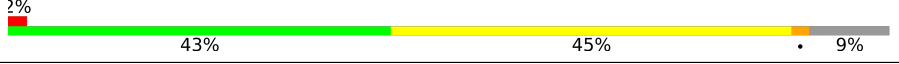
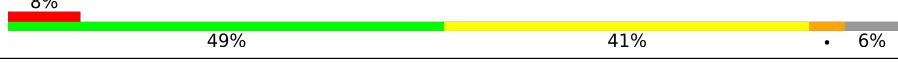
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	516	
2	B	323	
3	C	340	
4	D	353	

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Mol	Chain	Length	Quality of chain
5	E	354	
6	F	283	
6	G	283	
6	H	283	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19740 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 Activator 1 95 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	3345	2110	603	617	15	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	MET	-	expression tag	UNP P38630
A	271	GLY	-	expression tag	UNP P38630
A	272	SER	-	expression tag	UNP P38630
A	273	SER	-	expression tag	UNP P38630
A	274	HIS	-	expression tag	UNP P38630
A	275	HIS	-	expression tag	UNP P38630
A	276	HIS	-	expression tag	UNP P38630
A	277	HIS	-	expression tag	UNP P38630
A	278	HIS	-	expression tag	UNP P38630
A	279	HIS	-	expression tag	UNP P38630
A	280	SER	-	expression tag	UNP P38630
A	281	SER	-	expression tag	UNP P38630
A	282	GLY	-	expression tag	UNP P38630
A	283	LEU	-	expression tag	UNP P38630
A	284	GLU	-	expression tag	UNP P38630
A	285	VAL	-	expression tag	UNP P38630
A	286	LEU	-	expression tag	UNP P38630
A	287	PHE	-	expression tag	UNP P38630
A	288	GLN	-	expression tag	UNP P38630
A	289	GLY	-	expression tag	UNP P38630
A	290	PRO	-	expression tag	UNP P38630
A	291	HIS	-	expression tag	UNP P38630
A	292	MET	-	expression tag	UNP P38630
A	293	ALA	-	expression tag	UNP P38630
A	294	SER	-	expression tag	UNP P38630

- Molecule 2 is a protein called Activator 1 37 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	316	2482	1566	441	462	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLN	ARG	engineered mutation	UNP P40339

- Molecule 3 is a protein called Activator 1 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	322	2544	1604	443	489	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	160	GLN	ARG	engineered mutation	UNP P38629

- Molecule 4 is a protein called Activator 1 41 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	328	2597	1642	446	499	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	GLN	ARG	engineered mutation	UNP P40348

- Molecule 5 is a protein called Activator 1 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	317	2495	1582	428	468	17	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	184	GLN	ARG	engineered mutation	UNP P38251

- Molecule 6 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	258	Total 2021	C 1291	N 319	O 401	S 4	Se 6	0	0	0
6	G	258	Total 2022	C 1292	N 319	O 400	S 4	Se 7	5	0	0
6	H	267	Total 2079	C 1329	N 330	O 409	S 4	Se 7	0	0	0

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-24	MSE	-	expression tag	UNP P15873
F	-23	GLY	-	expression tag	UNP P15873
F	-22	SER	-	expression tag	UNP P15873
F	-21	SER	-	expression tag	UNP P15873
F	-20	HIS	-	expression tag	UNP P15873
F	-19	HIS	-	expression tag	UNP P15873
F	-18	HIS	-	expression tag	UNP P15873
F	-17	HIS	-	expression tag	UNP P15873
F	-16	HIS	-	expression tag	UNP P15873
F	-15	HIS	-	expression tag	UNP P15873
F	-14	SER	-	expression tag	UNP P15873
F	-13	SER	-	expression tag	UNP P15873
F	-12	GLY	-	expression tag	UNP P15873
F	-11	LEU	-	expression tag	UNP P15873
F	-10	GLU	-	expression tag	UNP P15873
F	-9	VAL	-	expression tag	UNP P15873
F	-8	LEU	-	expression tag	UNP P15873
F	-7	PHE	-	expression tag	UNP P15873
F	-6	GLN	-	expression tag	UNP P15873
F	-5	GLY	-	expression tag	UNP P15873
F	-4	PRO	-	expression tag	UNP P15873
F	-3	HIS	-	expression tag	UNP P15873
F	-2	MSE	-	expression tag	UNP P15873
F	-1	ALA	-	expression tag	UNP P15873
F	0	SER	-	expression tag	UNP P15873
F	1	MSE	MET	modified residue	UNP P15873
F	70	MSE	MET	modified residue	UNP P15873
F	119	MSE	MET	modified residue	UNP P15873
F	161	MSE	MET	modified residue	UNP P15873
F	188	MSE	MET	modified residue	UNP P15873
F	199	MSE	MET	modified residue	UNP P15873
G	-24	MSE	-	expression tag	UNP P15873
G	-23	GLY	-	expression tag	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-22	SER	-	expression tag	UNP P15873
G	-21	SER	-	expression tag	UNP P15873
G	-20	HIS	-	expression tag	UNP P15873
G	-19	HIS	-	expression tag	UNP P15873
G	-18	HIS	-	expression tag	UNP P15873
G	-17	HIS	-	expression tag	UNP P15873
G	-16	HIS	-	expression tag	UNP P15873
G	-15	HIS	-	expression tag	UNP P15873
G	-14	SER	-	expression tag	UNP P15873
G	-13	SER	-	expression tag	UNP P15873
G	-12	GLY	-	expression tag	UNP P15873
G	-11	LEU	-	expression tag	UNP P15873
G	-10	GLU	-	expression tag	UNP P15873
G	-9	VAL	-	expression tag	UNP P15873
G	-8	LEU	-	expression tag	UNP P15873
G	-7	PHE	-	expression tag	UNP P15873
G	-6	GLN	-	expression tag	UNP P15873
G	-5	GLY	-	expression tag	UNP P15873
G	-4	PRO	-	expression tag	UNP P15873
G	-3	HIS	-	expression tag	UNP P15873
G	-2	MSE	-	expression tag	UNP P15873
G	-1	ALA	-	expression tag	UNP P15873
G	0	SER	-	expression tag	UNP P15873
G	1	MSE	MET	modified residue	UNP P15873
G	70	MSE	MET	modified residue	UNP P15873
G	119	MSE	MET	modified residue	UNP P15873
G	161	MSE	MET	modified residue	UNP P15873
G	188	MSE	MET	modified residue	UNP P15873
G	199	MSE	MET	modified residue	UNP P15873
H	-24	MSE	-	expression tag	UNP P15873
H	-23	GLY	-	expression tag	UNP P15873
H	-22	SER	-	expression tag	UNP P15873
H	-21	SER	-	expression tag	UNP P15873
H	-20	HIS	-	expression tag	UNP P15873
H	-19	HIS	-	expression tag	UNP P15873
H	-18	HIS	-	expression tag	UNP P15873
H	-17	HIS	-	expression tag	UNP P15873
H	-16	HIS	-	expression tag	UNP P15873
H	-15	HIS	-	expression tag	UNP P15873
H	-14	SER	-	expression tag	UNP P15873
H	-13	SER	-	expression tag	UNP P15873
H	-12	GLY	-	expression tag	UNP P15873

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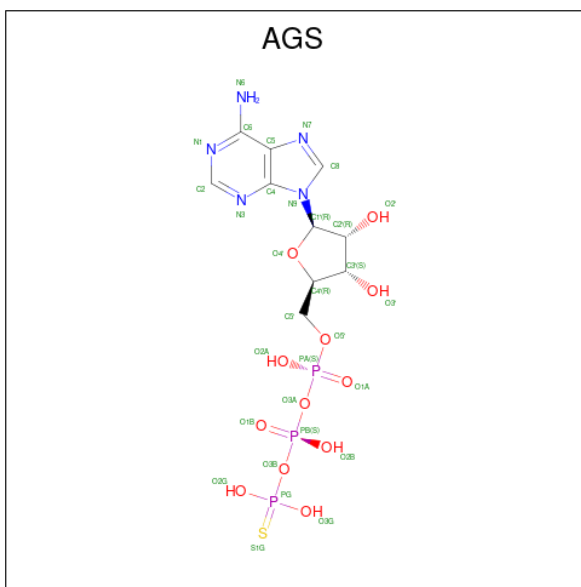
Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	LEU	-	expression tag	UNP P15873
H	-10	GLU	-	expression tag	UNP P15873
H	-9	VAL	-	expression tag	UNP P15873
H	-8	LEU	-	expression tag	UNP P15873
H	-7	PHE	-	expression tag	UNP P15873
H	-6	GLN	-	expression tag	UNP P15873
H	-5	GLY	-	expression tag	UNP P15873
H	-4	PRO	-	expression tag	UNP P15873
H	-3	HIS	-	expression tag	UNP P15873
H	-2	MSE	-	expression tag	UNP P15873
H	-1	ALA	-	expression tag	UNP P15873
H	0	SER	-	expression tag	UNP P15873
H	1	MSE	MET	modified residue	UNP P15873
H	70	MSE	MET	modified residue	UNP P15873
H	119	MSE	MET	modified residue	UNP P15873
H	161	MSE	MET	modified residue	UNP P15873
H	188	MSE	MET	modified residue	UNP P15873
H	199	MSE	MET	modified residue	UNP P15873

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

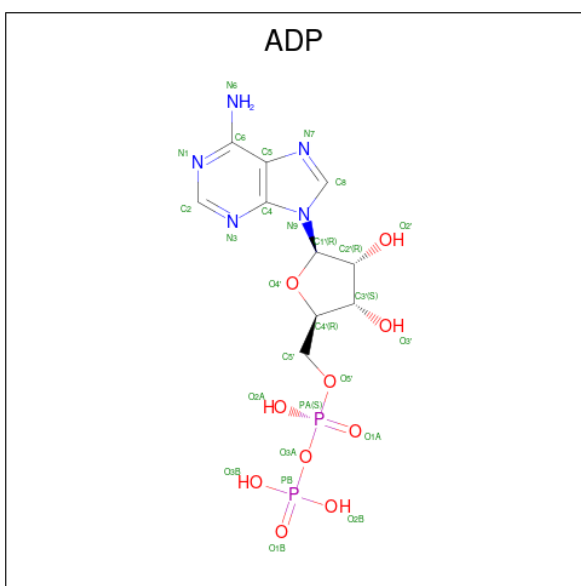
- Molecule 8 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).





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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

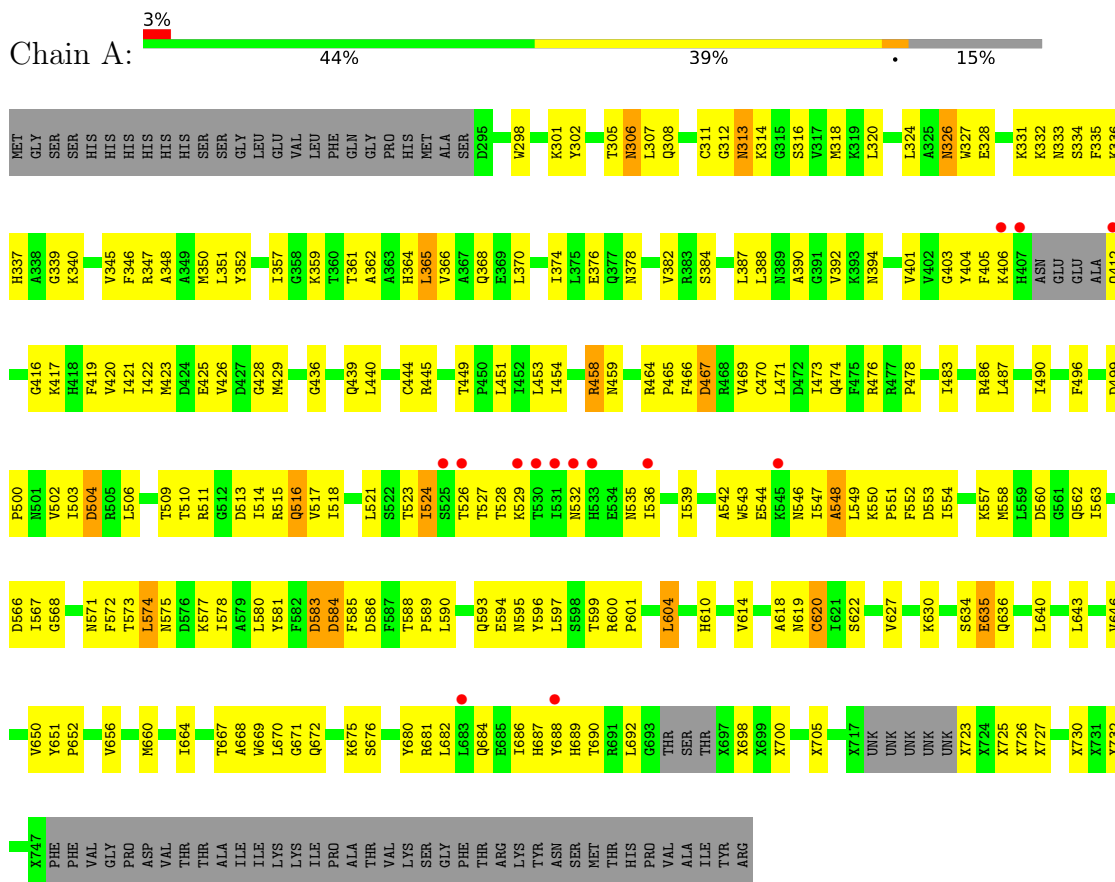


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	E	1	27	10	5	10	2	0	0

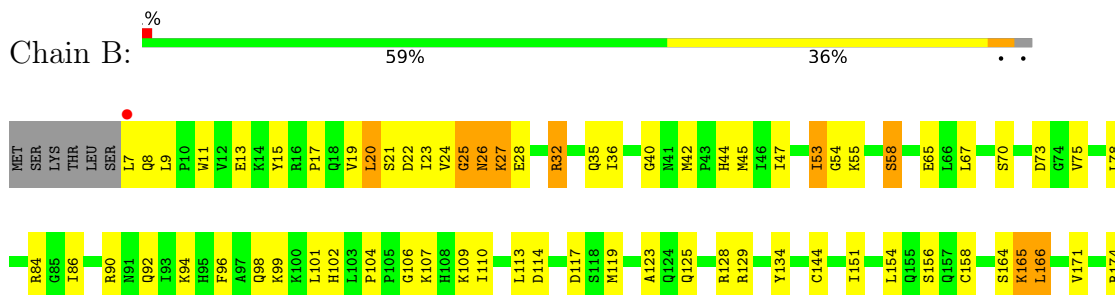
### 3 Residue-property plots

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

- Molecule 1: Activator 1 95 kDa subunit

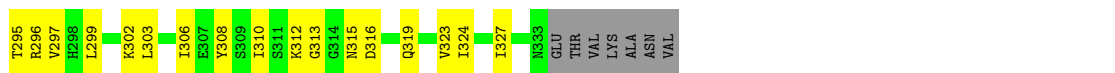
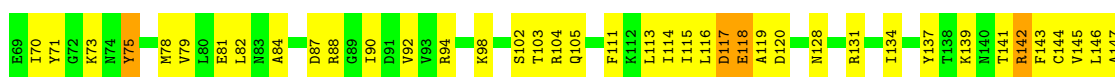


- Molecule 2: Activator 1 37 kDa subunit

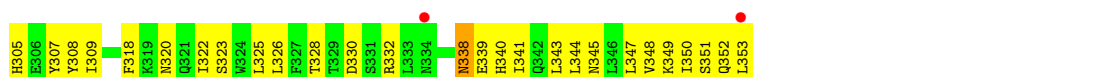
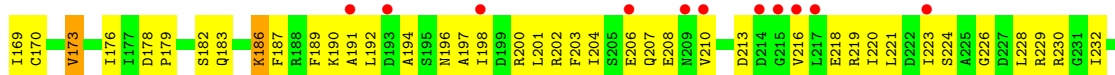
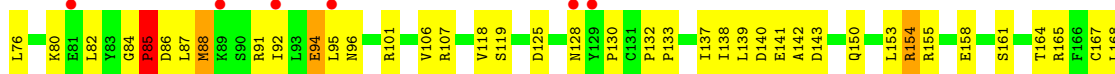
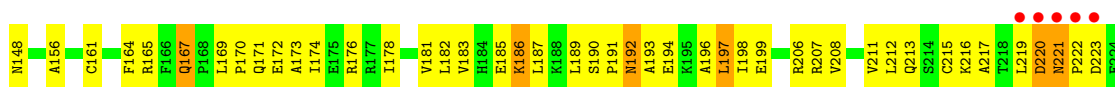
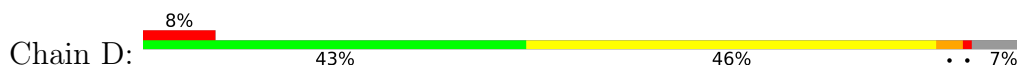




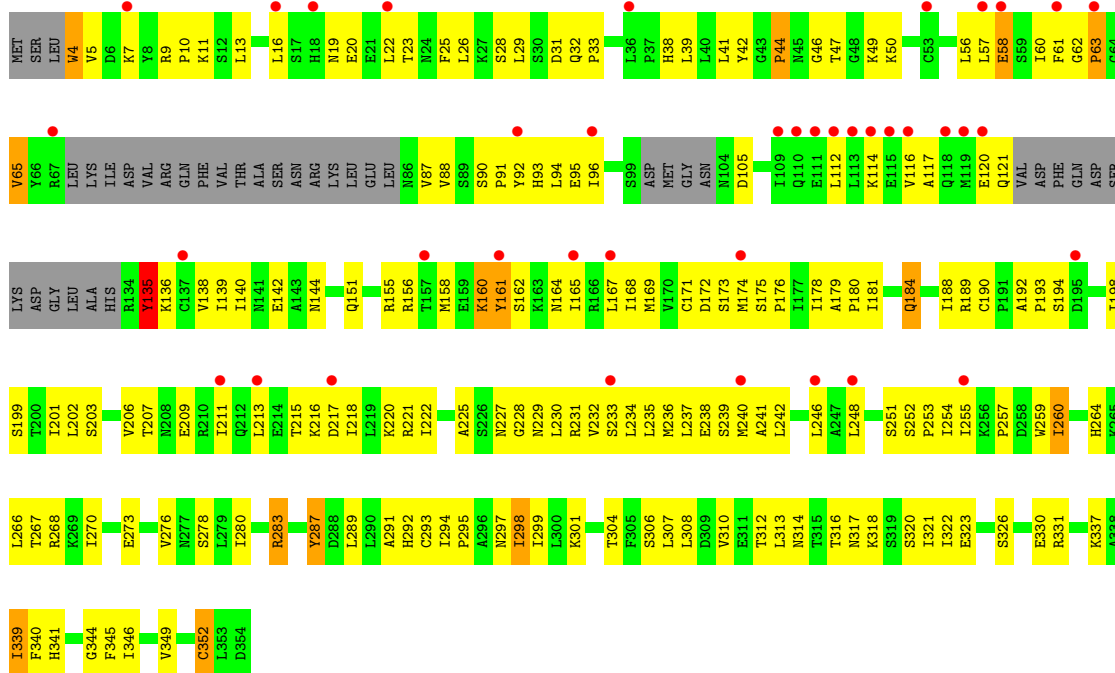
● Molecule 3: Activator 1 40 kDa subunit



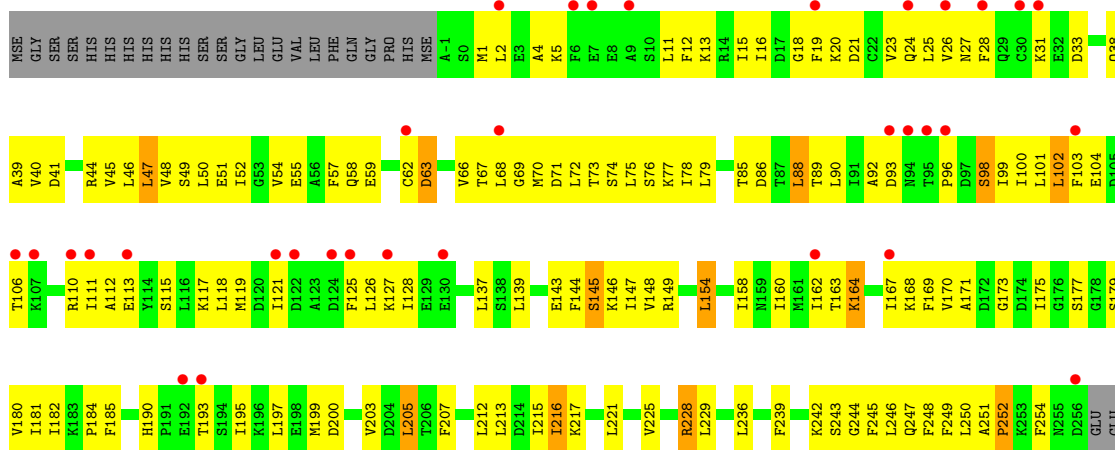
● Molecule 4: Activator 1 41 kDa subunit



● Molecule 5: Activator 1 40 kDa subunit

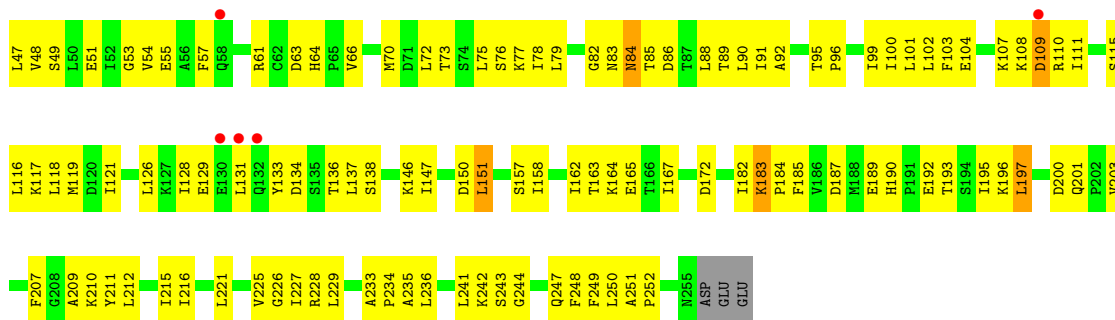


• Molecule 6: Proliferating cell nuclear antigen

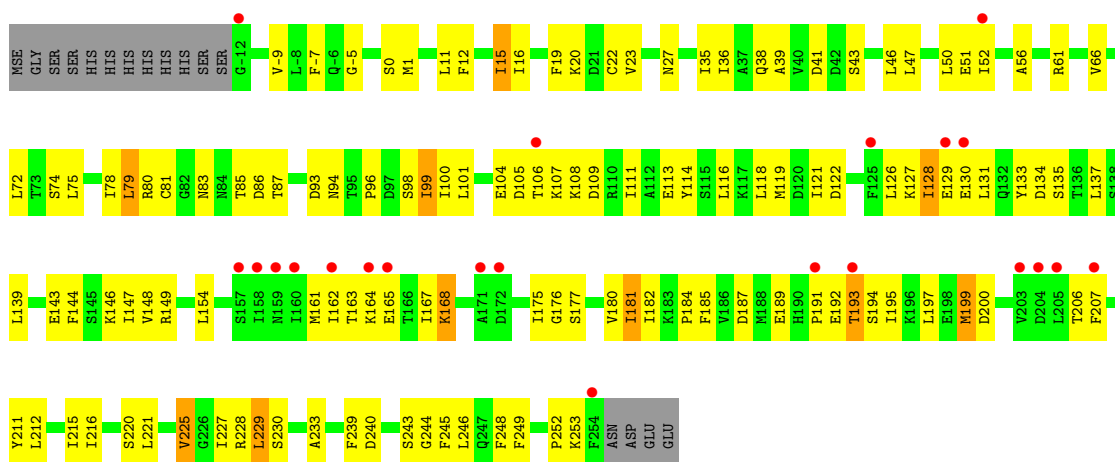


• Molecule 6: Proliferating cell nuclear antigen





● Molecule 6: Proliferating cell nuclear antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.21Å 110.48Å 268.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.85 48.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.81-2.85) 94.8 (48.81-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.251 , 0.306 0.241 , 0.295	Depositor DCC
$R_{free}$ test set	6077 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtrriage
Anisotropy	0.491	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, MG, AGS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/3173	0.59	0/4283
2	B	0.32	0/2517	0.58	0/3394
3	C	0.30	0/2584	0.56	0/3497
4	D	0.27	0/2642	0.53	0/3573
5	E	0.27	0/2529	0.52	0/3416
6	F	0.30	0/2045	0.55	0/2749
6	G	0.31	0/2046	0.56	0/2749
6	H	0.31	0/2105	0.56	0/2828
All	All	0.30	0/19641	0.56	0/26489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	3207	210	0
2	B	2482	0	2572	132	0
3	C	2544	0	2573	171	0
4	D	2597	0	2627	183	0
5	E	2495	0	2598	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	2021	0	2036	159	0
6	G	2022	0	2044	122	0
6	H	2079	0	2083	126	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	31	0	12	1	0
8	B	31	0	12	2	0
8	C	31	0	12	2	0
8	D	31	0	12	2	0
9	E	27	0	12	3	0
All	All	19740	0	19800	1225	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 31.

All (1225) 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:523:THR:HG21	1:A:547:ILE:HG21	1.30	1.09
4:D:138:ILE:HG22	4:D:167:CYS:HB3	1.39	1.04
3:C:221:ASN:HB2	3:C:222:PRO:HD3	1.33	1.03
5:E:39:LEU:HD21	5:E:41:LEU:HG	1.41	1.01
4:D:41:ALA:HB1	4:D:192:LEU:HD22	1.41	1.01
4:D:80:LYS:HG2	4:D:88:MET:HE3	1.45	0.99
5:E:229:ASN:ND2	5:E:232:VAL:HG23	1.80	0.97
3:C:207:ARG:HH21	3:C:236:CYS:HB2	1.29	0.96
2:B:26:ASN:N	2:B:26:ASN:HD22	1.64	0.94
2:B:23:ILE:HG22	2:B:25:GLY:H	1.32	0.92
1:A:516:GLN:HG2	2:B:156:SER:HA	1.50	0.92
4:D:192:LEU:HD12	4:D:228:LEU:HB2	1.52	0.91
6:H:131:LEU:HD23	6:H:233:ALA:HB2	1.49	0.91
4:D:130:PRO:O	4:D:132:PRO:HD3	1.72	0.90
3:C:172:GLU:HG3	3:C:173:ALA:H	1.34	0.89
5:E:206:VAL:HB	5:E:211:ILE:HB	1.52	0.89
6:F:16:ILE:HD12	6:F:79:LEU:HD22	1.55	0.89
6:F:115:SER:HB3	6:H:177:SER:HB3	1.55	0.88
1:A:357:ILE:HD11	1:A:359:LYS:HG3	1.56	0.88
5:E:94:LEU:HD21	5:E:138:VAL:HG22	1.55	0.87
2:B:99:LYS:HE3	6:G:117:LYS:HD3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:LEU:HD11	3:C:231:VAL:HG21	1.57	0.86
6:F:4:ALA:HB3	6:F:90:LEU:HB2	1.57	0.86
1:A:374:ILE:HG23	1:A:422:ILE:HD13	1.55	0.86
1:A:601:PRO:HB2	1:A:604:LEU:HD11	1.57	0.86
1:A:529:LYS:HB2	2:B:35:GLN:HE22	1.39	0.86
2:B:53:ILE:HG22	2:B:166:LEU:HD22	1.56	0.85
6:F:147:ILE:HD12	6:F:180:VAL:HG11	1.56	0.85
5:E:222:ILE:HD12	5:E:236:MET:HE2	1.57	0.84
3:C:244:LEU:HD21	3:C:280:GLY:HA3	1.60	0.84
5:E:240:MET:HE2	5:E:254:ILE:HA	1.60	0.82
5:E:273:GLU:HG3	5:E:278:SER:HB2	1.62	0.82
3:C:178:ILE:HD11	3:C:208:VAL:HG11	1.59	0.82
1:A:348:ALA:HB2	1:A:451:LEU:HB3	1.60	0.82
4:D:82:LEU:HD12	4:D:130:PRO:HG2	1.62	0.82
1:A:394:ASN:ND2	6:G:210:LYS:HD3	1.95	0.81
6:G:1:MSE:HE3	6:G:66:VAL:HB	1.61	0.81
3:C:167:GLN:H	3:C:167:GLN:HE21	1.29	0.81
5:E:295:PRO:HB2	5:E:298:ILE:HB	1.62	0.81
6:H:27:ASN:HD21	6:H:121:ILE:HB	1.46	0.81
5:E:58:GLU:HB2	5:E:63:PRO:HA	1.63	0.80
3:C:24:LEU:HB2	3:C:38:ARG:NH2	1.96	0.80
1:A:510:THR:HG22	1:A:513:ASP:HB3	1.63	0.80
5:E:254:ILE:HD12	5:E:254:ILE:H	1.46	0.79
2:B:151:ILE:HD11	2:B:154:LEU:HG	1.62	0.79
5:E:236:MET:HE3	5:E:254:ILE:HG23	1.63	0.79
4:D:158:GLU:HB2	4:D:183:GLN:HE22	1.46	0.79
6:H:147:ILE:HD12	6:H:180:VAL:HG11	1.65	0.79
1:A:333:ASN:HB3	1:A:337:HIS:HD2	1.48	0.78
1:A:563:ILE:HG22	1:A:577:LYS:HE2	1.65	0.77
3:C:90:ILE:HD12	3:C:94:ARG:NH2	1.99	0.77
3:C:220:ASP:OD1	3:C:223:ASP:HA	1.84	0.77
5:E:215:THR:HG22	5:E:216:LYS:H	1.49	0.76
6:F:90:LEU:HD22	6:F:99:ILE:HD11	1.66	0.76
4:D:33:PRO:HB3	4:D:38:GLU:HB2	1.66	0.76
6:F:68:LEU:HB3	6:F:70:MSE:HE3	1.68	0.76
6:G:78:ILE:HD12	6:G:116:LEU:HD12	1.68	0.75
5:E:266:LEU:O	5:E:270:ILE:HG12	1.85	0.75
2:B:44:HIS:HB2	2:B:158:CYS:HB3	1.68	0.74
1:A:500:PRO:O	1:A:504:ASP:HB2	1.85	0.74
6:F:41:ASP:OD2	6:F:46:LEU:HB3	1.86	0.74
6:G:70:MSE:HE2	6:G:75:LEU:HD22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:317:ASN:O	5:E:321:ILE:HG12	1.88	0.74
6:G:190:HIS:NE2	6:G:192:GLU:HB2	2.02	0.74
1:A:578:ILE:HD12	1:A:650:VAL:HG21	1.70	0.74
3:C:194:GLU:O	3:C:198:ILE:HG12	1.88	0.74
2:B:227:ILE:HD12	2:B:228:VAL:N	2.03	0.74
3:C:207:ARG:NH2	3:C:236:CYS:HB2	2.02	0.74
1:A:514:ILE:O	1:A:518:ILE:HG12	1.87	0.73
1:A:527:THR:HG21	2:B:32:ARG:NE	2.04	0.73
1:A:546:ASN:ND2	2:B:28:GLU:HB3	2.03	0.73
6:F:203:VAL:HG11	6:F:229:LEU:HB3	1.70	0.73
6:G:46:LEU:HD11	6:G:248:PHE:HB3	1.70	0.73
6:H:27:ASN:ND2	6:H:121:ILE:HB	2.03	0.73
1:A:646:VAL:HG21	2:B:289:ILE:HG21	1.70	0.73
4:D:192:LEU:CD1	4:D:228:LEU:HB2	2.18	0.73
6:F:13:LYS:HA	6:F:79:LEU:HD21	1.69	0.73
3:C:137:TYR:O	3:C:141:THR:HG22	1.89	0.73
5:E:47:THR:HG23	5:E:192:ALA:HA	1.71	0.73
5:E:229:ASN:HD22	5:E:232:VAL:HG23	1.53	0.73
4:D:345:ASN:HA	5:E:322:ILE:HD12	1.69	0.72
1:A:651:TYR:HB3	1:A:652:PRO:HD3	1.71	0.72
2:B:44:HIS:CB	2:B:158:CYS:HB3	2.20	0.72
6:G:27:ASN:HD21	6:G:121:ILE:HB	1.53	0.72
6:G:47:LEU:HD13	6:G:126:LEU:HD12	1.71	0.72
1:A:604:LEU:H	1:A:604:LEU:HD12	1.53	0.72
5:E:199:SER:HA	5:E:202:LEU:HD12	1.72	0.72
6:G:33:ASP:O	6:G:54:VAL:HB	1.90	0.72
6:H:16:ILE:HG23	6:H:72:LEU:HD22	1.71	0.72
1:A:326:ASN:N	1:A:326:ASN:HD22	1.86	0.71
5:E:287:TYR:CE2	5:E:339:ILE:HD13	2.25	0.71
5:E:16:LEU:HD12	5:E:23:THR:HG23	1.71	0.71
1:A:378:ASN:ND2	2:B:129:ARG:HG2	2.06	0.71
4:D:251:ILE:HG13	4:D:255:GLN:HG2	1.73	0.71
6:F:15:ILE:HA	6:F:221:LEU:HD13	1.73	0.71
3:C:82:LEU:HB3	3:C:88:ARG:HD3	1.73	0.70
5:E:229:ASN:HD21	5:E:231:ARG:HB3	1.54	0.70
3:C:24:LEU:HB2	3:C:38:ARG:HH21	1.54	0.70
4:D:154:ARG:HD3	4:D:179:PRO:HB3	1.73	0.70
6:H:168:LYS:NZ	6:H:181:ILE:HB	2.06	0.70
3:C:30:GLN:NE2	3:C:57:THR:HG22	2.06	0.70
4:D:345:ASN:OD1	4:D:349:LYS:HE3	1.92	0.70
1:A:348:ALA:O	1:A:470:CYS:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:HIS:O	1:A:368:GLN:HG3	1.91	0.70
1:A:544:GLU:HA	1:A:548:ALA:HB3	1.73	0.70
6:H:12:PHE:O	6:H:16:ILE:HD13	1.91	0.70
2:B:54:GLY:O	2:B:58:SER:HB2	1.92	0.70
6:F:16:ILE:HD13	6:F:75:LEU:HD21	1.72	0.70
6:G:55:GLU:HB3	6:G:243:SER:OG	1.92	0.70
3:C:299:LEU:HD11	3:C:327:ILE:HD13	1.72	0.70
5:E:47:THR:HG21	5:E:190:CYS:O	1.92	0.69
3:C:278:ILE:HG23	3:C:303:LEU:HD12	1.73	0.69
6:F:19:PHE:HZ	6:F:50:LEU:HB2	1.58	0.69
2:B:277:LEU:O	2:B:285:ARG:HD3	1.92	0.69
3:C:265:LYS:HG3	3:C:266:VAL:N	2.07	0.69
1:A:487:LEU:HD22	1:A:521:LEU:HD22	1.75	0.69
4:D:237:SER:HA	4:D:240:LYS:HE2	1.73	0.69
6:F:98:SER:HA	6:F:118:LEU:HG	1.74	0.69
6:G:4:ALA:HB1	6:G:57:PHE:CD2	2.27	0.69
2:B:253:ARG:HH21	2:B:258:LYS:NZ	1.91	0.68
5:E:252:SER:O	5:E:254:ILE:HD12	1.94	0.68
4:D:62:LEU:HD11	4:D:176:ILE:HD12	1.75	0.68
4:D:91:ARG:C	4:D:92:ILE:HD12	2.12	0.68
4:D:75:ILE:HD11	4:D:169:ILE:HG12	1.76	0.68
6:H:46:LEU:HD23	6:H:47:LEU:N	2.08	0.68
6:F:55:GLU:HB3	6:F:243:SER:HB3	1.74	0.68
1:A:568:GLY:HA2	1:A:571:ASN:HD22	1.58	0.68
5:E:41:LEU:HD23	5:E:188:ILE:HB	1.76	0.68
4:D:58:LEU:O	4:D:165:ARG:HD3	1.94	0.68
6:F:51:GLU:O	6:F:244:GLY:HA3	1.93	0.68
6:G:221:LEU:HB3	6:G:241:LEU:HD21	1.74	0.68
6:H:50:LEU:HD21	6:H:52:ILE:HD11	1.74	0.67
2:B:175:LEU:O	2:B:179:ILE:HG12	1.92	0.67
6:G:102:LEU:HG	6:G:104:GLU:HG3	1.76	0.67
2:B:274:THR:HG23	2:B:288:MET:HE3	1.77	0.67
6:F:1:MSE:HE3	6:F:66:VAL:HG22	1.75	0.67
3:C:117:ASP:C	3:C:118:GLU:HG2	2.14	0.67
4:D:263:VAL:HG12	4:D:303:GLN:HE22	1.59	0.67
4:D:274:LYS:HE3	4:D:274:LYS:HA	1.77	0.67
5:E:229:ASN:HD22	5:E:232:VAL:N	1.93	0.67
1:A:307:LEU:HD11	1:A:366:VAL:HG22	1.77	0.67
2:B:267:VAL:HG11	2:B:296:HIS:HB2	1.77	0.67
3:C:299:LEU:HD12	3:C:303:LEU:HD23	1.77	0.67
6:G:29:GLN:HB2	6:G:36:ILE:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ARG:HA	2:B:288:MET:HE3	1.75	0.67
6:H:229:LEU:N	6:H:229:LEU:HD12	2.10	0.67
1:A:550:LYS:O	1:A:554:ILE:HG12	1.95	0.67
5:E:215:THR:HG22	5:E:216:LYS:N	2.09	0.67
6:F:25:LEU:HD13	6:F:121:ILE:HD11	1.77	0.67
6:F:33:ASP:O	6:F:54:VAL:HG23	1.95	0.67
6:H:11:LEU:O	6:H:15:ILE:HG12	1.94	0.67
3:C:63:ILE:HD12	3:C:64:VAL:H	1.60	0.66
3:C:167:GLN:HE21	3:C:167:GLN:N	1.94	0.66
4:D:263:VAL:HG12	4:D:303:GLN:NE2	2.10	0.66
6:H:220:SER:O	6:H:221:LEU:HD23	1.96	0.66
2:B:274:THR:O	2:B:285:ARG:HD2	1.95	0.66
1:A:575:ASN:ND2	2:B:275:LYS:HE3	2.11	0.66
5:E:213:LEU:HD23	5:E:248:LEU:HD12	1.76	0.66
2:B:96:PHE:O	2:B:109:LYS:HE3	1.94	0.66
6:F:88:LEU:HD21	6:F:101:LEU:HB3	1.78	0.66
6:F:49:SER:HB2	6:F:247:GLN:HG3	1.76	0.66
6:F:46:LEU:HD11	6:F:248:PHE:HB3	1.77	0.66
6:H:225:VAL:HB	6:H:239:PHE:CE1	2.31	0.65
6:G:162:ILE:HB	6:G:203:VAL:CG2	2.26	0.65
3:C:174:ILE:O	3:C:178:ILE:HD13	1.95	0.65
3:C:174:ILE:HD11	3:C:208:VAL:HG21	1.78	0.65
4:D:318:PHE:O	4:D:322:ILE:HD13	1.97	0.65
5:E:222:ILE:HG23	5:E:236:MET:CE	2.26	0.65
2:B:284:VAL:O	2:B:288:MET:HG3	1.96	0.65
1:A:404:TYR:CD2	6:G:234:PRO:HD3	2.32	0.65
2:B:174:ARG:O	2:B:178:ILE:HG12	1.96	0.65
6:H:87:THR:OG1	6:H:104:GLU:HB3	1.97	0.65
5:E:234:LEU:O	5:E:238:GLU:HG3	1.96	0.64
6:G:91:ILE:O	6:G:99:ILE:HD12	1.97	0.64
3:C:38:ARG:O	3:C:41:VAL:HG22	1.97	0.64
4:D:45:ALA:HB1	4:D:187:PHE:HD2	1.61	0.64
6:F:40:VAL:HB	6:F:44:ARG:NH1	2.13	0.64
2:B:232:HIS:HE1	2:B:234:LEU:HD13	1.63	0.64
3:C:221:ASN:HB2	3:C:222:PRO:CD	2.20	0.64
6:H:98:SER:HA	6:H:118:LEU:HG	1.79	0.64
3:C:174:ILE:HD11	3:C:208:VAL:HG11	1.79	0.64
3:C:118:GLU:OE1	4:D:155:ARG:HG2	1.98	0.64
3:C:290:LEU:HD12	3:C:296:ARG:HD3	1.80	0.64
4:D:150:GLN:O	4:D:153:LEU:HB2	1.97	0.64
2:B:274:THR:HG23	2:B:288:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:HB3	1:A:337:HIS:CD2	2.30	0.64
5:E:39:LEU:CD2	5:E:41:LEU:HG	2.24	0.64
3:C:248:LEU:HD21	3:C:285:LEU:HD13	1.79	0.63
2:B:280:VAL:HG12	2:B:284:VAL:HB	1.81	0.63
5:E:198:ILE:O	5:E:202:LEU:HG	1.98	0.63
5:E:218:ILE:O	5:E:222:ILE:HG12	1.98	0.63
2:B:280:VAL:HG12	2:B:281:LYS:H	1.63	0.63
6:G:95:THR:N	6:G:96:PRO:HD3	2.11	0.63
3:C:172:GLU:HG3	3:C:173:ALA:N	2.09	0.63
3:C:270:LYS:HD3	3:C:272:LEU:HD11	1.79	0.63
2:B:26:ASN:N	2:B:26:ASN:ND2	2.37	0.63
5:E:42:TYR:HA	5:E:171:CYS:O	1.97	0.63
5:E:222:ILE:HA	5:E:236:MET:HE1	1.79	0.63
6:F:40:VAL:HG22	6:F:47:LEU:HB2	1.81	0.63
2:B:244:ASN:HB2	2:B:247:ASP:OD2	1.98	0.63
4:D:186:LYS:HZ2	4:D:186:LYS:H	1.46	0.63
1:A:311:CYS:SG	1:A:486:ARG:HD3	2.38	0.63
2:B:262:SER:HB3	2:B:265:ASP:OD2	1.99	0.63
3:C:78:MET:SD	3:C:105:GLN:HG2	2.39	0.63
5:E:13:LEU:HA	5:E:16:LEU:HG	1.81	0.63
2:B:53:ILE:CD1	2:B:55:LYS:HG3	2.29	0.62
4:D:271:ILE:HD13	4:D:286:TYR:CE2	2.34	0.62
6:H:23:VAL:HG11	6:H:39:ALA:HB3	1.81	0.62
4:D:39:VAL:HG23	8:D:804:AGS:N6	2.13	0.62
3:C:240:ARG:HG3	3:C:241:PRO:HD2	1.80	0.62
4:D:190:LYS:HG2	4:D:191:ALA:O	1.99	0.62
5:E:345:PHE:O	5:E:349:VAL:HG23	1.99	0.62
6:H:12:PHE:CE1	6:H:16:ILE:HD11	2.34	0.62
5:E:229:ASN:ND2	5:E:231:ARG:HB3	2.14	0.62
5:E:321:ILE:HD11	5:E:349:VAL:HG13	1.82	0.62
4:D:169:ILE:HD12	4:D:169:ILE:N	2.13	0.62
6:F:168:LYS:HG3	6:F:181:ILE:HG13	1.80	0.62
1:A:428:GLY:CA	2:B:125:GLN:HG2	2.29	0.62
2:B:23:ILE:HG22	2:B:25:GLY:N	2.10	0.62
6:F:5:LYS:HD3	6:F:58:GLN:NE2	2.15	0.62
6:F:110:ARG:HH21	6:H:195:ILE:HD11	1.64	0.62
4:D:96:ASN:HD22	5:E:156:ARG:HG3	1.63	0.62
1:A:428:GLY:HA2	2:B:125:GLN:HG2	1.82	0.62
1:A:526:THR:HG22	2:B:36:ILE:CD1	2.30	0.62
2:B:53:ILE:HG21	2:B:165:LYS:HA	1.82	0.62
6:G:226:GLY:C	6:G:227:ILE:HD12	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:LEU:HD21	3:C:280:GLY:CA	2.29	0.61
4:D:197:ALA:HB3	4:D:221:LEU:HD13	1.81	0.61
6:F:184:PRO:HG3	6:F:197:LEU:HB3	1.82	0.61
1:A:523:THR:HB	1:A:543:TRP:HE1	1.64	0.61
1:A:669:TRP:HD1	5:E:339:ILE:HD11	1.65	0.61
4:D:263:VAL:HG22	4:D:267:ILE:HG21	1.82	0.61
4:D:264:PRO:HB2	4:D:267:ILE:HG22	1.82	0.61
1:A:388:LEU:HD23	1:A:439:GLN:HB3	1.83	0.61
4:D:201:LEU:HD11	4:D:235:LEU:HD22	1.82	0.61
5:E:138:VAL:HB	5:E:167:LEU:HD23	1.81	0.61
6:G:150:ASP:OD1	6:H:81:CYS:HA	2.00	0.61
6:F:16:ILE:HD12	6:F:79:LEU:CD2	2.29	0.61
5:E:251:SER:O	5:E:253:PRO:HD3	2.00	0.61
6:H:16:ILE:H	6:H:16:ILE:HD12	1.64	0.61
1:A:320:LEU:HD23	1:A:366:VAL:HG21	1.83	0.61
1:A:535:ASN:HB3	1:A:539:ILE:HD11	1.83	0.61
6:H:16:ILE:HD12	6:H:16:ILE:N	2.16	0.61
4:D:203:PHE:O	4:D:207:GLN:HG2	2.00	0.61
5:E:19:ASN:HD22	5:E:22:LEU:HD12	1.64	0.61
6:G:11:LEU:O	6:G:15:ILE:HG12	2.01	0.61
6:G:27:ASN:ND2	6:G:121:ILE:HB	2.16	0.61
6:H:41:ASP:OD2	6:H:43:SER:HB2	1.99	0.61
4:D:75:ILE:HG21	4:D:138:ILE:HG21	1.83	0.60
4:D:200:ARG:O	4:D:204:ILE:HG12	2.00	0.60
5:E:297:ASN:O	5:E:301:LYS:HG3	2.01	0.60
3:C:60:THR:HA	3:C:63:ILE:HD11	1.83	0.60
3:C:90:ILE:HD12	3:C:94:ARG:HH21	1.66	0.60
3:C:174:ILE:CD1	3:C:208:VAL:HG21	2.31	0.60
1:A:302:TYR:CD1	1:A:490:ILE:HD12	2.37	0.60
2:B:307:LEU:HD13	3:C:282:VAL:HG21	1.81	0.60
3:C:254:ASP:HB3	3:C:258:THR:OG1	1.99	0.60
5:E:206:VAL:CB	5:E:211:ILE:HB	2.27	0.60
6:H:185:PHE:CZ	6:H:187:ASP:HB2	2.36	0.60
4:D:194:ALA:HA	4:D:221:LEU:HD13	1.83	0.60
4:D:300:VAL:O	4:D:304:LEU:HG	2.01	0.60
3:C:302:LYS:O	3:C:306:ILE:HG12	2.01	0.60
4:D:198:ILE:HD11	4:D:218:GLU:HG2	1.83	0.60
3:C:15:TRP:HA	3:C:18:LYS:HB3	1.83	0.60
5:E:240:MET:CE	5:E:254:ILE:HA	2.29	0.60
6:F:154:LEU:O	6:F:173:GLY:HA3	2.01	0.60
4:D:137:ILE:HD13	4:D:164:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:HB	1:A:589:PRO:HD3	1.82	0.60
4:D:325:LEU:HD12	4:D:353:LEU:HD11	1.84	0.60
6:G:70:MSE:HE2	6:G:75:LEU:HB2	1.84	0.60
4:D:137:ILE:HD13	4:D:164:THR:CG2	2.32	0.60
6:F:117:LYS:HD3	6:H:175:ILE:O	2.02	0.60
1:A:590:LEU:HB3	1:A:667:THR:HG21	1.84	0.60
3:C:15:TRP:CD2	3:C:213:GLN:HB3	2.37	0.60
6:G:111:ILE:HD12	6:G:111:ILE:N	2.17	0.60
2:B:11:TRP:CZ2	2:B:182:GLU:HG2	2.36	0.59
6:G:133:TYR:CD1	6:G:228:ARG:HD3	2.37	0.59
6:H:83:ASN:HB2	6:H:86:ASP:OD2	2.01	0.59
1:A:682:LEU:O	1:A:686:ILE:HG12	2.02	0.59
4:D:186:LYS:HB2	4:D:186:LYS:HZ3	1.67	0.59
6:G:146:LYS:HE2	6:G:150:ASP:OD1	2.01	0.59
6:H:128:ILE:O	6:H:128:ILE:HG22	2.02	0.59
6:F:13:LYS:HA	6:F:79:LEU:CD2	2.31	0.59
6:F:102:LEU:HD22	6:F:104:GLU:HG3	1.83	0.59
4:D:42:GLN:HE22	4:D:190:LYS:HB3	1.66	0.59
4:D:165:ARG:HH11	4:D:165:ARG:HG3	1.66	0.59
5:E:94:LEU:CD2	5:E:138:VAL:HG22	2.31	0.59
5:E:96:ILE:HD11	5:E:112:LEU:HD23	1.85	0.59
6:F:13:LYS:HD3	6:F:79:LEU:HG	1.83	0.59
6:H:107:LYS:O	6:H:109:ASP:N	2.36	0.59
4:D:297:ALA:O	4:D:300:VAL:HG23	2.03	0.59
6:F:12:PHE:CE2	6:F:16:ILE:HD11	2.37	0.59
6:H:195:ILE:N	6:H:195:ILE:HD12	2.18	0.59
4:D:216:VAL:O	4:D:220:ILE:HG13	2.03	0.58
5:E:236:MET:HG3	5:E:255:ILE:CG2	2.33	0.58
6:G:185:PHE:HE1	6:G:195:ILE:HG12	1.67	0.58
6:H:35:ILE:C	6:H:36:ILE:HD12	2.23	0.58
4:D:96:ASN:HD22	5:E:156:ARG:CG	2.16	0.58
5:E:235:LEU:HD23	5:E:235:LEU:O	2.03	0.58
5:E:292:HIS:O	5:E:294:ILE:HG13	2.03	0.58
6:H:78:ILE:HD12	6:H:114:TYR:HB3	1.85	0.58
3:C:60:THR:O	3:C:63:ILE:HD12	2.03	0.58
4:D:263:VAL:HG23	4:D:295:TRP:CD1	2.38	0.58
5:E:213:LEU:CD2	5:E:248:LEU:HD12	2.33	0.58
2:B:223:ASN:O	2:B:226:LYS:HB2	2.03	0.58
5:E:144:ASN:HD21	5:E:172:ASP:H	1.50	0.58
2:B:280:VAL:HG12	2:B:281:LYS:N	2.18	0.58
2:B:299:ILE:HD13	2:B:304:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:ASN:N	3:C:192:ASN:HD22	2.00	0.58
6:G:136:THR:HG23	6:G:228:ARG:HG2	1.85	0.58
6:H:131:LEU:CD2	6:H:233:ALA:HB2	2.29	0.58
6:G:88:LEU:HD13	6:G:103:PHE:CZ	2.38	0.58
6:H:99:ILE:HD13	6:H:100:ILE:N	2.19	0.58
6:H:137:LEU:HD22	6:H:167:ILE:HD13	1.84	0.58
2:B:287:GLU:HB3	2:B:319:LEU:HD13	1.85	0.58
5:E:158:MET:O	5:E:162:SER:HB3	2.03	0.58
6:F:66:VAL:HG12	6:F:67:THR:H	1.69	0.58
6:H:50:LEU:CD2	6:H:52:ILE:HD11	2.34	0.58
3:C:15:TRP:CE3	3:C:213:GLN:HB3	2.39	0.58
6:H:46:LEU:HD23	6:H:47:LEU:H	1.68	0.58
2:B:220:ASN:HB3	2:B:223:ASN:ND2	2.18	0.57
6:F:46:LEU:HD12	6:F:249:PHE:O	2.03	0.57
4:D:295:TRP:CE3	5:E:189:ARG:HD3	2.39	0.57
6:G:167:ILE:N	6:G:167:ILE:HD12	2.19	0.57
6:H:181:ILE:HD13	6:H:181:ILE:C	2.24	0.57
1:A:510:THR:HG23	1:A:516:GLN:HB3	1.86	0.57
3:C:178:ILE:O	3:C:182:LEU:HG	2.04	0.57
4:D:27:TRP:HA	4:D:30:LYS:HB2	1.87	0.57
5:E:194:SER:O	5:E:198:ILE:HG13	2.04	0.57
6:F:74:SER:HB3	6:H:175:ILE:HD12	1.85	0.57
1:A:347:ARG:HG2	1:A:347:ARG:HH11	1.70	0.57
3:C:197:LEU:HD11	3:C:212:LEU:HG	1.85	0.57
4:D:201:LEU:CD1	4:D:235:LEU:HD22	2.34	0.57
5:E:139:ILE:N	5:E:139:ILE:HD12	2.18	0.57
6:G:207:PHE:CZ	6:G:235:ALA:HB2	2.39	0.57
1:A:672:GLN:NE2	5:E:287:TYR:HB3	2.19	0.57
3:C:187:LEU:HD11	3:C:227:ILE:HD11	1.87	0.57
6:F:181:ILE:HD12	6:F:181:ILE:N	2.20	0.57
6:G:137:LEU:H	6:G:137:LEU:HD23	1.70	0.57
4:D:167:CYS:SG	4:D:169:ILE:HD11	2.45	0.57
5:E:255:ILE:HG13	5:E:257:PRO:HD3	1.86	0.57
6:H:16:ILE:H	6:H:16:ILE:CD1	2.17	0.57
3:C:63:ILE:HD12	3:C:64:VAL:N	2.20	0.57
6:F:40:VAL:HB	6:F:44:ARG:HH11	1.67	0.57
6:F:213:LEU:O	6:F:216:ILE:HG13	2.04	0.57
1:A:382:VAL:CG1	1:A:387:LEU:HD12	2.35	0.57
3:C:222:PRO:HD2	3:C:225:ASP:OD2	2.04	0.57
6:G:128:ILE:HD12	6:G:128:ILE:N	2.20	0.57
3:C:131:ARG:HD2	3:C:156:ALA:HB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:ILE:HG23	3:C:324:ILE:HG23	1.85	0.57
5:E:174:MET:O	5:E:174:MET:HG2	2.05	0.57
5:E:321:ILE:CD1	5:E:349:VAL:HG13	2.34	0.57
6:G:70:MSE:CE	6:G:75:LEU:HD22	2.35	0.57
1:A:580:LEU:O	1:A:583:ASP:HB2	2.04	0.56
6:F:16:ILE:HD13	6:F:75:LEU:CD2	2.35	0.56
3:C:104:ARG:HA	6:F:254:PHE:CZ	2.40	0.56
3:C:192:ASN:ND2	3:C:192:ASN:H	2.02	0.56
6:F:66:VAL:HG12	6:F:67:THR:N	2.20	0.56
6:F:103:PHE:HB2	6:F:112:ALA:HB3	1.86	0.56
6:F:146:LYS:HE2	6:G:83:ASN:OD1	2.06	0.56
6:F:12:PHE:O	6:F:79:LEU:HD21	2.05	0.56
6:H:206:THR:O	6:H:253:LYS:HG2	2.06	0.56
2:B:78:LEU:HB2	2:B:113:LEU:HD23	1.87	0.56
3:C:60:THR:O	3:C:64:VAL:HG23	2.05	0.56
3:C:228:SER:OG	3:C:231:VAL:HG23	2.06	0.56
6:G:157:SER:C	6:G:158:ILE:HD12	2.26	0.56
1:A:510:THR:CG2	1:A:513:ASP:HB3	2.36	0.56
5:E:267:THR:HG21	5:E:306:SER:O	2.05	0.56
6:F:184:PRO:HA	6:F:195:ILE:O	2.05	0.56
6:G:187:ASP:OD2	6:G:189:GLU:HB3	2.06	0.56
6:F:182:ILE:HG22	6:G:110:ARG:HG2	1.87	0.56
1:A:515:ARG:HD2	2:B:156:SER:O	2.05	0.56
5:E:238:GLU:O	5:E:242:LEU:HG	2.04	0.56
6:H:137:LEU:HD22	6:H:167:ILE:CD1	2.36	0.56
1:A:357:ILE:CD1	1:A:359:LYS:HG3	2.34	0.56
1:A:542:ALA:O	1:A:546:ASN:HB3	2.06	0.55
3:C:119:ALA:CB	3:C:145:VAL:HG13	2.36	0.55
3:C:219:LEU:HD11	3:C:231:VAL:CG2	2.30	0.55
4:D:252:THR:O	4:D:255:GLN:HB3	2.06	0.55
4:D:295:TRP:O	4:D:297:ALA:N	2.37	0.55
6:G:99:ILE:HG22	6:G:116:LEU:O	2.06	0.55
1:A:352:TYR:CZ	1:A:474:GLN:HB2	2.42	0.55
6:F:1:MSE:HE3	6:F:66:VAL:CG2	2.35	0.55
1:A:405:PHE:CE2	6:G:128:ILE:HG13	2.42	0.55
1:A:459:ASN:HB2	1:A:681:ARG:HD3	1.87	0.55
5:E:216:LYS:HB3	5:E:220:LYS:HE3	1.88	0.55
4:D:87:LEU:HB3	4:D:91:ARG:HD3	1.88	0.55
5:E:239:SER:CB	5:E:255:ILE:HD13	2.36	0.55
6:F:38:GLN:HB2	6:F:126:LEU:HD22	1.89	0.55
6:F:102:LEU:HG	6:F:113:GLU:CG	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:LEU:HD12	3:C:47:PRO:HD2	1.88	0.55
3:C:185:GLU:HG3	3:C:216:LYS:HE2	1.89	0.55
5:E:322:ILE:HG13	5:E:323:GLU:H	1.72	0.55
6:F:236:LEU:HD21	6:F:247:GLN:HB2	1.88	0.55
6:G:185:PHE:CE1	6:G:195:ILE:HG12	2.41	0.55
1:A:601:PRO:HB2	1:A:604:LEU:CD1	2.32	0.55
5:E:211:ILE:CD1	5:E:246:LEU:HD22	2.37	0.55
5:E:229:ASN:HD22	5:E:232:VAL:H	1.53	0.55
1:A:351:LEU:N	1:A:351:LEU:HD23	2.20	0.55
6:F:199:MSE:HG2	6:F:200:ASP:N	2.20	0.55
6:H:16:ILE:O	6:H:20:LYS:HB2	2.07	0.55
3:C:176:ARG:NH1	3:C:176:ARG:HB3	2.22	0.55
3:C:206:ARG:HD3	4:D:183:GLN:HA	1.89	0.55
4:D:41:ALA:CB	4:D:192:LEU:HD22	2.28	0.55
6:F:31:LYS:O	6:F:62:CYS:HB3	2.07	0.55
6:H:0:SER:HA	6:H:93:ASP:HA	1.88	0.55
6:H:143:GLU:O	6:H:147:ILE:HG12	2.07	0.55
4:D:33:PRO:HB3	4:D:38:GLU:CB	2.34	0.55
6:H:98:SER:CA	6:H:118:LEU:HG	2.38	0.55
1:A:574:LEU:CD2	1:A:578:ILE:HD13	2.37	0.54
2:B:45:MET:SD	2:B:47:ILE:HD11	2.47	0.54
4:D:64:TYR:HA	4:D:170:CYS:O	2.07	0.54
4:D:242:ALA:HB2	4:D:251:ILE:HD12	1.89	0.54
6:F:12:PHE:CZ	6:F:16:ILE:HD11	2.42	0.54
6:F:137:LEU:HD22	6:F:167:ILE:HD13	1.87	0.54
6:G:29:GLN:HB2	6:G:36:ILE:CG2	2.37	0.54
1:A:384:SER:O	1:A:388:LEU:HB2	2.07	0.54
3:C:215:CYS:C	3:C:217:ALA:H	2.10	0.54
6:H:52:ILE:HD12	6:H:52:ILE:N	2.21	0.54
5:E:25:PHE:O	5:E:29:LEU:HB2	2.06	0.54
6:F:15:ILE:HG12	6:F:221:LEU:HD11	1.90	0.54
6:H:207:PHE:CE2	6:H:252:PRO:HG3	2.42	0.54
2:B:262:SER:O	2:B:266:ILE:HG12	2.07	0.54
4:D:158:GLU:CB	4:D:183:GLN:HE22	2.17	0.54
5:E:87:VAL:HG13	5:E:95:GLU:O	2.06	0.54
5:E:167:LEU:C	5:E:168:ILE:HD12	2.28	0.54
6:F:19:PHE:O	6:F:21:ASP:N	2.41	0.54
6:H:119:MSE:HB2	6:H:121:ILE:HD11	1.88	0.54
6:H:121:ILE:HD12	6:H:121:ILE:N	2.23	0.54
3:C:82:LEU:HD23	3:C:88:ARG:HG2	1.90	0.54
4:D:42:GLN:HG2	4:D:189:PHE:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:325:LEU:CD1	4:D:353:LEU:HD11	2.37	0.54
1:A:459:ASN:CB	1:A:681:ARG:HD3	2.37	0.54
2:B:253:ARG:HH21	2:B:258:LYS:HZ3	1.55	0.54
5:E:206:VAL:HG11	5:E:213:LEU:HD21	1.90	0.54
4:D:26:PRO:HA	4:D:236:GLN:OE1	2.07	0.54
5:E:63:PRO:C	5:E:65:VAL:H	2.11	0.54
5:E:139:ILE:HA	5:E:168:ILE:O	2.07	0.54
5:E:218:ILE:HG21	5:E:248:LEU:HD13	1.89	0.54
6:G:72:LEU:O	6:G:76:SER:HB2	2.07	0.54
6:G:211:TYR:O	6:G:215:ILE:HG13	2.08	0.54
1:A:331:LYS:HA	1:A:335:PHE:CE1	2.43	0.54
2:B:24:VAL:HG22	8:B:802:AGS:N1	2.23	0.54
3:C:52:TYR:HA	3:C:147:ALA:O	2.08	0.54
4:D:140:ASP:OD2	4:D:169:ILE:HB	2.07	0.54
6:F:85:THR:O	6:F:85:THR:HG22	2.08	0.54
6:H:47:LEU:HB3	6:H:249:PHE:HB2	1.90	0.54
6:H:168:LYS:NZ	6:H:168:LYS:HB2	2.23	0.54
1:A:578:ILE:O	1:A:581:TYR:HB3	2.08	0.53
4:D:106:VAL:HG13	4:D:153:LEU:HD23	1.90	0.53
5:E:16:LEU:CD1	5:E:23:THR:HG23	2.38	0.53
5:E:322:ILE:HG13	5:E:323:GLU:N	2.22	0.53
6:F:160:ILE:HD13	6:F:207:PHE:CD1	2.43	0.53
6:H:162:ILE:HG22	6:H:199:MSE:HG2	1.88	0.53
1:A:594:GLU:O	5:E:283:ARG:NH2	2.41	0.53
6:F:110:ARG:HH12	6:H:143:GLU:CD	2.12	0.53
6:G:75:LEU:HA	6:G:116:LEU:HD11	1.89	0.53
6:H:35:ILE:O	6:H:36:ILE:HD12	2.08	0.53
1:A:306:ASN:C	1:A:308:GLN:H	2.11	0.53
2:B:17:PRO:HG3	2:B:174:ARG:HH12	1.72	0.53
2:B:253:ARG:O	2:B:258:LYS:HB2	2.09	0.53
3:C:84:ALA:H	3:C:118:GLU:HG3	1.73	0.53
4:D:94:GLU:O	4:D:95:LEU:HD12	2.09	0.53
5:E:13:LEU:HD22	5:E:16:LEU:HD11	1.90	0.53
6:G:133:TYR:CG	6:G:228:ARG:HB3	2.43	0.53
6:H:75:LEU:HG	6:H:79:LEU:HD22	1.89	0.53
6:H:131:LEU:HD23	6:H:233:ALA:CB	2.32	0.53
6:H:227:ILE:N	6:H:227:ILE:HD12	2.23	0.53
1:A:361:THR:O	1:A:365:LEU:HB2	2.08	0.53
3:C:216:LYS:O	3:C:216:LYS:HG3	2.09	0.53
3:C:170:PRO:HB2	3:C:172:GLU:HG2	1.89	0.53
3:C:192:ASN:N	3:C:192:ASN:ND2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:ILE:HG13	5:E:168:ILE:HB	1.90	0.53
5:E:222:ILE:HG23	5:E:236:MET:HE2	1.90	0.53
6:F:158:ILE:HD12	6:F:212:LEU:HD23	1.91	0.53
6:H:74:SER:HB3	6:H:116:LEU:HD11	1.91	0.53
3:C:103:THR:HG21	6:F:45:VAL:HG13	1.90	0.53
5:E:33:PRO:HB3	5:E:60:ILE:HG23	1.90	0.53
2:B:216:HIS:O	2:B:218:LEU:N	2.39	0.53
5:E:239:SER:HB3	5:E:255:ILE:HD13	1.91	0.53
1:A:563:ILE:CG2	1:A:577:LYS:HE2	2.37	0.53
2:B:299:ILE:CD1	2:B:304:GLY:HA2	2.38	0.53
6:F:195:ILE:HD11	6:G:110:ARG:HH21	1.74	0.53
1:A:553:ASP:O	1:A:557:LYS:HG3	2.08	0.53
3:C:174:ILE:HG23	3:C:198:ILE:HD12	1.90	0.53
3:C:221:ASN:CB	3:C:222:PRO:HD3	2.20	0.53
1:A:306:ASN:C	1:A:308:GLN:N	2.61	0.52
5:E:4:TRP:CH2	5:E:209:GLU:HG2	2.44	0.52
5:E:222:ILE:HD12	5:E:236:MET:CE	2.34	0.52
6:F:13:LYS:CD	6:F:79:LEU:HG	2.38	0.52
6:H:165:GLU:HG2	6:H:199:MSE:HB2	1.91	0.52
6:G:82:GLY:HA3	6:G:103:PHE:CE2	2.45	0.52
3:C:176:ARG:CA	3:C:176:ARG:HH11	2.22	0.52
4:D:27:TRP:CZ2	4:D:208:GLU:HG2	2.44	0.52
5:E:225:ALA:HB3	5:E:236:MET:HE1	1.90	0.52
6:H:163:THR:HG22	6:H:164:LYS:HG3	1.92	0.52
5:E:5:VAL:HG23	5:E:238:GLU:OE1	2.09	0.52
5:E:39:LEU:HD22	5:E:168:ILE:HG23	1.92	0.52
6:F:111:ILE:O	6:H:181:ILE:HG22	2.09	0.52
6:H:93:ASP:O	6:H:96:PRO:HD3	2.09	0.52
4:D:194:ALA:O	4:D:198:ILE:HG13	2.09	0.52
6:H:144:PHE:O	6:H:148:VAL:HG23	2.09	0.52
1:A:324:LEU:HG	1:A:370:LEU:HD12	1.91	0.52
1:A:543:TRP:HA	2:B:32:ARG:NH2	2.25	0.52
1:A:627:VAL:HG22	2:B:297:MET:SD	2.50	0.52
2:B:26:ASN:O	2:B:28:GLU:N	2.42	0.52
3:C:185:GLU:O	3:C:187:LEU:N	2.43	0.52
3:C:310:ILE:HG13	3:C:319:GLN:OE1	2.09	0.52
4:D:263:VAL:HG22	4:D:264:PRO:HD2	1.91	0.52
5:E:90:SER:OG	5:E:91:PRO:HD2	2.10	0.52
1:A:348:ALA:CB	1:A:451:LEU:HB3	2.36	0.52
5:E:289:LEU:O	5:E:294:ILE:HB	2.10	0.52
6:F:27:ASN:N	6:F:27:ASN:HD22	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:46:LEU:HD22	6:F:215:ILE:HD11	1.90	0.52
6:G:3:GLU:HB3	6:G:61:ARG:HD3	1.92	0.52
6:H:212:LEU:O	6:H:216:ILE:HG23	2.10	0.52
3:C:24:LEU:HD12	3:C:38:ARG:HE	1.74	0.52
4:D:289:THR:O	4:D:292:LYS:HB3	2.10	0.52
5:E:140:ILE:HG13	5:E:169:MET:HE3	1.90	0.52
6:F:228:ARG:HG3	6:F:236:LEU:HD12	1.91	0.52
3:C:81:GLU:O	3:C:82:LEU:HD12	2.10	0.52
3:C:244:LEU:CD2	3:C:280:GLY:HA3	2.36	0.52
3:C:315:ASN:HB3	4:D:330:ASP:OD1	2.08	0.52
4:D:26:PRO:O	4:D:30:LYS:HG2	2.10	0.52
4:D:304:LEU:O	4:D:308:TYR:HD1	1.92	0.52
3:C:131:ARG:HD2	3:C:156:ALA:CB	2.40	0.52
5:E:39:LEU:HD21	5:E:41:LEU:CG	2.27	0.52
6:F:160:ILE:HD12	6:F:160:ILE:N	2.25	0.52
1:A:445:ARG:HE	1:A:469:VAL:CG1	2.23	0.51
2:B:285:ARG:HA	2:B:288:MET:CE	2.39	0.51
3:C:189:LEU:HD12	3:C:227:ILE:HB	1.91	0.51
4:D:192:LEU:HG	4:D:226:GLY:O	2.10	0.51
5:E:235:LEU:HA	5:E:238:GLU:OE1	2.10	0.51
6:G:38:GLN:HA	6:G:48:VAL:O	2.10	0.51
1:A:593:GLN:HG3	5:E:340:PHE:CE2	2.44	0.51
3:C:190:SER:OG	3:C:193:ALA:HB2	2.09	0.51
2:B:19:VAL:HG23	2:B:21:SER:HB3	1.91	0.51
3:C:73:LYS:C	3:C:75:TYR:H	2.12	0.51
5:E:4:TRP:HB3	5:E:238:GLU:OE2	2.09	0.51
5:E:304:THR:O	5:E:308:LEU:HG	2.11	0.51
6:G:15:ILE:HD13	6:G:221:LEU:HD22	1.91	0.51
6:H:-7:PHE:HD2	6:H:113:GLU:HB3	1.75	0.51
4:D:305:HIS:HD2	4:D:309:ILE:HD13	1.74	0.51
5:E:237:LEU:O	5:E:241:ALA:HB2	2.11	0.51
6:F:26:VAL:HG12	6:F:39:ALA:HB2	1.93	0.51
1:A:454:ILE:N	1:A:454:ILE:HD12	2.25	0.51
1:A:643:LEU:HD13	2:B:293:GLY:HA3	1.91	0.51
1:A:669:TRP:CZ2	5:E:337:LYS:HG2	2.46	0.51
5:E:158:MET:HG2	5:E:167:LEU:HD12	1.91	0.51
5:E:232:VAL:O	5:E:236:MET:N	2.44	0.51
6:F:24:GLN:HG2	6:F:25:LEU:HG	1.91	0.51
6:F:55:GLU:HB3	6:F:243:SER:CB	2.40	0.51
6:F:163:THR:HG22	6:F:164:LYS:N	2.25	0.51
6:H:128:ILE:O	6:H:130:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ILE:CG2	3:C:198:ILE:HD12	2.40	0.51
5:E:203:SER:O	5:E:206:VAL:HG22	2.10	0.51
6:F:62:CYS:O	6:F:63:ASP:C	2.49	0.51
1:A:394:ASN:HD21	6:G:210:LYS:HD3	1.75	0.51
1:A:425:GLU:HG2	2:B:128:ARG:NH2	2.26	0.51
1:A:610:HIS:CD2	5:E:276:VAL:HG21	2.46	0.51
1:A:667:THR:HG22	1:A:669:TRP:H	1.75	0.51
1:A:676:SER:O	1:A:680:TYR:HD1	1.94	0.51
3:C:63:ILE:HG21	3:C:144:CYS:SG	2.50	0.51
4:D:28:VAL:HG11	4:D:229:ARG:HG3	1.93	0.51
1:A:302:TYR:CE1	1:A:490:ILE:HG23	2.46	0.51
1:A:351:LEU:HD22	1:A:473:ILE:HD11	1.93	0.51
3:C:87:ASP:HA	4:D:107:ARG:NH1	2.25	0.51
6:F:205:LEU:HD13	6:F:207:PHE:CE1	2.46	0.51
6:H:194:SER:C	6:H:195:ILE:HD12	2.31	0.51
6:G:165:GLU:HA	6:G:197:LEU:HD21	1.93	0.51
6:H:135:SER:OG	6:H:162:ILE:HG21	2.11	0.51
4:D:286:TYR:O	4:D:289:THR:HB	2.11	0.51
6:H:56:ALA:HB2	6:H:243:SER:CB	2.40	0.51
1:A:326:ASN:N	1:A:326:ASN:ND2	2.57	0.50
3:C:52:TYR:CE1	3:C:165:ARG:HG3	2.46	0.50
4:D:46:VAL:HA	4:D:49:LEU:HD12	1.92	0.50
4:D:264:PRO:HD2	4:D:267:ILE:HG21	1.92	0.50
6:F:4:ALA:O	6:F:89:THR:HA	2.11	0.50
1:A:445:ARG:HE	1:A:469:VAL:HG11	1.76	0.50
2:B:232:HIS:CE1	2:B:234:LEU:HD13	2.45	0.50
6:F:175:ILE:HD12	6:F:175:ILE:C	2.32	0.50
6:F:229:LEU:HD22	6:F:229:LEU:N	2.25	0.50
1:A:672:GLN:HG2	5:E:287:TYR:CD2	2.47	0.50
2:B:102:HIS:CD2	6:G:95:THR:HG22	2.46	0.50
3:C:197:LEU:HD21	3:C:208:VAL:HA	1.93	0.50
5:E:202:LEU:HD22	5:E:237:LEU:HD22	1.93	0.50
6:F:121:ILE:HG22	6:F:121:ILE:O	2.11	0.50
6:F:195:ILE:CD1	6:G:110:ARG:HH21	2.25	0.50
4:D:71:LYS:HE3	4:D:170:CYS:O	2.11	0.50
6:F:46:LEU:HD12	6:F:249:PHE:C	2.32	0.50
6:F:167:ILE:HG22	6:F:169:PHE:CE1	2.47	0.50
6:G:54:VAL:HG22	6:G:54:VAL:O	2.10	0.50
6:G:146:LYS:HG3	6:G:150:ASP:OD2	2.11	0.50
6:H:168:LYS:HZ2	6:H:181:ILE:HB	1.76	0.50
1:A:640:LEU:HD21	2:B:297:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:280:PHE:CE2	5:E:318:LYS:HB3	2.47	0.50
6:H:105:ASP:OD1	6:H:106:THR:N	2.45	0.50
4:D:91:ARG:NH2	4:D:132:PRO:O	2.44	0.50
4:D:224:SER:OG	4:D:230:ARG:HB3	2.11	0.50
4:D:338:ASN:HB2	5:E:301:LYS:HE2	1.94	0.50
5:E:61:PHE:HB3	5:E:92:TYR:CD2	2.47	0.50
5:E:217:ASP:O	5:E:221:ARG:HG3	2.12	0.50
6:F:26:VAL:HG23	6:F:28:PHE:CE2	2.47	0.50
6:F:145:SER:O	6:F:149:ARG:HG2	2.12	0.50
6:G:110:ARG:C	6:G:111:ILE:HD12	2.32	0.50
1:A:546:ASN:HD22	2:B:28:GLU:HB3	1.75	0.50
3:C:310:ILE:HD11	3:C:319:GLN:HB3	1.94	0.50
5:E:192:ALA:HB1	5:E:193:PRO:HD2	1.93	0.50
6:G:47:LEU:HB3	6:G:249:PHE:HB2	1.92	0.50
6:G:163:THR:HG22	6:G:164:LYS:HG2	1.94	0.50
2:B:47:ILE:HD12	2:B:47:ILE:N	2.27	0.49
2:B:151:ILE:CD1	2:B:154:LEU:HG	2.39	0.49
4:D:339:GLU:HG3	5:E:173:SER:OG	2.12	0.49
2:B:15:TYR:CG	2:B:178:ILE:HD12	2.46	0.49
4:D:41:ALA:HB3	8:D:804:AGS:N6	2.27	0.49
5:E:273:GLU:CG	5:E:278:SER:HB2	2.37	0.49
6:G:128:ILE:HD12	6:G:128:ILE:H	1.77	0.49
1:A:466:PHE:O	1:A:469:VAL:HG22	2.11	0.49
3:C:178:ILE:O	3:C:181:VAL:HG12	2.12	0.49
4:D:290:PHE:HD2	4:D:291:MET:CE	2.25	0.49
4:D:328:THR:O	4:D:332:ARG:HG2	2.12	0.49
5:E:13:LEU:HD11	5:E:56:LEU:HD12	1.93	0.49
5:E:112:LEU:O	5:E:116:VAL:HG23	2.12	0.49
6:G:167:ILE:CD1	6:G:197:LEU:HD22	2.42	0.49
1:A:511:ARG:NH1	1:A:670:LEU:HB3	2.28	0.49
5:E:88:VAL:HB	5:E:95:GLU:HB2	1.93	0.49
1:A:426:VAL:O	1:A:429:MET:HG3	2.13	0.49
2:B:298:ARG:HD2	3:C:308:TYR:CD1	2.48	0.49
6:F:11:LEU:O	6:F:15:ILE:HG13	2.12	0.49
1:A:563:ILE:HD12	1:A:572:PHE:CB	2.43	0.49
2:B:7:LEU:C	2:B:8:GLN:HG3	2.33	0.49
3:C:105:GLN:CD	3:C:105:GLN:H	2.15	0.49
3:C:183:VAL:C	3:C:185:GLU:H	2.16	0.49
4:D:27:TRP:CH2	4:D:208:GLU:HG2	2.47	0.49
5:E:114:LYS:O	5:E:117:ALA:HB3	2.13	0.49
6:H:137:LEU:C	6:H:137:LEU:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PHE:O	1:A:345:VAL:HA	2.12	0.49
1:A:425:GLU:HG2	2:B:128:ARG:CZ	2.43	0.49
3:C:230:ASP:OD1	3:C:240:ARG:NH1	2.46	0.49
3:C:262:THR:O	3:C:265:LYS:HG2	2.13	0.49
4:D:91:ARG:NH2	4:D:118:VAL:HG11	2.28	0.49
4:D:302:ASN:O	4:D:305:HIS:HB3	2.13	0.49
5:E:50:LYS:HB2	9:E:805:ADP:O2A	2.12	0.49
6:F:73:THR:O	6:F:77:LYS:HG3	2.12	0.49
6:H:107:LYS:C	6:H:109:ASP:H	2.16	0.49
6:F:69:GLY:HA3	6:F:119:MSE:O	2.12	0.49
6:G:107:LYS:C	6:G:109:ASP:H	2.14	0.49
1:A:634:SER:O	1:A:636:GLN:N	2.46	0.49
1:A:672:GLN:OE1	1:A:675:LYS:HD2	2.13	0.49
1:A:687:HIS:C	1:A:689:HIS:H	2.16	0.49
6:F:38:GLN:HG2	6:F:49:SER:HA	1.93	0.49
6:G:129:GLU:O	6:G:131:LEU:HG	2.13	0.49
6:G:167:ILE:HD11	6:G:197:LEU:HD22	1.95	0.49
1:A:301:LYS:HE2	1:A:302:TYR:CE2	2.48	0.49
4:D:274:LYS:O	4:D:283:ILE:HD11	2.13	0.49
3:C:178:ILE:HD11	3:C:208:VAL:CG1	2.36	0.48
3:C:319:GLN:O	3:C:323:VAL:HG23	2.13	0.48
4:D:228:LEU:HD23	4:D:228:LEU:O	2.13	0.48
4:D:301:VAL:HG13	4:D:326:LEU:HD22	1.95	0.48
4:D:305:HIS:HB2	4:D:326:LEU:HD13	1.95	0.48
4:D:344:LEU:O	4:D:348:VAL:HG23	2.13	0.48
6:F:110:ARG:NH2	6:H:195:ILE:HD11	2.26	0.48
6:G:91:ILE:HB	6:G:100:ILE:HB	1.94	0.48
6:G:227:ILE:HD12	6:G:227:ILE:N	2.28	0.48
1:A:453:LEU:N	1:A:453:LEU:HD12	2.28	0.48
3:C:20:ARG:HB2	8:C:803:AGS:O3'	2.14	0.48
3:C:114:ILE:HG22	3:C:116:LEU:CD1	2.43	0.48
3:C:169:LEU:HD22	3:C:169:LEU:H	1.79	0.48
5:E:320:SER:CB	5:E:352:CYS:SG	3.01	0.48
1:A:351:LEU:HD22	1:A:473:ILE:CD1	2.43	0.48
1:A:357:ILE:C	1:A:357:ILE:HD12	2.33	0.48
1:A:553:ASP:OD2	1:A:557:LYS:HE3	2.14	0.48
1:A:620:CYS:HB3	1:A:652:PRO:HG3	1.94	0.48
2:B:20:LEU:HB2	2:B:65:GLU:OE2	2.13	0.48
4:D:210:VAL:HG13	4:D:239:SER:HB2	1.94	0.48
4:D:322:ILE:HD12	4:D:353:LEU:HD13	1.95	0.48
6:F:92:ALA:HB1	6:F:96:PRO:HG3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:137:LEU:HB3	6:F:197:LEU:HD13	1.95	0.48
6:F:168:LYS:HE2	6:F:170:VAL:HG21	1.95	0.48
6:G:162:ILE:HB	6:G:203:VAL:HG22	1.95	0.48
1:A:374:ILE:CG2	1:A:422:ILE:HD13	2.36	0.48
1:A:524:ILE:HD11	1:A:543:TRP:CE3	2.48	0.48
1:A:535:ASN:HB3	1:A:539:ILE:CD1	2.43	0.48
3:C:247:VAL:O	3:C:251:ILE:HG13	2.13	0.48
4:D:263:VAL:HG22	4:D:267:ILE:CG2	2.44	0.48
5:E:184:GLN:O	5:E:184:GLN:HG2	2.14	0.48
6:G:147:ILE:O	6:G:151:LEU:HD22	2.14	0.48
1:A:458:ARG:HH22	1:A:467:ASP:HA	1.77	0.48
4:D:275:VAL:HG13	4:D:351:SER:HB3	1.94	0.48
1:A:730:UNK:C	1:A:732:UNK:N	2.74	0.48
2:B:182:GLU:HB3	2:B:184:VAL:HG23	1.96	0.48
3:C:64:VAL:HG12	3:C:68:ARG:NH1	2.28	0.48
3:C:250:SER:O	3:C:259:ALA:HB2	2.12	0.48
4:D:251:ILE:HG23	4:D:251:ILE:O	2.11	0.48
4:D:290:PHE:CE2	4:D:300:VAL:HG21	2.49	0.48
6:F:90:LEU:HD22	6:F:99:ILE:CD1	2.40	0.48
4:D:282:GLU:O	4:D:285:LYS:HB3	2.13	0.48
5:E:28:SER:HA	5:E:31:ASP:OD2	2.14	0.48
5:E:38:HIS:HB2	5:E:184:GLN:O	2.13	0.48
6:F:205:LEU:HD13	6:F:207:PHE:HE1	1.79	0.48
1:A:601:PRO:HG2	1:A:610:HIS:ND1	2.28	0.48
3:C:33:VAL:O	3:C:37:VAL:HG23	2.14	0.48
3:C:94:ARG:O	3:C:98:LYS:HB3	2.13	0.48
3:C:244:LEU:HD11	3:C:281:ILE:HG13	1.96	0.48
4:D:87:LEU:O	4:D:91:ARG:HG2	2.14	0.48
4:D:158:GLU:HB2	4:D:183:GLN:NE2	2.21	0.48
4:D:191:ALA:C	4:D:192:LEU:HD23	2.34	0.48
4:D:196:ASN:N	4:D:196:ASN:HD22	2.11	0.48
4:D:213:ASP:HB3	4:D:216:VAL:HG23	1.94	0.48
5:E:164:ASN:O	5:E:165:ILE:HD13	2.13	0.48
5:E:175:SER:HB3	5:E:176:PRO:HD3	1.95	0.48
1:A:401:VAL:HB	6:G:45:VAL:O	2.13	0.48
1:A:599:THR:O	1:A:601:PRO:HD3	2.13	0.48
1:A:640:LEU:HD21	2:B:297:MET:CG	2.43	0.48
3:C:53:GLY:O	3:C:148:ASN:HA	2.14	0.48
3:C:239:PRO:HG3	3:C:272:LEU:HD22	1.96	0.48
5:E:87:VAL:HG12	5:E:88:VAL:N	2.29	0.48
6:G:16:ILE:HD12	6:G:75:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:167:ILE:HB	6:G:182:ILE:HG12	1.95	0.48
6:G:241:LEU:O	6:G:243:SER:N	2.47	0.48
1:A:583:ASP:O	1:A:584:ASP:HB2	2.12	0.48
5:E:96:ILE:HB	5:E:140:ILE:HD13	1.96	0.48
5:E:168:ILE:HD12	5:E:168:ILE:N	2.28	0.48
5:E:206:VAL:HG21	5:E:213:LEU:HD11	1.96	0.48
6:F:106:THR:O	6:F:106:THR:HG22	2.13	0.48
6:H:168:LYS:HZ1	6:H:181:ILE:HB	1.78	0.48
2:B:25:GLY:C	2:B:26:ASN:HD22	2.15	0.47
2:B:90:ARG:O	2:B:94:LYS:HE2	2.14	0.47
2:B:219:VAL:HG12	2:B:219:VAL:O	2.13	0.47
5:E:287:TYR:CZ	5:E:339:ILE:HD13	2.48	0.47
6:G:212:LEU:O	6:G:216:ILE:HG23	2.14	0.47
6:H:16:ILE:HA	6:H:19:PHE:CE2	2.49	0.47
6:H:182:ILE:HG13	6:H:182:ILE:O	2.14	0.47
2:B:171:VAL:O	2:B:175:LEU:HB2	2.15	0.47
4:D:31:TYR:CD2	4:D:204:ILE:HD12	2.49	0.47
5:E:254:ILE:HG22	5:E:255:ILE:N	2.29	0.47
2:B:17:PRO:HB3	2:B:22:ASP:HB2	1.97	0.47
3:C:258:THR:O	3:C:261:TYR:HB3	2.14	0.47
6:F:128:ILE:HD12	6:F:128:ILE:O	2.13	0.47
6:G:99:ILE:CG2	6:G:116:LEU:HB3	2.44	0.47
3:C:59:LYS:HB3	3:C:146:LEU:HD23	1.97	0.47
3:C:90:ILE:O	3:C:94:ARG:HG3	2.13	0.47
4:D:64:TYR:CD1	4:D:173:VAL:HG13	2.49	0.47
4:D:192:LEU:H	4:D:226:GLY:HA2	1.80	0.47
5:E:65:VAL:O	5:E:65:VAL:HG22	2.14	0.47
6:H:51:GLU:O	6:H:244:GLY:HA3	2.14	0.47
6:H:139:LEU:N	6:H:139:LEU:HD23	2.29	0.47
1:A:499:ASP:HB2	1:A:502:VAL:HG23	1.94	0.47
1:A:535:ASN:O	1:A:539:ILE:HG13	2.15	0.47
1:A:560:ASP:OD2	1:A:562:GLN:HB2	2.14	0.47
2:B:174:ARG:NH1	8:B:802:AGS:H2	2.29	0.47
5:E:5:VAL:HG23	5:E:238:GLU:CD	2.34	0.47
3:C:290:LEU:HD22	3:C:295:THR:HG21	1.97	0.47
4:D:40:THR:O	4:D:41:ALA:C	2.53	0.47
4:D:118:VAL:HG12	4:D:119:SER:N	2.29	0.47
6:F:99:ILE:HG12	6:F:100:ILE:N	2.30	0.47
1:A:486:ARG:O	1:A:490:ILE:HG12	2.15	0.47
2:B:13:GLU:OE1	3:C:139:LYS:HE3	2.15	0.47
2:B:15:TYR:O	2:B:174:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ILE:HD13	2:B:123:ALA:HA	1.97	0.47
5:E:62:GLY:O	5:E:65:VAL:HB	2.15	0.47
5:E:93:HIS:HD2	5:E:139:ILE:HD13	1.80	0.47
6:F:162:ILE:HB	6:F:203:VAL:HB	1.97	0.47
2:B:26:ASN:O	2:B:27:LYS:C	2.52	0.47
2:B:220:ASN:HB3	2:B:223:ASN:HD22	1.79	0.47
6:F:46:LEU:HA	6:F:249:PHE:O	2.14	0.47
6:G:107:LYS:O	6:G:109:ASP:N	2.47	0.47
2:B:179:ILE:HG21	2:B:186:TYR:CD2	2.50	0.47
3:C:114:ILE:HG22	3:C:116:LEU:HD12	1.96	0.47
5:E:9:ARG:HE	5:E:11:LYS:HE2	1.78	0.47
1:A:428:GLY:HA3	2:B:125:GLN:CG	2.45	0.47
1:A:723:UNK:C	1:A:725:UNK:N	2.78	0.47
4:D:165:ARG:HG3	4:D:165:ARG:NH1	2.27	0.47
4:D:271:ILE:HD13	4:D:286:TYR:HE2	1.76	0.47
6:H:230:SER:HB3	6:H:233:ALA:HB3	1.97	0.47
3:C:250:SER:OG	3:C:262:THR:HG21	2.15	0.46
4:D:178:ASP:HB2	4:D:179:PRO:HD3	1.98	0.46
6:F:102:LEU:HG	6:F:113:GLU:HG2	1.96	0.46
6:G:2:LEU:HB3	6:G:92:ALA:HB3	1.97	0.46
6:G:158:ILE:HD13	6:G:209:ALA:HB2	1.96	0.46
6:G:190:HIS:CD2	6:G:192:GLU:HB2	2.50	0.46
6:H:-7:PHE:CD2	6:H:113:GLU:HB3	2.49	0.46
6:H:16:ILE:HA	6:H:19:PHE:CZ	2.51	0.46
1:A:422:ILE:HD12	1:A:422:ILE:N	2.30	0.46
1:A:511:ARG:NH1	1:A:671:GLY:N	2.63	0.46
1:A:630:LYS:HE2	2:B:301:GLU:HG2	1.97	0.46
1:A:676:SER:HB3	5:E:291:ALA:HA	1.97	0.46
3:C:222:PRO:HD2	3:C:225:ASP:CG	2.35	0.46
6:G:16:ILE:HG21	6:G:79:LEU:HD12	1.98	0.46
4:D:50:LYS:O	4:D:53:LEU:HB3	2.15	0.46
5:E:65:VAL:O	5:E:65:VAL:HG13	2.14	0.46
5:E:206:VAL:HG23	5:E:207:THR:N	2.31	0.46
6:F:68:LEU:HB3	6:F:70:MSE:CE	2.43	0.46
6:F:228:ARG:CG	6:F:236:LEU:HD12	2.46	0.46
6:G:51:GLU:O	6:G:244:GLY:HA3	2.15	0.46
6:H:133:TYR:CG	6:H:228:ARG:HB3	2.51	0.46
1:A:464:ARG:HB3	1:A:465:PRO:HD3	1.97	0.46
2:B:7:LEU:O	2:B:8:GLN:HG3	2.15	0.46
2:B:98:GLN:NE2	2:B:134:TYR:OH	2.48	0.46
3:C:41:VAL:HG23	3:C:42:ASP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:SER:HB3	3:C:137:TYR:CE2	2.50	0.46
4:D:251:ILE:HG13	4:D:255:GLN:CG	2.44	0.46
1:A:382:VAL:HG22	2:B:90:ARG:HH11	1.81	0.46
1:A:594:GLU:OE1	1:A:668:ALA:N	2.45	0.46
6:G:162:ILE:HB	6:G:203:VAL:HG23	1.97	0.46
6:H:127:LYS:C	6:H:129:GLU:H	2.18	0.46
1:A:528:THR:HG22	1:A:529:LYS:N	2.31	0.46
5:E:211:ILE:HD11	5:E:246:LEU:HD22	1.98	0.46
6:F:15:ILE:HG12	6:F:221:LEU:CD1	2.45	0.46
6:F:207:PHE:CD2	6:F:250:LEU:HD23	2.50	0.46
6:H:56:ALA:HB2	6:H:243:SER:HB3	1.96	0.46
2:B:271:PHE:C	2:B:271:PHE:CD2	2.89	0.46
4:D:84:GLY:O	4:D:86:ASP:N	2.47	0.46
4:D:309:ILE:HD12	4:D:309:ILE:N	2.31	0.46
6:F:98:SER:CA	6:F:118:LEU:HG	2.44	0.46
4:D:274:LYS:HA	4:D:274:LYS:CE	2.44	0.46
5:E:46:GLY:H	5:E:231:ARG:HH12	1.64	0.46
5:E:254:ILE:HD12	5:E:254:ILE:N	2.23	0.46
5:E:314:ASN:HD21	5:E:316:THR:HB	1.80	0.46
6:G:167:ILE:HB	6:G:182:ILE:CG1	2.45	0.46
6:H:139:LEU:HD23	6:H:139:LEU:H	1.81	0.46
1:A:359:LYS:HZ3	1:A:359:LYS:HB2	1.81	0.46
1:A:635:GLU:HG3	1:A:636:GLN:HG3	1.97	0.46
2:B:227:ILE:HD12	2:B:227:ILE:C	2.36	0.46
2:B:303:VAL:HG21	3:C:308:TYR:HD1	1.80	0.46
4:D:202:ARG:O	4:D:206:GLU:HG3	2.14	0.46
5:E:331:ARG:HB3	5:E:341:HIS:ND1	2.30	0.46
1:A:532:ASN:O	1:A:536:ILE:HG13	2.15	0.46
1:A:634:SER:C	1:A:636:GLN:N	2.70	0.46
2:B:242:ALA:HB3	2:B:248:SER:HB3	1.96	0.46
3:C:49:LEU:HD22	3:C:164:PHE:CE1	2.50	0.46
4:D:76:LEU:O	4:D:80:LYS:HG3	2.16	0.46
6:F:2:LEU:HD21	6:F:68:LEU:HD11	1.97	0.46
6:F:102:LEU:HD21	6:F:111:ILE:HG23	1.99	0.46
6:H:244:GLY:O	6:H:245:PHE:HB3	2.16	0.46
1:A:351:LEU:HD22	1:A:473:ILE:HG12	1.97	0.45
3:C:113:LEU:CD2	3:C:115:ILE:HD11	2.46	0.45
4:D:197:ALA:HB3	4:D:221:LEU:CD1	2.45	0.45
6:F:50:LEU:HD11	6:F:52:ILE:HD11	1.97	0.45
6:F:182:ILE:HD12	6:F:182:ILE:O	2.16	0.45
6:H:148:VAL:HG11	6:H:212:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:149:ARG:HH11	6:H:149:ARG:HB2	1.80	0.45
1:A:550:LYS:N	1:A:551:PRO:CD	2.80	0.45
3:C:30:GLN:HE22	3:C:57:THR:HG22	1.79	0.45
3:C:249:LYS:HE3	3:C:253:GLU:OE2	2.16	0.45
3:C:265:LYS:CG	3:C:266:VAL:N	2.78	0.45
6:G:75:LEU:HA	6:G:116:LEU:CD1	2.46	0.45
6:H:134:ASP:O	6:H:200:ASP:HB2	2.15	0.45
1:A:404:TYR:CE2	6:G:233:ALA:HA	2.51	0.45
2:B:45:MET:HA	2:B:158:CYS:HB2	1.98	0.45
2:B:117:ASP:OD2	2:B:144:CYS:HB2	2.16	0.45
3:C:243:ASP:O	3:C:246:ALA:HB3	2.16	0.45
4:D:247:ASP:C	4:D:249:LYS:H	2.19	0.45
5:E:201:ILE:O	5:E:201:ILE:HG22	2.16	0.45
6:F:25:LEU:HD23	6:F:71:ASP:HA	1.98	0.45
6:G:102:LEU:HD11	6:G:111:ILE:HG23	1.98	0.45
6:H:23:VAL:HG23	6:H:72:LEU:HD12	1.97	0.45
5:E:198:ILE:CD1	5:E:228:GLY:HA2	2.47	0.45
5:E:312:THR:O	5:E:313:LEU:HD23	2.17	0.45
6:F:27:ASN:HA	6:F:69:GLY:HA2	1.97	0.45
6:G:53:GLY:N	6:G:243:SER:O	2.48	0.45
6:G:221:LEU:HB3	6:G:241:LEU:CD2	2.46	0.45
6:H:23:VAL:HG23	6:H:72:LEU:CD1	2.46	0.45
5:E:254:ILE:H	5:E:254:ILE:CD1	2.21	0.45
1:A:596:TYR:O	1:A:656:VAL:HG21	2.17	0.45
3:C:134:ILE:HG12	3:C:143:PHE:CE1	2.52	0.45
5:E:202:LEU:HB3	5:E:237:LEU:HD22	1.98	0.45
6:F:68:LEU:HD13	6:F:99:ILE:HD12	1.97	0.45
6:H:228:ARG:C	6:H:229:LEU:HD12	2.36	0.45
1:A:634:SER:C	1:A:636:GLN:H	2.19	0.45
3:C:142:ARG:HD2	3:C:142:ARG:HA	1.79	0.45
3:C:206:ARG:HD2	4:D:182:SER:C	2.38	0.45
4:D:338:ASN:C	4:D:338:ASN:ND2	2.70	0.45
5:E:314:ASN:OD1	5:E:317:ASN:ND2	2.50	0.45
6:F:167:ILE:CG1	6:F:197:LEU:HD22	2.47	0.45
6:G:4:ALA:HB1	6:G:57:PHE:CE2	2.51	0.45
6:G:13:LYS:O	6:G:16:ILE:HG22	2.17	0.45
6:G:41:ASP:OD2	6:G:42:ASP:N	2.50	0.45
6:H:148:VAL:CG1	6:H:212:LEU:HB3	2.47	0.45
1:A:320:LEU:HD13	1:A:473:ILE:HD13	1.99	0.45
1:A:421:ILE:N	1:A:421:ILE:HD12	2.31	0.45
3:C:22:GLU:HB2	3:C:26:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:GLU:O	4:D:208:GLU:HG3	2.17	0.45
5:E:32:GLN:N	5:E:33:PRO:HD3	2.31	0.45
5:E:280:ILE:O	5:E:283:ARG:HB3	2.17	0.45
6:H:61:ARG:O	6:H:61:ARG:HG3	2.16	0.45
6:F:154:LEU:HD12	6:F:154:LEU:N	2.31	0.45
1:A:404:TYR:C	1:A:406:LYS:H	2.20	0.45
2:B:185:LYS:O	2:B:218:LEU:HD12	2.16	0.45
6:F:40:VAL:HG12	6:F:41:ASP:N	2.32	0.45
6:G:84:ASN:O	6:G:86:ASP:N	2.50	0.45
6:G:118:LEU:O	6:G:119:MSE:HE2	2.17	0.45
6:H:189:GLU:C	6:H:191:PRO:HD3	2.37	0.45
6:H:192:GLU:HG3	6:H:193:THR:N	2.32	0.45
1:A:302:TYR:HD1	1:A:490:ILE:HD12	1.79	0.44
1:A:618:ALA:HB1	5:E:344:GLY:HA2	1.98	0.44
3:C:244:LEU:HD21	3:C:280:GLY:C	2.38	0.44
4:D:338:ASN:CG	5:E:301:LYS:HE2	2.37	0.44
6:F:78:ILE:CD1	6:H:154:LEU:HD21	2.47	0.44
6:F:163:THR:HG22	6:F:164:LYS:H	1.82	0.44
6:F:225:VAL:HB	6:F:239:PHE:CE1	2.52	0.44
6:G:95:THR:N	6:G:96:PRO:CD	2.80	0.44
6:H:46:LEU:HD11	6:H:215:ILE:HD11	1.99	0.44
1:A:529:LYS:HB2	2:B:35:GLN:NE2	2.20	0.44
2:B:220:ASN:ND2	2:B:222:ASP:HB2	2.32	0.44
3:C:37:VAL:HG11	3:C:66:LEU:HD22	1.98	0.44
5:E:4:TRP:HH2	5:E:209:GLU:HG2	1.83	0.44
5:E:155:ARG:HB2	5:E:181:ILE:HD11	1.99	0.44
6:F:78:ILE:HG21	6:F:101:LEU:HD13	1.98	0.44
6:F:92:ALA:HB1	6:F:96:PRO:CG	2.47	0.44
6:G:227:ILE:CG2	6:G:229:LEU:HD21	2.47	0.44
1:A:705:UNK:O	5:E:235:LEU:HD11	2.18	0.44
5:E:179:ALA:N	5:E:180:PRO:CD	2.80	0.44
5:E:239:SER:C	5:E:241:ALA:H	2.21	0.44
6:F:184:PRO:CG	6:F:197:LEU:HB3	2.46	0.44
6:G:236:LEU:HD23	6:G:236:LEU:C	2.38	0.44
6:H:229:LEU:N	6:H:229:LEU:CD1	2.81	0.44
1:A:428:GLY:CA	2:B:125:GLN:CG	2.96	0.44
1:A:516:GLN:HG2	2:B:156:SER:CA	2.35	0.44
1:A:726:UNK:O	1:A:727:UNK:C	2.65	0.44
5:E:298:ILE:HG22	5:E:299:ILE:N	2.33	0.44
1:A:302:TYR:CD1	1:A:490:ILE:HG23	2.53	0.44
2:B:96:PHE:O	2:B:99:LYS:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:VAL:CG1	4:D:229:ARG:HG3	2.47	0.44
4:D:228:LEU:HD23	4:D:232:ILE:HG13	1.98	0.44
4:D:275:VAL:HG11	4:D:350:ILE:HG23	1.99	0.44
4:D:288:ASN:HD21	5:E:227:ASN:ND2	2.16	0.44
5:E:193:PRO:CG	5:E:198:ILE:HG12	2.47	0.44
6:F:16:ILE:HG23	6:F:72:LEU:HD22	1.98	0.44
6:H:19:PHE:O	6:H:23:VAL:HG22	2.17	0.44
6:H:78:ILE:HG21	6:H:101:LEU:HD22	2.00	0.44
1:A:340:LYS:O	1:A:340:LYS:HG2	2.18	0.44
1:A:680:TYR:O	1:A:684:GLN:HB2	2.18	0.44
4:D:53:LEU:CD1	4:D:82:LEU:HD13	2.48	0.44
4:D:318:PHE:CE2	4:D:322:ILE:HG12	2.52	0.44
5:E:151:GLN:OE1	5:E:178:ILE:HG23	2.17	0.44
5:E:229:ASN:HB3	5:E:232:VAL:HB	1.99	0.44
3:C:49:LEU:HD22	3:C:164:PHE:HE1	1.82	0.44
6:F:1:MSE:O	6:F:62:CYS:HA	2.18	0.44
6:F:160:ILE:HD13	6:F:207:PHE:CE1	2.53	0.44
1:A:510:THR:HG21	1:A:513:ASP:O	2.17	0.44
1:A:590:LEU:HB3	1:A:667:THR:CG2	2.47	0.44
3:C:48:HIS:CB	3:C:161:CYS:HB3	2.48	0.44
4:D:85:PRO:HA	4:D:88:MET:HB2	1.99	0.44
4:D:168:LEU:C	4:D:169:ILE:HD12	2.38	0.44
4:D:292:LYS:HG3	5:E:227:ASN:O	2.18	0.44
4:D:338:ASN:C	4:D:338:ASN:HD22	2.21	0.44
5:E:116:VAL:CG1	5:E:136:LYS:HD3	2.48	0.44
6:F:19:PHE:CZ	6:F:50:LEU:HB2	2.47	0.44
6:F:143:GLU:OE2	6:G:110:ARG:NH1	2.50	0.44
1:A:584:ASP:C	1:A:586:ASP:H	2.20	0.44
6:H:146:LYS:HG2	6:H:149:ARG:NH2	2.33	0.44
1:A:514:ILE:HA	1:A:517:VAL:CG2	2.48	0.43
5:E:57:LEU:O	5:E:61:PHE:HB2	2.18	0.43
6:F:102:LEU:HG	6:F:113:GLU:HG3	1.99	0.43
6:G:4:ALA:O	6:G:89:THR:HG23	2.17	0.43
1:A:328:GLU:O	1:A:332:LYS:HG2	2.17	0.43
1:A:524:ILE:HG12	1:A:543:TRP:CG	2.53	0.43
2:B:84:ARG:NH1	2:B:114:ASP:O	2.45	0.43
3:C:275:ILE:HG12	3:C:310:ILE:HG21	1.98	0.43
5:E:49:LYS:HG3	9:E:805:ADP:O2B	2.18	0.43
5:E:218:ILE:HD12	5:E:252:SER:HB3	2.00	0.43
6:F:16:ILE:CD1	6:F:75:LEU:HD21	2.44	0.43
6:H:121:ILE:HG22	6:H:122:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:147:ILE:CD1	6:H:180:VAL:HG11	2.41	0.43
1:A:549:LEU:HB3	1:A:552:PHE:CD1	2.53	0.43
3:C:207:ARG:O	3:C:211:VAL:HG13	2.18	0.43
4:D:348:VAL:O	4:D:352:GLN:HG2	2.18	0.43
5:E:158:MET:CG	5:E:167:LEU:HD12	2.48	0.43
5:E:198:ILE:HG23	5:E:230:LEU:CD2	2.48	0.43
5:E:270:ILE:HD12	5:E:346:ILE:HG23	1.98	0.43
6:F:242:LYS:HA	6:F:242:LYS:HD3	1.83	0.43
6:G:82:GLY:HA3	6:G:103:PHE:CD2	2.53	0.43
6:H:107:LYS:C	6:H:109:ASP:N	2.70	0.43
1:A:301:LYS:HE2	1:A:302:TYR:CZ	2.54	0.43
1:A:513:ASP:HB3	1:A:516:GLN:HB2	2.00	0.43
1:A:619:ASN:O	1:A:622:SER:HB3	2.18	0.43
2:B:67:LEU:O	2:B:70:SER:HB2	2.17	0.43
3:C:66:LEU:O	3:C:70:ILE:HG13	2.18	0.43
5:E:26:LEU:HD22	5:E:56:LEU:HD22	2.01	0.43
6:H:104:GLU:OE1	6:H:111:ILE:HD12	2.18	0.43
6:H:126:LEU:HD13	6:H:128:ILE:HD11	1.99	0.43
2:B:312:MET:O	2:B:316:ILE:HG12	2.18	0.43
5:E:198:ILE:HG23	5:E:230:LEU:HD23	2.00	0.43
1:A:515:ARG:NH1	8:A:801:AGS:H5'1	2.33	0.43
1:A:574:LEU:HD22	1:A:578:ILE:HD13	2.01	0.43
1:A:672:GLN:HE21	5:E:287:TYR:HB3	1.83	0.43
2:B:222:ASP:O	2:B:226:LYS:HG3	2.18	0.43
3:C:59:LYS:NZ	8:C:803:AGS:S1G	2.91	0.43
4:D:63:PHE:HB2	4:D:169:ILE:HG13	2.01	0.43
4:D:132:PRO:HA	4:D:133:PRO:HD3	1.90	0.43
4:D:139:LEU:O	4:D:142:ALA:HB2	2.19	0.43
4:D:161:SER:O	4:D:165:ARG:NH1	2.51	0.43
6:G:26:VAL:HG11	6:G:72:LEU:HD21	2.00	0.43
6:G:49:SER:HB3	6:G:247:GLN:HG3	2.00	0.43
6:G:190:HIS:ND1	6:G:193:THR:HG23	2.34	0.43
1:A:298:TRP:HA	1:A:301:LYS:HG2	2.00	0.43
1:A:347:ARG:HB2	1:A:444:CYS:O	2.18	0.43
2:B:232:HIS:CE1	2:B:234:LEU:HD22	2.54	0.43
4:D:254:THR:O	4:D:258:GLU:HG3	2.18	0.43
6:F:177:SER:OG	6:G:115:SER:HB3	2.18	0.43
1:A:312:GLY:O	1:A:314:LYS:N	2.52	0.43
1:A:546:ASN:O	1:A:550:LYS:HB2	2.18	0.43
2:B:40:GLY:O	2:B:106:GLY:O	2.37	0.43
3:C:260:HIS:CD2	4:D:309:ILE:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:LEU:CD2	6:F:68:LEU:HD11	2.49	0.43
6:G:30:CYS:C	6:G:31:LYS:HG3	2.39	0.43
2:B:67:LEU:HD12	2:B:75:VAL:HG23	2.01	0.43
2:B:102:HIS:NE2	6:G:95:THR:HG22	2.33	0.43
4:D:63:PHE:O	4:D:169:ILE:HA	2.17	0.43
6:H:56:ALA:HB2	6:H:243:SER:OG	2.19	0.43
1:A:573:THR:O	1:A:577:LYS:HG3	2.19	0.43
1:A:680:TYR:HA	5:E:293:CYS:SG	2.59	0.43
2:B:280:VAL:CG1	2:B:284:VAL:HB	2.47	0.43
3:C:172:GLU:CG	3:C:173:ALA:H	2.19	0.43
3:C:263:LEU:O	3:C:267:ARG:HG2	2.18	0.43
5:E:94:LEU:HD23	5:E:94:LEU:H	1.82	0.43
6:F:26:VAL:HG12	6:F:39:ALA:CB	2.49	0.43
6:F:110:ARG:HG2	6:H:182:ILE:HG22	2.01	0.43
6:F:182:ILE:HD13	6:F:195:ILE:HD13	1.99	0.43
1:A:690:THR:C	1:A:692:LEU:N	2.72	0.42
1:A:698:UNK:C	1:A:700:UNK:N	2.81	0.42
2:B:277:LEU:HA	2:B:277:LEU:HD12	1.77	0.42
4:D:27:TRP:O	4:D:31:TYR:HB2	2.19	0.42
4:D:42:GLN:NE2	4:D:190:LYS:HB3	2.32	0.42
5:E:320:SER:HB2	5:E:352:CYS:SG	2.59	0.42
1:A:348:ALA:HB1	1:A:451:LEU:O	2.19	0.42
1:A:405:PHE:N	1:A:405:PHE:CD1	2.87	0.42
1:A:510:THR:HG22	1:A:513:ASP:CB	2.40	0.42
2:B:113:LEU:HB3	2:B:119:MET:HE2	2.01	0.42
3:C:120:ASP:OD1	3:C:120:ASP:N	2.52	0.42
3:C:199:GLU:O	3:C:199:GLU:HG2	2.17	0.42
3:C:264:ASN:O	3:C:264:ASN:ND2	2.51	0.42
5:E:135:TYR:C	5:E:135:TYR:CD1	2.92	0.42
1:A:568:GLY:HA2	1:A:571:ASN:ND2	2.32	0.42
2:B:224:VAL:O	2:B:227:ILE:HG13	2.19	0.42
5:E:310:VAL:HB	5:E:313:LEU:HD12	2.01	0.42
6:F:72:LEU:O	6:F:76:SER:HB2	2.20	0.42
6:F:143:GLU:O	6:F:147:ILE:HG12	2.20	0.42
1:A:378:ASN:CG	2:B:129:ARG:HG2	2.40	0.42
1:A:390:ALA:O	6:G:210:LYS:HD2	2.20	0.42
1:A:483:ILE:HG12	1:A:514:ILE:HG12	2.01	0.42
1:A:667:THR:HG22	1:A:669:TRP:N	2.35	0.42
4:D:196:ASN:N	4:D:196:ASN:ND2	2.66	0.42
4:D:320:ASN:O	4:D:323:SER:HB3	2.19	0.42
5:E:20:GLU:HA	5:E:23:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:312:THR:O	5:E:312:THR:HG22	2.19	0.42
6:F:215:ILE:C	6:F:217:LYS:H	2.22	0.42
6:H:1:MSE:CE	6:H:66:VAL:HB	2.49	0.42
2:B:245:LEU:O	2:B:245:LEU:HD12	2.19	0.42
3:C:14:PRO:O	3:C:16:VAL:N	2.53	0.42
5:E:175:SER:HB3	5:E:176:PRO:CD	2.50	0.42
5:E:199:SER:O	5:E:202:LEU:HB2	2.19	0.42
5:E:215:THR:CG2	5:E:216:LYS:H	2.23	0.42
6:F:179:SER:OG	6:F:181:ILE:HD11	2.19	0.42
6:G:225:VAL:HG13	6:G:227:ILE:HD11	2.01	0.42
6:H:168:LYS:HB2	6:H:168:LYS:HZ2	1.84	0.42
1:A:361:THR:HG22	1:A:365:LEU:HD22	2.02	0.42
1:A:374:ILE:HD12	1:A:374:ILE:N	2.34	0.42
2:B:9:LEU:CD2	3:C:139:LYS:HE2	2.50	0.42
2:B:285:ARG:O	2:B:289:ILE:HG13	2.19	0.42
3:C:176:ARG:HB3	3:C:176:ARG:CZ	2.49	0.42
4:D:141:GLU:C	4:D:143:ASP:N	2.72	0.42
4:D:291:MET:CE	4:D:343:LEU:HD23	2.50	0.42
4:D:293:SER:CB	5:E:192:ALA:H	2.32	0.42
5:E:198:ILE:HD11	5:E:228:GLY:HA2	2.01	0.42
6:F:125:PHE:CE2	6:F:127:LYS:HG3	2.54	0.42
6:F:190:HIS:O	6:F:193:THR:HG22	2.19	0.42
6:G:137:LEU:HD13	6:G:167:ILE:HG12	2.00	0.42
1:A:334:SER:O	1:A:336:LYS:HG3	2.20	0.42
1:A:362:ALA:O	1:A:366:VAL:HG23	2.19	0.42
4:D:91:ARG:O	4:D:92:ILE:HD12	2.19	0.42
5:E:4:TRP:O	5:E:7:LYS:HB3	2.20	0.42
5:E:91:PRO:HG2	5:E:92:TYR:CD1	2.55	0.42
6:F:54:VAL:O	6:F:57:PHE:HB2	2.20	0.42
6:F:139:LEU:N	6:F:139:LEU:HD23	2.34	0.42
6:F:144:PHE:HE1	6:F:169:PHE:CE2	2.38	0.42
6:H:192:GLU:HG3	6:H:193:THR:H	1.85	0.42
1:A:312:GLY:C	1:A:314:LYS:H	2.23	0.42
1:A:420:VAL:HG12	1:A:422:ILE:CD1	2.49	0.42
1:A:574:LEU:HD12	2:B:285:ARG:HE	1.85	0.42
3:C:35:THR:HG22	3:C:39:LYS:HE3	2.01	0.42
3:C:50:LEU:CD1	3:C:52:TYR:CD2	3.03	0.42
3:C:79:VAL:CG1	3:C:115:ILE:HD13	2.50	0.42
4:D:347:LEU:HA	4:D:350:ILE:HG22	2.02	0.42
5:E:230:LEU:HA	5:E:233:SER:OG	2.20	0.42
1:A:451:LEU:HG	1:A:453:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:137:LEU:C	6:F:137:LEU:HD12	2.39	0.42
6:G:134:ASP:HB2	6:G:203:VAL:CG1	2.50	0.42
1:A:382:VAL:HG12	1:A:387:LEU:HD12	2.02	0.42
2:B:42:MET:SD	2:B:110:ILE:HD12	2.60	0.42
3:C:71:TYR:CD2	3:C:78:MET:HG2	2.55	0.42
3:C:215:CYS:C	3:C:217:ALA:N	2.73	0.42
4:D:27:TRP:CZ3	4:D:236:GLN:HA	2.55	0.42
4:D:291:MET:HG3	4:D:340:HIS:CG	2.55	0.42
5:E:142:GLU:C	5:E:144:ASN:H	2.23	0.42
5:E:218:ILE:CG2	5:E:248:LEU:HD13	2.50	0.42
6:H:146:LYS:O	6:H:147:ILE:C	2.57	0.42
1:A:313:ASN:O	1:A:316:SER:N	2.53	0.41
1:A:347:ARG:HH11	1:A:347:ARG:CG	2.30	0.41
1:A:412:GLN:O	1:A:412:GLN:HG3	2.20	0.41
4:D:154:ARG:HD3	4:D:179:PRO:CB	2.47	0.41
4:D:186:LYS:HD3	4:D:186:LYS:N	2.35	0.41
5:E:202:LEU:HD23	5:E:234:LEU:HD23	2.00	0.41
6:G:183:LYS:HA	6:G:184:PRO:HD3	1.95	0.41
1:A:350:MET:HB2	1:A:470:CYS:SG	2.60	0.41
4:D:186:LYS:HB2	4:D:186:LYS:NZ	2.34	0.41
4:D:270:GLU:O	4:D:274:LYS:HB2	2.20	0.41
6:F:251:ALA:HA	6:F:252:PRO:HD3	1.88	0.41
6:G:26:VAL:CG1	6:G:72:LEU:HD21	2.51	0.41
6:H:20:LYS:NZ	6:H:80:ARG:HH21	2.18	0.41
1:A:419:PHE:CZ	6:G:44:ARG:HB2	2.55	0.41
2:B:113:LEU:HD13	2:B:119:MET:CE	2.50	0.41
4:D:86:ASP:HB2	4:D:125:ASP:OD1	2.21	0.41
4:D:332:ARG:HA	5:E:330:GLU:OE2	2.20	0.41
5:E:114:LYS:HG2	5:E:161:TYR:CE1	2.55	0.41
5:E:218:ILE:HG21	5:E:248:LEU:HB3	2.01	0.41
6:F:88:LEU:HD23	6:F:89:THR:H	1.85	0.41
6:H:35:ILE:O	6:H:51:GLU:HA	2.20	0.41
6:H:50:LEU:HG	6:H:51:GLU:N	2.34	0.41
6:H:99:ILE:HD13	6:H:100:ILE:O	2.20	0.41
1:A:575:ASN:HD21	2:B:275:LYS:HE3	1.83	0.41
2:B:267:VAL:HG11	2:B:296:HIS:CB	2.49	0.41
3:C:67:ALA:CB	3:C:75:TYR:HE1	2.32	0.41
4:D:58:LEU:O	4:D:165:ARG:CD	2.65	0.41
5:E:120:GLU:HG3	5:E:121:GLN:HG3	2.01	0.41
5:E:231:ARG:O	5:E:235:LEU:HB2	2.21	0.41
6:F:38:GLN:HA	6:F:48:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:251:ALA:HA	6:G:252:PRO:HD3	1.84	0.41
6:H:161:MSE:HE3	6:H:168:LYS:HG2	2.01	0.41
1:A:305:THR:O	1:A:305:THR:HG22	2.20	0.41
3:C:113:LEU:HD23	3:C:115:ILE:HD11	2.02	0.41
4:D:137:ILE:HD12	4:D:137:ILE:N	2.35	0.41
5:E:90:SER:C	5:E:92:TYR:H	2.24	0.41
5:E:236:MET:HG3	5:E:255:ILE:HG22	2.01	0.41
5:E:267:THR:HG23	5:E:307:LEU:HD23	2.01	0.41
1:A:506:LEU:O	1:A:509:THR:N	2.53	0.41
2:B:225:PHE:CZ	2:B:233:PRO:HG2	2.56	0.41
3:C:186:LYS:O	3:C:216:LYS:NZ	2.50	0.41
4:D:94:GLU:C	4:D:95:LEU:HD12	2.41	0.41
4:D:95:LEU:HD23	4:D:101:ARG:HG2	2.03	0.41
5:E:61:PHE:HD2	5:E:92:TYR:HD2	1.67	0.41
5:E:160:LYS:HB3	5:E:161:TYR:H	1.58	0.41
6:H:137:LEU:HB3	6:H:197:LEU:HD13	2.03	0.41
2:B:256:LEU:HB3	2:B:266:ILE:HD12	2.02	0.41
5:E:264:HIS:O	5:E:268:ARG:HG3	2.20	0.41
6:F:1:MSE:HE2	6:F:93:ASP:O	2.21	0.41
6:F:23:VAL:HG11	6:F:39:ALA:HB3	2.03	0.41
6:F:148:VAL:HG21	6:F:216:ILE:HG21	2.01	0.41
6:G:196:LYS:O	6:G:197:LEU:HB2	2.20	0.41
1:A:684:GLN:O	1:A:688:TYR:HD1	2.03	0.41
2:B:274:THR:HG23	2:B:288:MET:HE1	2.01	0.41
3:C:196:ALA:HB1	3:C:233:TYR:CE2	2.56	0.41
4:D:219:ARG:O	4:D:223:ILE:HG13	2.21	0.41
5:E:259:TRP:O	5:E:260:ILE:C	2.59	0.41
6:G:146:LYS:HE2	6:G:150:ASP:CG	2.41	0.41
6:H:215:ILE:HG23	6:H:248:PHE:CG	2.56	0.41
1:A:496:PHE:CD1	1:A:496:PHE:C	2.94	0.41
2:B:151:ILE:HD12	2:B:154:LEU:H	1.85	0.41
3:C:189:LEU:HD21	3:C:194:GLU:HA	2.03	0.41
4:D:53:LEU:HD12	4:D:82:LEU:HD13	2.02	0.41
4:D:291:MET:O	4:D:292:LYS:C	2.59	0.41
5:E:46:GLY:N	5:E:231:ARG:HH12	2.18	0.41
5:E:120:GLU:HG3	5:E:121:GLN:N	2.36	0.41
5:E:193:PRO:HG2	5:E:198:ILE:HG12	2.03	0.41
5:E:193:PRO:HG2	5:E:198:ILE:HD11	2.02	0.41
5:E:320:SER:HB3	5:E:352:CYS:SG	2.60	0.41
6:F:28:PHE:HB2	6:F:68:LEU:HB2	2.02	0.41
6:F:170:VAL:HG12	6:F:171:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:73:THR:O	6:G:77:LYS:HG3	2.21	0.41
3:C:87:ASP:O	3:C:92:VAL:HG21	2.21	0.41
4:D:213:ASP:HB3	4:D:216:VAL:CG2	2.51	0.41
4:D:332:ARG:NH1	5:E:326:SER:OG	2.54	0.41
5:E:5:VAL:HG13	9:E:805:ADP:O2'	2.21	0.41
6:F:18:GLY:HA3	6:F:246:LEU:HD21	2.03	0.41
6:G:1:MSE:SE	6:G:64:HIS:HB2	2.71	0.41
1:A:403:GLY:O	1:A:417:LYS:HG2	2.21	0.40
1:A:503:ILE:HA	1:A:506:LEU:HD12	2.03	0.40
2:B:104:PRO:HB2	2:B:107:LYS:HG2	2.03	0.40
3:C:111:PHE:CD1	3:C:111:PHE:C	2.93	0.40
3:C:303:LEU:HD13	3:C:303:LEU:HA	1.94	0.40
5:E:116:VAL:HG12	5:E:116:VAL:O	2.20	0.40
1:A:346:PHE:CD1	1:A:471:LEU:HB2	2.56	0.40
1:A:436:GLY:O	1:A:440:LEU:HB2	2.21	0.40
1:A:610:HIS:O	1:A:614:VAL:HG23	2.21	0.40
1:A:688:TYR:O	1:A:689:HIS:ND1	2.49	0.40
1:A:690:THR:O	1:A:690:THR:HG22	2.22	0.40
3:C:19:TYR:CE2	3:C:181:VAL:HG23	2.56	0.40
3:C:170:PRO:O	3:C:171:GLN:C	2.58	0.40
3:C:265:LYS:HG3	3:C:266:VAL:H	1.85	0.40
5:E:160:LYS:HB3	5:E:161:TYR:CD1	2.56	0.40
6:G:75:LEU:CA	6:G:116:LEU:HD11	2.50	0.40
6:G:100:ILE:C	6:G:101:LEU:HD12	2.41	0.40
6:H:12:PHE:CZ	6:H:16:ILE:HD11	2.56	0.40
6:H:85:THR:HG22	6:H:85:THR:O	2.20	0.40
6:H:175:ILE:HG13	6:H:176:GLY:N	2.35	0.40
1:A:423:MET:HB2	1:A:453:LEU:HG	2.03	0.40
1:A:459:ASN:HB2	1:A:681:ARG:HH11	1.86	0.40
1:A:510:THR:CG2	1:A:516:GLN:HB3	2.50	0.40
1:A:660:MET:CE	1:A:664:ILE:HD11	2.52	0.40
3:C:131:ARG:CD	3:C:156:ALA:HB1	2.52	0.40
3:C:262:THR:O	3:C:266:VAL:HG23	2.22	0.40
3:C:310:ILE:C	3:C:312:LYS:H	2.23	0.40
4:D:42:GLN:NE2	4:D:42:GLN:HA	2.36	0.40
4:D:206:GLU:C	4:D:208:GLU:H	2.25	0.40
6:F:144:PHE:O	6:F:146:LYS:N	2.55	0.40
6:G:200:ASP:O	6:G:201:GLN:HG2	2.20	0.40
6:H:38:GLN:OE1	6:H:126:LEU:HD23	2.21	0.40
6:H:211:TYR:O	6:H:215:ILE:HG12	2.21	0.40
3:C:211:VAL:CG2	3:C:212:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:PRO:O	4:D:182:SER:HB3	2.21	0.40
4:D:262:VAL:HG12	4:D:263:VAL:N	2.37	0.40
4:D:292:LYS:O	5:E:44:PRO:HG2	2.21	0.40
5:E:234:LEU:C	5:E:236:MET:N	2.75	0.40
6:F:49:SER:HB2	6:F:247:GLN:HE21	1.87	0.40
6:F:86:ASP:HA	6:F:104:GLU:O	2.22	0.40
6:F:244:GLY:O	6:F:245:PHE:HB3	2.21	0.40
6:G:134:ASP:HB3	6:G:201:GLN:HB2	2.03	0.40
2:B:281:LYS:HB2	2:B:284:VAL:HG23	2.03	0.40
3:C:71:TYR:CE2	3:C:78:MET:HG2	2.56	0.40
3:C:165:ARG:HH21	3:C:167:GLN:HB2	1.87	0.40
3:C:231:VAL:O	3:C:235:CYS:HB2	2.21	0.40
5:E:13:LEU:HD11	5:E:56:LEU:CD1	2.51	0.40
5:E:155:ARG:O	5:E:158:MET:N	2.54	0.40
6:F:38:GLN:HB2	6:F:126:LEU:CD2	2.50	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	391/516 (76%)	324 (83%)	55 (14%)	12 (3%)	4	14
2	B	314/323 (97%)	279 (89%)	32 (10%)	3 (1%)	15	40
3	C	320/340 (94%)	257 (80%)	53 (17%)	10 (3%)	4	14
4	D	326/353 (92%)	268 (82%)	43 (13%)	15 (5%)	2	7
5	E	309/354 (87%)	244 (79%)	57 (18%)	8 (3%)	5	17
6	F	256/283 (90%)	216 (84%)	32 (12%)	8 (3%)	4	14
6	G	256/283 (90%)	219 (86%)	31 (12%)	6 (2%)	6	20
6	H	265/283 (94%)	224 (84%)	34 (13%)	7 (3%)	5	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2437/2735 (89%)	2031 (83%)	337 (14%)	69 (3%)	5 16

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	ASP
1	A	584	ASP
2	B	25	GLY
2	B	27	LYS
4	D	41	ALA
4	D	88	MET
4	D	252	THR
6	F	20	LYS
6	F	63	ASP
6	G	108	LYS
1	A	548	ALA
2	B	217	GLY
3	C	15	TRP
3	C	186	LYS
3	C	237	GLY
3	C	290	LEU
3	C	297	VAL
4	D	85	PRO
4	D	250	ASN
4	D	256	VAL
4	D	257	GLU
4	D	294	GLY
5	E	160	LYS
6	F	164	LYS
6	G	84	ASN
6	G	197	LEU
6	G	242	LYS
6	H	108	LYS
6	H	128	ILE
1	A	313	ASN
1	A	566	ASP
1	A	635	GLU
3	C	191	PRO
3	C	221	ASN
3	C	313	GLY
4	D	154	ARG
4	D	280	PHE

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Mol	Chain	Res	Type
4	D	295	TRP
4	D	307	TYR
5	E	105	ASP
6	F	98	SER
6	G	85	THR
1	A	478	PRO
1	A	585	PHE
3	C	75	TYR
4	D	281	ASP
4	D	296	SER
6	F	145	SER
6	F	216	ILE
6	F	252	PRO
6	H	94	ASN
1	A	339	GLY
3	C	316	ASP
5	E	10	PRO
5	E	135	TYR
5	E	260	ILE
6	F	59	GLU
6	G	63	ASP
6	H	-5	GLY
4	D	341	ILE
5	E	44	PRO
5	E	184	GLN
1	A	416	GLY
6	H	15	ILE
1	A	524	ILE
1	A	567	ILE
5	E	65	VAL
6	H	-9	VAL
6	H	184	PRO

### 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	340/400 (85%)	320 (94%)	20 (6%)	19	45
2	B	277/283 (98%)	263 (95%)	14 (5%)	24	52
3	C	279/296 (94%)	266 (95%)	13 (5%)	26	56
4	D	292/312 (94%)	282 (97%)	10 (3%)	37	67
5	E	290/324 (90%)	280 (97%)	10 (3%)	37	67
6	F	231/246 (94%)	224 (97%)	7 (3%)	41	72
6	G	232/246 (94%)	221 (95%)	11 (5%)	26	56
6	H	235/246 (96%)	224 (95%)	11 (5%)	26	56
All	All	2176/2353 (92%)	2080 (96%)	96 (4%)	28	58

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	318	MET
1	A	326	ASN
1	A	327	TRP
1	A	365	LEU
1	A	376	GLU
1	A	392	VAL
1	A	449	THR
1	A	458	ARG
1	A	476	ARG
1	A	504	ASP
1	A	516	GLN
1	A	558	MET
1	A	574	LEU
1	A	583	ASP
1	A	595	ASN
1	A	597	LEU
1	A	600	ARG
1	A	604	LEU
1	A	620	CYS
2	B	20	LEU
2	B	26	ASN
2	B	32	ARG
2	B	53	ILE
2	B	58	SER
2	B	73	ASP
2	B	92	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	101	LEU
2	B	164	SER
2	B	165	LYS
2	B	166	LEU
2	B	271	PHE
2	B	298	ARG
2	B	320	ASN
3	C	40	PHE
3	C	57	THR
3	C	63	ILE
3	C	117	ASP
3	C	118	GLU
3	C	128	ASN
3	C	142	ARG
3	C	167	GLN
3	C	192	ASN
3	C	197	LEU
3	C	220	ASP
3	C	255	ASP
3	C	264	ASN
4	D	85	PRO
4	D	94	GLU
4	D	128	ASN
4	D	173	VAL
4	D	186	LYS
4	D	274	LYS
4	D	284	LYS
4	D	288	ASN
4	D	295	TRP
4	D	338	ASN
5	E	4	TRP
5	E	58	GLU
5	E	63	PRO
5	E	135	TYR
5	E	161	TYR
5	E	283	ARG
5	E	287	TYR
5	E	298	ILE
5	E	339	ILE
5	E	352	CYS
6	F	47	LEU
6	F	88	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	F	102	LEU
6	F	154	LEU
6	F	185	PHE
6	F	205	LEU
6	F	228	ARG
6	G	17	ASP
6	G	20	LYS
6	G	26	VAL
6	G	42	ASP
6	G	90	LEU
6	G	109	ASP
6	G	138	SER
6	G	151	LEU
6	G	172	ASP
6	G	183	LYS
6	G	250	LEU
6	H	22	CYS
6	H	79	LEU
6	H	99	ILE
6	H	168	LYS
6	H	181	ILE
6	H	193	THR
6	H	199	MSE
6	H	225	VAL
6	H	229	LEU
6	H	240	ASP
6	H	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	326	ASN
1	A	337	HIS
1	A	394	ASN
1	A	442	GLN
1	A	459	ASN
1	A	474	GLN
1	A	508	GLN
1	A	562	GLN
1	A	571	ASN
1	A	575	ASN
1	A	665	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	35	GLN
2	B	41	ASN
2	B	91	ASN
2	B	98	GLN
2	B	220	ASN
2	B	223	ASN
2	B	276	ASN
2	B	296	HIS
3	C	140	ASN
3	C	167	GLN
3	C	192	ASN
3	C	221	ASN
3	C	264	ASN
3	C	317	GLN
4	D	42	GLN
4	D	96	ASN
4	D	112	ASN
4	D	128	ASN
4	D	183	GLN
4	D	196	ASN
4	D	288	ASN
4	D	302	ASN
4	D	303	GLN
4	D	334	ASN
4	D	340	HIS
5	E	19	ASN
5	E	24	ASN
5	E	93	HIS
5	E	144	ASN
5	E	229	ASN
5	E	243	ASN
5	E	314	ASN
5	E	317	ASN
6	F	27	ASN
6	F	29	GLN
6	F	38	GLN
6	F	58	GLN
6	F	153	GLN
6	F	247	GLN
6	F	255	ASN
6	G	27	ASN
6	G	153	GLN

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Mol	Chain	Res	Type
6	G	159	ASN
6	G	247	GLN
6	H	24	GLN
6	H	27	ASN
6	H	153	GLN
6	H	247	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
8	AGS	B	802	7	26,33,33	2.01	4 (15%)	26,52,52	1.34	3 (11%)
8	AGS	A	801	7	26,33,33	2.12	5 (19%)	26,52,52	1.52	3 (11%)
8	AGS	D	804	7	26,33,33	2.02	5 (19%)	26,52,52	1.50	4 (15%)
9	ADP	E	805	-	24,29,29	1.74	6 (25%)	29,45,45	1.36	4 (13%)
8	AGS	C	803	7	26,33,33	2.20	4 (15%)	26,52,52	1.46	4 (15%)

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
8	AGS	B	802	7	-	5/17/38/38	0/3/3/3
8	AGS	A	801	7	-	3/17/38/38	0/3/3/3
8	AGS	D	804	7	-	2/17/38/38	0/3/3/3
9	ADP	E	805	-	-	4/12/32/32	0/3/3/3
8	AGS	C	803	7	-	3/17/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	803	AGS	PG-S1G	-9.44	1.70	1.90
8	A	801	AGS	PG-S1G	-8.97	1.71	1.90
8	B	802	AGS	PG-S1G	-8.45	1.72	1.90
8	D	804	AGS	PG-S1G	-7.94	1.73	1.90
9	E	805	ADP	C2-N3	3.65	1.38	1.32
9	E	805	ADP	C4-N3	3.51	1.40	1.35
8	D	804	AGS	C2-N3	3.38	1.37	1.32
9	E	805	ADP	O4'-C1'	3.20	1.45	1.41
9	E	805	ADP	C2-N1	3.07	1.39	1.33
9	E	805	ADP	C2'-C1'	-2.93	1.49	1.53
8	C	803	AGS	C2-N3	2.78	1.36	1.32
8	D	804	AGS	O4'-C1'	2.68	1.44	1.41
8	B	802	AGS	C2-N3	2.68	1.36	1.32
8	A	801	AGS	C2-N3	2.51	1.36	1.32
8	D	804	AGS	C2-N1	2.49	1.38	1.33
8	A	801	AGS	C2-N1	2.32	1.38	1.33
8	A	801	AGS	C2'-C1'	-2.32	1.50	1.53
8	B	802	AGS	C2-N1	2.31	1.38	1.33
8	C	803	AGS	C2'-C1'	-2.27	1.50	1.53
8	C	803	AGS	C2-N1	2.21	1.38	1.33
8	B	802	AGS	C2'-C1'	-2.11	1.50	1.53
9	E	805	ADP	PB-O2B	-2.09	1.46	1.54
8	D	804	AGS	C4-N3	2.07	1.38	1.35
8	A	801	AGS	O4'-C1'	2.02	1.43	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	801	AGS	C1'-N9-C4	4.98	135.40	126.64
8	D	804	AGS	C1'-N9-C4	4.52	134.58	126.64
9	E	805	ADP	C1'-N9-C4	4.38	134.34	126.64
8	C	803	AGS	C1'-N9-C4	4.18	133.98	126.64
8	B	802	AGS	C1'-N9-C4	3.95	133.59	126.64
8	D	804	AGS	C3'-C2'-C1'	3.46	106.19	100.98
8	C	803	AGS	C3'-C2'-C1'	3.43	106.14	100.98
8	A	801	AGS	C3'-C2'-C1'	3.30	105.95	100.98
8	B	802	AGS	C3'-C2'-C1'	2.83	105.23	100.98
8	A	801	AGS	C5-C6-N6	2.53	124.20	120.35
8	B	802	AGS	C5-C6-N6	2.45	124.08	120.35
8	C	803	AGS	C5-C6-N6	2.43	124.05	120.35
9	E	805	ADP	C3'-C2'-C1'	2.39	104.57	100.98
8	D	804	AGS	C5-C6-N6	2.33	123.90	120.35
8	D	804	AGS	O3G-PG-O3B	2.32	112.38	104.64
8	C	803	AGS	O3G-PG-O3B	2.32	112.37	104.64
9	E	805	ADP	C5-C6-N6	2.27	123.80	120.35
9	E	805	ADP	O5'-C5'-C4'	2.02	115.96	108.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	AGS	C5'-O5'-PA-O1A
8	B	802	AGS	C5'-O5'-PA-O1A
8	C	803	AGS	C5'-O5'-PA-O1A
9	E	805	ADP	C5'-O5'-PA-O1A
9	E	805	ADP	O4'-C4'-C5'-O5'
9	E	805	ADP	C3'-C4'-C5'-O5'
8	A	801	AGS	C5'-O5'-PA-O3A
8	C	803	AGS	C5'-O5'-PA-O3A
9	E	805	ADP	PB-O3A-PA-O2A
8	B	802	AGS	C5'-O5'-PA-O2A
8	D	804	AGS	PA-O3A-PB-O2B
8	B	802	AGS	C5'-O5'-PA-O3A
8	B	802	AGS	PA-O3A-PB-O1B
8	B	802	AGS	PA-O3A-PB-O2B
8	D	804	AGS	PA-O3A-PB-O1B
8	A	801	AGS	C5'-O5'-PA-O2A
8	C	803	AGS	C5'-O5'-PA-O2A

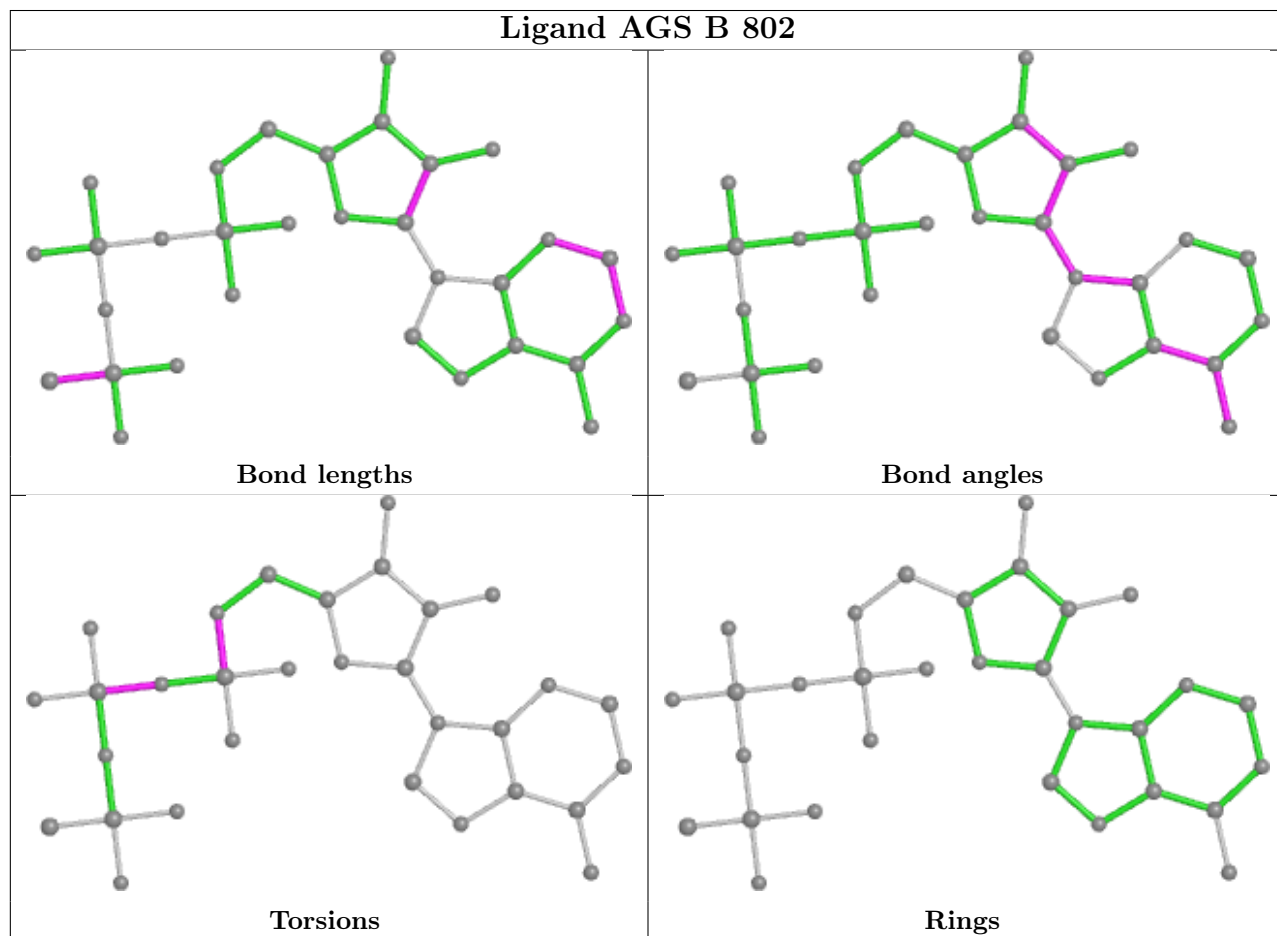
There are no ring outliers.

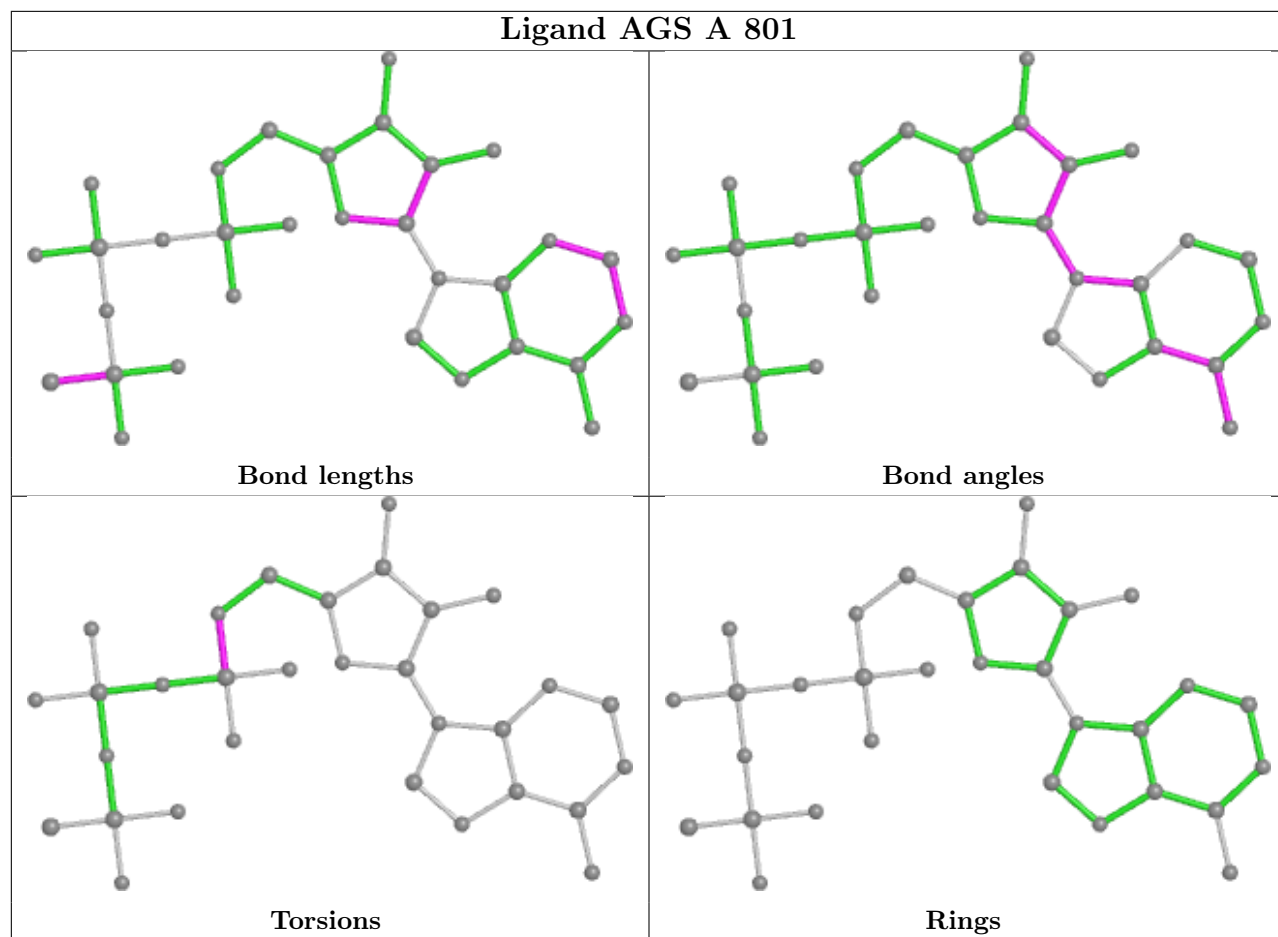
5 monomers are involved in 10 short contacts:

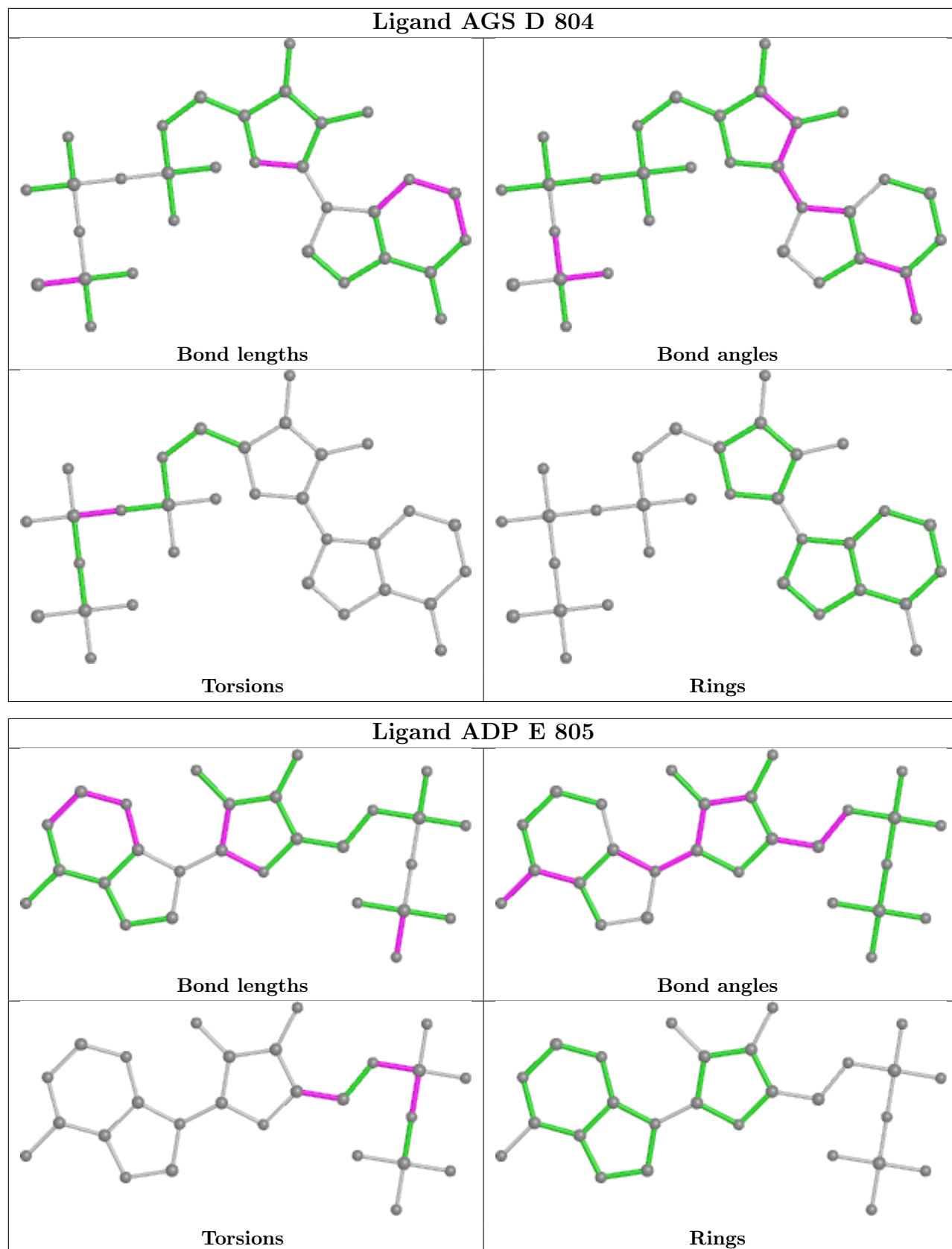


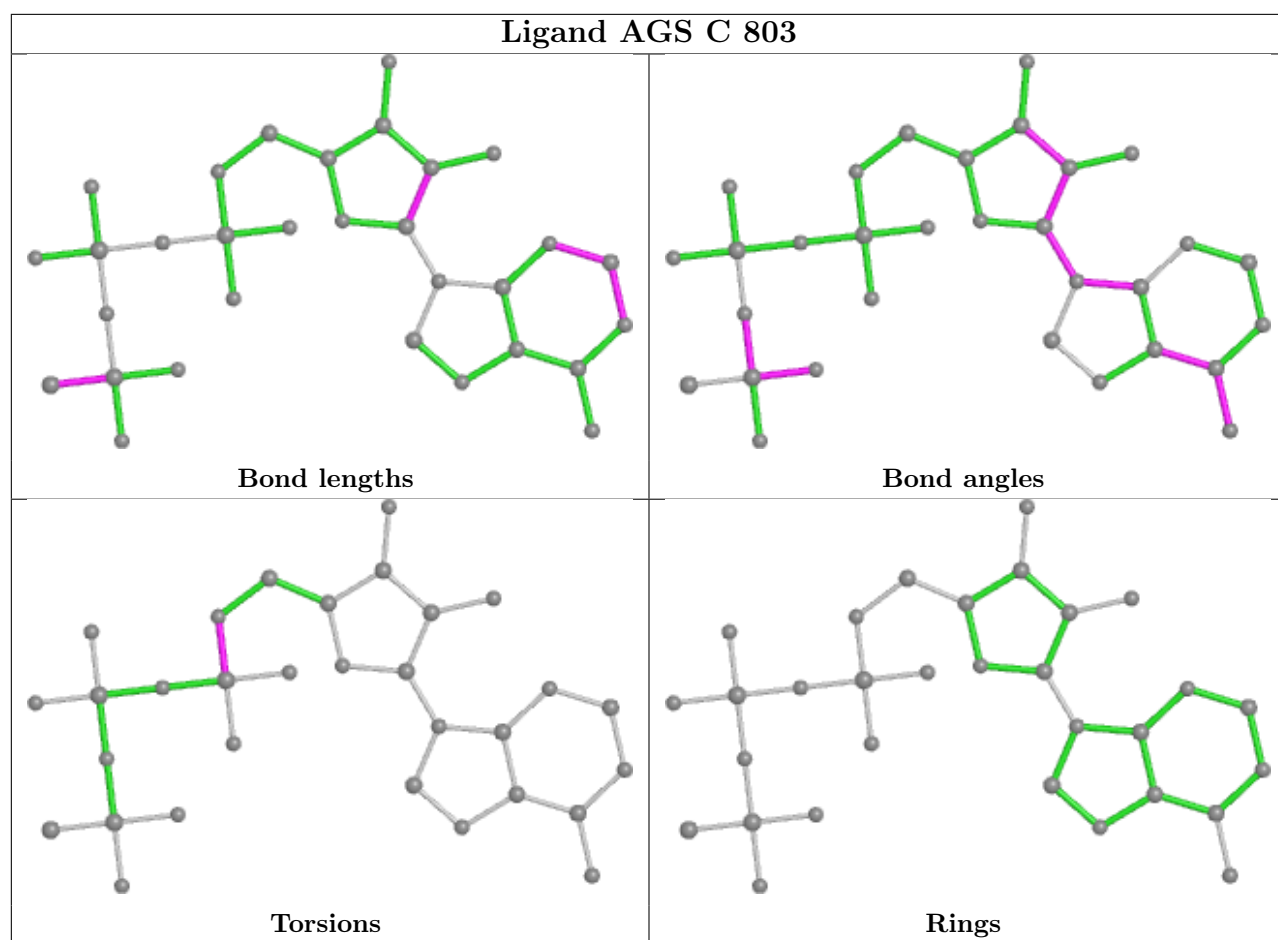
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	802	AGS	2	0
8	A	801	AGS	1	0
8	D	804	AGS	2	0
9	E	805	ADP	3	0
8	C	803	AGS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	395/516 (76%)	0.06	14 (3%) 44 38	37, 72, 130, 181	0
2	B	316/323 (97%)	-0.09	3 (0%) 84 84	32, 60, 99, 142	0
3	C	322/340 (94%)	0.05	8 (2%) 57 54	33, 76, 126, 178	0
4	D	328/353 (92%)	0.44	30 (9%) 9 6	53, 105, 167, 187	0
5	E	317/354 (89%)	0.65	39 (12%) 4 2	45, 113, 154, 181	0
6	F	252/283 (89%)	0.59	33 (13%) 3 2	48, 107, 154, 179	0
6	G	251/283 (88%)	0.09	7 (2%) 53 48	42, 77, 136, 165	0
6	H	260/283 (91%)	0.39	22 (8%) 10 7	44, 92, 148, 169	0
All	All	2441/2735 (89%)	0.26	156 (6%) 19 15	32, 85, 149, 187	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	122	ASP	11.8
6	H	158	ILE	8.2
1	A	533	HIS	6.0
6	F	193	THR	5.8
4	D	216	VAL	5.8
4	D	215	GLY	5.6
1	A	530	THR	5.5
4	D	247	ASP	5.2
6	H	125	PHE	5.1
6	G	131	LEU	4.9
5	E	217	ASP	4.9
4	D	128	ASN	4.7
6	G	130	GLU	4.7
6	F	192	GLU	4.6
5	E	213	LEU	4.4
6	H	193	THR	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	H	205	LEU	4.4
5	E	195	ASP	4.1
1	A	525	SER	4.1
6	F	130	GLU	3.9
6	H	130	GLU	3.9
5	E	255	ILE	3.8
1	A	526	THR	3.8
6	H	165	GLU	3.8
6	H	204	ASP	3.8
5	E	248	LEU	3.8
6	H	203	VAL	3.7
1	A	412	GLN	3.7
6	F	19	PHE	3.6
5	E	120	GLU	3.5
6	F	121	ILE	3.5
6	F	124	ASP	3.4
1	A	529	LYS	3.4
5	E	61	PHE	3.3
4	D	217	LEU	3.3
3	C	290	LEU	3.3
6	F	28	PHE	3.3
6	F	111	ILE	3.3
6	H	160	ILE	3.2
3	C	219	LEU	3.2
4	D	295	TRP	3.2
6	G	109	ASP	3.2
6	F	30	CYS	3.1
6	H	162	ILE	3.1
6	F	2	LEU	3.1
5	E	109	ILE	3.0
5	E	53	CYS	3.0
5	E	96	ILE	3.0
1	A	688	TYR	3.0
5	E	211	ILE	3.0
6	G	132	GLN	2.9
6	F	96	PRO	2.9
6	F	6	PHE	2.9
6	H	164	LYS	2.9
3	C	220	ASP	2.8
4	D	44	HIS	2.8
5	E	174	MET	2.8
5	E	165	ILE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	E	63	PRO	2.8
5	E	67	ARG	2.8
4	D	95	LEU	2.7
4	D	209	ASN	2.7
6	F	256	ASP	2.7
4	D	223	ILE	2.7
6	G	58	GLN	2.7
4	D	129	TYR	2.7
4	D	193	ASP	2.7
6	F	110	ARG	2.7
5	E	233	SER	2.6
3	C	222	PRO	2.6
5	E	137	CYS	2.6
1	A	407	HIS	2.6
6	H	129	GLU	2.6
6	F	24	GLN	2.6
4	D	206	GLU	2.6
4	D	214	ASP	2.6
5	E	161	TYR	2.6
3	C	12	ASN	2.6
5	E	7	LYS	2.5
4	D	242	ALA	2.5
4	D	353	LEU	2.5
5	E	18	HIS	2.5
1	A	536	ILE	2.5
5	E	16	LEU	2.5
5	E	57	LEU	2.5
5	E	246	LEU	2.5
6	F	62	CYS	2.5
6	H	159	ASN	2.5
1	A	545	LYS	2.5
6	H	106	THR	2.5
6	F	93	ASP	2.4
6	F	95	THR	2.4
5	E	22	LEU	2.4
3	C	223	ASP	2.4
5	E	58	GLU	2.4
5	E	119	MET	2.4
4	D	36	LEU	2.4
6	H	207	PHE	2.4
1	A	531	ILE	2.4
5	E	92	TYR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	322	LYS	2.4
6	F	127	LYS	2.4
4	D	293	SER	2.4
5	E	110	GLN	2.4
5	E	118	GLN	2.4
6	H	172	ASP	2.4
5	E	111	GLU	2.3
6	F	9	ALA	2.3
6	F	31	LYS	2.3
4	D	334	ASN	2.3
5	E	157	THR	2.3
2	B	184	VAL	2.3
4	D	239	SER	2.3
4	D	81	GLU	2.3
6	F	7	GLU	2.3
6	F	94	ASN	2.2
4	D	92	ILE	2.2
6	H	254	PHE	2.2
6	H	191	PRO	2.2
6	F	26	VAL	2.2
2	B	7	LEU	2.2
5	E	112	LEU	2.2
4	D	198	ILE	2.2
4	D	210	VAL	2.2
6	F	106	THR	2.2
4	D	191	ALA	2.2
6	F	103	PHE	2.2
4	D	298	ALA	2.2
6	H	171	ALA	2.2
6	F	167	ILE	2.2
6	H	157	SER	2.2
6	H	52	ILE	2.1
6	G	28	PHE	2.1
1	A	532	ASN	2.1
3	C	221	ASN	2.1
6	F	107	LYS	2.1
5	E	115	GLU	2.1
5	E	113	LEU	2.1
6	F	162	ILE	2.1
1	A	683	LEU	2.1
6	F	68	LEU	2.0
6	F	125	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	296	SER	2.0
3	C	273	ALA	2.0
5	E	114	LYS	2.0
5	E	116	VAL	2.0
4	D	273	GLU	2.0
6	G	7	GLU	2.0
5	E	240	MET	2.0
4	D	280	PHE	2.0
5	E	167	LEU	2.0
1	A	406	LYS	2.0
4	D	89	LYS	2.0
6	F	113	GLU	2.0
6	H	-12	GLY	2.0
5	E	36	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

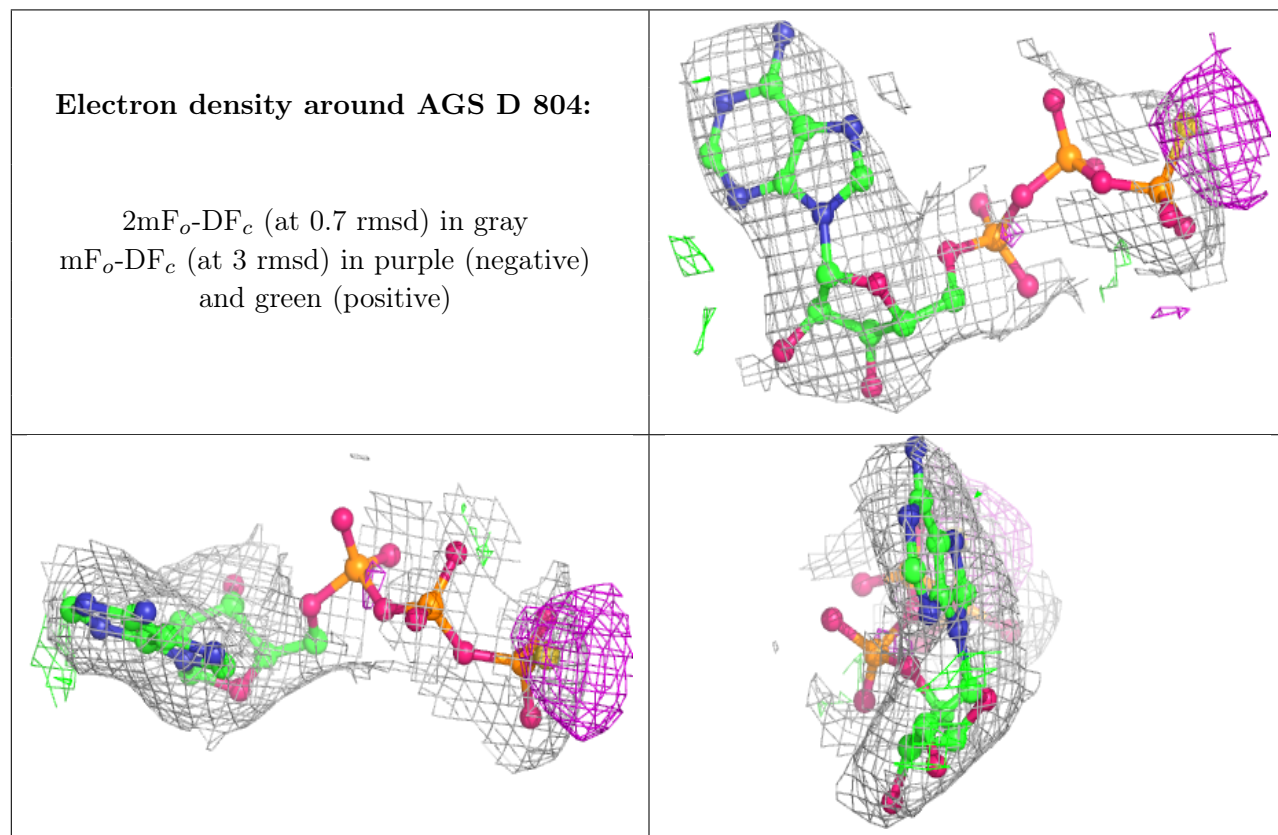
There are no monosaccharides in this entry.

## 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, 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.

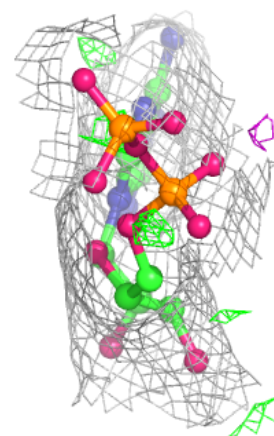
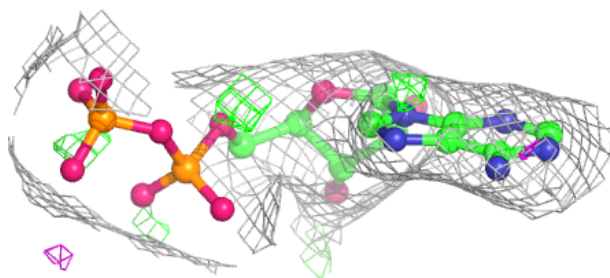
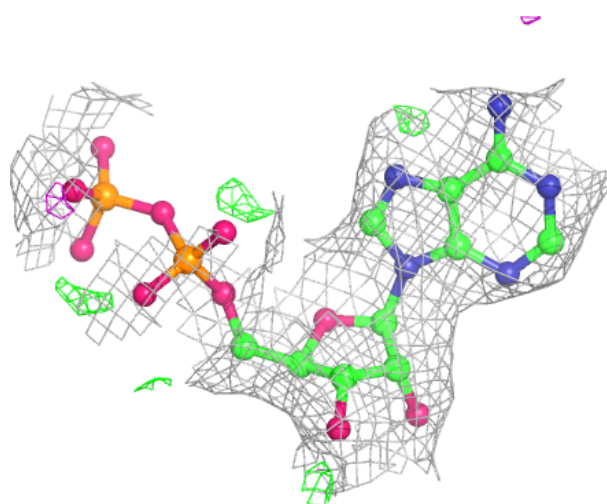
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MG	B	812	1/1	0.82	0.30	48,48,48,48	0
7	MG	A	811	1/1	0.89	0.43	56,56,56,56	0
7	MG	D	814	1/1	0.93	0.17	66,66,66,66	0
8	AGS	D	804	31/31	0.93	0.16	86,86,86,86	0
9	ADP	E	805	27/27	0.93	0.15	93,93,93,93	0
7	MG	C	813	1/1	0.94	0.30	40,40,40,40	0
8	AGS	B	802	31/31	0.94	0.18	51,51,51,51	0
8	AGS	A	801	31/31	0.96	0.17	51,51,51,51	0
8	AGS	C	803	31/31	0.96	0.18	50,50,50,50	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.



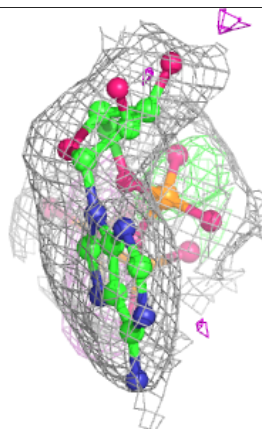
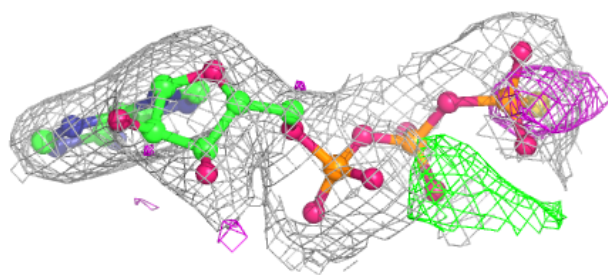
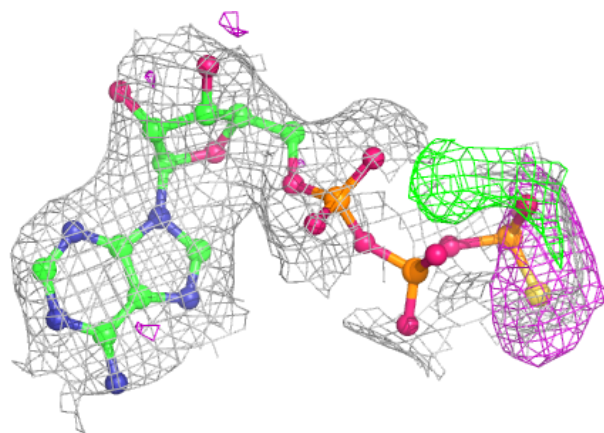
**Electron density around ADP E 805:**

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



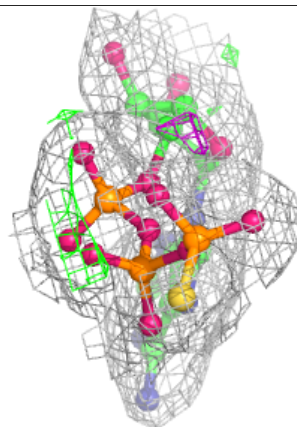
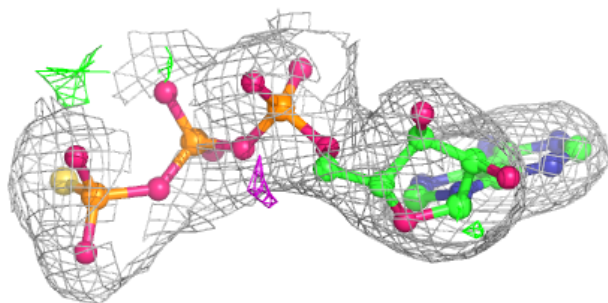
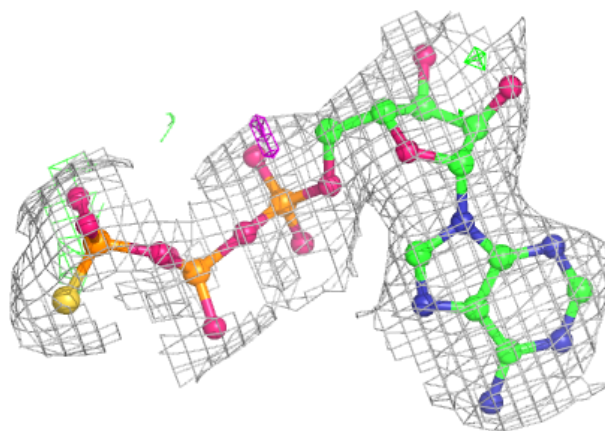
**Electron density around AGS B 802:**

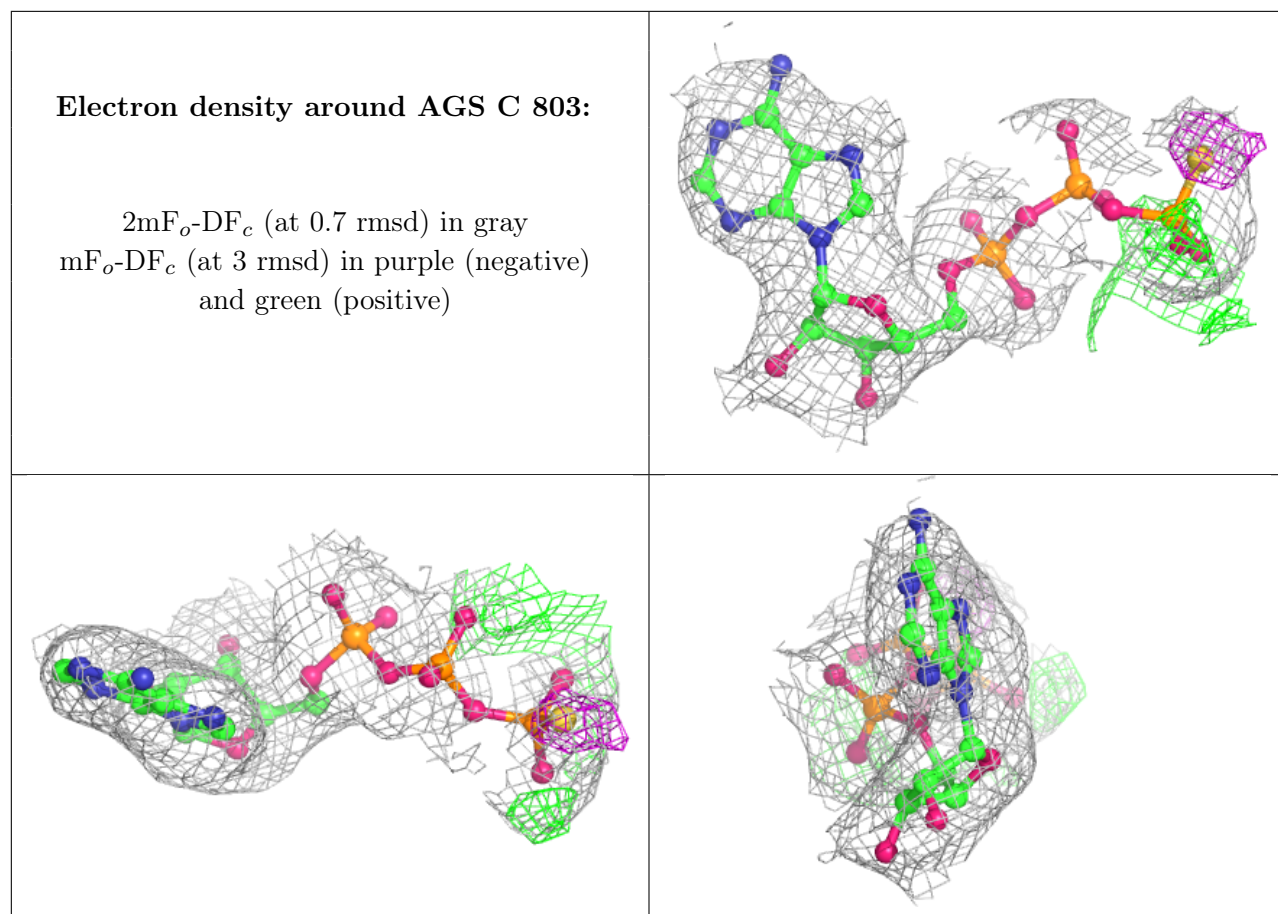
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AGS A 801:**

$2mF_o-DF_c$  (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.