



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:49 AM UTC

PDB ID : 8GJH / pdb_00008gjh
Title : Salmonella ArnA
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Deposited on : 2023-03-15
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

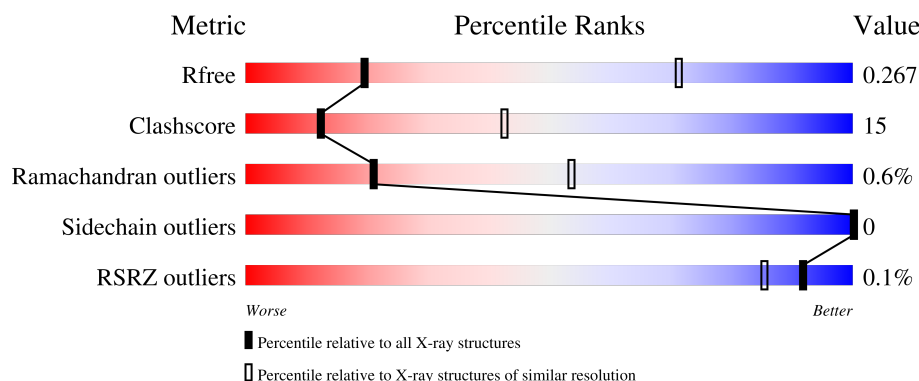
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	660	
1	B	660	
1	C	660	
1	D	660	
1	E	660	

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Mol	Chain	Length	Quality of chain
1	F	660	62% 34% ..

2 Entry composition [i](#)

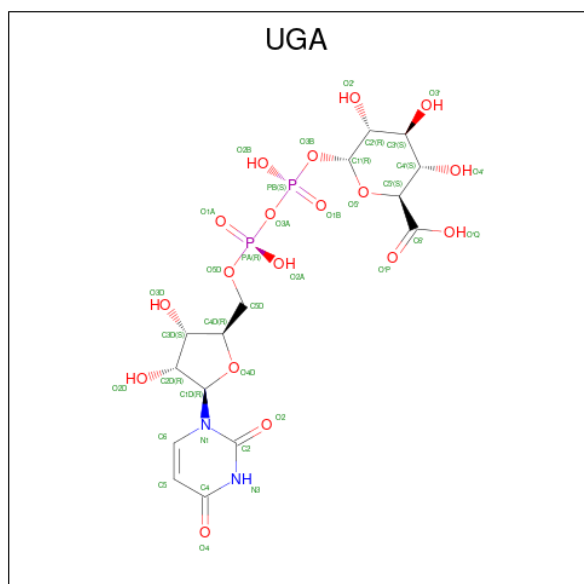
There are 2 unique types of molecules in this entry. The entry contains 30375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional polymyxin resistance protein ArnA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5028	3196	893	918	21			
1	B	638	Total	C	N	O	S	0	0	0
			5023	3193	892	917	21			
1	C	639	Total	C	N	O	S	0	0	0
			5028	3196	893	918	21			
1	D	638	Total	C	N	O	S	0	0	0
			5023	3193	892	917	21			
1	E	638	Total	C	N	O	S	0	0	0
			5023	3193	892	917	21			
1	F	639	Total	C	N	O	S	0	0	0
			5028	3196	893	918	21			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (CCD ID: UGA) (formula: $C_{15}H_{22}N_2O_{18}P_2$) (labeled as "Ligand of Interest" by depositor).

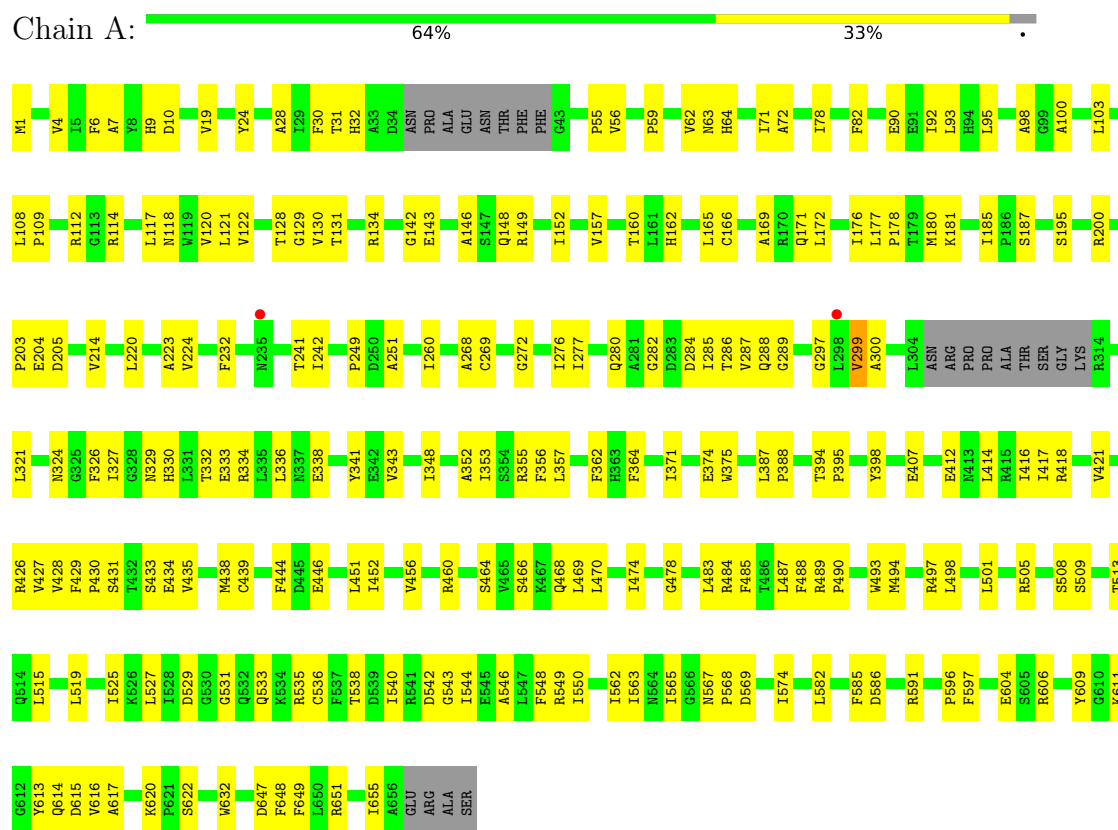


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	E	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	F	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

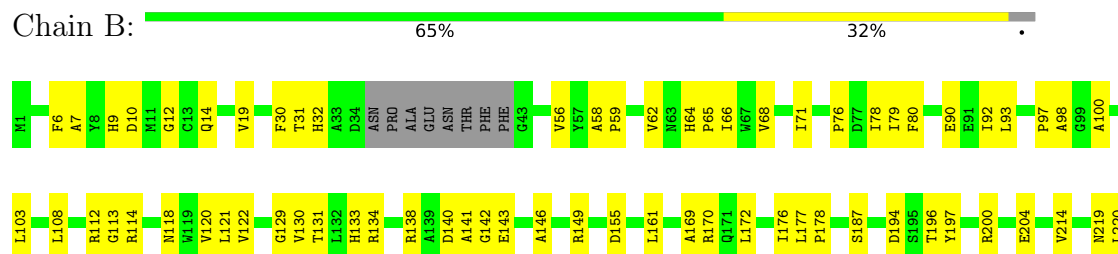
3 Residue-property plots

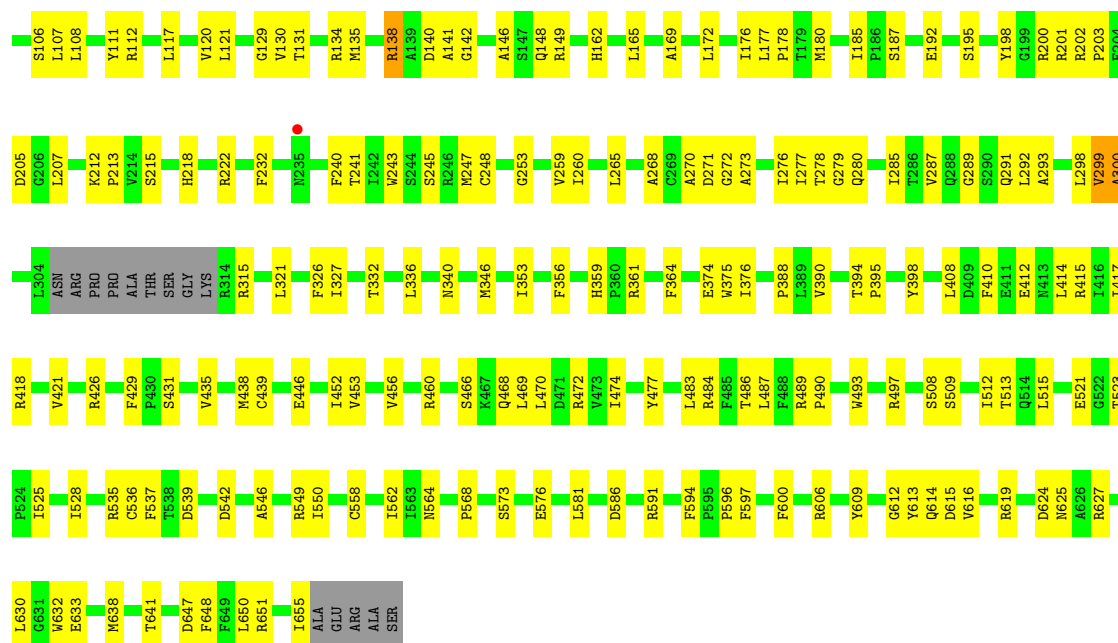
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



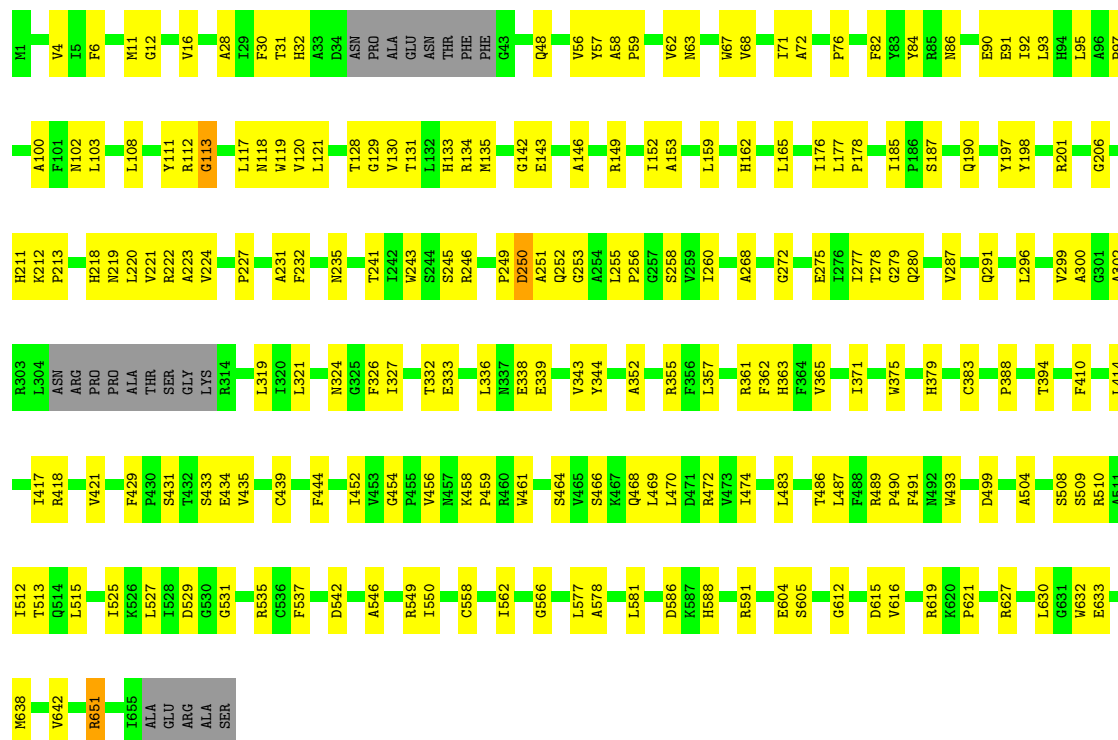
- Molecule 1: Bifunctional polymyxin resistance protein ArnA





- Molecule 1: Bifunctional polymyxin resistance protein ArnA

Chain E: 65% 31% .



- Molecule 1: Bifunctional polymyxin resistance protein ArnA

Chain F: 62% 34% . .

R619 R620 P621 L630 G631 W632 E633 P634 M638 R639 V642 L650 A656 GLU ARG ALA SER	W493	K494	L498	D499	G631	S500	A503	A504	S508	S509	R510	A511	I512	L527	G531	K534	R535	C536	F537	D542	G543	I544	E545	A546	L547	F548	R549	I550	I551	I563	N564	I565	G566	N567	P568	E571	A572	L580	L581	H588	P589	R606	G612	V613	Q614	D615	V616						
	L389	V390	T394	L408	L414	R415	I416	I417	R418	V421	R426	V427	V428	F429	P430	S431	T432	S433	E434	V435	M438	C439	I452	V453	G454	P455	V456	N457	K458	P459	R460	W461	S464	V465	S466	K467	Q468	L469	L470	I474	Q478	L483	R484	F485	T486	L487	P488	R489	P490				
	L304	ASN	ARG	PRO	PRO	ALA	THR	SER	GLY	LYS	R314	L319	I320	L321	N324	G325	F326	I327	L331	T332	E333	R334	L335	L336	N337	E338	Y344	A352	I353	S354	R355	F356	L357	F362	H363	F364	D368	I369	S370	I371	H372	W375	I376	E377	Y378	H379	V380	K381	V386	L387	P388		
	E192	S195	Y198	G199	R200	K212	P213	V214	R222	A223	F232	S233	Y234	N235	T241	I242	W243	S244	S245	R246	M247	C248	P249	D250	A251	Q252	I260	R266	G272	A273	L274	I277	T278	G279	Q280	I285	T286	V287	Q291	L296	G297	L298	V299	A300	G301	A302	R303						
	E90	E91	I92	L93	I5	F6	A7	Y8	H9	D10	M11	G12	I29	F30	T31	H32	A33	D34	ASN	PRO	ALA	GLU	ASN	THR	PHE	PHE	G43	S46	R47	Q48	A49	V56	Y57	A58	P59	V62	M63	H64	P65	I66	W67	V68	D69	R70	I71	D77	I78	I79	F80	S81	Y84	R85	N86
	L304	ASN	ARG	PRO	PRO	ALA	THR	SER	GLY	LYS	R314	L319	I320	L321	N324	G325	F326	I327	L331	T332	E333	R334	L335	L336	N337	E338	Y344	A352	I353	S354	R355	F356	L357	F362	H363	F364	D368	I369	S370	I371	H372	W375	I376	E377	Y378	H379	V380	K381	V386	L387	P388		
	E192	S195	Y198	G199	R200	K212	P213	V214	R222	A223	F232	S233	Y234	N235	T241	I242	W243	S244	S245	R246	M247	C248	P249	D250	A251	Q252	I260	R266	G272	A273	L274	I277	T278	G279	Q280	I285	T286	V287	Q291	L296	G297	L298	V299	A300	G301	A302	R303						
	E90	E91	I92	L93	I5	F6	A7	Y8	H9	D10	M11	G12	I29	F30	T31	H32	A33	D34	ASN	PRO	ALA	GLU	ASN	THR	PHE	PHE	G43	S46	R47	Q48	A49	V56	Y57	A58	P59	V62	M63	H64	P65	I66	W67	V68	D69	R70	I71	D77	I78	I79	F80	S81	Y84	R85	N86
	L304	ASN	ARG	PRO	PRO	ALA	THR	SER	GLY	LYS	R314	L319	I320	L321	N324	G325	F326	I327	L331	T332	E333	R334	L335	L336	N337	E338	Y344	A352	I353	S354	R355	F356	L357	F362	H363	F364	D368	I369	S370	I371	H372	W375	I376	E377	Y378	H379	V380	K381	V386	L387	P388		
	E192	S195	Y198	G199	R200	K212	P213	V214	R222	A223	F232	S233	Y234	N235	T241	I242	W243	S244	S245	R246	M247	C248	P249	D250	A251	Q252	I260	R266	G272	A273	L274	I277	T278	G279	Q280	I285	T286	V287	Q291	L296	G297	L298	V299	A300	G301	A302	R303						
E90	E91	I92	L93	I5	F6	A7	Y8	H9	D10	M11	G12	I29	F30	T31	H32	A33	D34	ASN	PRO	ALA	GLU	ASN	THR	PHE	PHE	G43	S46	R47	Q48	A49	V56	Y57	A58	P59	V62	M63	H64	P65	I66	W67	V68	D69	R70	I71	D77	I78	I79	F80	S81	Y84	R85	N86	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.83Å 129.44Å 140.19Å 62.99° 71.66° 77.76°	Depositor
Resolution (Å)	29.83 – 3.60 29.83 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.83-3.60) 95.0 (29.83-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.218 , 0.267 0.218 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	108.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30375	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UGA

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	0.15	0/5143	0.38	0/6984
1	B	0.14	0/5138	0.37	0/6977
1	C	0.17	0/5143	0.40	0/6984
1	D	0.17	0/5138	0.40	0/6977
1	E	0.16	0/5138	0.39	0/6977
1	F	0.16	0/5143	0.39	0/6984
All	All	0.16	0/30843	0.39	0/41883

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	138	ARG	Sidechain
1	E	651	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5028	0	4994	163	0
1	B	5023	0	4989	156	0
1	C	5028	0	4994	175	0
1	D	5023	0	4989	155	0
1	E	5023	0	4989	159	0
1	F	5028	0	4994	166	0
2	A	37	0	19	2	0
2	B	37	0	19	4	0
2	C	37	0	19	5	0
2	D	37	0	19	3	0
2	E	37	0	19	2	0
2	F	37	0	19	3	0
All	All	30375	0	30063	930	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 15.

All (930) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:181:LYS:NZ	2.16	1.17
1:A:129:GLY:HA3	1:A:149:ARG:HA	1.52	0.91
1:E:299:VAL:HG23	1:E:300:ALA:H	1.37	0.88
1:C:129:GLY:HA3	1:C:149:ARG:HA	1.55	0.86
1:A:582:LEU:HD11	1:A:597:PHE:CE2	2.10	0.85
1:B:321:LEU:HD22	1:B:346:MET:HE2	1.59	0.85
1:D:321:LEU:HD22	1:D:346:MET:HE2	1.60	0.84
1:D:394:THR:HG21	1:D:508:SER:HA	1.61	0.81
1:E:627:ARG:HD3	1:E:633:GLU:HG3	1.62	0.80
1:A:299:VAL:HG22	1:A:300:ALA:H	1.43	0.80
1:E:434:GLU:HG2	1:E:464:SER:HB2	1.66	0.78
1:D:326:PHE:HD2	1:D:327:ILE:HG13	1.50	0.77
1:C:245:SER:HB2	1:C:274:LEU:HD11	1.64	0.77
1:F:251:ALA:HA	1:F:272:GLY:HA2	1.67	0.77
1:E:326:PHE:HD1	1:E:327:ILE:HG13	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ALA:HA	1:E:272:GLY:HA2	1.66	0.76
1:A:326:PHE:HD1	1:A:327:ILE:HG13	1.49	0.76
1:C:134:ARG:HH21	1:C:187:SER:HB3	1.51	0.75
1:E:255:LEU:HD12	1:E:256:PRO:HD2	1.67	0.75
1:A:435:VAL:HG23	1:A:468:GLN:HB2	1.68	0.75
1:B:103:LEU:HD11	1:B:130:VAL:HB	1.69	0.74
1:E:102:ASN:HD22	1:E:133:HIS:HE1	1.36	0.74
1:E:112:ARG:NH2	1:E:190:GLN:OE1	2.19	0.73
1:B:515:LEU:HD22	1:B:525:ILE:HG23	1.70	0.73
1:D:176:ILE:HG22	1:D:180:MET:HE2	1.70	0.73
1:F:234:TYR:HD2	1:F:304:LEU:HD21	1.51	0.72
1:F:59:PRO:HG2	1:F:62:VAL:HG22	1.71	0.72
1:F:129:GLY:HA3	1:F:149:ARG:HA	1.73	0.71
1:B:434:GLU:HG2	1:B:464:SER:HB2	1.70	0.71
1:A:59:PRO:HG2	1:A:62:VAL:HG22	1.72	0.71
1:F:434:GLU:HG2	1:F:464:SER:HB2	1.73	0.71
1:F:619:ARG:HH12	2:F:1100:UGA:H5'1	1.57	0.70
1:B:108:LEU:HB2	1:B:131:THR:HG21	1.74	0.70
1:F:235:ASN:ND2	1:F:296:LEU:HB3	2.07	0.70
1:F:250:ASP:O	1:F:252:GLN:N	2.25	0.70
1:D:515:LEU:HD22	1:D:525:ILE:HG23	1.72	0.69
1:D:624:ASP:OD1	1:D:625:ASN:N	2.25	0.69
1:E:439:CYS:HA	1:E:452:ILE:HD13	1.73	0.69
1:F:390:VAL:HG12	1:F:408:LEU:HD21	1.74	0.69
1:A:251:ALA:HB2	1:A:272:GLY:HA2	1.75	0.68
1:C:435:VAL:HG23	1:C:468:GLN:HB2	1.76	0.68
1:E:235:ASN:HD22	1:E:296:LEU:HB3	1.56	0.68
1:E:578:ALA:HA	1:E:581:LEU:HD12	1.75	0.68
1:B:78:ILE:HG12	1:B:98:ALA:HB3	1.73	0.68
1:C:108:LEU:HB2	1:C:131:THR:HG21	1.75	0.68
1:A:134:ARG:HH22	1:A:185:ILE:HA	1.59	0.68
1:F:108:LEU:HB2	1:F:131:THR:HG21	1.76	0.68
1:B:414:LEU:HD21	1:B:418:ARG:HE	1.59	0.67
1:A:214:VAL:HG22	1:A:269:CYS:HB2	1.75	0.67
1:A:326:PHE:CD1	1:A:327:ILE:HG13	2.29	0.67
1:C:535:ARG:NH2	1:C:615:ASP:OD1	2.26	0.67
1:A:515:LEU:HD22	1:A:525:ILE:HG23	1.75	0.67
1:B:346:MET:HE1	1:B:376:ILE:HD12	1.76	0.67
1:F:588:HIS:HD2	1:F:589:PRO:HD2	1.59	0.67
1:E:16:VAL:HB	1:E:48:GLN:HE22	1.59	0.67
1:B:531:GLY:HA2	1:B:574:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:HIS:HB2	1:C:247:MET:HB3	1.78	0.66
1:E:535:ARG:HB2	1:E:537:PHE:HE1	1.58	0.66
1:B:535:ARG:NH2	1:B:615:ASP:OD1	2.28	0.66
1:B:64:HIS:CD2	1:E:604:GLU:HG2	2.29	0.66
1:B:375:TRP:HZ2	1:C:375:TRP:CZ2	2.14	0.66
1:D:594:PHE:HE2	1:D:650:LEU:HD22	1.61	0.66
1:A:562:ILE:HD12	1:D:456:VAL:HG21	1.78	0.66
1:A:439:CYS:HA	1:A:452:ILE:HD13	1.78	0.66
1:B:326:PHE:HD2	1:B:327:ILE:HG13	1.61	0.66
1:C:67:TRP:O	1:C:71:ILE:N	2.29	0.66
1:C:299:VAL:HG22	1:C:300:ALA:H	1.59	0.66
1:E:232:PHE:HB3	1:E:241:THR:HG22	1.76	0.66
1:C:615:ASP:OD1	1:C:616:VAL:N	2.28	0.65
1:E:581:LEU:HD23	1:E:642:VAL:HG13	1.78	0.65
1:C:323:VAL:HG22	1:C:353:ILE:HG21	1.78	0.65
1:D:232:PHE:HB3	1:D:241:THR:HG22	1.77	0.65
1:D:509:SER:HB2	1:D:513:THR:HG23	1.78	0.65
1:E:129:GLY:HA3	1:E:149:ARG:HA	1.78	0.65
1:F:394:THR:HG21	1:F:508:SER:HA	1.79	0.65
1:D:108:LEU:HB2	1:D:131:THR:HG21	1.77	0.65
1:A:108:LEU:HB2	1:A:131:THR:HG21	1.77	0.65
1:B:113:GLY:HA2	1:B:197:TYR:CD1	2.32	0.65
1:E:159:LEU:HD12	1:E:227:PRO:HD3	1.79	0.65
1:A:501:LEU:HD13	1:A:649:PHE:CD1	2.32	0.64
1:C:156:ASP:OD2	1:C:164:LYS:NZ	2.28	0.64
1:A:326:PHE:HD1	1:A:327:ILE:H	1.42	0.64
1:B:647:ASP:O	1:B:651:ARG:HG2	1.98	0.64
1:C:113:GLY:HA2	1:C:197:TYR:CD1	2.33	0.64
1:C:277:ILE:HG22	1:C:278:THR:HG23	1.78	0.64
1:D:609:TYR:OH	2:D:1100:UGA:H2A1	1.97	0.64
1:B:59:PRO:HG2	1:B:62:VAL:HG22	1.79	0.64
1:E:515:LEU:HD22	1:E:525:ILE:HG23	1.79	0.64
1:F:277:ILE:HG22	1:F:278:THR:HG23	1.80	0.64
1:B:439:CYS:HA	1:B:452:ILE:HD13	1.80	0.64
1:E:134:ARG:HH21	1:E:187:SER:HB3	1.64	0.64
1:C:214:VAL:HG23	1:C:247:MET:HE3	1.79	0.63
1:D:537:PHE:HB2	1:D:638:MET:HE2	1.80	0.63
1:D:417:ILE:HD11	1:D:470:LEU:HD21	1.80	0.63
1:C:434:GLU:HG2	1:C:464:SER:HB2	1.81	0.63
1:D:439:CYS:HA	1:D:452:ILE:HD13	1.80	0.63
1:E:535:ARG:NH2	1:E:615:ASP:OD1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ALA:HA	1:C:272:GLY:HA2	1.80	0.63
1:D:321:LEU:HB2	1:D:388:PRO:HA	1.79	0.63
1:E:108:LEU:HB2	1:E:131:THR:HG21	1.80	0.63
1:E:326:PHE:CD1	1:E:327:ILE:HG13	2.33	0.63
1:D:299:VAL:HG22	1:D:300:ALA:H	1.62	0.63
1:F:245:SER:HB2	1:F:274:LEU:HD11	1.81	0.63
1:A:19:VAL:HG22	1:A:177:LEU:HD21	1.79	0.63
1:D:265:LEU:HD23	1:D:276:ILE:HB	1.80	0.63
1:D:535:ARG:NH2	1:D:615:ASP:OD1	2.30	0.63
1:E:299:VAL:HG23	1:E:300:ALA:N	2.13	0.63
1:E:588:HIS:HE1	1:E:651:ARG:NH2	1.97	0.63
1:A:371:ILE:HD13	1:C:377:GLU:HG2	1.79	0.63
1:A:438:MET:SD	1:A:614:GLN:NE2	2.71	0.62
1:D:528:ILE:HD13	2:D:1100:UGA:HN3	1.63	0.62
1:F:260:ILE:HB	1:F:266:ARG:HB2	1.80	0.62
1:F:326:PHE:CD2	1:F:327:ILE:HG13	2.33	0.62
1:A:531:GLY:HA2	1:A:574:ILE:HD11	1.81	0.62
1:D:435:VAL:HG23	1:D:468:GLN:HB2	1.80	0.62
1:E:59:PRO:HG2	1:E:62:VAL:HG22	1.81	0.62
1:C:586:ASP:HA	1:C:591:ARG:HD3	1.80	0.62
1:E:117:LEU:HD13	1:E:165:LEU:HD12	1.82	0.62
1:F:332:THR:O	1:F:336:LEU:HB2	1.98	0.62
1:D:438:MET:SD	1:D:614:GLN:NE2	2.73	0.62
1:B:133:HIS:HD2	1:B:142:GLY:H	1.46	0.61
1:E:371:ILE:HD11	1:F:381:LYS:HD2	1.81	0.61
1:D:375:TRP:HE1	1:F:375:TRP:NE1	1.98	0.61
1:E:371:ILE:HD13	1:F:378:TYR:HA	1.81	0.61
1:D:615:ASP:OD1	1:D:616:VAL:N	2.33	0.61
1:A:103:LEU:HD11	1:A:130:VAL:HB	1.82	0.61
1:C:56:VAL:O	1:D:291:GLN:NE2	2.33	0.61
1:D:59:PRO:HG2	1:D:62:VAL:HG22	1.82	0.61
1:F:615:ASP:OD1	1:F:616:VAL:N	2.33	0.61
1:B:235:ASN:HB2	1:B:303:ARG:HH21	1.63	0.61
1:B:385:VAL:HG12	1:B:426:ARG:HB3	1.83	0.61
1:D:596:PRO:HB2	1:E:299:VAL:HG21	1.82	0.61
1:C:121:LEU:O	1:C:219:ASN:HB3	2.00	0.61
1:D:573:SER:HB3	1:D:576:GLU:OE1	2.01	0.61
1:F:354:SER:HA	1:F:357:LEU:HD23	1.81	0.61
1:B:433:SER:OG	2:B:1100:UGA:O'Q	2.19	0.61
1:A:509:SER:OG	1:A:513:THR:HG23	2.00	0.61
1:C:394:THR:HG21	1:C:508:SER:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:HG12	1:C:98:ALA:HB3	1.83	0.60
1:C:429:PHE:HB3	1:C:487:LEU:HD23	1.83	0.60
1:D:117:LEU:HD13	1:D:165:LEU:HD12	1.82	0.60
1:C:390:VAL:HG12	1:C:408:LEU:HD21	1.83	0.60
1:C:439:CYS:HA	1:C:452:ILE:HD13	1.82	0.60
1:C:153:ALA:O	1:C:222:ARG:NH2	2.33	0.60
1:C:321:LEU:HB2	1:C:388:PRO:HA	1.82	0.60
1:C:509:SER:OG	1:C:513:THR:HG23	2.01	0.60
1:F:299:VAL:HG12	1:F:300:ALA:H	1.67	0.60
1:A:128:THR:HG22	1:A:152:ILE:HD11	1.84	0.60
1:C:24:TYR:HE2	1:C:78:ILE:HD12	1.66	0.60
1:B:129:GLY:HA3	1:B:149:ARG:HA	1.82	0.60
1:D:107:LEU:HB2	1:D:129:GLY:H	1.66	0.60
1:F:71:ILE:HD12	1:F:92:ILE:HD11	1.83	0.60
1:B:435:VAL:HG23	1:B:468:GLN:HB2	1.84	0.60
1:C:647:ASP:OD2	1:C:651:ARG:NH2	2.34	0.60
1:F:478:GLY:HA2	1:F:483:LEU:H	1.67	0.60
1:B:401:ASN:HB3	1:B:404:ARG:HB3	1.83	0.60
1:F:438:MET:SD	1:F:614:GLN:NE2	2.75	0.59
1:A:333:GLU:OE1	1:A:355:ARG:NH2	2.36	0.59
1:A:562:ILE:CD1	1:D:456:VAL:HG21	2.32	0.59
1:A:591:ARG:HH22	1:A:596:PRO:HA	1.67	0.59
1:D:240:PHE:HZ	1:D:292:LEU:HD22	1.67	0.59
1:F:59:PRO:CG	1:F:62:VAL:HG22	2.33	0.59
1:B:343:VAL:HG23	1:B:362:PHE:HD1	1.67	0.59
1:C:103:LEU:HD11	1:C:130:VAL:HB	1.83	0.59
1:F:394:THR:OG1	1:F:510:ARG:NH2	2.35	0.59
1:F:511:ALA:HB2	2:F:1100:UGA:H5A1	1.85	0.59
1:A:4:VAL:HG22	1:A:28:ALA:HB3	1.83	0.59
1:A:232:PHE:HB3	1:A:241:THR:HG22	1.83	0.59
1:B:56:VAL:HG13	1:F:287:VAL:HG12	1.85	0.59
1:B:321:LEU:HB2	1:B:388:PRO:HA	1.84	0.59
1:D:103:LEU:HD11	1:D:130:VAL:HB	1.85	0.59
1:F:78:ILE:HG12	1:F:98:ALA:HB3	1.84	0.59
1:C:90:GLU:HA	1:C:93:LEU:HD23	1.84	0.59
1:E:338:GLU:N	1:E:338:GLU:OE1	2.36	0.59
1:C:355:ARG:HH12	1:C:497:ARG:NH1	2.00	0.59
1:E:435:VAL:HG23	1:E:468:GLN:HB2	1.84	0.59
1:F:235:ASN:HD22	1:F:296:LEU:HB3	1.68	0.59
1:B:284:ASP:OD1	1:B:285:ILE:N	2.35	0.58
1:D:277:ILE:HG22	1:D:278:THR:HG23	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ALA:O	1:E:222:ARG:NH2	2.35	0.58
1:F:6:PHE:CD1	1:F:30:PHE:HB2	2.38	0.58
1:A:527:LEU:HB3	1:A:531:GLY:HA3	1.84	0.58
1:B:242:ILE:HG23	1:B:276:ILE:HG23	1.84	0.58
1:D:90:GLU:HA	1:D:93:LEU:HD23	1.86	0.58
1:D:431:SER:HB3	1:D:489:ARG:HG2	1.84	0.58
1:F:243:TRP:HD1	1:F:279:GLY:HA2	1.68	0.58
1:A:284:ASP:OD1	1:A:285:ILE:N	2.34	0.58
1:A:606:ARG:HD2	1:A:611:LYS:HD3	1.85	0.58
1:E:615:ASP:OD1	1:E:616:VAL:N	2.36	0.58
1:B:365:VAL:HG22	1:B:375:TRP:HZ3	1.68	0.58
1:C:431:SER:HB3	1:C:489:ARG:HG2	1.85	0.58
1:E:357:LEU:HD23	1:E:362:PHE:HE2	1.68	0.58
1:A:249:PRO:HA	1:A:272:GLY:HA3	1.86	0.58
1:B:291:GLN:NE2	1:F:56:VAL:O	2.37	0.58
1:C:326:PHE:HD1	1:C:327:ILE:H	1.50	0.58
1:C:527:LEU:HB3	1:C:531:GLY:HA3	1.84	0.58
1:C:604:GLU:OE2	1:F:67:TRP:NE1	2.34	0.58
1:F:417:ILE:HD12	1:F:470:LEU:HD21	1.86	0.58
1:D:414:LEU:HD21	1:D:418:ARG:HE	1.69	0.58
1:A:6:PHE:HD1	1:A:30:PHE:HB2	1.69	0.58
1:C:529:ASP:HA	1:F:66:ILE:HD11	1.84	0.57
1:E:375:TRP:NE1	1:F:375:TRP:HE1	2.01	0.57
1:A:71:ILE:HD12	1:A:92:ILE:HD11	1.85	0.57
1:A:375:TRP:NE1	1:C:375:TRP:HE1	2.02	0.57
1:A:586:ASP:HA	1:A:591:ARG:HG2	1.86	0.57
1:D:6:PHE:HD1	1:D:30:PHE:HB2	1.69	0.57
1:F:588:HIS:CD2	1:F:589:PRO:HD2	2.38	0.57
1:C:252:GLN:HG2	1:C:260:ILE:HD13	1.86	0.57
1:E:470:LEU:O	1:E:474:ILE:HG13	2.05	0.57
1:F:157:VAL:N	1:F:160:THR:OG1	2.28	0.57
1:F:331:LEU:HB2	1:F:544:ILE:HD11	1.86	0.57
1:E:243:TRP:HD1	1:E:279:GLY:HA2	1.69	0.57
1:D:486:THR:HG21	1:D:558:CYS:HB3	1.86	0.57
1:E:235:ASN:ND2	1:E:296:LEU:HB3	2.19	0.57
1:A:535:ARG:NH2	1:A:615:ASP:OD1	2.35	0.57
1:B:538:THR:HG23	1:B:567:ASN:HB2	1.84	0.57
1:D:594:PHE:CE2	1:D:650:LEU:HD22	2.39	0.57
1:D:218:HIS:ND1	1:D:247:MET:HG3	2.20	0.57
1:D:460:ARG:HD3	1:D:613:TYR:CE1	2.39	0.57
1:E:212:LYS:HB3	1:E:213:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:HIS:HB2	1:A:544:ILE:HD11	1.87	0.56
1:D:148:GLN:HG2	1:D:172:LEU:HD12	1.87	0.56
1:E:537:PHE:HE2	1:E:577:LEU:HD22	1.69	0.56
1:C:490:PRO:HB3	1:C:493:TRP:CE2	2.41	0.56
1:A:130:VAL:HG23	1:A:172:LEU:HD13	1.87	0.56
1:E:529:ASP:OD1	1:E:605:SER:N	2.38	0.56
1:B:6:PHE:CD1	1:B:30:PHE:HB2	2.40	0.56
1:B:71:ILE:HD12	1:B:92:ILE:HD11	1.86	0.56
1:E:343:VAL:HG23	1:E:362:PHE:HD1	1.70	0.56
1:E:414:LEU:HD21	1:E:418:ARG:HE	1.70	0.56
1:F:537:PHE:HB2	1:F:638:MET:HE2	1.87	0.56
1:F:103:LEU:HD11	1:F:130:VAL:HB	1.86	0.56
1:C:359:HIS:HE1	1:C:361:ARG:HE	1.53	0.56
1:E:566:GLY:HA3	1:E:621:PRO:HG3	1.88	0.56
1:A:280:GLN:NE2	1:A:282:GLY:O	2.39	0.56
1:A:615:ASP:OD1	1:A:616:VAL:N	2.39	0.56
1:E:146:ALA:HB2	1:E:176:ILE:HG12	1.87	0.56
1:A:117:LEU:HD13	1:A:165:LEU:HD12	1.87	0.56
1:A:478:GLY:HA2	1:A:483:LEU:H	1.71	0.56
1:E:4:VAL:HG22	1:E:28:ALA:HB3	1.87	0.56
1:D:606:ARG:NH1	1:D:612:GLY:H	2.03	0.56
1:E:431:SER:HB3	1:E:489:ARG:HG2	1.88	0.56
1:F:512:ILE:HD11	1:F:581:LEU:HD11	1.88	0.56
1:C:72:ALA:HB2	1:C:95:LEU:HD13	1.88	0.55
1:C:134:ARG:O	1:C:142:GLY:HA3	2.05	0.55
1:F:387:LEU:HD11	1:F:551:ILE:HD11	1.88	0.55
1:C:210:TRP:HH2	1:C:233:SER:HB3	1.72	0.55
1:F:243:TRP:HE1	1:F:280:GLN:HG2	1.71	0.55
1:B:615:ASP:OD1	1:B:616:VAL:N	2.39	0.55
1:C:438:MET:SD	1:C:614:GLN:NE2	2.80	0.55
1:A:414:LEU:HD21	1:A:418:ARG:HE	1.70	0.55
1:D:326:PHE:CD2	1:D:327:ILE:HG13	2.36	0.55
1:F:107:LEU:HB2	1:F:129:GLY:H	1.72	0.55
1:A:280:GLN:HB3	1:A:286:THR:HA	1.89	0.55
1:B:19:VAL:HG22	1:B:177:LEU:HD21	1.89	0.55
1:A:117:LEU:HD21	1:A:162:HIS:HB2	1.88	0.54
1:B:466:SER:HA	1:E:469:LEU:HD11	1.88	0.54
1:C:619:ARG:HH12	2:C:1100:UGA:H5'1	1.72	0.54
1:D:655:ILE:HD12	1:D:655:ILE:H	1.71	0.54
1:E:332:THR:O	1:E:336:LEU:HB2	2.07	0.54
1:E:512:ILE:CD1	1:E:581:LEU:HD21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ASP:OD1	1:F:155:ASP:N	2.40	0.54
1:A:130:VAL:HG11	1:A:169:ALA:HB2	1.90	0.54
1:A:394:THR:HG21	1:A:508:SER:HA	1.90	0.54
1:C:6:PHE:CD1	1:C:30:PHE:HB2	2.42	0.54
1:C:59:PRO:HG2	1:C:62:VAL:HG22	1.88	0.54
1:D:117:LEU:HD21	1:D:162:HIS:HB2	1.90	0.54
1:D:129:GLY:HA3	1:D:149:ARG:HA	1.90	0.54
1:D:417:ILE:HD13	1:D:474:ILE:HG12	1.89	0.54
1:D:260:ILE:HD11	1:D:268:ALA:HB2	1.89	0.54
1:D:542:ASP:HB3	1:D:632:TRP:HZ2	1.73	0.54
1:F:84:TYR:HE2	1:F:86:ASN:HB2	1.73	0.54
1:F:433:SER:OG	1:F:490:PRO:O	2.25	0.54
1:F:439:CYS:HA	1:F:452:ILE:HD13	1.88	0.54
1:F:580:LEU:HD21	1:F:639:ARG:HA	1.90	0.54
1:C:11:MET:HB2	1:C:83:TYR:HB2	1.90	0.54
1:C:208:ILE:HD11	1:C:231:ALA:HB1	1.89	0.54
1:E:375:TRP:HE1	1:F:375:TRP:HE1	1.56	0.54
1:A:242:ILE:HG23	1:A:276:ILE:HG23	1.90	0.54
1:A:540:ILE:HG13	1:A:544:ILE:HD12	1.90	0.54
1:B:31:THR:OG1	1:B:32:HIS:N	2.41	0.54
1:B:114:ARG:NH2	1:B:200:ARG:HH21	2.06	0.54
1:C:387:LEU:HG	1:C:428:VAL:HB	1.89	0.54
1:D:271:ASP:CG	1:D:272:GLY:H	2.15	0.54
1:D:647:ASP:O	1:D:651:ARG:HG2	2.08	0.54
1:F:542:ASP:HB3	1:F:632:TRP:HZ2	1.73	0.54
1:A:357:LEU:HD23	1:A:362:PHE:HE2	1.72	0.53
1:A:549:ARG:HH11	1:A:632:TRP:HB2	1.73	0.53
1:C:332:THR:O	1:C:336:LEU:HB2	2.07	0.53
1:F:156:ASP:O	1:F:222:ARG:NH1	2.37	0.53
1:E:249:PRO:O	1:E:251:ALA:N	2.42	0.53
1:A:146:ALA:HB2	1:A:176:ILE:HG12	1.89	0.53
1:B:130:VAL:HG11	1:B:169:ALA:HB2	1.90	0.53
1:F:338:GLU:HG3	1:F:548:PHE:CZ	2.43	0.53
1:B:14:GLN:HB3	1:B:170:ARG:HD3	1.90	0.53
1:D:213:PRO:HA	1:D:270:ALA:HB3	1.91	0.53
1:A:582:LEU:HD11	1:A:597:PHE:CD2	2.43	0.53
1:D:71:ILE:HD12	1:D:92:ILE:HD11	1.90	0.53
1:E:490:PRO:HB3	1:E:493:TRP:CE2	2.44	0.53
1:F:500:SER:HB3	1:F:503:ALA:HB3	1.91	0.53
1:A:120:VAL:HG23	1:A:121:LEU:HD22	1.89	0.53
1:B:280:GLN:HG2	1:B:286:THR:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:ILE:HD11	1:E:268:ALA:HB2	1.91	0.53
1:E:277:ILE:HG22	1:E:278:THR:HG23	1.91	0.53
1:A:332:THR:HG23	1:A:343:VAL:HG21	1.90	0.53
1:B:134:ARG:O	1:B:142:GLY:HA3	2.09	0.53
1:C:146:ALA:HB2	1:C:176:ILE:HG12	1.91	0.53
1:A:387:LEU:HG	1:A:428:VAL:HB	1.90	0.53
1:B:438:MET:HA	1:B:616:VAL:HG13	1.91	0.53
1:C:537:PHE:HB2	1:C:638:MET:HE2	1.90	0.53
1:D:103:LEU:HD21	1:D:169:ALA:HB1	1.91	0.53
1:A:148:GLN:HG2	1:A:171:GLN:HE21	1.74	0.53
1:A:466:SER:HA	1:D:469:LEU:HD11	1.90	0.53
1:D:596:PRO:HB2	1:E:299:VAL:CG2	2.39	0.53
1:D:487:LEU:HD12	1:D:562:ILE:HG12	1.91	0.53
1:E:246:ARG:HB3	1:E:275:GLU:HB3	1.90	0.53
1:B:155:ASP:OD1	1:B:155:ASP:N	2.37	0.52
1:B:332:THR:O	1:B:336:LEU:HB2	2.09	0.52
1:B:478:GLY:HA2	1:B:483:LEU:H	1.73	0.52
1:C:71:ILE:HD12	1:C:92:ILE:HD11	1.92	0.52
1:E:71:ILE:HD12	1:E:92:ILE:HD11	1.90	0.52
1:B:410:PHE:HA	1:B:470:LEU:HD12	1.92	0.52
1:B:545:GLU:OE2	1:B:549:ARG:NH2	2.42	0.52
1:D:243:TRP:HD1	1:D:279:GLY:HA2	1.75	0.52
1:D:546:ALA:O	1:D:550:ILE:HG13	2.09	0.52
1:E:6:PHE:CD1	1:E:30:PHE:HB2	2.43	0.52
1:F:362:PHE:HE1	1:F:364:PHE:HB2	1.74	0.52
1:B:421:VAL:HG12	1:B:483:LEU:HD13	1.92	0.52
1:E:185:ILE:O	1:E:187:SER:N	2.42	0.52
1:F:572:ALA:HB3	1:F:638:MET:HE1	1.90	0.52
1:A:494:MET:HA	1:A:498:LEU:HD22	1.92	0.52
1:B:232:PHE:HB3	1:B:241:THR:HG22	1.91	0.52
1:C:212:LYS:HB3	1:C:213:PRO:HD2	1.90	0.52
1:C:287:VAL:HG12	1:D:56:VAL:HG13	1.92	0.52
1:E:454:GLY:H	1:E:461:TRP:NE1	2.07	0.52
1:E:326:PHE:HD1	1:E:327:ILE:H	1.57	0.52
1:E:439:CYS:HB3	1:E:444:PHE:CE1	2.43	0.52
1:A:321:LEU:HB2	1:A:388:PRO:HA	1.91	0.52
1:C:458:LYS:NZ	1:C:613:TYR:O	2.42	0.52
1:D:606:ARG:HH12	1:D:612:GLY:H	1.56	0.52
1:E:542:ASP:HB3	1:E:632:TRP:HZ2	1.74	0.52
1:A:56:VAL:HG13	1:E:287:VAL:HG12	1.92	0.52
1:A:343:VAL:HG23	1:A:362:PHE:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ILE:HB	1:B:419:TYR:HE2	1.75	0.52
1:C:414:LEU:CD2	1:C:418:ARG:HE	2.23	0.52
1:D:106:SER:HB2	1:D:111:TYR:HB2	1.92	0.52
1:D:287:VAL:CG1	1:D:291:GLN:HB3	2.40	0.52
1:E:118:ASN:ND2	1:E:223:ALA:O	2.39	0.51
1:F:588:HIS:ND1	1:F:650:LEU:HD12	2.26	0.51
1:A:429:PHE:HB3	1:A:487:LEU:HD23	1.92	0.51
1:B:296:LEU:HB3	1:B:298:LEU:HD13	1.93	0.51
1:A:56:VAL:O	1:E:291:GLN:NE2	2.41	0.51
1:B:591:ARG:HH22	1:B:596:PRO:HA	1.74	0.51
1:E:509:SER:OG	1:E:513:THR:HG23	2.11	0.51
1:F:93:LEU:HD22	1:F:100:ALA:HB3	1.91	0.51
1:F:117:LEU:HD21	1:F:162:HIS:HB2	1.92	0.51
1:F:490:PRO:HB3	1:F:493:TRP:CE2	2.45	0.51
1:F:79:ILE:HB	1:F:100:ALA:HB2	1.93	0.51
1:C:117:LEU:HD21	1:C:162:HIS:HB2	1.91	0.51
1:C:250:ASP:O	1:C:252:GLN:N	2.39	0.51
1:E:319:LEU:HD11	1:E:379:HIS:HB3	1.92	0.51
1:F:232:PHE:HB3	1:F:241:THR:HG22	1.90	0.51
1:C:259:VAL:HG22	1:C:267:VAL:HG22	1.93	0.51
1:C:458:LYS:NZ	1:C:606:ARG:HH21	2.09	0.51
1:D:240:PHE:CZ	1:D:292:LEU:HD13	2.46	0.51
1:F:299:VAL:HG12	1:F:300:ALA:N	2.25	0.51
1:F:550:ILE:HD11	1:F:565:ILE:HD11	1.91	0.51
1:B:527:LEU:HB3	1:B:531:GLY:HA3	1.92	0.51
1:F:114:ARG:HD3	1:F:200:ARG:HB3	1.92	0.51
1:B:138:ARG:HB3	1:B:141:ALA:HB3	1.93	0.51
1:B:329:ASN:ND2	1:B:352:ALA:O	2.43	0.51
1:D:410:PHE:CD1	1:D:470:LEU:HB2	2.45	0.51
1:E:68:VAL:HG22	1:E:92:ILE:HG13	1.93	0.51
1:A:543:GLY:HA2	1:A:565:ILE:HG21	1.92	0.51
1:D:412:GLU:O	1:D:415:ARG:HB2	2.10	0.51
1:E:421:VAL:HG12	1:E:483:LEU:HD13	1.93	0.51
1:F:303:ARG:O	1:F:304:LEU:HB2	2.11	0.51
1:E:68:VAL:HG13	1:E:95:LEU:HD11	1.92	0.51
1:F:344:TYR:CD1	1:F:363:HIS:HB2	2.46	0.51
1:B:93:LEU:HD12	1:B:100:ALA:HB3	1.93	0.50
1:C:243:TRP:HD1	1:C:279:GLY:HA2	1.75	0.50
1:E:527:LEU:HB3	1:E:531:GLY:HA3	1.93	0.50
1:A:529:ASP:HA	1:D:66:ILE:HD11	1.92	0.50
1:B:243:TRP:HZ3	1:F:47:ARG:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LEU:HD12	1:B:562:ILE:HG12	1.91	0.50
1:C:59:PRO:HB3	1:C:67:TRP:NE1	2.26	0.50
1:E:344:TYR:CD1	1:E:363:HIS:HB2	2.46	0.50
1:E:535:ARG:HB2	1:E:537:PHE:CE1	2.43	0.50
1:F:134:ARG:O	1:F:142:GLY:HA3	2.10	0.50
1:C:387:LEU:HD11	1:C:551:ILE:HD11	1.93	0.50
1:C:543:GLY:HA2	1:C:565:ILE:HG21	1.93	0.50
1:D:512:ILE:HD12	1:D:581:LEU:HD21	1.93	0.50
1:F:321:LEU:HB2	1:F:388:PRO:HA	1.92	0.50
1:F:368:ASP:H	1:F:372:HIS:HD2	1.59	0.50
1:F:456:VAL:C	1:F:458:LYS:H	2.19	0.50
1:B:9:HIS:CG	1:B:10:ASP:H	2.29	0.50
1:B:224:VAL:HB	1:B:230:GLY:H	1.76	0.50
1:B:359:HIS:CE1	1:B:361:ARG:HB2	2.47	0.50
1:F:280:GLN:HB3	1:F:286:THR:HA	1.94	0.50
1:A:469:LEU:HD11	1:D:466:SER:HA	1.93	0.50
1:B:394:THR:HG21	1:B:508:SER:HA	1.93	0.50
1:C:346:MET:SD	1:C:376:ILE:HG12	2.52	0.50
1:C:546:ALA:O	1:C:550:ILE:HG13	2.12	0.50
1:E:414:LEU:CD2	1:E:418:ARG:HE	2.24	0.50
1:A:542:ASP:HB3	1:A:632:TRP:HZ2	1.76	0.50
1:C:218:HIS:O	1:C:222:ARG:HG3	2.12	0.50
1:C:355:ARG:HH12	1:C:497:ARG:HH12	1.58	0.50
1:C:511:ALA:HB2	2:C:1100:UGA:H5A1	1.94	0.50
1:E:588:HIS:CE1	1:E:651:ARG:NH2	2.77	0.50
1:F:327:ILE:HB	1:F:389:LEU:HD13	1.93	0.50
1:A:426:ARG:NH2	1:A:550:ILE:O	2.40	0.50
1:B:454:GLY:O	1:E:472:ARG:NH2	2.44	0.50
1:C:459:PRO:HD2	1:C:612:GLY:HA3	1.94	0.50
1:D:490:PRO:HB3	1:D:493:TRP:CE2	2.46	0.50
1:F:421:VAL:HG12	1:F:483:LEU:HD13	1.94	0.50
1:A:439:CYS:HB3	1:A:444:PHE:CE1	2.47	0.50
1:B:177:LEU:HB3	1:B:178:PRO:HD3	1.94	0.50
1:D:112:ARG:NH2	1:D:195:SER:OG	2.45	0.50
1:D:315:ARG:HH11	1:D:340:ASN:HA	1.77	0.50
1:F:368:ASP:HB3	1:F:371:ILE:HD12	1.94	0.50
1:A:55:PRO:HA	1:E:291:GLN:OE1	2.12	0.49
1:B:79:ILE:O	1:B:100:ALA:HA	2.11	0.49
1:E:221:VAL:HG22	1:E:231:ALA:HB3	1.94	0.49
1:F:431:SER:HB3	1:F:489:ARG:HG2	1.94	0.49
1:A:535:ARG:HH12	1:A:616:VAL:HB	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:546:ALA:O	1:E:550:ILE:HG13	2.12	0.49
1:F:29:ILE:HD12	1:F:49:ALA:HB2	1.94	0.49
1:F:369:ILE:HA	1:F:376:ILE:HD11	1.94	0.49
1:B:56:VAL:O	1:F:291:GLN:NE2	2.37	0.49
1:C:588:HIS:NE2	1:C:647:ASP:OD1	2.45	0.49
1:D:146:ALA:HB2	1:D:176:ILE:HG12	1.94	0.49
1:D:521:GLU:HG3	1:D:523:THR:OG1	2.12	0.49
1:A:28:ALA:HB1	1:A:30:PHE:HE1	1.77	0.49
1:B:285:ILE:HB	1:F:46:SER:HB2	1.95	0.49
1:C:528:ILE:HG21	1:C:609:TYR:CE2	2.47	0.49
1:D:120:VAL:HG23	1:D:121:LEU:HD22	1.95	0.49
1:A:456:VAL:HG21	1:D:562:ILE:HD13	1.94	0.49
1:B:64:HIS:H	1:B:68:VAL:HG23	1.77	0.49
1:C:339:GLU:HG2	1:C:340:ASN:N	2.28	0.49
1:D:446:GLU:H	1:D:446:GLU:CD	2.21	0.49
1:E:255:LEU:CD1	1:E:256:PRO:HD2	2.41	0.49
1:E:627:ARG:HD3	1:E:633:GLU:CG	2.39	0.49
1:B:121:LEU:O	1:B:219:ASN:HB3	2.12	0.49
1:C:609:TYR:OH	2:C:1100:UGA:H2A1	2.12	0.49
1:E:321:LEU:HB2	1:E:388:PRO:HA	1.95	0.49
1:F:106:SER:HB2	1:F:111:TYR:HB2	1.94	0.49
1:F:458:LYS:NZ	1:F:606:ARG:HH21	2.10	0.49
1:A:338:GLU:HG3	1:A:548:PHE:CZ	2.48	0.49
1:B:143:GLU:HB3	1:B:187:SER:HB2	1.94	0.49
1:B:574:ILE:CD1	2:B:1100:UGA:H1A1	2.43	0.49
1:C:177:LEU:HB3	1:C:178:PRO:HD3	1.93	0.49
1:C:515:LEU:HD22	1:C:525:ILE:HG23	1.94	0.49
1:D:627:ARG:HD3	1:D:633:GLU:HG3	1.93	0.49
1:E:586:ASP:O	1:E:591:ARG:HD3	2.13	0.49
1:D:497:ARG:HD2	1:D:648:PHE:CZ	2.47	0.49
1:D:619:ARG:HH12	2:D:1100:UGA:H5'1	1.77	0.49
1:B:326:PHE:CD2	1:B:327:ILE:HG13	2.45	0.49
1:C:546:ALA:HB2	1:C:632:TRP:CE2	2.48	0.49
1:E:128:THR:HG22	1:E:152:ILE:HD11	1.94	0.49
1:C:19:VAL:HG22	1:C:177:LEU:HD21	1.95	0.48
1:C:46:SER:HB2	1:D:285:ILE:HB	1.95	0.48
1:C:185:ILE:O	1:C:187:SER:N	2.45	0.48
1:E:456:VAL:C	1:E:458:LYS:H	2.21	0.48
1:D:259:VAL:HG21	1:D:298:LEU:HD23	1.95	0.48
1:C:478:GLY:HA2	1:C:483:LEU:H	1.78	0.48
1:A:6:PHE:CD1	1:A:30:PHE:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ILE:O	1:B:415:ARG:NH2	2.47	0.48
1:B:393:ALA:HB1	2:B:1100:UGA:O3'	2.12	0.48
1:D:6:PHE:CD1	1:D:30:PHE:HB2	2.48	0.48
1:E:619:ARG:HH12	2:E:1100:UGA:H5'1	1.77	0.48
1:F:619:ARG:NH1	2:F:1100:UGA:H5'1	2.26	0.48
1:A:338:GLU:HB2	1:A:341:TYR:HD2	1.78	0.48
1:B:318:VAL:HG13	1:B:385:VAL:HG23	1.94	0.48
1:B:431:SER:HB3	1:B:489:ARG:HG2	1.95	0.48
1:C:31:THR:OG1	1:C:32:HIS:N	2.47	0.48
1:F:157:VAL:HG12	1:F:222:ARG:HG2	1.96	0.48
1:F:249:PRO:O	1:F:251:ALA:N	2.46	0.48
1:A:421:VAL:HG12	1:A:483:LEU:HD13	1.95	0.48
1:B:133:HIS:CD2	1:B:142:GLY:H	2.29	0.48
1:C:499:ASP:OD1	1:C:510:ARG:NH1	2.47	0.48
1:D:134:ARG:O	1:D:142:GLY:HA3	2.12	0.48
1:E:113:GLY:HA2	1:E:197:TYR:CD1	2.47	0.48
1:E:218:HIS:CD2	1:E:245:SER:HB3	2.49	0.48
1:E:220:LEU:O	1:E:224:VAL:HG22	2.13	0.48
1:F:146:ALA:HB2	1:F:176:ILE:HG12	1.95	0.48
1:A:277:ILE:O	1:A:289:GLY:N	2.45	0.48
1:A:470:LEU:O	1:A:474:ILE:HG13	2.13	0.48
1:B:509:SER:OG	1:B:513:THR:HG23	2.13	0.48
1:B:573:SER:O	1:B:577:LEU:N	2.38	0.48
1:C:469:LEU:HD11	1:F:466:SER:HA	1.94	0.48
1:F:112:ARG:HE	1:F:195:SER:HB2	1.77	0.48
1:A:326:PHE:HD1	1:A:327:ILE:N	2.11	0.48
1:A:332:THR:O	1:A:336:LEU:HB2	2.13	0.48
1:A:497:ARG:HD2	1:A:648:PHE:CZ	2.49	0.48
1:F:494:MET:HA	1:F:498:LEU:HD22	1.96	0.48
1:E:549:ARG:HD2	1:E:630:LEU:O	2.14	0.48
1:B:563:ILE:HG22	1:B:564:ASN:H	1.79	0.48
1:E:487:LEU:HD12	1:E:562:ILE:HG12	1.94	0.48
1:A:103:LEU:HD21	1:A:169:ALA:HB1	1.96	0.47
1:B:146:ALA:HB2	1:B:176:ILE:HG12	1.95	0.47
1:E:84:TYR:HE2	1:E:86:ASN:HB2	1.79	0.47
1:F:6:PHE:HB3	1:F:84:TYR:CD1	2.49	0.47
1:D:31:THR:OG1	1:D:32:HIS:N	2.45	0.47
1:E:6:PHE:HD1	1:E:30:PHE:HB2	1.80	0.47
1:A:24:TYR:HE2	1:A:78:ILE:HD12	1.79	0.47
1:A:134:ARG:O	1:A:142:GLY:HA3	2.14	0.47
1:C:470:LEU:O	1:C:474:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:HD21	1:E:162:HIS:HB2	1.96	0.47
1:F:81:SER:HB3	1:F:102:ASN:HA	1.96	0.47
1:F:431:SER:OG	1:F:432:THR:N	2.45	0.47
1:B:112:ARG:NH1	1:B:140:ASP:O	2.47	0.47
1:B:112:ARG:N	1:B:196:THR:O	2.48	0.47
1:B:130:VAL:HG23	1:B:172:LEU:HD13	1.96	0.47
1:C:478:GLY:HA2	1:C:483:LEU:N	2.29	0.47
1:A:434:GLU:HG2	1:A:464:SER:HB2	1.95	0.47
1:D:111:TYR:CE2	1:D:120:VAL:HG12	2.49	0.47
1:D:470:LEU:O	1:D:474:ILE:HG13	2.14	0.47
1:F:79:ILE:HB	1:F:100:ALA:CB	2.45	0.47
1:B:439:CYS:HB3	1:B:444:PHE:CE1	2.49	0.47
1:C:6:PHE:HD1	1:C:30:PHE:HB2	1.80	0.47
1:C:417:ILE:HD12	1:C:470:LEU:HD21	1.96	0.47
1:A:143:GLU:CB	1:A:187:SER:HB2	2.45	0.47
1:B:353:ILE:HB	1:B:356:PHE:CE1	2.50	0.47
1:B:469:LEU:HD11	1:E:466:SER:HA	1.95	0.47
1:C:55:PRO:HA	1:D:291:GLN:OE1	2.15	0.47
1:C:534:LYS:HD3	1:C:571:GLU:HG2	1.96	0.47
1:D:130:VAL:HG11	1:D:169:ALA:HB2	1.96	0.47
1:E:333:GLU:OE1	1:E:355:ARG:NH2	2.46	0.47
1:B:422:LYS:HG2	1:B:423:TYR:CE1	2.49	0.47
1:E:134:ARG:O	1:E:142:GLY:HA3	2.13	0.47
1:E:433:SER:HB3	1:E:491:PHE:CD1	2.49	0.47
1:F:458:LYS:HZ1	1:F:606:ARG:HH21	1.62	0.47
1:C:184:ASP:CG	1:C:186:PRO:HD3	2.40	0.47
1:D:212:LYS:HB3	1:D:213:PRO:HD2	1.97	0.47
1:D:346:MET:SD	1:D:376:ILE:HG22	2.55	0.47
1:E:119:TRP:CZ2	1:E:201:ARG:HG2	2.49	0.47
1:F:535:ARG:HB2	1:F:537:PHE:CE1	2.49	0.47
1:A:285:ILE:HD13	1:E:58:ALA:HB2	1.97	0.47
1:B:365:VAL:HG22	1:B:375:TRP:CZ3	2.48	0.47
1:B:375:TRP:CZ2	1:C:375:TRP:CZ2	3.01	0.47
1:B:542:ASP:HB3	1:B:632:TRP:HZ2	1.79	0.46
1:C:143:GLU:HB3	1:C:187:SER:HB2	1.97	0.46
1:C:369:ILE:HA	1:C:376:ILE:CD1	2.45	0.46
1:C:374:GLU:HG3	1:C:375:TRP:N	2.30	0.46
1:D:102:ASN:HB2	1:D:135:MET:SD	2.55	0.46
1:F:6:PHE:HD1	1:F:30:PHE:HB2	1.79	0.46
1:F:324:ASN:OD1	1:F:352:ALA:HB3	2.15	0.46
1:A:330:HIS:HB2	1:A:544:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLU:H	1:A:446:GLU:CD	2.23	0.46
1:C:280:GLN:HB2	1:C:284:ASP:O	2.15	0.46
1:D:332:THR:O	1:D:336:LEU:HB2	2.15	0.46
1:B:585:PHE:HA	1:B:646:LEU:HD21	1.97	0.46
1:C:79:ILE:O	1:C:100:ALA:HA	2.16	0.46
1:F:120:VAL:HG23	1:F:121:LEU:HD13	1.97	0.46
1:F:459:PRO:HD2	1:F:612:GLY:HA3	1.97	0.46
1:F:567:ASN:HA	1:F:634:PRO:HG3	1.96	0.46
1:B:344:TYR:CD1	1:B:363:HIS:HB2	2.50	0.46
1:B:7:ALA:HB1	1:B:12:GLY:HA3	1.98	0.46
1:B:417:ILE:HD12	1:B:470:LEU:HD21	1.97	0.46
1:C:528:ILE:HG21	1:C:609:TYR:HE2	1.80	0.46
1:D:185:ILE:HD12	1:D:185:ILE:O	2.15	0.46
1:D:205:ASP:C	1:D:207:LEU:H	2.23	0.46
1:E:206:GLY:O	1:E:231:ALA:HA	2.15	0.46
1:A:78:ILE:HG12	1:A:98:ALA:HB3	1.98	0.46
1:A:118:ASN:O	1:A:122:VAL:HG23	2.14	0.46
1:A:143:GLU:HB3	1:A:187:SER:HB2	1.98	0.46
1:B:490:PRO:HB3	1:B:493:TRP:CE2	2.51	0.46
1:C:458:LYS:HZ3	1:C:606:ARG:HH21	1.63	0.46
1:A:7:ALA:HA	1:A:82:PHE:O	2.15	0.46
1:A:260:ILE:HD11	1:A:268:ALA:HB2	1.97	0.46
1:A:326:PHE:CD1	1:A:327:ILE:N	2.78	0.46
1:B:567:ASN:HD21	1:B:569:ASP:HB2	1.81	0.46
1:D:285:ILE:O	1:D:287:VAL:HG23	2.15	0.46
1:E:31:THR:OG1	1:E:32:HIS:N	2.49	0.46
1:B:235:ASN:HB2	1:B:303:ARG:NH2	2.31	0.46
1:C:120:VAL:HG23	1:C:121:LEU:HD22	1.98	0.46
1:C:520:VAL:HG13	1:C:594:PHE:CE1	2.51	0.46
1:D:85:ARG:HH11	1:D:200:ARG:HH22	1.63	0.46
1:F:435:VAL:HG23	1:F:468:GLN:HB2	1.98	0.46
1:A:220:LEU:O	1:A:224:VAL:HG22	2.16	0.46
1:B:470:LEU:O	1:B:474:ILE:HG13	2.15	0.46
1:E:76:PRO:O	1:E:97:PRO:HD2	2.15	0.46
1:E:394:THR:HG21	1:E:509:SER:H	1.80	0.46
1:E:429:PHE:HB3	1:E:487:LEU:HD23	1.97	0.46
1:F:488:PHE:HA	1:F:563:ILE:O	2.15	0.46
1:A:490:PRO:HB3	1:A:493:TRP:CE2	2.51	0.45
1:A:546:ALA:O	1:A:550:ILE:HG13	2.17	0.45
1:B:319:LEU:HD11	1:B:379:HIS:HB3	1.98	0.45
1:B:458:LYS:HD2	1:B:614:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ALA:HB2	1:E:95:LEU:HD13	1.98	0.45
1:A:114:ARG:HD3	1:A:200:ARG:HB2	1.98	0.45
1:A:388:PRO:HB3	1:A:416:ILE:HG21	1.99	0.45
1:C:208:ILE:HD11	1:C:220:LEU:HD22	1.98	0.45
1:C:452:ILE:HG13	1:F:452:ILE:HG23	1.99	0.45
1:C:647:ASP:C	1:C:651:ARG:HH21	2.24	0.45
1:D:138:ARG:HB3	1:D:141:ALA:HB3	1.98	0.45
1:D:177:LEU:HB3	1:D:178:PRO:HD3	1.97	0.45
1:D:185:ILE:O	1:D:187:SER:N	2.47	0.45
1:F:353:ILE:HD11	1:F:364:PHE:HE2	1.82	0.45
1:B:14:GLN:OE1	1:B:170:ARG:NH1	2.49	0.45
1:B:214:VAL:HG22	1:B:269:CYS:SG	2.56	0.45
1:B:356:PHE:HD1	1:B:362:PHE:CD2	2.34	0.45
1:B:387:LEU:HG	1:B:428:VAL:HB	1.98	0.45
1:E:410:PHE:HA	1:E:470:LEU:HD12	1.98	0.45
1:C:516:ILE:HG12	1:C:581:LEU:HD11	1.97	0.45
1:E:299:VAL:CG2	1:E:300:ALA:H	2.18	0.45
1:A:353:ILE:HD11	1:A:364:PHE:CD1	2.51	0.45
1:A:519:LEU:HB3	1:A:585:PHE:CE2	2.51	0.45
1:A:536:CYS:SG	1:A:568:PRO:HA	2.56	0.45
1:B:252:GLN:HG2	1:B:260:ILE:CG2	2.47	0.45
1:C:159:LEU:HD23	1:C:227:PRO:HD2	1.98	0.45
1:C:421:VAL:HG12	1:C:483:LEU:HD13	1.99	0.45
1:D:395:PRO:HA	1:D:398:TYR:CD2	2.52	0.45
1:D:414:LEU:CD2	1:D:418:ARG:HE	2.30	0.45
1:A:134:ARG:HH12	1:A:185:ILE:HB	1.82	0.45
1:B:567:ASN:HA	1:B:634:PRO:HG3	1.99	0.45
1:C:150:VAL:HG11	1:C:164:LYS:HG2	1.99	0.45
1:C:492:ASN:H	2:C:1100:UGA:C6'	2.29	0.45
1:F:111:TYR:CE1	1:F:198:TYR:HE2	2.34	0.45
1:A:299:VAL:HG22	1:A:300:ALA:N	2.23	0.45
1:C:334:ARG:NH1	1:C:338:GLU:OE2	2.50	0.45
1:D:19:VAL:HA	1:D:177:LEU:HD21	1.99	0.45
1:D:218:HIS:CD2	1:D:245:SER:HB3	2.52	0.45
1:E:344:TYR:HD2	1:E:383:CYS:SG	2.39	0.45
1:E:365:VAL:HG21	1:E:379:HIS:NE2	2.32	0.45
1:F:185:ILE:O	1:F:187:SER:N	2.48	0.45
1:F:234:TYR:CD2	1:F:304:LEU:HD21	2.42	0.45
1:F:235:ASN:ND2	1:F:298:LEU:HD21	2.32	0.45
1:F:319:LEU:HD11	1:F:379:HIS:HB3	1.97	0.45
1:B:214:VAL:HG23	1:B:271:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLY:HA2	1:B:483:LEU:N	2.31	0.45
1:D:426:ARG:HA	1:D:484:ARG:O	2.16	0.45
1:E:102:ASN:HD22	1:E:133:HIS:CE1	2.25	0.45
1:A:203:PRO:C	1:A:205:ASP:H	2.25	0.45
1:B:435:VAL:HG11	1:B:489:ARG:CZ	2.46	0.45
1:C:210:TRP:HH2	1:C:233:SER:CB	2.30	0.45
1:C:488:PHE:HD1	1:C:490:PRO:HD3	1.82	0.45
1:C:519:LEU:HD11	1:C:581:LEU:HG	1.99	0.45
1:E:120:VAL:HG11	1:E:128:THR:HG21	1.99	0.45
1:A:324:ASN:OD1	1:A:352:ALA:HB3	2.17	0.45
1:A:348:ILE:HD12	1:C:378:TYR:CZ	2.52	0.45
1:E:103:LEU:HD11	1:E:130:VAL:HB	1.98	0.45
1:C:65:PRO:O	1:C:69:ASP:HB3	2.17	0.44
1:D:92:ILE:HA	1:D:95:LEU:HG	1.98	0.44
1:D:218:HIS:O	1:D:222:ARG:HG3	2.17	0.44
1:F:504:ALA:HA	1:F:509:SER:HB3	1.99	0.44
1:A:10:ASP:HB3	1:A:166:CYS:SG	2.58	0.44
1:E:11:MET:HE1	1:E:165:LEU:C	2.42	0.44
1:E:68:VAL:HG11	1:E:91:GLU:OE1	2.17	0.44
1:E:243:TRP:HE1	1:E:280:GLN:HG2	1.82	0.44
1:E:459:PRO:HD2	1:E:612:GLY:HA3	1.99	0.44
1:F:32:HIS:NE2	1:F:85:ARG:HB2	2.32	0.44
1:A:427:VAL:HG23	1:A:485:PHE:HB2	2.00	0.44
1:C:369:ILE:HA	1:C:376:ILE:HD11	1.99	0.44
1:E:177:LEU:HB3	1:E:178:PRO:HD3	1.98	0.44
1:E:499:ASP:OD2	1:E:510:ARG:NH1	2.43	0.44
1:F:355:ARG:H	1:F:355:ARG:HG2	1.64	0.44
1:A:417:ILE:HD13	1:A:474:ILE:HG12	2.00	0.44
1:C:529:ASP:OD2	1:C:605:SER:HB3	2.18	0.44
1:D:536:CYS:SG	1:D:568:PRO:HA	2.58	0.44
1:F:417:ILE:O	1:F:421:VAL:HG13	2.18	0.44
1:F:580:LEU:HD23	1:F:642:VAL:HG21	2.00	0.44
1:B:64:HIS:CD2	1:B:66:ILE:HB	2.52	0.44
1:B:500:SER:O	1:B:504:ALA:N	2.51	0.44
1:D:138:ARG:NH1	1:D:192:GLU:OE2	2.51	0.44
1:F:212:LYS:HB3	1:F:213:PRO:HD2	2.00	0.44
1:F:454:GLY:H	1:F:461:TRP:NE1	2.14	0.44
1:A:329:ASN:ND2	1:A:352:ALA:O	2.51	0.44
1:A:417:ILE:HD11	1:A:429:PHE:CD1	2.53	0.44
1:A:550:ILE:HG12	1:A:563:ILE:HD12	2.00	0.44
1:B:429:PHE:CZ	1:B:470:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:MET:HG3	1:B:641:THR:HG21	1.99	0.44
1:B:574:ILE:HD13	2:B:1100:UGA:H1A1	1.99	0.44
1:A:31:THR:OG1	1:A:32:HIS:N	2.50	0.44
1:B:76:PRO:O	1:B:97:PRO:HD2	2.17	0.44
1:B:90:GLU:HA	1:B:93:LEU:HD23	2.00	0.44
1:B:214:VAL:HG21	1:B:273:ALA:N	2.33	0.44
1:B:324:ASN:OD1	1:B:352:ALA:HB3	2.18	0.44
1:E:486:THR:HG21	1:E:558:CYS:HB3	2.00	0.44
1:F:157:VAL:HA	1:F:222:ARG:HB3	2.00	0.44
1:F:426:ARG:NH2	1:F:550:ILE:O	2.45	0.44
1:A:176:ILE:O	1:A:180:MET:HG3	2.18	0.44
1:C:239:LYS:HE2	1:C:241:THR:HG22	2.00	0.44
1:D:509:SER:HB2	1:D:513:THR:CG2	2.47	0.44
1:D:539:ASP:OD2	1:D:641:THR:OG1	2.32	0.44
1:E:344:TYR:HD1	1:E:363:HIS:HB2	1.82	0.44
1:F:546:ALA:O	1:F:550:ILE:HG13	2.18	0.44
1:A:433:SER:OG	2:A:1100:UGA:O'Q	2.33	0.44
1:A:478:GLY:HA2	1:A:483:LEU:N	2.32	0.44
1:A:567:ASN:HD21	1:A:569:ASP:HB2	1.83	0.44
1:B:6:PHE:HD1	1:B:30:PHE:HB2	1.79	0.44
1:B:288:GLN:O	1:B:292:LEU:N	2.45	0.44
1:C:648:PHE:HA	1:C:651:ARG:HE	1.83	0.44
1:D:11:MET:HE1	1:D:165:LEU:C	2.43	0.44
1:E:102:ASN:HB2	1:E:135:MET:SD	2.58	0.44
1:F:214:VAL:HG23	1:F:247:MET:HE3	1.99	0.44
1:F:353:ILE:HD11	1:F:364:PHE:CE2	2.53	0.44
1:D:112:ARG:NH1	1:D:140:ASP:O	2.51	0.43
1:D:271:ASP:CG	1:D:272:GLY:N	2.76	0.43
1:B:58:ALA:HB2	1:F:285:ILE:HG12	2.00	0.43
1:C:539:ASP:OD1	1:C:540:ILE:N	2.51	0.43
1:D:192:GLU:O	1:D:192:GLU:HG3	2.18	0.43
1:E:12:GLY:HA2	1:E:82:PHE:HB2	1.99	0.43
1:E:67:TRP:O	1:E:71:ILE:N	2.51	0.43
1:E:394:THR:HG21	1:E:508:SER:HA	2.00	0.43
1:A:353:ILE:HB	1:A:356:PHE:CE1	2.52	0.43
1:B:317:ARG:HB2	1:B:383:CYS:HA	2.00	0.43
1:C:398:TYR:HD2	1:C:460:ARG:HD2	1.83	0.43
1:C:455:PRO:HB2	1:C:457:ASN:OD1	2.18	0.43
1:D:550:ILE:HG12	1:D:630:LEU:HD21	2.01	0.43
1:F:430:PRO:HB3	1:F:488:PHE:CZ	2.53	0.43
1:A:582:LEU:HD21	1:A:597:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ARG:HB2	1:B:484:ARG:NH1	2.33	0.43
1:D:243:TRP:HE1	1:D:280:GLN:HG2	1.83	0.43
1:D:292:LEU:HD12	1:D:293:ALA:N	2.32	0.43
1:E:549:ARG:CB	1:E:630:LEU:HD22	2.48	0.43
1:F:79:ILE:HG13	1:F:96:ALA:HB2	2.00	0.43
1:A:9:HIS:CG	1:A:10:ASP:H	2.36	0.43
1:C:185:ILE:O	1:C:185:ILE:HD12	2.19	0.43
1:C:439:CYS:HB3	1:C:444:PHE:CE1	2.54	0.43
1:F:77:ASP:HA	1:F:97:PRO:HD2	2.00	0.43
1:F:247:MET:O	1:F:249:PRO:HD3	2.18	0.43
1:F:414:LEU:HD21	1:F:418:ARG:HE	1.82	0.43
1:F:527:LEU:HB3	1:F:531:GLY:HA3	2.00	0.43
1:F:549:ARG:HD2	1:F:630:LEU:O	2.18	0.43
1:B:284:ASP:OD1	1:B:285:ILE:HG12	2.18	0.43
1:C:329:ASN:ND2	1:C:352:ALA:O	2.43	0.43
1:B:445:ASP:O	1:B:449:SER:HB2	2.18	0.43
1:C:353:ILE:HB	1:C:356:PHE:CE1	2.53	0.43
1:C:546:ALA:HB2	1:C:632:TRP:CD2	2.53	0.43
1:C:594:PHE:HB3	1:C:595:PRO:HD2	2.01	0.43
1:D:93:LEU:HD12	1:D:100:ALA:HB3	2.01	0.43
1:D:418:ARG:HA	1:D:421:VAL:HG22	2.00	0.43
1:E:339:GLU:HA	1:E:361:ARG:NE	2.34	0.43
1:F:415:ARG:HE	1:F:415:ARG:HB3	1.67	0.43
1:A:451:LEU:HB2	1:D:453:VAL:HG23	2.01	0.43
1:D:549:ARG:HB3	1:D:630:LEU:HD22	2.00	0.43
1:E:243:TRP:CD1	1:E:279:GLY:HA2	2.52	0.43
1:E:417:ILE:HD12	1:E:470:LEU:HD21	2.00	0.43
1:B:78:ILE:HG21	1:B:80:PHE:CZ	2.54	0.43
1:C:339:GLU:HG2	1:C:340:ASN:H	1.83	0.43
1:C:497:ARG:HG3	1:C:648:PHE:CZ	2.54	0.43
1:D:84:TYR:CE2	1:D:86:ASN:HB2	2.54	0.43
1:E:435:VAL:HG11	1:E:489:ARG:CZ	2.49	0.43
1:F:512:ILE:CD1	1:F:581:LEU:HD11	2.48	0.43
1:A:426:ARG:HA	1:A:484:ARG:O	2.18	0.43
1:C:112:ARG:NH1	1:C:140:ASP:O	2.52	0.43
1:C:150:VAL:HG21	1:C:168:ALA:HB2	2.01	0.43
1:D:81:SER:HB3	1:D:102:ASN:HA	2.01	0.43
1:D:586:ASP:O	1:D:591:ARG:HD2	2.19	0.42
1:A:204:GLU:O	1:A:204:GLU:HG2	2.19	0.42
1:C:48:GLN:O	1:C:52:LEU:HG	2.19	0.42
1:C:133:HIS:HD2	1:C:142:GLY:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:VAL:HG23	1:E:121:LEU:HD22	2.01	0.42
1:E:324:ASN:OD1	1:E:352:ALA:HB3	2.19	0.42
1:F:90:GLU:H	1:F:90:GLU:CD	2.27	0.42
1:F:429:PHE:HB3	1:F:487:LEU:HD23	2.01	0.42
1:A:109:PRO:O	1:A:195:SER:HA	2.19	0.42
1:A:417:ILE:HD12	1:A:470:LEU:HD21	2.00	0.42
1:A:546:ALA:HB2	1:A:632:TRP:CE2	2.54	0.42
1:C:84:TYR:CE2	1:C:86:ASN:HB2	2.54	0.42
1:D:202:ARG:HB2	1:D:203:PRO:HD2	2.01	0.42
1:D:418:ARG:HD3	1:D:477:TYR:OH	2.18	0.42
1:E:211:HIS:HD2	1:E:256:PRO:HB2	1.84	0.42
1:F:344:TYR:HD1	1:F:363:HIS:HB2	1.85	0.42
1:F:369:ILE:HA	1:F:376:ILE:CD1	2.49	0.42
1:F:566:GLY:HA3	1:F:621:PRO:HG3	2.01	0.42
1:A:287:VAL:HG12	1:E:56:VAL:HG13	2.01	0.42
1:A:431:SER:HB3	1:A:489:ARG:HG2	2.00	0.42
1:E:504:ALA:HA	1:E:509:SER:HB2	2.02	0.42
1:F:121:LEU:HD23	1:F:223:ALA:HA	2.00	0.42
1:A:430:PRO:HB3	1:A:488:PHE:CZ	2.54	0.42
1:B:549:ARG:HH11	1:B:632:TRP:HB2	1.85	0.42
1:B:605:SER:HB2	1:B:613:TYR:HD2	1.84	0.42
1:C:2:LYS:HG2	1:C:25:GLU:OE1	2.19	0.42
1:C:84:TYR:HE2	1:C:86:ASN:HB2	1.84	0.42
1:D:76:PRO:O	1:D:97:PRO:HD2	2.19	0.42
1:D:279:GLY:O	1:D:287:VAL:N	2.51	0.42
1:E:121:LEU:O	1:E:219:ASN:HB3	2.20	0.42
1:E:394:THR:HG21	1:E:509:SER:N	2.35	0.42
1:E:537:PHE:HB2	1:E:638:MET:HE2	2.01	0.42
1:A:395:PRO:HA	1:A:398:TYR:CD2	2.55	0.42
1:A:398:TYR:HD2	1:A:460:ARG:HD2	1.85	0.42
1:C:344:TYR:CD1	1:C:363:HIS:HB2	2.55	0.42
1:C:415:ARG:HE	1:C:415:ARG:HB3	1.69	0.42
1:C:586:ASP:C	1:C:588:HIS:H	2.28	0.42
1:D:215:SER:HA	1:D:247:MET:HE3	2.01	0.42
1:D:277:ILE:O	1:D:289:GLY:N	2.49	0.42
1:A:157:VAL:HG12	1:A:160:THR:HG23	2.01	0.42
1:A:407:GLU:O	1:A:412:GLU:HG2	2.19	0.42
1:B:422:LYS:HG2	1:B:423:TYR:CD1	2.55	0.42
1:D:19:VAL:HG22	1:D:177:LEU:HD21	2.01	0.42
1:D:374:GLU:HG3	1:D:375:TRP:N	2.35	0.42
1:E:185:ILE:O	1:E:185:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:ILE:HD11	1:E:581:LEU:HD21	2.01	0.42
1:A:505:ARG:HE	1:A:505:ARG:HB2	1.68	0.42
1:B:194:ASP:OD1	1:B:194:ASP:N	2.53	0.42
1:C:59:PRO:CG	1:C:62:VAL:HG22	2.50	0.42
1:C:208:ILE:CD1	1:C:220:LEU:HD22	2.50	0.42
1:C:410:PHE:HA	1:C:470:LEU:HD12	2.02	0.42
1:D:359:HIS:CE1	1:D:361:ARG:HB2	2.54	0.42
1:E:549:ARG:HB2	1:E:630:LEU:HD22	2.01	0.42
1:F:427:VAL:HG23	1:F:485:PHE:HB2	2.01	0.42
1:A:334:ARG:O	1:A:338:GLU:HG2	2.20	0.42
1:A:431:SER:O	1:A:489:ARG:HA	2.19	0.42
1:B:435:VAL:HG11	1:B:489:ARG:NE	2.35	0.42
1:C:208:ILE:HD12	1:C:217:VAL:HG13	2.01	0.42
1:C:355:ARG:HG3	1:C:356:PHE:CD2	2.54	0.42
1:F:543:GLY:HA2	1:F:565:ILE:HG21	2.01	0.42
1:B:121:LEU:HD21	1:B:161:LEU:HD23	2.01	0.42
1:D:248:CYS:O	1:D:273:ALA:N	2.53	0.42
1:E:90:GLU:HA	1:E:93:LEU:HD23	2.02	0.42
1:F:4:VAL:O	1:F:79:ILE:HA	2.20	0.42
1:F:368:ASP:H	1:F:372:HIS:CD2	2.38	0.42
1:A:90:GLU:H	1:A:90:GLU:CD	2.29	0.41
1:A:417:ILE:O	1:A:421:VAL:HG13	2.19	0.41
1:A:444:PHE:O	1:A:622:SER:HB3	2.19	0.41
1:A:655:ILE:HD12	1:A:655:ILE:O	2.20	0.41
1:C:32:HIS:NE2	1:C:85:ARG:HB2	2.35	0.41
1:C:260:ILE:HG13	1:C:266:ARG:O	2.20	0.41
1:D:200:ARG:HG2	1:D:201:ARG:N	2.35	0.41
1:F:11:MET:HE1	1:F:166:CYS:HA	2.01	0.41
1:F:470:LEU:O	1:F:474:ILE:HG13	2.20	0.41
1:A:93:LEU:HD12	1:A:100:ALA:HB3	2.02	0.41
1:B:288:GLN:HG2	1:B:289:GLY:N	2.34	0.41
1:C:572:ALA:HB3	1:C:638:MET:HE1	2.01	0.41
1:D:468:GLN:O	1:D:472:ARG:HG3	2.20	0.41
1:F:9:HIS:CG	1:F:10:ASP:H	2.37	0.41
1:F:334:ARG:HD2	1:F:334:ARG:HA	1.89	0.41
1:F:535:ARG:NH2	1:F:615:ASP:OD1	2.52	0.41
1:B:427:VAL:HG12	1:B:429:PHE:HB2	2.01	0.41
1:C:426:ARG:HA	1:C:484:ARG:O	2.21	0.41
1:C:613:TYR:CE2	1:C:615:ASP:HB2	2.55	0.41
1:D:390:VAL:HG12	1:D:408:LEU:HD21	2.02	0.41
1:D:421:VAL:HG12	1:D:483:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ASP:O	1:E:252:GLN:N	2.46	0.41
1:F:2:LYS:O	1:F:77:ASP:HB2	2.20	0.41
1:F:299:VAL:O	1:F:301:GLY:N	2.53	0.41
1:A:604:GLU:HB3	1:D:64:HIS:CD2	2.56	0.41
1:B:64:HIS:ND1	1:B:65:PRO:HD2	2.36	0.41
1:B:368:ASP:HB3	1:B:371:ILE:HD12	2.03	0.41
1:B:519:LEU:HD13	1:B:585:PHE:CD2	2.55	0.41
1:B:605:SER:HB2	1:B:613:TYR:CD2	2.55	0.41
1:C:339:GLU:O	1:C:361:ARG:NH1	2.54	0.41
1:C:394:THR:HG22	1:C:396:ILE:HG22	2.01	0.41
1:B:220:LEU:O	1:B:224:VAL:HG22	2.20	0.41
1:D:6:PHE:HE1	1:D:30:PHE:CD2	2.38	0.41
1:F:84:TYR:CE2	1:F:86:ASN:HB2	2.54	0.41
1:A:177:LEU:HB3	1:A:178:PRO:HD3	2.03	0.41
1:B:416:ILE:O	1:B:419:TYR:HB2	2.20	0.41
1:C:148:GLN:HG2	1:C:172:LEU:HD12	2.02	0.41
1:D:353:ILE:HB	1:D:356:PHE:CE1	2.54	0.41
1:E:93:LEU:HD12	1:E:100:ALA:CB	2.51	0.41
1:E:638:MET:O	1:E:642:VAL:HG23	2.21	0.41
1:F:30:PHE:HA	1:F:57:TYR:O	2.20	0.41
1:A:62:VAL:O	1:A:64:HIS:N	2.54	0.41
1:A:242:ILE:HD13	1:A:276:ILE:HG12	2.02	0.41
1:A:288:GLN:HG2	1:A:289:GLY:N	2.35	0.41
1:A:374:GLU:HG3	1:A:375:TRP:N	2.35	0.41
1:C:77:ASP:HA	1:C:97:PRO:HD2	2.01	0.41
1:C:112:ARG:NH1	1:C:141:ALA:HA	2.36	0.41
1:C:429:PHE:CZ	1:C:470:LEU:HD22	2.56	0.41
1:D:456:VAL:H	1:D:456:VAL:HG22	1.58	0.41
2:E:1100:UGA:PB	2:E:1100:UGA:H5'2	2.60	0.41
1:F:536:CYS:SG	1:F:568:PRO:HA	2.60	0.41
1:A:536:CYS:SG	1:A:620:LYS:HA	2.61	0.41
1:D:78:ILE:HG12	1:D:98:ALA:HB3	2.02	0.41
1:F:386:VAL:HG12	1:F:388:PRO:HD3	2.02	0.41
1:F:534:LYS:HD3	1:F:571:GLU:HG2	2.02	0.41
1:A:112:ARG:HE	1:A:195:SER:HB2	1.86	0.41
1:A:118:ASN:ND2	1:A:223:ALA:O	2.48	0.41
1:A:493:TRP:CD1	1:A:538:THR:HB	2.55	0.41
1:B:118:ASN:O	1:B:122:VAL:HG23	2.21	0.41
1:B:120:VAL:HG23	1:B:121:LEU:HD22	2.02	0.41
1:B:204:GLU:HG3	1:B:204:GLU:O	2.21	0.41
1:B:332:THR:HG21	1:B:356:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TYR:HE1	1:C:198:TYR:HE2	1.69	0.41
1:C:426:ARG:NH2	1:C:550:ILE:O	2.49	0.41
1:C:466:SER:HA	1:F:469:LEU:HD11	2.01	0.41
1:C:471:ASP:HA	1:C:474:ILE:HD12	2.03	0.41
1:D:72:ALA:HB2	1:D:95:LEU:HD13	2.03	0.41
1:D:375:TRP:CZ2	1:E:375:TRP:HZ2	2.39	0.41
1:F:7:ALA:HB1	1:F:12:GLY:CA	2.51	0.41
1:F:78:ILE:HG21	1:F:80:PHE:CZ	2.56	0.41
1:A:609:TYR:OH	2:A:1100:UGA:H2A1	2.20	0.41
1:B:445:ASP:HA	1:B:622:SER:HB3	2.03	0.41
1:D:353:ILE:HD11	1:D:364:PHE:CE2	2.56	0.41
1:D:410:PHE:HD1	1:D:470:LEU:HB2	1.86	0.41
1:E:577:LEU:O	1:E:581:LEU:HG	2.21	0.41
1:E:581:LEU:HD23	1:E:642:VAL:CG1	2.49	0.41
1:F:549:ARG:HB3	1:F:630:LEU:HD22	2.03	0.41
1:B:429:PHE:HB3	1:B:487:LEU:HD23	2.02	0.40
1:C:143:GLU:CB	1:C:187:SER:HB2	2.50	0.40
1:C:431:SER:CB	1:C:489:ARG:HG2	2.50	0.40
1:F:192:GLU:O	1:F:192:GLU:HG3	2.22	0.40
1:A:446:GLU:OE1	1:A:446:GLU:N	2.43	0.40
1:A:533:GLN:HB2	1:A:617:ALA:O	2.22	0.40
1:B:343:VAL:HG23	1:B:362:PHE:CD1	2.52	0.40
1:B:365:VAL:HG21	1:B:379:HIS:CE1	2.57	0.40
1:C:2:LYS:O	1:C:77:ASP:HB2	2.21	0.40
1:C:184:ASP:OD1	1:C:185:ILE:N	2.54	0.40
1:E:417:ILE:HD11	1:E:429:PHE:CD1	2.55	0.40
1:F:64:HIS:ND1	1:F:65:PRO:HD2	2.36	0.40
1:F:65:PRO:O	1:F:69:ASP:HB2	2.21	0.40
1:A:460:ARG:NH1	1:A:613:TYR:OH	2.54	0.40
1:B:417:ILE:O	1:B:421:VAL:HG13	2.20	0.40
1:B:581:LEU:HA	1:B:642:VAL:HG11	2.03	0.40
1:C:129:GLY:HA2	1:C:165:LEU:HD11	2.03	0.40
1:C:357:LEU:HD23	1:C:357:LEU:HA	1.87	0.40
1:C:528:ILE:HD13	2:C:1100:UGA:N3	2.37	0.40
1:D:111:TYR:HD1	1:D:198:TYR:CE2	2.39	0.40
1:D:421:VAL:HG12	1:D:483:LEU:HD22	2.02	0.40
1:E:30:PHE:HA	1:E:57:TYR:O	2.22	0.40
1:E:143:GLU:HB3	1:E:187:SER:HB2	2.02	0.40
1:E:336:LEU:HA	1:E:336:LEU:HD12	1.83	0.40
1:A:72:ALA:HB2	1:A:95:LEU:HD13	2.03	0.40
1:B:346:MET:HA	1:B:365:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ALA:O	1:B:550:ILE:HG13	2.22	0.40
1:D:429:PHE:CZ	1:D:470:LEU:HD22	2.57	0.40
1:D:446:GLU:HG2	1:D:564:ASN:HB2	2.03	0.40
1:D:597:PHE:HZ	1:D:600:PHE:CE1	2.40	0.40
1:E:67:TRP:O	1:E:71:ILE:HG13	2.20	0.40
1:E:258:SER:HA	1:E:302:ALA:HA	2.03	0.40
1:A:647:ASP:OD1	1:A:651:ARG:NH2	2.53	0.40
1:B:468:GLN:O	1:B:471:ASP:HB2	2.21	0.40
1:C:303:ARG:C	1:C:304:LEU:HD22	2.47	0.40
1:C:317:ARG:HB2	1:C:383:CYS:HA	2.03	0.40
1:E:111:TYR:CE1	1:E:198:TYR:HE2	2.40	0.40
1:E:218:HIS:CD2	1:E:222:ARG:HG3	2.56	0.40
1:F:177:LEU:HB3	1:F:178:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	633/660 (96%)	578 (91%)	52 (8%)	3 (0%)	24	57
1	B	632/660 (96%)	574 (91%)	55 (9%)	3 (0%)	24	57
1	C	633/660 (96%)	568 (90%)	61 (10%)	4 (1%)	21	54
1	D	632/660 (96%)	564 (89%)	64 (10%)	4 (1%)	21	54
1	E	632/660 (96%)	571 (90%)	57 (9%)	4 (1%)	21	54
1	F	633/660 (96%)	567 (90%)	60 (10%)	6 (1%)	14	46
All	All	3795/3960 (96%)	3422 (90%)	349 (9%)	24 (1%)	21	54

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	GLY
1	E	250	ASP
1	F	251	ALA
1	F	300	ALA
1	A	63	ASN
1	C	253	GLY
1	D	253	GLY
1	D	300	ALA
1	E	63	ASN
1	F	63	ASN
1	F	250	ASP
1	B	300	ALA
1	C	252	GLN
1	D	63	ASN
1	E	113	GLY
1	F	183	GLY
1	C	251	ALA
1	C	299	VAL
1	B	236	GLY
1	F	589	PRO
1	E	253	GLY
1	A	297	GLY
1	A	299	VAL
1	D	299	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	538/555 (97%)	538 (100%)	0	100	100
1	B	538/555 (97%)	538 (100%)	0	100	100
1	C	538/555 (97%)	538 (100%)	0	100	100
1	D	538/555 (97%)	538 (100%)	0	100	100
1	E	538/555 (97%)	538 (100%)	0	100	100
1	F	538/555 (97%)	538 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3228/3330 (97%)	3228 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	17	GLN
1	A	123	ASN
1	A	171	GLN
1	A	174	ASN
1	A	238	GLN
1	A	280	GLN
1	A	337	ASN
1	A	363	HIS
1	A	401	ASN
1	A	450	ASN
1	A	502	ASN
1	B	174	ASN
1	B	238	GLN
1	B	280	GLN
1	B	372	HIS
1	B	379	HIS
1	B	401	ASN
1	B	518	ASN
1	B	567	ASN
1	B	588	HIS
1	C	102	ASN
1	C	123	ASN
1	C	174	ASN
1	C	238	GLN
1	C	379	HIS
1	C	401	ASN
1	C	450	ASN
1	C	492	ASN
1	C	518	ASN
1	C	570	ASN
1	C	614	GLN
1	D	174	ASN
1	D	211	HIS
1	D	363	HIS
1	D	450	ASN

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Mol	Chain	Res	Type
1	D	614	GLN
1	D	625	ASN
1	E	17	GLN
1	E	48	GLN
1	E	102	ASN
1	E	211	HIS
1	E	218	HIS
1	E	280	GLN
1	E	330	HIS
1	E	401	ASN
1	E	450	ASN
1	E	518	ASN
1	E	570	ASN
1	E	593	HIS
1	E	601	GLN
1	E	614	GLN
1	F	61	ASN
1	F	174	ASN
1	F	235	ASN
1	F	372	HIS
1	F	450	ASN
1	F	518	ASN
1	F	593	HIS
1	F	601	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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	$\# Z > 2$
2	UGA	E	1100	-	38,39,39	1.48	7 (18%)	56,60,60	1.75	8 (14%)
2	UGA	D	1100	-	38,39,39	1.46	7 (18%)	56,60,60	1.85	8 (14%)
2	UGA	A	1100	-	38,39,39	1.48	7 (18%)	56,60,60	1.84	9 (16%)
2	UGA	B	1100	-	38,39,39	1.51	7 (18%)	56,60,60	1.90	9 (16%)
2	UGA	F	1100	-	38,39,39	1.45	6 (15%)	56,60,60	1.80	9 (16%)
2	UGA	C	1100	-	38,39,39	1.48	7 (18%)	56,60,60	1.77	9 (16%)

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	UGA	E	1100	-	-	1/25/61/61	0/3/3/3
2	UGA	D	1100	-	-	3/25/61/61	0/3/3/3
2	UGA	A	1100	-	-	6/25/61/61	0/3/3/3
2	UGA	B	1100	-	-	0/25/61/61	0/3/3/3
2	UGA	F	1100	-	-	6/25/61/61	0/3/3/3
2	UGA	C	1100	-	-	6/25/61/61	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1100	UGA	C5-C4	-2.83	1.37	1.43
2	B	1100	UGA	C4-N3	-2.82	1.33	1.38
2	D	1100	UGA	C4-N3	-2.80	1.33	1.38
2	C	1100	UGA	C5-C4	-2.79	1.37	1.43
2	F	1100	UGA	C5-C4	-2.79	1.37	1.43
2	A	1100	UGA	C5-C4	-2.78	1.37	1.43
2	B	1100	UGA	C5-C4	-2.78	1.37	1.43
2	D	1100	UGA	C5-C4	-2.76	1.37	1.43
2	B	1100	UGA	C4'-C5'	-2.75	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1100	UGA	O5'-C5'	-2.73	1.38	1.43
2	F	1100	UGA	C4-N3	-2.70	1.34	1.38
2	C	1100	UGA	C4-N3	-2.69	1.34	1.38
2	A	1100	UGA	C4-N3	-2.65	1.34	1.38
2	C	1100	UGA	O5'-C5'	-2.64	1.38	1.43
2	D	1100	UGA	O5'-C5'	-2.63	1.38	1.43
2	E	1100	UGA	C4'-C5'	-2.63	1.48	1.53
2	E	1100	UGA	C4-N3	-2.62	1.34	1.38
2	A	1100	UGA	C4'-C5'	-2.58	1.49	1.53
2	B	1100	UGA	O5'-C5'	-2.58	1.38	1.43
2	A	1100	UGA	O5'-C5'	-2.54	1.38	1.43
2	F	1100	UGA	O5'-C5'	-2.42	1.38	1.43
2	B	1100	UGA	C2D-C3D	-2.31	1.47	1.53
2	C	1100	UGA	C4'-C5'	-2.31	1.49	1.53
2	C	1100	UGA	C2D-C3D	-2.31	1.47	1.53
2	B	1100	UGA	O3D-C3D	-2.28	1.37	1.43
2	C	1100	UGA	O3D-C3D	-2.27	1.37	1.43
2	F	1100	UGA	O3D-C3D	-2.25	1.37	1.43
2	D	1100	UGA	C4'-C5'	-2.25	1.49	1.53
2	E	1100	UGA	C2D-C3D	-2.24	1.47	1.53
2	F	1100	UGA	C2D-C3D	-2.22	1.47	1.53
2	D	1100	UGA	C2D-C3D	-2.22	1.47	1.53
2	A	1100	UGA	O3D-C3D	-2.21	1.37	1.43
2	D	1100	UGA	O3D-C3D	-2.20	1.37	1.43
2	E	1100	UGA	O3D-C3D	-2.20	1.37	1.43
2	A	1100	UGA	C2D-C3D	-2.19	1.47	1.53
2	C	1100	UGA	O4D-C4D	-2.19	1.40	1.45
2	E	1100	UGA	O4D-C4D	-2.17	1.40	1.45
2	A	1100	UGA	O4D-C4D	-2.17	1.40	1.45
2	B	1100	UGA	O4D-C4D	-2.15	1.40	1.45
2	F	1100	UGA	O4D-C4D	-2.15	1.40	1.45
2	D	1100	UGA	O4D-C4D	-2.13	1.40	1.45

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1100	UGA	O'Q-C6'-O'P	7.55	141.21	124.08
2	E	1100	UGA	O'Q-C6'-O'P	7.47	141.03	124.08
2	A	1100	UGA	O'Q-C6'-O'P	7.41	140.88	124.08
2	B	1100	UGA	O'Q-C6'-O'P	7.40	140.87	124.08
2	C	1100	UGA	O'Q-C6'-O'P	7.34	140.74	124.08
2	F	1100	UGA	O'Q-C6'-O'P	7.32	140.70	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1100	UGA	C4-N3-C2	-4.70	120.77	126.61
2	A	1100	UGA	C4-N3-C2	-4.57	120.94	126.61
2	B	1100	UGA	C1'-O5'-C5'	4.55	119.70	112.23
2	F	1100	UGA	C4-N3-C2	-4.55	120.97	126.61
2	B	1100	UGA	C4-N3-C2	-4.52	121.00	126.61
2	D	1100	UGA	N3-C2-N1	4.50	120.75	114.89
2	C	1100	UGA	C4-N3-C2	-4.48	121.05	126.61
2	E	1100	UGA	C4-N3-C2	-4.45	121.09	126.61
2	B	1100	UGA	N3-C2-N1	4.37	120.58	114.89
2	C	1100	UGA	N3-C2-N1	4.32	120.52	114.89
2	A	1100	UGA	N3-C2-N1	4.32	120.52	114.89
2	F	1100	UGA	N3-C2-N1	4.30	120.49	114.89
2	E	1100	UGA	N3-C2-N1	4.22	120.39	114.89
2	D	1100	UGA	C5-C4-N3	3.90	120.26	114.80
2	F	1100	UGA	C5-C4-N3	3.90	120.26	114.80
2	A	1100	UGA	C5-C4-N3	3.84	120.17	114.80
2	B	1100	UGA	C5-C4-N3	3.83	120.16	114.80
2	A	1100	UGA	C1'-O5'-C5'	3.83	118.51	112.23
2	C	1100	UGA	C5-C4-N3	3.79	120.11	114.80
2	E	1100	UGA	C5-C4-N3	3.73	120.03	114.80
2	B	1100	UGA	O5'-C1'-C2'	3.72	118.02	110.37
2	F	1100	UGA	O'P-C6'-C5'	-3.19	109.31	120.81
2	D	1100	UGA	O'P-C6'-C5'	-3.18	109.32	120.81
2	B	1100	UGA	C1'-C2'-C3'	3.12	116.57	110.01
2	C	1100	UGA	O'P-C6'-C5'	-3.09	109.66	120.81
2	E	1100	UGA	O4-C4-C5	-3.08	119.85	125.16
2	F	1100	UGA	C3'-C4'-C5'	3.06	114.56	109.30
2	A	1100	UGA	O'P-C6'-C5'	-3.06	109.77	120.81
2	E	1100	UGA	O'P-C6'-C5'	-3.05	109.81	120.81
2	B	1100	UGA	O'P-C6'-C5'	-2.99	110.02	120.81
2	A	1100	UGA	O4-C4-C5	-2.98	120.03	125.16
2	F	1100	UGA	O4-C4-C5	-2.91	120.15	125.16
2	C	1100	UGA	O4-C4-C5	-2.88	120.20	125.16
2	D	1100	UGA	O4-C4-C5	-2.78	120.37	125.16
2	B	1100	UGA	O4-C4-C5	-2.72	120.46	125.16
2	F	1100	UGA	O5'-C5'-C4'	2.51	114.43	109.48
2	C	1100	UGA	C1'-O5'-C5'	2.45	116.25	112.23
2	D	1100	UGA	C3D-C2D-C1D	2.41	106.03	101.46
2	C	1100	UGA	C1'-C2'-C3'	2.32	114.88	110.01
2	A	1100	UGA	O5'-C1'-C2'	2.24	114.97	110.37
2	E	1100	UGA	C1'-C2'-C3'	2.20	114.64	110.01
2	E	1100	UGA	O2-C2-N1	-2.17	119.97	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1100	UGA	C1D-N1-C2	2.12	121.39	117.59
2	A	1100	UGA	O2-C2-N1	-2.04	120.14	122.80
2	F	1100	UGA	C1'-O5'-C5'	2.04	115.58	112.23
2	C	1100	UGA	O2-C2-N1	-2.02	120.16	122.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1100	UGA	C5D-O5D-PA-O3A
2	C	1100	UGA	C5D-O5D-PA-O2A
2	F	1100	UGA	C1'-O3B-PB-O3A
2	F	1100	UGA	C5D-O5D-PA-O3A
2	F	1100	UGA	C5D-O5D-PA-O1A
2	F	1100	UGA	C5D-O5D-PA-O2A
2	F	1100	UGA	O4D-C4D-C5D-O5D
2	F	1100	UGA	C3D-C4D-C5D-O5D
2	C	1100	UGA	C3D-C4D-C5D-O5D
2	C	1100	UGA	O4D-C4D-C5D-O5D
2	A	1100	UGA	PA-O3A-PB-O1B
2	C	1100	UGA	C1'-O3B-PB-O3A
2	C	1100	UGA	C5D-O5D-PA-O1A
2	A	1100	UGA	O4D-C4D-C5D-O5D
2	A	1100	UGA	C3D-C4D-C5D-O5D
2	D	1100	UGA	C1'-O3B-PB-O1B
2	A	1100	UGA	O5'-C5'-C6'-O'P
2	A	1100	UGA	O5'-C5'-C6'-O'Q
2	D	1100	UGA	C2'-C1'-O3B-PB
2	E	1100	UGA	C2'-C1'-O3B-PB
2	D	1100	UGA	C2D-C1D-N1-C2
2	A	1100	UGA	PA-O3A-PB-O2B

There are no ring outliers.

6 monomers are involved in 19 short contacts:

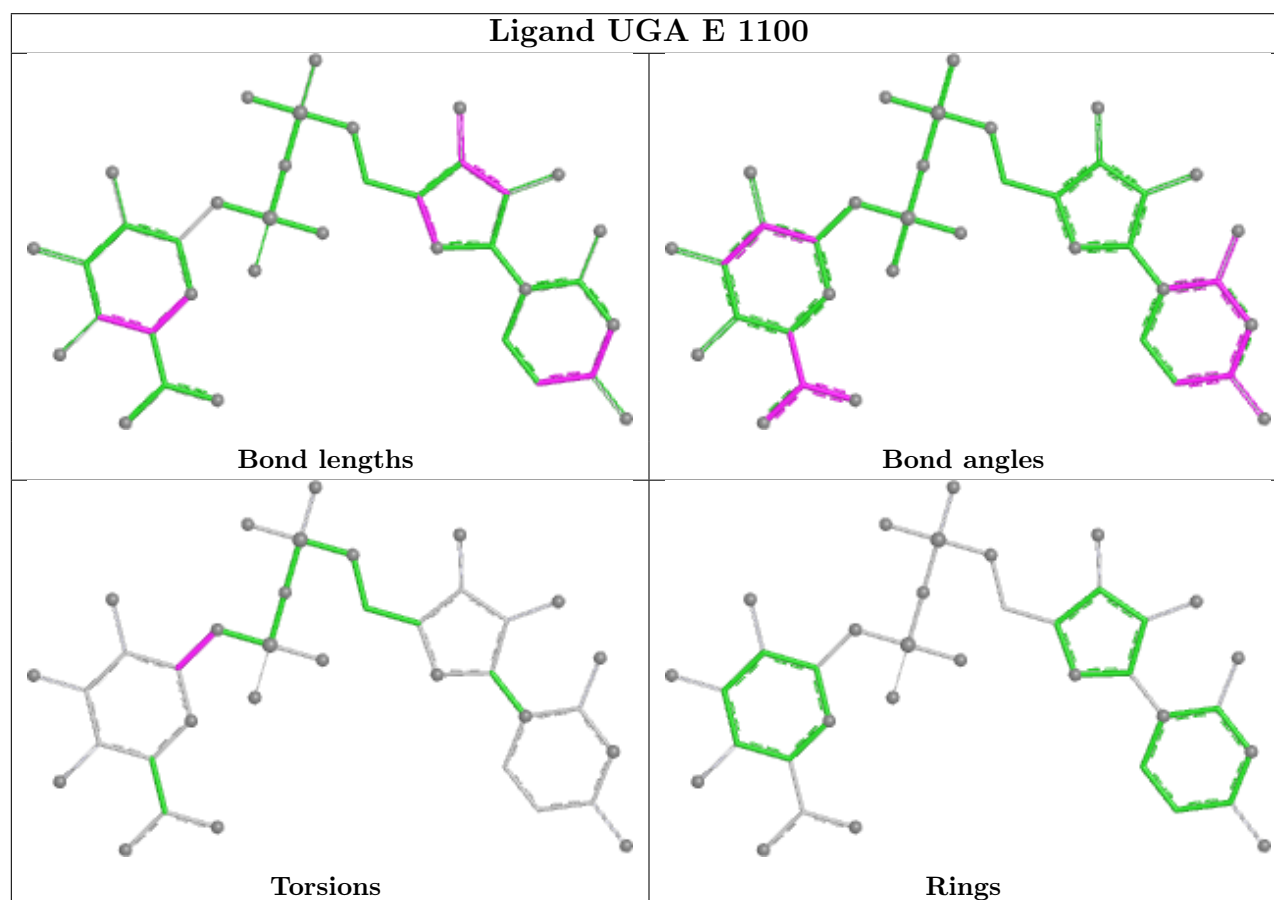
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1100	UGA	2	0
2	D	1100	UGA	3	0
2	A	1100	UGA	2	0
2	B	1100	UGA	4	0
2	F	1100	UGA	3	0

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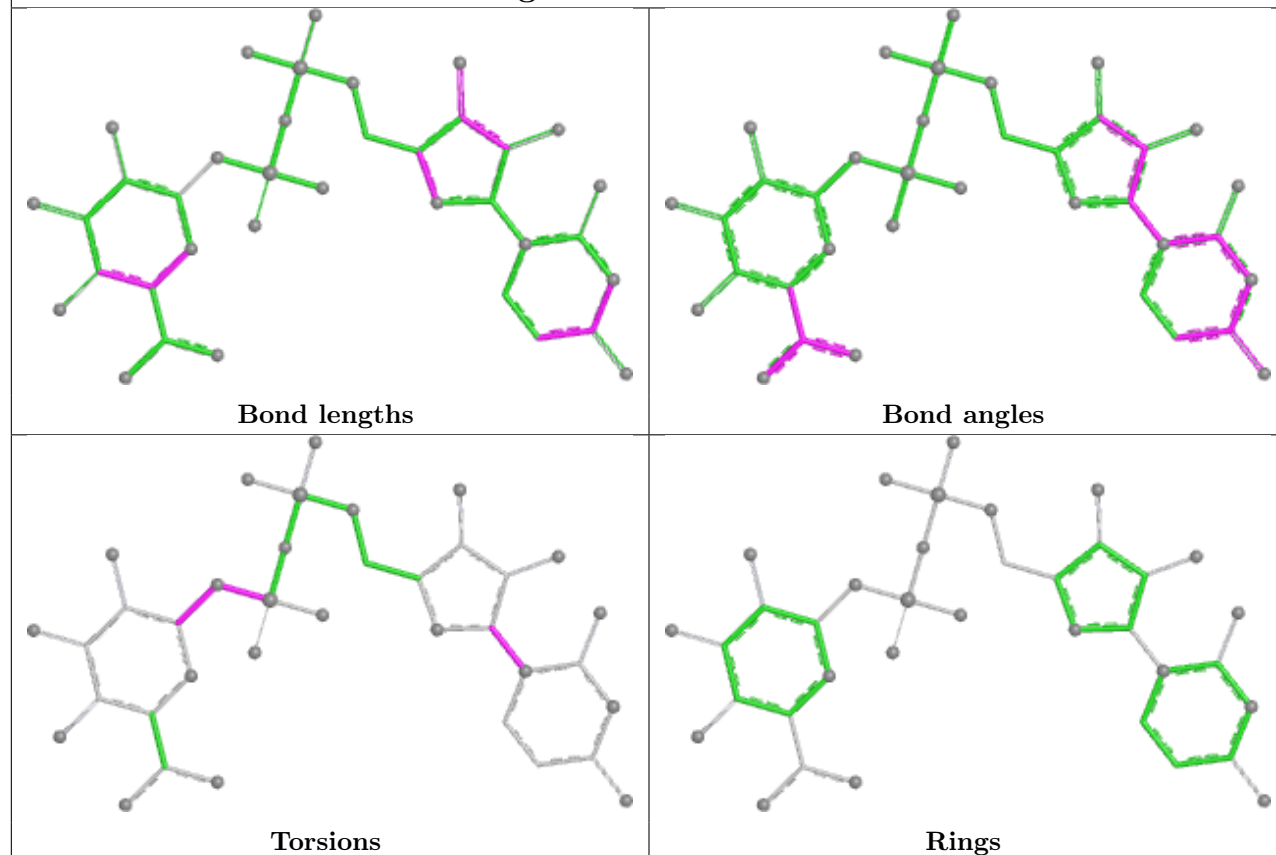
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1100	UGA	5	0

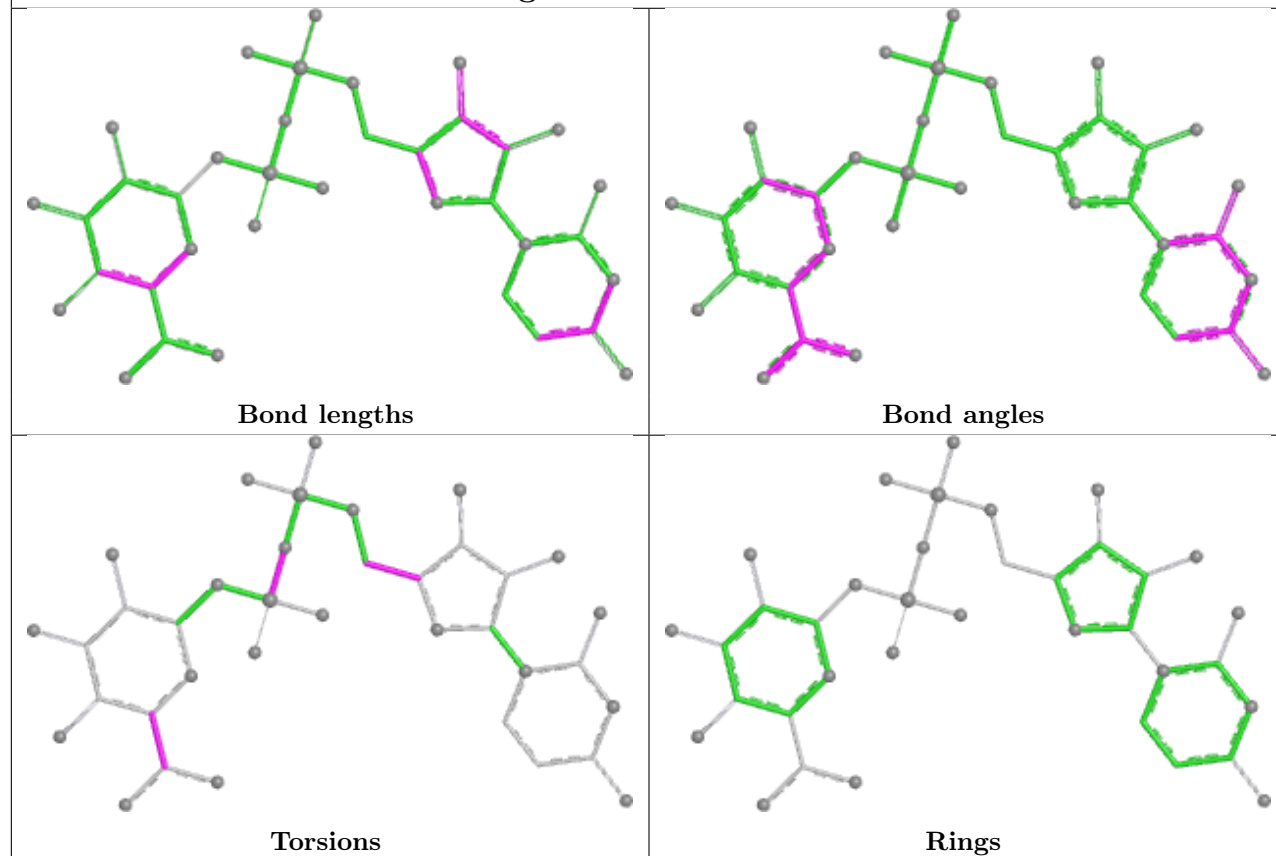
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



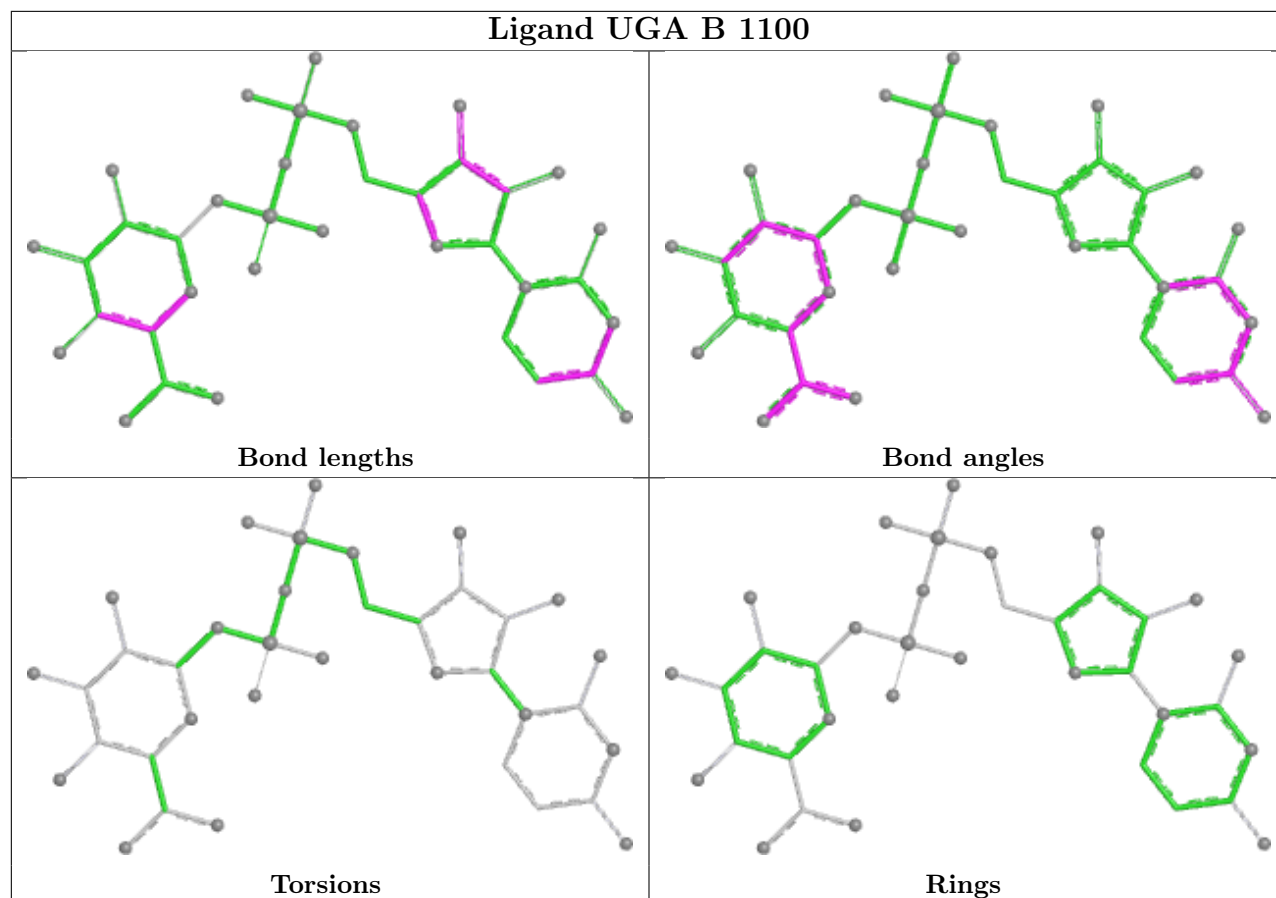
Ligand UGA D 1100



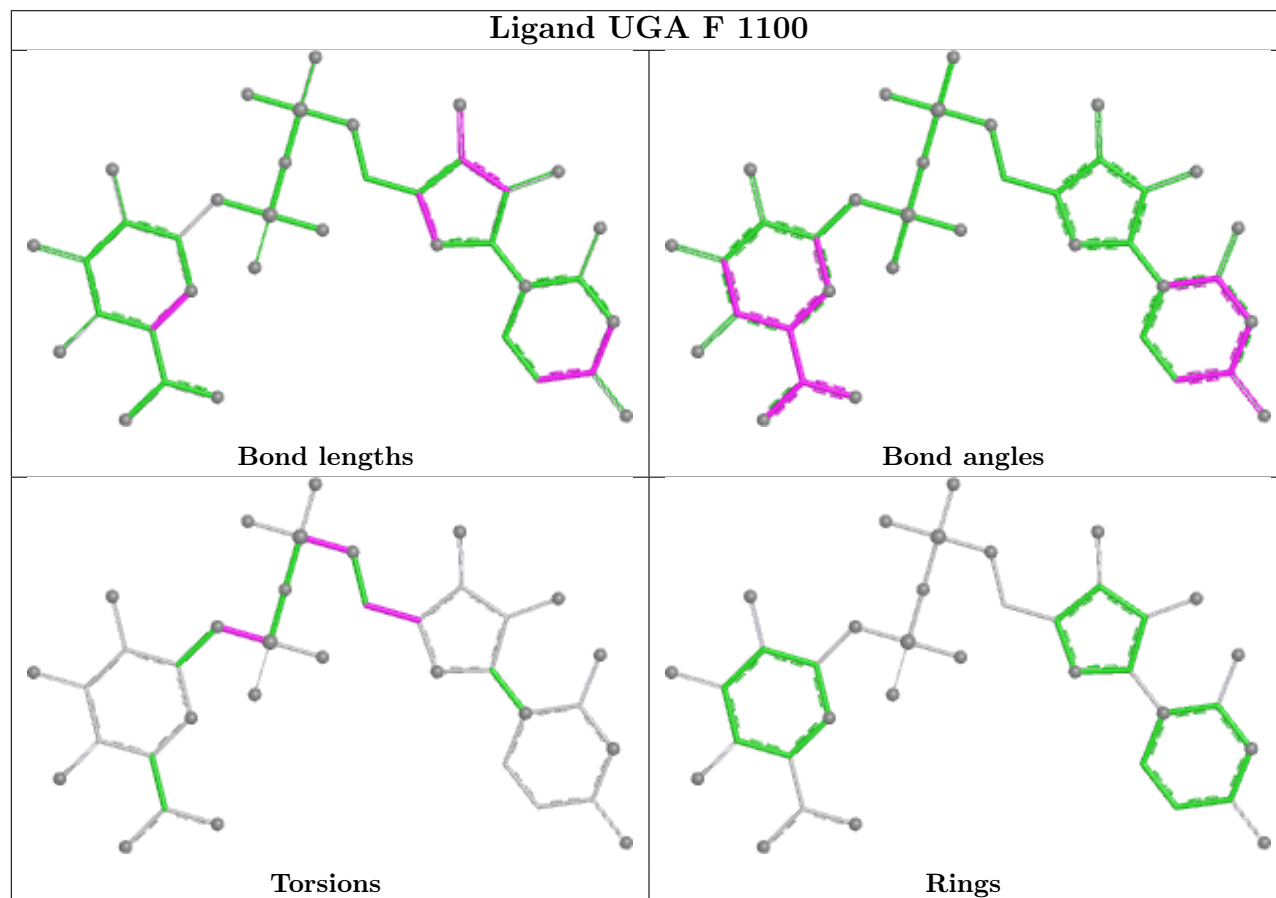
Ligand UGA A 1100

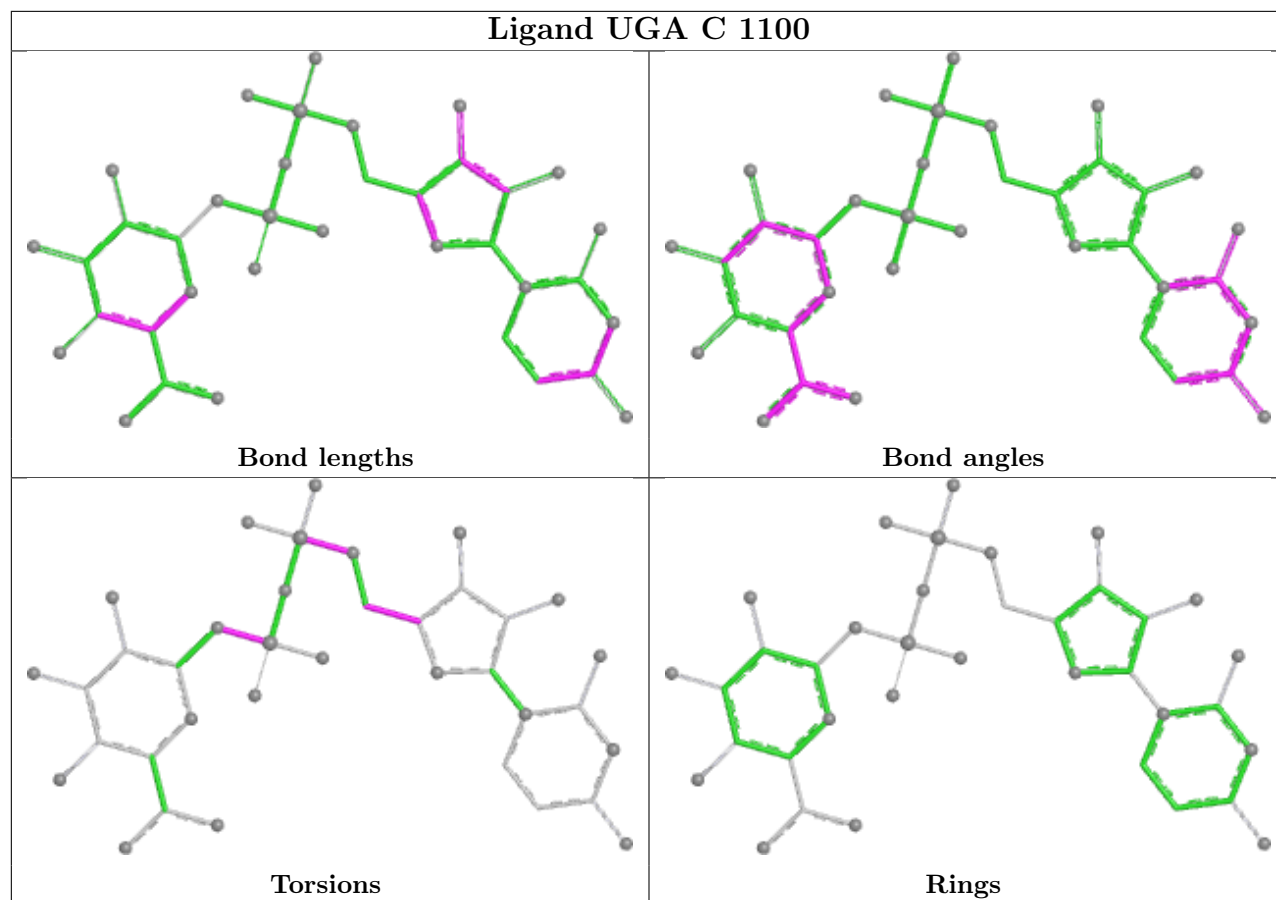


Ligand UGA B 1100



Ligand UGA F 1100





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	639/660 (96%)	-0.24	2 (0%) 90 75	63, 124, 164, 193	0
1	B	638/660 (96%)	-0.26	1 (0%) 91 80	61, 116, 158, 177	0
1	C	639/660 (96%)	-0.28	1 (0%) 91 80	61, 108, 162, 176	0
1	D	638/660 (96%)	-0.27	1 (0%) 91 80	66, 110, 140, 181	0
1	E	638/660 (96%)	-0.28	0 100 100	60, 106, 136, 158	0
1	F	639/660 (96%)	-0.27	0 100 100	60, 106, 136, 171	0
All	All	3831/3960 (96%)	-0.27	5 (0%) 92 85	60, 111, 155, 193	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ALA	3.0
1	D	235	ASN	2.6
1	C	303	ARG	2.4
1	A	235	ASN	2.1
1	A	298	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

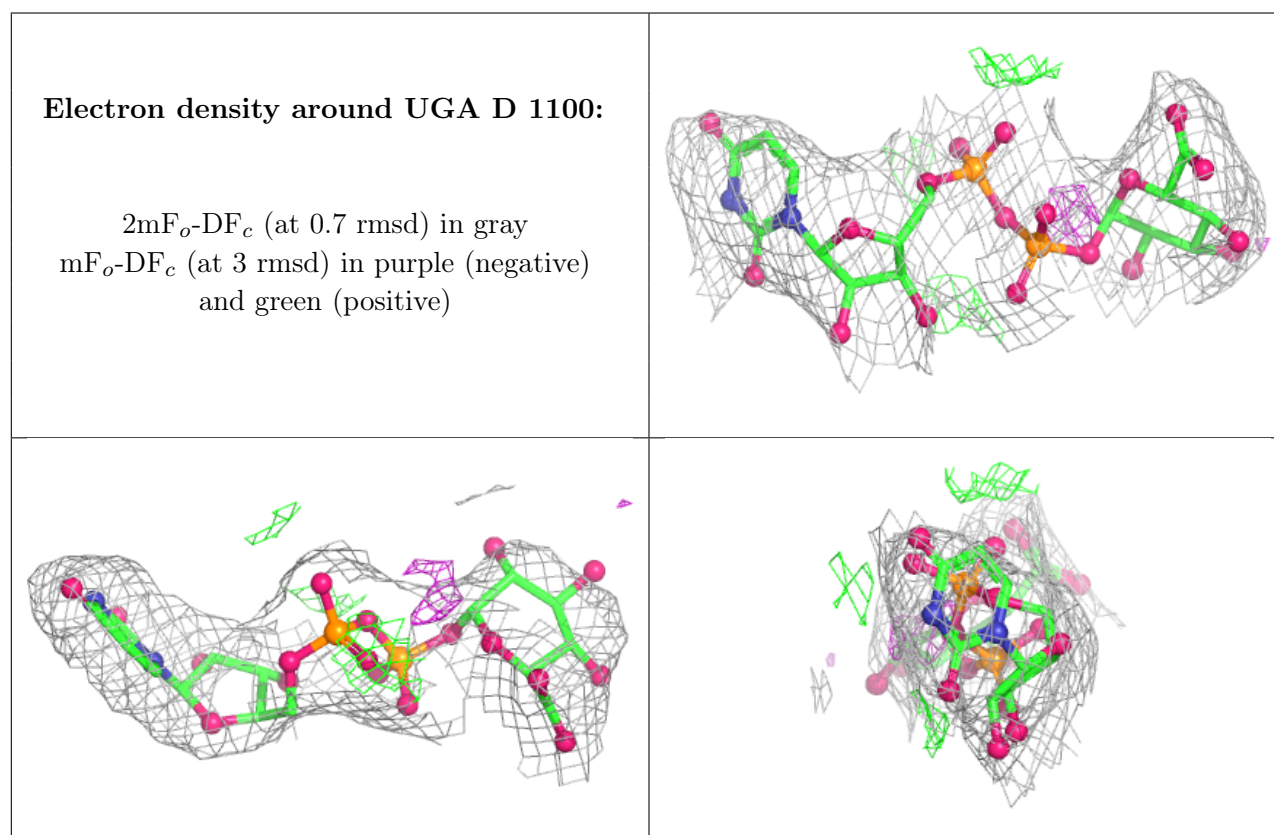
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

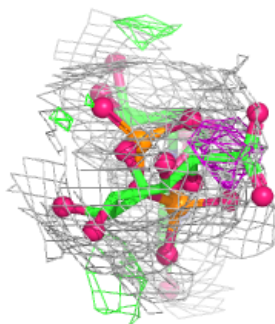
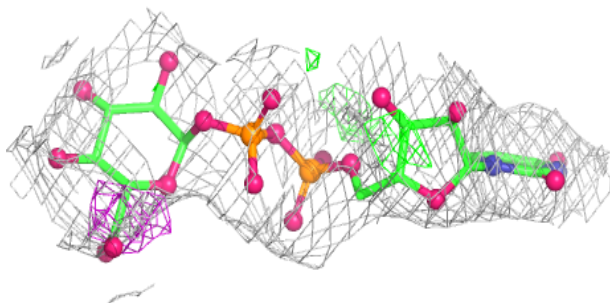
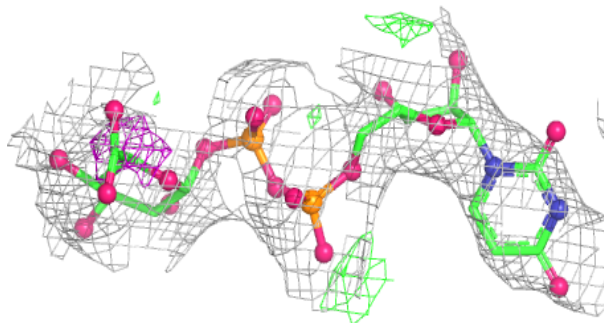
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UGA	D	1100	37/37	0.87	0.10	98,111,129,138	0
2	UGA	C	1100	37/37	0.89	0.10	84,94,107,110	0
2	UGA	E	1100	37/37	0.89	0.10	87,100,112,115	0
2	UGA	F	1100	37/37	0.89	0.09	101,114,123,130	0
2	UGA	B	1100	37/37	0.91	0.08	95,105,114,119	0
2	UGA	A	1100	37/37	0.93	0.09	102,109,128,132	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.

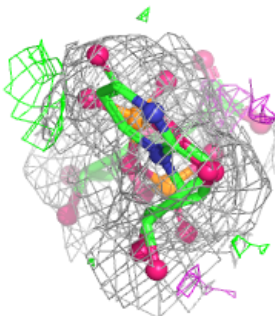
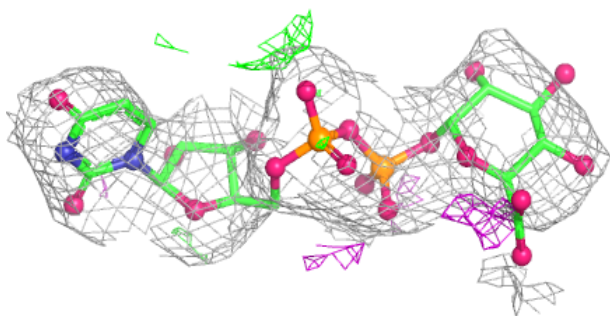
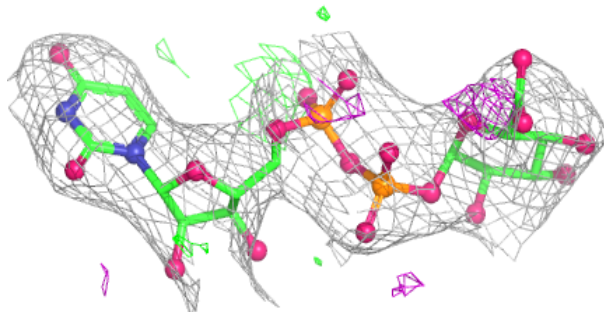


Electron density around UGA C 1100:

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

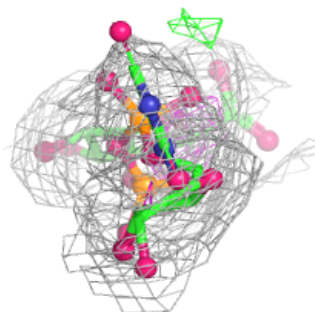
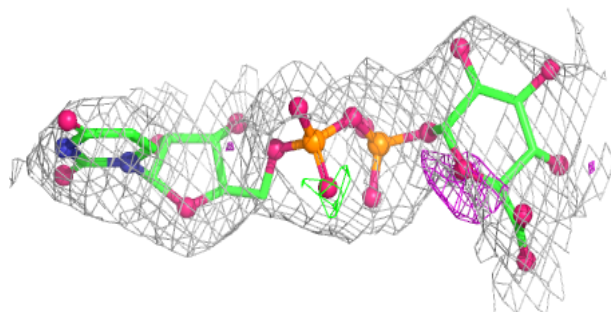
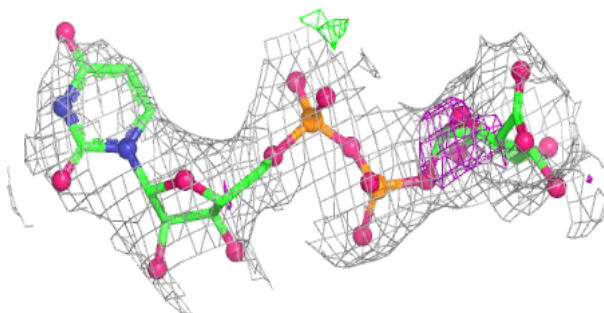
**Electron density around UGA E 1100:**

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

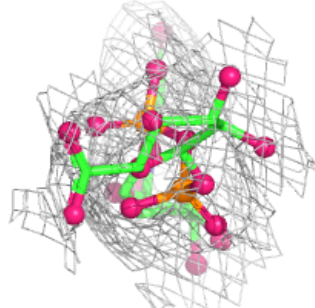
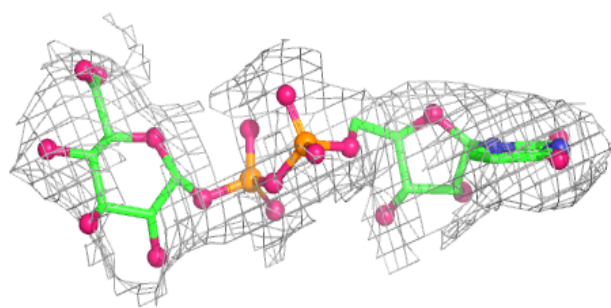
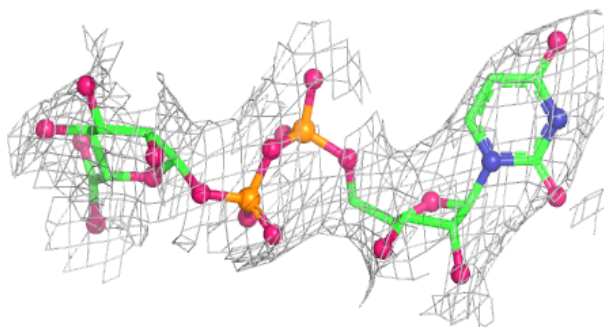


Electron density around UGA F 1100:

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

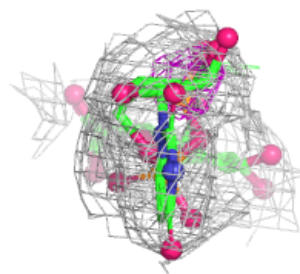
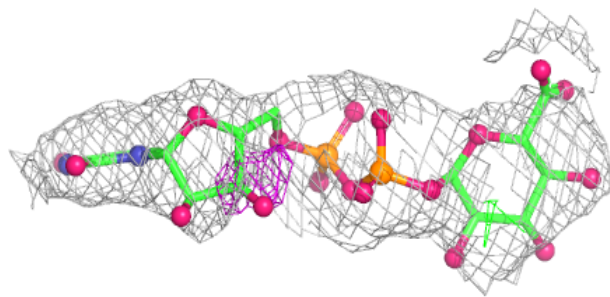
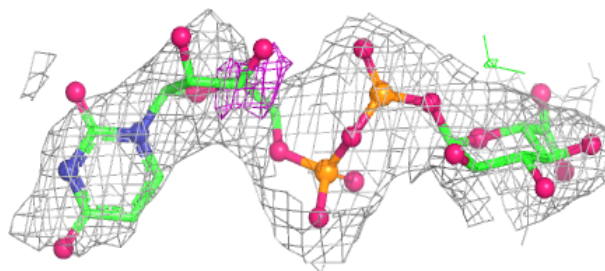
**Electron density around UGA B 1100:**

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



Electron density around UGA A 1100:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.