



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:53 AM BST

PDB ID : 5E9U
Title : Crystal structure of GtfA/B complex bound to UDP and GlcNAc
Authors : Chen, Y.; Rapoport, T.A.
Deposited on : 2015-10-15
Resolution : 3.84 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

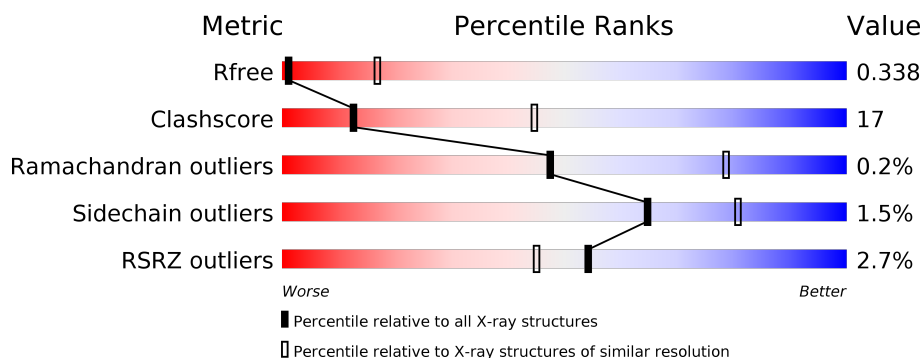
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

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 on 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	503	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>35%</div> </div> </div>
1	C	503	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>34%</div> </div> </div>
1	E	503	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>41%</div> </div> </div>
1	G	503	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>32%</div> </div> </div>
2	B	446	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>32%</div> </div> </div>
2	D	446	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>39%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	446	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>37%</div> <div></div> </div> </div>
2	H	446	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div></div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30948 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 Glycosyltransferase Gtf1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			
1	C	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			
1	E	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			
1	G	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9AET5
A	124	PHE	SER	conflict	UNP Q9AET5
C	1	SER	-	expression tag	UNP Q9AET5
C	124	PHE	SER	conflict	UNP Q9AET5
E	1	SER	-	expression tag	UNP Q9AET5
E	124	PHE	SER	conflict	UNP Q9AET5
G	1	SER	-	expression tag	UNP Q9AET5
G	124	PHE	SER	conflict	UNP Q9AET5

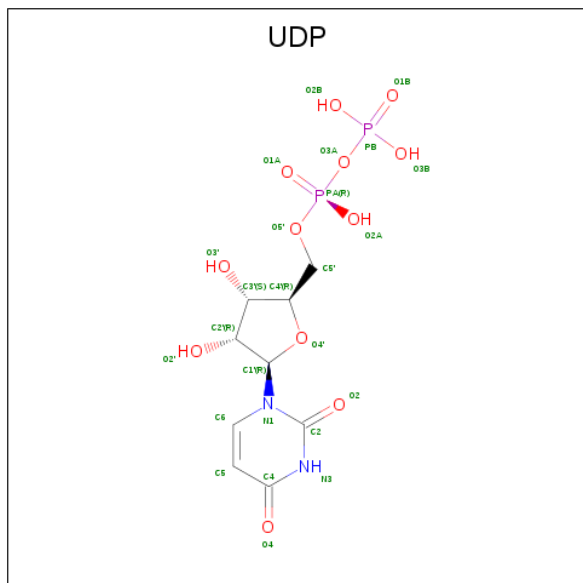
- Molecule 2 is a protein called Glycosyltransferase-stabilizing protein Gtf2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	445	Total	C	N	O	S	Se	0	0	0
			3607	2298	613	685	3	8			
2	D	446	Total	C	N	O	S	Se	0	0	0
			3611	2300	614	686	3	8			
2	F	445	Total	C	N	O	S	Se	0	0	0
			3607	2298	613	685	3	8			
2	H	445	Total	C	N	O	S	Se	0	0	0
			3607	2298	613	685	3	8			

There are 4 discrepancies between the modelled and reference sequences:

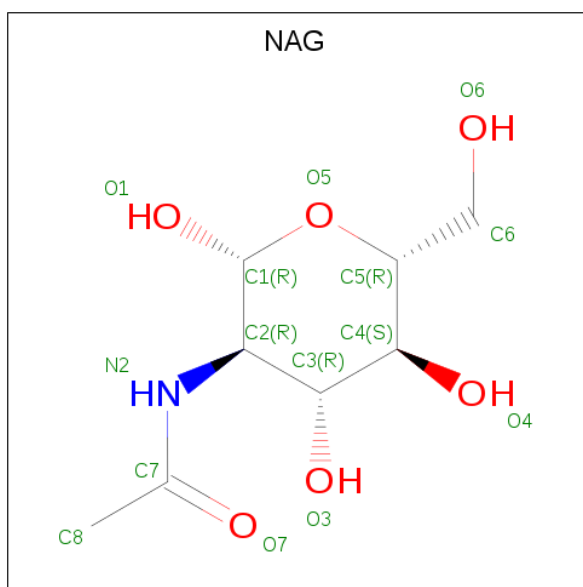
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP Q79T00
D	1	MSE	-	initiating methionine	UNP Q79T00
F	1	MSE	-	initiating methionine	UNP Q79T00
H	1	MSE	-	initiating methionine	UNP Q79T00

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

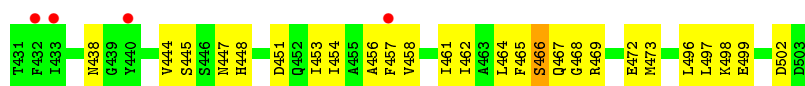
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



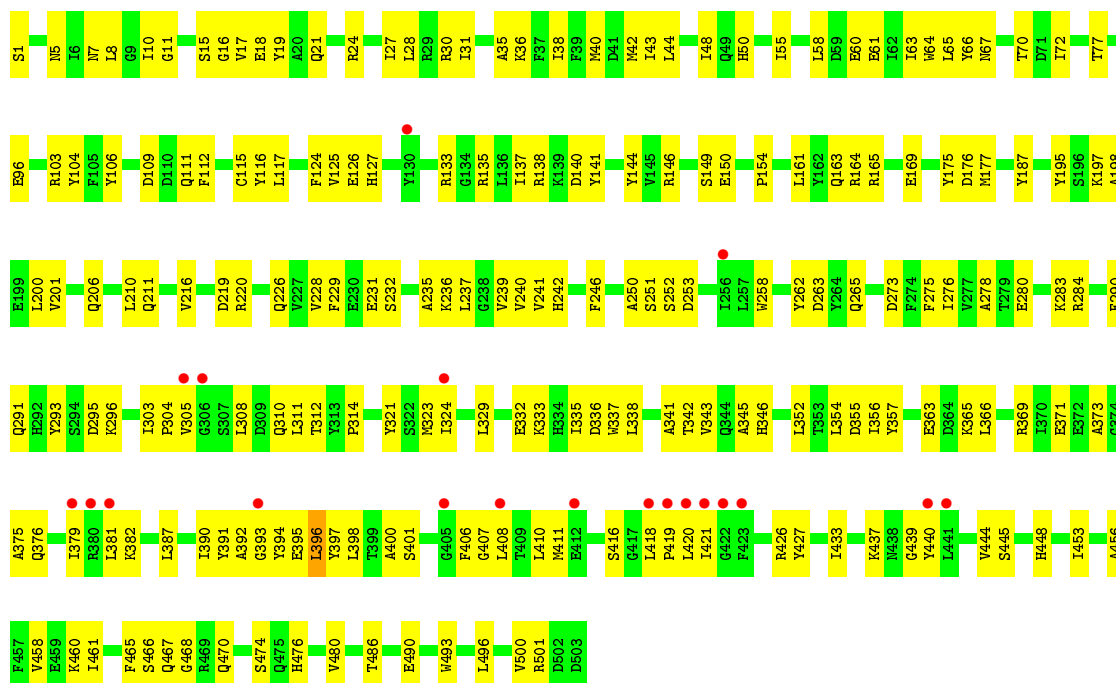
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	E	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

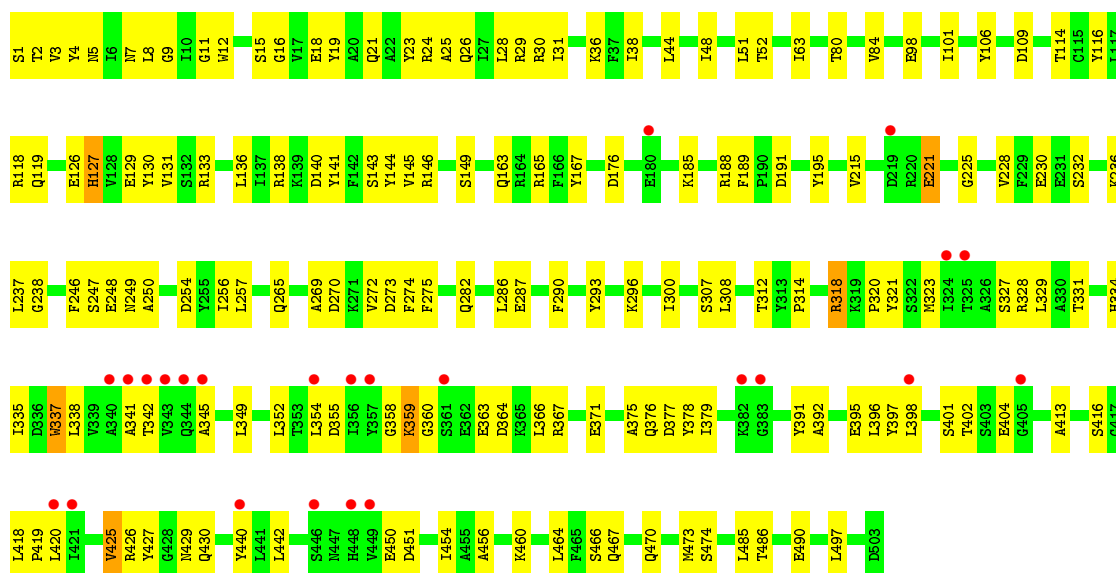
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		



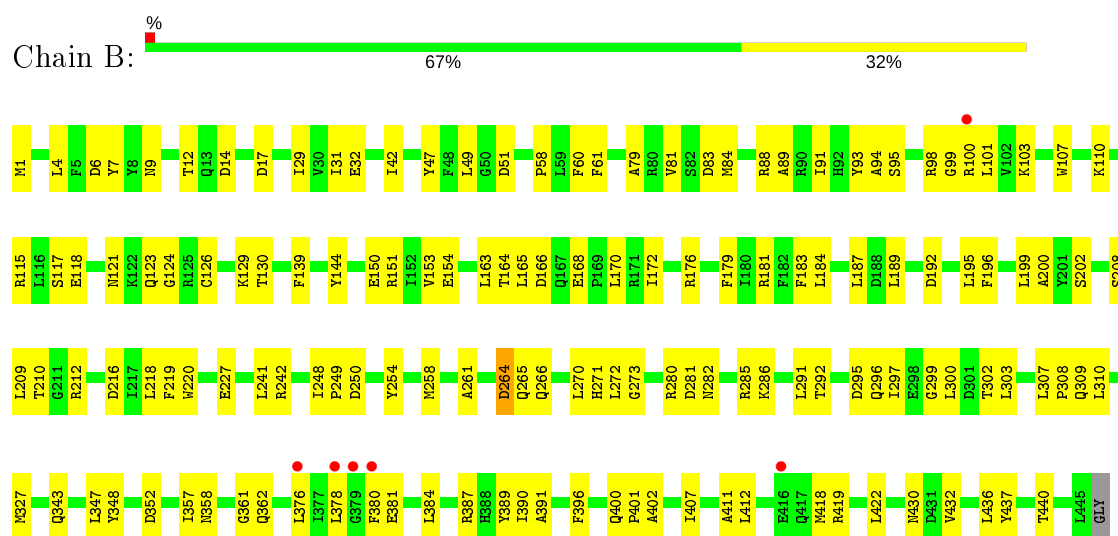
• Molecule 1: Glycosyltransferase Gtf1



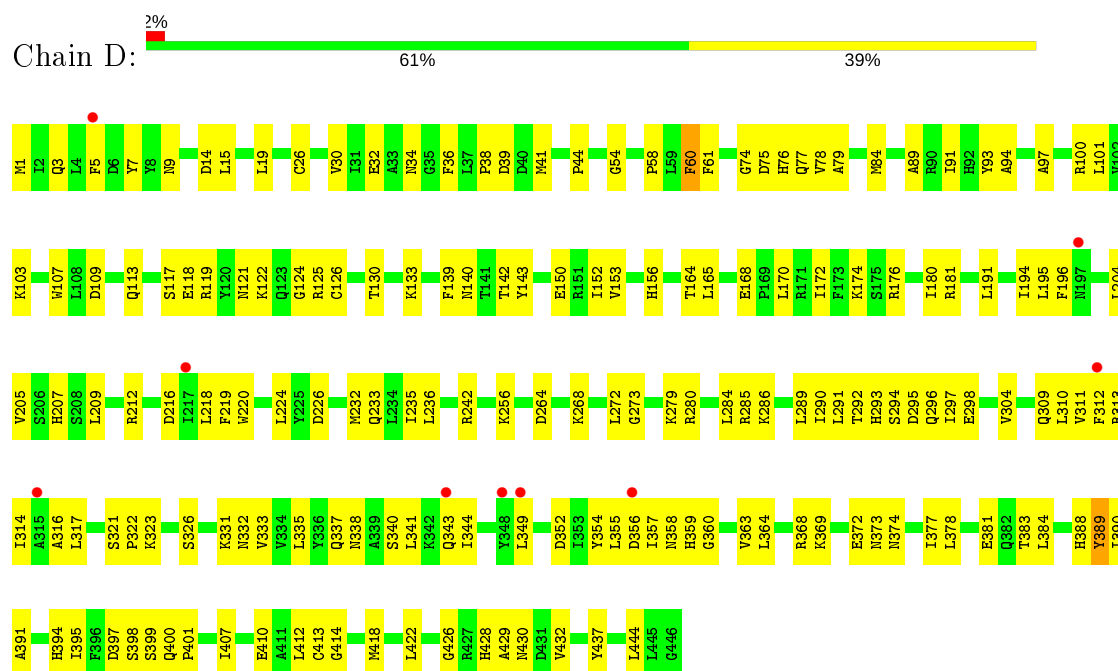
• Molecule 1: Glycosyltransferase Gtf1



• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2

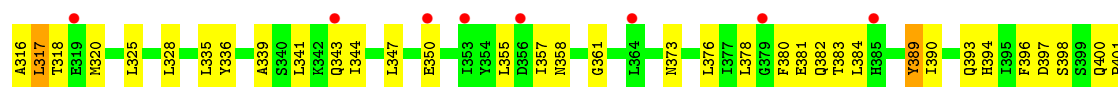


• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2





• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.97Å 196.00Å 215.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.48 – 3.84 145.05 – 3.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (94.48-3.84) 80.6 (145.05-3.84)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 3.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.269 , 0.337 0.270 , 0.338	Depositor DCC
R_{free} test set	2000 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	30948	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6915e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MG, NAG

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	0.30	0/4196	0.54	0/5678
1	C	0.29	0/4196	0.53	0/5678
1	E	0.30	0/4196	0.57	3/5678 (0.1%)
1	G	0.31	0/4196	0.54	0/5678
2	B	0.30	0/3678	0.55	0/4976
2	D	0.40	2/3682 (0.1%)	0.57	0/4981
2	F	0.31	0/3678	0.55	1/4976 (0.0%)
2	H	0.37	4/3678 (0.1%)	0.56	1/4976 (0.0%)
All	All	0.32	6/31500 (0.0%)	0.55	5/42621 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	E	0	1
1	G	0	2
2	B	0	1
2	D	0	1
2	F	0	2
2	H	0	2
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	60	PHE	CE1-CZ	-7.21	1.23	1.37
2	D	60	PHE	CE2-CZ	-7.13	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	389	TYR	CE2-CZ	-6.76	1.29	1.38
2	H	389	TYR	CE1-CZ	-6.21	1.30	1.38
2	H	389	TYR	CG-CD1	-5.97	1.31	1.39
2	H	389	TYR	CG-CD2	-5.90	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	396	LEU	CA-CB-CG	8.79	135.51	115.30
2	F	260	LEU	CA-CB-CG	-5.96	101.59	115.30
1	E	396	LEU	CB-CG-CD2	5.73	120.74	111.00
1	E	395	GLU	C-N-CA	5.23	134.77	121.70
2	H	317	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	GLU	Peptide
2	B	308	PRO	Peptide
1	C	314	PRO	Peptide
1	C	466	SER	Peptide
2	D	331	LYS	Peptide
1	E	466	SER	Peptide
2	F	225	TYR	Peptide
2	F	385	HIS	Peptide
1	G	221	GLU	Peptide
1	G	98	GLU	Peptide
2	H	396	PHE	Peptide
2	H	414	GLY	Peptide

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	4108	0	3965	140	0
1	C	4108	0	3965	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4108	0	3965	165	0
1	G	4108	0	3965	130	0
2	B	3607	0	3529	113	0
2	D	3611	0	3532	137	0
2	F	3607	0	3529	130	0
2	H	3607	0	3529	126	0
3	A	25	0	11	0	0
3	E	25	0	11	2	0
4	A	15	0	15	0	0
4	E	15	0	15	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
All	All	30948	0	30031	1019	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 17.

All (1019) 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)
2:B:272:LEU:HB2	2:B:436:LEU:HD21	1.39	1.02
2:H:280:ARG:HH12	2:H:373:ASN:HB3	1.28	0.97
1:G:364:ASP:HA	1:G:367:ARG:HG2	1.52	0.92
1:G:331:THR:O	1:G:334:HIS:ND1	2.01	0.92
2:H:412:LEU:HD23	2:H:418:MSE:HA	1.51	0.89
2:B:307:LEU:HD21	2:B:310:LEU:HG	1.55	0.88
1:E:355:ASP:HB2	1:E:394:TYR:HE2	1.36	0.88
1:E:133:ARG:NH2	2:F:174:LYS:O	2.05	0.88
1:A:150:GLU:HG2	1:A:164:ARG:HG2	1.55	0.87
2:F:362:GLN:HA	2:F:384:LEU:HD23	1.57	0.86
2:D:233:GLN:HA	2:D:236:LEU:HD12	1.58	0.86
2:F:261:ALA:HB1	2:F:265:GLN:HB2	1.57	0.86
2:F:286:LYS:HB3	2:F:310:LEU:HG	1.57	0.86
2:F:42:ILE:HG21	2:F:47:TYR:HD2	1.39	0.85
1:A:167:TYR:OH	2:B:150:GLU:OE2	1.95	0.85
1:G:26:GLN:HG2	1:G:29:ARG:HH12	1.42	0.84
2:H:280:ARG:NH1	2:H:373:ASN:HB3	1.92	0.84
2:D:220:TRP:HE1	2:D:224:LEU:HD21	1.42	0.84
2:B:81:VAL:HB	2:B:89:ALA:HB3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:LEU:HB2	1:E:61:GLU:HB2	1.59	0.82
2:H:172:ILE:O	2:H:174:LYS:NZ	2.12	0.82
2:D:397:ASP:HB3	2:D:400:GLN:HB2	1.61	0.82
1:E:164:ARG:HD2	1:E:177:MSE:HE3	1.61	0.82
2:F:81:VAL:HB	2:F:89:ALA:HB3	1.60	0.81
1:C:184:GLU:OE2	1:C:187:TYR:OH	1.97	0.81
1:C:408:LEU:HA	1:C:411:MSE:HB3	1.62	0.80
2:B:164:THR:HG22	2:B:170:LEU:HG	1.62	0.80
1:G:275:PHE:HB2	1:G:300:ILE:HG12	1.63	0.79
1:E:278:ALA:HB1	1:E:406:PHE:HD1	1.48	0.79
1:G:375:ALA:O	1:G:378:TYR:HB2	1.83	0.78
2:B:118:GLU:HG2	2:B:129:LYS:HG2	1.66	0.78
2:H:358:ASN:HD22	2:H:384:LEU:HD11	1.49	0.77
1:G:318:ARG:HD2	1:G:318:ARG:H	1.48	0.77
1:G:320:PRO:HB2	1:G:321:TYR:HD1	1.50	0.77
2:B:51:ASP:OD2	2:B:121:ASN:ND2	2.18	0.77
2:F:292:THR:HG22	2:F:358:ASN:HD22	1.48	0.77
1:G:419:PRO:HD3	1:G:474:SER:HB3	1.66	0.77
2:B:297:ILE:HB	2:B:300:LEU:HB2	1.67	0.76
1:C:138:ARG:HH22	1:C:146:ARG:NH1	1.83	0.76
1:E:329:LEU:HD21	1:E:363:GLU:HA	1.68	0.76
2:H:380:PHE:O	2:H:383:THR:OG1	2.04	0.75
2:H:6:ASP:HA	2:H:31:ILE:HB	1.68	0.75
2:D:236:LEU:HD23	2:D:268:LYS:HD2	1.69	0.75
1:G:11:GLY:HA2	1:G:51:LEU:HD13	1.68	0.75
2:H:397:ASP:HB3	2:H:400:GLN:HB2	1.69	0.75
2:B:286:LYS:HB3	2:B:310:LEU:HB3	1.68	0.75
2:H:400:GLN:HB3	2:H:401:PRO:HD2	1.68	0.75
1:C:397:TYR:HB3	1:C:420:LEU:HG	1.69	0.74
1:C:11:GLY:HA2	1:C:51:LEU:HD13	1.69	0.74
1:C:340:ALA:HA	1:C:343:VAL:HG12	1.68	0.74
2:D:36:PHE:HA	2:D:122:LYS:HB3	1.70	0.74
1:E:420:LEU:HB2	1:E:433:ILE:HD11	1.71	0.73
2:B:220:TRP:HB3	2:B:248:ILE:HG12	1.69	0.73
1:C:354:LEU:H	1:C:379:ILE:HD12	1.54	0.73
1:C:337:TRP:HH2	1:C:448:HIS:HB3	1.53	0.73
1:G:371:GLU:HA	1:G:376:GLN:HG3	1.70	0.73
2:D:280:ARG:NH1	2:D:349:LEU:HA	2.04	0.72
2:F:412:LEU:HA	2:F:417:GLN:HG3	1.71	0.72
1:G:163:GLN:OE1	2:H:140:ASN:ND2	2.22	0.72
2:D:280:ARG:HH12	2:D:349:LEU:HA	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:280:ARG:NH1	2:H:373:ASN:O	2.23	0.72
1:A:47:ASN:HB3	1:A:50:HIS:CD2	2.24	0.72
1:A:7:ASN:HB2	1:A:21:GLN:HE22	1.56	0.71
1:G:342:THR:HG21	1:G:379:ILE:HD11	1.72	0.71
2:H:317:LEU:HA	2:H:339:ALA:H	1.56	0.70
1:G:323:MSE:HB2	1:G:354:LEU:HD12	1.73	0.70
1:C:237:LEU:N	1:C:273:ASP:OD2	2.19	0.70
2:D:3:GLN:HE21	2:D:19:LEU:HD12	1.56	0.70
1:A:375:ALA:HB1	1:A:378:TYR:HB3	1.73	0.70
2:B:79:ALA:HB3	2:B:91:ILE:HB	1.74	0.70
2:F:191:LEU:O	2:F:242:ARG:NH2	2.25	0.69
1:C:327:SER:O	1:C:358:GLY:HA3	1.91	0.69
1:C:464:LEU:HD22	1:C:473:MSE:HE1	1.74	0.69
1:A:316:GLU:HB3	1:A:317:PRO:HD2	1.75	0.69
2:D:389:TYR:HD1	2:D:429:ALA:HB2	1.56	0.69
1:G:337:TRP:HB3	1:G:454:ILE:HG12	1.75	0.69
2:F:6:ASP:OD2	2:F:200:ALA:HB3	1.92	0.68
2:H:154:GLU:HG3	2:H:161:ILE:HG12	1.74	0.68
2:F:320:MSE:HE3	2:F:337:GLN:H	1.59	0.68
2:F:250:ASP:OD2	2:F:252:ALA:N	2.27	0.68
2:D:181:ARG:NH1	2:D:209:LEU:HD13	2.08	0.68
2:D:290:ILE:HB	2:D:314:ILE:HG22	1.75	0.68
1:C:5:ASN:OD1	1:C:24:ARG:NH2	2.28	0.67
1:E:387:LEU:HD12	3:E:602:UDP:H2'	1.76	0.67
1:A:265:GLN:OE1	1:A:265:GLN:N	2.27	0.67
2:B:285:ARG:N	2:B:352:ASP:OD2	2.24	0.67
2:D:58:PRO:HG2	2:D:101:LEU:HD13	1.76	0.67
1:E:329:LEU:HA	1:E:335:ILE:HD11	1.76	0.67
2:F:385:HIS:HB3	2:F:386:ASP:HA	1.76	0.67
2:B:303:LEU:HD21	2:B:402:ALA:HB1	1.76	0.67
1:A:424:ASP:HB2	1:A:441:LEU:HB3	1.76	0.67
2:D:79:ALA:HB3	2:D:91:ILE:HB	1.75	0.67
1:A:335:ILE:HD11	1:A:356:ILE:HD13	1.76	0.67
1:E:8:LEU:HB2	1:E:220:ARG:HD2	1.76	0.67
1:E:355:ASP:HB2	1:E:394:TYR:CE2	2.25	0.67
1:G:195:TYR:HE2	2:H:109:ASP:HA	1.59	0.67
1:C:188:ARG:NE	2:D:118:GLU:OE2	2.23	0.66
2:B:58:PRO:O	1:C:255:TYR:OH	2.09	0.66
1:C:162:TYR:HE1	2:D:133:LYS:HD3	1.60	0.66
2:F:118:GLU:HG2	2:F:129:LYS:HG2	1.77	0.66
2:F:220:TRP:HB3	2:F:248:ILE:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ALA:O	1:A:344:GLN:NE2	2.27	0.66
1:A:333:LYS:HE3	1:A:401:SER:HB3	1.78	0.66
1:C:138:ARG:NH2	1:C:146:ARG:HH11	1.93	0.66
1:A:258:TRP:HB2	1:A:263:ASP:OD2	1.96	0.65
1:A:322:SER:H	1:A:395:GLU:HB2	1.60	0.65
1:C:7:ASN:OD1	1:C:8:LEU:N	2.30	0.65
1:E:135:ARG:HD3	1:E:154:PRO:HG3	1.78	0.65
2:B:58:PRO:HB2	2:B:101:LEU:HD22	1.78	0.65
2:D:273:GLY:O	2:D:437:TYR:OH	2.09	0.65
2:F:236:LEU:O	2:F:268:LYS:NZ	2.27	0.65
2:B:83:ASP:HA	1:C:226:GLN:HE22	1.62	0.65
2:D:322:PRO:HG2	2:D:323:LYS:HE3	1.79	0.65
1:C:337:TRP:CH2	1:C:448:HIS:HB3	2.32	0.65
1:E:332:GLU:N	1:E:332:GLU:OE1	2.29	0.65
2:F:100:ARG:HH22	1:G:257:LEU:HD22	1.62	0.64
1:G:338:LEU:HD22	1:G:398:LEU:HD13	1.79	0.64
1:G:5:ASN:ND2	1:G:36:LYS:O	2.31	0.64
2:F:184:LEU:HD23	2:F:189:LEU:HD12	1.78	0.64
1:G:440:TYR:HD2	1:G:460:LYS:HB3	1.62	0.64
2:D:75:ASP:O	2:D:76:HIS:ND1	2.27	0.64
1:A:42:MSE:HG2	1:A:164:ARG:HH12	1.63	0.64
1:C:323:MSE:HG2	1:C:396:LEU:HD11	1.78	0.64
1:G:320:PRO:HB2	1:G:321:TYR:CD1	2.32	0.64
2:B:291:LEU:O	2:B:358:ASN:ND2	2.29	0.64
1:C:395:GLU:HG2	1:C:465:PHE:HE1	1.63	0.63
1:C:195:TYR:HE2	2:D:109:ASP:HA	1.63	0.63
2:B:199:LEU:HD23	2:B:220:TRP:CH2	2.34	0.63
1:G:450:GLU:HG2	1:G:451:ASP:H	1.63	0.63
1:E:305:VAL:HB	1:E:408:LEU:HD21	1.79	0.63
2:B:396:PHE:HB3	2:B:401:PRO:HG2	1.80	0.63
1:E:240:VAL:HG22	1:E:276:ILE:HD12	1.80	0.63
1:E:354:LEU:HB3	1:E:379:ILE:HG23	1.80	0.63
1:E:278:ALA:HB1	1:E:406:PHE:CD1	2.32	0.63
1:C:18:GLU:O	1:C:22:ALA:N	2.29	0.63
2:F:6:ASP:HA	2:F:31:ILE:HB	1.81	0.63
1:G:16:GLY:HA2	1:G:19:TYR:HB2	1.80	0.63
2:H:381:GLU:HB2	2:H:398:SER:HB3	1.80	0.63
1:G:307:SER:HB2	1:G:486:THR:HB	1.81	0.63
2:D:369:LYS:O	2:D:373:ASN:ND2	2.32	0.62
2:H:236:LEU:HD22	2:H:265:GLN:HB3	1.81	0.62
1:A:64:TRP:HB3	1:A:67:ASN:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:LEU:HD23	2:D:242:ARG:HH11	1.64	0.62
1:C:371:GLU:HA	1:C:376:GLN:CB	2.29	0.62
1:E:291:GLN:HA	1:E:295:ASP:HA	1.81	0.62
2:B:412:LEU:HD22	2:B:418:MSE:HA	1.81	0.62
1:E:7:ASN:HB2	1:E:21:GLN:HE22	1.64	0.62
2:F:250:ASP:OD2	2:F:253:THR:N	2.28	0.62
2:D:400:GLN:HB3	2:D:401:PRO:HD2	1.80	0.62
1:G:7:ASN:OD1	1:G:8:LEU:N	2.33	0.62
1:C:371:GLU:HA	1:C:376:GLN:HB3	1.82	0.61
2:D:280:ARG:HH12	2:D:349:LEU:CA	2.13	0.61
1:E:258:TRP:HB2	1:E:263:ASP:OD2	2.00	0.61
2:D:39:ASP:OD2	2:D:54:GLY:N	2.33	0.61
1:A:322:SER:HB2	1:A:395:GLU:H	1.64	0.61
2:D:220:TRP:NE1	2:D:224:LEU:HD21	2.14	0.61
2:D:298:GLU:OE1	2:D:359:HIS:NE2	2.33	0.61
1:G:451:ASP:HA	1:G:454:ILE:HB	1.82	0.61
2:B:199:LEU:HD23	2:B:220:TRP:HH2	1.65	0.61
1:E:357:TYR:HE1	1:E:382:LYS:HG3	1.65	0.60
1:A:305:VAL:HG23	1:A:408:LEU:HD11	1.83	0.60
2:H:176:ARG:HD2	2:H:201:TYR:CE1	2.36	0.60
2:D:181:ARG:HH11	2:D:209:LEU:HD13	1.66	0.60
2:D:397:ASP:CB	2:D:400:GLN:HB2	2.30	0.60
1:A:319:LYS:O	1:A:395:GLU:HG2	2.02	0.60
2:D:298:GLU:HB2	2:D:359:HIS:HE2	1.67	0.60
2:B:195:LEU:HB3	2:B:219:PHE:CE1	2.37	0.60
1:E:42:MSE:HE3	1:E:164:ARG:HH11	1.67	0.60
1:G:185:LYS:NZ	2:H:111:LYS:NZ	2.50	0.60
1:G:145:VAL:HG12	1:G:146:ARG:H	1.66	0.60
1:E:7:ASN:OD1	1:E:8:LEU:N	2.35	0.59
1:A:333:LYS:NZ	1:A:404:GLU:OE2	2.34	0.59
1:A:471:GLN:HG3	1:A:472:GLU:HG3	1.83	0.59
2:F:224:LEU:HD23	2:F:256:LYS:HB3	1.82	0.59
2:H:1:MSE:HE2	2:H:195:LEU:HD11	1.82	0.59
1:A:42:MSE:HE2	1:A:164:ARG:NH1	2.18	0.59
2:F:378:LEU:HB3	2:F:394:HIS:HB3	1.85	0.59
1:G:118:ARG:HG2	1:G:119:GLN:HG3	1.83	0.59
2:B:249:PRO:HA	2:B:272:LEU:O	2.02	0.59
2:B:272:LEU:HD12	2:B:437:TYR:CD1	2.38	0.59
2:D:195:LEU:HD22	2:D:219:PHE:HE2	1.68	0.59
1:C:138:ARG:NH2	1:C:146:ARG:NH1	2.51	0.59
1:G:314:PRO:HB3	1:G:392:ALA:HB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:218:LEU:HD23	2:H:246:ILE:HG12	1.83	0.59
2:H:393:GLN:NE2	2:H:393:GLN:O	2.35	0.59
1:A:323:MSE:HE3	1:A:352:LEU:HD13	1.85	0.59
2:B:181:ARG:HD2	2:B:209:LEU:HD21	1.84	0.59
2:B:258:MSE:SE	2:B:266:GLN:HB2	2.53	0.59
2:B:343:GLN:O	2:B:347:LEU:HG	2.01	0.59
1:A:387:LEU:HA	1:A:390:ILE:HB	1.85	0.59
2:B:210:THR:HA	2:B:242:ARG:HG3	1.84	0.59
2:H:397:ASP:CB	2:H:400:GLN:HB2	2.33	0.59
2:D:340:SER:HB3	2:D:343:GLN:HB2	1.83	0.58
1:A:129:GLU:HG2	1:A:139:LYS:HG3	1.85	0.58
1:C:36:LYS:HD2	1:C:63:ILE:HG13	1.86	0.58
2:F:297:ILE:HA	2:F:358:ASN:HA	1.85	0.58
1:G:114:THR:HB	1:G:129:GLU:HB2	1.84	0.58
2:H:1:MSE:HA	2:H:193:HIS:O	2.02	0.58
1:A:286:LEU:O	1:A:290:PHE:N	2.36	0.58
2:F:297:ILE:CG2	2:F:357:ILE:HG13	2.33	0.58
1:G:312:THR:HB	1:G:416:SER:HA	1.83	0.58
1:C:467:GLN:HG2	1:C:468:GLY:H	1.68	0.58
1:A:4:TYR:HB3	1:A:38:ILE:HD11	1.84	0.58
1:G:167:TYR:OH	2:H:150:GLU:OE2	2.19	0.58
2:B:254:TYR:CZ	2:B:271:HIS:HB3	2.37	0.58
1:E:66:TYR:O	1:E:175:TYR:OH	2.21	0.58
2:H:316:ALA:HB1	2:H:318:THR:HG22	1.84	0.58
2:H:93:TYR:CD1	2:H:100:ARG:HA	2.38	0.58
1:A:344:GLN:HE22	1:A:454:ILE:HD12	1.69	0.57
2:D:422:LEU:O	2:D:426:GLY:N	2.36	0.57
2:B:297:ILE:HD12	2:B:300:LEU:HD22	1.86	0.57
1:C:395:GLU:HG2	1:C:465:PHE:CE1	2.39	0.57
2:D:388:HIS:O	2:D:428:HIS:ND1	2.31	0.57
2:D:97:ALA:HB1	2:D:364:LEU:HD11	1.85	0.57
1:E:19:TYR:CE2	1:E:55:ILE:HD11	2.39	0.57
1:A:407:GLY:O	1:A:410:LEU:HG	2.05	0.57
1:E:314:PRO:HB3	1:E:392:ALA:HB1	1.85	0.57
1:G:464:LEU:HD13	1:G:473:MSE:HE1	1.84	0.57
2:F:285:ARG:N	2:F:352:ASP:OD2	2.35	0.57
2:F:362:GLN:OE1	2:F:366:ALA:N	2.38	0.57
2:F:391:ALA:HB2	2:F:425:GLN:HA	1.87	0.57
1:G:329:LEU:HD13	1:G:366:LEU:HD13	1.87	0.57
1:E:72:ILE:HA	1:E:144:TYR:OH	2.05	0.57
1:A:57:PHE:HB3	1:A:62:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:SER:HB3	1:G:257:LEU:HD11	1.87	0.56
1:G:44:LEU:HD22	1:G:141:TYR:CD2	2.39	0.56
2:H:325:LEU:HA	2:H:328:LEU:CD1	2.35	0.56
1:A:342:THR:O	1:A:346:HIS:N	2.37	0.56
1:A:308:LEU:HG	1:A:411:MSE:HE3	1.87	0.56
1:A:278:ALA:HB1	1:A:406:PHE:CD1	2.40	0.56
1:A:173:VAL:HG21	2:B:144:TYR:HE1	1.70	0.56
2:B:4:LEU:HD11	2:B:31:ILE:HD11	1.88	0.56
1:E:250:ALA:O	1:E:251:SER:OG	2.21	0.56
1:C:311:LEU:H	1:C:311:LEU:HD12	1.70	0.56
1:G:4:TYR:HB3	1:G:38:ILE:HD11	1.88	0.56
2:H:142:THR:HG22	2:H:153:VAL:HG22	1.88	0.56
2:H:195:LEU:HD22	2:H:219:PHE:HE1	1.70	0.56
1:C:195:TYR:CE2	2:D:109:ASP:HA	2.41	0.56
1:E:371:GLU:HA	1:E:376:GLN:HG2	1.88	0.56
2:F:117:SER:HB2	2:F:130:THR:HB	1.88	0.56
1:A:314:PRO:HG3	1:A:392:ALA:HB1	1.87	0.56
1:E:115:CYS:HB3	1:E:125:VAL:HG13	1.88	0.56
1:E:138:ARG:HH11	2:F:162:ILE:HG21	1.71	0.56
1:G:286:LEU:O	1:G:290:PHE:N	2.37	0.56
1:G:360:GLY:O	1:G:363:GLU:HB2	2.05	0.56
1:A:285:ILE:O	1:A:289:GLN:HG2	2.05	0.56
1:E:356:ILE:HD12	1:E:381:LEU:HD11	1.88	0.56
1:E:43:ILE:HD13	1:E:48:ILE:HD13	1.88	0.56
1:C:323:MSE:O	1:C:354:LEU:HA	2.06	0.56
2:D:407:ILE:HA	2:D:410:GLU:HB3	1.88	0.56
1:E:338:LEU:HD21	1:E:400:ALA:HB2	1.88	0.56
1:G:221:GLU:HG2	1:G:225:GLY:HA3	1.88	0.56
2:H:192:ASP:HB3	2:H:193:HIS:CE1	2.40	0.56
2:B:380:PHE:HD1	2:B:396:PHE:HB2	1.71	0.55
1:C:137:ILE:HD11	2:D:172:ILE:HD13	1.88	0.55
2:D:297:ILE:HG22	2:D:357:ILE:HB	1.87	0.55
1:E:324:ILE:HB	1:E:394:TYR:HD2	1.70	0.55
2:F:75:ASP:OD1	2:F:76:HIS:N	2.39	0.55
1:G:376:GLN:HG2	1:G:377:ASP:N	2.21	0.55
2:H:49:LEU:HD22	2:H:144:TYR:O	2.06	0.55
2:F:270:LEU:HD23	2:F:440:THR:HB	1.88	0.55
1:C:105:PHE:HB3	1:C:107:PRO:HD3	1.88	0.55
1:C:451:ASP:HA	1:C:454:ILE:HB	1.87	0.55
1:G:282:GLN:HG3	1:G:427:TYR:CZ	2.41	0.55
1:C:118:ARG:HG2	1:C:119:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:LEU:HB3	2:H:136:GLN:HG3	1.89	0.55
2:B:29:ILE:HD12	2:B:183:PHE:HE2	1.72	0.55
1:E:470:GLN:O	1:E:474:SER:HB3	2.06	0.55
1:E:111:GLN:NE2	2:F:172:ILE:HB	2.21	0.55
1:C:323:MSE:HB2	1:C:354:LEU:HB2	1.88	0.55
1:G:401:SER:HB3	1:G:404:GLU:OE2	2.06	0.55
2:H:6:ASP:OD2	2:H:198:SER:HB2	2.07	0.55
2:D:295:ASP:OD2	2:D:321:SER:HB3	2.06	0.55
1:E:17:VAL:HG11	1:E:220:ARG:HE	1.71	0.55
2:B:419:ARG:HA	2:B:422:LEU:HB2	1.87	0.55
1:C:398:LEU:HD12	1:C:421:ILE:HB	1.87	0.55
2:D:143:TYR:HB2	2:D:152:ILE:HB	1.88	0.55
2:H:3:GLN:HE21	2:H:19:LEU:HD12	1.71	0.55
1:A:93:GLU:HG2	1:A:94:ARG:H	1.72	0.55
2:D:381:GLU:HB3	2:D:398:SER:HB3	1.88	0.55
2:F:269:PHE:O	2:F:270:LEU:HD12	2.07	0.55
1:G:21:GLN:HG2	1:G:24:ARG:NH1	2.22	0.55
2:D:164:THR:HG22	2:D:170:LEU:HG	1.89	0.54
1:E:240:VAL:HG13	1:E:276:ILE:HB	1.89	0.54
1:E:342:THR:O	1:E:345:ALA:N	2.40	0.54
1:G:7:ASN:HD21	1:G:18:GLU:HG3	1.71	0.54
2:H:220:TRP:HE1	2:H:224:LEU:HD21	1.72	0.54
2:H:341:LEU:HD23	2:H:344:ILE:HD12	1.88	0.54
2:D:125:ARG:HG3	2:D:126:CYS:N	2.21	0.54
1:E:106:TYR:HB2	1:E:111:GLN:HB2	1.88	0.54
2:F:281:ASP:HB2	2:F:283:TYR:CZ	2.41	0.54
1:G:329:LEU:HD12	1:G:363:GLU:HG2	1.89	0.54
2:B:362:GLN:HA	2:B:384:LEU:HD23	1.89	0.54
2:F:42:ILE:HG21	2:F:47:TYR:CD2	2.31	0.54
2:B:285:ARG:HB2	2:B:352:ASP:HB2	1.88	0.54
1:E:211:GLN:O	1:E:235:ALA:HB2	2.07	0.54
2:H:176:ARG:HD2	2:H:201:TYR:HE1	1.72	0.54
2:B:261:ALA:HB1	2:B:265:GLN:CB	2.37	0.54
1:C:496:LEU:HD12	1:C:499:GLU:HB3	1.89	0.54
2:B:261:ALA:HB1	2:B:265:GLN:HB3	1.88	0.54
2:D:232:MSE:O	2:D:235:ILE:HG22	2.07	0.54
1:E:58:LEU:H	1:E:58:LEU:HD12	1.73	0.54
1:E:280:GLU:HG3	1:E:283:LYS:HD3	1.90	0.54
1:A:349:LEU:HB3	1:A:352:LEU:HD23	1.88	0.54
1:A:392:ALA:HA	1:A:416:SER:HB3	1.89	0.54
1:E:60:GLU:HA	1:E:60:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:TYR:HA	2:F:32:GLU:HB2	1.88	0.54
1:E:226:GLN:HG3	2:H:69:PHE:HB3	1.90	0.54
1:A:58:LEU:HB2	1:A:61:GLU:HG3	1.90	0.53
2:D:121:ASN:OD1	2:D:124:GLY:N	2.40	0.53
1:E:104:TYR:O	1:E:112:PHE:HB2	2.08	0.53
1:G:355:ASP:N	1:G:355:ASP:OD1	2.41	0.53
1:A:79:VAL:HG21	1:A:142:PHE:HD2	1.73	0.53
2:D:280:ARG:HH12	2:D:349:LEU:C	2.11	0.53
1:E:241:VAL:HA	1:E:262:TYR:CE2	2.43	0.53
1:G:195:TYR:CE2	2:H:109:ASP:HA	2.43	0.53
1:A:330:ALA:HA	1:A:361:SER:HB2	1.90	0.53
1:A:417:GLY:O	1:A:474:SER:HA	2.07	0.53
1:A:7:ASN:HB2	1:A:21:GLN:NE2	2.23	0.53
1:C:399:THR:HG22	1:C:401:SER:H	1.73	0.53
2:H:4:LEU:HG	2:H:202:SER:HB3	1.91	0.53
2:B:6:ASP:HA	2:B:31:ILE:HB	1.90	0.53
1:E:35:ALA:HB3	1:E:61:GLU:OE2	2.08	0.53
2:H:94:ALA:HA	2:H:103:LYS:HB2	1.90	0.53
2:D:109:ASP:OD2	2:D:113:GLN:HB3	2.08	0.53
2:F:151:ARG:HD3	2:F:164:THR:O	2.09	0.53
1:G:360:GLY:H	1:G:363:GLU:HB2	1.73	0.53
1:G:359:LYS:HA	1:G:363:GLU:HG3	1.89	0.53
2:B:400:GLN:HB2	2:B:401:PRO:HD3	1.91	0.53
2:D:32:GLU:HG2	2:D:34:ASN:H	1.74	0.53
1:E:336:ASP:N	1:E:336:ASP:OD1	2.41	0.53
2:B:212:ARG:O	2:B:242:ARG:NH1	2.41	0.53
2:D:291:LEU:HG	2:D:354:TYR:HE2	1.74	0.53
2:F:5:PHE:HE1	2:F:15:LEU:HD23	1.74	0.53
2:F:308:PRO:HA	2:F:332:ASN:OD1	2.09	0.53
2:F:9:ASN:OD1	2:F:12:THR:N	2.42	0.53
2:H:78:VAL:HG12	2:H:79:ALA:H	1.74	0.53
1:C:163:GLN:OE1	2:D:140:ASN:ND2	2.25	0.52
1:C:469:ARG:HA	1:C:472:GLU:HB2	1.90	0.52
1:E:426:ARG:HD2	1:E:427:TYR:CE1	2.44	0.52
1:G:21:GLN:O	1:G:25:ALA:N	2.36	0.52
2:B:151:ARG:HD3	2:B:165:LEU:HD23	1.90	0.52
1:C:43:ILE:HD12	1:C:48:ILE:HD13	1.91	0.52
1:G:126:GLU:HB3	1:G:127:HIS:ND1	2.23	0.52
2:F:340:SER:HA	1:G:249:ASN:O	2.09	0.52
2:H:292:THR:OG1	2:H:358:ASN:OD1	2.15	0.52
2:H:6:ASP:OD2	2:H:200:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:LEU:HD22	1:E:398:LEU:HD13	1.91	0.52
1:G:101:ILE:HG23	1:G:114:THR:HG23	1.90	0.52
2:H:287:ASP:OD2	2:H:350:GLU:O	2.27	0.52
2:H:89:ALA:HB2	2:H:107:TRP:CE3	2.44	0.52
1:E:140:ASP:OD1	1:E:149:SER:OG	2.19	0.52
2:F:79:ALA:HB3	2:F:91:ILE:HB	1.92	0.52
1:A:356:ILE:HD12	1:A:381:LEU:HD11	1.91	0.52
1:C:352:LEU:HD12	1:C:352:LEU:O	2.10	0.52
1:E:150:GLU:OE2	1:E:164:ARG:NH2	2.37	0.52
2:H:109:ASP:HB3	2:H:115:ARG:HG3	1.92	0.52
1:A:440:TYR:HE2	1:A:464:LEU:HD21	1.75	0.52
1:E:7:ASN:HB2	1:E:21:GLN:NE2	2.24	0.52
1:E:444:VAL:HG22	1:E:445:SER:O	2.09	0.52
1:E:138:ARG:NH1	2:F:162:ILE:HG21	2.25	0.52
2:F:11:GLU:HB3	2:F:221:GLN:HE21	1.74	0.52
1:C:70:THR:HA	1:C:168:HIS:CE1	2.45	0.52
2:D:317:LEU:HA	2:D:338:ASN:H	1.75	0.52
2:F:229:PRO:HG2	2:F:232:MSE:HE3	1.91	0.52
1:G:1:SER:O	1:G:2:THR:OG1	2.26	0.52
2:H:151:ARG:NH2	2:H:166:ASP:HB2	2.25	0.52
2:B:88:ARG:NH2	2:B:110:LYS:HD2	2.25	0.52
1:C:94:ARG:HB2	1:C:105:PHE:HB2	1.92	0.52
1:E:18:GLU:N	1:E:18:GLU:OE1	2.37	0.52
1:G:256:ILE:HB	1:G:293:TYR:CD1	2.45	0.52
1:A:278:ALA:HB1	1:A:406:PHE:HD1	1.75	0.51
1:E:407:GLY:O	1:E:410:LEU:HG	2.09	0.51
1:E:137:ILE:HD12	2:F:162:ILE:HD11	1.92	0.51
1:A:241:VAL:HA	1:A:262:TYR:CZ	2.45	0.51
1:C:109:ASP:HB3	2:D:174:LYS:HZ1	1.75	0.51
2:F:386:ASP:HB3	2:F:388:HIS:CE1	2.45	0.51
1:G:397:TYR:HB3	1:G:420:LEU:HD22	1.91	0.51
2:H:407:ILE:HA	2:H:410:GLU:HB3	1.90	0.51
1:A:233:GLN:NE2	1:A:271:LYS:O	2.30	0.51
1:A:278:ALA:HA	1:A:303:ILE:O	2.10	0.51
1:A:437:LYS:HB3	1:A:476:HIS:CG	2.44	0.51
1:C:323:MSE:HE3	1:C:352:LEU:HD22	1.91	0.51
2:D:293:HIS:HB2	2:D:363:VAL:CG2	2.41	0.51
1:E:252:SER:O	1:E:293:TYR:OH	2.24	0.51
1:G:360:GLY:O	1:G:363:GLU:N	2.44	0.51
1:A:398:LEU:HD23	1:A:421:ILE:HB	1.91	0.51
2:D:180:ILE:HG21	2:D:205:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:PHE:CE2	2:D:218:LEU:HB2	2.46	0.51
1:E:426:ARG:HB3	1:E:427:TYR:CD1	2.46	0.51
1:E:5:ASN:ND2	1:E:24:ARG:HH21	2.08	0.51
2:F:171:ARG:NH1	2:F:182:PHE:CE1	2.78	0.51
1:A:7:ASN:O	1:A:39:PHE:HA	2.11	0.51
1:C:2:THR:HG22	1:C:3:VAL:H	1.75	0.51
2:F:118:GLU:OE2	2:F:129:LYS:HE2	2.11	0.51
2:F:397:ASP:HB2	2:F:401:PRO:HD3	1.91	0.51
2:H:236:LEU:HB3	2:H:265:GLN:HG2	1.93	0.51
1:A:47:ASN:OD1	1:A:48:ILE:N	2.44	0.51
2:D:391:ALA:HB3	2:D:394:HIS:CD2	2.46	0.51
2:F:320:MSE:HG3	2:F:337:GLN:HA	1.92	0.51
2:B:79:ALA:HB2	2:B:93:TYR:OH	2.10	0.51
1:C:27:ILE:O	1:C:31:ILE:HG12	2.11	0.51
1:E:323:MSE:HB2	1:E:354:LEU:HG	1.90	0.51
1:G:464:LEU:HD22	1:G:473:MSE:HE1	1.93	0.51
1:A:186:LEU:HA	1:A:194:PHE:O	2.11	0.51
2:B:14:ASP:HA	2:B:17:ASP:HB2	1.93	0.51
1:E:21:GLN:HE21	1:E:219:ASP:CG	2.15	0.51
1:E:280:GLU:O	1:E:284:ARG:N	2.42	0.51
2:F:24:TYR:HE2	2:F:441:LEU:HD12	1.76	0.51
2:F:362:GLN:CA	2:F:384:LEU:HD23	2.37	0.51
1:G:456:ALA:O	1:G:460:LYS:HG2	2.11	0.51
2:H:249:PRO:HB3	2:H:274:TYR:CE2	2.46	0.51
2:H:80:ARG:HD3	2:H:82:SER:OG	2.11	0.51
1:G:331:THR:O	1:G:334:HIS:CE1	2.64	0.51
1:C:295:ASP:OD1	1:C:297:GLN:NE2	2.44	0.50
1:C:278:ALA:HB1	1:C:406:PHE:HB2	1.93	0.50
1:C:87:GLN:O	2:D:170:LEU:N	2.36	0.50
2:D:165:LEU:HB2	2:D:168:GLU:HG2	1.92	0.50
1:E:228:VAL:O	1:E:232:SER:OG	2.15	0.50
2:H:201:TYR:O	2:H:205:VAL:HG23	2.11	0.50
2:D:209:LEU:CD2	2:D:242:ARG:HH11	2.24	0.50
2:F:100:ARG:HH22	1:G:257:LEU:CD2	2.23	0.50
1:G:442:LEU:HD21	1:G:460:LYS:HG3	1.93	0.50
1:G:30:ARG:HD2	1:G:490:GLU:OE2	2.11	0.50
2:H:81:VAL:HB	2:H:89:ALA:HB3	1.93	0.50
1:C:144:TYR:CD1	1:C:145:VAL:HG23	2.47	0.50
1:E:343:VAL:O	1:E:346:HIS:ND1	2.44	0.50
2:F:199:LEU:O	2:F:199:LEU:HD12	2.11	0.50
1:G:327:SER:O	1:G:358:GLY:HA3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:317:LEU:HD23	2:H:344:ILE:HD11	1.92	0.50
1:A:270:ASP:OD1	1:A:296:LYS:HD3	2.11	0.50
2:B:154:GLU:OE2	2:B:176:ARG:NE	2.35	0.50
1:E:357:TYR:HE2	1:E:390:ILE:HG21	1.76	0.50
1:G:36:LYS:HB3	1:G:63:ILE:HD11	1.93	0.50
2:H:181:ARG:HH11	2:H:209:LEU:HD21	1.76	0.50
2:H:3:GLN:NE2	2:H:19:LEU:HD12	2.26	0.50
2:D:38:PRO:HG2	2:D:41:MSE:SE	2.61	0.50
1:G:185:LYS:HZ1	2:H:111:LYS:NZ	2.09	0.50
1:G:26:GLN:HG2	1:G:29:ARG:NH1	2.20	0.50
2:H:151:ARG:HD3	2:H:164:THR:O	2.12	0.50
2:H:2:ILE:HG12	2:H:194:ILE:HG12	1.93	0.50
1:E:396:LEU:HG	1:E:397:TYR:H	1.76	0.50
2:H:151:ARG:HA	2:H:164:THR:O	2.11	0.50
2:D:377:ILE:HG22	2:D:390:ILE:HD13	1.93	0.50
2:D:78:VAL:HG12	2:D:79:ALA:N	2.27	0.50
1:E:15:SER:OG	1:E:16:GLY:N	2.43	0.50
2:F:400:GLN:HB3	2:F:401:PRO:HD3	1.92	0.50
2:F:193:HIS:NE2	2:F:445:LEU:O	2.37	0.50
1:G:246:PHE:HE2	1:G:248:GLU:HB2	1.76	0.50
1:A:81:LEU:HG	1:A:123:ASP:O	2.12	0.50
1:E:165:ARG:NH1	2:F:142:THR:HG21	2.27	0.50
1:E:19:TYR:CE2	3:E:602:UDP:H1'	2.47	0.50
2:F:216:ASP:OD1	2:F:242:ARG:NE	2.39	0.50
2:F:69:PHE:CD2	1:G:230:GLU:HG2	2.47	0.50
1:A:358:GLY:N	1:A:383:GLY:O	2.45	0.49
2:F:94:ALA:HA	2:F:103:LYS:HB2	1.94	0.49
2:F:154:GLU:OE2	2:F:176:ARG:HG3	2.12	0.49
2:F:388:HIS:HD1	2:F:389:TYR:HD1	1.60	0.49
1:A:406:PHE:CD2	1:A:408:LEU:HD12	2.46	0.49
1:C:239:VAL:HG11	1:C:265:GLN:HG2	1.93	0.49
1:C:329:LEU:HD22	1:C:366:LEU:HD13	1.94	0.49
2:D:264:ASP:N	2:D:264:ASP:OD1	2.43	0.49
1:E:420:LEU:O	1:E:439:GLY:HA3	2.12	0.49
1:E:135:ARG:HG2	1:E:135:ARG:HH11	1.78	0.49
1:E:42:MSE:HE3	1:E:164:ARG:NH1	2.25	0.49
1:E:27:ILE:HG21	1:E:493:TRP:HD1	1.77	0.49
2:H:59:LEU:HD12	2:H:120:TYR:CE2	2.47	0.49
1:A:486:THR:OG1	1:A:490:GLU:OE2	2.31	0.49
2:D:142:THR:HG23	2:D:153:VAL:HG22	1.93	0.49
1:E:239:VAL:HB	1:E:275:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:PHE:HB3	1:E:296:LYS:O	2.13	0.49
1:E:310:GLN:NE2	1:E:311:LEU:O	2.45	0.49
1:E:333:LYS:HZ3	1:E:400:ALA:H	1.61	0.49
1:E:440:TYR:CD2	1:E:460:LYS:HB3	2.47	0.49
1:A:302:THR:C	1:A:303:ILE:HD12	2.33	0.49
2:B:29:ILE:HD13	2:B:42:ILE:HG13	1.93	0.49
2:D:294:SER:OG	2:D:360:GLY:HA3	2.13	0.49
1:A:104:TYR:O	1:A:112:PHE:HB2	2.12	0.49
2:B:9:ASN:HB2	2:B:12:THR:H	1.75	0.49
2:F:247:VAL:HG11	2:F:272:LEU:HD12	1.93	0.49
1:A:241:VAL:HG22	1:A:262:TYR:CD1	2.48	0.49
2:B:196:PHE:CE2	2:B:218:LEU:HD13	2.48	0.49
1:C:410:LEU:HA	1:C:413:ALA:HB3	1.93	0.49
1:E:237:LEU:O	1:E:273:ASP:HB3	2.13	0.49
1:C:165:ARG:HD2	2:D:150:GLU:OE2	2.13	0.49
2:B:273:GLY:H	2:B:432:VAL:HG21	1.78	0.49
1:E:36:LYS:HD2	1:E:63:ILE:HG13	1.94	0.49
2:F:139:PHE:CD2	2:F:140:ASN:HB3	2.48	0.49
2:H:125:ARG:NH1	2:H:145:SER:O	2.45	0.49
1:A:184:GLU:OE2	1:A:187:TYR:OH	2.26	0.49
2:B:99:GLY:O	2:B:100:ARG:HG2	2.13	0.49
1:C:137:ILE:HG13	1:C:138:ARG:N	2.27	0.49
1:C:320:PRO:HB2	1:C:321:TYR:HD2	1.78	0.49
2:F:78:VAL:HG22	2:F:79:ALA:N	2.28	0.49
2:H:154:GLU:OE2	2:H:176:ARG:NH2	2.43	0.49
1:C:302:THR:O	1:C:303:ILE:HG13	2.13	0.48
1:C:364:ASP:HA	1:C:367:ARG:HG2	1.94	0.48
1:C:453:ILE:HA	1:C:456:ALA:HB3	1.94	0.48
1:E:312:THR:O	1:E:416:SER:HA	2.13	0.48
2:H:140:ASN:HA	2:H:156:HIS:HD2	1.78	0.48
2:D:7:TYR:HD1	2:D:32:GLU:HB2	1.76	0.48
1:E:333:LYS:O	1:E:400:ALA:HB3	2.13	0.48
1:E:27:ILE:HG21	1:E:493:TRP:CD1	2.49	0.48
2:B:121:ASN:OD1	2:B:124:GLY:N	2.43	0.48
1:C:116:TYR:CD2	1:C:127:HIS:CE1	3.01	0.48
1:E:138:ARG:NH2	1:E:146:ARG:NH1	2.61	0.48
1:G:130:TYR:HB2	1:G:138:ARG:HB3	1.95	0.48
1:A:162:TYR:O	1:A:179:ILE:N	2.40	0.48
2:D:292:THR:O	2:D:316:ALA:HB2	2.13	0.48
1:A:42:MSE:HE2	1:A:164:ARG:HH11	1.79	0.48
1:C:33:GLN:HG2	1:C:497:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:GLN:HG2	2:H:236:LEU:HD12	1.95	0.48
2:H:325:LEU:HA	2:H:328:LEU:HD13	1.95	0.48
2:B:254:TYR:CE2	2:B:271:HIS:HB3	2.48	0.48
2:F:15:LEU:O	2:F:19:LEU:HD13	2.14	0.48
1:A:245:HIS:CG	1:A:286:LEU:HD12	2.49	0.48
2:B:376:LEU:HG	2:B:378:LEU:HD23	1.95	0.48
1:E:64:TRP:HB3	1:E:67:ASN:HB2	1.95	0.48
1:E:96:GLU:O	1:E:103:ARG:HG2	2.13	0.48
1:G:237:LEU:O	1:G:273:ASP:HB2	2.13	0.48
1:A:15:SER:OG	1:A:16:GLY:N	2.45	0.48
2:D:284:LEU:HD11	2:D:414:GLY:O	2.14	0.48
2:F:218:LEU:HD23	2:F:246:ILE:HG23	1.95	0.48
1:G:426:ARG:HA	1:G:427:TYR:HA	1.61	0.48
1:A:151:TYR:CE2	2:B:153:VAL:HG11	2.49	0.48
2:D:355:LEU:HA	2:D:378:LEU:O	2.14	0.48
1:E:398:LEU:HD23	1:E:421:ILE:HB	1.96	0.48
2:B:292:THR:HG22	2:B:358:ASN:HB3	1.94	0.48
2:B:7:TYR:HA	2:B:32:GLU:HB2	1.95	0.48
1:C:371:GLU:HA	1:C:376:GLN:HB2	1.96	0.48
2:D:216:ASP:OD1	2:D:242:ARG:NH2	2.47	0.48
2:D:165:LEU:HD12	2:D:168:GLU:HG2	1.96	0.47
2:F:417:GLN:O	2:F:420:SER:OG	2.31	0.47
1:C:354:LEU:N	1:C:379:ILE:HD12	2.27	0.47
1:E:323:MSE:CE	1:E:352:LEU:HD21	2.45	0.47
2:F:38:PRO:HD2	2:F:41:MSE:SE	2.64	0.47
1:G:133:ARG:NH2	2:H:160:ASP:OD1	2.46	0.47
1:E:396:LEU:HA	1:E:419:PRO:HG2	1.96	0.47
1:G:426:ARG:HB3	1:G:427:TYR:CD2	2.50	0.47
2:H:13:GLN:O	2:H:17:ASP:N	2.46	0.47
1:A:130:TYR:O	1:A:136:LEU:HD12	2.14	0.47
1:A:370:ILE:HG23	1:A:375:ALA:HB3	1.95	0.47
1:A:444:VAL:HG22	1:A:445:SER:O	2.14	0.47
2:B:296:GLN:HG2	2:B:297:ILE:H	1.80	0.47
1:C:395:GLU:O	1:C:419:PRO:HD2	2.14	0.47
1:C:466:SER:HA	1:C:467:GLN:HB2	1.96	0.47
2:D:94:ALA:N	2:D:101:LEU:O	2.41	0.47
1:E:393:GLY:C	1:E:394:TYR:HD1	2.17	0.47
1:E:426:ARG:HB3	1:E:427:TYR:CG	2.50	0.47
2:F:30:VAL:HG21	2:F:37:LEU:HD22	1.96	0.47
1:A:498:LYS:HA	1:A:501:ARG:HG3	1.97	0.47
2:B:196:PHE:CZ	2:B:218:LEU:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ASP:OD2	2:B:242:ARG:HB3	2.15	0.47
1:C:404:GLU:HG2	1:C:406:PHE:O	2.14	0.47
1:E:116:TYR:O	1:E:125:VAL:HA	2.15	0.47
1:G:188:ARG:NH1	1:G:189:PHE:O	2.47	0.47
2:B:407:ILE:O	2:B:411:ALA:N	2.46	0.47
2:B:6:ASP:O	2:B:32:GLU:HB2	2.15	0.47
2:D:311:VAL:HG23	2:D:332:ASN:O	2.15	0.47
1:G:413:ALA:HB1	1:G:420:LEU:HD21	1.96	0.47
2:H:310:LEU:HD11	2:H:312:PHE:CZ	2.49	0.47
1:A:342:THR:HG21	1:A:354:LEU:HD13	1.96	0.47
1:A:421:ILE:HD13	1:A:461:ILE:HG12	1.97	0.47
1:C:252:SER:OG	1:C:253:ASP:N	2.47	0.47
2:D:292:THR:HA	2:D:358:ASN:ND2	2.29	0.47
1:G:23:TYR:OH	1:G:307:SER:HB3	2.15	0.47
2:B:6:ASP:OD2	2:B:200:ALA:HB3	2.15	0.47
2:F:35:GLY:O	2:F:122:LYS:HG2	2.14	0.47
2:H:120:TYR:CZ	2:H:126:CYS:HB2	2.49	0.47
2:B:195:LEU:HB3	2:B:219:PHE:HE1	1.78	0.47
1:G:140:ASP:OD1	1:G:146:ARG:HD2	2.15	0.47
2:H:280:ARG:HD3	2:H:281:ASP:O	2.15	0.47
2:B:117:SER:O	2:B:130:THR:N	2.47	0.47
2:B:412:LEU:HD13	2:B:418:MSE:SE	2.65	0.47
2:D:74:GLY:HA2	2:D:79:ALA:HA	1.97	0.47
1:E:38:ILE:HA	1:E:63:ILE:O	2.15	0.47
2:F:176:ARG:HD2	2:F:201:TYR:CE1	2.50	0.47
2:F:297:ILE:HG22	2:F:357:ILE:HG13	1.97	0.47
2:F:394:HIS:HE1	2:F:424:ALA:HB3	1.80	0.47
1:A:367:ARG:HG2	1:A:381:LEU:HD22	1.97	0.46
2:B:192:ASP:OD1	2:B:192:ASP:N	2.48	0.46
1:C:316:GLU:HB3	1:C:317:PRO:HD2	1.97	0.46
1:C:349:LEU:HD11	1:C:462:ILE:HG22	1.97	0.46
2:F:328:LEU:HD13	2:F:335:LEU:HG	1.96	0.46
2:F:343:GLN:O	2:F:347:LEU:HG	2.15	0.46
2:H:113:GLN:NE2	2:H:134:SER:O	2.42	0.46
1:A:245:HIS:CE1	1:A:246:PHE:CD2	3.02	0.46
2:B:6:ASP:O	2:B:32:GLU:N	2.48	0.46
2:B:94:ALA:HA	2:B:103:LYS:HB2	1.97	0.46
1:E:391:TYR:O	1:E:418:LEU:HD11	2.15	0.46
2:D:165:LEU:HB2	2:D:168:GLU:HB3	1.97	0.46
1:E:392:ALA:HA	1:E:416:SER:OG	2.14	0.46
1:G:425:VAL:O	1:G:430:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HG22	1:A:375:ALA:O	2.16	0.46
2:D:444:LEU:HD22	2:D:444:LEU:N	2.30	0.46
2:F:412:LEU:HB3	2:F:418:MSE:HA	1.97	0.46
1:C:346:HIS:HB2	1:C:378:TYR:CZ	2.50	0.46
2:F:292:THR:HG22	2:F:358:ASN:ND2	2.23	0.46
2:H:320:MSE:HE3	2:H:335:LEU:HB3	1.97	0.46
1:A:163:GLN:HE22	1:A:165:ARG:NH2	2.14	0.46
1:A:346:HIS:ND1	1:A:346:HIS:O	2.40	0.46
2:D:93:TYR:CE1	2:D:100:ARG:HA	2.50	0.46
2:D:94:ALA:HA	2:D:103:LYS:HB3	1.97	0.46
1:G:321:TYR:HE2	1:G:349:LEU:HD11	1.81	0.46
1:A:44:LEU:HD13	1:A:141:TYR:CZ	2.51	0.46
2:B:84:MSE:H	1:C:226:GLN:CD	2.18	0.46
1:C:179:ILE:HA	1:C:183:GLN:O	2.16	0.46
1:E:210:LEU:HD11	1:E:216:VAL:HG21	1.97	0.46
2:F:236:LEU:HD13	2:F:265:GLN:HB3	1.98	0.46
1:G:323:MSE:HE2	1:G:352:LEU:HD11	1.96	0.46
2:H:165:LEU:HB2	2:H:168:GLU:HB2	1.98	0.46
1:A:49:GLN:NE2	1:A:53:GLU:OE1	2.39	0.46
2:B:280:ARG:HD2	2:B:281:ASP:O	2.15	0.46
1:E:324:ILE:HB	1:E:394:TYR:CD2	2.48	0.46
2:F:321:SER:O	2:F:325:LEU:HB2	2.15	0.46
1:E:335:ILE:HG21	1:E:366:LEU:HD13	1.98	0.46
1:G:131:VAL:HG22	1:G:136:LEU:HA	1.96	0.46
1:G:466:SER:HA	1:G:467:GLN:HG3	1.97	0.46
2:H:297:ILE:CG2	2:H:300:LEU:HB2	2.46	0.46
1:A:440:TYR:CE2	1:A:464:LEU:HD21	2.50	0.46
1:A:111:GLN:OE1	2:B:172:ILE:HB	2.16	0.46
2:B:163:LEU:HD22	2:B:179:PHE:HE1	1.81	0.46
2:D:94:ALA:HA	2:D:103:LYS:HD2	1.96	0.46
2:D:332:ASN:OD1	2:D:333:VAL:HG23	2.16	0.46
1:E:337:TRP:O	1:E:341:ALA:N	2.47	0.46
2:F:381:GLU:HG3	2:F:382:GLN:H	1.81	0.46
1:A:226:GLN:OE1	2:D:84:MSE:N	2.49	0.45
1:E:50:HIS:HE1	1:E:77:THR:H	1.65	0.45
1:G:401:SER:HB2	1:G:429:ASN:HD21	1.80	0.45
1:A:426:ARG:HA	1:A:427:TYR:HA	1.78	0.45
1:A:440:TYR:CD1	1:A:460:LYS:HD3	2.52	0.45
1:C:464:LEU:CD2	1:C:473:MSE:HE1	2.43	0.45
2:D:295:ASP:HA	2:D:296:GLN:HA	1.77	0.45
2:D:304:VAL:HA	2:D:312:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:GLU:O	2:D:357:ILE:HG21	2.16	0.45
1:E:144:TYR:HE2	1:E:169:GLU:HG2	1.81	0.45
1:E:396:LEU:HD22	1:E:465:PHE:CZ	2.51	0.45
2:F:2:ILE:HG22	2:F:27:PRO:CG	2.46	0.45
2:F:10:GLN:OE1	2:F:368:ARG:NH1	2.50	0.45
1:G:395:GLU:O	1:G:419:PRO:HD2	2.16	0.45
1:A:173:VAL:HG21	2:B:144:TYR:CE1	2.49	0.45
1:A:323:MSE:HE2	1:A:396:LEU:HD21	1.98	0.45
1:A:63:ILE:HG23	1:A:68:TYR:HB2	1.98	0.45
1:C:108:GLN:HG3	1:C:109:ASP:H	1.81	0.45
1:C:151:TYR:CE1	2:D:153:VAL:HG11	2.51	0.45
2:H:195:LEU:HD22	2:H:219:PHE:CE1	2.51	0.45
1:A:416:SER:HB2	1:A:418:LEU:HG	1.98	0.45
2:B:264:ASP:N	2:B:264:ASP:OD1	2.49	0.45
1:C:473:MSE:HB2	1:C:473:MSE:HE3	1.71	0.45
1:E:64:TRP:HB3	1:E:67:ASN:CB	2.46	0.45
2:F:304:VAL:HG13	2:F:332:ASN:HB2	1.98	0.45
1:A:458:VAL:HG12	1:A:461:ILE:HD12	1.97	0.45
1:C:10:ILE:HB	1:C:39:PHE:CE2	2.52	0.45
1:E:5:ASN:ND2	1:E:24:ARG:HD2	2.30	0.45
1:E:30:ARG:HD3	1:E:30:ARG:HA	1.74	0.45
1:E:354:LEU:HD23	1:E:355:ASP:N	2.31	0.45
1:E:406:PHE:CD2	1:E:407:GLY:N	2.84	0.45
1:E:195:TYR:CE1	2:F:109:ASP:HA	2.52	0.45
1:G:323:MSE:O	1:G:354:LEU:HA	2.16	0.45
1:G:3:VAL:O	1:G:36:LYS:N	2.50	0.45
1:G:395:GLU:OE2	1:G:470:GLN:HG2	2.17	0.45
1:G:308:LEU:O	1:G:485:LEU:HD12	2.17	0.45
1:A:49:GLN:NE2	1:A:53:GLU:HB2	2.32	0.45
2:B:273:GLY:HA3	2:B:430:ASN:O	2.16	0.45
2:D:368:ARG:NH1	2:D:389:TYR:OH	2.49	0.45
2:H:339:ALA:HB1	2:H:343:GLN:HG2	1.99	0.45
1:A:17:VAL:HG13	1:A:242:HIS:ND1	2.30	0.45
1:A:342:THR:HB	1:A:378:TYR:HE2	1.81	0.45
2:B:115:ARG:HD3	2:B:115:ARG:HA	1.76	0.45
2:B:250:ASP:OD1	2:B:430:ASN:ND2	2.49	0.45
2:B:295:ASP:HB2	2:B:296:GLN:HB2	1.99	0.45
2:D:341:LEU:HA	2:D:344:ILE:HD12	1.99	0.45
1:E:341:ALA:O	1:E:458:VAL:HG12	2.17	0.45
2:F:252:ALA:O	2:F:255:GLU:HB2	2.16	0.45
2:F:281:ASP:HB2	2:F:283:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:TYR:OH	2:F:176:ARG:NE	2.49	0.45
2:H:181:ARG:NH1	2:H:209:LEU:HD21	2.32	0.45
2:H:436:LEU:HA	2:H:439:GLU:HB2	1.97	0.45
1:G:116:TYR:HB2	1:G:127:HIS:HB2	1.99	0.45
2:H:127:PHE:O	2:H:144:TYR:N	2.46	0.45
2:H:341:LEU:HA	2:H:344:ILE:HD12	1.99	0.45
2:H:34:ASN:OD1	2:H:36:PHE:N	2.49	0.45
1:A:24:ARG:HH22	1:A:217:ILE:HG21	1.82	0.45
1:C:246:PHE:HB2	1:C:257:LEU:O	2.17	0.45
2:F:404:LEU:HA	2:F:407:ILE:HG12	1.99	0.45
1:G:15:SER:N	1:G:18:GLU:OE1	2.50	0.45
1:C:438:ASN:HA	1:C:473:MSE:HB3	1.99	0.45
1:E:24:ARG:O	1:E:28:LEU:HG	2.16	0.45
1:G:286:LEU:HD12	1:G:287:GLU:N	2.32	0.45
2:H:314:ILE:O	2:H:335:LEU:HD22	2.17	0.45
1:A:375:ALA:CB	1:A:378:TYR:HB3	2.44	0.44
1:C:109:ASP:HB3	2:D:174:LYS:NZ	2.32	0.44
1:C:303:ILE:HA	1:C:304:PRO:HD3	1.83	0.44
2:D:298:GLU:HB2	2:D:359:HIS:NE2	2.30	0.44
2:D:14:ASP:CG	2:D:368:ARG:HH22	2.21	0.44
2:D:383:THR:OG1	2:D:384:LEU:N	2.50	0.44
1:G:440:TYR:CD2	1:G:460:LYS:HB3	2.48	0.44
1:A:136:LEU:O	1:A:152:PHE:HB2	2.16	0.44
1:A:249:ASN:O	2:D:340:SER:HB2	2.18	0.44
1:C:179:ILE:HD13	1:C:184:GLU:HA	1.97	0.44
2:D:289:LEU:HA	2:D:313:ARG:O	2.18	0.44
2:B:272:LEU:HD12	2:B:437:TYR:HD1	1.81	0.44
2:D:412:LEU:HD23	2:D:418:MSE:SE	2.67	0.44
1:E:135:ARG:HG2	1:E:135:ARG:NH1	2.32	0.44
2:B:292:THR:HG22	2:B:358:ASN:CB	2.48	0.44
1:C:18:GLU:N	1:C:18:GLU:OE1	2.50	0.44
1:C:47:ASN:OD1	1:C:48:ILE:N	2.51	0.44
1:C:64:TRP:HB3	1:C:67:ASN:HB3	1.99	0.44
1:E:486:THR:O	1:E:490:GLU:HG3	2.18	0.44
2:F:49:LEU:HD22	2:F:144:TYR:O	2.17	0.44
1:A:486:THR:HA	1:A:489:VAL:HB	1.99	0.44
2:D:204:LEU:HD12	2:D:207:HIS:HB3	1.99	0.44
2:D:9:ASN:OD1	2:D:9:ASN:N	2.49	0.44
1:G:44:LEU:HD13	1:G:141:TYR:CZ	2.52	0.44
2:H:382:GLN:OE1	2:H:382:GLN:N	2.50	0.44
1:A:329:LEU:HD21	1:A:363:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LEU:HD22	2:B:440:THR:HG23	1.99	0.44
2:B:299:GLY:O	2:B:303:LEU:HG	2.18	0.44
1:C:161:LEU:C	1:C:162:TYR:HD2	2.21	0.44
1:C:7:ASN:OD1	1:C:220:ARG:HD2	2.18	0.44
1:G:165:ARG:HA	1:G:176:ASP:HA	2.00	0.44
1:G:318:ARG:O	1:G:320:PRO:HD3	2.18	0.44
2:H:313:ARG:HD3	2:H:347:LEU:HD22	2.00	0.44
1:A:50:HIS:O	1:A:54:ASN:HB2	2.17	0.44
2:B:181:ARG:HA	2:B:184:LEU:HD12	1.99	0.44
1:C:427:TYR:O	1:C:430:GLN:N	2.46	0.44
2:D:209:LEU:HG	2:D:212:ARG:HB3	1.99	0.44
2:D:391:ALA:O	2:D:395:ILE:HG13	2.18	0.44
1:G:12:TRP:CE3	1:G:12:TRP:HA	2.53	0.44
1:G:329:LEU:HD22	1:G:335:ILE:HD11	1.99	0.44
2:H:397:ASP:HB3	2:H:400:GLN:CB	2.44	0.44
1:A:313:TYR:HA	1:A:314:PRO:HD3	1.89	0.44
1:A:42:MSE:HG2	1:A:164:ARG:NH1	2.32	0.44
1:C:66:TYR:O	1:C:175:TYR:OH	2.35	0.44
1:E:117:LEU:HA	1:E:124:PHE:O	2.18	0.44
2:F:6:ASP:OD2	2:F:200:ALA:CB	2.62	0.44
2:H:120:TYR:CE1	2:H:126:CYS:HB2	2.53	0.44
2:D:5:PHE:HE1	2:D:15:LEU:HD23	1.82	0.44
2:F:220:TRP:CZ2	2:F:222:GLU:HB2	2.53	0.44
2:F:301:ASP:O	2:F:305:GLN:HG2	2.18	0.44
2:F:320:MSE:HE3	2:F:337:GLN:N	2.29	0.44
1:G:391:TYR:O	1:G:418:LEU:HD21	2.18	0.44
2:H:203:PHE:CE2	2:H:231:ASN:HB3	2.53	0.44
2:H:70:TRP:CD2	2:H:83:ASP:HB2	2.53	0.44
1:A:165:ARG:HA	1:A:176:ASP:HA	2.00	0.43
1:C:135:ARG:HD3	1:C:154:PRO:HG3	1.99	0.43
1:E:236:LYS:HD3	1:E:273:ASP:CG	2.38	0.43
1:E:496:LEU:O	1:E:500:VAL:HG23	2.18	0.43
1:A:38:ILE:HA	1:A:63:ILE:O	2.18	0.43
1:G:185:LYS:NZ	2:H:111:LYS:HZ1	2.14	0.43
1:G:191:ASP:OD1	1:G:191:ASP:N	2.37	0.43
1:A:241:VAL:HA	1:A:262:TYR:CE1	2.54	0.43
1:A:426:ARG:HG3	1:A:426:ARG:H	1.43	0.43
1:C:14:SER:HB3	1:C:19:TYR:HE1	1.82	0.43
1:C:2:THR:N	1:C:214:ASP:OD1	2.52	0.43
1:C:444:VAL:HG22	1:C:445:SER:O	2.18	0.43
1:E:109:ASP:N	1:E:109:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:MSE:SE	1:E:65:LEU:HD22	2.68	0.43
1:E:96:GLU:HB2	1:E:103:ARG:HG3	2.00	0.43
1:G:228:VAL:O	1:G:232:SER:OG	2.30	0.43
2:H:235:ILE:HD11	2:H:243:THR:O	2.19	0.43
2:H:45:TYR:HB3	2:H:143:TYR:CD2	2.53	0.43
1:A:100:LYS:HE2	1:A:117:LEU:O	2.17	0.43
1:A:343:VAL:O	1:A:346:HIS:HB3	2.18	0.43
1:C:232:SER:HB2	1:C:237:LEU:HD22	2.00	0.43
1:C:327:SER:OG	1:C:328:ARG:N	2.51	0.43
1:E:365:LYS:O	1:E:369:ARG:HG3	2.19	0.43
1:G:307:SER:HB2	1:G:486:THR:CB	2.48	0.43
1:A:188:ARG:HD2	1:A:188:ARG:HA	1.82	0.43
1:A:402:THR:O	1:A:425:VAL:HG21	2.19	0.43
2:B:390:ILE:HD12	2:B:391:ALA:H	1.83	0.43
1:C:260:ASN:OD1	1:C:260:ASN:N	2.51	0.43
2:D:314:ILE:HG13	2:D:335:LEU:CD2	2.49	0.43
2:F:397:ASP:HB2	2:F:401:PRO:CD	2.48	0.43
2:H:315:ALA:HA	2:H:336:TYR:O	2.18	0.43
2:B:1:MSE:HE2	2:B:195:LEU:HD11	2.01	0.43
2:B:381:GLU:OE2	2:B:387:ARG:NH1	2.51	0.43
1:C:137:ILE:HG13	1:C:138:ARG:H	1.84	0.43
1:C:245:HIS:HB2	1:C:266:PHE:HE2	1.84	0.43
2:D:279:LYS:HE2	2:D:372:GLU:OE1	2.18	0.43
1:E:197:LYS:O	1:E:201:VAL:HG23	2.19	0.43
1:G:28:LEU:HD21	1:G:497:LEU:HD11	2.00	0.43
2:H:226:ASP:HB2	2:H:227:GLU:OE2	2.19	0.43
2:B:358:ASN:OD1	2:B:358:ASN:N	2.52	0.43
1:C:143:SER:OG	1:C:144:TYR:N	2.50	0.43
1:C:177:MSE:HA	1:C:186:LEU:O	2.19	0.43
2:D:1:MSE:HG3	2:D:26:CYS:HB3	2.01	0.43
2:D:390:ILE:O	2:D:428:HIS:CE1	2.72	0.43
1:E:396:LEU:HD22	1:E:465:PHE:HZ	1.82	0.43
2:F:216:ASP:CG	2:F:242:ARG:HE	2.21	0.43
1:G:106:TYR:O	1:G:109:ASP:O	2.36	0.43
1:G:26:GLN:HA	1:G:29:ARG:NH1	2.33	0.43
1:A:44:LEU:HA	1:A:44:LEU:HD23	1.62	0.43
1:A:482:GLU:HA	1:A:485:LEU:HD11	2.00	0.43
2:B:195:LEU:HD22	2:B:219:PHE:HZ	1.84	0.43
1:C:33:GLN:NE2	1:C:497:LEU:HD21	2.33	0.43
2:F:226:ASP:O	2:F:260:LEU:HD13	2.18	0.43
2:H:376:LEU:HD11	2:H:394:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ILE:HD11	1:E:490:GLU:HB3	2.01	0.43
1:E:329:LEU:O	1:E:329:LEU:HD23	2.18	0.43
1:E:476:HIS:O	1:E:480:VAL:HG23	2.19	0.43
2:F:385:HIS:HB3	2:F:386:ASP:CA	2.47	0.43
2:F:38:PRO:HB2	2:F:40:ASP:H	1.83	0.43
2:B:110:LYS:HG2	2:B:110:LYS:H	1.64	0.43
2:B:300:LEU:HD23	2:B:327:MSE:HE3	2.00	0.43
2:B:60:PHE:HE1	2:B:100:ARG:HE	1.65	0.43
1:C:324:ILE:O	1:C:397:TYR:HA	2.19	0.43
1:C:42:MSE:HE3	1:C:164:ARG:HD2	2.01	0.43
2:D:286:LYS:HD2	2:D:310:LEU:HD11	2.00	0.43
2:D:280:ARG:NH1	2:D:349:LEU:O	2.51	0.43
1:E:117:LEU:HD23	1:E:124:PHE:O	2.19	0.43
2:F:1:MSE:HA	2:F:193:HIS:O	2.19	0.43
2:F:200:ALA:H	2:F:203:PHE:HB3	1.82	0.43
1:C:21:GLN:HG3	1:C:24:ARG:NH1	2.34	0.42
1:C:360:GLY:O	1:C:363:GLU:HB2	2.19	0.42
2:D:430:ASN:O	2:D:432:VAL:HG13	2.19	0.42
1:E:308:LEU:HG	1:E:411:MSE:HE2	2.01	0.42
2:H:361:GLY:O	2:H:384:LEU:HD22	2.19	0.42
1:A:52:THR:OG1	1:A:53:GLU:N	2.53	0.42
1:A:188:ARG:NE	2:B:118:GLU:OE2	2.49	0.42
2:B:212:ARG:C	2:B:242:ARG:NH1	2.72	0.42
1:C:153:ALA:HB2	2:D:139:PHE:HE1	1.83	0.42
2:D:165:LEU:HB2	2:D:168:GLU:CB	2.49	0.42
2:D:354:TYR:HE1	2:D:356:ASP:OD1	2.02	0.42
1:E:453:ILE:HA	1:E:456:ALA:HB3	2.01	0.42
1:E:55:ILE:HD12	1:E:55:ILE:HA	1.79	0.42
1:E:36:LYS:HD2	1:E:63:ILE:CG1	2.50	0.42
2:F:184:LEU:HD22	2:F:191:LEU:HD21	1.99	0.42
1:G:48:ILE:O	1:G:52:THR:HG23	2.19	0.42
2:H:297:ILE:HG22	2:H:300:LEU:HB2	2.01	0.42
1:A:240:VAL:HG22	1:A:242:HIS:CD2	2.55	0.42
1:C:323:MSE:HE2	1:C:461:ILE:HG21	2.02	0.42
2:D:117:SER:HB2	2:D:130:THR:HB	2.01	0.42
1:E:67:ASN:O	1:E:70:THR:OG1	2.31	0.42
2:F:367:VAL:HG13	2:F:377:ILE:HD13	2.00	0.42
2:F:78:VAL:HG22	2:F:79:ALA:H	1.84	0.42
1:G:256:ILE:HB	1:G:293:TYR:CG	2.54	0.42
1:G:396:LEU:HD12	1:G:419:PRO:HG2	2.00	0.42
2:H:427:ARG:C	2:H:430:ASN:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TYR:HB2	2:B:139:PHE:CZ	2.54	0.42
2:B:187:LEU:HB3	2:B:189:LEU:HD21	2.02	0.42
1:E:176:ASP:OD1	1:E:176:ASP:N	2.48	0.42
2:F:391:ALA:HA	2:F:428:HIS:ND1	2.35	0.42
2:H:390:ILE:HD13	2:H:390:ILE:HA	1.83	0.42
1:A:93:GLU:HG2	1:A:94:ARG:N	2.34	0.42
1:C:345:ALA:HB2	1:C:458:VAL:HG13	2.00	0.42
1:C:41:ASP:O	1:C:43:ILE:HG13	2.19	0.42
2:D:337:GLN:HG2	2:D:338:ASN:OD1	2.20	0.42
2:D:297:ILE:CG2	2:D:357:ILE:HB	2.49	0.42
1:E:187:TYR:CE2	1:E:200:LEU:HD22	2.54	0.42
2:F:389:TYR:O	2:F:425:GLN:NE2	2.50	0.42
2:F:432:VAL:HG21	2:F:436:LEU:HD23	2.02	0.42
1:G:327:SER:OG	1:G:328:ARG:N	2.52	0.42
2:H:132:TYR:CD2	2:H:138:ALA:HA	2.55	0.42
2:H:44:PRO:HB2	2:H:179:PHE:HE2	1.85	0.42
1:A:321:TYR:H	1:A:395:GLU:HG3	1.84	0.42
2:B:303:LEU:CD2	2:B:402:ALA:HB1	2.49	0.42
1:E:338:LEU:O	1:E:342:THR:HG23	2.20	0.42
2:F:235:ILE:HG23	2:F:243:THR:O	2.20	0.42
1:G:349:LEU:HD12	1:G:349:LEU:HA	1.75	0.42
1:G:44:LEU:HD23	1:G:44:LEU:HA	1.72	0.42
2:H:107:TRP:HB2	2:H:116:LEU:HB2	2.01	0.42
2:H:59:LEU:HG	2:H:124:GLY:O	2.20	0.42
1:A:94:ARG:HH21	1:A:107:PRO:HG2	1.85	0.42
1:A:116:TYR:CD1	1:A:127:HIS:HB2	2.55	0.42
1:C:246:PHE:CZ	1:C:248:GLU:HB2	2.55	0.42
2:D:391:ALA:HB3	2:D:394:HIS:HD2	1.83	0.42
2:D:75:ASP:OD2	2:D:77:GLN:N	2.42	0.42
1:E:437:LYS:HD2	1:E:437:LYS:N	2.35	0.42
2:H:117:SER:OG	2:H:132:TYR:HE1	2.02	0.42
1:E:198:ALA:HB1	2:H:84:MSE:HE3	2.02	0.42
1:A:303:ILE:HG21	1:A:493:TRP:CE2	2.54	0.42
2:B:282:ASN:OD1	2:B:418:MSE:HG2	2.20	0.42
2:B:299:GLY:O	2:B:302:THR:HG22	2.20	0.42
2:D:272:LEU:HD23	2:D:437:TYR:CE1	2.55	0.42
1:E:137:ILE:HG21	2:F:160:ASP:OD2	2.20	0.42
1:G:250:ALA:HB3	1:G:257:LEU:CD2	2.50	0.42
1:A:366:LEU:O	1:A:370:ILE:HD12	2.19	0.42
1:A:391:TYR:O	1:A:418:LEU:HD11	2.20	0.42
1:A:396:LEU:HD23	1:A:465:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:LYS:O	2:D:326:SER:OG	2.36	0.42
1:E:200:LEU:HD12	1:E:200:LEU:HA	1.80	0.42
2:F:248:ILE:HB	2:F:254:TYR:HD1	1.84	0.42
2:H:36:PHE:HE2	2:H:103:LYS:HA	1.85	0.42
1:A:94:ARG:HB3	1:A:94:ARG:HE	1.52	0.42
1:C:3:VAL:HG22	1:C:215:VAL:HB	2.02	0.42
2:D:61:PHE:CE1	2:D:100:ARG:HD3	2.55	0.42
1:E:406:PHE:HD2	1:E:407:GLY:N	2.17	0.42
2:H:93:TYR:CZ	2:H:100:ARG:HG2	2.55	0.42
2:D:285:ARG:HB2	2:D:352:ASP:OD2	2.20	0.41
1:E:126:GLU:HB3	1:E:127:HIS:CE1	2.55	0.41
1:G:236:LYS:HA	1:G:273:ASP:OD2	2.20	0.41
1:G:341:ALA:O	1:G:345:ALA:HB2	2.19	0.41
2:H:32:GLU:HG2	2:H:34:ASN:H	1.84	0.41
2:H:78:VAL:HG12	2:H:79:ALA:N	2.35	0.41
1:A:48:ILE:O	1:A:52:THR:HG23	2.19	0.41
2:D:216:ASP:OD2	2:D:242:ARG:HB3	2.19	0.41
2:D:298:GLU:OE2	2:D:399:SER:HB2	2.20	0.41
2:F:236:LEU:HD22	2:F:265:GLN:HB3	2.01	0.41
1:G:143:SER:OG	1:G:144:TYR:N	2.52	0.41
1:C:100:LYS:HA	1:C:117:LEU:HB2	2.01	0.41
1:E:262:TYR:HA	1:E:265:GLN:NE2	2.35	0.41
1:E:467:GLN:CD	1:E:468:GLY:H	2.24	0.41
1:E:96:GLU:HB2	1:E:103:ARG:CG	2.50	0.41
2:F:296:GLN:HG3	2:F:297:ILE:N	2.35	0.41
2:F:53:GLU:HG2	2:F:53:GLU:H	1.68	0.41
2:H:222:GLU:HB3	2:H:223:PRO:HD2	2.02	0.41
2:B:210:THR:HG22	2:B:241:LEU:HA	2.03	0.41
2:D:30:VAL:O	2:D:44:PRO:HD2	2.20	0.41
2:D:89:ALA:HB2	2:D:107:TRP:CE3	2.55	0.41
2:D:93:TYR:CD1	2:D:100:ARG:HA	2.55	0.41
1:E:150:GLU:HG2	1:E:164:ARG:HE	1.85	0.41
1:E:303:ILE:HG22	1:E:304:PRO:O	2.20	0.41
1:E:373:ALA:C	1:E:375:ALA:H	2.24	0.41
1:G:3:VAL:HG22	1:G:215:VAL:HB	2.01	0.41
2:H:292:THR:HG21	2:H:297:ILE:HD11	2.02	0.41
2:B:196:PHE:HB2	2:B:202:SER:HB3	2.03	0.41
2:B:285:ARG:HG3	2:B:352:ASP:OD2	2.20	0.41
2:D:377:ILE:O	2:D:378:LEU:HD23	2.20	0.41
1:G:265:GLN:N	1:G:265:GLN:OE1	2.38	0.41
1:G:28:LEU:HA	1:G:31:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD22	1:A:141:TYR:CD2	2.55	0.41
2:B:94:ALA:N	2:B:101:LEU:O	2.52	0.41
1:E:44:LEU:HD13	1:E:141:TYR:CZ	2.55	0.41
2:F:192:ASP:OD1	2:F:193:HIS:N	2.54	0.41
2:F:295:ASP:HA	2:F:296:GLN:HA	1.77	0.41
2:H:355:LEU:HA	2:H:378:LEU:O	2.20	0.41
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.90	0.41
2:B:295:ASP:HA	2:B:296:GLN:HA	1.84	0.41
1:C:325:THR:HA	1:C:397:TYR:CE2	2.56	0.41
1:C:10:ILE:HB	1:C:39:PHE:HE2	1.84	0.41
1:C:498:LYS:O	1:C:502:ASP:HB2	2.20	0.41
1:C:52:THR:O	1:C:57:PHE:N	2.50	0.41
2:D:309:GLN:H	2:D:309:GLN:HG3	1.47	0.41
1:E:337:TRP:HZ2	1:E:448:HIS:CD2	2.38	0.41
1:A:268:ASN:O	1:A:271:LYS:HG2	2.21	0.41
2:B:49:LEU:HD22	2:B:144:TYR:O	2.21	0.41
1:C:28:LEU:HA	1:C:31:ILE:HG12	2.02	0.41
1:A:226:GLN:CD	2:D:84:MSE:H	2.23	0.41
1:E:163:GLN:OE1	2:F:140:ASN:ND2	2.52	0.41
1:E:210:LEU:HA	1:E:210:LEU:HD23	1.85	0.41
2:F:152:ILE:HG12	2:F:163:LEU:HD13	2.03	0.41
1:G:237:LEU:HD23	1:G:272:VAL:HA	2.03	0.41
1:G:334:HIS:CD2	1:G:402:THR:HG21	2.56	0.41
2:H:176:ARG:NH1	2:H:201:TYR:CE1	2.89	0.41
1:A:458:VAL:HA	1:A:461:ILE:HB	2.03	0.41
2:B:60:PHE:CE1	2:B:100:ARG:HG3	2.55	0.41
2:B:297:ILE:HG23	2:B:357:ILE:HB	2.03	0.41
2:F:226:ASP:OD1	2:F:226:ASP:N	2.53	0.41
2:F:290:ILE:HG22	2:F:292:THR:HG22	2.01	0.41
2:F:351:SER:HB2	2:F:375:LEU:HD21	2.03	0.41
1:A:221:GLU:HG2	1:A:225:GLY:HA3	2.02	0.41
1:A:303:ILE:HG21	1:A:493:TRP:CZ2	2.56	0.41
1:A:25:ALA:HB2	1:A:57:PHE:HE1	1.86	0.41
1:C:221:GLU:HG2	1:C:225:GLY:HA3	2.03	0.41
1:C:244:GLU:OE2	1:C:244:GLU:HA	2.21	0.41
1:E:165:ARG:HD2	2:F:150:GLU:OE2	2.21	0.41
2:F:11:GLU:HB3	2:F:221:GLN:NE2	2.36	0.41
1:G:167:TYR:HE2	2:H:150:GLU:HG3	1.86	0.41
1:A:408:LEU:HA	1:A:411:MSE:HB3	2.03	0.41
2:B:84:MSE:HE3	1:C:202:ARG:HH12	1.86	0.41
1:C:100:LYS:HG2	1:C:120:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:MSE:HB2	1:C:354:LEU:CB	2.51	0.41
2:D:272:LEU:HB3	2:D:273:GLY:H	1.79	0.41
2:F:295:ASP:HB2	2:F:296:GLN:HB2	2.02	0.41
2:F:394:HIS:NE2	2:F:421:ALA:HB1	2.36	0.41
1:G:270:ASP:N	1:G:270:ASP:OD1	2.53	0.41
1:G:8:LEU:HD23	1:G:9:GLY:N	2.36	0.41
2:H:201:TYR:CD2	2:H:201:TYR:N	2.89	0.41
2:H:232:MSE:O	2:H:235:ILE:HG22	2.21	0.41
1:A:191:ASP:C	1:A:192:ARG:HG2	2.41	0.40
2:B:166:ASP:O	2:B:168:GLU:HG3	2.21	0.40
2:D:89:ALA:HB2	2:D:107:TRP:CZ3	2.56	0.40
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.70	0.40
1:E:321:TYR:HA	1:E:465:PHE:CE2	2.56	0.40
2:F:306:SER:HB2	2:F:307:LEU:HD12	2.02	0.40
2:F:290:ILE:HG22	2:F:358:ASN:HD22	1.85	0.40
1:G:140:ASP:OD1	1:G:149:SER:OG	2.21	0.40
1:G:321:TYR:O	1:G:352:LEU:HD12	2.21	0.40
2:H:299:GLY:HA3	2:H:357:ILE:HD11	2.03	0.40
2:H:400:GLN:HB3	2:H:401:PRO:CD	2.43	0.40
1:A:44:LEU:HD22	1:A:141:TYR:CE2	2.56	0.40
1:E:161:LEU:HD21	1:E:164:ARG:NH2	2.36	0.40
1:E:229:PHE:HB3	2:H:69:PHE:CE2	2.56	0.40
2:F:330:TYR:HB2	2:F:333:VAL:HG23	2.02	0.40
2:H:145:SER:OG	2:H:146:THR:N	2.54	0.40
2:H:220:TRP:HE1	2:H:224:LEU:CD2	2.34	0.40
2:B:227:GLU:OE1	2:B:227:GLU:N	2.54	0.40
2:B:89:ALA:HB2	2:B:107:TRP:CE3	2.57	0.40
1:C:15:SER:OG	1:C:16:GLY:N	2.54	0.40
1:C:346:HIS:HB2	1:C:378:TYR:CE1	2.56	0.40
1:C:44:LEU:HA	1:C:44:LEU:HD23	1.76	0.40
2:D:140:ASN:HA	2:D:156:HIS:HD2	1.86	0.40
2:D:5:PHE:CE1	2:D:15:LEU:HD23	2.55	0.40
2:D:191:LEU:HD23	2:D:194:ILE:HD11	2.03	0.40
2:D:209:LEU:HD23	2:D:242:ARG:NH1	2.33	0.40
2:D:78:VAL:CG1	2:D:79:ALA:N	2.85	0.40
1:E:10:ILE:HG22	1:E:11:GLY:N	2.37	0.40
1:E:252:SER:OG	1:E:253:ASP:N	2.55	0.40
1:E:323:MSE:HE1	1:E:461:ILE:HG21	2.02	0.40
2:H:31:ILE:HA	2:H:31:ILE:HD13	1.91	0.40
2:H:79:ALA:HB2	2:H:93:TYR:OH	2.21	0.40
1:A:103:ARG:HA	1:A:113:ILE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLN:HA	1:A:131:VAL:O	2.22	0.40
2:B:361:GLY:HA2	2:B:384:LEU:HG	2.03	0.40
2:D:374:ASN:OD1	2:D:422:LEU:HD11	2.21	0.40
1:E:1:SER:HB2	1:E:501:ARG:HH21	1.87	0.40
1:E:206:GLN:HE21	1:E:231:GLU:CD	2.25	0.40
2:F:280:ARG:HD3	2:F:280:ARG:HA	1.66	0.40
1:G:238:GLY:HA2	1:G:274:PHE:O	2.21	0.40
1:G:80:THR:O	1:G:84:VAL:HG23	2.21	0.40
2:H:341:LEU:H	2:H:341:LEU:HG	1.70	0.40
2:H:358:ASN:ND2	2:H:384:LEU:HD11	2.28	0.40
1:C:338:LEU:HA	1:C:338:LEU:HD23	1.94	0.40
2:D:256:LYS:HE2	2:D:256:LYS:HB2	1.84	0.40
1:E:27:ILE:O	1:E:31:ILE:HG12	2.21	0.40
1:E:343:VAL:HA	1:E:346:HIS:HD1	1.85	0.40
2:F:231:ASN:O	2:F:235:ILE:HG13	2.21	0.40
1:G:470:GLN:O	1:G:474:SER:OG	2.38	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	501/503 (100%)	463 (92%)	37 (7%)	1 (0%)	47	78
1	C	501/503 (100%)	475 (95%)	25 (5%)	1 (0%)	47	78
1	E	501/503 (100%)	471 (94%)	30 (6%)	0	100	100
1	G	501/503 (100%)	466 (93%)	33 (7%)	2 (0%)	34	70
2	B	443/446 (99%)	408 (92%)	35 (8%)	0	100	100
2	D	444/446 (100%)	414 (93%)	30 (7%)	0	100	100
2	F	443/446 (99%)	419 (95%)	21 (5%)	3 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	443/446 (99%)	410 (93%)	33 (7%)	0	100	100
All	All	3777/3796 (100%)	3526 (93%)	244 (6%)	7 (0%)	47	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	200	ALA
1	C	447	ASN
1	G	269	ALA
2	F	78	VAL
1	A	145	VAL
2	F	401	PRO
1	G	425	VAL

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	435/429 (101%)	432 (99%)	3 (1%)	84	91
1	C	435/429 (101%)	429 (99%)	6 (1%)	67	81
1	E	435/429 (101%)	432 (99%)	3 (1%)	84	91
1	G	435/429 (101%)	429 (99%)	6 (1%)	67	81
2	B	392/384 (102%)	381 (97%)	11 (3%)	43	67
2	D	392/384 (102%)	386 (98%)	6 (2%)	65	81
2	F	392/384 (102%)	386 (98%)	6 (2%)	65	81
2	H	392/384 (102%)	384 (98%)	8 (2%)	55	74
All	All	3308/3252 (102%)	3259 (98%)	49 (2%)	65	81

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	PHE

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Mol	Chain	Res	Type
1	A	295	ASP
1	A	457	PHE
2	B	47	TYR
2	B	61	PHE
2	B	95	SER
2	B	98	ARG
2	B	123	GLN
2	B	126	CYS
2	B	208	SER
2	B	264	ASP
2	B	309	GLN
2	B	348	TYR
2	B	389	TYR
1	C	41	ASP
1	C	127	HIS
1	C	135	ARG
1	C	246	PHE
1	C	378	TYR
1	C	457	PHE
2	D	60	PHE
2	D	119	ARG
2	D	176	ARG
2	D	226	ASP
2	D	389	TYR
2	D	413	CYS
1	E	242	HIS
1	E	246	PHE
1	E	401	SER
2	F	26	CYS
2	F	127	PHE
2	F	133	LYS
2	F	227	GLU
2	F	388	HIS
2	F	418	MSE
1	G	127	HIS
1	G	254	ASP
1	G	296	LYS
1	G	318	ARG
1	G	337	TRP
1	G	359	LYS
2	H	57	HIS
2	H	60	PHE

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Mol	Chain	Res	Type
2	H	126	CYS
2	H	133	LYS
2	H	280	ARG
2	H	293	HIS
2	H	389	TYR
2	H	430	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	HIS
1	C	297	GLN
1	E	242	HIS
2	F	221	GLN
2	H	393	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	UDP	E	602	-	20,26,26	1.12	1 (5%)	25,40,40	1.13	2 (8%)
4	NAG	A	602	-	15,15,15	0.26	0	21,21,21	0.21	0
3	UDP	A	601	-	20,26,26	1.12	1 (5%)	25,40,40	1.23	2 (8%)
4	NAG	E	603	-	15,15,15	0.26	0	21,21,21	0.24	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
3	UDP	E	602	-	-	4/14/32/32	0/2/2/2
4	NAG	A	602	-	-	0/6/26/26	0/1/1/1
3	UDP	A	601	-	-	5/14/32/32	0/2/2/2
4	NAG	E	603	-	-	2/6/26/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	UDP	C4-N3	3.25	1.38	1.33
3	E	602	UDP	C4-N3	3.20	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	UDP	C3'-C2'-C1'	3.22	105.83	100.98
3	A	601	UDP	PA-O3A-PB	-3.21	121.81	132.83
3	E	602	UDP	C3'-C2'-C1'	2.78	105.17	100.98
3	E	602	UDP	PA-O3A-PB	-2.58	123.99	132.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	603	NAG	C1-C2-N2-C7
3	E	602	UDP	C3'-C4'-C5'-O5'
3	E	602	UDP	O4'-C4'-C5'-O5'
3	A	601	UDP	O4'-C4'-C5'-O5'
3	E	602	UDP	PB-O3A-PA-O2A
4	E	603	NAG	C3-C2-N2-C7

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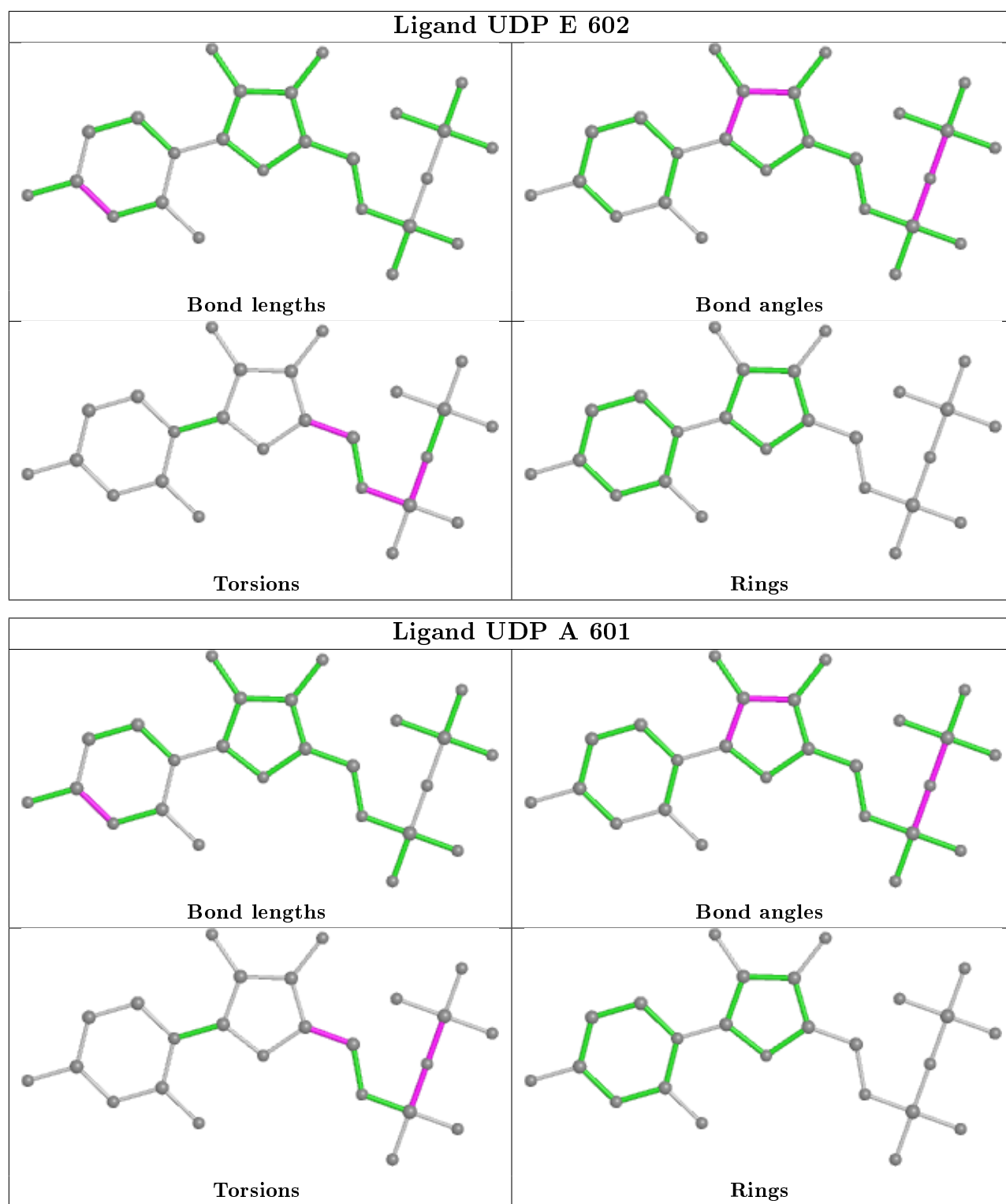
Mol	Chain	Res	Type	Atoms
3	A	601	UDP	PB-O3A-PA-O1A
3	A	601	UDP	C3'-C4'-C5'-O5'
3	A	601	UDP	PA-O3A-PB-O2B
3	A	601	UDP	PA-O3A-PB-O3B
3	E	602	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	UDP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å ²)	Q<0.9
1	A	497/503 (98%)	0.22	14 (2%) 53 43	70, 113, 158, 173	0
1	C	497/503 (98%)	0.14	9 (1%) 68 61	71, 109, 162, 181	0
1	E	497/503 (98%)	0.23	20 (4%) 38 31	73, 114, 162, 174	0
1	G	497/503 (98%)	0.27	24 (4%) 30 26	66, 112, 163, 175	0
2	B	437/446 (97%)	0.18	6 (1%) 75 67	70, 114, 147, 168	0
2	D	438/446 (98%)	0.23	9 (2%) 63 55	68, 112, 139, 161	0
2	F	437/446 (97%)	0.05	4 (0%) 84 78	64, 119, 149, 171	0
2	H	437/446 (97%)	0.21	14 (3%) 47 38	66, 113, 146, 166	0
All	All	3737/3796 (98%)	0.19	100 (2%) 54 45	64, 114, 157, 181	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	344	GLN	6.0
1	G	448	HIS	5.1
1	A	359	LYS	4.7
1	G	356	ILE	4.6
2	H	385	HIS	4.4
1	G	449	VAL	4.2
1	G	325	THR	4.2
1	G	383	GLY	4.0
1	E	418	LEU	4.0
1	C	399	THR	4.0
1	G	398	LEU	4.0
1	G	343	VAL	3.9
2	H	289	LEU	3.8
1	G	357	TYR	3.7
2	D	312	PHE	3.7
2	F	437	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	420	LEU	3.6
1	A	448	HIS	3.6
1	G	342	THR	3.5
1	E	419	PRO	3.4
2	H	356	ASP	3.4
1	C	422	GLY	3.2
2	H	379	GLY	3.1
1	E	305	VAL	3.1
1	E	379	ILE	3.1
1	A	440	TYR	3.0
1	E	423	PHE	2.9
1	A	10	ILE	2.9
2	D	217	ILE	2.9
1	C	433	ILE	2.9
2	H	343	GLN	2.9
2	F	152	ILE	2.9
1	C	357	TYR	2.9
1	E	441	LEU	2.9
1	E	324	ILE	2.8
1	G	361	SER	2.8
1	A	457	PHE	2.8
1	G	324	ILE	2.8
2	H	290	ILE	2.8
1	A	324	ILE	2.7
1	G	340	ALA	2.7
1	G	180	GLU	2.6
1	E	256	ILE	2.6
1	G	354	LEU	2.6
2	D	197	ASN	2.6
1	E	306	GLY	2.6
1	C	398	LEU	2.6
1	A	439	GLY	2.5
1	G	420	LEU	2.5
2	H	313	ARG	2.5
1	E	421	ILE	2.5
2	D	356	ASP	2.5
2	B	378	LEU	2.5
2	B	100	ARG	2.5
1	G	345	ALA	2.5
1	A	423	PHE	2.5
1	C	432	PHE	2.5
1	G	341	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	343	GLN	2.4
2	B	379	GLY	2.4
1	E	381	LEU	2.4
2	B	416	GLU	2.4
1	E	412	GLU	2.4
2	H	315	ALA	2.4
1	G	219	ASP	2.4
1	G	421	ILE	2.4
2	F	183	PHE	2.4
2	B	376	LEU	2.3
1	A	335	ILE	2.3
1	A	397	TYR	2.3
1	G	440	TYR	2.3
2	H	350	GLU	2.3
1	G	446	SER	2.3
1	A	301	ALA	2.3
1	E	380	ARG	2.3
2	B	380	PHE	2.3
1	A	493	TRP	2.2
1	G	405	GLY	2.2
1	C	440	TYR	2.2
1	E	440	TYR	2.2
2	H	364	LEU	2.2
1	E	405	GLY	2.2
2	H	217	ILE	2.2
2	D	315	ALA	2.2
2	H	353	ILE	2.2
1	A	464	LEU	2.1
1	E	393	GLY	2.1
2	H	228	LEU	2.1
1	E	422	GLY	2.1
2	F	220	TRP	2.1
1	E	130	TYR	2.1
2	D	348	TYR	2.1
2	D	5	PHE	2.1
1	C	457	PHE	2.1
1	C	337	TRP	2.1
1	G	382	LYS	2.0
2	D	349	LEU	2.0
1	E	408	LEU	2.0
2	H	319	GLU	2.0
1	A	398	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

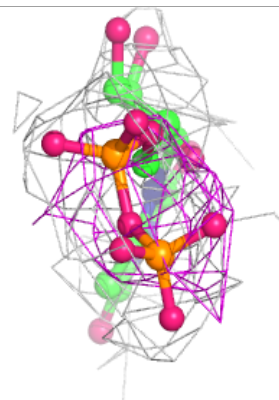
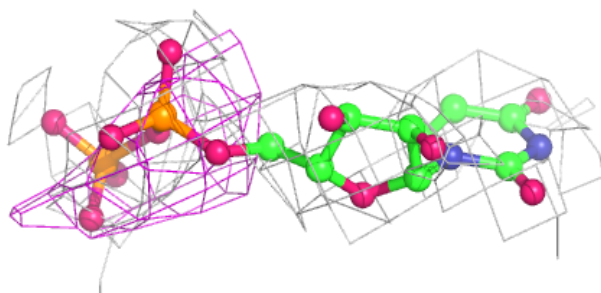
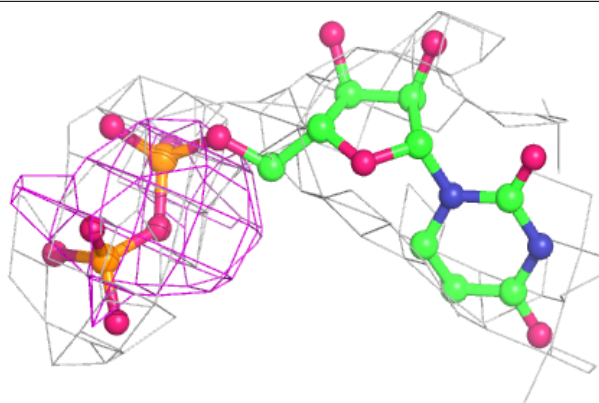
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	603	15/15	0.78	0.59	111,121,132,133	0
5	MG	B	501	1/1	0.79	0.35	40,40,40,40	0
3	UDP	E	602	25/25	0.80	0.38	122,136,143,147	0
5	MG	E	601	1/1	0.86	0.19	40,40,40,40	0
5	MG	G	601	1/1	0.87	0.39	31,31,31,31	0
4	NAG	A	602	15/15	0.89	0.37	108,118,127,127	0
3	UDP	A	601	25/25	0.90	0.36	120,131,139,141	0
5	MG	D	501	1/1	0.92	0.42	41,41,41,41	0

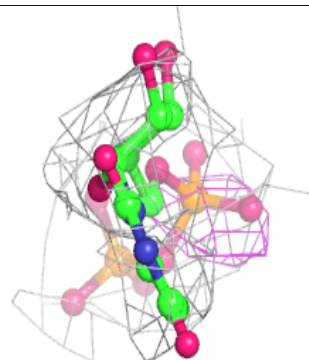
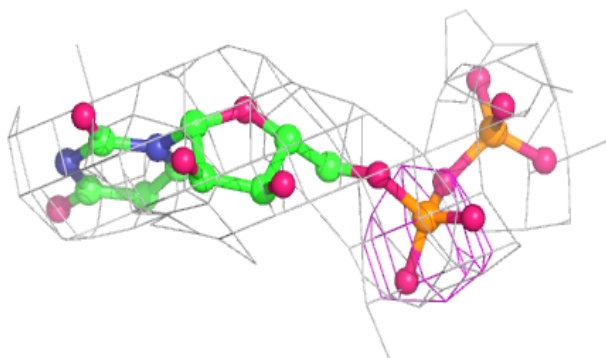
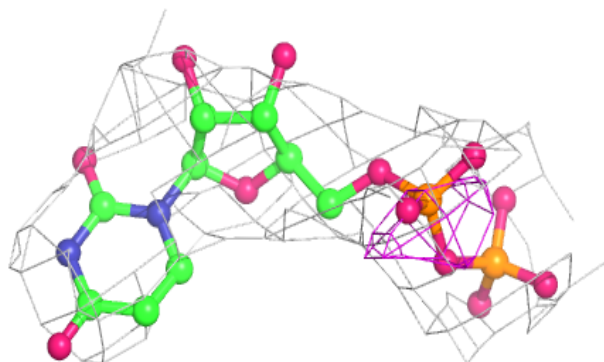
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP E 602:

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

**Electron density around UDP A 601:**

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



6.5 Other polymers

There are no such residues in this entry.