Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 08:44 PM EDT

PDB ID	:	3KDO
Title	:	Crystal structure of Type III Rubisco SP6 mutant complexed with 2-CABP
Authors	:	Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on	:	2009-10-23
Resolution	:	2.36 Å(reported)

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

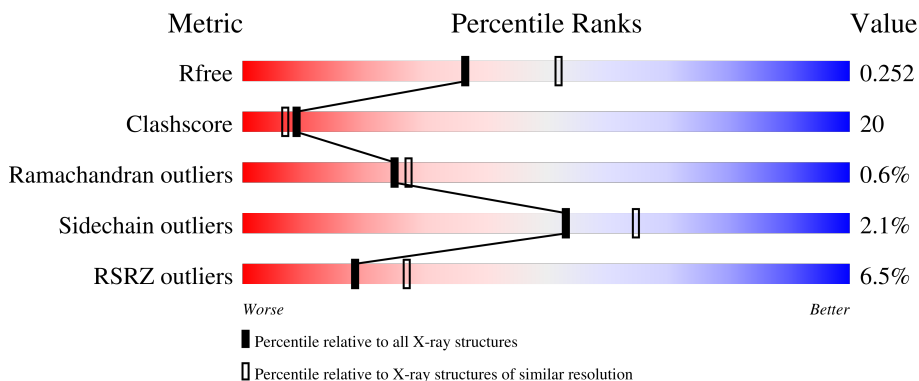|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1　Overall quality at a glance　ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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.
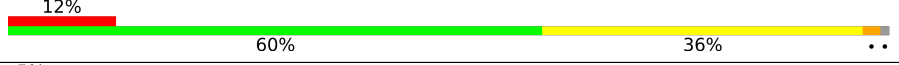
Metric	Percentile Ranks	Value
Rfree		0.252
Clashscore		20
Ramachandran outliers		0.6%
Sidechain outliers		2.1%
RSRZ outliers		6.5%

Worse　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	444	10% / 54% 42% ··
1	B	444	8% / 67% 30% ··
1	C	444	4% / 74% 23% ··
1	D	444	2% / 74% 24% ··
1	E	444	9% / 72% 27% ··

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	F	444	5% 70% 27%
1	G	444	2% 70% 27%
1	H	444	12% 60% 36%
1	I	444	5% 70% 28%
1	J	444	8% 69% 29%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 36065 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 Ribulose bisphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3341	2146	569	616	10			
1	B	438	Total	C	N	O	S	0	0	0
			3391	2179	575	627	10			
1	C	440	Total	C	N	O	S	0	0	0
			3420	2196	580	634	10			
1	D	437	Total	C	N	O	S	0	0	0
			3419	2195	582	632	10			
1	E	440	Total	C	N	O	S	0	0	0
			3418	2198	582	628	10			
1	F	437	Total	C	N	O	S	0	0	0
			3415	2195	581	629	10			
1	G	437	Total	C	N	O	S	0	0	0
			3423	2200	582	631	10			
1	H	438	Total	C	N	O	S	0	0	0
			3382	2178	574	620	10			
1	I	438	Total	C	N	O	S	0	0	0
			3410	2190	582	628	10			
1	J	438	Total	C	N	O	S	0	0	0
			3415	2195	581	629	10			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	engineered mutation	UNP O93627
A	327	ARG	LYS	engineered mutation	UNP O93627
A	328	ASP	TRP	engineered mutation	UNP O93627
A	329	ILE	ASP	engineered mutation	UNP O93627
A	330	THR	VAL	engineered mutation	UNP O93627
A	331	LEU	ILE	engineered mutation	UNP O93627
A	332	GLY	GLN	engineered mutation	UNP O93627
A	333	PHE	ASN	engineered mutation	UNP O93627
A	334	VAL	ALA	engineered mutation	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ASP	ARG	engineered mutation	UNP O93627
A	336	LEU	ILE	engineered mutation	UNP O93627
B	326	GLU	GLY	engineered mutation	UNP O93627
B	327	ARG	LYS	engineered mutation	UNP O93627
B	328	ASP	TRP	engineered mutation	UNP O93627
B	329	ILE	ASP	engineered mutation	UNP O93627
B	330	THR	VAL	engineered mutation	UNP O93627
B	331	LEU	ILE	engineered mutation	UNP O93627
B	332	GLY	GLN	engineered mutation	UNP O93627
B	333	PHE	ASN	engineered mutation	UNP O93627
B	334	VAL	ALA	engineered mutation	UNP O93627
B	335	ASP	ARG	engineered mutation	UNP O93627
B	336	LEU	ILE	engineered mutation	UNP O93627
C	326	GLU	GLY	engineered mutation	UNP O93627
C	327	ARG	LYS	engineered mutation	UNP O93627
C	328	ASP	TRP	engineered mutation	UNP O93627
C	329	ILE	ASP	engineered mutation	UNP O93627
C	330	THR	VAL	engineered mutation	UNP O93627
C	331	LEU	ILE	engineered mutation	UNP O93627
C	332	GLY	GLN	engineered mutation	UNP O93627
C	333	PHE	ASN	engineered mutation	UNP O93627
C	334	VAL	ALA	engineered mutation	UNP O93627
C	335	ASP	ARG	engineered mutation	UNP O93627
C	336	LEU	ILE	engineered mutation	UNP O93627
D	326	GLU	GLY	engineered mutation	UNP O93627
D	327	ARG	LYS	engineered mutation	UNP O93627
D	328	ASP	TRP	engineered mutation	UNP O93627
D	329	ILE	ASP	engineered mutation	UNP O93627
D	330	THR	VAL	engineered mutation	UNP O93627
D	331	LEU	ILE	engineered mutation	UNP O93627
D	332	GLY	GLN	engineered mutation	UNP O93627
D	333	PHE	ASN	engineered mutation	UNP O93627
D	334	VAL	ALA	engineered mutation	UNP O93627
D	335	ASP	ARG	engineered mutation	UNP O93627
D	336	LEU	ILE	engineered mutation	UNP O93627
E	326	GLU	GLY	engineered mutation	UNP O93627
E	327	ARG	LYS	engineered mutation	UNP O93627
E	328	ASP	TRP	engineered mutation	UNP O93627
E	329	ILE	ASP	engineered mutation	UNP O93627
E	330	THR	VAL	engineered mutation	UNP O93627
E	331	LEU	ILE	engineered mutation	UNP O93627
E	332	GLY	GLN	engineered mutation	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
E	333	PHE	ASN	engineered mutation	UNP O93627
E	334	VAL	ALA	engineered mutation	UNP O93627
E	335	ASP	ARG	engineered mutation	UNP O93627
E	336	LEU	ILE	engineered mutation	UNP O93627
F	326	GLU	GLY	engineered mutation	UNP O93627
F	327	ARG	LYS	engineered mutation	UNP O93627
F	328	ASP	TRP	engineered mutation	UNP O93627
F	329	ILE	ASP	engineered mutation	UNP O93627
F	330	THR	VAL	engineered mutation	UNP O93627
F	331	LEU	ILE	engineered mutation	UNP O93627
F	332	GLY	GLN	engineered mutation	UNP O93627
F	333	PHE	ASN	engineered mutation	UNP O93627
F	334	VAL	ALA	engineered mutation	UNP O93627
F	335	ASP	ARG	engineered mutation	UNP O93627
F	336	LEU	ILE	engineered mutation	UNP O93627
G	326	GLU	GLY	engineered mutation	UNP O93627
G	327	ARG	LYS	engineered mutation	UNP O93627
G	328	ASP	TRP	engineered mutation	UNP O93627
G	329	ILE	ASP	engineered mutation	UNP O93627
G	330	THR	VAL	engineered mutation	UNP O93627
G	331	LEU	ILE	engineered mutation	UNP O93627
G	332	GLY	GLN	engineered mutation	UNP O93627
G	333	PHE	ASN	engineered mutation	UNP O93627
G	334	VAL	ALA	engineered mutation	UNP O93627
G	335	ASP	ARG	engineered mutation	UNP O93627
G	336	LEU	ILE	engineered mutation	UNP O93627
H	326	GLU	GLY	engineered mutation	UNP O93627
H	327	ARG	LYS	engineered mutation	UNP O93627
H	328	ASP	TRP	engineered mutation	UNP O93627
H	329	ILE	ASP	engineered mutation	UNP O93627
H	330	THR	VAL	engineered mutation	UNP O93627
H	331	LEU	ILE	engineered mutation	UNP O93627
H	332	GLY	GLN	engineered mutation	UNP O93627
H	333	PHE	ASN	engineered mutation	UNP O93627
H	334	VAL	ALA	engineered mutation	UNP O93627
H	335	ASP	ARG	engineered mutation	UNP O93627
H	336	LEU	ILE	engineered mutation	UNP O93627
I	326	GLU	GLY	engineered mutation	UNP O93627
I	327	ARG	LYS	engineered mutation	UNP O93627
I	328	ASP	TRP	engineered mutation	UNP O93627
I	329	ILE	ASP	engineered mutation	UNP O93627
I	330	THR	VAL	engineered mutation	UNP O93627

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Chain	Residue	Modelled	Actual	Comment	Reference
I	331	LEU	ILE	engineered mutation	UNP O93627
I	332	GLY	GLN	engineered mutation	UNP O93627
I	333	PHE	ASN	engineered mutation	UNP O93627
I	334	VAL	ALA	engineered mutation	UNP O93627
I	335	ASP	ARG	engineered mutation	UNP O93627
I	336	LEU	ILE	engineered mutation	UNP O93627
J	326	GLU	GLY	engineered mutation	UNP O93627
J	327	ARG	LYS	engineered mutation	UNP O93627
J	328	ASP	TRP	engineered mutation	UNP O93627
J	329	ILE	ASP	engineered mutation	UNP O93627
J	330	THR	VAL	engineered mutation	UNP O93627
J	331	LEU	ILE	engineered mutation	UNP O93627
J	332	GLY	GLN	engineered mutation	UNP O93627
J	333	PHE	ASN	engineered mutation	UNP O93627
J	334	VAL	ALA	engineered mutation	UNP O93627
J	335	ASP	ARG	engineered mutation	UNP O93627
J	336	LEU	ILE	engineered mutation	UNP O93627

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).
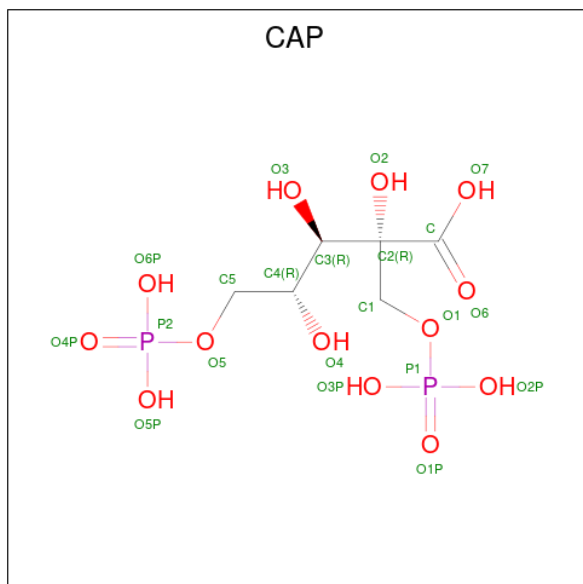
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			21	6	13	2		
2	B	1	Total	C	O	P	0	0
			21	6	13	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 21	C 6	O 13	P 2	0	0
2	D	1	Total 21	C 6	O 13	P 2	0	0
2	E	1	Total 21	C 6	O 13	P 2	0	0
2	F	1	Total 21	C 6	O 13	P 2	0	0
2	G	1	Total 21	C 6	O 13	P 2	0	0
2	H	1	Total 21	C 6	O 13	P 2	0	0
2	I	1	Total 21	C 6	O 13	P 2	0	0
2	J	1	Total 21	C 6	O 13	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0
3	I	1	Total 1	Mg 1	0	0
3	J	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total 97	O 97	0	0
4	B	175	Total 175	O 175	0	0
4	C	226	Total 226	O 226	0	0
4	D	239	Total 239	O 239	0	0
4	E	197	Total 197	O 197	0	0
4	F	179	Total 179	O 179	0	0
4	G	174	Total 174	O 174	0	0
4	H	123	Total 123	O 123	0	0
4	I	192	Total 192	O 192	0	0
4	J	209	Total 209	O 209	0	0

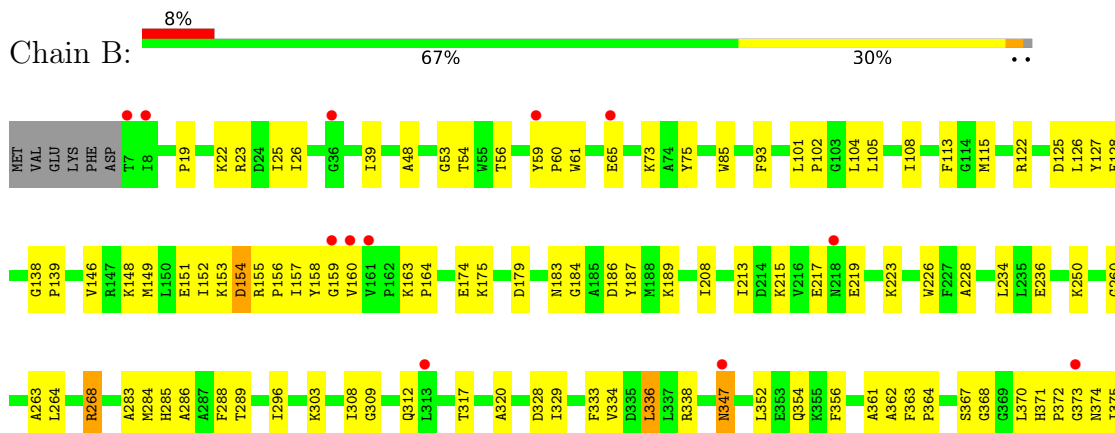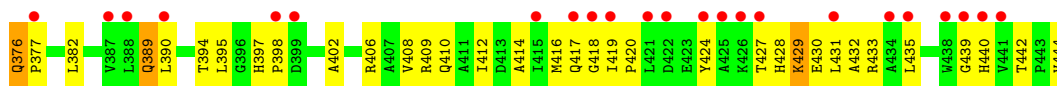# 3 Residue-property plots ⓘ

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.

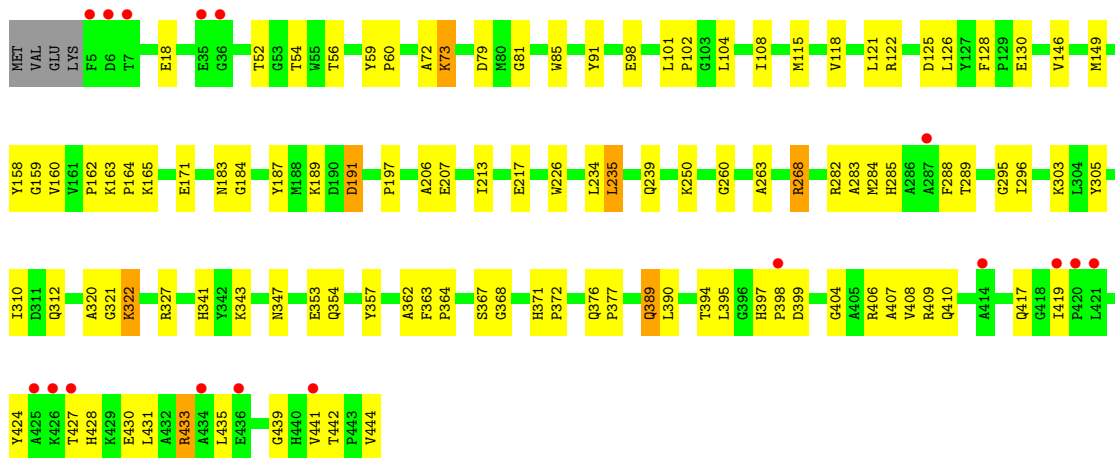- Molecule 1: Ribulose bisphosphate carboxylase
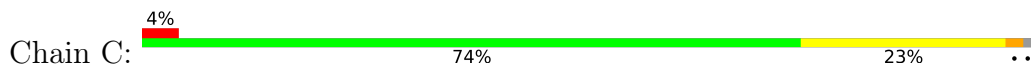

- Molecule 1: Ribulose bisphosphate carboxylase

• Molecule 1: Ribulose bisphosphate carboxylase

Chain C:

• Molecule 1: Ribulose bisphosphate carboxylase

Chain D:

• Molecule 1: Ribulose bisphosphate carboxylase

Chain E:

The residue sequence blocks for chains appear here.

- Molecule 1: Ribulose bisphosphate carboxylase

Chain F:

- Molecule 1: Ribulose bisphosphate carboxylase

Chain G:

- Molecule 1: Ribulose bisphosphate carboxylase
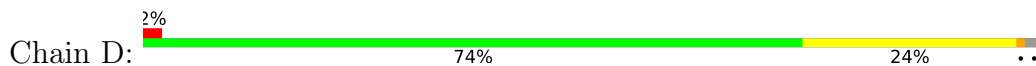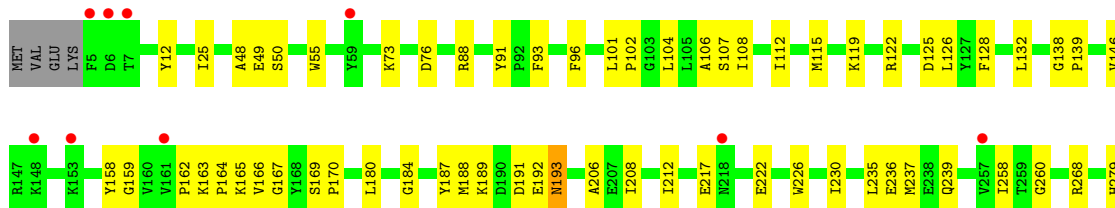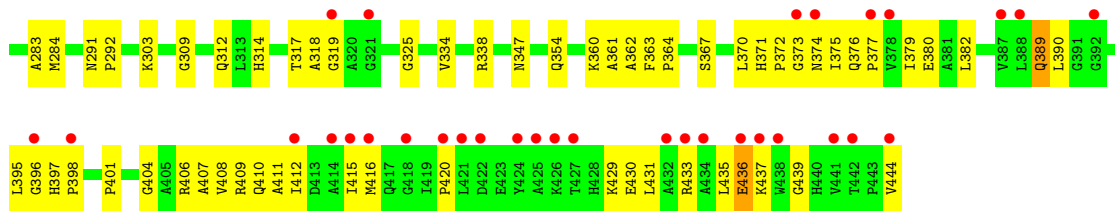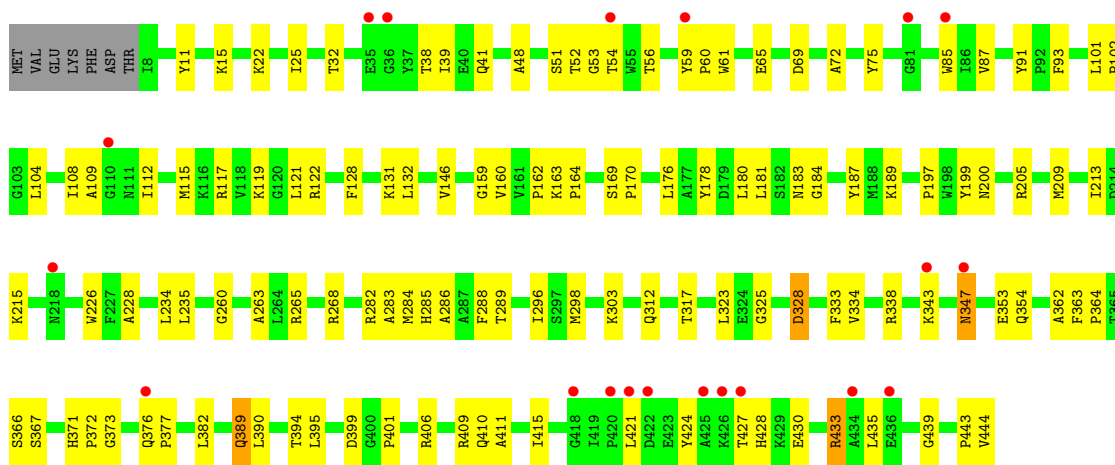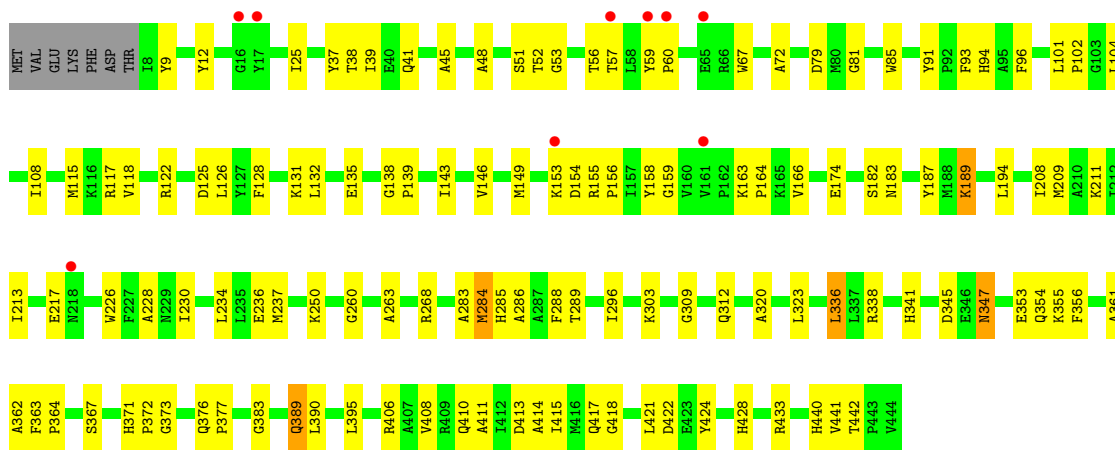
Chain H:

• Molecule 1: Ribulose bisphosphate carboxylase

Chain I:

• Molecule 1: Ribulose bisphosphate carboxylase

Chain J:
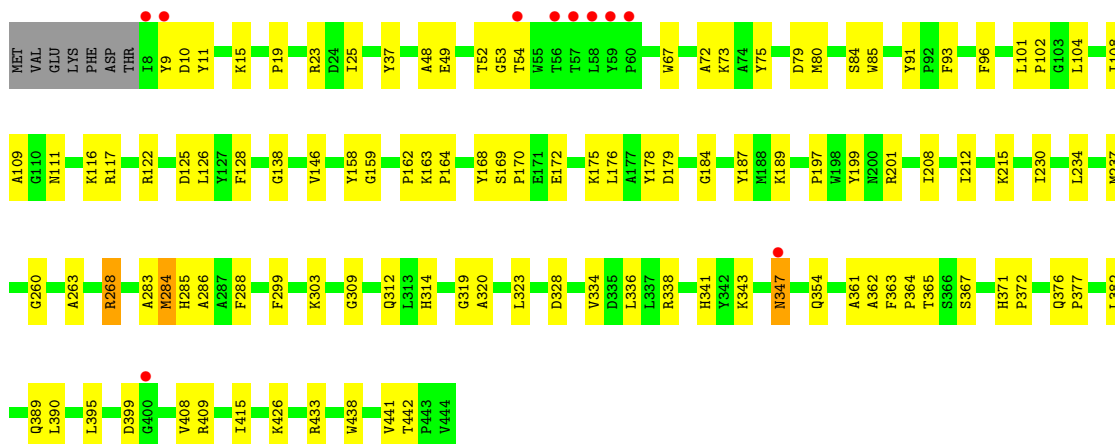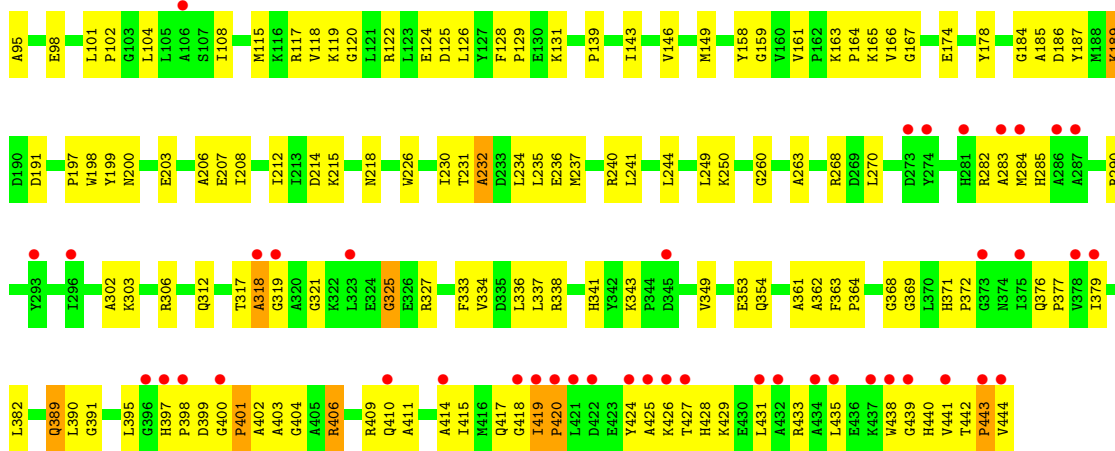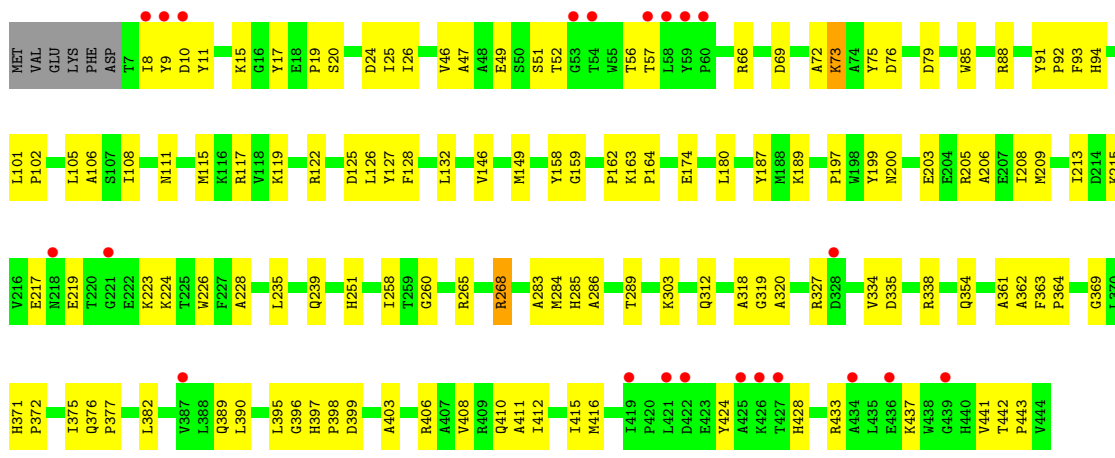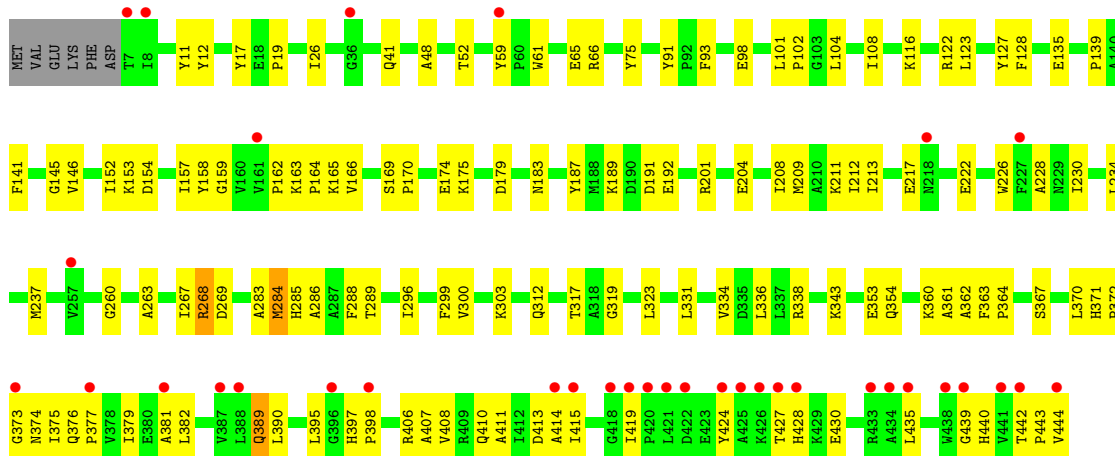
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.48Å 246.57Å 134.83Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	38.46 – 2.36 38.46 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.46-2.36) 99.4 (38.46-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.219 , 0.264 0.213 , 0.252	Depositor DCC
R_{free} test set	12530 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.7	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36065	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, CAP, KCX

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	0.21	0/3415	0.36	0/4642
1	B	0.22	0/3467	0.37	0/4712
1	C	0.22	0/3496	0.38	0/4750
1	D	0.22	0/3494	0.39	0/4739
1	E	0.22	0/3494	0.38	0/4744
1	F	0.22	0/3491	0.38	0/4738
1	G	0.21	0/3499	0.38	0/4747
1	H	0.21	0/3458	0.37	0/4700
1	I	0.22	0/3485	0.38	0/4730
1	J	0.22	0/3491	0.39	0/4738
All	All	0.22	0/34790	0.38	0/47240

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	3341	0	3185	218	0
1	B	3391	0	3252	153	0
1	C	3420	0	3289	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3419	0	3317	102	0
1	E	3418	0	3303	121	0
1	F	3415	0	3313	126	0
1	G	3423	0	3328	129	0
1	H	3382	0	3257	207	0
1	I	3410	0	3301	112	0
1	J	3415	0	3310	143	0
2	A	21	0	8	0	0
2	B	21	0	7	1	0
2	C	21	0	9	1	0
2	D	21	0	8	0	0
2	E	21	0	8	2	0
2	F	21	0	8	0	0
2	G	21	0	8	1	0
2	H	21	0	8	0	0
2	I	21	0	8	0	0
2	J	21	0	7	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	97	0	0	12	0
4	B	175	0	0	10	0
4	C	226	0	0	7	0
4	D	239	0	0	4	0
4	E	197	0	0	9	0
4	F	179	0	0	9	0
4	G	174	0	0	8	0
4	H	123	0	0	6	0
4	I	192	0	0	7	0
4	J	209	0	0	15	0
All	All	36065	0	32934	1362	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 20.

All (1362) 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:H:397:HIS:ND1	1:H:398:PRO:HD2	1.29	1.44
1:H:397:HIS:CG	1:H:398:PRO:HD2	1.61	1.32
1:A:149:MET:HE3	1:A:250:LYS:CB	1.65	1.26
1:H:397:HIS:ND1	1:H:398:PRO:CD	2.06	1.18
1:I:72:ALA:O	1:I:73:LYS:HD2	1.43	1.17
1:H:282:ARG:HD2	1:H:285:HIS:CD2	1.81	1.15
1:H:397:HIS:CE1	1:H:398:PRO:HD2	1.81	1.15
1:A:108:ILE:CD1	1:A:126:LEU:HD11	1.80	1.11
1:F:433:ARG:HG2	1:F:433:ARG:HH11	1.01	1.10
1:E:91:TYR:CZ	1:E:108:ILE:HD11	1.88	1.08
1:B:317:THR:HG21	1:B:370:LEU:HD11	1.35	1.08
1:B:149:MET:HE3	1:B:250:LYS:HB2	1.36	1.07
1:A:108:ILE:HD11	1:A:126:LEU:HD11	1.36	1.07
1:A:149:MET:HE2	1:A:250:LYS:HD2	1.36	1.07
1:C:433:ARG:HG2	1:C:433:ARG:HH11	0.98	1.06
1:A:149:MET:HE3	1:A:250:LYS:HB3	1.04	1.04
1:J:343:LYS:HE2	1:J:353:GLU:OE2	1.57	1.03
1:E:91:TYR:CE2	1:E:108:ILE:HD11	1.94	1.03
1:C:433:ARG:HH11	1:C:433:ARG:CG	1.72	1.03
1:A:108:ILE:HD12	1:A:126:LEU:HD21	1.40	1.03
1:F:433:ARG:HH11	1:F:433:ARG:CG	1.72	1.03
1:A:444:VAL:O	1:H:117:ARG:HD2	1.60	1.02
1:A:282:ARG:HD2	1:A:285:HIS:CD2	1.96	1.01
1:I:159:GLY:HA3	1:I:187:TYR:CZ	1.96	1.00
1:H:149:MET:HE1	1:H:250:LYS:HB2	1.41	1.00
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.44	0.99
1:C:397:HIS:CG	1:C:398:PRO:HD2	1.99	0.98
1:E:319:GLY:HA2	4:E:496:HOH:O	1.61	0.97
1:A:86:ILE:CD1	1:A:349:VAL:HG23	1.95	0.97
1:F:131:LYS:HE2	4:F:1817:HOH:O	1.65	0.95
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.00	0.95
1:H:302:ALA:HB1	1:H:337:LEU:HD11	1.48	0.95
1:C:163:LYS:H	1:C:395:LEU:CD2	1.78	0.95
1:A:149:MET:CE	1:A:250:LYS:HB3	1.96	0.95
1:H:397:HIS:CG	1:H:398:PRO:CD	2.47	0.95
1:E:193:ASN:H	1:E:193:ASN:HD22	1.13	0.93
1:A:366:SER:HA	4:A:1262:HOH:O	1.68	0.92
1:C:433:ARG:HG2	1:C:433:ARG:NH1	1.79	0.91
1:I:209:MET:O	1:I:213:ILE:HG13	1.69	0.91
1:H:159:GLY:HA3	1:H:187:TYR:CZ	2.06	0.91
1:H:424:TYR:O	1:H:427:THR:HG22	1.71	0.91
1:E:91:TYR:CZ	1:E:108:ILE:CD1	2.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:ARG:HG2	1:F:433:ARG:NH1	1.82	0.91
1:H:334:VAL:CG1	1:H:338:ARG:NH2	2.33	0.90
1:G:347:ASN:H	1:G:347:ASN:ND2	1.70	0.90
1:G:38:THR:HG23	1:G:41:GLN:OE1	1.72	0.90
1:D:116:LYS:HE2	4:J:1843:HOH:O	1.69	0.90
1:B:371:HIS:O	1:B:375:ILE:HG23	1.72	0.89
1:H:334:VAL:HG11	1:H:338:ARG:NH2	1.87	0.89
1:A:86:ILE:CD1	1:A:349:VAL:CG2	2.50	0.89
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.08	0.89
1:A:86:ILE:HD13	1:A:349:VAL:HG23	1.53	0.88
1:B:183:ASN:ND2	1:B:402:ALA:HB1	1.89	0.88
1:C:149:MET:HE1	1:C:250:LYS:HB2	1.53	0.88
1:B:317:THR:CG2	1:B:370:LEU:HD11	2.04	0.87
1:G:347:ASN:H	1:G:347:ASN:HD22	0.88	0.87
1:B:303:LYS:HZ3	1:B:354:GLN:HE21	1.23	0.87
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.10	0.86
1:H:397:HIS:CE1	1:H:398:PRO:CD	2.56	0.86
1:A:149:MET:CE	1:A:250:LYS:CB	2.52	0.86
1:E:180:LEU:HD12	1:E:188:MET:CE	2.04	0.86
1:C:399:ASP:OD2	1:C:433:ARG:HD3	1.75	0.86
1:B:149:MET:HE2	1:B:250:LYS:HD2	1.56	0.85
1:A:108:ILE:CD1	1:A:126:LEU:CD1	2.55	0.85
1:A:108:ILE:CD1	1:A:126:LEU:HD21	2.06	0.85
1:F:32:THR:HG21	1:F:119:LYS:HE2	1.58	0.85
1:A:14:ASP:CB	4:A:2019:HOH:O	2.25	0.85
1:H:149:MET:HE1	1:H:250:LYS:CB	2.06	0.85
1:J:443:PRO:O	1:J:444:VAL:HG23	1.76	0.85
1:B:149:MET:HE3	1:B:250:LYS:CB	2.07	0.85
1:A:381:ALA:O	1:A:382:LEU:HD12	1.76	0.85
1:J:353:GLU:HB3	4:J:1285:HOH:O	1.76	0.85
1:F:347:ASN:H	1:F:347:ASN:HD22	1.25	0.85
1:J:413:ASP:HA	4:J:1924:HOH:O	1.77	0.84
1:A:76:ASP:OD1	1:A:77:PHE:N	2.10	0.84
1:A:438:TRP:O	1:A:441:VAL:HG12	1.76	0.84
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.12	0.84
1:F:159:GLY:HA3	1:F:187:TYR:CZ	2.13	0.84
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.13	0.84
1:B:373:GLY:O	1:B:440:HIS:HA	1.77	0.84
1:J:397:HIS:CG	1:J:398:PRO:HD2	2.13	0.84
1:H:32:THR:HG22	1:H:119:LYS:HB3	1.59	0.83
1:G:411:ALA:O	1:G:415:ILE:HG13	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:PHE:O	1:H:337:LEU:HD13	1.79	0.83
1:B:371:HIS:CE1	1:B:373:GLY:C	2.52	0.83
1:C:389:GLN:C	1:C:390:LEU:HD12	1.98	0.83
1:A:444:VAL:O	1:H:117:ARG:CD	2.27	0.83
1:F:32:THR:CG2	1:F:119:LYS:HE2	2.08	0.82
1:I:15:LYS:HG3	4:I:468:HOH:O	1.79	0.82
1:A:108:ILE:HD12	1:A:126:LEU:HD11	1.60	0.82
1:A:14:ASP:HB2	4:A:2019:HOH:O	1.78	0.82
1:C:347:ASN:HB3	4:C:1690:HOH:O	1.80	0.82
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.14	0.82
1:J:303:LYS:NZ	1:J:354:GLN:HE21	1.78	0.81
1:G:153:LYS:HG2	1:G:154:ASP:OD1	1.80	0.81
1:H:419:ILE:HD12	1:H:419:ILE:N	1.94	0.81
1:I:376:GLN:HB3	1:I:377:PRO:HD3	1.61	0.81
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.16	0.81
1:G:347:ASN:HD22	1:G:347:ASN:N	1.68	0.81
1:F:376:GLN:HB3	1:F:377:PRO:HD3	1.62	0.80
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.16	0.80
1:C:397:HIS:CD2	1:C:398:PRO:HD2	2.16	0.80
1:H:163:LYS:HA	1:H:164:PRO:O	1.82	0.80
1:J:153:LYS:CE	1:J:154:ASP:OD1	2.29	0.80
1:J:427:THR:HB	4:J:2029:HOH:O	1.81	0.80
1:A:149:MET:HE3	1:A:250:LYS:HB2	1.64	0.79
1:H:417:GLN:CB	1:H:419:ILE:HD13	2.13	0.79
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.18	0.79
1:C:149:MET:HE1	1:C:250:LYS:CB	2.13	0.79
1:G:128:PHE:H	1:G:354:GLN:HE22	1.27	0.79
1:H:149:MET:HE3	1:H:250:LYS:CD	2.11	0.79
1:H:406:ARG:O	1:H:410:GLN:HG3	1.83	0.79
1:J:165:LYS:HB3	1:J:191:ASP:OD1	1.82	0.79
1:F:427:THR:HG22	4:F:494:HOH:O	1.82	0.79
1:A:149:MET:HE2	1:A:250:LYS:CD	2.11	0.79
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.18	0.79
1:F:163:LYS:H	1:F:395:LEU:HD13	1.48	0.78
1:B:317:THR:HG21	1:B:370:LEU:CD1	2.13	0.78
1:H:397:HIS:CE1	1:H:398:PRO:HG2	2.19	0.78
1:D:37:TYR:OH	1:J:444:VAL:HG12	1.84	0.77
1:A:76:ASP:C	1:A:77:PHE:CD2	2.58	0.77
1:I:128:PHE:H	1:I:354:GLN:HE22	1.31	0.77
1:B:371:HIS:ND1	1:B:373:GLY:N	2.33	0.77
1:H:397:HIS:CD2	1:H:398:PRO:HD2	2.18	0.77

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ASP:HB2	1:G:85:TRP:CZ3	2.20	0.77
1:A:149:MET:CE	1:A:250:LYS:HD2	2.14	0.77
1:A:376:GLN:HA	1:A:415:ILE:HD13	1.65	0.77
1:C:419:ILE:HD12	1:C:419:ILE:H	1.50	0.77
1:J:331:LEU:HD13	1:J:381:ALA:O	1.85	0.77
1:C:149:MET:HE3	1:C:250:LYS:HD2	1.65	0.76
1:B:60:PRO:HA	4:B:2001:HOH:O	1.84	0.76
1:E:180:LEU:HD12	1:E:188:MET:HE2	1.65	0.76
1:A:108:ILE:HD12	1:A:126:LEU:CD2	2.14	0.76
1:E:159:GLY:HA3	1:E:187:TYR:CZ	2.21	0.76
1:A:334:VAL:CG1	1:A:338:ARG:NH2	2.48	0.76
1:C:419:ILE:HD12	1:C:419:ILE:N	2.01	0.76
1:A:424:TYR:CZ	1:A:428:HIS:CE1	2.74	0.75
1:J:443:PRO:O	1:J:444:VAL:CG2	2.34	0.75
1:D:176:LEU:HD11	1:D:395:LEU:HD21	1.67	0.75
1:H:371:HIS:HB2	1:H:372:PRO:CD	2.16	0.75
1:J:303:LYS:HZ3	1:J:354:GLN:HE21	1.34	0.75
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.21	0.75
1:B:149:MET:HE2	1:B:250:LYS:CD	2.16	0.75
1:A:334:VAL:HG21	1:A:382:LEU:HG	1.67	0.75
1:A:14:ASP:CG	4:A:2019:HOH:O	2.24	0.75
1:B:371:HIS:HE1	1:B:373:GLY:C	1.90	0.75
1:C:149:MET:HE3	1:C:250:LYS:CD	2.17	0.75
1:H:334:VAL:HG12	1:H:338:ARG:HH21	1.52	0.75
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.35	0.74
1:B:371:HIS:CE1	1:B:373:GLY:CA	2.70	0.74
1:J:397:HIS:ND1	1:J:398:PRO:HD2	2.03	0.74
1:A:406:ARG:O	1:A:410:GLN:HG3	1.87	0.74
1:G:163:LYS:H	1:G:395:LEU:HD22	1.52	0.74
1:A:108:ILE:HD11	1:A:126:LEU:CD1	2.14	0.74
1:H:125:ASP:OD1	1:H:126:LEU:N	2.21	0.74
1:H:334:VAL:CG1	1:H:338:ARG:HH21	1.98	0.74
1:A:268:ARG:HD3	1:A:268:ARG:C	2.08	0.74
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.23	0.73
1:H:410:GLN:HE21	1:H:431:LEU:HB2	1.52	0.73
1:F:376:GLN:CB	1:F:377:PRO:HD3	2.18	0.73
1:A:159:GLY:HA3	1:A:187:TYR:CE2	2.23	0.73
1:E:163:LYS:H	1:E:395:LEU:CD1	2.02	0.73
1:C:163:LYS:H	1:C:395:LEU:HD22	1.51	0.73
1:B:149:MET:CE	1:B:250:LYS:HD2	2.17	0.73
1:H:163:LYS:HA	1:H:164:PRO:C	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:H	1:D:395:LEU:HD13	1.54	0.73
1:C:263:ALA:HB2	1:F:263:ALA:HB2	1.71	0.73
1:F:25:ILE:HD11	1:F:132:LEU:HD21	1.69	0.73
1:H:282:ARG:NH1	1:H:285:HIS:CE1	2.56	0.73
1:H:410:GLN:HE22	1:H:431:LEU:H	1.35	0.73
1:B:429:LYS:O	1:B:432:ALA:N	2.22	0.72
1:G:104:LEU:HD23	1:G:104:LEU:O	1.89	0.72
1:A:424:TYR:CE2	1:A:428:HIS:CE1	2.77	0.72
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.17	0.72
1:D:117:ARG:NH2	1:J:444:VAL:O	2.22	0.72
1:D:108:ILE:HD12	1:D:108:ILE:C	2.10	0.72
1:F:347:ASN:HD22	1:F:347:ASN:N	1.87	0.72
1:H:208:ILE:O	1:H:212:ILE:HG13	1.90	0.72
1:F:399:ASP:OD2	1:F:433:ARG:HD3	1.89	0.72
1:A:125:ASP:OD1	1:A:126:LEU:N	2.23	0.72
1:A:334:VAL:HG11	1:A:338:ARG:NH2	2.03	0.72
1:B:373:GLY:HA3	1:B:439:GLY:O	1.89	0.72
1:G:389:GLN:C	1:G:390:LEU:HD12	2.09	0.72
1:H:128:PHE:H	1:H:354:GLN:HE22	1.37	0.72
1:H:400:GLY:O	1:H:403:ALA:HB3	1.90	0.71
1:J:153:LYS:HE2	1:J:154:ASP:OD1	1.89	0.71
1:H:425:ALA:C	1:H:427:THR:H	1.92	0.71
1:D:268:ARG:C	1:D:268:ARG:HD3	2.11	0.71
1:G:376:GLN:HB3	1:G:377:PRO:HD3	1.71	0.71
1:G:104:LEU:HD23	1:G:104:LEU:C	2.11	0.71
1:B:419:ILE:N	1:B:419:ILE:HD12	2.06	0.71
1:H:349:VAL:HG12	1:H:349:VAL:O	1.90	0.70
1:H:397:HIS:CE1	1:H:398:PRO:CG	2.73	0.70
1:H:318:ALA:HA	1:H:325:GLY:O	1.91	0.70
1:H:371:HIS:HB2	1:H:372:PRO:HD2	1.73	0.70
1:B:397:HIS:ND1	1:B:398:PRO:HD2	2.06	0.70
1:C:128:PHE:H	1:C:354:GLN:HE22	1.40	0.70
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.25	0.70
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.25	0.70
1:I:319:GLY:HA2	4:I:459:HOH:O	1.90	0.70
1:J:268:ARG:HD3	1:J:268:ARG:C	2.10	0.70
1:J:362:ALA:O	1:J:364:PRO:HD3	1.91	0.70
1:C:79:ASP:HB2	1:C:85:TRP:CZ3	2.26	0.70
1:H:318:ALA:HB1	1:H:327:ARG:HA	1.73	0.70
1:B:236:GLU:N	1:B:236:GLU:OE1	2.24	0.70
1:J:370:LEU:HA	1:J:374:ASN:HD21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.26	0.70
1:I:285:HIS:HD2	1:I:289:THR:OG1	1.75	0.70
1:G:79:ASP:HB2	1:G:85:TRP:CH2	2.27	0.69
1:A:367:SER:N	4:A:1262:HOH:O	2.23	0.69
1:H:419:ILE:HD12	1:H:419:ILE:H	1.55	0.69
1:I:406:ARG:O	1:I:410:GLN:HG3	1.92	0.69
1:J:153:LYS:HE3	1:J:154:ASP:OD1	1.91	0.69
1:I:72:ALA:C	1:I:73:LYS:HD2	2.11	0.69
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.28	0.69
1:B:303:LYS:NZ	1:B:354:GLN:HE21	1.90	0.69
1:C:417:GLN:CB	1:C:419:ILE:HD13	2.21	0.69
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.28	0.69
1:B:389:GLN:C	1:B:390:LEU:HD12	2.13	0.69
1:J:411:ALA:O	1:J:415:ILE:HG13	1.93	0.68
1:A:376:GLN:HB3	1:A:377:PRO:HD3	1.75	0.68
1:J:98:GLU:HG3	1:J:135:GLU:OE2	1.93	0.68
1:A:260:GLY:HA3	1:H:260:GLY:HA3	1.75	0.68
1:C:162:PRO:HA	1:C:395:LEU:HD21	1.74	0.68
1:F:54:THR:HG23	1:F:56:THR:O	1.94	0.68
1:I:376:GLN:HA	1:I:415:ILE:HD13	1.74	0.68
1:I:268:ARG:HD3	1:I:268:ARG:C	2.13	0.68
1:F:362:ALA:O	1:F:364:PRO:HD3	1.93	0.68
1:H:178:TYR:CE1	1:H:215:LYS:HE3	2.29	0.68
1:F:38:THR:OG1	1:F:41:GLN:HG3	1.92	0.68
1:I:163:LYS:H	1:I:395:LEU:HD12	1.58	0.68
1:J:104:LEU:C	1:J:104:LEU:HD23	2.13	0.68
1:A:444:VAL:O	1:H:117:ARG:HB2	1.93	0.68
1:B:54:THR:HG23	1:B:56:THR:O	1.93	0.68
1:B:183:ASN:HD21	1:B:402:ALA:HB1	1.56	0.68
1:B:268:ARG:HD3	1:B:268:ARG:C	2.15	0.68
1:A:139:PRO:HD3	1:A:306:ARG:O	1.94	0.68
1:B:125:ASP:OD1	1:B:126:LEU:N	2.27	0.68
1:H:391:GLY:O	1:H:395:LEU:HD23	1.94	0.68
1:H:397:HIS:CD2	1:H:404:GLY:HA2	2.29	0.68
1:E:435:LEU:O	1:E:439:GLY:N	2.25	0.67
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.29	0.67
1:H:427:THR:HG23	1:H:428:HIS:ND1	2.09	0.67
1:A:128:PHE:H	1:A:354:GLN:HE22	1.41	0.67
1:A:175:LYS:CG	4:A:1729:HOH:O	2.43	0.67
1:C:376:GLN:HB3	1:C:377:PRO:HD3	1.75	0.67
1:E:279:HIS:NE2	1:E:314:HIS:HE1	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:407:ALA:O	1:J:410:GLN:HB2	1.94	0.67
1:H:425:ALA:O	1:H:427:THR:N	2.28	0.67
1:B:424:TYR:HE1	4:B:963:HOH:O	1.77	0.67
1:E:371:HIS:ND1	1:E:373:GLY:N	2.42	0.67
1:F:159:GLY:HA3	1:F:187:TYR:CE1	2.29	0.67
1:G:376:GLN:CB	1:G:377:PRO:HD3	2.25	0.67
1:B:328:ASP:CB	4:B:1794:HOH:O	2.43	0.67
1:E:389:GLN:C	1:E:390:LEU:HD12	2.15	0.67
1:H:282:ARG:HD2	1:H:285:HIS:NE2	2.10	0.67
1:I:25:ILE:HD11	1:I:132:LEU:HD21	1.75	0.67
1:A:413:ASP:O	1:A:417:GLN:HG3	1.95	0.66
1:B:60:PRO:CA	4:B:2001:HOH:O	2.42	0.66
1:A:334:VAL:CG1	1:A:338:ARG:CZ	2.74	0.66
1:H:376:GLN:HA	1:H:415:ILE:HD13	1.76	0.66
1:B:334:VAL:HG21	1:B:382:LEU:HD22	1.78	0.66
1:C:283:ALA:O	1:C:284:MET:HB3	1.95	0.66
1:J:334:VAL:HG21	1:J:382:LEU:HD22	1.78	0.66
1:B:424:TYR:CE1	4:B:963:HOH:O	2.49	0.66
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.30	0.66
1:A:66:ARG:HD2	1:H:167:GLY:O	1.96	0.65
1:B:444:VAL:O	1:G:117:ARG:NH2	2.22	0.65
1:I:72:ALA:O	1:I:73:LYS:CD	2.32	0.65
1:I:162:PRO:HA	1:I:395:LEU:HD11	1.78	0.65
1:I:163:LYS:H	1:I:395:LEU:CD1	2.09	0.65
1:I:319:GLY:CA	4:I:459:HOH:O	2.43	0.65
1:A:175:LYS:HE3	1:A:179:ASP:OD2	1.96	0.65
1:H:104:LEU:C	1:H:104:LEU:HD23	2.16	0.65
1:I:215:LYS:HE2	1:I:219:GLU:OE2	1.97	0.65
1:E:371:HIS:CE1	1:E:373:GLY:CA	2.79	0.65
1:F:54:THR:HA	4:F:492:HOH:O	1.96	0.65
1:A:122:ARG:HD3	1:A:292:PRO:O	1.95	0.65
1:H:283:ALA:O	1:H:284:MET:HB3	1.96	0.65
1:I:371:HIS:HB2	1:I:372:PRO:HD2	1.79	0.65
1:A:283:ALA:O	1:A:284:MET:HB3	1.96	0.65
1:C:59:TYR:CD1	1:C:60:PRO:HD2	2.32	0.65
1:J:343:LYS:HG2	1:J:353:GLU:HG3	1.78	0.65
1:C:320:ALA:O	1:C:442:THR:HG23	1.97	0.65
1:F:430:GLU:OE1	1:F:430:GLU:N	2.25	0.65
1:I:389:GLN:C	1:I:390:LEU:HD12	2.15	0.65
1:E:128:PHE:H	1:E:354:GLN:HE22	1.45	0.64
1:H:334:VAL:HG12	1:H:338:ARG:NH2	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396:GLY:O	1:I:437:LYS:NZ	2.24	0.64
1:H:54:THR:HG23	1:H:56:THR:H	1.61	0.64
1:H:418:GLY:O	1:H:420:PRO:HD3	1.97	0.64
1:B:215:LYS:HE2	1:B:219:GLU:OE2	1.97	0.64
1:H:108:ILE:HG22	1:H:108:ILE:O	1.96	0.64
1:J:317:THR:HG21	1:J:370:LEU:HD11	1.78	0.64
1:A:376:GLN:HA	1:A:415:ILE:CD1	2.27	0.64
1:B:158:TYR:O	1:B:186:ASP:HB2	1.97	0.64
1:G:338:ARG:HA	1:G:361:ALA:HB1	1.78	0.64
1:E:260:GLY:HA3	1:I:260:GLY:HA3	1.79	0.64
1:H:334:VAL:CG1	1:H:338:ARG:CZ	2.76	0.64
1:I:410:GLN:NE2	1:I:428:HIS:HB3	2.13	0.64
1:B:371:HIS:HE1	1:B:373:GLY:CA	2.10	0.64
1:F:343:LYS:HE2	1:F:353:GLU:OE2	1.97	0.64
1:A:108:ILE:CD1	1:A:126:LEU:CD2	2.74	0.64
1:B:163:LYS:HA	1:B:164:PRO:C	2.18	0.64
1:C:160:VAL:HG11	1:C:395:LEU:HD11	1.78	0.64
1:D:376:GLN:HB3	1:D:377:PRO:HD3	1.80	0.64
1:H:419:ILE:H	1:H:419:ILE:CD1	2.09	0.64
1:B:234:LEU:HD21	1:G:234:LEU:HD21	1.80	0.64
1:D:117:ARG:HH21	1:J:444:VAL:C	2.01	0.64
1:F:159:GLY:HA3	1:F:187:TYR:CE2	2.33	0.64
1:D:168:TYR:HA	1:J:66:ARG:HH21	1.63	0.64
1:E:125:ASP:OD1	1:E:126:LEU:N	2.31	0.63
1:B:283:ALA:O	1:B:284:MET:HB3	1.99	0.63
1:C:410:GLN:HE22	1:C:431:LEU:H	1.45	0.63
1:F:433:ARG:CG	1:F:433:ARG:NH1	2.43	0.63
1:B:376:GLN:HB3	1:B:377:PRO:HD3	1.80	0.63
1:D:263:ALA:HB2	1:J:263:ALA:HB2	1.78	0.63
1:H:149:MET:CE	1:H:250:LYS:HB2	2.24	0.63
1:H:419:ILE:N	1:H:419:ILE:CD1	2.61	0.63
1:E:371:HIS:CE1	1:E:373:GLY:C	2.72	0.63
1:E:429:LYS:CB	4:E:2023:HOH:O	2.46	0.63
1:H:149:MET:CE	1:H:250:LYS:CB	2.77	0.63
1:C:260:GLY:HA3	1:F:260:GLY:HA3	1.80	0.63
1:H:417:GLN:CB	1:H:419:ILE:CD1	2.77	0.63
1:C:419:ILE:H	1:C:419:ILE:CD1	2.11	0.63
1:J:128:PHE:H	1:J:354:GLN:HE22	1.45	0.63
1:A:362:ALA:O	1:A:364:PRO:HD3	1.99	0.63
1:H:303:LYS:HZ1	1:H:354:GLN:HE21	1.47	0.63
1:H:441:VAL:HG12	1:H:442:THR:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ALA:HB1	1:G:115:MET:CE	2.28	0.63
1:G:48:ALA:HB1	1:G:53:GLY:HA3	1.80	0.63
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.28	0.63
1:H:101:LEU:HB3	1:H:102:PRO:HD3	1.81	0.63
1:D:128:PHE:H	1:D:354:GLN:HE22	1.47	0.63
1:H:341:HIS:NE2	1:H:353:GLU:OE2	2.28	0.62
1:J:406:ARG:O	1:J:410:GLN:HG3	1.99	0.62
1:B:149:MET:CE	1:B:250:LYS:CD	2.77	0.62
1:H:282:ARG:HH11	1:H:285:HIS:CE1	2.15	0.62
1:B:128:PHE:H	1:B:354:GLN:HE22	1.48	0.62
1:F:25:ILE:HD11	1:F:132:LEU:CD2	2.29	0.62
1:H:41:GLN:HB3	1:H:117:ARG:HH11	1.61	0.62
1:A:381:ALA:C	1:A:382:LEU:HD12	2.20	0.62
1:B:184:GLY:HA3	1:B:409:ARG:HG3	1.82	0.62
1:D:389:GLN:C	1:D:390:LEU:HD12	2.20	0.62
1:H:399:ASP:HB2	1:H:403:ALA:CB	2.30	0.62
1:A:46:VAL:HG22	1:A:115:MET:CE	2.29	0.62
1:B:419:ILE:HD12	1:B:419:ILE:H	1.64	0.62
1:I:213:ILE:O	1:I:217:GLU:HG3	1.99	0.62
1:I:283:ALA:O	1:I:284:MET:HB3	2.00	0.62
1:F:389:GLN:C	1:F:390:LEU:HD12	2.19	0.62
1:B:412:ILE:O	1:B:416:MET:HG2	1.99	0.62
1:E:444:VAL:O	1:I:117:ARG:NH2	2.25	0.62
1:F:289:THR:HG22	1:F:296:ILE:O	2.00	0.62
1:H:302:ALA:HB1	1:H:337:LEU:CD1	2.27	0.62
1:H:435:LEU:O	1:H:439:GLY:N	2.33	0.62
1:A:86:ILE:HG21	1:A:349:VAL:O	2.00	0.61
1:C:371:HIS:HB2	1:C:372:PRO:HD2	1.81	0.61
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.81	0.61
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.82	0.61
1:A:376:GLN:CB	1:A:377:PRO:HD3	2.28	0.61
1:E:180:LEU:CD1	1:E:188:MET:HE1	2.28	0.61
1:F:268:ARG:HD3	1:F:268:ARG:C	2.20	0.61
1:F:347:ASN:H	1:F:347:ASN:ND2	1.97	0.61
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.35	0.61
1:E:303:LYS:NZ	1:E:354:GLN:HE21	1.97	0.61
1:G:371:HIS:HB2	1:G:372:PRO:HD2	1.83	0.61
1:F:32:THR:HG21	1:F:119:LYS:CE	2.29	0.61
1:H:319:GLY:N	1:H:325:GLY:O	2.33	0.61
1:A:214:ASP:O	1:A:218:ASN:HB2	2.00	0.61
1:H:268:ARG:HD3	1:H:268:ARG:C	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:376:GLN:N	1:H:377:PRO:CD	2.63	0.61
1:D:37:TYR:CZ	1:J:444:VAL:HG12	2.35	0.61
1:F:163:LYS:HA	1:F:164:PRO:C	2.21	0.61
1:A:143:ILE:HD11	1:A:338:ARG:HG2	1.83	0.60
1:B:159:GLY:HA3	1:B:187:TYR:CD1	2.35	0.60
1:E:163:LYS:HA	1:E:164:PRO:C	2.20	0.60
1:G:163:LYS:H	1:G:395:LEU:CD2	2.14	0.60
1:A:115:MET:O	1:A:118:VAL:HG22	2.00	0.60
1:E:268:ARG:HD3	1:E:268:ARG:C	2.21	0.60
1:H:174:GLU:HG3	1:H:212:ILE:HD11	1.82	0.60
1:B:430:GLU:OE1	1:B:430:GLU:N	2.34	0.60
1:B:260:GLY:HA3	1:G:260:GLY:HA3	1.83	0.60
1:E:180:LEU:CD1	1:E:188:MET:CE	2.79	0.60
1:E:370:LEU:HB2	4:E:1679:HOH:O	2.01	0.60
1:G:345:ASP:HB3	1:G:347:ASN:HD21	1.66	0.60
1:B:263:ALA:HB2	1:G:263:ALA:HB2	1.83	0.60
1:E:410:GLN:NE2	1:E:430:GLU:HB2	2.15	0.60
1:G:38:THR:H	1:G:41:GLN:CD	2.05	0.60
1:B:427:THR:HG23	1:B:428:HIS:ND1	2.17	0.60
1:H:410:GLN:NE2	1:H:431:LEU:H	1.99	0.60
1:B:427:THR:HG23	1:B:428:HIS:CE1	2.37	0.60
1:D:108:ILE:C	1:D:108:ILE:CD1	2.70	0.60
1:D:172:GLU:OE1	1:J:66:ARG:NH2	2.35	0.60
1:G:336:LEU:CD2	1:G:356:PHE:HZ	2.15	0.60
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.37	0.60
1:C:163:LYS:HA	1:C:164:PRO:C	2.22	0.60
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.36	0.60
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.31	0.60
1:E:396:GLY:O	1:E:437:LYS:NZ	2.35	0.60
1:F:163:LYS:H	1:F:395:LEU:CD1	2.13	0.60
1:A:80:MET:SD	1:A:86:ILE:CD1	2.90	0.59
1:A:203:GLU:O	1:A:207:GLU:HG2	2.01	0.59
1:A:345:ASP:O	1:A:348:ASP:N	2.32	0.59
1:J:317:THR:CG2	1:J:370:LEU:HD11	2.32	0.59
1:H:395:LEU:N	1:H:395:LEU:HD22	2.17	0.59
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.37	0.59
1:F:427:THR:HG23	1:F:428:HIS:ND1	2.16	0.59
1:A:86:ILE:HD11	1:A:349:VAL:HG23	1.81	0.59
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.38	0.59
1:B:183:ASN:ND2	1:B:402:ALA:CB	2.63	0.59
1:A:182:SER:C	1:A:183:ASN:HD22	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLY:O	1:A:437:LYS:NZ	2.27	0.59
1:B:158:TYR:CE1	1:B:408:VAL:HG11	2.37	0.59
1:C:424:TYR:CE2	1:C:428:HIS:CE1	2.90	0.59
1:F:104:LEU:C	1:F:104:LEU:HD23	2.23	0.59
1:J:162:PRO:HA	1:J:395:LEU:HD11	1.85	0.59
1:A:80:MET:SD	1:A:86:ILE:HD11	2.42	0.59
1:B:371:HIS:HB2	1:B:372:PRO:HD2	1.84	0.59
1:D:37:TYR:OH	1:J:444:VAL:CG1	2.51	0.59
1:C:108:ILE:O	1:C:108:ILE:CG2	2.51	0.59
1:D:320:ALA:O	1:D:442:THR:HG23	2.03	0.59
1:H:17:TYR:CE1	1:H:73:LYS:HE3	2.37	0.59
1:A:108:ILE:HD12	1:A:126:LEU:CD1	2.28	0.58
1:B:406:ARG:O	1:B:410:GLN:HG3	2.03	0.58
1:H:149:MET:CE	1:H:250:LYS:HD2	2.27	0.58
1:C:427:THR:HG23	1:C:428:HIS:CE1	2.39	0.58
1:I:72:ALA:HB2	1:I:91:TYR:CD1	2.38	0.58
1:I:285:HIS:CD2	1:I:289:THR:OG1	2.56	0.58
1:C:165:LYS:NZ	1:C:191:ASP:OD1	2.20	0.58
1:I:159:GLY:CA	1:I:187:TYR:CZ	2.80	0.58
1:A:375:ILE:O	1:A:378:VAL:N	2.32	0.58
1:H:231:THR:O	1:H:232:ALA:HB2	2.02	0.58
1:H:317:THR:O	1:H:318:ALA:HB3	2.02	0.58
1:I:371:HIS:HB2	1:I:372:PRO:CD	2.33	0.58
1:J:319:GLY:CA	4:J:1255:HOH:O	2.52	0.58
1:E:165:LYS:HG2	1:E:191:ASP:OD2	2.04	0.58
1:H:439:GLY:O	1:H:440:HIS:CD2	2.57	0.58
1:J:183:ASN:OD1	1:J:406:ARG:NH1	2.36	0.58
1:J:373:GLY:O	1:J:440:HIS:HA	2.04	0.58
1:B:410:GLN:OE1	1:B:431:LEU:HB2	2.04	0.58
1:D:283:ALA:O	1:D:284:MET:HB3	2.04	0.58
1:B:175:LYS:HE3	1:B:179:ASP:OD2	2.04	0.58
1:A:282:ARG:HD2	1:A:285:HIS:NE2	2.18	0.58
1:B:183:ASN:HD22	1:B:402:ALA:CA	2.17	0.58
2:E:600:CAP:H4	2:E:600:CAP:O7	2.04	0.58
1:H:191:ASP:HB2	4:H:470:HOH:O	2.04	0.57
1:I:362:ALA:O	1:I:364:PRO:HD3	2.04	0.57
1:G:149:MET:HE3	1:G:250:LYS:HD2	1.85	0.57
1:J:397:HIS:ND1	1:J:398:PRO:CD	2.67	0.57
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.86	0.57
1:B:213:ILE:O	1:B:217:GLU:HG3	2.05	0.57
1:I:163:LYS:HA	1:I:164:PRO:C	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ALA:HB1	1:B:53:GLY:HA3	1.85	0.57
1:B:59:TYR:O	1:B:61:TRP:HD1	1.87	0.57
1:F:104:LEU:HD23	1:F:104:LEU:O	2.04	0.57
1:G:289:THR:HG22	1:G:296:ILE:O	2.05	0.57
1:J:108:ILE:CG2	1:J:108:ILE:O	2.52	0.57
1:B:215:LYS:CE	1:B:219:GLU:OE2	2.52	0.57
1:B:347:ASN:C	1:B:347:ASN:HD22	2.08	0.57
1:G:149:MET:HE1	1:G:250:LYS:HB3	1.87	0.57
1:H:118:VAL:HG22	1:H:120:GLY:H	1.70	0.57
1:J:443:PRO:C	1:J:444:VAL:HG23	2.24	0.57
1:E:180:LEU:HD12	1:E:188:MET:HE1	1.85	0.57
4:E:722:HOH:O	1:I:265:ARG:HB3	2.04	0.57
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.86	0.57
1:G:414:ALA:HB2	1:G:424:TYR:CG	2.40	0.57
1:H:159:GLY:HA3	1:H:187:TYR:CD1	2.40	0.57
1:A:86:ILE:HD13	1:A:349:VAL:CG2	2.26	0.57
1:B:370:LEU:HB2	4:B:1246:HOH:O	2.05	0.57
1:C:389:GLN:O	1:C:390:LEU:HD12	2.04	0.57
1:G:373:GLY:O	1:G:440:HIS:CD2	2.58	0.57
1:F:128:PHE:H	1:F:354:GLN:HE22	1.52	0.56
1:H:178:TYR:CE1	1:H:215:LYS:CE	2.88	0.56
1:J:283:ALA:O	1:J:284:MET:HB3	2.05	0.56
1:A:282:ARG:NH1	1:A:285:HIS:CE1	2.74	0.56
1:A:283:ALA:O	1:A:284:MET:CB	2.53	0.56
1:B:362:ALA:O	1:B:364:PRO:HD3	2.04	0.56
1:H:425:ALA:C	1:H:427:THR:N	2.57	0.56
1:I:338:ARG:HA	1:I:361:ALA:HB1	1.87	0.56
1:J:108:ILE:O	1:J:108:ILE:HG22	2.03	0.56
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.87	0.56
1:B:226:TRP:CZ3	1:B:228:ALA:HB2	2.40	0.56
1:C:149:MET:CE	1:C:250:LYS:HD2	2.36	0.56
1:C:343:LYS:HG2	1:C:353:GLU:HG3	1.86	0.56
1:E:376:GLN:N	1:E:377:PRO:HD2	2.21	0.56
1:H:184:GLY:CA	1:H:409:ARG:HG3	2.36	0.56
1:C:433:ARG:CG	1:C:433:ARG:NH1	2.43	0.56
1:D:260:GLY:HA3	1:J:260:GLY:HA3	1.86	0.56
1:A:330:THR:CG2	1:A:382:LEU:HD21	2.35	0.56
1:B:419:ILE:CG2	1:B:424:TYR:HB2	2.36	0.56
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.36	0.56
1:E:283:ALA:O	1:E:284:MET:HB3	2.06	0.56
1:A:442:THR:O	1:A:444:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.88	0.56
1:D:67:TRP:CD1	1:J:164:PRO:HG3	2.41	0.56
1:J:158:TYR:CE1	1:J:408:VAL:HG11	2.41	0.56
1:J:163:LYS:H	1:J:395:LEU:CD1	2.19	0.56
1:B:431:LEU:O	1:B:435:LEU:HG	2.06	0.56
1:C:79:ASP:HB2	1:C:85:TRP:CH2	2.41	0.56
1:D:376:GLN:HA	1:D:415:ILE:HD13	1.87	0.56
1:G:38:THR:N	1:G:41:GLN:OE1	2.33	0.56
1:H:184:GLY:HA3	1:H:409:ARG:HG3	1.88	0.56
1:B:288:PHE:HB3	1:G:288:PHE:HB3	1.87	0.56
1:H:290:ARG:N	4:H:461:HOH:O	2.27	0.56
1:J:163:LYS:HA	1:J:164:PRO:C	2.26	0.56
1:J:201:ARG:HB2	1:J:204:GLU:HG3	1.88	0.56
1:A:163:LYS:HA	1:A:164:PRO:C	2.27	0.56
1:F:395:LEU:HD23	1:F:401:PRO:HG3	1.88	0.56
1:I:203:GLU:HG3	4:I:448:HOH:O	2.05	0.55
1:J:442:THR:HG23	1:J:442:THR:O	2.07	0.55
1:B:347:ASN:C	1:B:347:ASN:ND2	2.59	0.55
1:E:319:GLY:CA	4:E:496:HOH:O	2.32	0.55
1:F:334:VAL:CG1	1:F:338:ARG:CZ	2.84	0.55
1:A:305:TYR:O	1:A:310:ILE:HG12	2.06	0.55
1:G:341:HIS:ND1	1:G:355:LYS:HG2	2.21	0.55
1:H:236:GLU:OE1	1:H:236:GLU:N	2.38	0.55
1:B:22:LYS:HD3	1:F:65:GLU:HG3	1.87	0.55
1:J:375:ILE:O	1:J:379:ILE:HG13	2.06	0.55
1:E:101:LEU:HB3	1:E:102:PRO:HD3	1.88	0.55
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.87	0.55
1:F:424:TYR:CE2	1:F:428:HIS:CE1	2.94	0.55
1:A:209:MET:O	1:A:213:ILE:HG13	2.07	0.55
1:C:362:ALA:O	1:C:364:PRO:HD3	2.06	0.55
1:G:45:ALA:HB1	1:G:115:MET:HE1	1.87	0.55
1:H:397:HIS:ND1	1:H:398:PRO:N	2.54	0.55
1:B:368:GLY:O	1:B:370:LEU:CD1	2.54	0.55
1:C:52:THR:O	1:F:164:PRO:HB3	2.07	0.55
1:C:441:VAL:HG12	1:C:442:THR:N	2.22	0.55
1:J:289:THR:HG22	1:J:296:ILE:O	2.07	0.55
1:A:76:ASP:O	1:A:77:PHE:CD2	2.59	0.55
1:C:419:ILE:N	1:C:419:ILE:CD1	2.70	0.55
1:D:48:ALA:HB1	1:D:53:GLY:HA3	1.89	0.55
1:D:163:LYS:HA	1:D:164:PRO:C	2.27	0.55
1:G:174:GLU:OE2	1:G:211:LYS:NZ	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:318:ALA:CA	1:H:325:GLY:O	2.54	0.55
1:J:376:GLN:CB	1:J:377:PRO:HD3	2.36	0.55
1:A:92:PRO:HG2	1:A:95:ALA:HB2	1.87	0.55
1:C:160:VAL:HG11	1:C:395:LEU:CD1	2.37	0.55
1:D:362:ALA:O	1:D:364:PRO:HD3	2.08	0.54
1:A:51:SER:OG	1:A:52:THR:N	2.39	0.54
1:G:209:MET:O	1:G:213:ILE:HG13	2.06	0.54
1:H:397:HIS:HD2	1:H:404:GLY:HA2	1.71	0.54
1:J:165:LYS:CB	1:J:191:ASP:OD1	2.54	0.54
1:B:183:ASN:HD22	1:B:402:ALA:HA	1.73	0.54
1:B:226:TRP:CH2	1:B:228:ALA:HB2	2.42	0.54
1:C:59:TYR:CG	1:C:60:PRO:HD2	2.43	0.54
1:G:149:MET:HE1	1:G:250:LYS:CB	2.38	0.54
1:H:427:THR:HG23	1:H:428:HIS:HD1	1.72	0.54
1:A:55:TRP:O	1:A:55:TRP:CE3	2.60	0.54
1:A:183:ASN:HD22	1:A:183:ASN:N	2.05	0.54
1:G:79:ASP:OD1	1:G:81:GLY:N	2.34	0.54
1:G:158:TYR:CE1	1:G:408:VAL:HG11	2.43	0.54
1:E:193:ASN:H	1:E:193:ASN:ND2	1.95	0.54
1:H:165:LYS:NZ	1:H:191:ASP:OD2	2.35	0.54
1:H:244:LEU:HD23	1:H:249:LEU:HD12	1.89	0.54
1:I:9:TYR:C	1:I:11:TYR:N	2.60	0.54
1:E:49:GLU:HG3	1:E:115:MET:SD	2.48	0.54
1:G:104:LEU:C	1:G:104:LEU:CD2	2.76	0.54
1:H:143:ILE:HD11	1:H:338:ARG:HG2	1.87	0.54
1:H:343:LYS:HG2	1:H:353:GLU:HG3	1.89	0.54
1:H:395:LEU:HD22	1:H:395:LEU:H	1.71	0.54
1:H:410:GLN:NE2	1:H:431:LEU:HB2	2.22	0.54
1:F:93:PHE:CD2	4:F:496:HOH:O	2.61	0.54
1:I:162:PRO:HA	1:I:395:LEU:CD1	2.38	0.54
1:J:317:THR:HG21	1:J:370:LEU:CD1	2.37	0.54
1:A:184:GLY:HA3	1:A:409:ARG:HG3	1.89	0.54
1:A:285:HIS:CG	1:A:286:ALA:N	2.76	0.54
1:A:330:THR:HG21	1:A:382:LEU:HD21	1.88	0.54
1:A:435:LEU:O	1:A:439:GLY:HA2	2.08	0.54
1:B:397:HIS:CE1	1:B:398:PRO:HD2	2.43	0.54
1:C:163:LYS:N	1:C:395:LEU:HD22	2.21	0.54
1:E:314:HIS:HD2	2:E:600:CAP:O6P	1.91	0.54
1:E:371:HIS:O	1:E:375:ILE:HG23	2.08	0.54
1:G:38:THR:CG2	1:G:41:GLN:OE1	2.53	0.54
1:G:138:GLY:C	1:G:309:GLY:HA2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:GLY:CA	1:H:187:TYR:CZ	2.86	0.54
1:A:86:ILE:HD11	1:A:349:VAL:CG2	2.35	0.54
1:C:424:TYR:CZ	1:C:428:HIS:CE1	2.96	0.54
1:D:341:HIS:NE2	1:D:343:LYS:HE2	2.23	0.54
1:G:45:ALA:CB	1:G:117:ARG:HD2	2.38	0.54
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.04	0.54
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.89	0.54
1:C:397:HIS:ND1	1:C:398:PRO:HD2	2.23	0.54
1:E:380:GLU:HA	4:E:1249:HOH:O	2.08	0.54
1:F:32:THR:HG22	1:F:119:LYS:HE2	1.87	0.54
1:G:303:LYS:NZ	1:G:354:GLN:HE21	2.06	0.54
1:I:411:ALA:O	1:I:415:ILE:HG13	2.08	0.54
1:A:76:ASP:C	1:A:77:PHE:HD2	2.08	0.53
1:A:424:TYR:CE2	1:A:428:HIS:ND1	2.76	0.53
1:C:321:GLY:HA3	1:C:368:GLY:O	2.07	0.53
1:F:160:VAL:HG21	1:F:394:THR:HG21	1.90	0.53
1:F:406:ARG:O	1:F:410:GLN:HG3	2.06	0.53
1:I:180:LEU:HD11	1:I:395:LEU:HD21	1.89	0.53
1:H:429:LYS:O	1:H:433:ARG:N	2.26	0.53
1:I:76:ASP:HB3	1:I:88:ARG:HG3	1.90	0.53
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.43	0.53
1:A:356:PHE:HB3	1:A:359:ILE:HB	1.90	0.53
1:C:79:ASP:OD1	1:C:81:GLY:N	2.38	0.53
1:A:175:LYS:HG3	4:A:1729:HOH:O	2.06	0.53
1:D:172:GLU:CD	1:J:66:ARG:HH22	2.11	0.53
1:I:108:ILE:HD12	1:I:108:ILE:C	2.29	0.53
1:A:86:ILE:CD1	1:A:349:VAL:HG21	2.35	0.53
1:A:381:ALA:C	1:A:382:LEU:CD1	2.77	0.53
1:E:165:LYS:HE2	1:I:49:GLU:O	2.09	0.53
1:F:101:LEU:HB3	1:F:102:PRO:HD3	1.89	0.53
1:D:288:PHE:HB3	1:J:288:PHE:HB3	1.90	0.53
1:H:139:PRO:HD3	1:H:306:ARG:O	2.08	0.53
1:A:115:MET:O	1:A:118:VAL:CG2	2.57	0.53
1:B:105:LEU:HD23	1:B:108:ILE:HD11	1.90	0.53
1:E:192:GLU:OE2	1:I:111:ASN:ND2	2.42	0.53
1:C:163:LYS:NZ	1:C:191:ASP:OD2	2.42	0.53
1:F:72:ALA:HB2	1:F:91:TYR:CD1	2.44	0.53
1:I:101:LEU:HB3	1:I:102:PRO:HD3	1.90	0.53
1:J:174:GLU:OE1	1:J:211:LYS:CE	2.57	0.53
1:C:441:VAL:CG1	1:C:442:THR:N	2.72	0.53
1:D:9:TYR:CD2	1:D:117:ARG:NH1	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:HB2	1:D:199:TYR:CE2	2.44	0.53
1:E:430:GLU:OE1	1:E:430:GLU:N	2.27	0.53
1:F:176:LEU:HD11	1:F:395:LEU:HD21	1.91	0.53
1:J:435:LEU:O	1:J:439:GLY:N	2.41	0.53
1:A:116:LYS:O	1:A:118:VAL:N	2.43	0.52
1:A:225:THR:HG1	1:A:251:HIS:HD1	1.57	0.52
1:H:284:MET:O	1:H:284:MET:HG2	2.09	0.52
1:B:334:VAL:CG1	1:B:338:ARG:CZ	2.88	0.52
1:D:299:PHE:CZ	1:D:336:LEU:HD22	2.44	0.52
1:F:421:LEU:HD13	4:F:1429:HOH:O	2.08	0.52
1:B:429:LYS:O	1:B:430:GLU:C	2.48	0.52
1:G:345:ASP:HB3	1:G:347:ASN:ND2	2.24	0.52
1:H:59:TYR:O	1:H:61:TRP:HD1	1.93	0.52
1:A:11:TYR:CZ	1:A:73:LYS:HE2	2.45	0.52
1:A:337:LEU:HD22	1:A:362:ALA:HB3	1.89	0.52
1:D:367:SER:HB2	1:D:389:GLN:HB3	1.92	0.52
1:E:397:HIS:ND1	1:E:398:PRO:HD2	2.23	0.52
1:F:112:ILE:HD12	1:F:121:LEU:HD21	1.89	0.52
1:G:163:LYS:HA	1:G:164:PRO:C	2.29	0.52
1:H:22:LYS:HE3	4:H:1185:HOH:O	2.10	0.52
1:D:117:ARG:NE	1:J:444:VAL:O	2.43	0.52
1:D:347:ASN:C	1:D:347:ASN:HD22	2.11	0.52
1:G:428:HIS:HA	4:G:852:HOH:O	2.09	0.52
1:H:283:ALA:O	1:H:284:MET:CB	2.57	0.52
1:J:371:HIS:CE1	1:J:373:GLY:C	2.83	0.52
1:A:324:GLU:OE1	1:A:325:GLY:N	2.42	0.52
1:C:417:GLN:CB	1:C:419:ILE:CD1	2.88	0.52
1:D:15:LYS:HD2	4:D:948:HOH:O	2.09	0.52
1:D:371:HIS:HB2	1:D:372:PRO:HD2	1.92	0.52
1:F:178:TYR:HE1	1:F:215:LYS:CD	2.23	0.52
1:F:283:ALA:O	1:F:284:MET:HB3	2.09	0.52
1:G:226:TRP:CZ3	1:G:228:ALA:HB2	2.44	0.52
1:G:283:ALA:O	1:G:284:MET:HB3	2.08	0.52
1:H:104:LEU:HD23	1:H:104:LEU:O	2.08	0.52
1:B:336:LEU:HD23	1:B:336:LEU:O	2.10	0.52
1:G:336:LEU:CD2	1:G:356:PHE:CZ	2.92	0.52
1:A:180:LEU:O	1:A:183:ASN:N	2.30	0.52
1:F:399:ASP:OD2	1:F:433:ARG:CD	2.57	0.52
1:F:427:THR:HG23	1:F:428:HIS:CE1	2.44	0.52
1:H:8:ILE:HG12	1:H:8:ILE:O	2.08	0.52
1:A:37:TYR:OH	1:H:444:VAL:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:HD3	1:C:268:ARG:C	2.30	0.52
1:F:59:TYR:O	1:F:61:TRP:HD1	1.93	0.52
1:D:49:GLU:O	1:J:165:LYS:HE3	2.08	0.52
1:D:328:ASP:HB2	4:D:457:HOH:O	2.10	0.52
1:E:370:LEU:HA	1:E:374:ASN:HD21	1.74	0.52
1:J:209:MET:O	1:J:213:ILE:HG13	2.10	0.52
1:D:283:ALA:O	1:D:284:MET:CB	2.58	0.51
1:G:341:HIS:NE2	1:G:353:GLU:OE2	2.36	0.51
1:B:264:LEU:HD23	1:B:308:ILE:CD1	2.39	0.51
1:H:203:GLU:O	1:H:207:GLU:HG3	2.09	0.51
1:I:26:ILE:HD13	1:I:75:TYR:OH	2.11	0.51
1:A:26:ILE:HB	1:A:127:TYR:HB3	1.92	0.51
1:A:366:SER:CA	4:A:1262:HOH:O	2.40	0.51
1:E:338:ARG:HA	1:E:361:ALA:HB1	1.92	0.51
1:C:104:LEU:C	1:C:104:LEU:HD23	2.31	0.51
1:G:413:ASP:O	1:G:417:GLN:HG3	2.10	0.51
1:H:9:TYR:CE1	1:H:54:THR:O	2.64	0.51
1:H:338:ARG:HA	1:H:361:ALA:HB1	1.93	0.51
1:J:226:TRP:CZ3	1:J:228:ALA:HB2	2.45	0.51
1:A:268:ARG:HD3	1:A:268:ARG:O	2.11	0.51
1:B:104:LEU:HD23	1:B:108:ILE:HG13	1.92	0.51
1:E:410:GLN:NE2	1:E:431:LEU:H	2.09	0.51
1:A:207:GLU:OE1	1:A:247:LEU:HD21	2.11	0.51
1:F:285:HIS:CG	1:F:286:ALA:N	2.78	0.51
1:H:400:GLY:O	1:H:403:ALA:N	2.44	0.51
1:J:371:HIS:ND1	1:J:373:GLY:N	2.56	0.51
1:A:217:GLU:HG2	1:A:222:GLU:O	2.11	0.51
1:E:404:GLY:O	1:E:407:ALA:HB3	2.11	0.51
1:H:349:VAL:O	1:H:349:VAL:CG1	2.56	0.51
1:I:11:TYR:O	1:I:73:LYS:HE2	2.11	0.51
1:D:116:LYS:HE3	1:J:323:LEU:O	2.11	0.51
1:H:159:GLY:HA3	1:H:187:TYR:CD2	2.46	0.51
1:I:397:HIS:CE1	1:I:399:ASP:HB2	2.46	0.51
1:I:399:ASP:OD2	1:I:433:ARG:HG3	2.10	0.51
1:A:289:THR:HG22	1:A:296:ILE:O	2.11	0.51
1:B:390:LEU:HD12	1:B:390:LEU:N	2.26	0.51
1:C:234:LEU:HD21	1:F:234:LEU:HD21	1.93	0.51
1:E:334:VAL:CG1	1:E:338:ARG:CZ	2.89	0.51
1:G:174:GLU:HG3	1:G:208:ILE:HG23	1.93	0.51
1:H:158:TYR:O	1:H:186:ASP:HB2	2.11	0.51
1:J:319:GLY:HA2	4:J:1255:HOH:O	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HD12	1:B:108:ILE:C	2.32	0.51
1:D:23:ARG:NE	1:I:69:ASP:OD1	2.44	0.51
1:H:439:GLY:C	1:H:440:HIS:CD2	2.84	0.51
1:C:149:MET:HE3	1:C:250:LYS:HD3	1.92	0.50
1:C:158:TYR:CE1	1:C:408:VAL:HG11	2.46	0.50
1:C:435:LEU:O	1:C:439:GLY:HA2	2.11	0.50
1:D:303:LYS:HZ3	1:D:354:GLN:HE21	1.58	0.50
1:E:166:VAL:HG23	1:I:52:THR:HG22	1.93	0.50
1:A:389:GLN:C	1:A:390:LEU:HD12	2.31	0.50
1:A:427:THR:O	1:A:427:THR:HG22	2.11	0.50
1:A:443:PRO:O	1:A:444:VAL:CG2	2.60	0.50
1:D:9:TYR:HD2	1:D:117:ARG:NH1	2.09	0.50
1:E:106:ALA:HA	1:I:258:ILE:CD1	2.41	0.50
1:F:169:SER:HB2	1:F:170:PRO:HD2	1.91	0.50
1:B:320:ALA:O	1:B:442:THR:HG23	2.11	0.50
1:E:180:LEU:HD21	1:E:401:PRO:HB3	1.92	0.50
1:G:236:GLU:N	1:G:236:GLU:OE1	2.45	0.50
1:G:418:GLY:HA2	4:G:1310:HOH:O	2.10	0.50
1:D:178:TYR:CE1	1:D:215:LYS:HD3	2.47	0.50
1:G:362:ALA:O	1:G:364:PRO:HD3	2.11	0.50
1:H:334:VAL:HG21	1:H:382:LEU:HD22	1.93	0.50
4:B:1128:HOH:O	1:F:65:GLU:HG2	2.11	0.50
1:E:138:GLY:C	1:E:309:GLY:HA2	2.32	0.50
1:E:371:HIS:HB2	1:E:372:PRO:HD2	1.93	0.50
1:G:115:MET:O	1:G:118:VAL:HG22	2.11	0.50
1:B:283:ALA:O	1:B:284:MET:CB	2.60	0.50
1:E:334:VAL:HG21	1:E:382:LEU:HD22	1.93	0.50
1:H:93:PHE:CD1	1:H:93:PHE:C	2.84	0.50
1:I:335:ASP:HA	4:I:1735:HOH:O	2.11	0.50
1:J:338:ARG:HA	1:J:361:ALA:HB1	1.93	0.50
1:B:104:LEU:HD23	1:B:104:LEU:O	2.12	0.50
1:C:18:GLU:HG3	4:C:1961:HOH:O	2.12	0.50
1:C:108:ILE:O	1:C:108:ILE:HG22	2.12	0.50
1:E:376:GLN:H	1:E:377:PRO:HD2	1.76	0.50
1:I:390:LEU:HD12	1:I:390:LEU:N	2.27	0.50
1:I:412:ILE:O	1:I:416:MET:HG2	2.11	0.50
1:B:153:LYS:CB	1:B:154:ASP:OD1	2.60	0.50
1:A:319:GLY:N	1:A:325:GLY:O	2.45	0.49
1:D:230:ILE:O	1:D:237:MET:HG2	2.12	0.49
1:B:152:ILE:HD12	1:B:157:ILE:HD12	1.93	0.49
1:B:371:HIS:HA	1:B:390:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:TYR:C	1:I:11:TYR:H	2.15	0.49
1:I:371:HIS:O	1:I:375:ILE:HG23	2.12	0.49
1:D:303:LYS:NZ	1:D:354:GLN:HE21	2.09	0.49
1:H:51:SER:OG	1:H:52:THR:N	2.46	0.49
1:H:230:ILE:O	1:H:237:MET:HG2	2.13	0.49
1:H:402:ALA:O	1:H:406:ARG:NH1	2.45	0.49
1:H:441:VAL:CG1	1:H:442:THR:N	2.74	0.49
1:J:159:GLY:HA3	1:J:187:TYR:CD1	2.48	0.49
1:A:116:LYS:C	1:A:118:VAL:H	2.14	0.49
1:B:104:LEU:HD23	1:B:104:LEU:C	2.32	0.49
1:B:183:ASN:HD22	1:B:402:ALA:CB	2.24	0.49
1:C:419:ILE:HG22	1:C:424:TYR:HB2	1.95	0.49
1:D:72:ALA:O	1:D:73:LYS:HD3	2.12	0.49
1:D:176:LEU:HD11	1:D:395:LEU:CD2	2.39	0.49
1:E:362:ALA:O	1:E:364:PRO:HD3	2.11	0.49
1:E:371:HIS:HE1	1:E:373:GLY:C	2.14	0.49
1:E:390:LEU:HD12	1:E:390:LEU:N	2.27	0.49
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.95	0.49
1:A:77:PHE:N	1:A:77:PHE:CD2	2.80	0.49
1:A:226:TRP:CZ3	1:A:228:ALA:HB2	2.47	0.49
1:H:411:ALA:O	1:H:414:ALA:HB3	2.13	0.49
1:I:47:ALA:O	1:I:51:SER:HB2	2.13	0.49
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.77	0.49
1:A:80:MET:HB2	1:A:84:SER:O	2.11	0.49
1:A:299:PHE:CE2	1:A:351:HIS:CD2	3.00	0.49
1:E:193:ASN:HD22	1:E:193:ASN:N	1.87	0.49
1:F:347:ASN:ND2	4:F:1415:HOH:O	2.45	0.49
1:H:108:ILE:O	1:H:108:ILE:CG2	2.61	0.49
1:I:235:LEU:O	1:I:239:GLN:HG3	2.13	0.49
1:I:318:ALA:HB1	1:I:327:ARG:HA	1.95	0.49
1:B:26:ILE:HB	1:B:127:TYR:HB3	1.94	0.49
1:B:444:VAL:HG12	1:G:117:ARG:HB3	1.94	0.49
1:D:347:ASN:C	1:D:347:ASN:ND2	2.66	0.49
1:E:406:ARG:O	1:E:410:GLN:HG2	2.13	0.49
1:F:303:LYS:NZ	1:F:354:GLN:HE21	2.10	0.49
1:A:411:ALA:O	1:A:414:ALA:HB3	2.12	0.49
1:C:397:HIS:CG	1:C:398:PRO:CD	2.84	0.49
1:E:217:GLU:HG2	1:E:222:GLU:O	2.11	0.49
1:J:371:HIS:HB2	1:J:372:PRO:HD2	1.95	0.49
1:C:404:GLY:O	1:C:408:VAL:HG23	2.13	0.49
1:C:427:THR:HG23	1:C:428:HIS:ND1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:ILE:O	1:J:212:ILE:HG12	2.13	0.49
1:J:353:GLU:CG	4:J:1285:HOH:O	2.61	0.49
1:F:54:THR:CG2	1:F:56:THR:O	2.60	0.49
1:B:25:ILE:N	1:B:25:ILE:HD12	2.28	0.48
1:E:158:TYR:CE1	1:E:408:VAL:HG11	2.48	0.48
1:E:165:LYS:HB3	1:E:191:ASP:OD2	2.13	0.48
1:E:367:SER:HB2	1:E:389:GLN:HB3	1.93	0.48
1:G:213:ILE:O	1:G:217:GLU:HG3	2.13	0.48
1:G:373:GLY:O	1:G:440:HIS:HD2	1.96	0.48
1:J:26:ILE:HB	1:J:127:TYR:HB3	1.95	0.48
1:A:86:ILE:HD13	1:A:349:VAL:O	2.13	0.48
1:A:345:ASP:O	1:A:346:GLU:C	2.51	0.48
1:C:303:LYS:NZ	1:C:354:GLN:HE21	2.11	0.48
1:H:79:ASP:HB2	1:H:85:TRP:CZ3	2.48	0.48
1:H:391:GLY:O	1:H:395:LEU:CD2	2.59	0.48
1:I:15:LYS:CB	4:I:468:HOH:O	2.61	0.48
1:E:371:HIS:HE1	1:E:373:GLY:CA	2.22	0.48
1:A:54:THR:HG23	1:A:56:THR:H	1.78	0.48
1:A:93:PHE:CE1	1:A:131:LYS:HD3	2.49	0.48
1:B:419:ILE:N	1:B:419:ILE:CD1	2.76	0.48
1:C:149:MET:CE	1:C:250:LYS:CD	2.89	0.48
1:C:410:GLN:HE21	1:C:431:LEU:HB2	1.78	0.48
1:F:178:TYR:CE1	1:F:215:LYS:HD2	2.47	0.48
1:H:371:HIS:CB	1:H:372:PRO:CD	2.88	0.48
1:A:158:TYR:O	1:A:186:ASP:HB2	2.14	0.48
1:B:368:GLY:O	1:B:370:LEU:HD12	2.13	0.48
1:C:410:GLN:NE2	1:C:431:LEU:H	2.11	0.48
1:D:111:ASN:ND2	1:J:192:GLU:OE2	2.46	0.48
1:E:412:ILE:O	1:E:416:MET:HG2	2.14	0.48
1:G:45:ALA:HB1	1:G:115:MET:HE2	1.94	0.48
1:I:223:LYS:O	1:I:224:LYS:HD3	2.13	0.48
1:J:146:VAL:HG21	1:J:312:GLN:HE21	1.77	0.48
1:J:371:HIS:O	1:J:374:ASN:OD1	2.31	0.48
1:J:397:HIS:CE1	1:J:398:PRO:HD2	2.48	0.48
1:A:330:THR:O	1:A:334:VAL:HG23	2.13	0.48
1:A:441:VAL:HG22	1:A:442:THR:N	2.28	0.48
1:B:174:GLU:HG3	1:B:208:ILE:HG23	1.95	0.48
1:C:122:ARG:HD2	4:C:448:HOH:O	2.11	0.48
1:G:283:ALA:O	1:G:284:MET:CB	2.62	0.48
1:J:41:GLN:HA	4:J:1290:HOH:O	2.13	0.48
1:J:153:LYS:HB3	1:J:154:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:MET:O	1:A:284:MET:HG2	2.13	0.48
1:A:435:LEU:O	1:A:439:GLY:N	2.46	0.48
1:B:54:THR:CG2	1:B:56:THR:O	2.59	0.48
1:C:283:ALA:O	1:C:284:MET:CB	2.61	0.48
1:C:399:ASP:OD2	1:C:433:ARG:CD	2.56	0.48
1:F:39:ILE:HG12	1:F:85:TRP:CG	2.48	0.48
1:F:209:MET:O	1:F:213:ILE:HG13	2.14	0.48
1:I:334:VAL:HG21	1:I:382:LEU:HD22	1.96	0.48
1:A:282:ARG:CD	1:A:285:HIS:CD2	2.85	0.48
1:D:72:ALA:HB2	1:D:91:TYR:CD1	2.48	0.48
1:A:20:SER:N	1:A:24:ASP:OD2	2.38	0.48
1:A:116:LYS:C	1:A:118:VAL:N	2.66	0.48
1:A:334:VAL:HG12	1:A:338:ARG:NH2	2.26	0.48
1:D:371:HIS:HB2	1:D:372:PRO:CD	2.44	0.48
1:H:98:GLU:OE2	1:H:131:LYS:NZ	2.47	0.48
1:H:159:GLY:CA	1:H:187:TYR:CE2	2.95	0.48
1:A:46:VAL:HG22	1:A:115:MET:HE1	1.95	0.48
1:A:324:GLU:OE1	1:A:324:GLU:C	2.52	0.48
1:D:178:TYR:CE1	1:D:215:LYS:CE	2.97	0.48
1:D:197:PRO:O	1:D:201:ARG:HD3	2.14	0.48
1:E:159:GLY:HA3	1:E:187:TYR:CD1	2.49	0.48
1:H:197:PRO:HB2	1:H:199:TYR:CE2	2.48	0.48
1:B:419:ILE:H	1:B:419:ILE:CD1	2.27	0.47
1:D:159:GLY:CA	1:D:187:TYR:CZ	2.89	0.47
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.43	0.47
1:G:108:ILE:C	1:G:108:ILE:HD12	2.34	0.47
1:J:323:LEU:HB2	4:J:455:HOH:O	2.14	0.47
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.14	0.47
1:F:443:PRO:O	1:F:444:VAL:CG2	2.62	0.47
1:I:226:TRP:CZ3	1:I:228:ALA:HB2	2.49	0.47
1:J:370:LEU:HA	1:J:374:ASN:ND2	2.28	0.47
1:B:234:LEU:CD2	1:G:234:LEU:HD21	2.44	0.47
1:B:338:ARG:HA	1:B:361:ALA:HB1	1.96	0.47
1:C:130:GLU:OE1	1:J:66:ARG:HD3	2.14	0.47
1:E:371:HIS:CE1	1:E:373:GLY:HA3	2.47	0.47
1:G:367:SER:HB2	1:G:389:GLN:HB3	1.96	0.47
1:H:9:TYR:CZ	1:H:55:TRP:HA	2.50	0.47
1:J:139:PRO:O	1:J:360:LYS:HD2	2.13	0.47
1:J:343:LYS:O	4:J:2115:HOH:O	2.20	0.47
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.79	0.47
1:A:397:HIS:CE1	1:A:399:ASP:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:O	1:A:416:MET:HG2	2.14	0.47
1:B:164:PRO:HG3	1:G:67:TRP:CD1	2.50	0.47
1:I:399:ASP:HB2	1:I:403:ALA:CB	2.45	0.47
1:E:25:ILE:HD11	1:E:132:LEU:HD21	1.97	0.47
1:H:362:ALA:O	1:H:364:PRO:HD3	2.14	0.47
1:A:79:ASP:HA	1:A:85:TRP:NE1	2.30	0.47
1:D:175:LYS:HE3	1:D:179:ASP:OD2	2.14	0.47
1:H:163:LYS:CA	1:H:164:PRO:O	2.58	0.47
1:H:206:ALA:HA	1:H:226:TRP:CH2	2.50	0.47
1:H:250:LYS:HE2	4:H:624:HOH:O	2.15	0.47
1:I:441:VAL:O	1:I:443:PRO:HD3	2.14	0.47
1:J:283:ALA:O	1:J:284:MET:CB	2.61	0.47
1:J:410:GLN:HG2	4:J:456:HOH:O	2.13	0.47
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.95	0.47
1:A:187:TYR:CE1	1:A:227:PHE:CE2	3.03	0.47
1:A:399:ASP:HB2	1:A:403:ALA:CB	2.44	0.47
4:E:722:HOH:O	1:I:265:ARG:CB	2.62	0.47
1:H:118:VAL:HG22	1:H:120:GLY:N	2.29	0.47
1:H:197:PRO:HD2	1:H:200:ASN:O	2.15	0.47
1:H:226:TRP:CZ3	1:H:249:LEU:HD13	2.50	0.47
1:H:400:GLY:O	1:H:403:ALA:CB	2.61	0.47
1:H:410:GLN:NE2	1:H:428:HIS:HB3	2.29	0.47
2:B:600:CAP:O6P	4:B:482:HOH:O	2.21	0.47
1:D:9:TYR:HD2	1:D:117:ARG:HH12	1.62	0.47
1:D:108:ILE:HD12	1:D:109:ALA:N	2.30	0.47
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.80	0.47
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.49	0.47
1:F:178:TYR:CE1	1:F:215:LYS:CD	2.97	0.47
1:F:180:LEU:HD21	1:F:401:PRO:HB3	1.97	0.47
1:I:46:VAL:HG22	1:I:115:MET:HE1	1.97	0.47
1:J:334:VAL:CG1	1:J:338:ARG:CZ	2.93	0.47
1:C:444:VAL:O	1:F:117:ARG:NH2	2.32	0.47
1:F:328:ASP:OD2	1:F:328:ASP:N	2.48	0.47
1:H:161:VAL:CG2	1:H:189:KCX:HD2	2.44	0.47
1:H:395:LEU:H	1:H:395:LEU:CD2	2.28	0.47
1:J:226:TRP:CH2	1:J:228:ALA:HB2	2.50	0.47
1:A:216:VAL:C	1:A:218:ASN:N	2.69	0.47
1:A:441:VAL:CG2	1:A:442:THR:N	2.77	0.47
1:B:138:GLY:C	1:B:309:GLY:HA2	2.35	0.47
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.80	0.47
1:B:159:GLY:CA	1:B:187:TYR:CZ	2.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:MET:O	1:E:284:MET:HG2	2.14	0.47
1:E:411:ALA:O	1:E:415:ILE:HG12	2.15	0.47
1:G:59:TYR:CD1	1:G:60:PRO:HD2	2.50	0.47
1:C:213:ILE:O	1:C:217:GLU:HG3	2.15	0.46
1:F:376:GLN:CB	1:F:377:PRO:CD	2.89	0.46
1:I:17:TYR:CE2	1:I:19:PRO:HA	2.50	0.46
1:J:353:GLU:CB	4:J:1285:HOH:O	2.49	0.46
1:A:108:ILE:HD12	1:A:126:LEU:CG	2.45	0.46
1:A:376:GLN:HG3	1:A:377:PRO:N	2.31	0.46
1:C:98:GLU:CD	4:C:1818:HOH:O	2.53	0.46
1:F:226:TRP:CZ3	1:F:228:ALA:HB2	2.50	0.46
1:G:126:LEU:O	1:G:303:LYS:NZ	2.48	0.46
1:A:282:ARG:HH11	1:A:285:HIS:CE1	2.33	0.46
1:D:111:ASN:HD21	1:J:192:GLU:CD	2.18	0.46
1:G:125:ASP:OD1	1:G:126:LEU:N	2.48	0.46
1:H:93:PHE:CD1	1:H:94:HIS:N	2.83	0.46
1:B:376:GLN:N	1:B:377:PRO:CD	2.79	0.46
1:C:184:GLY:HA3	1:C:409:ARG:HG3	1.98	0.46
1:E:236:GLU:HA	1:E:239:GLN:HE21	1.81	0.46
1:G:159:GLY:CA	1:G:187:TYR:CZ	2.87	0.46
1:H:438:TRP:O	1:H:441:VAL:HG23	2.15	0.46
1:A:407:ALA:O	1:A:410:GLN:HB2	2.15	0.46
1:B:22:LYS:HD3	1:F:65:GLU:CG	2.45	0.46
1:E:375:ILE:O	1:E:379:ILE:HG13	2.16	0.46
1:G:226:TRP:CH2	1:G:228:ALA:HB2	2.51	0.46
1:G:395:LEU:N	1:G:395:LEU:HD12	2.30	0.46
1:H:9:TYR:OH	1:H:55:TRP:HA	2.16	0.46
1:J:303:LYS:HZ2	1:J:354:GLN:HE21	1.58	0.46
1:A:54:THR:HG21	1:A:56:THR:O	2.15	0.46
1:E:139:PRO:O	1:E:360:LYS:HD2	2.15	0.46
1:G:285:HIS:CG	1:G:286:ALA:N	2.82	0.46
1:H:427:THR:HG23	1:H:428:HIS:CE1	2.50	0.46
1:J:152:ILE:HD12	1:J:157:ILE:HD12	1.96	0.46
1:A:334:VAL:HG12	1:A:338:ARG:HH21	1.81	0.46
1:B:22:LYS:CG	1:F:65:GLU:HG3	2.46	0.46
1:A:159:GLY:CA	1:A:187:TYR:CE2	2.96	0.46
1:A:180:LEU:HD21	1:A:401:PRO:HB3	1.97	0.46
1:B:148:LYS:HB3	4:B:1301:HOH:O	2.16	0.46
1:B:371:HIS:HB2	1:B:372:PRO:HD3	1.97	0.46
1:D:441:VAL:HG22	1:D:442:THR:N	2.31	0.46
1:E:396:GLY:O	1:E:397:HIS:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:GLY:HA3	1:F:409:ARG:HG3	1.98	0.46
1:E:91:TYR:CE1	1:E:108:ILE:CD1	2.98	0.46
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.80	0.46
1:E:379:ILE:HD12	1:E:415:ILE:HG21	1.97	0.46
1:G:336:LEU:CD2	1:G:336:LEU:O	2.64	0.46
1:G:389:GLN:O	1:G:390:LEU:HD12	2.16	0.46
1:I:25:ILE:HD11	1:I:132:LEU:CD2	2.42	0.46
1:A:443:PRO:C	1:A:444:VAL:HG23	2.36	0.46
1:B:433:ARG:CB	4:B:1637:HOH:O	2.63	0.46
1:C:322:LYS:O	1:C:322:LYS:HG2	2.16	0.46
1:E:279:HIS:NE2	1:E:314:HIS:CE1	2.80	0.46
1:I:159:GLY:HA3	1:I:187:TYR:CD1	2.49	0.46
1:I:283:ALA:O	1:I:284:MET:CB	2.62	0.46
1:J:59:TYR:O	1:J:61:TRP:HD1	1.99	0.46
1:A:234:LEU:HD21	1:H:234:LEU:HD21	1.96	0.45
1:A:329:ILE:HG22	1:A:333:PHE:CE2	2.51	0.45
1:C:122:ARG:NH1	4:C:1829:HOH:O	2.24	0.45
1:C:160:VAL:CG1	1:C:395:LEU:HD11	2.46	0.45
1:D:163:LYS:H	1:D:395:LEU:CD1	2.25	0.45
1:D:399:ASP:OD2	1:D:433:ARG:HG3	2.17	0.45
1:F:159:GLY:CA	1:F:187:TYR:CZ	2.95	0.45
1:F:265:ARG:NH1	4:F:501:HOH:O	2.49	0.45
1:G:155:ARG:HB2	1:G:156:PRO:HD2	1.98	0.45
1:G:376:GLN:HG3	1:G:377:PRO:N	2.30	0.45
1:H:17:TYR:CD1	1:H:73:LYS:CD	2.99	0.45
1:H:399:ASP:HB2	1:H:403:ALA:HB1	1.98	0.45
1:I:215:LYS:CE	1:I:219:GLU:OE2	2.64	0.45
1:C:115:MET:HA	1:F:323:LEU:HD23	1.98	0.45
1:C:322:LYS:NZ	2:C:600:CAP:O3P	2.47	0.45
1:E:371:HIS:HE1	1:E:373:GLY:HA3	1.80	0.45
1:A:27:ALA:HB1	1:A:29:PHE:CE2	2.52	0.45
1:B:395:LEU:N	1:B:395:LEU:HD12	2.32	0.45
1:D:117:ARG:CZ	1:J:444:VAL:O	2.64	0.45
1:D:376:GLN:N	1:D:377:PRO:CD	2.80	0.45
1:E:158:TYR:CD1	1:E:408:VAL:HG11	2.51	0.45
1:G:104:LEU:HD23	1:G:108:ILE:HG13	1.98	0.45
1:H:39:ILE:HG23	1:H:40:GLU:N	2.31	0.45
1:A:149:MET:CE	1:A:250:LYS:CD	2.83	0.45
1:A:370:LEU:HA	1:A:374:ASN:HD21	1.81	0.45
1:B:263:ALA:CB	1:G:263:ALA:HB2	2.46	0.45
1:C:305:TYR:O	1:C:310:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:GLY:O	1:D:409:ARG:HD3	2.17	0.45
1:H:369:GLY:HA3	1:H:443:PRO:HG2	1.97	0.45
1:H:389:GLN:C	1:H:390:LEU:HD12	2.37	0.45
1:H:390:LEU:HD12	1:H:390:LEU:N	2.32	0.45
1:J:101:LEU:HB3	1:J:102:PRO:HD3	1.98	0.45
1:J:101:LEU:N	1:J:102:PRO:CD	2.79	0.45
1:J:299:PHE:CZ	1:J:336:LEU:HD22	2.52	0.45
1:J:424:TYR:CZ	1:J:428:HIS:CE1	3.04	0.45
1:B:65:GLU:HG3	1:F:22:LYS:CG	2.47	0.45
1:D:234:LEU:HD21	1:J:234:LEU:HD21	1.99	0.45
1:G:93:PHE:CD1	1:G:94:HIS:N	2.84	0.45
1:H:424:TYR:O	1:H:427:THR:CG2	2.53	0.45
1:J:123:LEU:HG	1:J:300:VAL:HG21	1.99	0.45
1:A:25:ILE:HD12	1:A:96:PHE:CE2	2.52	0.45
1:A:285:HIS:ND1	1:A:286:ALA:N	2.65	0.45
1:A:435:LEU:O	1:A:439:GLY:CA	2.65	0.45
1:B:419:ILE:HG22	1:B:424:TYR:HB2	1.99	0.45
1:C:130:GLU:HG3	1:C:357:TYR:CE2	2.51	0.45
1:D:138:GLY:C	1:D:309:GLY:HA2	2.37	0.45
1:H:240:ARG:NH1	4:H:697:HOH:O	2.48	0.45
1:J:108:ILE:N	1:J:108:ILE:HD12	2.32	0.45
1:A:111:ASN:HA	4:A:464:HOH:O	2.17	0.45
1:A:268:ARG:C	1:A:268:ARG:CD	2.78	0.45
1:B:149:MET:HE2	1:B:250:LYS:HD3	1.97	0.45
1:D:52:THR:HG22	1:J:166:VAL:HG23	1.99	0.45
1:F:334:VAL:HG21	1:F:382:LEU:HG	1.97	0.45
1:G:320:ALA:O	1:G:442:THR:HG23	2.16	0.45
1:H:343:LYS:HE2	1:H:353:GLU:OE2	2.17	0.45
1:I:105:LEU:HD23	1:I:108:ILE:HD11	1.97	0.45
1:J:263:ALA:O	1:J:267:ILE:HG12	2.17	0.45
1:A:138:GLY:C	1:A:309:GLY:HA2	2.37	0.45
1:C:122:ARG:HA	1:C:295:GLY:O	2.17	0.45
1:F:433:ARG:HH11	1:F:433:ARG:CB	2.26	0.45
1:G:39:ILE:HG12	1:G:85:TRP:CG	2.52	0.45
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.82	0.45
1:I:424:TYR:CZ	1:I:428:HIS:CE1	3.05	0.45
1:B:139:PRO:N	1:B:309:GLY:HA2	2.32	0.45
1:B:160:VAL:HG21	1:B:394:THR:HG21	1.98	0.45
1:E:435:LEU:O	1:E:437:LYS:N	2.50	0.45
1:H:424:TYR:CE2	1:H:428:HIS:CE1	3.05	0.45
1:J:19:PRO:HG3	1:J:75:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:PHE:O	1:J:145:GLY:HA3	2.16	0.45
1:A:299:PHE:CD2	1:A:351:HIS:CD2	3.05	0.45
1:C:407:ALA:HB2	1:C:430:GLU:HB3	1.98	0.45
1:F:183:ASN:OD1	1:F:406:ARG:NH1	2.50	0.45
1:F:435:LEU:O	1:F:439:GLY:N	2.48	0.45
1:G:183:ASN:N	1:G:183:ASN:HD22	2.15	0.45
1:H:12:TYR:CD2	1:H:48:ALA:HB2	2.51	0.45
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.52	0.45
1:J:371:HIS:CE1	1:J:373:GLY:CA	3.00	0.45
1:J:371:HIS:N	1:J:374:ASN:OD1	2.27	0.45
1:A:82:ASP:OD1	1:A:82:ASP:C	2.56	0.44
1:A:166:VAL:HG23	1:H:52:THR:HG22	1.99	0.44
1:E:283:ALA:O	1:E:284:MET:CB	2.65	0.44
1:F:108:ILE:HD12	1:F:109:ALA:N	2.32	0.44
1:H:206:ALA:HA	1:H:226:TRP:CZ3	2.52	0.44
1:H:282:ARG:NH1	1:H:285:HIS:NE2	2.64	0.44
1:H:442:THR:O	1:H:443:PRO:O	2.35	0.44
1:I:284:MET:O	1:I:284:MET:HG2	2.17	0.44
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.82	0.44
1:B:39:ILE:CD1	1:B:85:TRP:HB2	2.47	0.44
1:D:159:GLY:HA3	1:D:187:TYR:CD2	2.52	0.44
1:D:285:HIS:CG	1:D:286:ALA:N	2.85	0.44
1:E:347:ASN:OD1	1:E:347:ASN:N	2.37	0.44
1:G:38:THR:OG1	1:G:41:GLN:HG2	2.18	0.44
1:I:285:HIS:CG	1:I:286:ALA:N	2.86	0.44
1:A:288:PHE:CD1	1:A:289:THR:HG23	2.53	0.44
1:C:206:ALA:HA	1:C:226:TRP:CH2	2.52	0.44
1:C:288:PHE:HB3	1:F:288:PHE:HB3	2.00	0.44
1:D:9:TYR:HE1	1:D:54:THR:O	2.00	0.44
1:E:106:ALA:HA	1:I:258:ILE:HD11	1.99	0.44
1:E:112:ILE:HG23	4:E:1890:HOH:O	2.16	0.44
1:F:15:LYS:HA	1:F:75:TYR:O	2.17	0.44
1:G:376:GLN:CB	1:G:377:PRO:CD	2.94	0.44
1:H:8:ILE:O	1:H:8:ILE:CG1	2.65	0.44
1:B:289:THR:HG22	1:B:296:ILE:O	2.18	0.44
1:C:73:LYS:HE2	4:J:641:HOH:O	2.18	0.44
1:E:163:LYS:H	1:E:395:LEU:HD11	1.81	0.44
1:G:421:LEU:HD13	4:G:1150:HOH:O	2.18	0.44
1:A:47:ALA:HB2	1:A:89:ILE:HD13	1.98	0.44
1:A:136:PHE:HB3	1:A:307:LEU:O	2.17	0.44
1:A:185:ALA:O	1:A:224:LYS:NZ	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ASP:HB3	1:E:88:ARG:HG3	2.00	0.44
1:E:192:GLU:CD	1:I:111:ASN:HD21	2.20	0.44
1:G:406:ARG:O	1:G:410:GLN:HG3	2.16	0.44
1:A:375:ILE:O	1:A:376:GLN:C	2.55	0.44
1:C:54:THR:HG23	1:C:56:THR:H	1.82	0.44
1:F:433:ARG:NH1	1:F:433:ARG:CB	2.80	0.44
1:I:174:GLU:HB2	1:I:208:ILE:HD13	2.00	0.44
1:A:46:VAL:CG2	1:A:115:MET:HE3	2.48	0.44
1:B:93:PHE:CD1	1:B:93:PHE:C	2.91	0.44
1:D:11:TYR:CE2	1:D:73:LYS:NZ	2.85	0.44
1:D:299:PHE:CE2	1:D:336:LEU:HD22	2.53	0.44
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.83	0.44
1:F:283:ALA:O	1:F:284:MET:CB	2.66	0.44
1:I:206:ALA:HA	1:I:226:TRP:CZ3	2.53	0.44
1:J:268:ARG:C	1:J:268:ARG:CD	2.84	0.44
1:A:411:ALA:O	1:A:414:ALA:N	2.50	0.44
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.83	0.44
1:C:341:HIS:NE2	1:C:353:GLU:OE2	2.40	0.44
1:D:438:TRP:O	1:D:441:VAL:HG12	2.17	0.44
1:F:39:ILE:CD1	1:F:85:TRP:HB2	2.48	0.44
1:F:93:PHE:CE2	4:F:496:HOH:O	2.56	0.44
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.48	0.44
1:I:20:SER:O	1:I:24:ASP:HB2	2.17	0.44
1:A:79:ASP:HA	1:A:85:TRP:CD1	2.52	0.44
1:A:281:HIS:CE1	1:A:283:ALA:HB2	2.53	0.44
1:A:285:HIS:O	1:A:287:ALA:N	2.51	0.44
1:C:289:THR:HG22	1:C:296:ILE:O	2.18	0.44
1:F:197:PRO:HB2	1:F:199:TYR:CE2	2.53	0.44
1:F:373:GLY:HA3	1:F:439:GLY:O	2.17	0.44
1:B:23:ARG:NE	1:F:69:ASP:OD1	2.49	0.43
1:B:285:HIS:CG	1:B:286:ALA:N	2.86	0.43
1:D:184:GLY:HA3	1:D:409:ARG:HG3	2.00	0.43
1:A:216:VAL:O	1:A:218:ASN:N	2.51	0.43
1:B:374:ASN:C	1:B:374:ASN:OD1	2.57	0.43
1:C:235:LEU:O	1:C:239:GLN:HG3	2.18	0.43
1:C:397:HIS:CE1	1:C:398:PRO:HD2	2.52	0.43
1:E:208:ILE:O	1:E:212:ILE:HG12	2.18	0.43
1:F:162:PRO:HA	1:F:395:LEU:HD11	2.00	0.43
1:G:139:PRO:N	1:G:309:GLY:HA2	2.32	0.43
1:J:389:GLN:C	1:J:390:LEU:HD12	2.38	0.43
1:J:430:GLU:OE1	1:J:430:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:OH	1:A:53:GLY:HA2	2.18	0.43
1:A:49:GLU:O	1:H:165:LYS:HE2	2.19	0.43
1:A:159:GLY:HA3	1:A:187:TYR:CD2	2.52	0.43
1:B:371:HIS:CB	1:B:372:PRO:CD	2.87	0.43
1:A:216:VAL:O	1:A:219:GLU:N	2.44	0.43
1:C:118:VAL:HG11	1:C:121:LEU:HB2	2.00	0.43
1:C:163:LYS:N	1:C:395:LEU:CD2	2.62	0.43
1:D:80:MET:HB2	1:D:84:SER:O	2.18	0.43
1:D:93:PHE:CD1	1:D:93:PHE:C	2.91	0.43
1:D:208:ILE:O	1:D:212:ILE:HG12	2.18	0.43
1:D:338:ARG:HA	1:D:361:ALA:HB1	2.01	0.43
1:F:51:SER:OG	1:F:52:THR:N	2.52	0.43
1:F:59:TYR:CD2	1:F:60:PRO:HD2	2.54	0.43
1:G:131:LYS:O	1:G:135:GLU:HG3	2.19	0.43
1:G:441:VAL:CG1	1:G:442:THR:N	2.82	0.43
1:I:79:ASP:HB2	1:I:85:TRP:CZ3	2.54	0.43
1:I:251:HIS:NE2	1:I:312:GLN:NE2	2.64	0.43
1:J:159:GLY:CA	1:J:187:TYR:CZ	2.96	0.43
1:A:123:LEU:HG	1:A:300:VAL:HG21	2.00	0.43
1:A:373:GLY:O	1:A:440:HIS:HA	2.18	0.43
1:B:371:HIS:CE1	1:B:373:GLY:N	2.84	0.43
1:C:72:ALA:HB2	1:C:91:TYR:CD1	2.53	0.43
1:G:51:SER:OG	1:G:52:THR:N	2.52	0.43
1:G:166:VAL:HG12	1:G:194:LEU:HD13	2.00	0.43
1:J:93:PHE:CD1	1:J:93:PHE:C	2.91	0.43
1:J:175:LYS:HE3	1:J:179:ASP:OD2	2.19	0.43
1:A:122:ARG:HD3	1:A:292:PRO:C	2.39	0.43
1:B:155:ARG:HB2	1:B:156:PRO:HD2	2.00	0.43
1:D:159:GLY:HA3	1:D:187:TYR:CD1	2.53	0.43
1:E:165:LYS:CB	1:E:191:ASP:OD2	2.65	0.43
1:E:230:ILE:O	1:E:237:MET:HG2	2.19	0.43
1:E:407:ALA:O	1:E:410:GLN:HG2	2.18	0.43
1:F:11:TYR:CD2	1:F:11:TYR:C	2.92	0.43
1:F:317:THR:HA	1:F:366:SER:HG	1.82	0.43
1:H:427:THR:CG2	1:H:428:HIS:HD1	2.32	0.43
1:A:401:PRO:O	1:A:404:GLY:N	2.51	0.43
1:B:417:GLN:CB	1:B:419:ILE:HD13	2.49	0.43
1:C:159:GLY:HA3	1:C:187:TYR:CD2	2.52	0.43
1:D:19:PRO:HG3	1:D:75:TYR:CZ	2.53	0.43
1:G:336:LEU:HD21	1:G:356:PHE:HZ	1.82	0.43
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:LYS:HG3	1:J:212:ILE:N	2.33	0.43
1:A:174:GLU:CG	1:A:212:ILE:HD11	2.49	0.43
1:A:263:ALA:HA	4:A:1589:HOH:O	2.19	0.43
1:C:125:ASP:OD1	1:C:126:LEU:N	2.49	0.43
1:C:376:GLN:N	1:C:377:PRO:CD	2.80	0.43
1:E:398:PRO:CG	1:E:433:ARG:HB3	2.49	0.43
1:F:38:THR:HA	4:F:476:HOH:O	2.18	0.43
1:F:200:ASN:OD1	1:F:205:ARG:CG	2.66	0.43
1:G:118:VAL:HG23	1:G:118:VAL:O	2.17	0.43
1:I:56:THR:OG1	1:I:57:THR:N	2.52	0.43
1:I:209:MET:HG3	1:I:226:TRP:CG	2.54	0.43
1:J:374:ASN:N	4:J:1683:HOH:O	2.51	0.43
1:A:338:ARG:HA	1:A:361:ALA:HB1	2.00	0.43
1:D:169:SER:HB2	1:D:170:PRO:HD2	2.00	0.43
1:F:376:GLN:HA	1:F:415:ILE:HD13	2.01	0.43
1:F:443:PRO:C	1:F:444:VAL:HG23	2.39	0.43
1:I:125:ASP:OD1	1:I:126:LEU:N	2.52	0.43
1:B:104:LEU:HD23	1:B:108:ILE:CG1	2.49	0.43
1:C:390:LEU:HD12	1:C:390:LEU:N	2.31	0.43
1:D:54:THR:CB	4:D:1771:HOH:O	2.67	0.43
1:F:178:TYR:HE1	1:F:215:LYS:HD2	1.84	0.43
1:H:32:THR:CG2	1:H:119:LYS:HB3	2.40	0.43
1:I:101:LEU:N	1:I:102:PRO:CD	2.82	0.43
1:D:25:ILE:CD1	1:D:93:PHE:HA	2.49	0.42
1:F:443:PRO:O	1:F:444:VAL:HG23	2.19	0.42
1:G:96:PHE:HB3	4:G:1180:HOH:O	2.19	0.42
1:G:104:LEU:HD21	1:G:108:ILE:HG12	2.01	0.42
1:H:101:LEU:N	1:H:102:PRO:CD	2.81	0.42
1:I:15:LYS:CG	4:I:468:HOH:O	2.50	0.42
1:D:389:GLN:O	1:D:390:LEU:HD12	2.19	0.42
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.83	0.42
1:I:159:GLY:CA	1:I:187:TYR:CE2	3.00	0.42
1:C:183:ASN:OD1	1:C:406:ARG:NH1	2.43	0.42
1:D:125:ASP:OD1	1:D:126:LEU:N	2.47	0.42
1:E:55:TRP:CD1	1:I:369:GLY:HA2	2.54	0.42
1:E:184:GLY:HA3	1:E:409:ARG:HG3	2.01	0.42
1:D:9:TYR:CE1	1:D:54:THR:O	2.72	0.42
1:E:25:ILE:HD12	1:E:96:PHE:CE2	2.54	0.42
1:G:25:ILE:HD13	1:G:93:PHE:HA	2.01	0.42
1:G:48:ALA:O	1:G:53:GLY:N	2.50	0.42
1:G:56:THR:OG1	1:G:57:THR:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:ARG:HG2	1:H:124:GLU:OE2	2.19	0.42
1:A:184:GLY:CA	1:A:409:ARG:HG3	2.50	0.42
1:B:336:LEU:CD2	1:B:356:PHE:HZ	2.32	0.42
1:B:444:VAL:HB	1:G:37:TYR:OH	2.19	0.42
1:D:319:GLY:HA2	4:D:468:HOH:O	2.20	0.42
1:E:101:LEU:N	1:E:102:PRO:CD	2.82	0.42
1:E:119:LYS:HE2	4:E:2010:HOH:O	2.18	0.42
1:E:159:GLY:CA	1:E:187:TYR:CZ	2.97	0.42
1:H:379:ILE:HD12	1:H:415:ILE:HD12	2.02	0.42
1:A:161:VAL:HG23	1:A:389:GLN:CG	2.50	0.42
1:A:376:GLN:CB	1:A:377:PRO:CD	2.97	0.42
1:B:367:SER:HB2	1:B:389:GLN:HB3	2.00	0.42
1:E:93:PHE:CD1	1:E:93:PHE:C	2.93	0.42
1:E:317:THR:O	1:E:318:ALA:C	2.58	0.42
1:F:298:MET:HB3	1:F:333:PHE:CZ	2.54	0.42
1:H:70:LEU:HD22	1:H:95:ALA:HA	2.00	0.42
1:H:214:ASP:O	1:H:218:ASN:HB2	2.19	0.42
1:J:269:ASP:OD2	4:J:1488:HOH:O	2.21	0.42
1:G:9:TYR:CD1	1:G:45:ALA:HA	2.55	0.42
1:G:182:SER:C	1:G:183:ASN:HD22	2.23	0.42
1:H:158:TYR:CD2	1:H:185:ALA:HA	2.55	0.42
1:H:341:HIS:HB2	4:H:1700:HOH:O	2.20	0.42
1:J:158:TYR:CD1	1:J:408:VAL:HG11	2.55	0.42
1:J:414:ALA:HB1	1:J:419:ILE:O	2.19	0.42
1:A:195:THR:OG1	1:A:196:SER:N	2.52	0.42
1:B:395:LEU:N	1:B:395:LEU:CD1	2.83	0.42
1:D:164:PRO:HB3	1:J:52:THR:O	2.19	0.42
1:E:162:PRO:HA	1:E:395:LEU:HD11	2.02	0.42
1:G:45:ALA:HB2	1:G:117:ARG:HD2	2.00	0.42
1:H:79:ASP:OD1	1:H:81:GLY:N	2.52	0.42
1:H:241:LEU:HD12	1:H:270:LEU:HD23	2.02	0.42
1:H:395:LEU:N	1:H:395:LEU:CD2	2.83	0.42
1:I:209:MET:HG3	1:I:226:TRP:CD2	2.55	0.42
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.49	0.42
1:A:27:ALA:CB	1:A:29:PHE:CE2	3.03	0.42
1:A:46:VAL:HG22	1:A:115:MET:HE3	2.02	0.42
1:C:367:SER:HB2	1:C:389:GLN:HB3	2.02	0.42
1:C:433:ARG:HH11	1:C:433:ARG:CB	2.29	0.42
1:G:159:GLY:HA3	1:G:187:TYR:CD1	2.55	0.42
1:I:303:LYS:NZ	1:I:354:GLN:HE21	2.17	0.42
1:A:72:ALA:HB1	1:A:90:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:O	1:C:285:HIS:HB3	2.19	0.42
1:D:158:TYR:CE1	1:D:408:VAL:HG11	2.55	0.42
1:E:291:ASN:HA	1:E:292:PRO:HD3	1.81	0.42
1:E:319:GLY:N	1:E:325:GLY:O	2.53	0.42
1:G:143:ILE:HD11	1:G:338:ARG:HG2	2.02	0.42
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.55	0.42
1:G:149:MET:CE	1:G:250:LYS:HB3	2.48	0.41
1:A:52:THR:HG22	1:H:166:VAL:O	2.20	0.41
1:B:329:ILE:HG22	1:B:333:PHE:CZ	2.55	0.41
1:C:197:PRO:HG3	4:C:565:HOH:O	2.19	0.41
1:D:314:HIS:HA	1:D:365:THR:O	2.20	0.41
1:F:108:ILE:HD12	1:F:108:ILE:C	2.40	0.41
1:F:390:LEU:HD12	1:F:390:LEU:N	2.35	0.41
1:G:12:TYR:CD2	1:G:48:ALA:HB2	2.55	0.41
1:H:104:LEU:C	1:H:104:LEU:CD2	2.87	0.41
1:H:334:VAL:CG1	1:H:338:ARG:NE	2.84	0.41
1:J:65:GLU:CD	1:J:65:GLU:H	2.21	0.41
1:B:113:PHE:HB2	1:G:286:ALA:HB3	2.01	0.41
1:B:397:HIS:ND1	1:B:398:PRO:CD	2.78	0.41
1:J:11:TYR:CD2	1:J:11:TYR:C	2.93	0.41
1:J:169:SER:HB2	1:J:170:PRO:CD	2.49	0.41
1:A:128:PHE:H	1:A:354:GLN:NE2	2.14	0.41
1:A:167:GLY:O	1:H:66:ARG:HD2	2.19	0.41
1:A:282:ARG:O	1:A:283:ALA:C	2.58	0.41
1:B:115:MET:HA	1:G:323:LEU:HD23	2.03	0.41
1:B:371:HIS:HE1	1:B:373:GLY:HA3	1.83	0.41
1:E:397:HIS:ND1	1:E:398:PRO:CD	2.83	0.41
1:G:230:ILE:O	1:G:237:MET:HG2	2.19	0.41
1:G:433:ARG:NH1	4:G:1446:HOH:O	2.25	0.41
1:I:9:TYR:O	1:I:11:TYR:N	2.52	0.41
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.56	0.41
1:J:91:TYR:N	1:J:91:TYR:CD2	2.88	0.41
1:A:128:PHE:HA	1:A:129:PRO:HD2	1.97	0.41
1:A:240:ARG:NH1	4:A:467:HOH:O	2.47	0.41
1:B:226:TRP:CH2	1:B:228:ALA:CB	3.04	0.41
1:B:264:LEU:HD23	1:B:308:ILE:HD12	2.02	0.41
1:D:323:LEU:O	1:J:116:LYS:HE3	2.19	0.41
1:E:169:SER:HB2	1:E:170:PRO:HD2	2.03	0.41
1:F:424:TYR:CZ	1:F:428:HIS:CE1	3.08	0.41
1:G:12:TYR:OH	1:G:53:GLY:HA2	2.20	0.41
1:G:159:GLY:CA	1:G:187:TYR:CE2	3.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:ILE:HB	1:I:127:TYR:HB3	2.02	0.41
1:I:93:PHE:CD1	1:I:93:PHE:C	2.93	0.41
1:I:119:LYS:HB2	1:I:119:LYS:HE3	1.78	0.41
1:J:367:SER:HB2	1:J:389:GLN:HB3	2.02	0.41
1:J:414:ALA:HB2	1:J:424:TYR:CG	2.54	0.41
1:A:151:GLU:OE1	1:A:223:LYS:HE2	2.21	0.41
1:D:96:PHE:CE1	1:D:104:LEU:HD12	2.56	0.41
1:G:383:GLY:HA2	4:G:1439:HOH:O	2.20	0.41
1:J:12:TYR:CD2	1:J:48:ALA:HB2	2.56	0.41
1:J:285:HIS:CG	1:J:286:ALA:N	2.88	0.41
1:A:390:LEU:HD12	1:A:390:LEU:N	2.35	0.41
1:C:433:ARG:NH1	1:C:433:ARG:CB	2.83	0.41
1:D:334:VAL:HG21	1:D:382:LEU:HD22	2.03	0.41
1:F:104:LEU:HD23	1:F:108:ILE:HG13	2.02	0.41
1:H:435:LEU:O	1:H:439:GLY:CA	2.69	0.41
1:E:12:TYR:CD2	1:E:48:ALA:HB2	2.56	0.41
1:F:112:ILE:O	1:F:115:MET:HE2	2.21	0.41
1:F:421:LEU:HD12	1:F:421:LEU:N	2.36	0.41
1:G:433:ARG:NH2	4:G:1446:HOH:O	2.50	0.41
1:H:401:PRO:C	1:H:403:ALA:N	2.74	0.41
1:J:163:LYS:H	1:J:395:LEU:HD12	1.85	0.41
1:A:263:ALA:O	1:A:267:ILE:HG12	2.21	0.41
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.93	0.41
1:B:151:GLU:OE2	1:B:223:LYS:HE2	2.21	0.41
1:D:79:ASP:HB2	1:D:85:TRP:CZ3	2.56	0.41
1:D:101:LEU:HB3	1:D:102:PRO:HD3	2.01	0.41
1:E:167:GLY:O	1:I:66:ARG:HD2	2.21	0.41
1:F:101:LEU:N	1:F:102:PRO:CD	2.83	0.41
1:F:433:ARG:NH1	1:F:433:ARG:HB3	2.36	0.41
1:G:101:LEU:N	1:G:102:PRO:CD	2.83	0.41
1:G:108:ILE:HD13	1:G:126:LEU:HD11	2.01	0.41
1:H:49:GLU:HG3	1:H:115:MET:SD	2.61	0.41
1:H:159:GLY:HA3	1:H:187:TYR:CG	2.56	0.41
1:H:161:VAL:HG22	1:H:189:KCX:HB2	2.02	0.41
1:H:198:TRP:CZ3	1:H:199:TYR:HB3	2.56	0.41
1:H:231:THR:O	1:H:232:ALA:CB	2.68	0.41
1:H:399:ASP:HB2	1:H:403:ALA:HB2	2.02	0.41
1:H:429:LYS:O	1:H:433:ARG:CB	2.69	0.41
1:I:17:TYR:HE2	1:I:19:PRO:HA	1.85	0.41
1:A:443:PRO:O	1:A:444:VAL:HG23	2.21	0.41
1:I:320:ALA:O	1:I:442:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:424:TYR:CE2	1:I:428:HIS:CE1	3.09	0.41
1:J:169:SER:HB2	1:J:170:PRO:HD2	2.03	0.41
1:J:230:ILE:O	1:J:237:MET:HG2	2.20	0.41
1:J:407:ALA:O	1:J:410:GLN:N	2.54	0.41
1:C:159:GLY:CA	1:C:187:TYR:CE2	3.02	0.40
1:C:171:GLU:H	1:C:171:GLU:CD	2.24	0.40
1:E:317:THR:HG23	1:E:367:SER:O	2.22	0.40
1:F:178:TYR:CE1	1:F:215:LYS:HD3	2.56	0.40
1:H:24:ASP:O	1:H:129:PRO:HG3	2.20	0.40
1:H:54:THR:HG23	1:H:55:TRP:N	2.36	0.40
1:I:376:GLN:N	1:I:377:PRO:CD	2.84	0.40
1:J:390:LEU:HD12	1:J:390:LEU:N	2.36	0.40
1:A:160:VAL:HG21	1:A:394:THR:HG21	2.03	0.40
1:A:428:HIS:HA	4:A:1965:HOH:O	2.22	0.40
1:B:264:LEU:HD23	1:B:308:ILE:HD13	2.03	0.40
1:C:395:LEU:N	1:C:395:LEU:HD12	2.36	0.40
1:D:162:PRO:HA	1:D:395:LEU:HD11	2.03	0.40
1:D:268:ARG:HD3	1:D:268:ARG:O	2.21	0.40
1:G:72:ALA:HB2	1:G:91:TYR:CD1	2.56	0.40
1:A:263:ALA:HB2	1:H:263:ALA:HB2	2.03	0.40
1:B:22:LYS:CD	1:F:65:GLU:HG3	2.51	0.40
1:C:160:VAL:HG21	1:C:394:THR:HG21	2.03	0.40
1:E:191:ASP:HB3	1:E:193:ASN:ND2	2.35	0.40
1:F:411:ALA:O	1:F:415:ILE:HG13	2.20	0.40
1:G:183:ASN:OD1	1:G:406:ARG:NH1	2.51	0.40
1:H:63:GLU:HG2	1:H:66:ARG:H	1.86	0.40
1:I:92:PRO:HB2	1:I:94:HIS:CE1	2.56	0.40
1:I:197:PRO:HB2	1:I:199:TYR:CE2	2.56	0.40
1:J:268:ARG:HD3	1:J:268:ARG:O	2.21	0.40
1:B:414:ALA:O	1:B:418:GLY:N	2.44	0.40
1:C:149:MET:CE	1:C:250:LYS:CB	2.91	0.40
1:E:50:SER:O	1:E:107:SER:OG	2.38	0.40
1:E:435:LEU:O	1:E:436:GLU:C	2.59	0.40
1:F:282:ARG:O	1:F:285:HIS:HB3	2.22	0.40
1:H:78:HIS:CD2	1:H:349:VAL:HG11	2.56	0.40
1:H:79:ASP:OD1	1:H:79:ASP:C	2.60	0.40
1:H:321:GLY:HA3	1:H:368:GLY:O	2.22	0.40
1:I:115:MET:HB2	1:I:115:MET:HE2	1.91	0.40
1:J:174:GLU:OE1	1:J:211:LYS:HE2	2.20	0.40
1:A:331:LEU:HD13	1:A:381:ALA:O	2.22	0.40
1:B:19:PRO:HG3	1:B:75:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:O	1:B:336:LEU:CD2	2.69	0.40
1:C:18:GLU:HB2	4:C:612:HOH:O	2.22	0.40
1:E:104:LEU:HD21	1:E:128:PHE:CE1	2.56	0.40
1:E:258:ILE:HD11	1:I:106:ALA:HA	2.04	0.40
1:F:38:THR:HG1	1:F:41:GLN:HG3	1.86	0.40
1:G:132:LEU:HG	4:G:1820:HOH:O	2.22	0.40
1:G:189:KCX:OQ1	2:G:600:CAP:O3	2.38	0.40
1:J:217:GLU:HG2	1:J:222:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

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	433/444 (98%)	386 (89%)	40 (9%)	7 (2%)	9	8
1	B	435/444 (98%)	408 (94%)	25 (6%)	2 (0%)	29	32
1	C	437/444 (98%)	420 (96%)	16 (4%)	1 (0%)	47	56
1	D	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	47	56
1	E	437/444 (98%)	410 (94%)	25 (6%)	2 (0%)	29	32
1	F	434/444 (98%)	414 (95%)	19 (4%)	1 (0%)	47	56
1	G	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	47	56
1	H	435/444 (98%)	389 (89%)	39 (9%)	7 (2%)	9	8
1	I	435/444 (98%)	415 (95%)	18 (4%)	2 (0%)	29	32
1	J	435/444 (98%)	414 (95%)	20 (5%)	1 (0%)	47	56
All	All	4349/4440 (98%)	4086 (94%)	238 (6%)	25 (1%)	25	27

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	426	LYS
1	B	429	LYS
1	A	34	ALA
1	A	82	ASP
1	A	117	ARG
1	D	284	MET
1	E	420	PRO
1	H	232	ALA
1	H	443	PRO
1	A	286	ALA
1	E	436	GLU
1	H	318	ALA
1	H	420	PRO
1	I	10	ASP
1	C	327	ARG
1	G	284	MET
1	J	284	MET
1	A	51	SER
1	B	420	PRO
1	H	325	GLY
1	A	325	GLY
1	F	325	GLY
1	H	401	PRO
1	I	8	ILE
1	A	344	PRO

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/356 (90%)	313 (98%)	8 (2%)	47	58
1	B	331/356 (93%)	322 (97%)	9 (3%)	44	55
1	C	336/356 (94%)	327 (97%)	9 (3%)	44	55
1	D	339/356 (95%)	333 (98%)	6 (2%)	59	70
1	E	335/356 (94%)	329 (98%)	6 (2%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	338/356 (95%)	329 (97%)	9 (3%)	44	55
1	G	340/356 (96%)	333 (98%)	7 (2%)	53	65
1	H	329/356 (92%)	322 (98%)	7 (2%)	53	65
1	I	336/356 (94%)	331 (98%)	5 (2%)	65	76
1	J	337/356 (95%)	333 (99%)	4 (1%)	71	82
All	All	3342/3560 (94%)	3272 (98%)	70 (2%)	53	65

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	PHE
1	A	85	TRP
1	A	183	ASN
1	A	235	LEU
1	A	268	ARG
1	A	324	GLU
1	A	363	PHE
1	A	389	GLN
1	B	122	ARG
1	B	154	ASP
1	B	268	ARG
1	B	336	LEU
1	B	347	ASN
1	B	352	LEU
1	B	363	PHE
1	B	376	GLN
1	B	389	GLN
1	C	73	LYS
1	C	191	ASP
1	C	207	GLU
1	C	235	LEU
1	C	268	ARG
1	C	322	LYS
1	C	363	PHE
1	C	389	GLN
1	C	433	ARG
1	D	10	ASP
1	D	122	ARG
1	D	268	ARG
1	D	347	ASN

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Mol	Chain	Res	Type
1	D	363	PHE
1	D	426	LYS
1	E	73	LYS
1	E	122	ARG
1	E	193	ASN
1	E	235	LEU
1	E	363	PHE
1	E	389	GLN
1	F	87	VAL
1	F	122	ARG
1	F	181	LEU
1	F	235	LEU
1	F	328	ASP
1	F	347	ASN
1	F	363	PHE
1	F	389	GLN
1	F	433	ARG
1	G	122	ARG
1	G	268	ARG
1	G	336	LEU
1	G	347	ASN
1	G	363	PHE
1	G	389	GLN
1	G	422	ASP
1	H	7	THR
1	H	235	LEU
1	H	336	LEU
1	H	363	PHE
1	H	389	GLN
1	H	406	ARG
1	H	419	ILE
1	I	73	LYS
1	I	122	ARG
1	I	149	MET
1	I	268	ARG
1	I	363	PHE
1	J	122	ARG
1	J	268	ARG
1	J	363	PHE
1	J	389	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	183	ASN
1	A	312	GLN
1	A	354	GLN
1	A	417	GLN
1	B	183	ASN
1	B	312	GLN
1	B	347	ASN
1	B	354	GLN
1	B	376	GLN
1	C	312	GLN
1	C	354	GLN
1	C	376	GLN
1	C	410	GLN
1	C	440	HIS
1	D	312	GLN
1	D	347	ASN
1	D	354	GLN
1	D	417	GLN
1	D	440	HIS
1	E	193	ASN
1	E	239	GLN
1	E	312	GLN
1	E	314	HIS
1	E	354	GLN
1	E	410	GLN
1	F	64	GLN
1	F	239	GLN
1	F	312	GLN
1	F	347	ASN
1	F	354	GLN
1	G	239	GLN
1	G	312	GLN
1	G	347	ASN
1	G	354	GLN
1	G	417	GLN
1	G	440	HIS
1	H	78	HIS
1	H	312	GLN
1	H	354	GLN
1	H	410	GLN
1	H	440	HIS
1	I	218	ASN

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Mol	Chain	Res	Type
1	I	239	GLN
1	I	285	HIS
1	I	312	GLN
1	I	354	GLN
1	I	376	GLN
1	I	410	GLN
1	J	64	GLN
1	J	239	GLN
1	J	312	GLN
1	J	354	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#|Z| > 2$
1	KCX	E	189	3,1	9,11,12	0.86	0	5,12,14	1.57	1 (20%)
1	KCX	I	189	3,1	9,11,12	0.88	0	5,12,14	1.36	1 (20%)
1	KCX	A	189	3,1	9,11,12	0.85	0	5,12,14	1.63	1 (20%)
1	KCX	C	189	3,1	9,11,12	0.85	0	5,12,14	1.34	1 (20%)
1	KCX	G	189	3,1	9,11,12	0.86	0	5,12,14	1.44	1 (20%)
1	KCX	F	189	3,1	9,11,12	0.80	0	5,12,14	1.64	1 (20%)
1	KCX	D	189	3,1	9,11,12	0.83	0	5,12,14	1.51	1 (20%)
1	KCX	H	189	3,1	9,11,12	0.85	0	5,12,14	1.49	1 (20%)
1	KCX	J	189	3,1	9,11,12	0.84	0	5,12,14	1.60	1 (20%)
1	KCX	B	189	3,1	9,11,12	0.86	0	5,12,14	1.60	1 (20%)

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
1	KCX	E	189	3,1	-	0/9/10/12	-
1	KCX	I	189	3,1	-	0/9/10/12	-
1	KCX	A	189	3,1	-	0/9/10/12	-
1	KCX	C	189	3,1	-	0/9/10/12	-
1	KCX	G	189	3,1	-	0/9/10/12	-
1	KCX	F	189	3,1	-	0/9/10/12	-
1	KCX	D	189	3,1	-	0/9/10/12	-
1	KCX	H	189	3,1	-	0/9/10/12	-
1	KCX	J	189	3,1	-	0/9/10/12	-
1	KCX	B	189	3,1	-	0/9/10/12	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	189	KCX	OQ1-CX-NZ	-3.36	119.75	124.96
1	J	189	KCX	OQ1-CX-NZ	-3.32	119.81	124.96
1	A	189	KCX	OQ1-CX-NZ	-3.31	119.83	124.96
1	B	189	KCX	OQ1-CX-NZ	-3.27	119.89	124.96
1	E	189	KCX	OQ1-CX-NZ	-3.23	119.94	124.96
1	D	189	KCX	OQ1-CX-NZ	-3.21	119.99	124.96
1	G	189	KCX	OQ1-CX-NZ	-3.06	120.21	124.96
1	H	189	KCX	OQ1-CX-NZ	-3.02	120.28	124.96
1	I	189	KCX	OQ1-CX-NZ	-2.88	120.50	124.96
1	C	189	KCX	OQ1-CX-NZ	-2.82	120.59	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	189	KCX	1	0
1	H	189	KCX	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#|Z| > 2$
2	CAP	J	600	3	17,20,20	0.88	0	22,31,31	0.80	0
2	CAP	F	600	3	17,20,20	0.85	0	22,31,31	0.80	0
2	CAP	D	600	3	17,20,20	0.86	0	22,31,31	0.78	0
2	CAP	I	600	3	17,20,20	0.84	0	22,31,31	0.81	0
2	CAP	E	600	3	17,20,20	0.88	0	22,31,31	0.80	0
2	CAP	A	600	3	17,20,20	0.86	0	22,31,31	0.80	0
2	CAP	G	600	3	17,20,20	0.86	0	22,31,31	0.80	0
2	CAP	B	600	3	17,20,20	0.85	0	22,31,31	0.78	0
2	CAP	C	600	3	17,20,20	0.84	0	22,31,31	0.76	0
2	CAP	H	600	3	17,20,20	0.83	0	22,31,31	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	J	600	3	-	8/29/29/29	-
2	CAP	F	600	3	-	6/29/29/29	-
2	CAP	D	600	3	-	6/29/29/29	-
2	CAP	I	600	3	-	6/29/29/29	-
2	CAP	E	600	3	-	8/29/29/29	-
2	CAP	A	600	3	-	6/29/29/29	-
2	CAP	G	600	3	-	6/29/29/29	-
2	CAP	B	600	3	-	7/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	C	600	3	-	7/29/29/29	-
2	CAP	H	600	3	-	9/29/29/29	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	CAP	O6-C-C2-C1
2	A	600	CAP	O7-C-C2-C1
2	A	600	CAP	O6-C-C2-O2
2	A	600	CAP	O7-C-C2-O2
2	A	600	CAP	O3-C3-C4-O4
2	B	600	CAP	O6-C-C2-C1
2	B	600	CAP	O7-C-C2-C1
2	B	600	CAP	O6-C-C2-O2
2	B	600	CAP	O7-C-C2-O2
2	B	600	CAP	O3-C3-C4-O4
2	C	600	CAP	O6-C-C2-C1
2	C	600	CAP	O7-C-C2-C1
2	C	600	CAP	O6-C-C2-O2
2	C	600	CAP	O7-C-C2-O2
2	C	600	CAP	C2-C3-C4-O4
2	C	600	CAP	O3-C3-C4-O4
2	D	600	CAP	O6-C-C2-C1
2	D	600	CAP	O7-C-C2-C1
2	D	600	CAP	O6-C-C2-O2
2	D	600	CAP	O7-C-C2-O2
2	E	600	CAP	O1-C1-C2-C
2	E	600	CAP	O1-C1-C2-O2
2	E	600	CAP	C2-C3-C4-O4
2	E	600	CAP	O3-C3-C4-O4
2	F	600	CAP	O6-C-C2-C1
2	F	600	CAP	O7-C-C2-C1
2	F	600	CAP	O6-C-C2-O2
2	F	600	CAP	O7-C-C2-O2
2	F	600	CAP	O3-C3-C4-O4
2	G	600	CAP	O6-C-C2-C1
2	G	600	CAP	O7-C-C2-C1

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Mol	Chain	Res	Type	Atoms
2	G	600	CAP	O6-C-C2-O2
2	G	600	CAP	O7-C-C2-O2
2	H	600	CAP	O6-C-C2-C1
2	H	600	CAP	O7-C-C2-C1
2	H	600	CAP	O6-C-C2-O2
2	H	600	CAP	O7-C-C2-O2
2	H	600	CAP	C2-C3-C4-O4
2	H	600	CAP	O3-C3-C4-O4
2	I	600	CAP	O6-C-C2-C1
2	I	600	CAP	O7-C-C2-C1
2	I	600	CAP	O6-C-C2-O2
2	I	600	CAP	O7-C-C2-O2
2	I	600	CAP	O3-C3-C4-O4
2	J	600	CAP	O6-C-C2-C3
2	J	600	CAP	O6-C-C2-O2
2	J	600	CAP	O7-C-C2-O2
2	J	600	CAP	O6-C-C2-C1
2	J	600	CAP	O7-C-C2-C1
2	A	600	CAP	O2-C2-C3-C4
2	B	600	CAP	O2-C2-C3-C4
2	C	600	CAP	O2-C2-C3-C4
2	D	600	CAP	O2-C2-C3-C4
2	E	600	CAP	O2-C2-C3-C4
2	F	600	CAP	O2-C2-C3-C4
2	G	600	CAP	O2-C2-C3-C4
2	H	600	CAP	O2-C2-C3-C4
2	I	600	CAP	O2-C2-C3-C4
2	J	600	CAP	O2-C2-C3-C4
2	D	600	CAP	O3-C3-C4-O4
2	G	600	CAP	O3-C3-C4-O4
2	E	600	CAP	C5-O5-P2-O4P
2	J	600	CAP	O7-C-C2-C3
2	H	600	CAP	C1-O1-P1-O2P
2	J	600	CAP	O3-C3-C4-O4
2	B	600	CAP	C5-O5-P2-O4P
2	E	600	CAP	O1-C1-C2-C3
2	H	600	CAP	C2-C3-C4-C5
2	E	600	CAP	O4-C4-C5-O5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

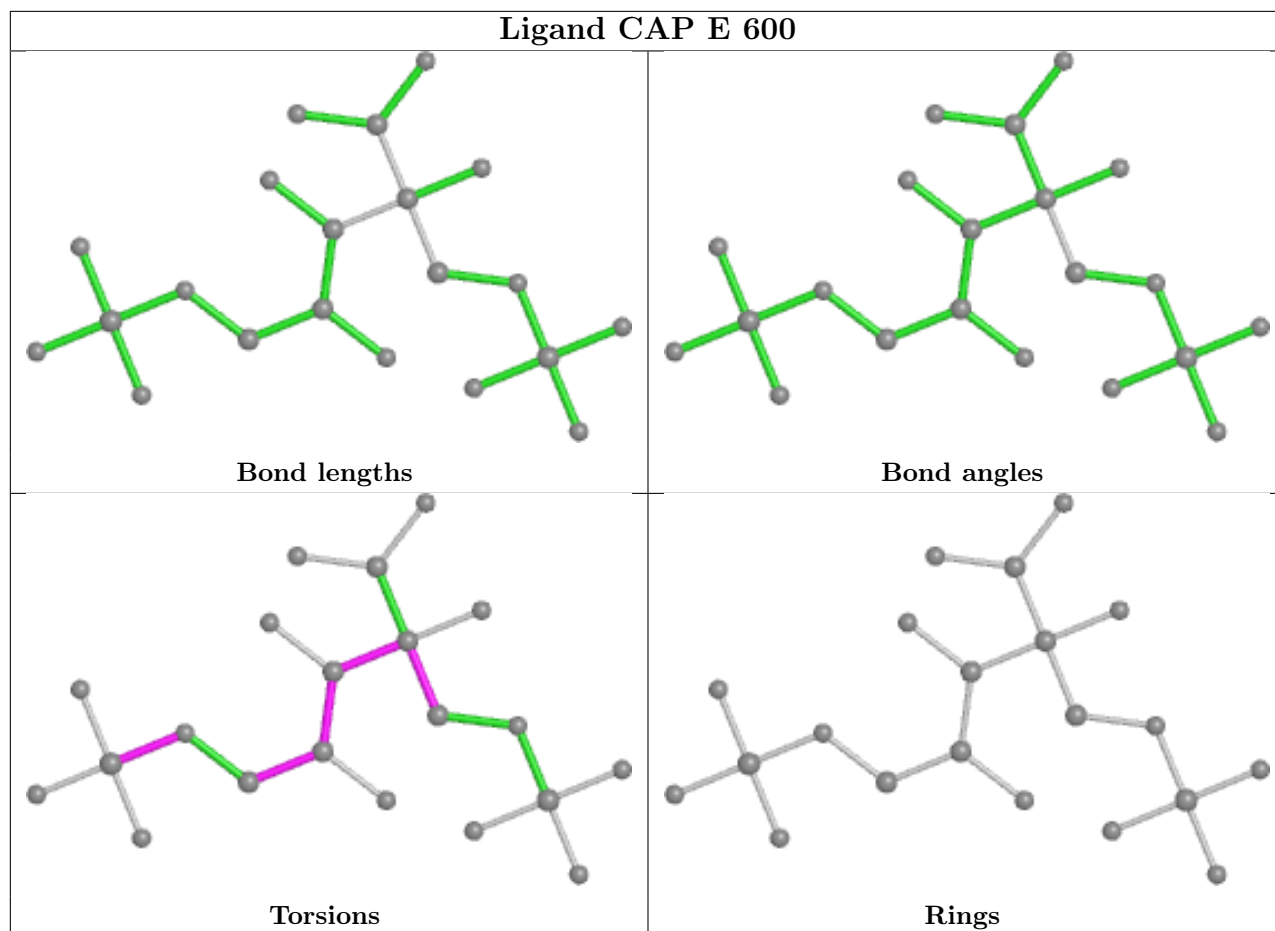| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	600	CAP	2	0
2	G	600	CAP	1	0
2	B	600	CAP	1	0
2	C	600	CAP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
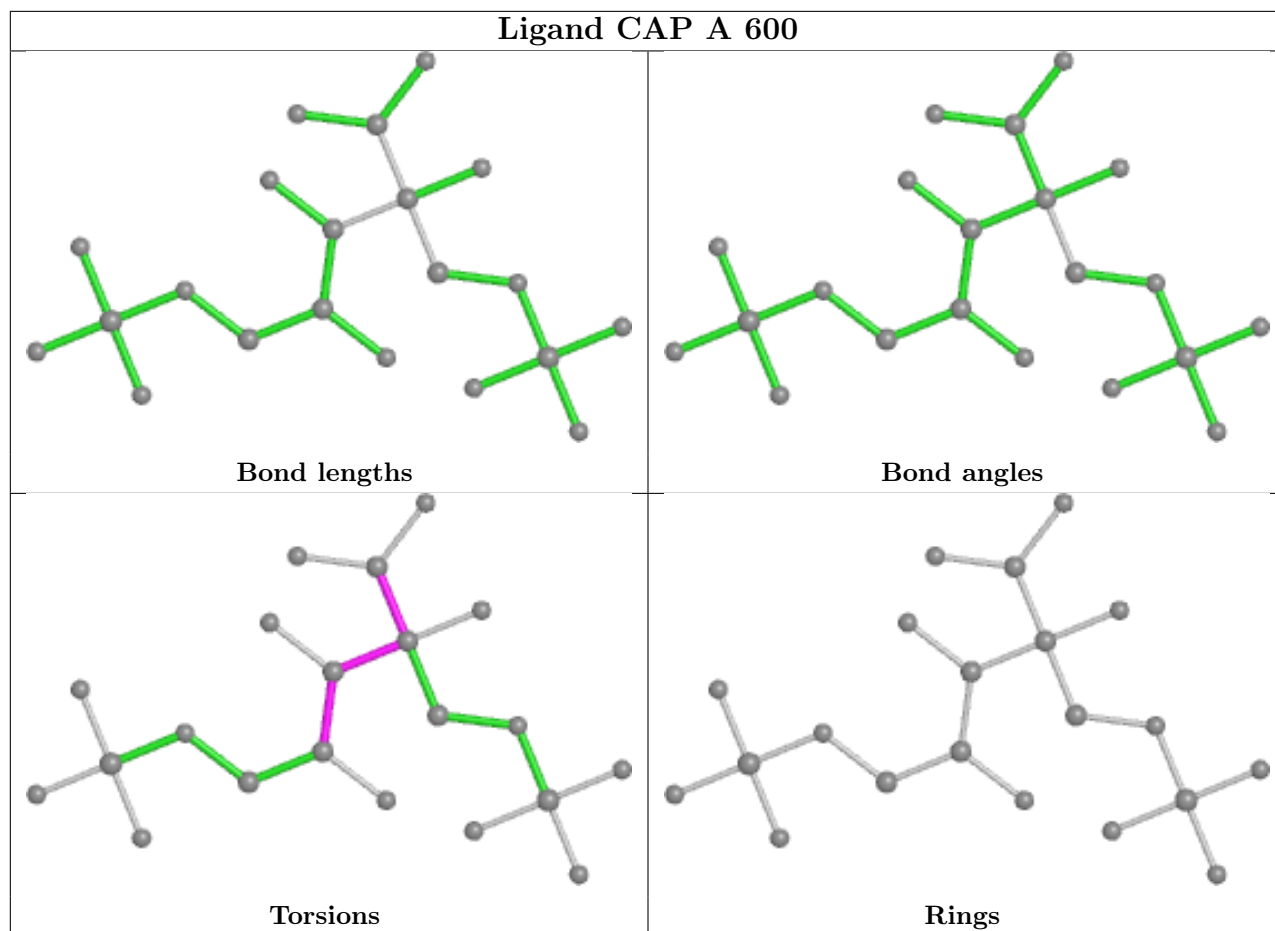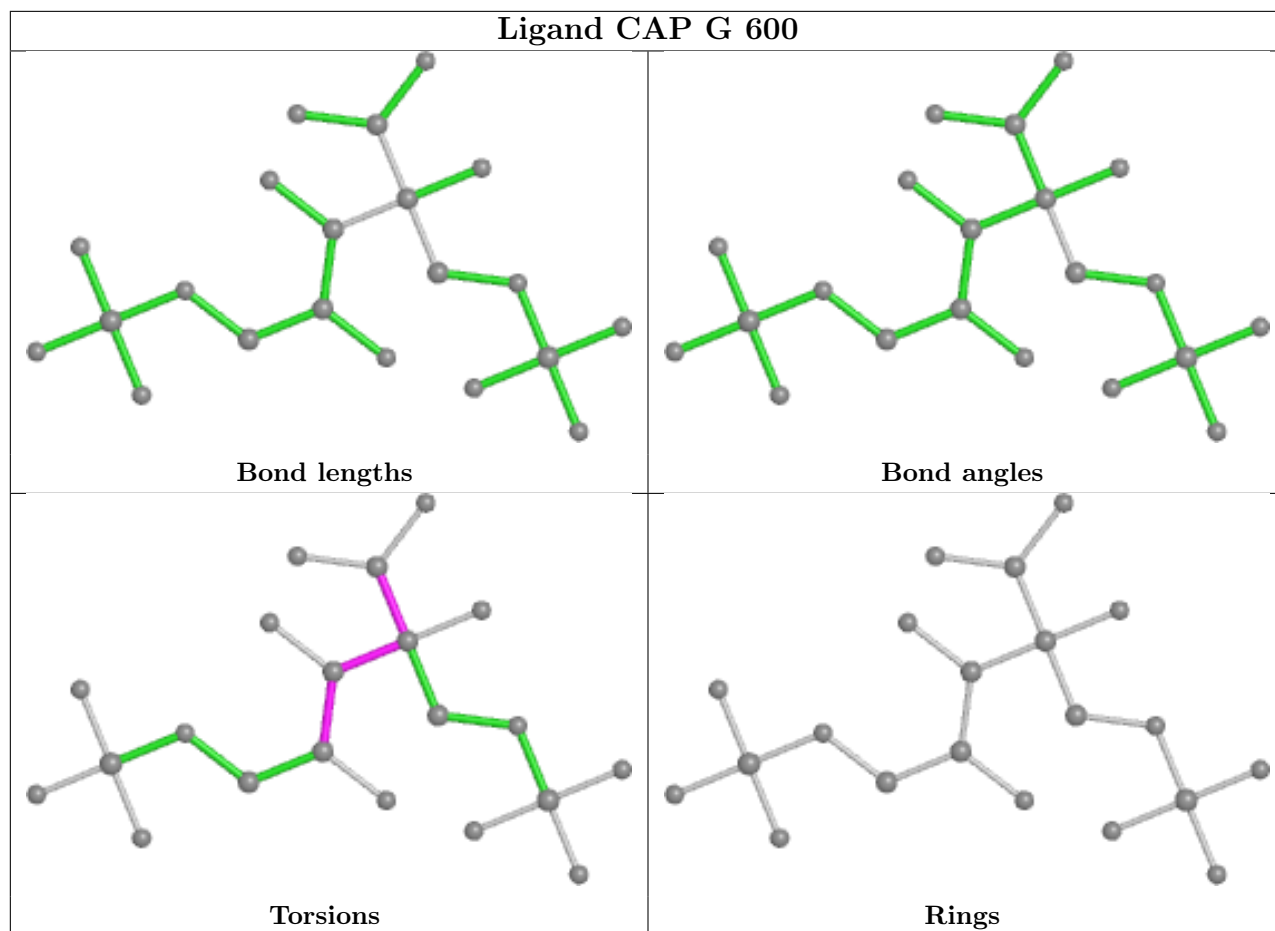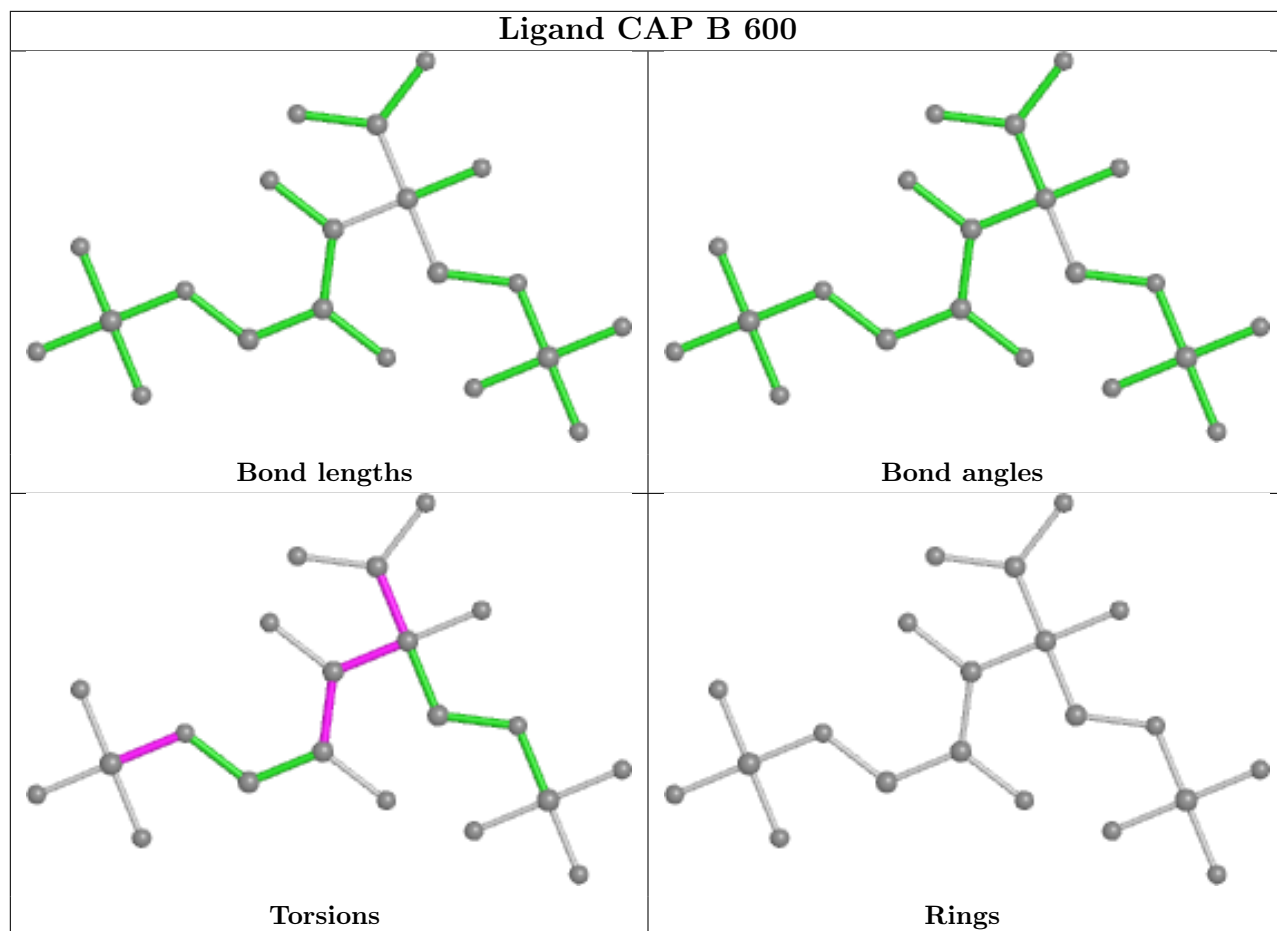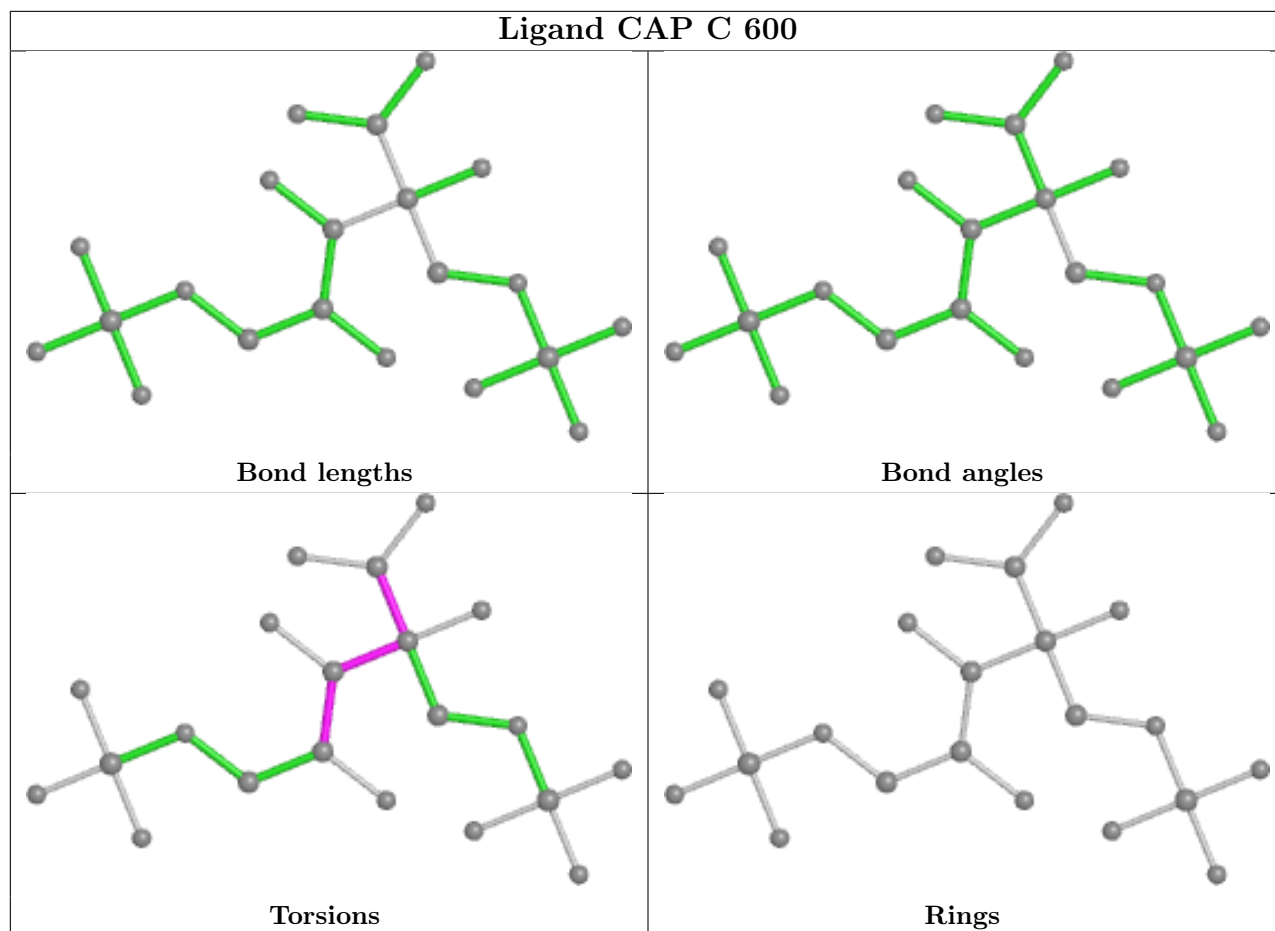
Ligand CAP J 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP F 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP D 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP I 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP E 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP G 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CAP H 600

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	435/444 (97%)	0.83	43 (9%)	7	11	28, 41, 56, 60	0
1	B	437/444 (98%)	0.50	35 (8%)	12	18	19, 32, 62, 65	0
1	C	439/444 (98%)	0.27	17 (3%)	39	52	17, 27, 49, 52	0
1	D	436/444 (98%)	0.11	10 (2%)	60	70	16, 24, 35, 42	0
1	E	439/444 (98%)	0.46	41 (9%)	8	14	18, 28, 58, 60	0
1	F	436/444 (98%)	0.32	20 (4%)	32	45	18, 29, 45, 51	0
1	G	436/444 (98%)	0.26	9 (2%)	63	74	18, 31, 44, 48	0
1	H	437/444 (98%)	0.79	52 (11%)	4	7	27, 37, 66, 66	0
1	I	437/444 (98%)	0.23	22 (5%)	28	41	17, 28, 47, 53	0
1	J	437/444 (98%)	0.39	35 (8%)	12	18	16, 25, 59, 60	0
All	All	4369/4440 (98%)	0.42	284 (6%)	18	27	16, 30, 52, 66	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	7.3
1	J	434	ALA	6.6
1	E	441	VAL	6.4
1	E	425	ALA	6.2
1	E	415	ILE	6.1
1	J	425	ALA	5.7
1	J	421	LEU	5.7
1	E	418	GLY	5.6
1	B	421	LEU	5.6
1	E	421	LEU	5.5
1	E	434	ALA	5.5
1	A	59	TYR	5.1
1	B	441	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	398	PRO	4.9
1	A	54	THR	4.9
1	H	421	LEU	4.8
1	H	426	LYS	4.7
1	H	441	VAL	4.7
1	J	424	TYR	4.6
1	D	59	TYR	4.5
1	B	424	TYR	4.4
1	I	57	THR	4.3
1	E	377	PRO	4.3
1	I	434	ALA	4.3
1	C	5	PHE	4.2
1	F	59	TYR	4.2
1	A	85	TRP	4.1
1	G	59	TYR	4.1
1	E	414	ALA	4.0
1	H	425	ALA	4.0
1	J	7	THR	4.0
1	H	434	ALA	4.0
1	B	59	TYR	4.0
1	A	36	GLY	4.0
1	A	13	VAL	4.0
1	I	59	TYR	3.9
1	J	381	ALA	3.9
1	H	36	GLY	3.9
1	E	433	ARG	3.9
1	E	426	LYS	3.8
1	I	421	LEU	3.8
1	H	398	PRO	3.8
1	I	425	ALA	3.8
1	J	414	ALA	3.8
1	G	57	THR	3.8
1	J	427	THR	3.8
1	E	424	TYR	3.8
1	C	7	THR	3.8
1	H	8	ILE	3.7
1	B	419	ILE	3.7
1	E	427	THR	3.7
1	F	427	THR	3.6
1	E	5	PHE	3.6
1	E	422	ASP	3.6
1	H	422	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	58	LEU	3.6
1	H	85	TRP	3.6
1	E	7	THR	3.5
1	H	396	GLY	3.5
1	J	422	ASP	3.4
1	C	421	LEU	3.4
1	D	54	THR	3.4
1	J	420	PRO	3.4
1	I	10	ASP	3.4
1	A	414	ALA	3.4
1	H	431	LEU	3.4
1	H	414	ALA	3.4
1	C	441	VAL	3.3
1	J	426	LYS	3.3
1	J	398	PRO	3.3
1	F	426	LYS	3.3
1	E	387	VAL	3.3
1	F	421	LEU	3.2
1	I	58	LEU	3.2
1	E	396	GLY	3.2
1	E	420	PRO	3.2
1	D	58	LEU	3.2
1	D	9	TYR	3.2
1	I	9	TYR	3.2
1	E	218	ASN	3.2
1	A	57	THR	3.2
1	C	6	ASP	3.2
1	B	398	PRO	3.1
1	A	78	HIS	3.1
1	C	425	ALA	3.1
1	J	415	ILE	3.1
1	A	11	TYR	3.1
1	J	387	VAL	3.1
1	F	418	GLY	3.1
1	H	435	LEU	3.1
1	J	377	PRO	3.1
1	B	435	LEU	3.0
1	E	432	ALA	3.0
1	E	59	TYR	3.0
1	B	417	GLN	3.0
1	C	420	PRO	3.0
1	A	418	GLY	3.0

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	J	418	GLY	3.0
1	J	396	GLY	3.0
1	B	427	THR	2.9
1	A	37	TYR	2.9
1	B	8	ILE	2.9
1	A	56	THR	2.9
1	H	7	THR	2.9
1	H	373	GLY	2.9
1	I	8	ILE	2.9
1	J	161	VAL	2.9
1	B	422	ASP	2.8
1	F	425	ALA	2.8
1	I	427	THR	2.8
1	J	433	ARG	2.8
1	H	283	ALA	2.8
1	B	373	GLY	2.8
1	J	439	GLY	2.8
1	B	160	VAL	2.8
1	F	420	PRO	2.8
1	H	438	TRP	2.8
1	E	6	ASP	2.8
1	G	65	GLU	2.8
1	H	274	TYR	2.8
1	E	444	VAL	2.8
1	H	418	GLY	2.8
1	H	293	TYR	2.8
1	H	432	ALA	2.7
1	J	444	VAL	2.7
1	H	35	GLU	2.7
1	A	35	GLU	2.7
1	B	418	GLY	2.7
1	A	40	GLU	2.7
1	C	35	GLU	2.7
1	A	29	PHE	2.7
1	A	426	LYS	2.7
1	B	439	GLY	2.7
1	H	379	ILE	2.7
1	A	43	ALA	2.7
1	C	434	ALA	2.7
1	H	424	TYR	2.7
1	B	438	TRP	2.6
1	B	218	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	426	LYS	2.6
1	A	16	GLY	2.6
1	B	161	VAL	2.6
1	H	420	PRO	2.6
1	E	392	GLY	2.6
1	A	419	ILE	2.6
1	A	427	THR	2.6
1	J	59	TYR	2.6
1	I	426	LYS	2.6
1	J	373	GLY	2.6
1	F	218	ASN	2.6
1	I	436	GLU	2.6
1	E	412	ILE	2.6
1	A	87	VAL	2.5
1	A	115	MET	2.5
1	J	441	VAL	2.5
1	F	36	GLY	2.5
1	A	318	ALA	2.5
1	A	50	SER	2.5
1	B	415	ILE	2.5
1	I	422	ASP	2.5
1	J	438	TRP	2.5
1	D	400	GLY	2.5
1	G	218	ASN	2.5
1	A	109	ALA	2.5
1	H	419	ILE	2.5
1	B	65	GLU	2.5
1	E	438	TRP	2.5
1	G	60	PRO	2.5
1	B	431	LEU	2.5
1	A	376	GLN	2.5
1	C	414	ALA	2.5
1	F	347	ASN	2.5
1	I	53	GLY	2.5
1	A	351	HIS	2.5
1	H	296	ILE	2.5
1	I	419	ILE	2.5
1	B	426	LYS	2.4
1	E	374	ASN	2.4
1	E	442	THR	2.4
1	H	319	GLY	2.4
1	A	417	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	284	MET	2.4
1	D	347	ASN	2.4
1	A	106	ALA	2.4
1	H	443	PRO	2.4
1	I	54	THR	2.4
1	J	442	THR	2.4
1	F	434	ALA	2.4
1	H	287	ALA	2.4
1	H	439	GLY	2.4
1	C	427	THR	2.4
1	H	345	ASP	2.4
1	G	17	TYR	2.4
1	A	347	ASN	2.4
1	B	313	LEU	2.4
1	E	388	LEU	2.4
1	B	377	PRO	2.4
1	F	35	GLU	2.4
1	B	425	ALA	2.4
1	B	434	ALA	2.4
1	E	416	MET	2.4
1	A	31	VAL	2.4
1	I	439	GLY	2.3
1	A	388	LEU	2.3
1	H	58	LEU	2.3
1	J	435	LEU	2.3
1	I	218	ASN	2.3
1	B	440	HIS	2.3
1	D	8	ILE	2.3
1	A	345	ASP	2.3
1	E	436	GLU	2.3
1	F	436	GLU	2.3
1	A	110	GLY	2.3
1	J	227	PHE	2.3
1	D	57	THR	2.3
1	H	323	LEU	2.3
1	E	321	GLY	2.3
1	B	387	VAL	2.3
1	A	283	ALA	2.3
1	H	59	TYR	2.2
1	C	287	ALA	2.2
1	H	286	ALA	2.2
1	B	7	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	352	LEU	2.2
1	C	36	GLY	2.2
1	H	397	HIS	2.2
1	F	343	LYS	2.2
1	B	388	LEU	2.2
1	F	422	ASP	2.2
1	A	284	MET	2.2
1	A	441	VAL	2.2
1	I	387	VAL	2.2
1	H	273	ASP	2.2
1	F	376	GLN	2.2
1	E	161	VAL	2.2
1	G	161	VAL	2.2
1	H	318	ALA	2.2
1	H	437	LYS	2.2
1	J	428	HIS	2.2
1	C	419	ILE	2.2
1	J	8	ILE	2.2
1	B	399	ASP	2.1
1	E	153	LYS	2.1
1	C	436	GLU	2.1
1	E	257	VAL	2.1
1	H	106	ALA	2.1
1	E	148	LYS	2.1
1	B	36	GLY	2.1
1	A	17	TYR	2.1
1	A	274	TYR	2.1
1	I	328	ASP	2.1
1	E	319	GLY	2.1
1	H	81	GLY	2.1
1	I	221	GLY	2.1
1	H	34	ALA	2.1
1	H	378	VAL	2.1
1	B	347	ASN	2.1
1	B	159	GLY	2.1
1	I	60	PRO	2.1
1	H	375	ILE	2.1
1	D	56	THR	2.1
1	F	85	TRP	2.1
1	A	420	PRO	2.1
1	J	218	ASN	2.1
1	G	153	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	110	GLY	2.1
1	J	36	GLY	2.1
1	D	60	PRO	2.1
1	J	388	LEU	2.0
1	E	437	LYS	2.0
1	F	54	THR	2.0
1	J	257	VAL	2.0
1	H	281	HIS	2.0
1	B	390	LEU	2.0
1	G	16	GLY	2.0
1	H	427	THR	2.0
1	C	398	PRO	2.0
1	E	378	VAL	2.0
1	A	75	TYR	2.0
1	J	419	ILE	2.0
1	E	373	GLY	2.0
1	F	81	GLY	2.0
1	H	400	GLY	2.0
1	H	410	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	C	189	12/13	0.96	0.20	24,24,24,24	0
1	KCX	H	189	12/13	0.96	0.20	35,36,37,37	0
1	KCX	A	189	12/13	0.97	0.22	33,33,33,34	0
1	KCX	E	189	12/13	0.97	0.21	22,23,24,24	0
1	KCX	B	189	12/13	0.97	0.23	30,31,32,33	0
1	KCX	I	189	12/13	0.97	0.19	24,25,26,26	0
1	KCX	J	189	12/13	0.97	0.23	22,23,23,24	0
1	KCX	D	189	12/13	0.98	0.20	16,18,19,19	0
1	KCX	F	189	12/13	0.98	0.20	22,22,22,22	0
1	KCX	G	189	12/13	0.98	0.21	21,21,22,23	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CAP	H	600	21/21	0.89	0.22	41,42,42,43	0
2	CAP	E	600	21/21	0.92	0.24	31,37,40,41	0
3	MG	B	500	1/1	0.93	0.10	31,31,31,31	0
2	CAP	A	600	21/21	0.94	0.17	36,38,38,39	0
3	MG	C	500	1/1	0.94	0.17	28,28,28,28	0
3	MG	H	500	1/1	0.94	0.16	37,37,37,37	0
3	MG	I	500	1/1	0.94	0.10	20,20,20,20	0
2	CAP	J	600	21/21	0.95	0.21	31,35,38,38	0
3	MG	G	500	1/1	0.97	0.09	20,20,20,20	0
2	CAP	C	600	21/21	0.97	0.18	30,31,32,32	0
2	CAP	B	600	21/21	0.97	0.16	31,35,36,37	0
2	CAP	G	600	21/21	0.98	0.17	22,25,26,26	0
2	CAP	D	600	21/21	0.98	0.13	16,20,21,21	0
3	MG	E	500	1/1	0.98	0.23	26,26,26,26	0
2	CAP	I	600	21/21	0.98	0.10	18,21,21,22	0
2	CAP	F	600	21/21	0.98	0.12	22,24,24,25	0
3	MG	A	500	1/1	0.98	0.14	28,28,28,28	0
3	MG	F	500	1/1	0.99	0.10	25,25,25,25	0
3	MG	D	500	1/1	0.99	0.08	15,15,15,15	0
3	MG	J	500	1/1	0.99	0.13	19,19,19,19	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.
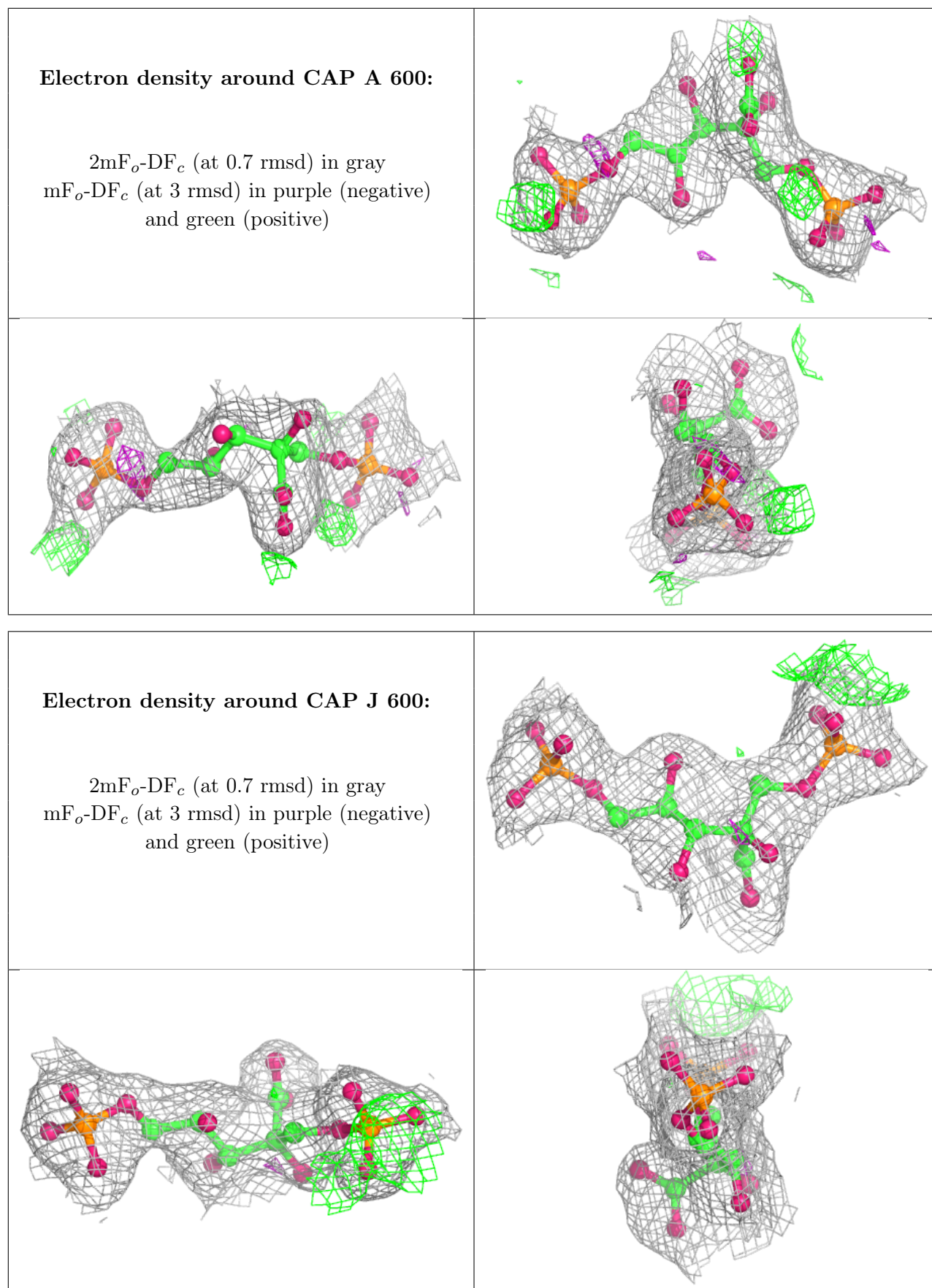
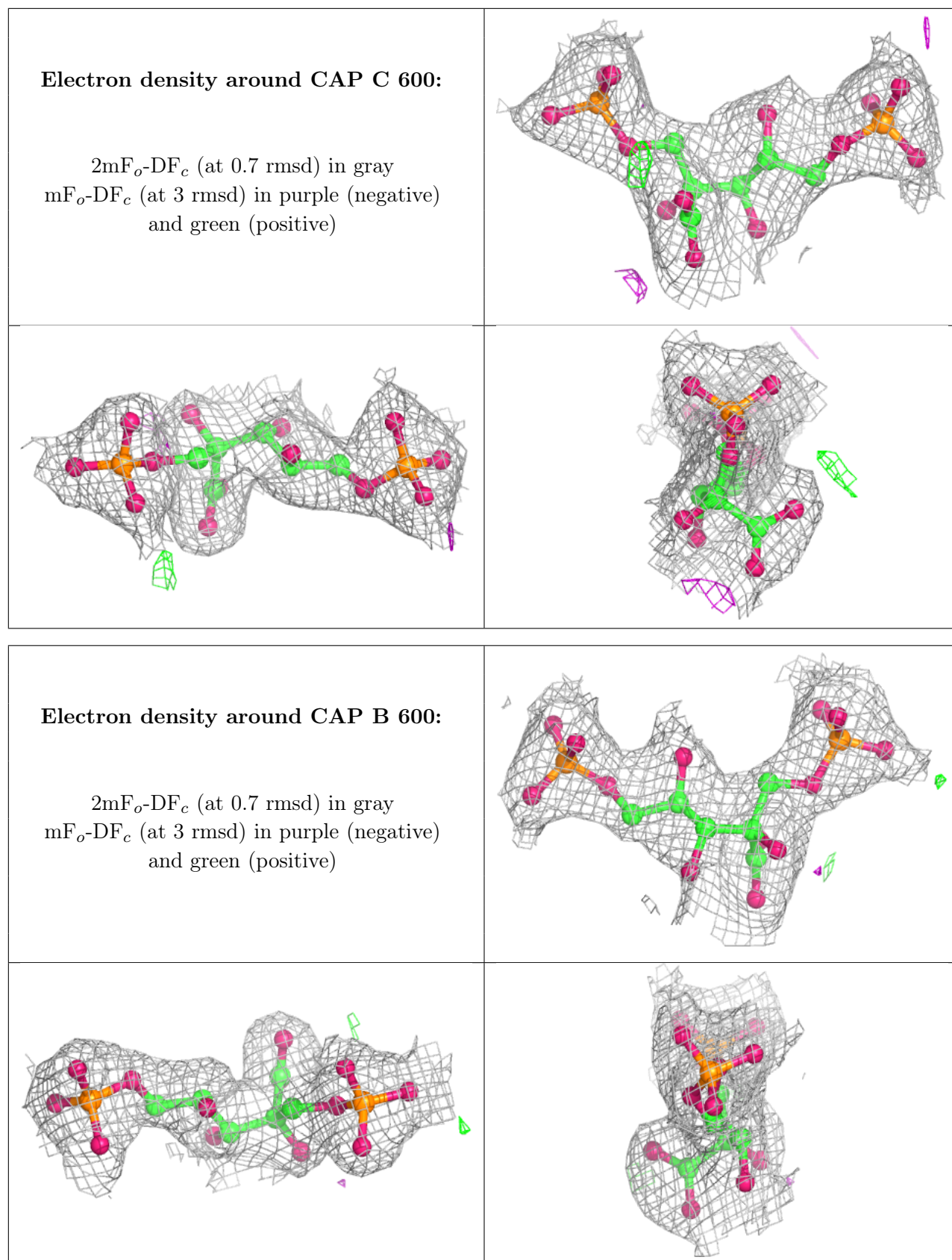**Electron density around CAP H 600:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
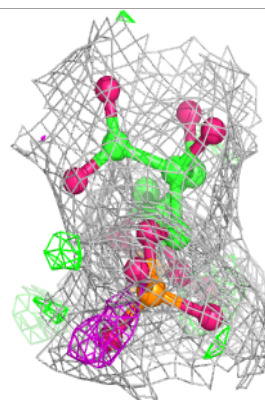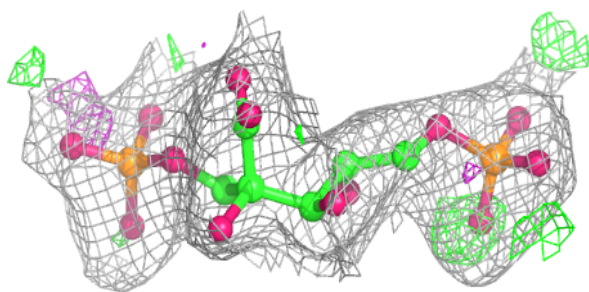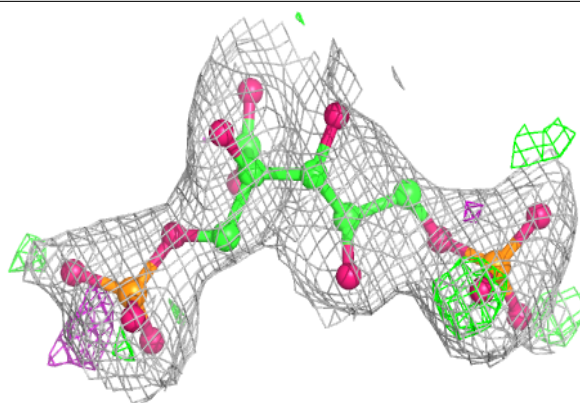
Electron density around CAP E 600:

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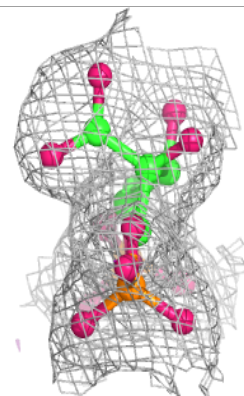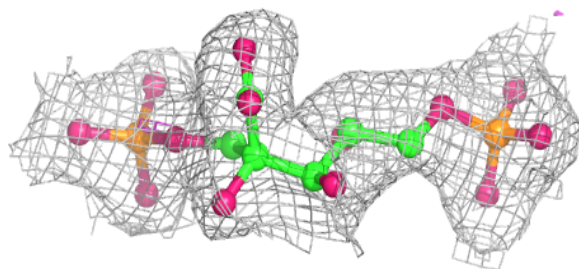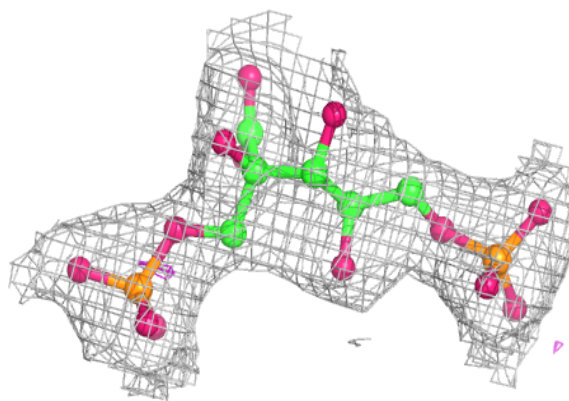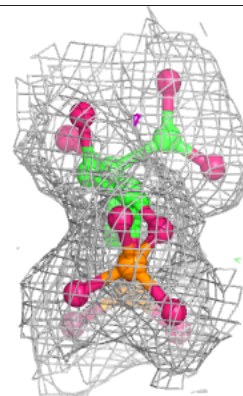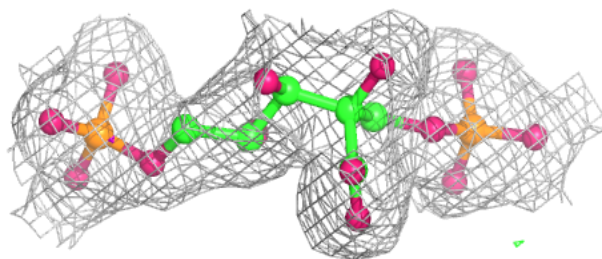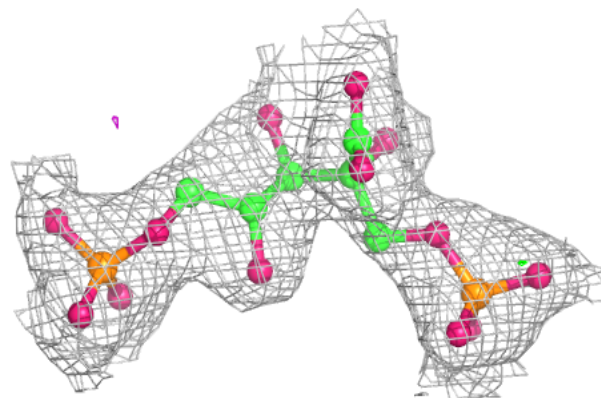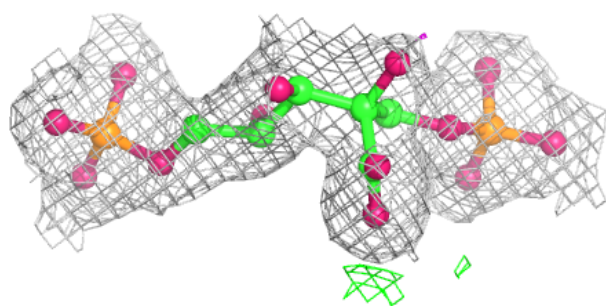$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CAP A 600:

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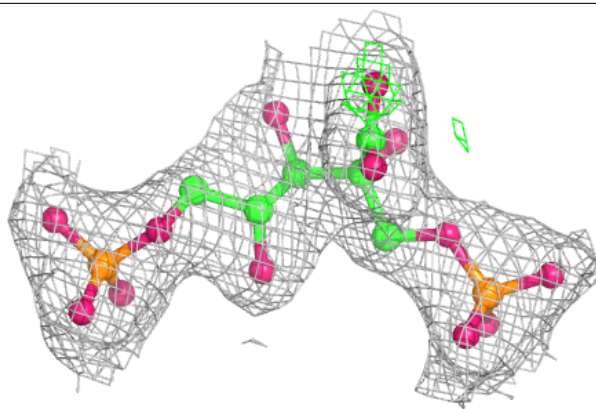and green (positive)

Electron density around CAP J 600:

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

Electron density around CAP C 600:

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

Electron density around CAP B 600:

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

Electron density around CAP G 600:

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

Electron density around CAP D 600:

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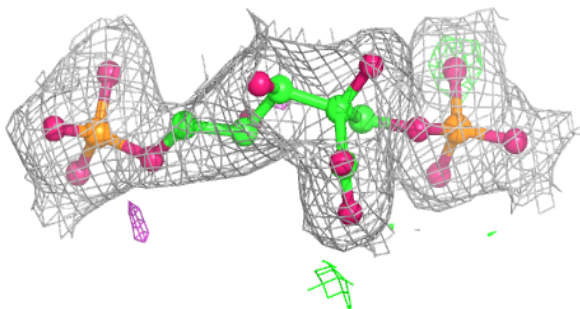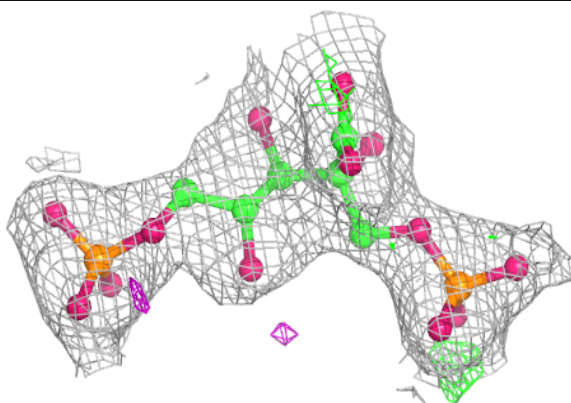and green (positive)

Electron density around CAP I 600:

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

Electron density around CAP F 600:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.