



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2020 – 01:08 PM EST

PDB ID : 6TS2
Title : Truncated version of Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) lacking domain TRXL2 (417-650).
Authors : Roversi, P.; Zitzmann, N.
Deposited on : 2019-12-19
Resolution : 5.74 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

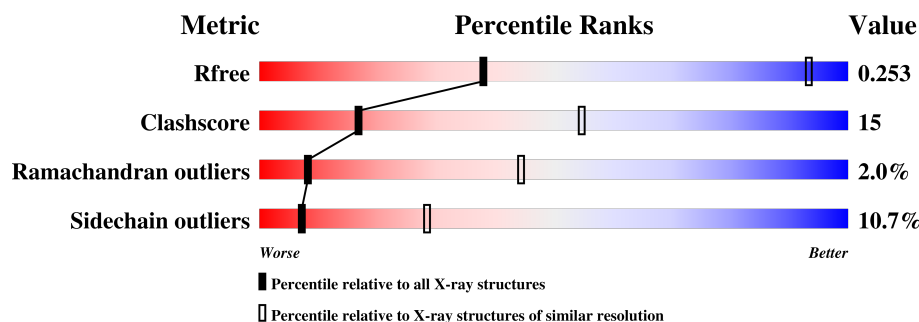
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.74 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}	111664	1035 (7.66-3.80)
Clashscore	122126	1112 (7.66-3.80)
Ramachandran outliers	120053	1039 (7.60-3.80)
Sidechain outliers	120020	1010 (7.60-3.80)

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. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1260	<div> <div>62%</div> <div>24%</div> <div>•</div> <div>12%</div> </div>
1	B	1260	<div> <div>52%</div> <div>31%</div> <div>5%</div> <div>11%</div> </div>
1	C	1260	<div> <div>58%</div> <div>26%</div> <div>•</div> <div>12%</div> </div>
1	D	1260	<div> <div>58%</div> <div>28%</div> <div>•</div> <div>11%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36079 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 UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1111	Total	C	N	O	S	0	0	0
			8882	5671	1509	1675	27			
1	B	1120	Total	C	N	O	S	0	0	0
			8955	5718	1522	1688	27			
1	C	1113	Total	C	N	O	S	0	0	0
			8898	5680	1512	1678	28			
1	D	1123	Total	C	N	O	S	0	0	0
			8983	5735	1529	1691	28			

There are 48 discrepancies between the modelled and reference sequences:

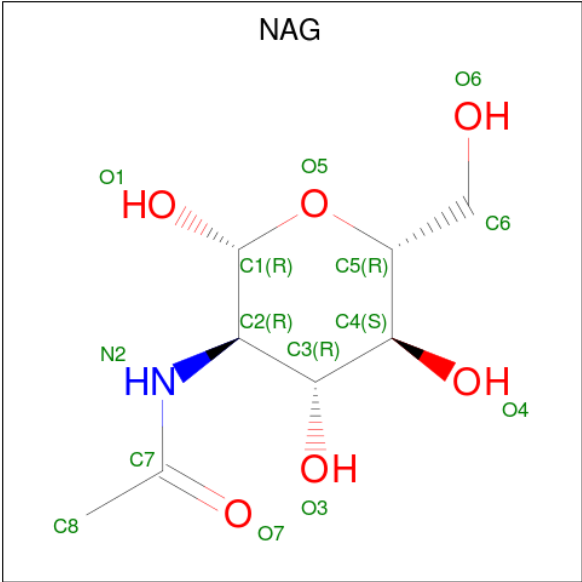
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58
B	21	GLU	-	expression tag	UNP G0SB58
B	22	THR	-	expression tag	UNP G0SB58
B	23	GLY	-	expression tag	UNP G0SB58
B	1506	GLY	-	expression tag	UNP G0SB58
B	1507	THR	-	expression tag	UNP G0SB58
B	1508	LYS	-	expression tag	UNP G0SB58
B	1509	HIS	-	expression tag	UNP G0SB58
B	1510	HIS	-	expression tag	UNP G0SB58

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1511	HIS	-	expression tag	UNP G0SB58
B	1512	HIS	-	expression tag	UNP G0SB58
B	1513	HIS	-	expression tag	UNP G0SB58
B	1514	HIS	-	expression tag	UNP G0SB58
C	21	GLU	-	expression tag	UNP G0SB58
C	22	THR	-	expression tag	UNP G0SB58
C	23	GLY	-	expression tag	UNP G0SB58
C	1506	GLY	-	expression tag	UNP G0SB58
C	1507	THR	-	expression tag	UNP G0SB58
C	1508	LYS	-	expression tag	UNP G0SB58
C	1509	HIS	-	expression tag	UNP G0SB58
C	1510	HIS	-	expression tag	UNP G0SB58
C	1511	HIS	-	expression tag	UNP G0SB58
C	1512	HIS	-	expression tag	UNP G0SB58
C	1513	HIS	-	expression tag	UNP G0SB58
C	1514	HIS	-	expression tag	UNP G0SB58
D	21	GLU	-	expression tag	UNP G0SB58
D	22	THR	-	expression tag	UNP G0SB58
D	23	GLY	-	expression tag	UNP G0SB58
D	1506	GLY	-	expression tag	UNP G0SB58
D	1507	THR	-	expression tag	UNP G0SB58
D	1508	LYS	-	expression tag	UNP G0SB58
D	1509	HIS	-	expression tag	UNP G0SB58
D	1510	HIS	-	expression tag	UNP G0SB58
D	1511	HIS	-	expression tag	UNP G0SB58
D	1512	HIS	-	expression tag	UNP G0SB58
D	1513	HIS	-	expression tag	UNP G0SB58
D	1514	HIS	-	expression tag	UNP G0SB58

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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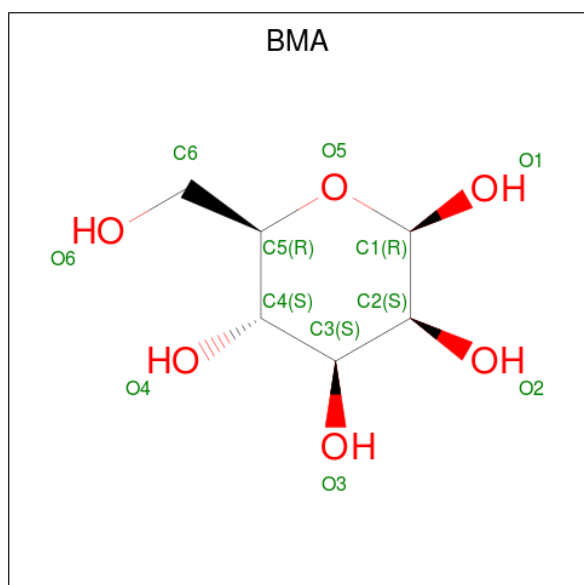
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

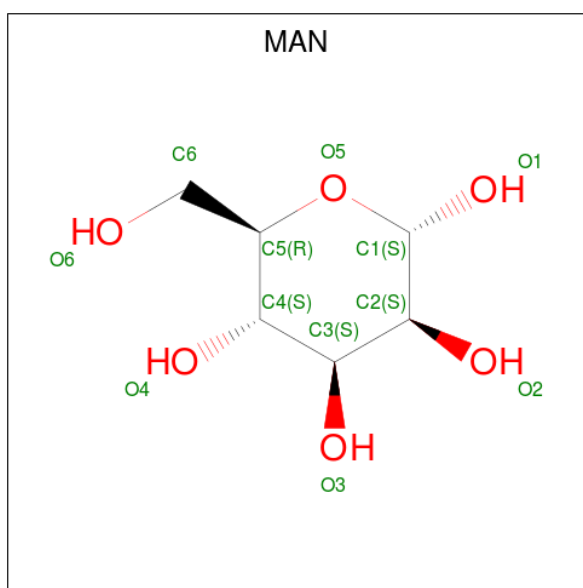
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

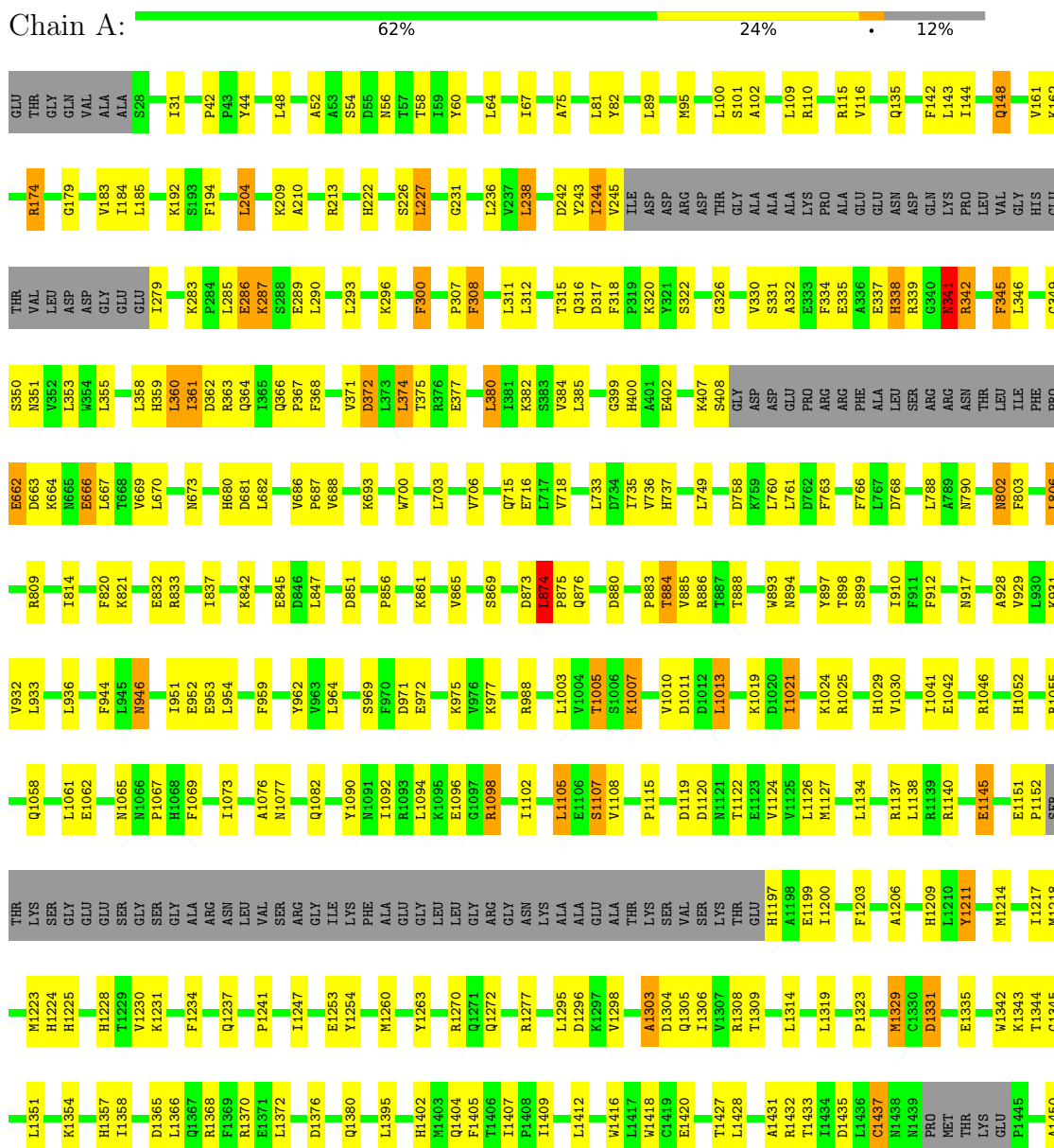


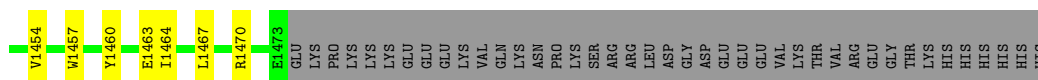
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

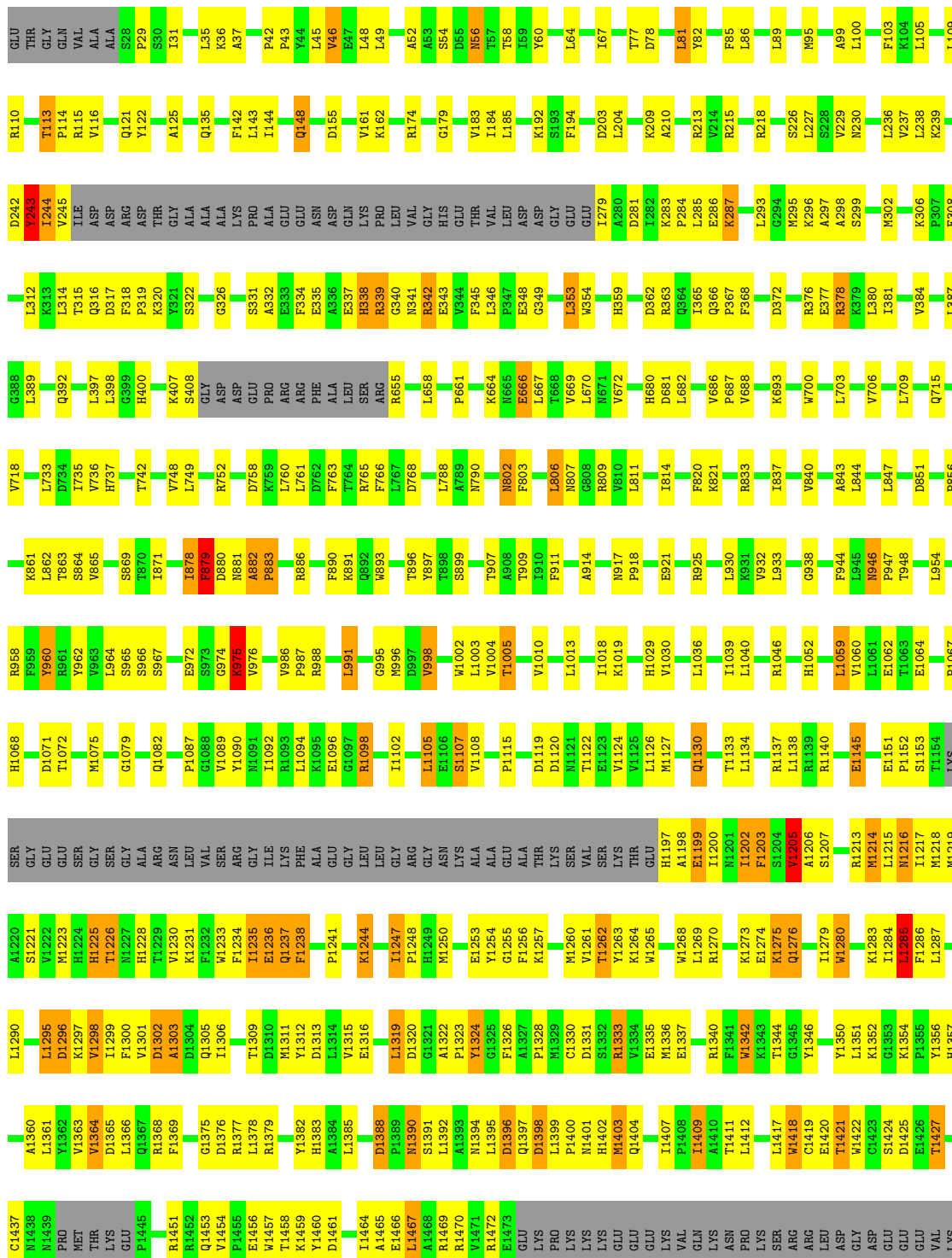
- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein





• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein, UDP-glucose-glycoprotein glucosyltransferase-like protein

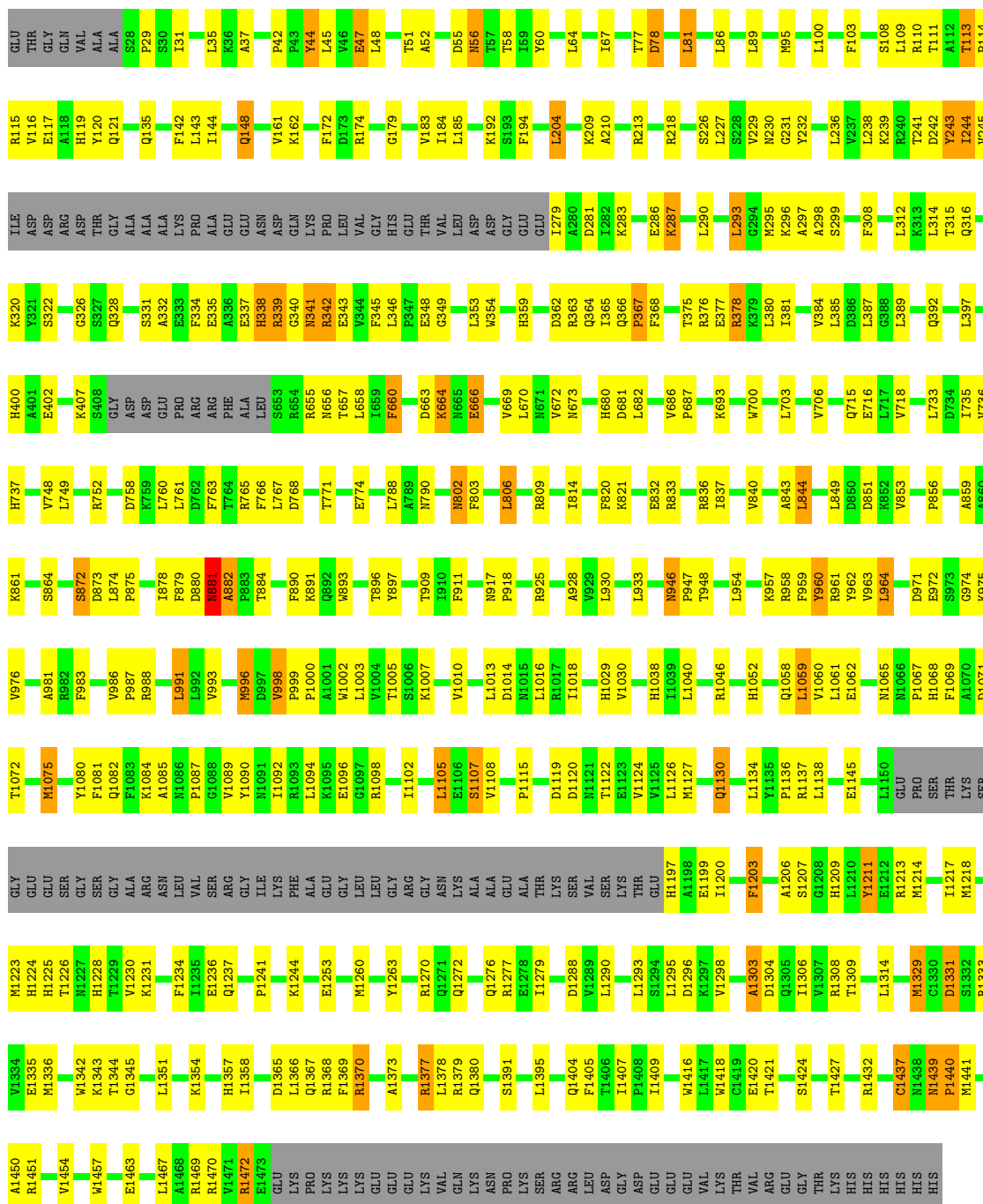
Chain B: 52% 31% 5% 11%





- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein,UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.15Å 191.01Å 158.81Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	140.60 – 5.74 140.61 – 5.73	Depositor EDS
% Data completeness (in resolution range)	74.9 (140.60-5.74) 63.9 (140.61-5.73)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 5.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.174 , 0.249 0.187 , 0.253	Depositor DCC
R_{free} test set	829 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	290.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 185.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	36079	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: CA, BMA, NAG, MAN

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	0.45	0/9087	0.66	1/12325 (0.0%)
1	B	0.46	0/9162	0.68	3/12428 (0.0%)
1	C	0.42	0/9104	0.64	2/12349 (0.0%)
1	D	0.43	0/9191	0.65	2/12467 (0.0%)
All	All	0.44	0/36544	0.66	8/49569 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	871	ILE	C-N-CA	5.99	136.68	121.70
1	D	875	PRO	C-N-CA	5.67	135.87	121.70
1	D	243	TYR	C-N-CA	5.33	135.04	121.70
1	B	1274	GLU	C-N-CA	5.23	134.77	121.70
1	A	341	ASN	CA-CB-CG	5.15	124.72	113.40
1	C	243	TYR	C-N-CA	5.06	134.35	121.70
1	B	243	TYR	C-N-CA	5.04	134.30	121.70
1	C	1020	ASP	C-N-CA	5.04	134.30	121.70

There are no chirality outliers.

There are no planarity outliers.

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	8882	0	8770	226	0
1	B	8955	0	8846	326	0
1	C	8898	0	8788	270	0
1	D	8983	0	8881	287	0
2	A	70	0	63	4	0
2	B	70	0	63	0	0
2	C	70	0	63	0	0
2	D	70	0	63	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	8	0	0
4	B	11	0	10	0	0
4	C	11	0	9	0	0
4	D	11	0	10	0	0
5	A	22	0	20	0	0
5	C	11	0	10	0	0
All	All	36079	0	35604	1080	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 (1080) 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:D:78:ASP:HB2	1:D:975:LYS:HA	1.23	1.16
1:B:1376:ASP:HA	1:B:1379:ARG:HD3	1.26	1.15
1:B:1333:ARG:HG3	1:B:1424:SER:HA	1.17	1.13
1:D:1241:PRO:HA	1:D:1244:LYS:HB2	1.32	1.12
1:B:869:SER:HB2	1:B:886:ARG:HE	1.07	1.10
1:D:364:GLN:HG2	1:D:880:ASP:HB2	1.32	1.10
1:B:921:GLU:HB3	1:B:958:ARG:HE	1.03	1.09
1:B:1107:SER:HB2	1:B:1120:ASP:HA	1.35	1.08
1:D:42:PRO:HB3	1:D:116:VAL:HG11	1.31	1.07
1:D:1107:SER:HB2	1:D:1120:ASP:HA	1.38	1.04
1:A:673:ASN:HA	1:A:861:LYS:HE2	1.39	1.04
1:C:1107:SER:HB2	1:C:1120:ASP:HA	1.36	1.03
1:A:243:TYR:HB3	1:A:285:LEU:HG	1.41	1.03
1:A:1107:SER:HB2	1:A:1120:ASP:HA	1.39	1.01
1:A:1270:ARG:HH12	1:C:821:LYS:NZ	1.57	1.00
1:A:296:LYS:HD2	1:A:326:GLY:HA2	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:LEU:H	1:A:875:PRO:HA	1.27	1.00
1:A:1105:LEU:HA	1:A:1138:LEU:HG	1.44	0.99
1:D:1367:GLN:HE22	1:D:1370:ARG:HH11	1.05	0.99
1:B:1202:ILE:HG12	1:B:1299:ILE:HB	1.44	0.98
1:B:1105:LEU:HA	1:B:1138:LEU:HG	1.43	0.98
1:B:1404:GLN:HG3	1:B:1409:ILE:HB	1.46	0.97
1:D:1105:LEU:HA	1:D:1138:LEU:HG	1.47	0.97
1:D:1439:ASN:HB3	1:D:1440:PRO:HA	1.47	0.97
1:B:1197:HIS:N	1:B:1257:LYS:HZ3	1.63	0.96
1:C:1439:ASN:HB3	1:C:1440:PRO:HA	1.47	0.96
1:C:1105:LEU:HA	1:C:1138:LEU:HG	1.46	0.96
1:D:387:LEU:HD21	1:D:861:LYS:HB2	1.46	0.96
1:D:115:ARG:NH2	1:D:174:ARG:HH21	1.62	0.95
1:B:1466:GLU:HA	1:B:1469:ARG:HD2	1.46	0.94
1:A:1270:ARG:HH12	1:C:821:LYS:HZ1	1.05	0.94
1:B:869:SER:HB2	1:B:886:ARG:NE	1.83	0.93
1:B:1357:HIS:NE2	1:B:1411:THR:HG22	1.82	0.93
1:C:878:ILE:HG23	1:C:1044:HIS:HE1	1.32	0.93
1:B:1270:ARG:HH12	1:D:821:LYS:NZ	1.66	0.92
1:B:921:GLU:HB3	1:B:958:ARG:NE	1.84	0.91
1:C:878:ILE:HG23	1:C:1044:HIS:CE1	2.07	0.90
1:D:1416:TRP:HA	1:D:1432:ARG:HB2	1.53	0.90
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.53	0.89
1:B:1340:ARG:HE	1:B:1422:TRP:HD1	1.19	0.89
1:B:802:ASN:HB2	1:B:814:ILE:HB	1.52	0.89
1:B:78:ASP:HB2	1:B:975:LYS:HA	1.54	0.89
1:D:1367:GLN:NE2	1:D:1370:ARG:HH11	1.69	0.89
1:D:672:VAL:HB	1:D:861:LYS:HA	1.52	0.89
1:B:1302:ASP:O	1:B:1302:ASP:OD1	1.90	0.88
1:A:1098:ARG:HE	1:A:1152:PRO:HD3	1.40	0.87
1:D:77:THR:HB	1:D:974:GLY:HA3	1.55	0.87
1:C:802:ASN:HB2	1:C:814:ILE:HB	1.55	0.87
1:D:802:ASN:HB2	1:D:814:ILE:HB	1.54	0.86
1:C:858:SER:HA	1:C:861:LYS:HE2	1.58	0.86
1:C:1416:TRP:HA	1:C:1432:ARG:HB2	1.57	0.85
1:D:673:ASN:HA	1:D:861:LYS:HD2	1.57	0.85
1:B:880:ASP:HB3	1:B:881:ASN:HA	1.57	0.84
1:C:79:LYS:NZ	1:C:972:GLU:HA	1.92	0.84
1:A:1416:TRP:HA	1:A:1432:ARG:HB2	1.57	0.84
1:B:349:GLY:HA3	1:B:948:THR:HB	1.60	0.84
1:B:879:PHE:HB2	1:B:880:ASP:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:OD1	1:C:1142:PRO:HG3	1.78	0.83
1:C:79:LYS:HE3	1:C:970:PHE:HB3	1.60	0.83
1:B:1270:ARG:HH12	1:D:821:LYS:HZ3	1.22	0.82
1:C:105:LEU:HG	1:C:966:SER:HA	1.61	0.82
1:A:1062:GLU:HB2	1:A:1067:PRO:HA	1.61	0.82
1:B:1062:GLU:HB2	1:B:1067:PRO:HA	1.62	0.82
1:D:117:GLU:HA	1:D:120:TYR:HB2	1.60	0.82
2:A:1605:NAG:H61	2:A:1606:NAG:N2	1.95	0.82
1:B:1270:ARG:NH1	1:D:821:LYS:NZ	2.27	0.82
1:B:296:LYS:HD3	1:B:326:GLY:HA2	1.62	0.81
1:C:349:GLY:HA3	1:C:948:THR:HB	1.62	0.81
1:B:1276:GLN:HA	1:B:1279:ILE:HB	1.60	0.81
1:B:1469:ARG:HA	1:B:1472:ARG:HD2	1.63	0.81
1:B:77:THR:HB	1:B:974:GLY:HA3	1.62	0.80
1:C:296:LYS:HD3	1:C:326:GLY:HA2	1.64	0.80
1:D:339:ARG:HH12	1:D:946:ASN:HB2	1.46	0.80
1:A:345:PHE:HB3	1:A:893:TRP:HE1	1.46	0.80
1:D:1062:GLU:HB2	1:D:1067:PRO:HA	1.62	0.80
1:B:338:HIS:CD2	1:B:341:ASN:HD21	2.00	0.80
1:D:349:GLY:HA3	1:D:948:THR:HB	1.63	0.80
1:C:77:THR:HB	1:C:974:GLY:HA3	1.64	0.79
1:B:245:VAL:HB	1:B:287:LYS:HA	1.63	0.79
1:C:1062:GLU:HB2	1:C:1067:PRO:HA	1.63	0.79
1:C:245:VAL:HB	1:C:287:LYS:HA	1.65	0.79
1:C:338:HIS:CD2	1:C:341:ASN:HD21	2.00	0.79
1:B:1382:TYR:HA	1:B:1385:LEU:HG	1.64	0.79
1:A:296:LYS:HE2	1:A:331:SER:HA	1.64	0.78
1:B:239:LYS:HZ1	1:B:1275:LYS:HZ1	1.30	0.78
1:C:693:LYS:H	1:C:693:LYS:NZ	1.80	0.78
1:B:1333:ARG:HG3	1:B:1424:SER:CA	2.07	0.78
1:C:692:SER:HA	1:C:693:LYS:NZ	1.97	0.78
1:D:338:HIS:CD2	1:D:341:ASN:HD21	2.01	0.78
1:C:339:ARG:HH12	1:C:946:ASN:HB2	1.49	0.78
1:A:1418:TRP:NE1	1:A:1427:THR:HB	1.99	0.78
1:A:821:LYS:HZ1	1:C:1270:ARG:HH12	1.30	0.78
1:B:339:ARG:HH12	1:B:946:ASN:HB2	1.48	0.77
1:D:1418:TRP:NE1	1:D:1427:THR:HB	1.98	0.77
1:A:821:LYS:NZ	1:C:1270:ARG:HH12	1.82	0.77
1:C:1418:TRP:NE1	1:C:1427:THR:HB	1.99	0.77
1:D:296:LYS:HD3	1:D:326:GLY:HA2	1.67	0.77
1:D:1418:TRP:HE1	1:D:1427:THR:HB	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:HA3	1:A:210:ALA:HA	1.68	0.76
1:B:1323:PRO:HB3	1:B:1369:PHE:HA	1.68	0.76
1:B:1197:HIS:N	1:B:1257:LYS:NZ	2.34	0.76
1:C:79:LYS:HZ2	1:C:972:GLU:HA	1.51	0.76
1:A:1270:ARG:NH1	1:C:821:LYS:HZ1	1.81	0.76
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.51	0.76
1:A:842:LYS:HA	1:A:845:GLU:HG2	1.68	0.76
1:D:245:VAL:HB	1:D:287:LYS:HA	1.68	0.75
1:B:1451:ARG:HE	1:B:1457:TRP:HH2	1.32	0.75
1:C:1253:GLU:HG3	1:C:1467:LEU:HD11	1.68	0.75
1:C:179:GLY:HA3	1:C:210:ALA:HA	1.69	0.75
1:B:49:LEU:HD21	1:B:64:LEU:HD13	1.67	0.74
1:A:296:LYS:CD	1:A:326:GLY:HA2	2.18	0.74
1:C:338:HIS:CE1	1:C:896:THR:HB	2.23	0.74
1:D:1418:TRP:CD1	1:D:1427:THR:HB	2.21	0.74
1:A:1214:MET:HE2	1:A:1457:TRP:HE1	1.51	0.74
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.52	0.74
1:D:1331:ASP:HB3	1:D:1343:LYS:HZ1	1.51	0.74
1:B:1402:HIS:NE2	1:D:767:LEU:HD13	2.02	0.73
1:B:179:GLY:HA3	1:B:210:ALA:HA	1.68	0.73
1:D:179:GLY:HA3	1:D:210:ALA:HA	1.69	0.73
1:D:78:ASP:CB	1:D:975:LYS:HA	2.12	0.73
1:D:1367:GLN:HE22	1:D:1370:ARG:NH1	1.86	0.73
1:C:1418:TRP:HE1	1:C:1427:THR:HB	1.51	0.73
1:D:338:HIS:CE1	1:D:896:THR:HB	2.24	0.73
1:B:1467:LEU:HD13	1:B:1470:ARG:HE	1.54	0.73
1:C:1306:ILE:HD11	1:C:1457:TRP:HD1	1.53	0.73
1:C:380:LEU:HD11	1:C:869:SER:HA	1.70	0.73
1:D:1214:MET:HE2	1:D:1457:TRP:HE1	1.53	0.73
1:A:1253:GLU:HG3	1:A:1467:LEU:HD11	1.71	0.72
1:B:1202:ILE:CG1	1:B:1299:ILE:HB	2.19	0.72
1:A:1418:TRP:CD1	1:A:1427:THR:HB	2.24	0.72
1:B:239:LYS:HZ1	1:B:1275:LYS:NZ	1.86	0.72
1:C:1418:TRP:CD1	1:C:1427:THR:HB	2.24	0.72
1:A:969:SER:HB2	1:A:977:LYS:HB3	1.70	0.72
1:B:1460:TYR:O	1:B:1464:ILE:HG12	1.88	0.72
1:B:338:HIS:CE1	1:B:896:THR:HB	2.25	0.72
1:A:399:GLY:O	1:A:888:THR:HB	1.90	0.72
1:C:1331:ASP:HB3	1:C:1343:LYS:HZ1	1.53	0.72
1:C:135:GLN:HE22	1:C:148:GLN:NE2	1.88	0.71
1:D:335:GLU:HA	1:D:338:HIS:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:873:ASP:HB3	1:D:874:LEU:HA	1.73	0.71
1:D:95:MET:HB3	1:D:100:LEU:HG	1.72	0.71
1:D:296:LYS:NZ	1:D:326:GLY:HA2	2.05	0.71
1:A:1354:LYS:HZ3	1:A:1405:PHE:HD1	1.38	0.71
1:D:1253:GLU:HG3	1:D:1467:LEU:HD11	1.72	0.71
1:B:239:LYS:NZ	1:B:1275:LYS:NZ	2.38	0.71
1:B:335:GLU:HA	1:B:338:HIS:HB2	1.71	0.71
1:D:1306:ILE:HD11	1:D:1457:TRP:HD1	1.55	0.71
1:B:52:ALA:HB1	1:B:89:LEU:HD21	1.73	0.71
1:C:335:GLU:HA	1:C:338:HIS:HB2	1.72	0.71
1:D:961:ARG:NE	1:D:983:PHE:HA	2.05	0.70
1:C:1306:ILE:HG21	1:C:1454:VAL:HG11	1.71	0.70
1:D:115:ARG:HG2	1:D:1127:MET:HB2	1.73	0.70
1:B:1284:ILE:O	1:B:1285:LEU:HB2	1.91	0.70
1:A:236:LEU:HB2	1:A:959:PHE:HB2	1.74	0.70
1:D:44:TYR:HE2	1:D:110:ARG:NH2	1.88	0.70
1:C:1214:MET:HE2	1:C:1457:TRP:HE1	1.56	0.70
1:C:358:LEU:HD22	1:C:884:THR:HG22	1.73	0.69
1:C:296:LYS:HE2	1:C:331:SER:HA	1.74	0.69
1:D:872:SER:HA	1:D:878:ILE:HB	1.73	0.69
1:D:342:ARG:HG2	1:D:346:LEU:O	1.93	0.69
1:D:135:GLN:HE22	1:D:148:GLN:NE2	1.91	0.69
1:B:1299:ILE:HD11	1:B:1315:VAL:HG22	1.73	0.69
1:C:35:LEU:HD23	1:C:229:VAL:HG23	1.74	0.69
1:D:1197:HIS:HE1	1:D:1231:LYS:NZ	1.91	0.69
1:B:135:GLN:HE22	1:B:148:GLN:NE2	1.89	0.69
1:A:135:GLN:HE22	1:A:148:GLN:NE2	1.91	0.69
1:A:374:LEU:HG	1:A:375:THR:N	2.08	0.69
1:A:1306:ILE:HG21	1:A:1454:VAL:HG11	1.75	0.69
1:B:342:ARG:HG2	1:B:346:LEU:O	1.93	0.69
1:C:387:LEU:HD21	1:C:861:LYS:HB2	1.75	0.69
1:B:1298:VAL:HG12	1:B:1364:VAL:HG13	1.73	0.68
1:C:1060:VAL:HG22	1:C:1071:ASP:HB3	1.75	0.68
1:B:1385:LEU:HD22	1:B:1392:LEU:HD12	1.75	0.68
1:C:342:ARG:HG2	1:C:346:LEU:O	1.93	0.68
1:D:1060:VAL:HG22	1:D:1071:ASP:HB3	1.75	0.68
1:A:874:LEU:N	1:A:875:PRO:HA	2.07	0.68
1:B:296:LYS:HE2	1:B:331:SER:HA	1.74	0.68
1:A:1331:ASP:HB3	1:A:1343:LYS:HZ1	1.59	0.68
1:D:1306:ILE:HG21	1:D:1454:VAL:HG11	1.74	0.68
1:B:239:LYS:NZ	1:B:1275:LYS:HZ1	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:HH22	1:D:174:ARG:HH21	1.41	0.67
1:A:243:TYR:O	1:A:244:ILE:HG13	1.94	0.67
1:D:296:LYS:HE2	1:D:331:SER:HA	1.77	0.67
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.77	0.67
1:B:998:VAL:HG13	1:B:1002:TRP:HB2	1.76	0.67
1:B:1265:TRP:CE2	1:B:1269:LEU:HD23	2.29	0.67
1:C:1197:HIS:HE1	1:C:1231:LYS:NZ	1.93	0.67
1:D:844:LEU:HD12	1:D:849:LEU:HB2	1.77	0.67
1:B:1060:VAL:HG22	1:B:1071:ASP:HB3	1.75	0.67
1:B:1270:ARG:NH1	1:D:821:LYS:HZ1	1.91	0.67
1:D:364:GLN:CG	1:D:880:ASP:HB2	2.17	0.67
1:C:296:LYS:NZ	1:C:326:GLY:HA2	2.08	0.67
1:D:1197:HIS:HE1	1:D:1231:LYS:HZ2	1.41	0.67
1:C:1439:ASN:HB3	1:C:1440:PRO:CA	2.25	0.66
1:B:1203:PHE:HB2	1:B:1233:TRP:O	1.96	0.66
1:B:1324:TYR:HB3	1:B:1364:VAL:HB	1.78	0.66
1:D:334:PHE:O	1:D:337:GLU:HG2	1.95	0.66
1:B:1376:ASP:HA	1:B:1379:ARG:CD	2.17	0.66
1:D:1236:GLU:HG2	1:D:1244:LYS:HZ1	1.60	0.66
1:A:75:ALA:HB1	1:A:81:LEU:HB2	1.78	0.66
1:B:1467:LEU:HD13	1:B:1470:ARG:NE	2.11	0.65
1:B:1383:HIS:HD2	1:D:716:GLU:OE1	1.79	0.65
1:A:345:PHE:CB	1:A:893:TRP:HE1	2.08	0.65
1:A:1270:ARG:NH1	1:C:821:LYS:NZ	2.39	0.65
1:D:238:LEU:HD13	1:D:283:LYS:HD3	1.79	0.65
1:B:1270:ARG:CZ	1:D:821:LYS:HZ1	2.09	0.65
1:B:238:LEU:HD13	1:B:283:LYS:HD3	1.78	0.65
1:B:334:PHE:O	1:B:337:GLU:HG2	1.97	0.65
1:D:999:PRO:HB2	1:D:1002:TRP:CD1	2.32	0.65
1:A:1197:HIS:HE1	1:A:1231:LYS:NZ	1.95	0.65
1:C:998:VAL:HG13	1:C:1002:TRP:HB2	1.79	0.65
1:C:52:ALA:HB1	1:C:89:LEU:HD21	1.78	0.65
1:C:319:PRO:HA	1:C:322:SER:HB2	1.79	0.65
1:B:296:LYS:NZ	1:B:326:GLY:HA2	2.12	0.65
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.79	0.64
1:B:1218:MET:HG3	1:B:1301:VAL:HG11	1.79	0.64
1:B:672:VAL:HB	1:B:861:LYS:HA	1.78	0.64
1:A:382:LYS:HA	1:A:385:LEU:HG	1.79	0.64
1:A:399:GLY:HA2	1:A:886:ARG:HB3	1.79	0.64
1:D:241:THR:HG21	1:D:957:LYS:HE2	1.79	0.64
1:A:300:PHE:CD2	1:A:330:VAL:HG21	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:SER:CB	1:B:1120:ASP:HA	2.22	0.64
2:A:1605:NAG:H61	2:A:1606:NAG:HN2	1.60	0.64
1:D:397:LEU:HD11	1:D:840:VAL:HG13	1.80	0.64
1:C:317:ASP:HB3	1:C:320:LYS:HB3	1.78	0.64
1:C:334:PHE:O	1:C:337:GLU:HG2	1.98	0.64
1:B:1241:PRO:HA	1:B:1244:LYS:HB2	1.79	0.63
1:B:821:LYS:NZ	1:D:1270:ARG:HH12	1.97	0.63
1:B:35:LEU:HD23	1:B:229:VAL:HG23	1.80	0.63
1:C:1329:MET:HG2	1:C:1358:ILE:HD11	1.81	0.63
1:A:1450:ALA:HB1	1:A:1457:TRP:CD2	2.34	0.63
1:D:1207:SER:CB	1:D:1279:ILE:HD11	2.29	0.63
1:A:238:LEU:HD13	1:A:283:LYS:HD3	1.81	0.63
1:B:1333:ARG:CG	1:B:1424:SER:HA	2.11	0.63
1:C:1354:LYS:HD2	1:C:1404:GLN:HG3	1.79	0.63
1:B:1465:ALA:HB1	1:B:1469:ARG:HH21	1.64	0.63
1:D:387:LEU:HD21	1:D:861:LYS:CB	2.25	0.63
1:C:296:LYS:HZ3	1:C:326:GLY:HA2	1.63	0.62
1:D:1272:GLN:HB3	1:D:1277:ARG:HB2	1.80	0.62
1:D:1354:LYS:HD2	1:D:1404:GLN:HG3	1.81	0.62
1:A:346:LEU:HG	1:A:893:TRP:HZ2	1.64	0.62
1:C:1197:HIS:HE1	1:C:1231:LYS:HZ2	1.47	0.62
1:C:238:LEU:HD13	1:C:283:LYS:HD3	1.81	0.62
1:C:833:ARG:HA	1:C:837:ILE:HB	1.81	0.62
1:C:316:GLN:HB2	1:C:961:ARG:CD	2.29	0.62
1:D:1439:ASN:HB3	1:D:1440:PRO:CA	2.25	0.62
1:A:1197:HIS:HE1	1:A:1231:LYS:HZ2	1.48	0.62
1:B:400:HIS:CD2	1:B:843:ALA:HB2	2.33	0.62
1:B:1454:VAL:CG1	1:B:1456:GLU:HG2	2.30	0.62
1:B:95:MET:HB3	1:B:100:LEU:HG	1.82	0.62
1:B:833:ARG:HA	1:B:837:ILE:HB	1.82	0.62
1:D:1329:MET:HG2	1:D:1358:ILE:HD11	1.81	0.62
1:D:963:VAL:HG22	1:D:981:ALA:HB2	1.80	0.62
1:A:339:ARG:HD3	1:A:342:ARG:HB2	1.82	0.62
1:C:1234:PHE:HD1	1:C:1260:MET:SD	2.22	0.62
1:C:400:HIS:CD2	1:C:843:ALA:HB2	2.35	0.62
1:D:1107:SER:CB	1:D:1120:ASP:HA	2.24	0.62
1:B:1237:GLN:NE2	1:B:1262:THR:OG1	2.33	0.61
1:C:1272:GLN:HB3	1:C:1277:ARG:HB2	1.82	0.61
1:B:1351:LEU:HA	1:B:1354:LYS:NZ	2.15	0.61
1:A:1351:LEU:HA	1:A:1354:LYS:HE3	1.82	0.61
1:D:1450:ALA:HB1	1:D:1457:TRP:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ILE:HD11	1:D:1018:ILE:HD11	1.80	0.61
1:D:833:ARG:HA	1:D:837:ILE:HB	1.83	0.61
1:A:1041:ILE:HG12	1:A:1126:LEU:HD23	1.83	0.61
1:C:1450:ALA:HB1	1:C:1457:TRP:CD2	2.35	0.61
1:D:400:HIS:CD2	1:D:843:ALA:HB2	2.35	0.61
1:C:1351:LEU:HA	1:C:1354:LYS:HE3	1.83	0.61
1:A:1357:HIS:CE1	1:A:1409:ILE:HG21	2.36	0.61
1:B:1419:CYS:SG	1:B:1422:TRP:HE3	2.24	0.61
1:D:1234:PHE:HD1	1:D:1260:MET:SD	2.23	0.61
1:D:239:LYS:HD2	1:D:991:LEU:HD22	1.82	0.61
1:D:231:GLY:HA2	1:D:367:PRO:HG3	1.82	0.61
1:B:1059:LEU:HG	1:B:1094:LEU:HA	1.83	0.61
1:A:345:PHE:CD2	1:A:893:TRP:NE1	2.69	0.60
1:B:1247:ILE:HD12	1:B:1248:PRO:HD3	1.82	0.60
1:B:397:LEU:HD11	1:B:840:VAL:HG13	1.83	0.60
1:C:706:VAL:HB	1:C:803:PHE:HB2	1.83	0.60
1:A:1329:MET:HG2	1:A:1358:ILE:HD11	1.82	0.60
1:B:1068:HIS:NE2	1:B:1071:ASP:OD2	2.34	0.60
1:B:1337:GLU:HA	1:B:1340:ARG:HG3	1.84	0.60
1:B:1340:ARG:NE	1:B:1422:TRP:HD1	1.96	0.60
1:D:706:VAL:HB	1:D:803:PHE:HB2	1.82	0.60
1:C:1354:LYS:HZ3	1:C:1405:PHE:HD1	1.49	0.60
1:D:1351:LEU:HA	1:D:1354:LYS:HE3	1.83	0.60
1:A:1214:MET:HA	1:A:1217:ILE:HD12	1.84	0.60
1:A:353:LEU:HD23	1:A:360:LEU:HD22	1.83	0.60
1:A:833:ARG:HA	1:A:837:ILE:HB	1.83	0.60
1:D:1354:LYS:HZ3	1:D:1405:PHE:HD1	1.50	0.60
1:B:1328:PRO:HA	1:B:1357:HIS:HA	1.82	0.60
1:C:1059:LEU:HG	1:C:1094:LEU:HA	1.83	0.60
1:D:279:ILE:HD13	1:D:320:LYS:HE3	1.83	0.60
1:D:1059:LEU:HG	1:D:1094:LEU:HA	1.82	0.60
1:D:290:LEU:HD23	1:D:293:LEU:HD13	1.82	0.60
1:D:35:LEU:HD23	1:D:229:VAL:HG23	1.84	0.60
1:D:718:VAL:HG13	1:D:735:ILE:HD13	1.82	0.60
1:B:1214:MET:HA	1:B:1217:ILE:HD12	1.83	0.60
1:D:1357:HIS:CE1	1:D:1409:ILE:HG21	2.37	0.60
1:B:1090:TYR:HB2	1:B:1124:VAL:HG23	1.84	0.59
1:B:1402:HIS:NE2	1:D:767:LEU:CD1	2.65	0.59
1:C:387:LEU:HD21	1:C:861:LYS:CB	2.30	0.59
1:B:239:LYS:HD2	1:B:991:LEU:HD22	1.84	0.59
1:C:49:LEU:HD21	1:C:64:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:ASN:ND2	1:C:818:ASP:OD2	2.35	0.59
1:C:1044:HIS:O	1:C:1136:PRO:HD2	2.02	0.59
1:C:858:SER:HA	1:C:861:LYS:CE	2.30	0.59
1:A:1234:PHE:HD1	1:A:1260:MET:SD	2.25	0.59
1:B:122:TYR:HE2	1:B:215:ARG:NH1	2.00	0.59
1:C:971:ASP:HB3	1:C:975:LYS:O	2.03	0.59
1:D:1061:LEU:O	1:D:1069:PHE:HB3	2.02	0.59
1:A:296:LYS:CE	1:A:331:SER:HA	2.33	0.59
1:B:1270:ARG:HH22	1:D:821:LYS:NZ	2.00	0.59
1:A:308:PHE:CE2	1:A:931:LYS:HA	2.38	0.59
1:C:1306:ILE:HD11	1:C:1457:TRP:CD1	2.36	0.59
1:C:1357:HIS:CE1	1:C:1409:ILE:HG21	2.37	0.59
1:B:1351:LEU:HA	1:B:1354:LYS:HZ1	1.66	0.59
1:B:706:VAL:HB	1:B:803:PHE:HB2	1.83	0.59
1:C:105:LEU:HD11	1:C:936:LEU:HD21	1.83	0.59
1:D:316:GLN:HB3	1:D:960:TYR:O	2.01	0.59
1:B:1216:ASN:HA	1:B:1219:MET:SD	2.43	0.59
1:B:1342:TRP:HB3	1:B:1356:TYR:CD1	2.38	0.59
1:A:407:LYS:HD3	1:A:885:VAL:HG22	1.85	0.58
1:B:1388:ASP:OD2	1:B:1390:ASN:ND2	2.36	0.58
1:B:99:ALA:HA	1:B:378:ARG:HD3	1.84	0.58
1:B:1268:TRP:CH2	1:B:1379:ARG:NH2	2.71	0.58
1:D:1306:ILE:HD11	1:D:1457:TRP:CD1	2.37	0.58
1:A:243:TYR:HB3	1:A:285:LEU:CG	2.25	0.58
1:B:1351:LEU:HB3	1:B:1354:LYS:HB2	1.84	0.58
1:B:340:GLY:HA2	1:B:343:GLU:HB2	1.84	0.58
1:C:397:LEU:HD11	1:C:840:VAL:HG13	1.84	0.58
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	2.19	0.58
1:C:1068:HIS:NE2	1:C:1071:ASP:OD2	2.36	0.58
1:C:1107:SER:CB	1:C:1120:ASP:HA	2.23	0.58
1:C:840:VAL:HG12	1:C:844:LEU:HD22	1.85	0.58
1:C:1214:MET:HA	1:C:1217:ILE:HD12	1.85	0.58
1:D:1214:MET:HA	1:D:1217:ILE:HD12	1.85	0.58
1:D:1225:HIS:ND1	1:D:1308:ARG:HA	2.18	0.58
1:D:998:VAL:HG13	1:D:1002:TRP:HB2	1.85	0.58
1:B:31:ILE:HD11	1:B:1018:ILE:HD11	1.85	0.58
1:C:64:LEU:HD12	1:C:67:ILE:HD11	1.85	0.58
1:C:693:LYS:H	1:C:693:LYS:HZ2	1.50	0.58
1:D:42:PRO:CB	1:D:116:VAL:HG11	2.20	0.58
1:A:1380:GLN:HG3	1:C:712:ILE:HG21	1.85	0.58
1:D:340:GLY:HA2	1:D:343:GLU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.36	0.58
1:A:706:VAL:HB	1:A:803:PHE:HB2	1.84	0.58
1:C:239:LYS:HD2	1:C:991:LEU:HD22	1.86	0.58
1:C:963:VAL:HG22	1:C:981:ALA:HB2	1.85	0.58
1:A:231:GLY:HA2	1:A:367:PRO:HG2	1.86	0.58
1:D:1331:ASP:HB3	1:D:1343:LYS:NZ	2.19	0.58
1:D:853:VAL:HG12	1:D:859:ALA:HA	1.86	0.57
1:B:1205:VAL:HB	1:B:1235:ILE:HG12	1.86	0.57
1:A:1272:GLN:HB3	1:A:1277:ARG:HB2	1.84	0.57
1:B:353:LEU:HG	1:B:914:ALA:HA	1.85	0.57
1:D:1068:HIS:NE2	1:D:1071:ASP:OD2	2.37	0.57
1:C:692:SER:HA	1:C:693:LYS:HZ2	1.68	0.57
1:D:110:ARG:NH1	1:D:976:VAL:HG21	2.20	0.57
1:B:1198:ALA:HB3	1:B:1231:LYS:HB2	1.86	0.57
1:C:1214:MET:CE	1:C:1457:TRP:HE1	2.18	0.57
1:C:122:TYR:OH	1:C:215:ARG:NH1	2.38	0.57
1:B:1075:MET:HB3	1:B:1379:ARG:NH2	2.20	0.57
1:C:1331:ASP:HB3	1:C:1343:LYS:NZ	2.19	0.57
1:C:238:LEU:HD21	1:C:959:PHE:HE2	1.69	0.57
1:A:1082:GLN:HG2	1:A:1263:TYR:CZ	2.39	0.57
1:B:718:VAL:HG13	1:B:735:ILE:HD13	1.86	0.57
1:A:718:VAL:HG13	1:A:735:ILE:HD13	1.86	0.57
1:B:1270:ARG:NH2	1:D:821:LYS:NZ	2.53	0.56
1:A:346:LEU:HG	1:A:893:TRP:CZ2	2.39	0.56
1:B:930:LEU:HD23	1:B:933:LEU:HD12	1.86	0.56
1:D:119:HIS:CE1	1:D:172:PHE:HB2	2.40	0.56
1:D:1214:MET:CE	1:D:1457:TRP:HE1	2.18	0.56
1:B:821:LYS:HZ1	1:D:1270:ARG:HH12	1.54	0.56
1:A:1021:ILE:HG23	1:A:1025:ARG:HG3	1.86	0.56
1:B:666:GLU:OE1	1:D:664:LYS:O	2.23	0.56
1:C:1275:LYS:O	1:C:1279:ILE:HG13	2.05	0.56
1:C:718:VAL:HG13	1:C:735:ILE:HD13	1.85	0.56
1:B:237:VAL:HA	1:B:958:ARG:HA	1.88	0.56
1:C:340:GLY:HA2	1:C:343:GLU:HB2	1.87	0.56
1:D:387:LEU:CD2	1:D:861:LYS:HB2	2.30	0.56
1:D:1288:ASP:HB3	1:D:1369:PHE:HD2	1.69	0.56
1:D:64:LEU:HD12	1:D:67:ILE:HD11	1.87	0.56
1:B:64:LEU:HD12	1:B:67:ILE:HD11	1.87	0.56
1:C:1197:HIS:CE1	1:C:1231:LYS:NZ	2.74	0.56
1:C:1225:HIS:ND1	1:C:1308:ARG:HA	2.20	0.56
1:C:78:ASP:HB2	1:C:975:LYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:993:VAL:HG13	1:D:1014:ASP:HA	1.87	0.56
1:A:1214:MET:CE	1:A:1457:TRP:HE1	2.16	0.56
1:B:1287:LEU:HD22	1:B:1364:VAL:HG11	1.88	0.56
2:A:1605:NAG:H61	2:A:1606:NAG:C7	2.36	0.56
1:A:64:LEU:HD12	1:A:67:ILE:HD11	1.86	0.56
1:B:1280:TRP:HA	1:B:1283:LYS:HD3	1.87	0.56
1:B:1404:GLN:CG	1:B:1409:ILE:HB	2.30	0.56
1:A:1013:LEU:HD21	1:A:1241:PRO:HD3	1.86	0.56
1:A:361:ILE:HG13	1:A:364:GLN:HB2	1.87	0.56
1:B:703:LEU:HB2	1:B:806:LEU:HD12	1.88	0.56
1:B:1253:GLU:HG3	1:B:1467:LEU:HD11	1.86	0.55
1:B:46:VAL:HG13	1:B:116:VAL:HG21	1.88	0.55
1:D:975:LYS:HG3	1:D:976:VAL:H	1.70	0.55
1:B:1270:ARG:HH22	1:D:821:LYS:HZ2	1.54	0.55
1:C:378:ARG:HD2	1:C:909:THR:HG21	1.88	0.55
1:D:1207:SER:HB2	1:D:1279:ILE:HD11	1.89	0.55
1:C:1374:ALA:HA	1:C:1377:ARG:HE	1.71	0.55
1:C:853:VAL:HG12	1:C:859:ALA:HA	1.88	0.55
1:C:105:LEU:CG	1:C:966:SER:HA	2.34	0.55
1:A:1309:THR:HG21	1:A:1432:ARG:HD3	1.87	0.55
1:A:338:HIS:CE1	1:A:897:TYR:H	2.24	0.55
1:D:1236:GLU:HG2	1:D:1244:LYS:NZ	2.22	0.55
1:B:1270:ARG:NH2	1:D:821:LYS:HZ1	2.04	0.55
1:A:380:LEU:HD21	1:A:869:SER:CB	2.37	0.55
1:C:1040:LEU:HD22	1:C:1082:GLN:HB2	1.89	0.55
1:C:397:LEU:HD13	1:C:844:LEU:HD13	1.88	0.55
1:D:703:LEU:HB2	1:D:806:LEU:HD12	1.89	0.55
1:A:308:PHE:HE2	1:A:931:LYS:HA	1.72	0.55
1:B:1302:ASP:HB3	1:B:1360:ALA:HB1	1.88	0.55
1:C:1134:LEU:O	1:C:1136:PRO:HD3	2.07	0.55
1:D:1225:HIS:CE1	1:D:1308:ARG:HA	2.42	0.55
1:C:1224:HIS:HE1	1:C:1463:GLU:OE1	1.90	0.55
1:C:703:LEU:HB2	1:C:806:LEU:HD12	1.88	0.55
1:D:52:ALA:HB1	1:D:89:LEU:HD21	1.89	0.55
1:A:1094:LEU:HD11	1:A:1105:LEU:H	1.71	0.55
1:D:1197:HIS:CE1	1:D:1231:LYS:NZ	2.74	0.55
1:C:1374:ALA:HA	1:C:1377:ARG:HG3	1.89	0.55
1:A:1107:SER:CB	1:A:1120:ASP:HA	2.26	0.54
1:B:296:LYS:HZ3	1:B:326:GLY:HA2	1.71	0.54
1:B:882:ALA:H	1:B:883:PRO:CD	2.20	0.54
1:D:930:LEU:HD23	1:D:933:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1357:HIS:CE1	1:B:1404:GLN:NE2	2.76	0.54
1:B:1454:VAL:HG13	1:B:1456:GLU:HG2	1.88	0.54
1:B:765:ARG:HD2	1:D:1391:SER:HB3	1.88	0.54
1:A:312:LEU:O	1:A:316:GLN:HG2	2.07	0.54
1:B:1094:LEU:HD11	1:B:1105:LEU:H	1.72	0.54
1:A:703:LEU:HB2	1:A:806:LEU:HD12	1.88	0.54
1:B:1205:VAL:HB	1:B:1235:ILE:CG1	2.37	0.54
1:B:666:GLU:O	1:B:667:LEU:HB2	2.07	0.54
1:C:1450:ALA:HB1	1:C:1457:TRP:CG	2.42	0.54
1:B:837:ILE:HG12	1:B:863:THR:HG21	1.88	0.54
1:C:279:ILE:HD13	1:C:320:LYS:HE3	1.88	0.54
1:D:1309:THR:HG21	1:D:1432:ARG:HD3	1.89	0.54
1:D:1450:ALA:HB1	1:D:1457:TRP:CG	2.43	0.54
1:D:78:ASP:HB2	1:D:975:LYS:CA	2.16	0.54
1:D:376:ARG:HH22	1:D:874:LEU:N	2.05	0.54
1:D:230:ASN:HD22	1:D:964:LEU:HG	1.72	0.54
1:B:279:ILE:HD13	1:B:320:LYS:HE3	1.90	0.54
1:D:1094:LEU:HD11	1:D:1105:LEU:H	1.73	0.54
1:D:999:PRO:O	1:D:1002:TRP:HB2	2.08	0.54
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.43	0.54
1:A:1450:ALA:HB1	1:A:1457:TRP:CG	2.42	0.54
1:A:279:ILE:HD13	1:A:320:LYS:HE3	1.90	0.54
1:B:669:VAL:HG22	1:B:809:ARG:HG3	1.90	0.54
1:A:339:ARG:HH12	1:A:946:ASN:HB2	1.73	0.54
1:B:1352:LYS:H	1:B:1354:LYS:NZ	2.06	0.53
1:C:1044:HIS:N	1:C:1044:HIS:CD2	2.75	0.53
1:D:715:GLN:HG3	1:D:766:PHE:HZ	1.73	0.53
1:B:1361:LEU:HD22	1:B:1417:LEU:HD13	1.90	0.53
1:C:1309:THR:HG21	1:C:1432:ARG:HD3	1.89	0.53
1:A:245:VAL:HB	1:A:287:LYS:HA	1.89	0.53
1:C:1374:ALA:HB2	1:C:1377:ARG:HH21	1.73	0.53
1:A:1368:ARG:HD3	1:A:1368:ARG:O	2.09	0.53
1:D:673:ASN:CA	1:D:861:LYS:HD2	2.33	0.53
1:B:988:ARG:HG2	1:B:1018:ILE:HG22	1.89	0.53
1:C:31:ILE:HD12	1:C:236:LEU:HD11	1.90	0.53
1:A:1007:LYS:O	1:A:1241:PRO:HB3	2.09	0.53
1:B:1299:ILE:HG23	1:B:1363:VAL:HG22	1.91	0.53
1:C:1225:HIS:CE1	1:C:1308:ARG:HA	2.43	0.53
1:C:1467:LEU:HD12	1:C:1470:ARG:HE	1.73	0.53
1:C:79:LYS:HZ2	1:C:972:GLU:CA	2.21	0.53
1:A:929:VAL:O	1:A:933:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1270:ARG:CZ	1:D:821:LYS:NZ	2.71	0.53
1:C:1286:PHE:HB3	1:C:1290:LEU:HD13	1.91	0.53
1:B:179:GLY:HA3	1:B:210:ALA:CA	2.39	0.53
1:B:686:VAL:HG11	1:B:736:VAL:HG22	1.91	0.53
1:C:354:TRP:CZ3	1:C:890:PHE:HB3	2.44	0.53
1:C:363:ARG:NH1	1:C:879:PHE:CE1	2.77	0.53
1:D:657:THR:HG21	1:D:884:THR:HG22	1.91	0.53
1:C:316:GLN:HB2	1:C:961:ARG:HD3	1.90	0.53
1:D:1038:HIS:CD2	1:D:1085:ALA:HA	2.43	0.53
1:D:354:TRP:CZ3	1:D:890:PHE:HB3	2.44	0.53
1:B:122:TYR:CE2	1:B:215:ARG:NH1	2.77	0.53
1:D:37:ALA:O	1:D:226:SER:OG	2.27	0.53
1:D:375:THR:O	1:D:378:ARG:HB3	2.09	0.53
1:A:1467:LEU:HD12	1:A:1470:ARG:HE	1.74	0.52
1:A:308:PHE:CZ	1:A:931:LYS:HG3	2.44	0.52
1:B:237:VAL:HG22	1:B:958:ARG:HB3	1.91	0.52
1:B:125:ALA:O	1:B:1064:GLU:HB2	2.08	0.52
1:C:1094:LEU:HD11	1:C:1105:LEU:H	1.73	0.52
1:B:354:TRP:CZ3	1:B:890:PHE:HB3	2.45	0.52
1:D:763:PHE:HD1	1:D:768:ASP:HB3	1.74	0.52
1:A:109:LEU:HD21	1:A:964:LEU:CD1	2.40	0.52
1:A:1197:HIS:CE1	1:A:1231:LYS:NZ	2.77	0.52
1:A:179:GLY:HA3	1:A:210:ALA:CA	2.37	0.52
1:D:660:PHE:O	1:D:663:ASP:OD1	2.28	0.52
1:B:1392:LEU:HD22	1:B:1398:ASP:HB3	1.91	0.52
1:B:879:PHE:CD1	1:B:879:PHE:N	2.75	0.52
1:B:349:GLY:CA	1:B:948:THR:HB	2.37	0.52
1:C:874:LEU:HB3	1:C:879:PHE:HD2	1.74	0.52
1:D:1134:LEU:C	1:D:1136:PRO:HD3	2.30	0.52
1:D:669:VAL:HG22	1:D:809:ARG:HG3	1.91	0.52
1:A:60:TYR:CD1	1:A:174:ARG:NH1	2.78	0.52
1:B:60:TYR:CD1	1:B:174:ARG:NH1	2.78	0.52
1:B:965:SER:OG	1:B:967:SER:O	2.24	0.52
1:D:115:ARG:NH2	1:D:174:ARG:NH2	2.45	0.52
1:A:1094:LEU:HG	1:A:1105:LEU:HD23	1.91	0.52
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.75	0.52
1:C:930:LEU:HD23	1:C:933:LEU:HD12	1.92	0.52
1:C:992:LEU:O	1:C:1014:ASP:O	2.28	0.52
1:A:244:ILE:HD11	1:A:954:LEU:HB2	1.92	0.52
1:B:384:VAL:HG12	1:B:389:LEU:HB2	1.91	0.52
1:C:1016:LEU:HD11	1:C:1030:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1467:LEU:HD12	1:D:1470:ARG:HE	1.75	0.52
1:A:338:HIS:CE1	1:A:894:ASN:O	2.63	0.51
1:C:144:ILE:HG12	1:C:183:VAL:HG12	1.92	0.51
1:C:693:LYS:H	1:C:693:LYS:HZ3	1.55	0.51
1:A:296:LYS:CD	1:A:331:SER:HA	2.40	0.51
1:D:381:ILE:HG21	1:D:909:THR:HA	1.92	0.51
1:B:1234:PHE:HB2	1:B:1260:MET:HG2	1.92	0.51
1:D:334:PHE:HB3	1:D:897:TYR:CZ	2.46	0.51
1:D:60:TYR:CD1	1:D:174:ARG:NH1	2.79	0.51
1:D:700:TRP:HB3	1:D:856:PRO:HA	1.92	0.51
1:D:45:LEU:HA	1:D:81:LEU:HD21	1.91	0.51
1:A:48:LEU:HD21	1:A:82:TYR:HA	1.91	0.51
1:B:1219:MET:O	1:B:1223:MET:HG2	2.11	0.51
1:B:1418:TRP:NE1	1:B:1427:THR:OG1	2.29	0.51
1:B:400:HIS:CD2	1:B:843:ALA:CB	2.94	0.51
1:C:963:VAL:CG1	1:C:979:LEU:HB3	2.41	0.51
1:D:1040:LEU:HD22	1:D:1082:GLN:HB2	1.92	0.51
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.92	0.51
1:B:1235:ILE:HB	1:B:1238:PHE:HE2	1.75	0.51
1:B:879:PHE:HB2	1:B:880:ASP:CA	2.37	0.51
1:B:995:GLY:O	1:B:996:MET:HG3	2.10	0.51
1:C:119:HIS:ND1	1:C:216:TYR:CD2	2.78	0.51
1:C:1416:TRP:CZ2	1:C:1432:ARG:NH1	2.79	0.51
1:D:1288:ASP:HB3	1:D:1369:PHE:CD2	2.45	0.51
1:A:1416:TRP:CZ2	1:A:1432:ARG:NH1	2.79	0.51
1:B:144:ILE:HG12	1:B:183:VAL:HG12	1.93	0.51
1:C:998:VAL:HG21	1:C:1004:VAL:HG21	1.93	0.51
1:C:392:GLN:HE22	1:C:891:LYS:NZ	2.09	0.51
1:C:763:PHE:HD1	1:C:768:ASP:HB3	1.75	0.51
1:D:958:ARG:NH1	1:D:960:TYR:CE1	2.79	0.51
1:C:686:VAL:HG11	1:C:736:VAL:HG22	1.93	0.51
1:B:1213:ARG:NH2	1:B:1451:ARG:HH12	2.09	0.51
1:B:381:ILE:HG21	1:B:909:THR:HA	1.93	0.51
1:C:313:LYS:O	1:C:316:GLN:HG2	2.11	0.51
1:C:715:GLN:HG3	1:C:766:PHE:HZ	1.74	0.51
1:B:296:LYS:HE2	1:B:331:SER:CA	2.41	0.51
2:A:1605:NAG:C6	2:A:1606:NAG:HN2	2.23	0.50
1:B:1199:GLU:OE2	1:B:1228:HIS:ND1	2.37	0.50
1:C:737:HIS:NE2	1:C:749:LEU:HD12	2.25	0.50
1:D:400:HIS:HD2	1:D:402:GLU:HB2	1.76	0.50
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1296:ASP:O	1:B:1366:LEU:HB2	2.11	0.50
1:B:932:VAL:HG11	1:B:964:LEU:HG	1.92	0.50
1:C:119:HIS:ND1	1:C:216:TYR:HD2	2.09	0.50
1:C:296:LYS:HE2	1:C:331:SER:CA	2.41	0.50
1:A:1331:ASP:HB3	1:A:1343:LYS:NZ	2.26	0.50
1:B:1108:VAL:HG12	1:B:1134:LEU:HD22	1.93	0.50
1:B:1265:TRP:NE1	1:B:1269:LEU:HD23	2.26	0.50
1:B:1319:LEU:HG	1:B:1320:ASP:N	2.26	0.50
1:B:244:ILE:HD11	1:B:954:LEU:HB2	1.93	0.50
1:C:60:TYR:CD1	1:C:174:ARG:NH1	2.79	0.50
1:D:881:ASN:OD1	1:D:881:ASN:O	2.28	0.50
1:D:963:VAL:CG2	1:D:981:ALA:HB2	2.42	0.50
1:C:1342:TRP:HE1	1:C:1343:LYS:HE3	1.77	0.50
1:D:682:LEU:HD22	1:D:788:LEU:HA	1.92	0.50
1:B:1094:LEU:HG	1:B:1105:LEU:HD23	1.93	0.50
1:B:143:LEU:HD13	1:B:161:VAL:HG21	1.94	0.50
1:C:700:TRP:HB3	1:C:856:PRO:HA	1.93	0.50
1:D:1224:HIS:HE1	1:D:1463:GLU:OE1	1.95	0.50
1:D:1416:TRP:CZ2	1:D:1432:ARG:NH1	2.79	0.50
1:D:316:GLN:NE2	1:D:961:ARG:HH11	2.09	0.50
1:B:42:PRO:HB3	1:B:116:VAL:HG11	1.94	0.50
1:C:381:ILE:HG21	1:C:909:THR:HA	1.94	0.50
1:D:1134:LEU:O	1:D:1136:PRO:HD3	2.11	0.50
1:D:111:THR:O	1:D:114:PRO:HD2	2.12	0.50
1:B:700:TRP:HB3	1:B:856:PRO:HA	1.94	0.50
1:C:75:ALA:HB1	1:C:81:LEU:HG	1.94	0.50
1:C:334:PHE:HB3	1:C:897:TYR:CZ	2.47	0.50
1:D:1199:GLU:OE2	1:D:1228:HIS:ND1	2.44	0.50
1:A:1098:ARG:NE	1:A:1152:PRO:HD3	2.19	0.50
1:B:312:LEU:O	1:B:316:GLN:HB3	2.11	0.50
1:B:715:GLN:HG3	1:B:766:PHE:HZ	1.76	0.50
1:B:78:ASP:CB	1:B:975:LYS:HA	2.36	0.50
1:C:1058:GLN:HB3	1:C:1293:LEU:CD1	2.42	0.50
1:B:1352:LYS:NZ	1:D:774:GLU:HB3	2.27	0.50
1:B:334:PHE:HB3	1:B:897:TYR:CZ	2.47	0.50
1:A:686:VAL:HG11	1:A:736:VAL:HG22	1.93	0.49
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.94	0.49
1:B:1319:LEU:HG	1:B:1320:ASP:H	1.77	0.49
1:C:400:HIS:CD2	1:C:843:ALA:CB	2.95	0.49
1:D:179:GLY:HA3	1:D:210:ALA:CA	2.39	0.49
1:D:316:GLN:NE2	1:D:961:ARG:NH1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:THR:HG22	1:A:1237:GLN:HB3	1.94	0.49
1:A:1224:HIS:HE1	1:A:1463:GLU:OE1	1.95	0.49
1:B:1087:PRO:HA	1:B:1126:LEU:HG	1.94	0.49
1:B:1295:LEU:HD11	1:B:1298:VAL:HB	1.93	0.49
1:C:244:ILE:HD11	1:C:954:LEU:HB2	1.93	0.49
1:D:1351:LEU:HA	1:D:1354:LYS:CE	2.42	0.49
1:B:1270:ARG:NH1	1:D:821:LYS:HZ3	1.99	0.49
1:A:1351:LEU:HA	1:A:1354:LYS:CE	2.42	0.49
1:B:115:ARG:HA	1:B:1127:MET:HB2	1.94	0.49
1:B:45:LEU:HA	1:B:48:LEU:HD12	1.94	0.49
1:D:110:ARG:O	1:D:113:THR:OG1	2.27	0.49
1:D:737:HIS:NE2	1:D:749:LEU:HD12	2.27	0.49
1:A:1105:LEU:CA	1:A:1138:LEU:HG	2.30	0.49
1:A:715:GLN:HG3	1:A:766:PHE:HZ	1.77	0.49
1:B:1323:PRO:CB	1:B:1369:PHE:HA	2.41	0.49
1:B:763:PHE:HD1	1:B:768:ASP:HB3	1.76	0.49
1:C:1467:LEU:HD12	1:C:1470:ARG:NE	2.27	0.49
1:C:143:LEU:HD13	1:C:161:VAL:HG21	1.95	0.49
1:D:1081:PHE:HE2	1:D:1134:LEU:HD12	1.76	0.49
1:D:686:VAL:HG11	1:D:736:VAL:HG22	1.94	0.49
1:A:1450:ALA:HB1	1:A:1457:TRP:CE2	2.47	0.49
1:C:179:GLY:HA3	1:C:210:ALA:CA	2.39	0.49
1:D:44:TYR:CE2	1:D:110:ARG:NH2	2.77	0.49
1:C:1199:GLU:OE2	1:C:1228:HIS:ND1	2.46	0.49
1:C:349:GLY:CA	1:C:948:THR:HB	2.38	0.49
1:D:109:LEU:HD21	1:D:964:LEU:HD21	1.93	0.49
1:D:1342:TRP:HE1	1:D:1343:LYS:HE3	1.77	0.49
1:A:384:VAL:HG22	1:A:865:VAL:HG11	1.95	0.49
1:D:120:TYR:CE1	1:D:218:ARG:HA	2.48	0.49
1:B:1098:ARG:HE	1:B:1152:PRO:HB3	1.77	0.49
1:C:1331:ASP:CB	1:C:1343:LYS:HZ1	2.21	0.49
1:C:89:LEU:HD22	1:C:95:MET:HG3	1.94	0.49
1:A:339:ARG:HH22	1:A:946:ASN:HB2	1.78	0.49
1:A:669:VAL:HG22	1:A:809:ARG:HG3	1.94	0.48
1:B:1352:LYS:N	1:B:1354:LYS:NZ	2.61	0.48
1:B:1375:GLY:O	1:B:1379:ARG:HD2	2.13	0.48
1:A:339:ARG:NH1	1:A:946:ASN:HB2	2.27	0.48
1:A:380:LEU:HD21	1:A:869:SER:HB3	1.95	0.48
1:C:407:LYS:HE3	1:C:870:THR:HG21	1.94	0.48
1:C:682:LEU:HD22	1:C:788:LEU:HA	1.95	0.48
1:D:349:GLY:HA2	1:D:917:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ASP:OD2	1:A:1021:ILE:HG12	2.13	0.48
1:A:1199:GLU:OE2	1:A:1228:HIS:ND1	2.45	0.48
1:A:315:THR:HG23	1:A:316:GLN:HE21	1.77	0.48
1:A:358:LEU:HD22	1:A:884:THR:HB	1.95	0.48
1:B:1040:LEU:HD22	1:B:1082:GLN:HB2	1.94	0.48
1:B:737:HIS:NE2	1:B:749:LEU:HD12	2.27	0.48
1:A:1376:ASP:O	1:A:1380:GLN:HG2	2.12	0.48
1:B:29:PRO:HB2	1:B:986:VAL:O	2.14	0.48
1:B:78:ASP:HA	1:B:81:LEU:HD23	1.94	0.48
1:C:349:GLY:HA2	1:C:917:ASN:HB2	1.96	0.48
1:D:1094:LEU:HG	1:D:1105:LEU:HD23	1.94	0.48
1:D:392:GLN:HE22	1:D:891:LYS:NZ	2.10	0.48
1:A:368:PHE:O	1:A:372:ASP:OD1	2.32	0.48
1:B:1357:HIS:H	1:B:1401:ASN:HD21	1.60	0.48
1:B:1459:LYS:HZ3	1:B:1460:TYR:HE1	1.62	0.48
1:B:682:LEU:HD22	1:B:788:LEU:HA	1.94	0.48
1:D:1377:ARG:HA	1:D:1380:GLN:CG	2.44	0.48
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.95	0.48
1:A:334:PHE:O	1:A:337:GLU:HG2	2.12	0.48
1:B:1376:ASP:CA	1:B:1379:ARG:HD3	2.18	0.48
1:C:363:ARG:NH1	1:C:879:PHE:CZ	2.82	0.48
1:C:353:LEU:HG	1:C:914:ALA:HA	1.95	0.48
1:D:1087:PRO:HA	1:D:1126:LEU:HG	1.95	0.48
1:D:1377:ARG:HA	1:D:1380:GLN:HG2	1.94	0.48
1:D:1450:ALA:HB1	1:D:1457:TRP:CE2	2.49	0.48
1:A:700:TRP:HB3	1:A:856:PRO:HA	1.96	0.48
1:B:372:ASP:O	1:B:376:ARG:HG3	2.13	0.48
1:C:1197:HIS:CE1	1:C:1231:LYS:HZ3	2.31	0.48
1:D:56:ASN:OD1	1:D:58:THR:OG1	2.32	0.48
1:A:334:PHE:HB3	1:A:897:TYR:CZ	2.48	0.48
1:D:1357:HIS:CE1	1:D:1409:ILE:CG2	2.97	0.48
1:A:1357:HIS:CE1	1:A:1409:ILE:CG2	2.97	0.48
1:A:110:ARG:CZ	1:A:227:LEU:HD11	2.44	0.48
1:A:371:VAL:HA	1:A:374:LEU:HD23	1.96	0.48
1:B:184:ILE:HG12	1:B:213:ARG:HG3	1.96	0.48
1:C:1206:ALA:HB1	1:C:1211:TYR:HB3	1.96	0.48
1:C:1276:GLN:HA	1:C:1279:ILE:HD12	1.94	0.48
1:C:1357:HIS:CE1	1:C:1409:ILE:CG2	2.97	0.48
1:D:244:ILE:HD11	1:D:954:LEU:HB2	1.94	0.48
1:C:345:PHE:HB3	1:C:893:TRP:HE1	1.79	0.48
1:A:874:LEU:H	1:A:875:PRO:CA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1280:TRP:CD1	1:B:1283:LYS:NZ	2.82	0.47
1:B:664:LYS:HB3	1:D:666:GLU:OE2	2.14	0.47
1:A:143:LEU:HD13	1:A:161:VAL:HG21	1.96	0.47
1:B:392:GLN:HE22	1:B:891:LYS:HZ1	1.62	0.47
1:C:669:VAL:HG22	1:C:809:ARG:HG3	1.95	0.47
1:A:1402:HIS:HE1	1:C:770:GLU:OE1	1.97	0.47
1:A:737:HIS:NE2	1:A:749:LEU:HD12	2.28	0.47
1:D:1467:LEU:HD12	1:D:1470:ARG:NE	2.29	0.47
1:D:296:LYS:HE2	1:D:331:SER:CA	2.42	0.47
1:D:47:GLU:O	1:D:51:THR:OG1	2.26	0.47
1:B:230:ASN:HD22	1:B:964:LEU:HA	1.78	0.47
1:C:1450:ALA:HB1	1:C:1457:TRP:CE2	2.49	0.47
1:C:988:ARG:HB3	1:C:1019:LYS:HB2	1.95	0.47
1:A:184:ILE:HG12	1:A:213:ARG:HG3	1.96	0.47
1:B:1301:VAL:HG13	1:B:1305:GLN:HB2	1.95	0.47
1:B:1335:GLU:HG2	1:B:1336:MET:SD	2.55	0.47
1:B:392:GLN:HE22	1:B:891:LYS:NZ	2.11	0.47
1:B:387:LEU:HD22	1:B:862:LEU:HG	1.96	0.47
1:C:311:LEU:HG	1:C:927:VAL:HG11	1.97	0.47
1:A:52:ALA:HB1	1:A:89:LEU:HD21	1.97	0.47
1:C:1336:MET:SD	1:C:1421:THR:O	2.73	0.47
1:C:184:ILE:HG12	1:C:213:ARG:HG3	1.96	0.47
1:D:988:ARG:HG2	1:D:1018:ILE:HG22	1.96	0.47
1:D:143:LEU:HD13	1:D:161:VAL:HG21	1.96	0.47
1:D:144:ILE:HG12	1:D:183:VAL:HG12	1.95	0.47
1:A:296:LYS:HE2	1:A:331:SER:CA	2.41	0.47
1:A:951:ILE:HG22	1:A:953:GLU:O	2.15	0.47
1:B:1357:HIS:NE2	1:B:1411:THR:CG2	2.68	0.47
1:C:1108:VAL:HG23	1:C:1122:THR:HA	1.97	0.47
1:C:924:GLN:HE22	1:C:956:VAL:HG11	1.79	0.47
1:C:963:VAL:HG12	1:C:979:LEU:HB3	1.97	0.47
1:D:1080:TYR:OH	1:D:1082:GLN:NE2	2.29	0.47
1:D:1206:ALA:HB1	1:D:1211:TYR:HB3	1.97	0.47
1:D:1336:MET:SD	1:D:1421:THR:O	2.73	0.47
1:D:349:GLY:CA	1:D:948:THR:HB	2.38	0.47
1:A:682:LEU:HD22	1:A:788:LEU:HA	1.95	0.47
1:C:1094:LEU:HG	1:C:1105:LEU:HD23	1.95	0.47
1:D:29:PRO:HB2	1:D:986:VAL:O	2.14	0.47
1:B:297:ALA:HB1	1:B:314:LEU:HD21	1.97	0.47
1:B:43:PRO:O	1:B:46:VAL:HG12	2.15	0.47
1:B:907:THR:O	1:B:938:GLY:HA2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:ILE:O	1:D:882:ALA:O	2.32	0.47
1:A:1296:ASP:O	1:A:1366:LEU:HB2	2.14	0.47
1:B:1466:GLU:HA	1:B:1469:ARG:CD	2.32	0.47
1:B:917:ASN:OD1	1:B:947:PRO:HA	2.15	0.47
1:D:296:LYS:HZ2	1:D:326:GLY:HA2	1.75	0.47
1:D:298:ALA:HB2	1:D:918:PRO:HG2	1.96	0.47
1:A:1467:LEU:HD12	1:A:1470:ARG:NE	2.29	0.46
1:B:109:LEU:HB3	1:B:368:PHE:CE1	2.50	0.46
1:B:1352:LYS:N	1:B:1354:LYS:HZ3	2.12	0.46
1:B:348:GLU:HB2	1:B:947:PRO:O	2.15	0.46
1:D:184:ILE:HG12	1:D:213:ARG:HG3	1.97	0.46
1:B:1090:TYR:HB2	1:B:1124:VAL:O	2.15	0.46
1:B:1108:VAL:HG23	1:B:1122:THR:HA	1.96	0.46
1:B:1357:HIS:HE1	1:B:1404:GLN:HE22	1.63	0.46
1:B:345:PHE:HB3	1:B:893:TRP:HE1	1.81	0.46
1:B:349:GLY:HA2	1:B:917:ASN:HB2	1.98	0.46
1:C:135:GLN:HE22	1:C:148:GLN:HE21	1.63	0.46
1:D:917:ASN:OD1	1:D:947:PRO:HA	2.15	0.46
1:B:1105:LEU:CA	1:B:1138:LEU:HG	2.30	0.46
1:D:384:VAL:HG12	1:D:389:LEU:HB2	1.97	0.46
1:A:109:LEU:HD21	1:A:964:LEU:HD13	1.97	0.46
1:B:687:PRO:HD2	1:B:735:ILE:O	2.15	0.46
1:C:281:ASP:OD1	1:C:988:ARG:NH1	2.44	0.46
1:D:110:ARG:HH12	1:D:976:VAL:HG21	1.80	0.46
1:A:286:GLU:HB2	1:A:289:GLU:OE2	2.16	0.46
1:B:1420:GLU:N	1:B:1437:CYS:SG	2.89	0.46
1:C:1319:LEU:HD12	1:C:1365:ASP:HB2	1.98	0.46
1:C:672:VAL:HB	1:C:861:LYS:HA	1.97	0.46
1:B:1391:SER:HB3	1:D:765:ARG:HD2	1.97	0.46
1:C:384:VAL:HG12	1:C:389:LEU:HB2	1.98	0.46
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.98	0.46
1:B:1302:ASP:O	1:B:1302:ASP:CG	2.54	0.46
1:B:1324:TYR:HA	1:B:1364:VAL:HA	1.98	0.46
1:B:398:LEU:HB3	1:B:886:ARG:HD3	1.98	0.46
1:C:1295:LEU:HD21	1:C:1298:VAL:HG22	1.97	0.46
1:D:1236:GLU:CG	1:D:1244:LYS:NZ	2.79	0.46
1:D:1276:GLN:HA	1:D:1279:ILE:HD12	1.98	0.46
1:A:335:GLU:HA	1:A:338:HIS:HB2	1.97	0.46
1:D:110:ARG:CZ	1:D:227:LEU:HD11	2.45	0.46
1:D:345:PHE:HB3	1:D:893:TRP:HE1	1.81	0.46
1:D:400:HIS:CD2	1:D:843:ALA:CB	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:TRP:HE1	1:A:1343:LYS:HE3	1.80	0.46
1:B:1351:LEU:HD22	1:B:1354:LYS:HE2	1.97	0.46
1:B:56:ASN:OD1	1:B:58:THR:OG1	2.30	0.46
1:C:1092:ILE:O	1:C:1122:THR:OG1	2.34	0.46
1:C:115:ARG:HA	1:C:1127:MET:HB2	1.98	0.46
1:C:1314:LEU:HD11	1:C:1412:LEU:HD13	1.98	0.46
1:D:878:ILE:HA	1:D:879:PHE:HA	1.77	0.46
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.46	0.46
1:C:31:ILE:HG12	1:C:1030:VAL:HB	1.96	0.46
1:C:45:LEU:HD12	1:C:81:LEU:HD21	1.97	0.46
1:D:998:VAL:HG13	1:D:1002:TRP:CB	2.46	0.46
1:A:666:GLU:O	1:A:667:LEU:HB2	2.15	0.45
1:C:1335:GLU:HG2	1:C:1336:MET:SD	2.56	0.45
1:C:348:GLU:HB2	1:C:947:PRO:O	2.16	0.45
1:D:1331:ASP:CB	1:D:1343:LYS:HZ1	2.26	0.45
1:B:1092:ILE:O	1:B:1122:THR:OG1	2.33	0.45
1:D:1115:PRO:HG3	1:D:1137:ARG:NE	2.31	0.45
1:B:338:HIS:CD2	1:B:341:ASN:ND2	2.79	0.45
1:C:1234:PHE:CD1	1:C:1260:MET:SD	3.08	0.45
1:C:1351:LEU:HA	1:C:1354:LYS:CE	2.44	0.45
1:D:297:ALA:HB1	1:D:314:LEU:HD21	1.98	0.45
1:D:296:LYS:HZ3	1:D:326:GLY:HA2	1.80	0.45
1:D:375:THR:HA	1:D:378:ARG:HB2	1.98	0.45
1:A:75:ALA:HB1	1:A:81:LEU:CB	2.46	0.45
1:B:1319:LEU:H	1:B:1319:LEU:HD23	1.82	0.45
1:D:1108:VAL:HG23	1:D:1122:THR:HA	1.98	0.45
1:A:687:PRO:HD2	1:A:735:ILE:O	2.16	0.45
1:B:1295:LEU:HB3	1:B:1366:LEU:HG	1.98	0.45
1:C:1469:ARG:HA	1:C:1472:ARG:HB2	1.98	0.45
1:D:1469:ARG:HA	1:D:1472:ARG:HB2	1.97	0.45
1:A:1092:ILE:O	1:A:1122:THR:OG1	2.34	0.45
1:A:311:LEU:O	1:A:315:THR:HG22	2.16	0.45
1:B:1223:MET:HA	1:B:1226:THR:HG22	1.98	0.45
1:B:1396:ASP:O	1:B:1400:PRO:HD2	2.16	0.45
1:D:1296:ASP:O	1:D:1366:LEU:HB2	2.17	0.45
1:A:115:ARG:HA	1:A:1127:MET:HB2	1.98	0.45
1:D:760:LEU:O	1:D:761:LEU:HG	2.16	0.45
1:A:339:ARG:NH2	1:A:946:ASN:HB2	2.31	0.45
1:B:1250:MET:SD	1:B:1256:PHE:HZ	2.40	0.45
1:B:135:GLN:HE22	1:B:148:GLN:HE21	1.65	0.45
1:B:31:ILE:HG12	1:B:1030:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASP:OD1	1:B:988:ARG:NH1	2.44	0.45
1:B:807:ASN:O	1:B:864:SER:HB2	2.17	0.45
1:D:1081:PHE:CE2	1:D:1134:LEU:HD12	2.52	0.45
1:A:317:ASP:O	1:A:320:LYS:HB3	2.17	0.45
1:B:879:PHE:HD1	1:B:879:PHE:N	2.15	0.45
1:B:925:ARG:NH1	1:B:960:TYR:OH	2.50	0.45
1:C:49:LEU:CD2	1:C:64:LEU:HD13	2.45	0.45
1:C:687:PRO:HD2	1:C:735:ILE:O	2.17	0.45
1:D:1092:ILE:O	1:D:1122:THR:OG1	2.35	0.45
1:D:232:TYR:CD2	1:D:996:MET:SD	3.10	0.45
1:B:1036:LEU:HD21	1:B:1039:ILE:HG12	1.99	0.44
1:B:397:LEU:HD13	1:B:844:LEU:HD13	1.98	0.44
1:C:693:LYS:N	1:C:693:LYS:NZ	2.58	0.44
1:D:338:HIS:CD2	1:D:341:ASN:ND2	2.80	0.44
1:A:1323:PRO:CA	1:A:1368:ARG:HG3	2.47	0.44
1:B:1398:ASP:HA	1:B:1401:ASN:HB2	1.99	0.44
1:B:1357:HIS:CE1	1:B:1404:GLN:HE22	2.35	0.44
1:D:31:ILE:HD12	1:D:236:LEU:HD13	1.98	0.44
1:A:349:GLY:HA2	1:A:917:ASN:HB2	1.99	0.44
1:B:1247:ILE:HG13	1:B:1247:ILE:H	1.62	0.44
1:C:296:LYS:CD	1:C:326:GLY:HA2	2.42	0.44
1:C:863:THR:O	1:C:866:THR:OG1	2.31	0.44
1:B:1200:ILE:HG13	1:B:1230:VAL:HG22	1.99	0.44
1:C:112:ALA:O	1:C:116:VAL:HG23	2.16	0.44
1:D:1295:LEU:HD21	1:D:1298:VAL:HG22	1.98	0.44
1:D:362:ASP:HA	1:D:365:ILE:HB	1.99	0.44
1:A:703:LEU:HD23	1:A:733:LEU:HD13	2.00	0.44
1:A:345:PHE:HD2	1:A:893:TRP:NE1	2.15	0.44
1:D:316:GLN:HE21	1:D:961:ARG:NH1	2.16	0.44
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.99	0.44
1:B:1215:LEU:HB3	1:B:1303:ALA:HB1	2.00	0.44
1:B:1382:TYR:HA	1:B:1385:LEU:CG	2.40	0.44
1:D:1075:MET:SD	1:D:1379:ARG:CZ	3.06	0.44
1:D:1197:HIS:CE1	1:D:1231:LYS:HZ3	2.36	0.44
1:D:296:LYS:NZ	1:D:326:GLY:CA	2.78	0.44
1:A:1214:MET:HB3	1:A:1304:ASP:HA	2.00	0.44
1:B:296:LYS:CD	1:B:326:GLY:HA2	2.41	0.44
1:C:104:LYS:HD3	1:C:967:SER:HA	1.99	0.44
1:A:1206:ALA:HB1	1:A:1211:TYR:HB3	2.00	0.44
1:B:1115:PRO:HG3	1:B:1137:ARG:NE	2.32	0.44
1:B:363:ARG:NH1	1:B:879:PHE:CE1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1105:LEU:CA	1:C:1138:LEU:HG	2.32	0.44
1:C:760:LEU:O	1:C:761:LEU:HG	2.18	0.44
1:B:1378:LEU:HB3	1:B:1399:LEU:HD21	1.99	0.44
1:D:135:GLN:HE22	1:D:148:GLN:HE21	1.66	0.44
1:C:362:ASP:HA	1:C:365:ILE:HB	1.98	0.43
1:B:1231:LYS:NZ	1:B:1233:TRP:CH2	2.78	0.43
1:B:387:LEU:HD13	1:B:862:LEU:HD23	1.99	0.43
1:C:1058:GLN:HB3	1:C:1293:LEU:HD13	2.00	0.43
1:C:29:PRO:HB2	1:C:986:VAL:O	2.18	0.43
1:C:56:ASN:OD1	1:C:58:THR:OG1	2.33	0.43
1:D:1061:LEU:HD11	1:D:1090:TYR:HB3	1.99	0.43
1:D:296:LYS:HZ2	1:D:326:GLY:CA	2.31	0.43
1:B:105:LEU:HD12	1:B:966:SER:HA	2.00	0.43
1:C:1115:PRO:HG3	1:C:1137:ARG:NE	2.34	0.43
1:D:1130:GLN:N	1:D:1130:GLN:HE21	2.16	0.43
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.54	0.43
1:B:113:THR:H	1:B:114:PRO:CD	2.30	0.43
1:B:1215:LEU:O	1:B:1219:MET:SD	2.75	0.43
1:B:49:LEU:CD2	1:B:64:LEU:HD13	2.43	0.43
1:C:1140:ARG:CZ	1:C:1145:GLU:HA	2.47	0.43
1:C:961:ARG:NH2	1:C:983:PHE:CD2	2.86	0.43
1:A:1366:LEU:O	1:A:1370:ARG:HG3	2.19	0.43
1:A:339:ARG:HH11	1:A:898:THR:HG21	1.82	0.43
1:B:1263:TYR:HB2	1:B:1290:LEU:HD12	2.00	0.43
1:C:925:ARG:HB2	1:C:960:TYR:CE2	2.53	0.43
1:A:243:TYR:O	1:A:244:ILE:CG1	2.65	0.43
1:A:31:ILE:HA	1:A:1030:VAL:HB	1.99	0.43
1:A:341:ASN:HB2	1:A:893:TRP:CG	2.53	0.43
1:B:988:ARG:HA	1:B:1018:ILE:HB	1.99	0.43
1:B:703:LEU:HD23	1:B:733:LEU:HD13	1.99	0.43
1:B:880:ASP:HB3	1:B:881:ASN:CA	2.40	0.43
1:C:316:GLN:HB2	1:C:961:ARG:HD2	1.98	0.43
1:D:117:GLU:CA	1:D:120:TYR:HB2	2.41	0.43
1:D:687:PRO:HD2	1:D:735:ILE:O	2.18	0.43
1:A:928:ALA:HB1	1:A:962:TYR:HB2	2.01	0.43
1:C:1134:LEU:C	1:C:1136:PRO:HD3	2.39	0.43
1:C:1331:ASP:CB	1:C:1343:LYS:NZ	2.81	0.43
1:D:1130:GLN:HE21	1:D:1130:GLN:H	1.67	0.43
1:A:1331:ASP:CB	1:A:1343:LYS:HZ1	2.28	0.43
1:A:204:LEU:HD12	1:A:209:LYS:HB2	1.99	0.43
1:A:345:PHE:CD1	1:A:345:PHE:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1306:ILE:HD13	1:B:1457:TRP:HB3	2.00	0.43
1:C:878:ILE:CG2	1:C:1044:HIS:CE1	2.93	0.43
1:C:1226:THR:HG21	1:C:1230:VAL:HG21	2.01	0.43
1:D:142:PHE:CE1	1:D:185:LEU:HB2	2.54	0.43
1:A:312:LEU:HA	1:A:315:THR:HG22	2.01	0.43
1:B:110:ARG:CZ	1:B:227:LEU:HD11	2.48	0.43
1:C:42:PRO:HB3	1:C:116:VAL:HG11	2.01	0.43
1:C:53:ALA:HB1	1:C:60:TYR:HB2	2.00	0.43
1:B:1152:PRO:HA	1:B:1153:SER:HA	1.70	0.43
1:B:1004:VAL:H	1:B:1264:LYS:HZ1	1.67	0.43
1:B:408:SER:HB2	1:B:655:ARG:NH2	2.34	0.43
1:C:1130:GLN:N	1:C:1130:GLN:HE21	2.17	0.43
1:C:392:GLN:HE22	1:C:891:LYS:HZ1	1.66	0.43
1:C:737:HIS:NE2	1:C:749:LEU:CD1	2.82	0.43
1:C:95:MET:HB3	1:C:100:LEU:HG	2.01	0.43
1:D:988:ARG:HA	1:D:1018:ILE:HB	2.01	0.43
1:D:1107:SER:HB2	1:D:1120:ASP:CA	2.29	0.43
1:D:1058:GLN:HB3	1:D:1293:LEU:CD1	2.48	0.43
1:D:1331:ASP:CB	1:D:1343:LYS:NZ	2.81	0.43
1:D:231:GLY:HA2	1:D:367:PRO:CG	2.49	0.43
1:D:281:ASP:O	1:D:987:PRO:HB3	2.18	0.43
1:D:806:LEU:HD23	1:D:832:GLU:HG2	2.01	0.43
1:A:1115:PRO:HG3	1:A:1137:ARG:NE	2.34	0.42
1:A:56:ASN:OD1	1:A:58:THR:OG1	2.33	0.42
1:C:105:LEU:H	1:C:105:LEU:HD12	1.84	0.42
1:D:48:LEU:HD12	1:D:81:LEU:HD22	2.00	0.42
1:D:348:GLU:HB2	1:D:947:PRO:O	2.18	0.42
1:A:1323:PRO:HA	1:A:1368:ARG:HG3	2.00	0.42
1:B:1200:ILE:HB	1:B:1230:VAL:HG13	2.01	0.42
1:B:1394:ASN:HB2	1:B:1398:ASP:HB2	2.01	0.42
1:B:1361:LEU:HB3	1:B:1417:LEU:HD22	2.00	0.42
1:B:686:VAL:O	1:B:688:VAL:HG23	2.20	0.42
1:C:957:LYS:HZ3	1:C:957:LYS:N	2.17	0.42
1:D:840:VAL:HG12	1:D:844:LEU:HD22	2.00	0.42
1:C:1333:ARG:HE	1:C:1424:SER:HA	1.85	0.42
1:C:142:PHE:CE1	1:C:185:LEU:HB2	2.54	0.42
1:D:339:ARG:HH12	1:D:946:ASN:CB	2.26	0.42
1:A:1055:ARG:HD3	1:A:1076:ALA:HB2	2.01	0.42
1:A:1368:ARG:HD2	1:A:1372:LEU:HD22	2.00	0.42
1:A:929:VAL:HG12	1:A:933:LEU:HD11	2.02	0.42
1:B:105:LEU:HB2	1:B:966:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1280:TRP:HA	1:B:1283:LYS:CD	2.49	0.42
1:B:239:LYS:HZ1	1:B:1275:LYS:CE	2.31	0.42
1:B:298:ALA:HB2	1:B:918:PRO:HG2	2.00	0.42
1:C:811:LEU:HD23	1:C:811:LEU:HA	1.93	0.42
1:A:42:PRO:HB3	1:A:116:VAL:HG11	2.01	0.42
1:A:1416:TRP:O	1:A:1433:THR:OG1	2.29	0.42
1:A:1450:ALA:HB1	1:A:1457:TRP:CD1	2.54	0.42
1:A:355:LEU:HD11	1:A:910:ILE:HG23	2.00	0.42
1:B:318:PHE:HB3	1:B:319:PRO:HD3	2.01	0.42
1:C:283:LYS:HA	1:C:284:PRO:HD3	1.93	0.42
1:C:917:ASN:OD1	1:C:947:PRO:HA	2.20	0.42
1:A:1197:HIS:CE1	1:A:1231:LYS:HZ3	2.35	0.42
1:A:1218:MET:HB2	1:A:1303:ALA:O	2.19	0.42
1:A:1323:PRO:HB3	1:A:1368:ARG:HG3	2.02	0.42
1:B:142:PHE:CE1	1:B:185:LEU:HB2	2.55	0.42
1:B:737:HIS:NE2	1:B:749:LEU:CD1	2.82	0.42
1:A:142:PHE:CE1	1:A:185:LEU:HB2	2.54	0.42
1:A:110:ARG:HD3	1:A:227:LEU:HD21	2.02	0.42
1:B:1319:LEU:HB2	1:B:1322:ALA:O	2.20	0.42
1:B:1403:MET:HB3	1:B:1407:ILE:HD12	2.02	0.42
1:B:760:LEU:O	1:B:761:LEU:HG	2.20	0.42
1:C:1416:TRP:O	1:C:1433:THR:OG1	2.29	0.42
1:C:1450:ALA:HB1	1:C:1457:TRP:CD1	2.54	0.42
1:C:317:ASP:OD1	1:C:961:ARG:NH2	2.52	0.42
1:C:760:LEU:HD23	1:C:763:PHE:HE2	1.85	0.42
1:D:1335:GLU:HG2	1:D:1336:MET:SD	2.60	0.42
1:D:703:LEU:HD23	1:D:733:LEU:HD13	2.02	0.42
1:D:737:HIS:NE2	1:D:749:LEU:CD1	2.83	0.42
1:D:109:LEU:HD21	1:D:964:LEU:HD11	2.02	0.42
1:B:1454:VAL:O	1:B:1454:VAL:HG12	2.20	0.42
1:B:36:LYS:HD2	1:B:226:SER:HB3	2.00	0.42
1:B:302:MET:SD	1:B:897:TYR:O	2.78	0.42
1:C:1314:LEU:HD13	1:C:1416:TRP:CE2	2.54	0.42
1:D:1214:MET:HB3	1:D:1304:ASP:HA	2.01	0.42
1:D:1218:MET:HB2	1:D:1303:ALA:O	2.20	0.42
1:D:1225:HIS:HD1	1:D:1308:ARG:HA	1.84	0.42
1:D:1333:ARG:HE	1:D:1424:SER:HA	1.84	0.42
1:D:1450:ALA:HB1	1:D:1457:TRP:CD1	2.55	0.42
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	2.02	0.42
1:B:1130:GLN:N	1:B:1130:GLN:HE21	2.18	0.42
1:B:1336:MET:SD	1:B:1421:THR:O	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:861:LYS:O	1:C:865:VAL:HG23	2.20	0.42
1:C:669:VAL:HB	1:C:868:LEU:HD21	2.00	0.42
1:D:31:ILE:HG12	1:D:1030:VAL:HB	2.00	0.42
1:D:281:ASP:OD1	1:D:988:ARG:NH1	2.45	0.42
1:B:281:ASP:O	1:B:987:PRO:HB3	2.20	0.42
1:C:1218:MET:HB2	1:C:1303:ALA:O	2.20	0.42
1:C:204:LEU:HD12	1:C:209:LYS:HB2	2.02	0.42
1:C:44:TYR:HB3	1:C:81:LEU:HD13	2.02	0.42
1:D:999:PRO:HA	1:D:1000:PRO:HD3	1.93	0.42
1:D:1200:ILE:HD12	1:D:1230:VAL:HG22	2.00	0.42
1:A:1061:LEU:HD23	1:A:1069:PHE:HD2	1.84	0.41
1:A:1105:LEU:HG	1:A:1105:LEU:O	2.20	0.41
1:A:353:LEU:HG	1:A:360:LEU:HD13	2.00	0.41
1:B:243:TYR:O	1:B:244:ILE:HG13	2.19	0.41
1:B:811:LEU:HA	1:B:811:LEU:HD23	1.92	0.41
1:C:1084:LYS:HG3	1:C:1084:LYS:H	1.69	0.41
1:C:1354:LYS:NZ	1:C:1405:PHE:HD1	2.16	0.41
1:C:958:ARG:HH21	1:C:1273:LYS:NZ	2.18	0.41
1:D:367:PRO:HB2	1:D:368:PHE:H	1.74	0.41
1:B:1005:THR:HB	1:B:1237:GLN:HA	2.01	0.41
1:B:204:LEU:HD12	1:B:209:LYS:HB2	2.02	0.41
1:C:1213:ARG:HH22	1:C:1451:ARG:NH1	2.18	0.41
1:C:686:VAL:O	1:C:688:VAL:HG23	2.20	0.41
1:A:1200:ILE:HD12	1:A:1230:VAL:HG22	2.02	0.41
1:B:42:PRO:HG2	1:B:113:THR:HG22	2.02	0.41
1:B:1457:TRP:HA	1:B:1460:TYR:CD2	2.55	0.41
1:C:319:PRO:HD2	1:C:959:PHE:CE1	2.54	0.41
1:A:1225:HIS:HD1	1:A:1308:ARG:HA	1.85	0.41
1:A:662:GLU:O	1:A:663:ASP:CG	2.58	0.41
1:A:988:ARG:HB3	1:A:1019:LYS:HB2	2.02	0.41
1:B:1205:VAL:CG1	1:B:1235:ILE:HG13	2.51	0.41
1:B:362:ASP:HA	1:B:365:ILE:HB	2.01	0.41
1:C:1209:HIS:CE1	1:C:1242:SER:HB2	2.55	0.41
1:A:760:LEU:O	1:A:761:LEU:HG	2.20	0.41
1:B:1105:LEU:O	1:B:1105:LEU:HG	2.20	0.41
1:C:1105:LEU:HG	1:C:1105:LEU:O	2.20	0.41
1:C:296:LYS:NZ	1:C:326:GLY:CA	2.80	0.41
1:C:284:PRO:HB2	1:C:323:ASN:HB2	2.02	0.41
1:C:235:GLU:HG2	1:C:995:GLY:O	2.20	0.41
1:A:1428:LEU:HA	1:A:1431:ALA:HB2	2.03	0.41
1:A:686:VAL:O	1:A:688:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:TYR:O	1:C:285:LEU:HG	2.21	0.41
1:D:392:GLN:HE22	1:D:891:LYS:HZ1	1.67	0.41
1:A:1140:ARG:CZ	1:A:1145:GLU:HA	2.50	0.41
1:A:737:HIS:NE2	1:A:749:LEU:CD1	2.83	0.41
1:B:1140:ARG:CZ	1:B:1145:GLU:HA	2.51	0.41
1:B:1465:ALA:C	1:B:1469:ARG:HE	2.23	0.41
1:C:1059:LEU:HD11	1:C:1094:LEU:HD23	2.02	0.41
1:A:1305:GLN:HG2	1:A:1435:ASP:HA	2.02	0.41
1:A:48:LEU:CD2	1:A:82:TYR:HA	2.50	0.41
1:B:1098:ARG:NE	1:B:1152:PRO:HB3	2.36	0.41
1:B:1215:LEU:O	1:B:1218:MET:HB3	2.21	0.41
1:B:1420:GLU:HB2	1:B:1453:GLN:OE1	2.21	0.41
1:B:296:LYS:NZ	1:B:326:GLY:CA	2.82	0.41
1:B:899:SER:HB2	1:B:944:PHE:CE2	2.56	0.41
1:C:1203:PHE:HB3	1:C:1298:VAL:CG1	2.51	0.41
1:C:1223:MET:HG3	1:C:1254:TYR:HB3	2.03	0.41
1:D:1059:LEU:HD11	1:D:1094:LEU:HD23	2.03	0.41
1:D:1203:PHE:HB3	1:D:1298:VAL:HG11	2.03	0.41
1:D:204:LEU:HD12	1:D:209:LYS:HB2	2.01	0.41
1:D:961:ARG:CD	1:D:983:PHE:HA	2.50	0.41
1:A:95:MET:HB3	1:A:100:LEU:HG	2.02	0.41
1:B:748:VAL:O	1:B:752:ARG:HG2	2.21	0.41
1:B:975:LYS:HE3	1:B:976:VAL:HB	2.03	0.41
1:D:1404:GLN:HA	1:D:1407:ILE:O	2.19	0.41
1:A:1214:MET:CE	1:A:1457:TRP:NE1	2.83	0.41
1:A:399:GLY:HA2	1:A:886:ARG:CB	2.50	0.41
1:B:243:TYR:O	1:B:285:LEU:HG	2.21	0.41
1:C:692:SER:CA	1:C:693:LYS:NZ	2.78	0.41
1:D:1213:ARG:HH22	1:D:1451:ARG:NH1	2.19	0.41
1:A:1319:LEU:HD12	1:A:1365:ASP:HB2	2.03	0.41
1:A:1404:GLN:HA	1:A:1407:ILE:O	2.21	0.41
1:A:400:HIS:CD2	1:A:402:GLU:OE2	2.74	0.41
1:A:806:LEU:HD23	1:A:832:GLU:HG2	2.03	0.41
1:B:878:ILE:HD13	1:B:1133:THR:HG21	2.03	0.41
1:C:31:ILE:HA	1:C:1030:VAL:HB	2.03	0.41
1:C:1108:VAL:HG11	1:C:1124:VAL:CG1	2.51	0.41
1:C:1342:TRP:CD1	1:C:1343:LYS:HG3	2.56	0.41
1:D:349:GLY:HA2	1:D:917:ASN:CB	2.51	0.41
1:D:52:ALA:HB1	1:D:89:LEU:CD2	2.50	0.41
1:A:1342:TRP:CD1	1:A:1343:LYS:HG3	2.56	0.40
1:B:1326:PHE:HB2	1:B:1357:HIS:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1333:ARG:HB2	1:B:1422:TRP:O	2.21	0.40
1:B:709:LEU:H	1:B:737:HIS:HD1	1.70	0.40
1:C:1404:GLN:HA	1:C:1407:ILE:O	2.21	0.40
1:C:969:SER:HB2	1:C:977:LYS:HB3	2.03	0.40
1:D:1105:LEU:HG	1:D:1105:LEU:O	2.22	0.40
1:D:31:ILE:HA	1:D:1030:VAL:HB	2.03	0.40
1:B:1350:TYR:HD2	1:D:771:THR:HG22	1.86	0.40
1:A:1314:LEU:HD11	1:A:1412:LEU:HD13	2.02	0.40
1:A:1460:TYR:O	1:A:1464:ILE:HG12	2.21	0.40
1:B:946:ASN:HA	1:B:947:PRO:HD3	1.87	0.40
1:C:281:ASP:O	1:C:987:PRO:HB3	2.21	0.40
1:D:1314:LEU:HD13	1:D:1416:TRP:CE2	2.56	0.40
1:D:748:VAL:O	1:D:752:ARG:HG2	2.22	0.40
1:A:1234:PHE:CD1	1:A:1260:MET:SD	3.10	0.40
1:B:1458:THR:O	1:B:1461:ASP:HB3	2.21	0.40
1:B:37:ALA:O	1:B:226:SER:OG	2.38	0.40
1:C:1223:MET:HA	1:C:1226:THR:HG22	2.03	0.40
1:C:1200:ILE:HD12	1:C:1230:VAL:HG22	2.03	0.40
1:A:716:GLU:CD	1:C:1384:ALA:HB2	2.42	0.40
1:C:338:HIS:CD2	1:C:341:ASN:ND2	2.78	0.40
1:C:899:SER:HB2	1:C:944:PHE:CE2	2.56	0.40
1:D:1090:TYR:HB2	1:D:1124:VAL:HG23	2.03	0.40
1:D:760:LEU:HD23	1:D:763:PHE:HE2	1.85	0.40
1:A:102:ALA:HB1	1:A:374:LEU:HD21	2.03	0.40
1:A:760:LEU:HD23	1:A:763:PHE:HE2	1.86	0.40
1:A:899:SER:HB2	1:A:944:PHE:CE2	2.57	0.40
1:B:998:VAL:HG21	1:B:1004:VAL:HG21	2.02	0.40
1:C:1090:TYR:HB2	1:C:1124:VAL:O	2.20	0.40
1:C:664:LYS:HD3	1:C:664:LYS:HA	1.92	0.40
1:D:1416:TRP:CD2	1:D:1432:ARG:HD2	2.57	0.40
1:D:312:LEU:HD13	1:D:928:ALA:HA	2.04	0.40
1:A:101:SER:OG	1:A:936:LEU:HA	2.22	0.40
1:B:1221:SER:O	1:B:1225:HIS:HB2	2.22	0.40
1:B:1319:LEU:HD13	1:B:1368:ARG:HB2	2.02	0.40
1:B:48:LEU:HD13	1:B:85:PHE:CD1	2.56	0.40
1:C:703:LEU:HD23	1:C:733:LEU:HD13	2.03	0.40
1:D:1223:MET:HA	1:D:1226:THR:HG22	2.03	0.40
1:D:1263:TYR:HB2	1:D:1290:LEU:HD12	2.03	0.40
1:D:44:TYR:HB3	1:D:81:LEU:HD13	2.04	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	1101/1260 (87%)	1009 (92%)	78 (7%)	14 (1%)	13	54
1	B	1110/1260 (88%)	947 (85%)	134 (12%)	29 (3%)	6	38
1	C	1105/1260 (88%)	991 (90%)	98 (9%)	16 (1%)	12	52
1	D	1115/1260 (88%)	987 (88%)	100 (9%)	28 (2%)	6	39
All	All	4431/5040 (88%)	3934 (89%)	410 (9%)	87 (2%)	8	44

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	ALA
1	A	873	ASP
1	A	874	LEU
1	A	876	GLN
1	A	883	PRO
1	A	1303	ALA
1	B	332	ALA
1	B	367	PRO
1	B	882	ALA
1	B	1199	GLU
1	B	1225	HIS
1	B	1236	GLU
1	B	1237	GLN
1	B	1275	LYS
1	B	1285	LEU
1	B	1388	ASP
1	C	332	ALA
1	C	367	PRO
1	C	1303	ALA
1	D	332	ALA
1	D	367	PRO
1	D	655	ARG

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Mol	Chain	Res	Type
1	D	656	ASN
1	D	881	ASN
1	D	1303	ALA
1	D	1437	CYS
1	A	244	ILE
1	A	884	THR
1	A	1345	GLY
1	A	1437	CYS
1	B	661	PRO
1	B	883	PRO
1	B	1079	GLY
1	B	1205	VAL
1	B	1206	ALA
1	B	1255	GLY
1	C	1127	MET
1	C	1345	GLY
1	C	1368	ARG
1	C	1437	CYS
1	C	1439	ASN
1	D	55	ASP
1	D	244	ILE
1	D	287	LYS
1	D	1345	GLY
1	D	1439	ASN
1	A	287	LYS
1	B	244	ILE
1	B	287	LYS
1	B	407	LYS
1	B	879	PHE
1	B	1303	ALA
1	B	1396	ASP
1	C	244	ILE
1	C	287	LYS
1	C	407	LYS
1	C	875	PRO
1	D	56	ASN
1	D	407	LYS
1	D	660	PHE
1	D	872	SER
1	D	1373	ALA
1	B	56	ASN
1	B	113	THR

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Mol	Chain	Res	Type
1	B	1427	THR
1	C	1440	PRO
1	D	658	LEU
1	D	1368	ARG
1	D	1440	PRO
1	A	162	LYS
1	A	880	ASP
1	B	162	LYS
1	B	218	ARG
1	B	975	LYS
1	C	54	SER
1	D	162	LYS
1	D	664	LYS
1	D	1377	ARG
1	C	162	LYS
1	D	882	ALA
1	D	971	ASP
1	D	1472	ARG
1	D	366	GLN
1	B	366	GLN
1	A	307	PRO
1	C	967	SER
1	D	113	THR

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	965/1088 (89%)	880 (91%)	85 (9%)	11	37
1	B	974/1088 (90%)	844 (87%)	130 (13%)	4	22
1	C	967/1088 (89%)	864 (89%)	103 (11%)	7	28
1	D	977/1088 (90%)	881 (90%)	96 (10%)	9	32
All	All	3883/4352 (89%)	3469 (89%)	414 (11%)	7	28

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR
1	A	54	SER
1	A	148	GLN
1	A	174	ARG
1	A	192	LYS
1	A	194	PHE
1	A	204	LEU
1	A	222	HIS
1	A	226	SER
1	A	227	LEU
1	A	238	LEU
1	A	242	ASP
1	A	286	GLU
1	A	300	PHE
1	A	308	PHE
1	A	318	PHE
1	A	322	SER
1	A	338	HIS
1	A	341	ASN
1	A	342	ARG
1	A	345	PHE
1	A	350	SER
1	A	351	ASN
1	A	359	HIS
1	A	360	LEU
1	A	361	ILE
1	A	362	ASP
1	A	363	ARG
1	A	366	GLN
1	A	372	ASP
1	A	374	LEU
1	A	377	GLU
1	A	380	LEU
1	A	408	SER
1	A	662	GLU
1	A	664	LYS
1	A	666	GLU
1	A	670	LEU
1	A	680	HIS
1	A	681	ASP
1	A	693	LYS
1	A	758	ASP
1	A	790	ASN

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Mol	Chain	Res	Type
1	A	802	ASN
1	A	806	LEU
1	A	820	PHE
1	A	847	LEU
1	A	851	ASP
1	A	874	LEU
1	A	946	ASN
1	A	952	GLU
1	A	971	ASP
1	A	972	GLU
1	A	975	LYS
1	A	1003	LEU
1	A	1005	THR
1	A	1007	LYS
1	A	1010	VAL
1	A	1013	LEU
1	A	1021	ILE
1	A	1024	LYS
1	A	1029	HIS
1	A	1042	GLU
1	A	1046	ARG
1	A	1052	HIS
1	A	1065	ASN
1	A	1096	GLU
1	A	1098	ARG
1	A	1102	ILE
1	A	1105	LEU
1	A	1107	SER
1	A	1119	ASP
1	A	1145	GLU
1	A	1151	GLU
1	A	1203	PHE
1	A	1209	HIS
1	A	1211	TYR
1	A	1247	ILE
1	A	1329	MET
1	A	1331	ASP
1	A	1335	GLU
1	A	1344	THR
1	A	1395	LEU
1	A	1420	GLU
1	A	1437	CYS

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Mol	Chain	Res	Type
1	B	46	VAL
1	B	54	SER
1	B	81	LEU
1	B	82	TYR
1	B	86	LEU
1	B	103	PHE
1	B	121	GLN
1	B	148	GLN
1	B	192	LYS
1	B	194	PHE
1	B	203	ASP
1	B	236	LEU
1	B	242	ASP
1	B	243	TYR
1	B	284	PRO
1	B	286	GLU
1	B	293	LEU
1	B	295	MET
1	B	299	SER
1	B	306	LYS
1	B	308	PHE
1	B	315	THR
1	B	317	ASP
1	B	322	SER
1	B	338	HIS
1	B	339	ARG
1	B	342	ARG
1	B	353	LEU
1	B	359	HIS
1	B	377	GLU
1	B	378	ARG
1	B	380	LEU
1	B	658	LEU
1	B	666	GLU
1	B	670	LEU
1	B	680	HIS
1	B	681	ASP
1	B	693	LYS
1	B	742	THR
1	B	758	ASP
1	B	790	ASN
1	B	802	ASN

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Mol	Chain	Res	Type
1	B	806	LEU
1	B	820	PHE
1	B	847	LEU
1	B	851	ASP
1	B	865	VAL
1	B	878	ILE
1	B	879	PHE
1	B	911	PHE
1	B	946	ASN
1	B	960	TYR
1	B	962	TYR
1	B	972	GLU
1	B	975	LYS
1	B	991	LEU
1	B	998	VAL
1	B	1003	LEU
1	B	1005	THR
1	B	1010	VAL
1	B	1013	LEU
1	B	1019	LYS
1	B	1029	HIS
1	B	1046	ARG
1	B	1052	HIS
1	B	1059	LEU
1	B	1072	THR
1	B	1089	VAL
1	B	1096	GLU
1	B	1098	ARG
1	B	1102	ILE
1	B	1105	LEU
1	B	1107	SER
1	B	1119	ASP
1	B	1130	GLN
1	B	1145	GLU
1	B	1151	GLU
1	B	1202	ILE
1	B	1203	PHE
1	B	1205	VAL
1	B	1207	SER
1	B	1214	MET
1	B	1216	ASN
1	B	1226	THR

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Mol	Chain	Res	Type
1	B	1235	ILE
1	B	1236	GLU
1	B	1238	PHE
1	B	1244	LYS
1	B	1247	ILE
1	B	1254	TYR
1	B	1261	VAL
1	B	1262	THR
1	B	1273	LYS
1	B	1276	GLN
1	B	1280	TRP
1	B	1285	LEU
1	B	1286	PHE
1	B	1295	LEU
1	B	1296	ASP
1	B	1297	LYS
1	B	1298	VAL
1	B	1300	PHE
1	B	1302	ASP
1	B	1309	THR
1	B	1311	MET
1	B	1312	TYR
1	B	1313	ASP
1	B	1316	GLU
1	B	1319	LEU
1	B	1324	TYR
1	B	1330	CYS
1	B	1331	ASP
1	B	1333	ARG
1	B	1342	TRP
1	B	1344	THR
1	B	1346	TYR
1	B	1364	VAL
1	B	1365	ASP
1	B	1377	ARG
1	B	1390	ASN
1	B	1395	LEU
1	B	1397	GLN
1	B	1398	ASP
1	B	1403	MET
1	B	1409	ILE
1	B	1412	LEU

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Mol	Chain	Res	Type
1	B	1418	TRP
1	B	1421	THR
1	B	1425	ASP
1	B	1467	LEU
1	C	44	TYR
1	C	54	SER
1	C	82	TYR
1	C	86	LEU
1	C	103	PHE
1	C	107	LEU
1	C	148	GLN
1	C	174	ARG
1	C	192	LYS
1	C	194	PHE
1	C	204	LEU
1	C	239	LYS
1	C	242	ASP
1	C	243	TYR
1	C	286	GLU
1	C	293	LEU
1	C	295	MET
1	C	299	SER
1	C	306	LYS
1	C	308	PHE
1	C	315	THR
1	C	338	HIS
1	C	339	ARG
1	C	342	ARG
1	C	353	LEU
1	C	359	HIS
1	C	363	ARG
1	C	370	LEU
1	C	377	GLU
1	C	378	ARG
1	C	380	LEU
1	C	407	LYS
1	C	664	LYS
1	C	666	GLU
1	C	670	LEU
1	C	680	HIS
1	C	681	ASP
1	C	693	LYS

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Mol	Chain	Res	Type
1	C	729	ASP
1	C	742	THR
1	C	758	ASP
1	C	790	ASN
1	C	798	LYS
1	C	802	ASN
1	C	806	LEU
1	C	820	PHE
1	C	836	ARG
1	C	844	LEU
1	C	847	LEU
1	C	851	ASP
1	C	862	LEU
1	C	886	ARG
1	C	911	PHE
1	C	925	ARG
1	C	937	GLU
1	C	946	ASN
1	C	957	LYS
1	C	960	TYR
1	C	961	ARG
1	C	962	TYR
1	C	966	SER
1	C	972	GLU
1	C	975	LYS
1	C	979	LEU
1	C	991	LEU
1	C	998	VAL
1	C	1003	LEU
1	C	1007	LYS
1	C	1010	VAL
1	C	1013	LEU
1	C	1016	LEU
1	C	1021	ILE
1	C	1029	HIS
1	C	1044	HIS
1	C	1046	ARG
1	C	1052	HIS
1	C	1059	LEU
1	C	1065	ASN
1	C	1072	THR
1	C	1084	LYS

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Mol	Chain	Res	Type
1	C	1089	VAL
1	C	1096	GLU
1	C	1098	ARG
1	C	1102	ILE
1	C	1105	LEU
1	C	1107	SER
1	C	1119	ASP
1	C	1126	LEU
1	C	1130	GLN
1	C	1145	GLU
1	C	1203	PHE
1	C	1209	HIS
1	C	1211	TYR
1	C	1247	ILE
1	C	1263	TYR
1	C	1329	MET
1	C	1331	ASP
1	C	1344	THR
1	C	1376	ASP
1	C	1395	LEU
1	C	1420	GLU
1	C	1437	CYS
1	C	1441	MET
1	D	44	TYR
1	D	47	GLU
1	D	78	ASP
1	D	81	LEU
1	D	86	LEU
1	D	103	PHE
1	D	108	SER
1	D	121	GLN
1	D	148	GLN
1	D	192	LYS
1	D	194	PHE
1	D	204	LEU
1	D	242	ASP
1	D	243	TYR
1	D	286	GLU
1	D	293	LEU
1	D	295	MET
1	D	299	SER
1	D	308	PHE

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Mol	Chain	Res	Type
1	D	315	THR
1	D	322	SER
1	D	328	GLN
1	D	338	HIS
1	D	339	ARG
1	D	341	ASN
1	D	342	ARG
1	D	353	LEU
1	D	359	HIS
1	D	363	ARG
1	D	377	GLU
1	D	378	ARG
1	D	380	LEU
1	D	385	LEU
1	D	666	GLU
1	D	670	LEU
1	D	680	HIS
1	D	681	ASP
1	D	693	LYS
1	D	758	ASP
1	D	790	ASN
1	D	802	ASN
1	D	806	LEU
1	D	820	PHE
1	D	836	ARG
1	D	844	LEU
1	D	851	ASP
1	D	864	SER
1	D	881	ASN
1	D	911	PHE
1	D	925	ARG
1	D	946	ASN
1	D	959	PHE
1	D	960	TYR
1	D	962	TYR
1	D	964	LEU
1	D	972	GLU
1	D	991	LEU
1	D	996	MET
1	D	998	VAL
1	D	1003	LEU
1	D	1005	THR

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Mol	Chain	Res	Type
1	D	1007	LYS
1	D	1010	VAL
1	D	1013	LEU
1	D	1016	LEU
1	D	1029	HIS
1	D	1046	ARG
1	D	1052	HIS
1	D	1059	LEU
1	D	1065	ASN
1	D	1072	THR
1	D	1075	MET
1	D	1084	LYS
1	D	1089	VAL
1	D	1096	GLU
1	D	1098	ARG
1	D	1102	ILE
1	D	1105	LEU
1	D	1107	SER
1	D	1119	ASP
1	D	1130	GLN
1	D	1145	GLU
1	D	1203	PHE
1	D	1209	HIS
1	D	1211	TYR
1	D	1237	GLN
1	D	1329	MET
1	D	1331	ASP
1	D	1344	THR
1	D	1365	ASP
1	D	1370	ARG
1	D	1378	LEU
1	D	1395	LEU
1	D	1420	GLU
1	D	1437	CYS
1	D	1441	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	230	ASN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	392	GLN
1	A	738	ASN
1	A	1077	ASN
1	A	1197	HIS
1	A	1224	HIS
1	A	1267	HIS
1	A	1402	HIS
1	B	148	GLN
1	B	338	HIS
1	B	392	GLN
1	B	400	HIS
1	B	738	ASN
1	B	876	GLN
1	B	881	ASN
1	B	1077	ASN
1	B	1201	ASN
1	B	1216	ASN
1	B	1237	GLN
1	B	1267	HIS
1	B	1380	GLN
1	B	1383	HIS
1	B	1390	ASN
1	B	1404	GLN
1	C	148	GLN
1	C	230	ASN
1	C	338	HIS
1	C	392	GLN
1	C	400	HIS
1	C	738	ASN
1	C	924	GLN
1	C	1044	HIS
1	C	1197	HIS
1	C	1224	HIS
1	D	148	GLN
1	D	316	GLN
1	D	338	HIS
1	D	392	GLN
1	D	400	HIS
1	D	738	ASN
1	D	807	ASN
1	D	881	ASN

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Mol	Chain	Res	Type
1	D	1029	HIS
1	D	1038	HIS
1	D	1197	HIS
1	D	1224	HIS
1	D	1267	HIS
1	D	1367	GLN
1	D	1402	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1601	-	14,14,15	0.34	0	17,19,21	0.69	0
2	NAG	A	1602	1	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
2	NAG	A	1603	1	14,14,15	0.34	0	17,19,21	0.78	1 (5%)
2	NAG	A	1605	1,2	14,14,15	0.31	0	17,19,21	1.12	2 (11%)
2	NAG	A	1606	2,4	14,14,15	0.45	0	17,19,21	2.47	3 (17%)
4	BMA	A	1607	2,5	11,11,12	0.40	0	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	1608	4	11,11,12	0.94	0	15,15,17	1.95	2 (13%)
5	MAN	A	1609	4	11,11,12	0.79	0	15,15,17	1.91	2 (13%)
2	NAG	B	1601	-	14,14,15	0.30	0	17,19,21	0.50	0
2	NAG	B	1602	1	14,14,15	0.35	0	17,19,21	1.16	1 (5%)
2	NAG	B	1603	1	14,14,15	0.36	0	17,19,21	0.98	2 (11%)
2	NAG	B	1605	1,2	14,14,15	0.29	0	17,19,21	1.20	2 (11%)
2	NAG	B	1606	2,4	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
4	BMA	B	1607	2	11,11,12	0.31	0	15,15,17	0.49	0
2	NAG	C	1601	-	14,14,15	0.50	0	17,19,21	0.80	0
2	NAG	C	1602	1,2	14,14,15	0.28	0	17,19,21	1.06	2 (11%)
2	NAG	C	1603	2,4	14,14,15	0.28	0	17,19,21	1.50	4 (23%)
4	BMA	C	1604	2,5	11,11,12	0.36	0	15,15,17	0.91	1 (6%)
5	MAN	C	1605	4	11,11,12	0.74	0	15,15,17	1.37	2 (13%)
2	NAG	C	1606	1	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
2	NAG	C	1607	1	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	D	1601	-	14,14,15	0.30	0	17,19,21	0.65	0
2	NAG	D	1602	1,2	14,14,15	0.29	0	17,19,21	1.05	2 (11%)
2	NAG	D	1603	2,4	14,14,15	0.29	0	17,19,21	1.00	2 (11%)
4	BMA	D	1604	2	11,11,12	0.30	0	15,15,17	0.42	0
2	NAG	D	1605	1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
2	NAG	D	1606	1	14,14,15	0.29	0	17,19,21	0.75	1 (5%)

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	NAG	A	1601	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1603	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1606	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1607	2,5	-	0/2/19/22	0/1/1/1
5	MAN	A	1608	4	-	0/2/19/22	1/1/1/1
5	MAN	A	1609	4	-	1/2/19/22	0/1/1/1
2	NAG	B	1601	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1603	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1606	2,4	-	4/6/23/26	0/1/1/1
4	BMA	B	1607	2	-	1/2/19/22	0/1/1/1
2	NAG	C	1601	-	-	0/6/23/26	0/1/1/1
2	NAG	C	1602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1603	2,4	-	3/6/23/26	0/1/1/1
4	BMA	C	1604	2,5	-	0/2/19/22	0/1/1/1
5	MAN	C	1605	4	-	1/2/19/22	0/1/1/1
2	NAG	C	1606	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1607	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1601	-	-	0/6/23/26	0/1/1/1
2	NAG	D	1602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1603	2,4	-	4/6/23/26	0/1/1/1
4	BMA	D	1604	2	-	1/2/19/22	0/1/1/1
2	NAG	D	1605	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1606	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1608	MAN	C1-O5-C5	6.06	120.44	112.20
2	A	1606	NAG	O5-C1-C2	-5.90	102.10	111.36
5	A	1609	MAN	C1-O5-C5	5.84	120.13	112.20
2	A	1606	NAG	C1-C2-N2	5.72	120.27	110.49
2	A	1606	NAG	C1-O5-C5	4.95	118.93	112.20
2	B	1602	NAG	C1-O5-C5	4.00	117.64	112.20
2	B	1605	NAG	O5-C1-C2	-3.86	105.30	111.36
2	C	1603	NAG	C1-C2-N2	3.71	116.83	110.49
5	C	1605	MAN	C1-O5-C5	3.64	117.15	112.20
5	A	1609	MAN	C1-C2-C3	3.56	114.03	109.66
2	B	1606	NAG	C1-C2-N2	3.46	116.39	110.49
2	A	1605	NAG	O5-C1-C2	-3.39	106.04	111.36
5	A	1608	MAN	C1-C2-C3	3.30	113.72	109.66
4	C	1604	BMA	C1-O5-C5	3.20	116.55	112.20
2	D	1602	NAG	O5-C1-C2	-3.09	106.51	111.36
2	D	1603	NAG	C1-C2-N2	3.08	115.74	110.49
2	C	1606	NAG	C1-O5-C5	3.01	116.29	112.20
2	A	1602	NAG	C1-O5-C5	2.92	116.17	112.20
2	B	1603	NAG	C1-O5-C5	2.92	116.17	112.20
2	C	1602	NAG	O5-C1-C2	-2.91	106.79	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1605	MAN	C1-C2-C3	2.77	113.06	109.66
2	C	1603	NAG	C1-O5-C5	2.77	115.97	112.20
2	A	1603	NAG	C1-O5-C5	2.76	115.96	112.20
2	C	1602	NAG	C1-O5-C5	2.65	115.81	112.20
2	D	1605	NAG	C1-O5-C5	2.64	115.78	112.20
2	B	1605	NAG	C1-O5-C5	2.60	115.73	112.20
2	D	1602	NAG	C1-O5-C5	2.59	115.73	112.20
2	C	1603	NAG	O5-C1-C2	-2.55	107.35	111.36
2	A	1605	NAG	C1-O5-C5	2.50	115.61	112.20
2	D	1606	NAG	C1-O5-C5	2.47	115.56	112.20
4	A	1607	BMA	O3-C3-C4	2.46	116.04	110.34
2	C	1603	NAG	C2-N2-C7	2.44	126.42	122.92
4	A	1607	BMA	C1-C2-C3	-2.11	107.06	109.66
2	B	1603	NAG	C1-C2-N2	2.11	114.09	110.49
2	D	1603	NAG	C2-N2-C7	2.00	125.80	122.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1606	NAG	O5-C5-C6-O6
2	D	1603	NAG	O5-C5-C6-O6
5	A	1609	MAN	O5-C5-C6-O6
5	C	1605	MAN	O5-C5-C6-O6
2	C	1603	NAG	O5-C5-C6-O6
4	B	1607	BMA	O5-C5-C6-O6
4	D	1604	BMA	O5-C5-C6-O6
2	D	1603	NAG	C4-C5-C6-O6
2	B	1606	NAG	C4-C5-C6-O6
2	B	1606	NAG	C3-C2-N2-C7
2	C	1603	NAG	C3-C2-N2-C7
2	D	1603	NAG	C1-C2-N2-C7
2	C	1603	NAG	C1-C2-N2-C7
2	D	1603	NAG	C3-C2-N2-C7
2	B	1606	NAG	C1-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1608	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1605	NAG	4	0
2	A	1606	NAG	4	0

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.