



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:18 PM EDT

PDB ID : 3MX0 / pdb_00003mx0
Title : Crystal Structure of EphA2 ectodomain in complex with ephrin-A5
Authors : Himanen, J.P.; Yermekbayeva, L.; Janes, P.W.; Walker, J.R.; Xu, K.; Atapattu, L.; Rajashankar, K.R.; Mensinga, A.; Lackmann, M.; Nikolov, D.B.; Dhe-Paganon, S.
Deposited on : 2010-05-06
Resolution : 3.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

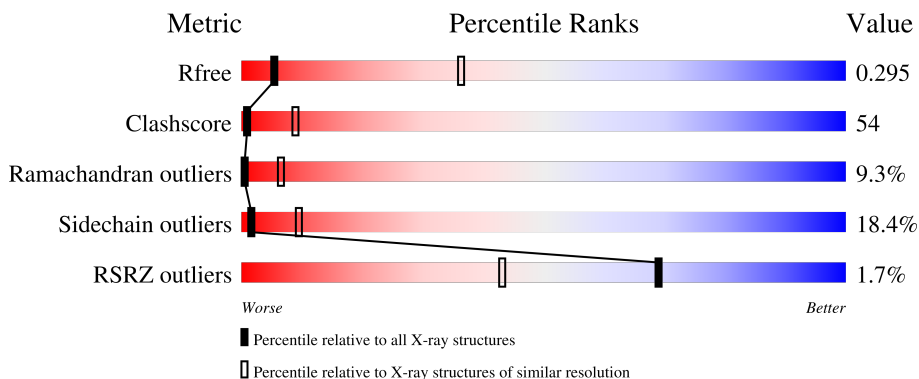
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 Å.

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



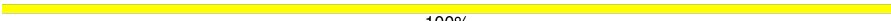
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	409	 29% 50% 19% ..
1	C	409	 30% 49% 18% ..
2	B	138	 37% 51% 10% .
2	D	138	 27% 59% 13% .
3	E	3	 33% 67%

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Mol	Chain	Length	Quality of chain
3	F	3	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8574 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.

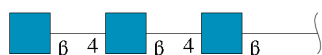
- Molecule 1 is a protein called Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	406	Total 3080	C 1944	N 511	O 597	S 28	0	0	0
1	C	406	Total 3080	C 1944	N 511	O 597	S 28	0	0	0

- Molecule 2 is a protein called Ephrin-A5.

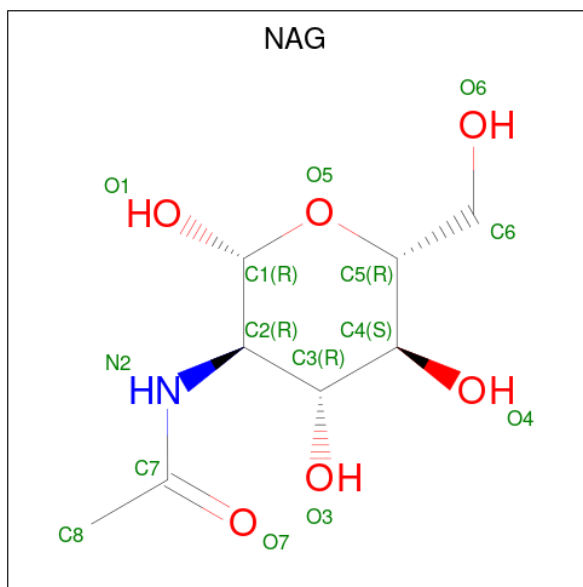
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	138	Total 1151	C 736	N 198	O 209	S 8	0	0	0
2	D	138	Total 1151	C 736	N 198	O 209	S 8	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	3	Total 42	C 24	N 3	O 15	0	0	0
3	F	3	Total 42	C 24	N 3	O 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

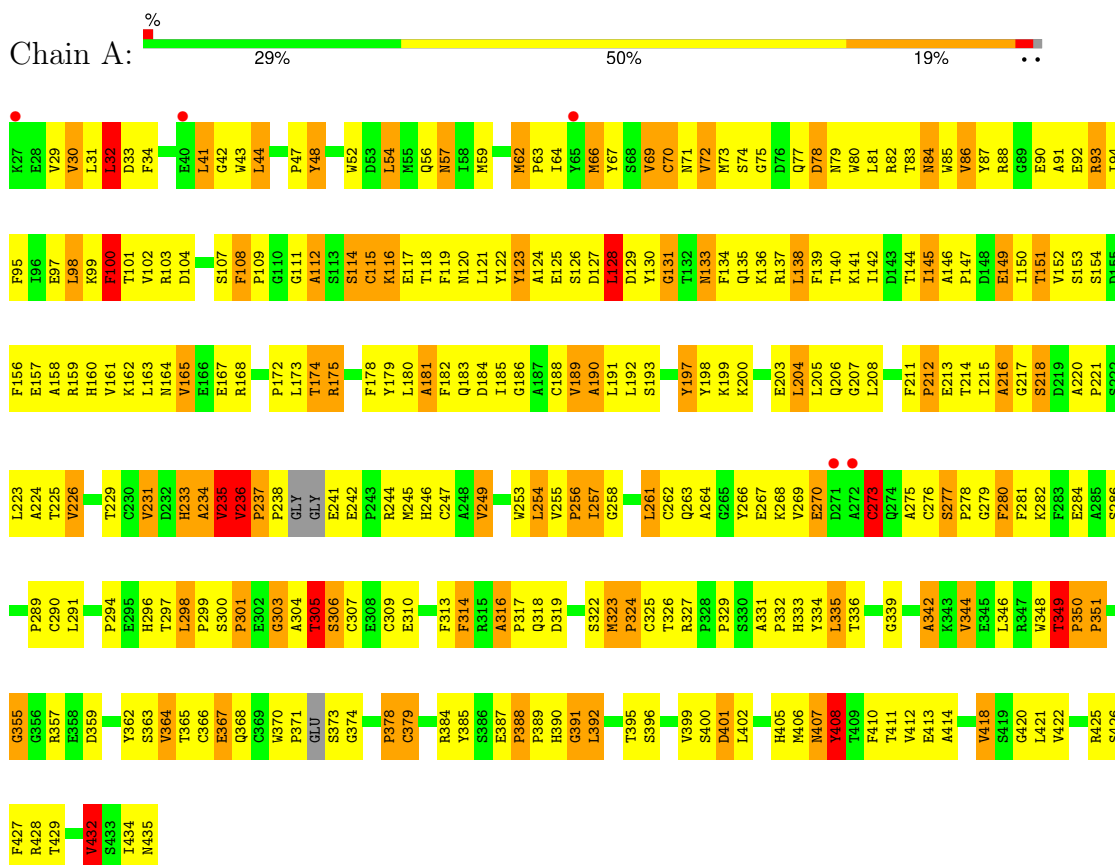


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots i

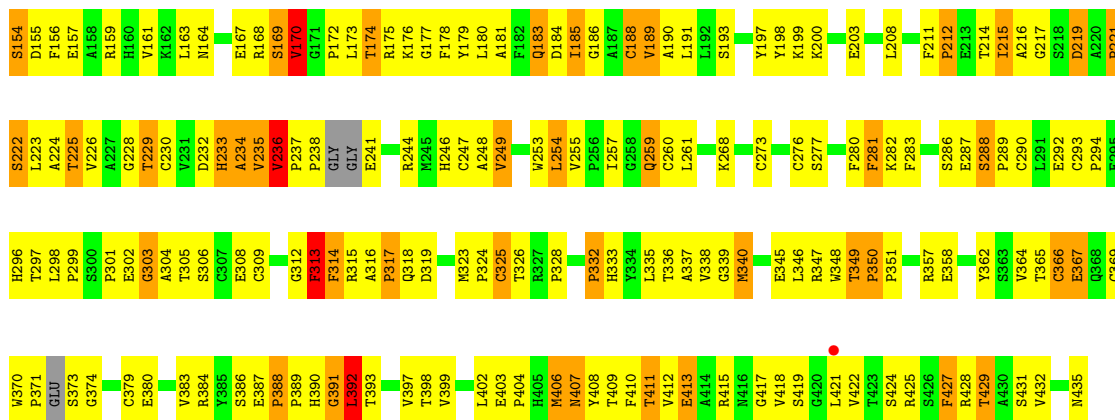
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Ephrin type-A receptor 2



• Molecule 1: Ephrin type-A receptor 2





MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.86Å 89.05Å 198.15Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	45.03 – 3.51 45.03 – 3.51	Depositor EDS
% Data completeness (in resolution range)	88.1 (45.03-3.51) 88.1 (45.03-3.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.234 , 0.295 0.228 , 0.295	Depositor DCC
R_{free} test set	1157 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtrriage
Anisotropy	1.284	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 99.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.065 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8574	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	2/3163 (0.1%)	1.19	36/4314 (0.8%)
1	C	0.64	0/3163	1.14	24/4314 (0.6%)
2	B	0.52	0/1190	1.05	5/1610 (0.3%)
2	D	0.54	0/1190	0.96	3/1610 (0.2%)
All	All	0.63	2/8706 (0.0%)	1.12	68/11848 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	PRO	CA-C	6.02	1.55	1.51
1	A	237	PRO	CA-C	5.18	1.56	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	107	SER	CA-C-N	11.67	132.63	119.32
2	B	107	SER	C-N-CA	11.67	132.63	119.32
1	A	236	VAL	CA-C-N	9.87	130.55	120.38
1	A	236	VAL	C-N-CA	9.87	130.55	120.38
1	A	237	PRO	N-CA-C	8.56	121.14	110.70
1	C	254	LEU	N-CA-C	8.55	124.08	111.34
1	C	288	SER	CA-C-N	8.45	130.40	119.84
1	C	288	SER	C-N-CA	8.45	130.40	119.84
1	C	40	GLU	N-CA-C	-8.35	103.58	112.93
1	A	350	PRO	CA-C-N	8.34	130.26	119.84
1	A	350	PRO	C-N-CA	8.34	130.26	119.84
1	C	314	PHE	N-CA-C	8.32	118.92	108.19
1	C	235	VAL	N-CA-C	8.04	119.17	107.75
1	A	314	PHE	N-CA-C	7.92	118.43	108.45
1	A	62	MET	CA-C-N	7.60	127.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	MET	C-N-CA	7.60	127.89	119.90
1	A	236	VAL	N-CA-C	6.89	114.72	107.76
1	A	432	VAL	N-CA-C	6.79	117.25	107.88
1	A	82	ARG	N-CA-C	6.56	120.54	107.62
2	D	159	ARG	CA-C-N	6.55	128.03	119.84
2	D	159	ARG	C-N-CA	6.55	128.03	119.84
1	C	236	VAL	CA-C-N	6.49	127.07	120.38
1	C	236	VAL	C-N-CA	6.49	127.07	120.38
1	C	96	ILE	CB-CA-C	-6.45	103.06	110.73
1	C	146	ALA	CA-C-N	6.37	127.33	120.13
1	C	146	ALA	C-N-CA	6.37	127.33	120.13
1	A	100	PHE	N-CA-C	6.24	117.88	108.46
1	C	350	PRO	O-C-N	5.96	123.95	121.15
1	A	199	LYS	N-CA-C	5.84	117.91	108.34
1	A	30	VAL	N-CA-C	5.83	116.97	108.58
1	C	56	GLN	N-CA-C	5.76	117.77	107.80
1	A	254	LEU	N-CA-C	5.57	122.66	110.80
1	A	213	GLU	N-CA-C	-5.47	100.33	109.24
1	A	316	ALA	CA-C-N	5.45	125.12	119.56
1	A	316	ALA	C-N-CA	5.45	125.12	119.56
1	A	270	GLU	CB-CA-C	-5.44	110.29	116.54
1	C	391	GLY	N-CA-C	-5.40	107.52	115.30
1	A	108	PHE	CA-C-N	5.37	126.56	119.84
1	A	108	PHE	C-N-CA	5.37	126.56	119.84
1	A	298	LEU	CA-C-N	5.36	126.55	119.84
1	A	298	LEU	C-N-CA	5.36	126.55	119.84
1	C	348	TRP	N-CA-C	5.36	118.18	109.24
1	C	413	GLU	N-CA-C	5.32	118.12	109.24
1	A	218	SER	N-CA-C	5.29	117.86	111.40
1	A	323	MET	CA-C-N	5.29	126.45	119.84
1	A	323	MET	C-N-CA	5.29	126.45	119.84
1	A	133	ASN	N-CA-C	-5.28	102.47	110.28
1	C	388	PRO	CA-C-N	5.26	126.41	119.84
1	C	388	PRO	C-N-CA	5.26	126.41	119.84
1	C	328	PRO	CA-C-N	5.24	125.00	119.76
1	C	328	PRO	C-N-CA	5.24	125.00	119.76
1	A	322	SER	N-CA-C	-5.24	106.58	113.12
1	C	350	PRO	CA-C-N	5.22	126.37	119.84
1	C	350	PRO	C-N-CA	5.22	126.37	119.84
1	A	349	THR	CA-C-N	5.16	125.69	120.38
1	A	349	THR	C-N-CA	5.16	125.69	120.38
1	C	349	THR	CA-C-N	5.12	123.34	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	349	THR	C-N-CA	5.12	123.34	119.66
1	A	355	GLY	N-CA-C	-5.10	105.22	114.46
2	B	156	VAL	N-CA-C	5.09	115.37	107.78
1	A	174	THR	N-CA-C	5.08	116.62	111.14
1	A	342	ALA	N-CA-C	-5.03	107.82	114.31
2	B	134	ARG	N-CA-C	-5.03	102.74	110.14
2	D	125	SER	N-CA-C	-5.03	107.20	113.19
1	A	175	ARG	N-CA-C	5.03	117.93	110.48
1	A	235	VAL	CA-C-N	5.03	126.21	122.59
1	A	235	VAL	C-N-CA	5.03	126.21	122.59
2	B	101	GLU	N-CA-C	5.01	116.33	107.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3080	0	2863	336	0
1	C	3080	0	2863	323	0
2	B	1151	0	1067	120	0
2	D	1151	0	1067	152	0
3	E	42	0	37	1	0
3	F	42	0	37	0	0
4	A	14	0	13	2	0
4	C	14	0	13	1	0
All	All	8574	0	7960	886	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 54.

All (886) 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:C:103:ARG:HD2	1:C:156:PHE:CZ	1.74	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB1	2:B:124:PHE:CZ	1.79	1.18
1:C:71:ASN:HB3	1:C:77:GLN:NE2	1.67	1.09
1:A:200:LYS:HB3	1:A:215:ILE:HD13	1.35	1.05
1:C:139:PHE:HE1	1:C:181:ALA:HB2	1.19	1.04
1:C:103:ARG:HD2	1:C:156:PHE:HZ	0.93	1.04
1:C:224:ALA:HB3	1:C:247:CYS:HB3	1.39	1.04
1:C:370:TRP:HB3	1:C:373:SER:HB3	1.36	1.02
1:A:224:ALA:HB3	1:A:247:CYS:HB3	1.41	1.02
1:C:120:ASN:HB3	1:C:122:TYR:HE1	1.27	0.99
2:B:43:PHE:HB3	2:B:152:LEU:HD21	1.50	0.94
1:C:139:PHE:CE1	1:C:181:ALA:HB2	2.02	0.93
1:C:43:TRP:CD1	1:C:83:THR:HA	2.04	0.93
1:C:67:TYR:CD1	1:C:81:LEU:HD11	2.05	0.92
1:C:100:PHE:CE2	1:C:164:ASN:HB2	2.05	0.92
1:C:59:MET:HB2	1:C:64:ILE:HD13	1.50	0.92
1:C:223:LEU:HD21	1:C:254:LEU:HD12	1.52	0.90
1:A:408:TYR:HB2	1:A:432:VAL:O	1.72	0.90
2:D:81:MET:HG3	2:D:138:TYR:CE2	2.09	0.88
1:C:103:ARG:CD	1:C:156:PHE:HZ	1.84	0.88
1:A:192:LEU:HD21	2:B:124:PHE:HE1	1.38	0.87
1:C:72:VAL:HG21	1:C:108:PHE:CE1	2.09	0.86
1:C:55:MET:HE3	2:D:117:LYS:HD3	1.57	0.86
1:C:94:ILE:HG12	1:C:173:LEU:HD11	1.58	0.86
1:A:71:ASN:HB3	1:A:77:GLN:HE22	1.39	0.85
1:C:365:THR:OG1	1:C:411:THR:HG23	1.76	0.85
1:C:53:ASP:HB2	1:C:55:MET:HE1	1.59	0.85
2:D:149:ARG:HG2	2:D:150:SER:N	1.91	0.85
1:A:103:ARG:HD2	1:A:156:PHE:CZ	2.12	0.85
2:D:100:TRP:CD2	2:D:114:PHE:HB3	2.12	0.85
1:C:71:ASN:CB	1:C:77:GLN:NE2	2.41	0.84
1:A:72:VAL:HG11	1:A:108:PHE:CE1	2.13	0.84
2:D:60:VAL:HG11	2:D:79:LEU:HD11	1.59	0.83
2:D:51:ASP:HB3	2:D:159:ARG:HD3	1.62	0.82
2:B:81:MET:HG3	2:B:138:TYR:CE2	2.14	0.82
1:C:87:TYR:HD2	1:C:176:LYS:O	1.64	0.81
2:D:131:ARG:HH11	2:D:134:ARG:NH2	1.77	0.81
1:A:93:ARG:HG2	1:A:95:PHE:HE2	1.45	0.80
1:C:122:TYR:HD2	1:C:139:PHE:O	1.65	0.80
1:C:72:VAL:HG21	1:C:108:PHE:HE1	1.47	0.80
1:A:371:PRO:C	1:A:373:SER:N	2.40	0.80
1:C:52:TRP:CD1	1:C:80:TRP:O	2.36	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ALA:HB2	1:C:198:TYR:CG	2.19	0.78
1:A:103:ARG:CZ	2:B:121:PHE:CZ	2.67	0.78
1:C:208:LEU:HD11	1:C:268:LYS:HG3	1.66	0.78
1:C:107:SER:HB3	1:C:153:SER:OG	1.84	0.77
1:C:32:LEU:HD12	1:C:33:ASP:N	1.98	0.77
2:D:34:VAL:HG12	2:D:34:VAL:O	1.83	0.77
1:A:335:LEU:HD12	1:A:336:THR:H	1.47	0.77
1:A:212:PRO:HB2	1:A:214:THR:HG23	1.67	0.77
2:B:118:PHE:HA	2:B:130:PHE:CD1	2.20	0.77
1:C:71:ASN:HB3	1:C:77:GLN:HE22	1.50	0.77
1:A:41:LEU:HD21	1:A:84:ASN:HD22	1.50	0.76
1:A:71:ASN:HB3	1:A:77:GLN:NE2	2.01	0.76
1:A:335:LEU:HD12	1:A:336:THR:N	2.01	0.76
1:C:31:LEU:O	1:C:32:LEU:HB3	1.85	0.76
1:C:82:ARG:HB2	1:C:134:PHE:HE1	1.50	0.76
1:A:188:CYS:SG	2:B:123:PRO:HB3	2.26	0.76
1:C:100:PHE:HE2	1:C:164:ASN:HB2	1.51	0.75
2:D:40:ASN:HB3	2:D:43:PHE:HD2	1.51	0.75
2:D:87:TYR:CD1	2:D:137:PHE:HB3	2.21	0.75
1:C:93:ARG:HD3	1:C:95:PHE:HE2	1.51	0.74
2:D:122:THR:HG23	2:D:124:PHE:CD1	2.22	0.74
1:A:43:TRP:CG	1:A:83:THR:HA	2.22	0.74
1:A:226:VAL:HG21	1:A:253:TRP:HZ3	1.52	0.74
1:C:134:PHE:HD2	1:C:134:PHE:O	1.70	0.74
1:C:389:PRO:HB2	1:C:390:HIS:CD2	2.23	0.74
2:D:40:ASN:HD22	2:D:43:PHE:HE2	1.35	0.74
1:A:100:PHE:CE1	1:A:119:PHE:HE2	2.05	0.73
1:A:399:VAL:HG12	1:A:402:LEU:HD21	1.69	0.73
1:C:406:MET:HB3	1:C:408:TYR:CD1	2.23	0.73
1:C:95:PHE:HB2	1:C:197:TYR:CE1	2.22	0.73
1:A:43:TRP:CD1	1:A:84:ASN:H	2.06	0.73
1:A:208:LEU:HD11	1:A:268:LYS:HD2	1.70	0.73
1:C:276:CYS:HB2	1:C:303:GLY:HA2	1.70	0.73
1:C:80:TRP:CE2	1:C:183:GLN:HB2	2.23	0.73
1:C:120:ASN:HB3	1:C:122:TYR:CE1	2.18	0.73
1:C:223:LEU:HD23	1:C:248:ALA:HB2	1.70	0.73
1:C:413:GLU:OE1	1:C:425:ARG:HD2	1.88	0.73
2:B:144:PRO:HB2	2:B:146:ASN:HD21	1.51	0.73
1:C:188:CYS:SG	2:D:121:PHE:CE2	2.82	0.73
1:A:167:GLU:O	1:A:168:ARG:HG2	1.89	0.73
1:C:137:ARG:O	1:C:138:LEU:HD23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ARG:HH22	1:C:257:ILE:HG21	1.54	0.72
2:D:51:ASP:OD1	2:D:157:PHE:HB3	1.89	0.72
1:C:108:PHE:CZ	2:D:121:PHE:CE1	2.77	0.72
1:C:134:PHE:O	1:C:134:PHE:CD2	2.43	0.72
1:A:100:PHE:O	1:A:164:ASN:HB2	1.89	0.72
2:D:149:ARG:HG2	2:D:150:SER:H	1.51	0.72
1:A:384:ARG:H	1:A:401:ASP:HB3	1.54	0.72
2:B:87:TYR:HE1	2:B:153:LYS:HB2	1.55	0.72
1:C:226:VAL:HG21	1:C:253:TRP:CH2	2.25	0.72
1:A:41:LEU:HD21	1:A:84:ASN:ND2	2.05	0.71
1:A:411:THR:CB	1:A:429:THR:HG22	2.20	0.71
1:A:54:LEU:HD22	1:A:67:TYR:CE2	2.26	0.71
1:C:357:ARG:O	1:C:358:GLU:HG3	1.90	0.71
1:C:129:ASP:O	1:C:130:TYR:CD2	2.43	0.71
1:A:56:GLN:O	1:A:57:ASN:HB2	1.92	0.70
1:A:314:PHE:CD1	1:A:421:LEU:HD13	2.25	0.70
1:A:246:HIS:HB2	1:A:255:VAL:H	1.57	0.70
1:A:413:GLU:OE1	1:A:425:ARG:HD2	1.92	0.70
1:C:203:GLU:HA	1:C:212:PRO:O	1.91	0.70
2:B:87:TYR:CE1	2:B:153:LYS:HB2	2.25	0.70
1:C:46:HIS:C	1:C:46:HIS:CD2	2.70	0.70
1:C:80:TRP:CD2	1:C:183:GLN:HB2	2.27	0.70
1:C:95:PHE:CD2	1:C:169:SER:HB3	2.27	0.70
1:C:99:LYS:HB2	1:C:193:SER:HB3	1.73	0.70
2:D:87:TYR:HB2	2:D:137:PHE:HB3	1.73	0.70
1:A:52:TRP:HA	1:A:69:VAL:HG23	1.74	0.70
1:C:123:TYR:HA	1:C:179:TYR:O	1.90	0.70
2:D:100:TRP:CG	2:D:114:PHE:HB3	2.26	0.69
2:D:59:ASP:HB3	2:D:61:PHE:CE1	2.26	0.69
2:D:121:PHE:CD2	2:D:122:THR:N	2.61	0.69
1:A:32:LEU:HD12	1:A:33:ASP:N	2.07	0.69
1:C:92:GLU:O	1:C:172:PRO:HA	1.91	0.69
1:C:135:GLN:HG3	1:C:137:ARG:HG2	1.74	0.69
1:A:91:ALA:HB2	1:A:198:TYR:CG	2.28	0.69
2:B:31:ARG:HG2	2:B:57:TYR:HB2	1.73	0.69
1:C:137:ARG:C	1:C:138:LEU:HD23	2.17	0.69
1:C:200:LYS:HB3	1:C:215:ILE:HG23	1.74	0.69
1:C:366:CYS:HB2	1:C:410:PHE:CE2	2.27	0.69
1:C:411:THR:HB	1:C:429:THR:HG22	1.73	0.69
1:A:167:GLU:C	1:A:168:ARG:HG2	2.16	0.69
1:A:66:MET:SD	2:B:124:PHE:CZ	2.86	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:TYR:HD1	2:D:137:PHE:HB3	1.57	0.69
1:A:72:VAL:HG11	1:A:108:PHE:HE1	1.53	0.69
1:A:235:VAL:HG13	1:A:236:VAL:N	2.08	0.69
1:A:167:GLU:HG3	1:A:168:ARG:N	2.09	0.68
1:A:411:THR:HB	1:A:429:THR:HG22	1.76	0.68
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.59	0.68
1:C:103:ARG:NH2	2:D:121:PHE:CE1	2.62	0.68
1:C:406:MET:O	1:C:408:TYR:N	2.27	0.68
1:A:103:ARG:HD2	1:A:156:PHE:HZ	1.59	0.68
1:A:224:ALA:CB	1:A:247:CYS:HB3	2.23	0.68
1:A:234:ALA:HA	1:A:261:LEU:O	1.93	0.68
1:A:120:ASN:HB3	1:A:122:TYR:HE1	1.59	0.68
1:A:172:PRO:HB3	1:A:218:SER:CB	2.24	0.67
1:C:415:ARG:NH1	1:C:419:SER:HB3	2.09	0.67
1:C:244:ARG:NH2	1:C:257:ILE:HG21	2.10	0.67
1:A:102:VAL:HG11	1:A:117:GLU:HB3	1.76	0.67
1:A:192:LEU:HD21	2:B:124:PHE:CE1	2.26	0.67
1:A:226:VAL:HG21	1:A:253:TRP:CZ3	2.29	0.67
1:A:316:ALA:O	1:A:319:ASP:HB2	1.95	0.67
1:C:47:PRO:HD2	1:C:79:ASN:HA	1.76	0.66
1:C:326:THR:O	1:C:418:VAL:HG21	1.96	0.66
1:A:276:CYS:HB2	1:A:303:GLY:HA2	1.77	0.66
1:C:337:ALA:HB2	1:C:346:LEU:HD23	1.76	0.66
1:A:84:ASN:O	1:A:179:TYR:CE1	2.48	0.66
1:A:253:TRP:O	1:A:254:LEU:HD23	1.96	0.66
2:D:131:ARG:NH1	2:D:134:ARG:NH2	2.44	0.66
1:A:334:TYR:HB2	1:A:349:THR:HB	1.75	0.66
1:C:406:MET:HB3	1:C:408:TYR:CE1	2.30	0.66
1:A:103:ARG:NE	2:B:121:PHE:CZ	2.64	0.66
2:D:48:TYR:HD1	2:D:49:HIS:N	1.93	0.65
1:A:30:VAL:HG12	1:A:32:LEU:H	1.61	0.65
2:D:82:VAL:HG11	2:D:139:ILE:HD11	1.78	0.65
1:A:242:GLU:O	1:A:258:GLY:HA3	1.96	0.65
1:C:34:PHE:HB2	1:C:43:TRP:CH2	2.30	0.65
1:C:139:PHE:CE1	1:C:181:ALA:CB	2.79	0.65
2:D:89:ALA:O	2:D:90:CYS:C	2.38	0.65
1:C:143:ASP:OD1	1:C:144:THR:N	2.29	0.65
1:A:335:LEU:HD13	1:A:348:TRP:HB3	1.78	0.65
1:A:77:GLN:O	1:A:78:ASP:HB2	1.96	0.65
1:A:100:PHE:CE1	1:A:119:PHE:CE2	2.85	0.65
1:C:200:LYS:HA	1:C:215:ILE:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ALA:HA	1:C:261:LEU:O	1.97	0.64
2:B:150:SER:O	2:B:151:CYS:HB3	1.97	0.64
1:C:103:ARG:CZ	2:D:121:PHE:CE1	2.80	0.64
1:A:182:PHE:CE1	1:A:191:LEU:HD11	2.33	0.64
1:A:296:HIS:HB2	1:A:325:CYS:HB2	1.79	0.64
2:D:76:ARG:HG3	2:D:76:ARG:HH11	1.62	0.64
2:B:62:CYS:HB3	2:B:63:PRO:HD2	1.79	0.64
1:A:94:ILE:HG23	1:A:173:LEU:HD12	1.79	0.64
1:C:74:SER:HB2	1:C:77:GLN:HE22	1.61	0.64
1:A:314:PHE:HD1	1:A:421:LEU:HD13	1.61	0.64
2:B:100:TRP:CH2	2:B:116:GLU:HB2	2.32	0.64
2:D:100:TRP:HB3	2:D:114:PHE:CG	2.32	0.64
2:B:164:CYS:O	2:B:165:MET:HB2	1.98	0.64
1:A:269:VAL:HG12	1:A:270:GLU:HG2	1.80	0.63
1:A:313:PHE:HB3	1:A:325:CYS:HB3	1.79	0.63
1:A:406:MET:C	1:A:408:TYR:H	2.05	0.63
1:C:362:TYR:HB2	1:C:392:LEU:HB3	1.79	0.63
1:A:134:PHE:CD2	1:A:135:GLN:N	2.66	0.63
1:C:87:TYR:CD2	1:C:176:LYS:O	2.49	0.63
1:A:348:TRP:O	1:A:395:THR:HB	1.97	0.63
2:B:120:LEU:HD12	2:B:120:LEU:H	1.63	0.63
1:C:237:PRO:HB2	1:C:238:PRO:HD3	1.81	0.63
2:B:82:VAL:HG12	2:B:96:GLY:HA3	1.81	0.63
1:C:82:ARG:HB2	1:C:134:PHE:CE1	2.32	0.63
2:B:105:PRO:HG2	2:B:106:HIS:CD2	2.33	0.63
1:C:127:ASP:OD1	1:C:175:ARG:HB3	1.99	0.63
1:C:137:ARG:HG3	1:C:138:LEU:HD23	1.81	0.63
1:A:235:VAL:HG22	1:A:236:VAL:H	1.62	0.63
2:B:43:PHE:HB3	2:B:152:LEU:CD2	2.25	0.63
1:C:121:LEU:HB2	1:C:145:ILE:HD11	1.80	0.63
1:C:151:THR:HG21	2:D:125:SER:OG	1.99	0.63
1:C:333:HIS:O	1:C:428:ARG:NH1	2.31	0.63
2:D:40:ASN:OD1	2:D:41:PRO:HD2	1.98	0.63
2:D:65:TYR:HB3	2:D:69:VAL:HG21	1.79	0.63
1:A:93:ARG:CG	1:A:95:PHE:HE2	2.09	0.62
1:A:367:GLU:HA	1:A:378:PRO:HA	1.80	0.62
1:A:103:ARG:NE	2:B:121:PHE:HZ	1.97	0.62
1:C:369:CYS:HB2	1:C:407:ASN:HB3	1.82	0.62
1:A:313:PHE:C	1:A:314:PHE:CD2	2.77	0.62
2:D:33:ALA:O	2:D:34:VAL:HG23	1.98	0.62
2:D:52:VAL:HA	2:D:159:ARG:NH2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:TRP:HB3	2:D:114:PHE:CD1	2.34	0.62
1:C:246:HIS:ND1	1:C:255:VAL:HG23	2.14	0.62
1:A:277:SER:HB3	1:A:278:PRO:CD	2.30	0.62
2:D:82:VAL:CG1	2:D:139:ILE:HD11	2.30	0.62
1:C:93:ARG:HG3	1:C:93:ARG:O	1.99	0.62
2:D:98:LYS:HD3	2:D:98:LYS:C	2.25	0.62
2:D:43:PHE:C	2:D:45:ARG:H	2.08	0.61
1:A:147:PRO:HB3	1:A:164:ASN:HD21	1.65	0.61
1:C:103:ARG:NE	2:D:121:PHE:CZ	2.69	0.61
1:C:217:GLY:O	1:C:249:VAL:HG13	2.00	0.61
1:C:119:PHE:CE2	1:C:189:VAL:HG11	2.36	0.61
1:C:221:PRO:HG2	1:C:222:SER:H	1.65	0.61
1:C:314:PHE:O	1:C:315:ARG:HG3	2.01	0.61
1:A:71:ASN:CB	1:A:77:GLN:NE2	2.63	0.61
1:C:103:ARG:CZ	2:D:121:PHE:CZ	2.83	0.61
1:C:316:ALA:HB3	1:C:319:ASP:OD1	2.00	0.61
1:A:95:PHE:HB3	1:A:197:TYR:CE2	2.36	0.61
1:C:219:ASP:HB2	1:C:222:SER:HB2	1.81	0.61
1:A:102:VAL:HG21	1:A:147:PRO:HG3	1.82	0.61
2:B:100:TRP:CG	2:B:114:PHE:HB3	2.36	0.61
1:C:198:TYR:CE1	1:C:215:ILE:HG21	2.35	0.61
2:D:77:TYR:O	2:D:143:ILE:HD11	2.01	0.61
1:A:69:VAL:HG21	1:A:79:ASN:HD22	1.65	0.61
1:A:178:PHE:CD1	1:A:178:PHE:C	2.79	0.61
2:B:161:THR:O	2:B:162:ASN:HB3	1.99	0.61
1:A:200:LYS:HB3	1:A:215:ILE:CD1	2.21	0.60
1:A:384:ARG:N	1:A:401:ASP:HB3	2.16	0.60
1:C:411:THR:HB	1:C:429:THR:CG2	2.30	0.60
1:C:85:TRP:CZ2	1:C:177:GLY:HA3	2.37	0.60
1:A:29:VAL:HG12	1:A:198:TYR:CE2	2.37	0.60
1:A:224:ALA:HB3	1:A:247:CYS:CB	2.25	0.60
2:B:100:TRP:CD1	2:B:114:PHE:CD2	2.90	0.60
1:C:32:LEU:HD12	1:C:32:LEU:C	2.27	0.60
1:A:52:TRP:CG	1:A:81:LEU:HB2	2.37	0.60
1:A:192:LEU:CD2	2:B:124:PHE:HE1	2.14	0.60
1:C:46:HIS:HA	1:C:47:PRO:C	2.27	0.60
1:A:119:PHE:CD2	1:A:189:VAL:HG11	2.37	0.60
1:C:223:LEU:CD2	1:C:254:LEU:HD12	2.29	0.60
1:C:298:LEU:HB2	1:C:308:GLU:O	2.01	0.59
1:C:226:VAL:HG21	1:C:253:TRP:HH2	1.66	0.59
1:C:338:VAL:HG12	1:C:339:GLY:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:CD1	1:A:81:LEU:HB2	2.37	0.59
2:D:79:LEU:HD12	2:D:100:TRP:CE3	2.37	0.59
1:C:123:TYR:CD1	1:C:123:TYR:C	2.80	0.59
2:D:79:LEU:HD12	2:D:100:TRP:HE3	1.67	0.59
2:B:98:LYS:O	2:B:98:LYS:HD3	2.02	0.59
1:A:233:HIS:O	1:A:234:ALA:HB2	2.03	0.59
1:A:399:VAL:O	1:A:402:LEU:HD11	2.03	0.59
1:A:77:GLN:O	1:A:78:ASP:CB	2.49	0.59
1:A:246:HIS:ND1	1:A:255:VAL:HG22	2.18	0.59
1:C:107:SER:O	1:C:109:PRO:HD3	2.03	0.59
1:C:233:HIS:O	1:C:273:CYS:SG	2.60	0.59
2:D:91:ASP:OD2	2:D:94:SER:HB2	2.01	0.59
1:A:204:LEU:HD22	1:A:205:LEU:N	2.17	0.59
1:A:217:GLY:O	1:A:249:VAL:HG13	2.03	0.59
1:A:282:LYS:HE2	1:A:286:SER:OG	2.02	0.59
2:B:161:THR:O	2:B:162:ASN:CB	2.51	0.59
1:A:43:TRP:CD1	1:A:83:THR:HA	2.38	0.59
1:A:246:HIS:O	1:A:254:LEU:N	2.36	0.59
2:B:100:TRP:CD1	2:B:114:PHE:HB3	2.38	0.59
2:D:54:ILE:O	2:D:55:ASN:HB2	2.01	0.59
1:A:44:LEU:HD23	1:A:44:LEU:C	2.28	0.58
2:B:160:PRO:HD2	2:B:163:SER:HB2	1.83	0.58
2:D:122:THR:HG22	2:D:124:PHE:H	1.68	0.58
1:A:71:ASN:CB	1:A:77:GLN:HE22	2.12	0.58
1:A:370:TRP:CD1	1:A:373:SER:HB3	2.39	0.58
1:C:128:LEU:HD12	1:C:130:TYR:CE2	2.39	0.58
2:D:82:VAL:HG12	2:D:96:GLY:HA3	1.83	0.58
1:A:84:ASN:O	1:A:179:TYR:CD1	2.56	0.58
1:C:84:ASN:O	1:C:85:TRP:C	2.46	0.58
1:A:182:PHE:CD2	1:A:182:PHE:N	2.70	0.58
1:A:167:GLU:HG3	1:A:168:ARG:H	1.67	0.58
1:C:93:ARG:CD	1:C:95:PHE:HE2	2.14	0.58
1:C:223:LEU:CD2	1:C:248:ALA:HB2	2.33	0.58
2:D:52:VAL:HG13	2:D:156:VAL:HG13	1.86	0.58
2:B:43:PHE:CD1	2:B:48:TYR:HD2	2.21	0.58
1:A:95:PHE:CB	1:A:197:TYR:CE2	2.87	0.58
1:C:91:ALA:HB2	1:C:198:TYR:CD1	2.39	0.58
1:C:167:GLU:O	1:C:168:ARG:HD3	2.03	0.58
1:A:329:PRO:HG2	1:A:414:ALA:O	2.04	0.58
2:D:99:ARG:HG3	2:D:99:ARG:HH11	1.69	0.58
1:C:68:SER:HB3	2:D:124:PHE:HZ	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TRP:CZ2	2:D:140:SER:HB3	2.39	0.57
1:A:145:ILE:HD13	1:A:145:ILE:N	2.19	0.57
1:C:122:TYR:CD2	1:C:139:PHE:O	2.51	0.57
2:B:36:TRP:CZ2	2:B:140:SER:HB3	2.39	0.57
1:C:152:VAL:O	1:C:155:ASP:HB2	2.03	0.57
1:A:41:LEU:HD22	1:A:43:TRP:CD1	2.39	0.57
1:A:88:ARG:HG2	1:A:88:ARG:NH1	2.18	0.57
1:A:332:PRO:HG2	1:A:412:VAL:HG13	1.86	0.57
1:A:31:LEU:O	1:A:32:LEU:HB2	2.04	0.57
1:A:175:ARG:HG3	1:A:175:ARG:HH11	1.69	0.57
2:B:132:PRO:HA	2:B:158:VAL:HG11	1.86	0.57
2:D:120:LEU:HD23	2:D:130:PHE:O	2.04	0.57
1:A:134:PHE:HE2	1:A:136:LYS:HG3	1.68	0.57
1:A:236:VAL:O	1:A:236:VAL:HG22	2.04	0.57
1:C:392:LEU:HD21	1:C:397:VAL:HG11	1.87	0.57
2:D:34:VAL:O	2:D:34:VAL:CG1	2.53	0.57
1:A:57:ASN:HD21	2:B:127:GLY:N	2.03	0.57
1:C:73:MET:SD	1:C:112:ALA:HB3	2.43	0.57
1:A:108:PHE:CZ	2:B:121:PHE:CZ	2.92	0.57
1:A:114:SER:O	1:A:116:LYS:HE2	2.04	0.57
2:B:133:GLY:H	2:B:158:VAL:HB	1.69	0.57
1:A:66:MET:HE2	1:A:192:LEU:HD11	1.86	0.57
1:A:108:PHE:CE2	2:B:121:PHE:CZ	2.93	0.57
1:C:391:GLY:O	1:C:393:THR:HG23	2.04	0.57
2:D:48:TYR:HD1	2:D:49:HIS:H	1.52	0.57
1:A:346:LEU:HB3	1:A:348:TRP:HZ3	1.70	0.56
2:B:52:VAL:HG21	2:B:118:PHE:CD2	2.39	0.56
1:A:103:ARG:NH1	1:A:156:PHE:CE2	2.73	0.56
1:A:59:MET:HE2	1:A:64:ILE:HG21	1.86	0.56
1:A:333:HIS:HB3	1:A:349:THR:CG2	2.35	0.56
1:C:33:ASP:OD1	1:C:35:ALA:HB3	2.06	0.56
1:C:282:LYS:NZ	1:C:286:SER:H	2.03	0.56
2:D:104:ARG:HB2	2:D:112:LEU:HD21	1.87	0.56
2:D:122:THR:CG2	2:D:124:PHE:H	2.18	0.56
1:C:59:MET:HE3	1:C:60:ASN:ND2	2.20	0.56
1:C:98:LEU:HD11	1:C:121:LEU:CD2	2.36	0.56
2:B:74:THR:HG22	2:B:76:ARG:HH11	1.71	0.56
2:B:99:ARG:HG3	2:B:99:ARG:HH11	1.71	0.56
2:D:87:TYR:HB2	2:D:137:PHE:CB	2.35	0.56
1:A:79:ASN:HB2	1:A:184:ASP:HB3	1.88	0.56
1:C:318:GLN:CD	1:C:318:GLN:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:THR:HG22	2:B:74:THR:O	2.05	0.56
1:A:412:VAL:O	1:A:427:PHE:HB2	2.05	0.56
1:C:188:CYS:SG	2:D:121:PHE:CD2	2.98	0.56
1:A:103:ARG:NH1	1:A:156:PHE:HE2	2.04	0.56
1:C:43:TRP:HB3	1:C:82:ARG:O	2.05	0.56
2:D:43:PHE:CE1	2:D:48:TYR:HD2	2.23	0.56
1:C:314:PHE:CD1	1:C:421:LEU:HD22	2.41	0.56
1:A:80:TRP:HA	1:A:182:PHE:O	2.06	0.55
1:A:124:ALA:O	1:A:178:PHE:HA	2.06	0.55
1:C:111:GLY:O	1:C:112:ALA:O	2.25	0.55
1:C:198:TYR:HE1	1:C:215:ILE:HG21	1.71	0.55
1:C:370:TRP:HB3	1:C:373:SER:CB	2.23	0.55
2:D:131:ARG:HH11	2:D:134:ARG:HH21	1.52	0.55
1:C:94:ILE:CG1	1:C:173:LEU:HD11	2.33	0.55
1:A:348:TRP:CZ3	1:A:396:SER:HA	2.41	0.55
2:B:81:MET:HB2	2:B:99:ARG:HG3	1.87	0.55
2:D:122:THR:HG22	2:D:122:THR:O	2.05	0.55
1:A:316:ALA:HB1	1:A:317:PRO:HD2	1.87	0.55
1:C:82:ARG:HG3	1:C:139:PHE:CZ	2.42	0.55
2:D:121:PHE:CD2	2:D:121:PHE:C	2.84	0.55
1:C:31:LEU:HD21	1:C:198:TYR:CD2	2.42	0.55
2:D:149:ARG:CG	2:D:150:SER:N	2.64	0.55
1:A:91:ALA:HB2	1:A:198:TYR:CD2	2.41	0.55
1:A:116:LYS:HG2	1:A:186:GLY:O	2.06	0.55
2:B:142:ALA:HB1	2:B:144:PRO:HD2	1.89	0.55
1:C:184:ASP:CG	1:C:186:GLY:H	2.15	0.55
1:A:406:MET:C	1:A:408:TYR:N	2.65	0.55
2:D:36:TRP:HZ2	2:D:140:SER:HB3	1.71	0.55
1:C:224:ALA:CB	1:C:247:CYS:HB3	2.27	0.55
1:C:318:GLN:O	1:C:318:GLN:HG2	2.06	0.55
2:B:70:PRO:HG2	2:B:73:LYS:HE3	1.89	0.54
2:B:121:PHE:HA	2:B:129:GLU:HG2	1.89	0.54
1:C:169:SER:O	1:C:170:VAL:HB	2.05	0.54
1:C:323:MET:HG3	1:C:324:PRO:HD2	1.89	0.54
1:A:29:VAL:CG1	1:A:198:TYR:CE2	2.90	0.54
1:A:66:MET:SD	2:B:124:PHE:CE2	3.00	0.54
1:A:344:VAL:HG23	1:A:399:VAL:HB	1.88	0.54
1:C:88:ARG:HD3	1:C:173:LEU:HB2	1.89	0.54
2:D:98:LYS:NZ	2:D:101:GLU:HB2	2.21	0.54
2:D:40:ASN:HB3	2:D:43:PHE:CD2	2.38	0.54
1:A:134:PHE:CD2	1:A:134:PHE:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ASN:N	2:B:118:PHE:O	2.36	0.54
2:B:87:TYR:HB2	2:B:137:PHE:HB3	1.89	0.54
1:C:211:PHE:CE1	1:C:228:GLY:HA3	2.42	0.54
1:A:120:ASN:HB2	1:A:183:GLN:HB3	1.89	0.54
1:C:104:ASP:HB3	1:C:107:SER:OG	2.08	0.54
1:A:127:ASP:C	1:A:128:LEU:HD23	2.31	0.54
1:A:246:HIS:ND1	1:A:255:VAL:CG2	2.71	0.54
1:A:277:SER:HB3	1:A:278:PRO:HD2	1.90	0.54
1:A:57:ASN:HD21	2:B:127:GLY:HA2	1.73	0.54
1:A:399:VAL:CG1	1:A:402:LEU:HD21	2.37	0.54
1:C:29:VAL:HB	1:C:198:TYR:CE2	2.43	0.54
1:C:415:ARG:CZ	1:C:419:SER:HB3	2.37	0.54
1:A:104:ASP:HB2	1:A:150:ILE:HG22	1.91	0.53
1:A:172:PRO:HB3	1:A:218:SER:HB2	1.90	0.53
2:B:132:PRO:HA	2:B:158:VAL:CG1	2.38	0.53
1:A:245:MET:HE1	1:A:256:PRO:HG3	1.90	0.53
1:A:280:PHE:CD1	1:A:280:PHE:N	2.75	0.53
2:D:57:TYR:CE2	2:D:117:LYS:HD2	2.43	0.53
2:D:74:THR:HG21	2:D:105:PRO:HG3	1.89	0.53
2:B:100:TRP:CZ2	2:B:116:GLU:HB2	2.44	0.53
2:B:149:ARG:HG3	2:B:150:SER:H	1.72	0.53
1:C:124:ALA:O	1:C:178:PHE:HA	2.08	0.53
1:A:66:MET:SD	2:B:124:PHE:CE1	3.02	0.53
1:A:92:GLU:O	1:A:172:PRO:HA	2.09	0.53
1:A:203:GLU:HA	1:A:212:PRO:O	2.09	0.53
1:A:280:PHE:N	1:A:280:PHE:HD1	2.07	0.53
1:C:47:PRO:HB2	1:C:50:LYS:CB	2.39	0.53
1:A:411:THR:OG1	1:A:427:PHE:HD1	1.91	0.53
1:A:34:PHE:C	1:A:34:PHE:CD2	2.87	0.53
1:A:80:TRP:HH2	1:A:122:TYR:CE2	2.25	0.53
1:C:211:PHE:CD1	1:C:228:GLY:HA3	2.45	0.52
1:C:226:VAL:HG21	1:C:253:TRP:CZ3	2.43	0.52
1:A:103:ARG:HD3	2:B:121:PHE:CE2	2.45	0.52
1:C:43:TRP:CD1	1:C:83:THR:CA	2.87	0.52
2:D:161:THR:O	2:D:162:ASN:HB3	2.08	0.52
1:A:247:CYS:HB2	1:A:253:TRP:CZ3	2.44	0.52
1:A:279:GLY:C	1:A:280:PHE:HD1	2.17	0.52
1:C:100:PHE:HA	1:C:190:ALA:O	2.09	0.52
1:A:84:ASN:O	1:A:179:TYR:HE1	1.92	0.52
1:A:411:THR:HG1	1:A:427:PHE:HD1	1.55	0.52
2:B:121:PHE:C	2:B:121:PHE:CD2	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:PHE:CZ	2:D:121:PHE:HE1	2.26	0.52
1:C:370:TRP:C	1:C:374:GLY:H	2.18	0.52
2:D:128:PHE:HD2	2:D:130:PHE:CE2	2.28	0.52
1:A:346:LEU:O	1:A:396:SER:HB2	2.09	0.52
2:D:100:TRP:CD1	2:D:114:PHE:CD2	2.98	0.52
2:D:104:ARG:HB2	2:D:112:LEU:HD11	1.92	0.52
1:A:75:GLY:O	1:A:77:GLN:HG2	2.10	0.52
1:A:167:GLU:CG	1:A:168:ARG:N	2.73	0.52
1:C:52:TRP:HD1	1:C:80:TRP:O	1.87	0.52
2:D:98:LYS:C	2:D:98:LYS:CD	2.83	0.52
1:A:316:ALA:HB1	1:A:318:GLN:HE21	1.73	0.52
1:A:317:PRO:HG2	1:A:318:GLN:HE22	1.75	0.52
1:C:85:TRP:CE2	1:C:177:GLY:HA3	2.45	0.52
1:C:104:ASP:OD2	1:C:152:VAL:HG13	2.09	0.52
2:D:62:CYS:HB3	2:D:63:PRO:HD2	1.92	0.52
1:C:337:ALA:CB	1:C:346:LEU:HD23	2.38	0.52
1:C:365:THR:HG1	1:C:411:THR:HG23	1.73	0.52
2:D:76:ARG:HG3	2:D:76:ARG:NH1	2.25	0.51
2:D:124:PHE:C	2:D:126:LEU:H	2.17	0.51
1:A:316:ALA:HB1	1:A:318:GLN:NE2	2.25	0.51
2:B:100:TRP:HB3	2:B:114:PHE:CD1	2.45	0.51
1:C:68:SER:CB	2:D:124:PHE:HZ	2.23	0.51
1:A:212:PRO:CB	1:A:214:THR:HG23	2.38	0.51
1:C:67:TYR:CD1	1:C:81:LEU:CD1	2.86	0.51
1:C:413:GLU:HG3	1:C:427:PHE:HB3	1.91	0.51
1:C:357:ARG:NH2	1:C:417:GLY:HA3	2.26	0.51
1:C:281:PHE:HB2	1:C:304:ALA:O	2.11	0.51
2:D:76:ARG:HB2	2:D:144:PRO:HD3	1.92	0.51
1:A:98:LEU:HA	1:A:193:SER:O	2.11	0.51
1:A:101:THR:HG22	1:A:162:LYS:O	2.10	0.51
1:A:119:PHE:C	1:A:120:ASN:OD1	2.54	0.51
1:A:137:ARG:HG3	1:A:138:LEU:HD23	1.93	0.51
1:C:48:TYR:C	1:C:50:LYS:H	2.19	0.51
1:A:154:SER:C	1:A:156:PHE:H	2.19	0.51
1:C:197:TYR:CD1	1:C:197:TYR:C	2.89	0.51
1:A:95:PHE:HB3	1:A:197:TYR:HE2	1.75	0.51
1:A:103:ARG:HH11	1:A:156:PHE:HE2	1.59	0.51
2:B:160:PRO:HG2	2:B:163:SER:HB2	1.91	0.51
1:C:221:PRO:O	1:C:222:SER:C	2.54	0.51
1:A:52:TRP:HD1	1:A:80:TRP:O	1.94	0.51
1:A:94:ILE:HG23	1:A:173:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:OE2	1:A:150:ILE:HD12	2.11	0.51
1:A:32:LEU:HD12	1:A:32:LEU:C	2.36	0.51
1:A:111:GLY:O	1:A:112:ALA:C	2.52	0.51
1:A:276:CYS:O	1:A:277:SER:O	2.29	0.51
2:D:133:GLY:HA2	2:D:160:PRO:HD3	1.92	0.51
1:A:208:LEU:O	1:A:231:VAL:HG13	2.10	0.50
1:A:420:GLY:C	1:A:422:VAL:H	2.19	0.50
1:C:98:LEU:HD11	1:C:121:LEU:HD22	1.91	0.50
2:D:124:PHE:HB3	2:D:126:LEU:HD12	1.92	0.50
1:A:220:ALA:HB3	1:A:221:PRO:HD3	1.92	0.50
2:B:66:GLU:C	2:B:68:SER:H	2.19	0.50
1:C:33:ASP:O	1:C:34:PHE:C	2.53	0.50
1:A:56:GLN:NE2	2:B:114:PHE:CD2	2.79	0.50
1:A:57:ASN:HD21	2:B:127:GLY:CA	2.24	0.50
1:A:411:THR:OG1	1:A:429:THR:HG22	2.12	0.50
1:C:144:THR:C	1:C:145:ILE:HD13	2.36	0.50
1:C:335:LEU:HB3	1:C:428:ARG:HG2	1.92	0.50
1:A:124:ALA:HB3	1:A:179:TYR:HB2	1.93	0.50
1:A:418:VAL:HG23	1:A:418:VAL:O	2.12	0.50
2:B:77:TYR:O	2:B:143:ILE:HG13	2.11	0.50
2:D:102:CYS:HA	2:D:112:LEU:HD12	1.94	0.50
1:A:29:VAL:HG11	1:A:198:TYR:OH	2.12	0.50
2:B:100:TRP:HH2	2:B:116:GLU:HB2	1.74	0.50
1:C:135:GLN:CG	1:C:137:ARG:HG2	2.40	0.50
2:D:160:PRO:HB2	2:D:163:SER:HB2	1.94	0.50
1:A:317:PRO:HG2	1:A:318:GLN:NE2	2.27	0.50
1:A:331:ALA:O	1:A:332:PRO:C	2.55	0.50
1:C:384:ARG:O	1:C:399:VAL:HA	2.12	0.50
1:A:149:GLU:CD	1:A:162:LYS:HG3	2.37	0.50
1:A:370:TRP:CD1	1:A:370:TRP:C	2.89	0.50
2:B:40:ASN:OD1	2:B:41:PRO:HD2	2.11	0.50
1:A:104:ASP:HB2	1:A:150:ILE:CG2	2.42	0.50
3:E:1:NAG:H61	3:E:2:NAG:C7	2.42	0.50
1:A:208:LEU:C	1:A:231:VAL:HG13	2.37	0.49
1:C:338:VAL:HG12	1:C:339:GLY:H	1.77	0.49
1:A:99:LYS:HA	1:A:164:ASN:O	2.12	0.49
1:C:82:ARG:NE	1:C:83:THR:O	2.45	0.49
1:C:409:THR:HG23	1:C:431:SER:OG	2.11	0.49
2:D:57:TYR:HE2	2:D:117:LYS:HD2	1.77	0.49
1:A:125:GLU:HB3	1:A:175:ARG:HB2	1.94	0.49
1:A:167:GLU:O	1:A:168:ARG:NH1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HD3	1:A:362:TYR:OH	2.13	0.49
1:C:88:ARG:HD2	1:C:91:ALA:O	2.13	0.49
1:A:147:PRO:HB3	1:A:164:ASN:ND2	2.27	0.49
1:A:326:THR:OG1	1:A:418:VAL:HG11	2.13	0.49
1:C:129:ASP:O	1:C:130:TYR:HD2	1.91	0.49
1:C:286:SER:OG	1:C:288:SER:HB2	2.13	0.49
1:C:72:VAL:HG11	1:C:108:PHE:CE1	2.48	0.49
1:C:236:VAL:O	1:C:236:VAL:HG22	2.13	0.49
1:C:323:MET:HG3	1:C:324:PRO:CD	2.43	0.49
2:D:118:PHE:HA	2:D:130:PHE:CD1	2.47	0.49
1:C:95:PHE:HD2	1:C:169:SER:HB3	1.75	0.49
1:C:152:VAL:HG12	1:C:153:SER:H	1.78	0.49
2:D:59:ASP:OD1	2:D:115:SER:HB2	2.13	0.49
2:D:131:ARG:NH1	2:D:134:ARG:HH21	2.09	0.49
1:A:73:MET:SD	1:A:112:ALA:HB3	2.53	0.49
1:A:134:PHE:CE2	1:A:136:LYS:HG3	2.47	0.49
1:A:123:TYR:HA	1:A:179:TYR:O	2.13	0.48
1:C:74:SER:HB2	1:C:77:GLN:NE2	2.28	0.48
2:D:43:PHE:O	2:D:45:ARG:N	2.44	0.48
1:A:72:VAL:HG21	1:A:108:PHE:CE1	2.48	0.48
1:A:93:ARG:CG	1:A:95:PHE:CE2	2.93	0.48
1:A:190:ALA:HB1	2:B:124:PHE:HZ	1.64	0.48
2:B:65:TYR:HE1	2:B:75:GLU:H	1.60	0.48
1:C:221:PRO:CG	1:C:222:SER:H	2.25	0.48
1:C:282:LYS:HE2	1:C:288:SER:O	2.13	0.48
1:A:267:GLU:OE1	1:A:290:CYS:HB2	2.13	0.48
1:C:82:ARG:HD2	1:C:179:TYR:CD1	2.49	0.48
1:C:145:ILE:HD13	1:C:145:ILE:N	2.28	0.48
2:D:43:PHE:CZ	2:D:48:TYR:CD2	3.01	0.48
1:A:149:GLU:OE1	1:A:162:LYS:HG3	2.13	0.48
1:A:366:CYS:SG	1:A:410:PHE:HE2	2.36	0.48
1:C:41:LEU:HD21	1:C:84:ASN:HD21	1.79	0.48
1:C:102:VAL:HG23	1:C:189:VAL:HG13	1.95	0.48
1:C:130:TYR:O	1:C:132:THR:N	2.40	0.48
1:A:120:ASN:OD1	1:A:144:THR:HG23	2.13	0.48
1:A:159:ARG:NH2	2:B:126:LEU:O	2.46	0.48
1:A:237:PRO:HB2	1:A:238:PRO:HD3	1.95	0.48
1:A:332:PRO:O	1:A:428:ARG:HD2	2.12	0.48
1:C:69:VAL:HG12	1:C:189:VAL:HG23	1.95	0.48
1:C:108:PHE:CE1	2:D:121:PHE:CE1	3.01	0.48
1:C:357:ARG:C	1:C:358:GLU:HG3	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:VAL:HG21	2:D:118:PHE:CE2	2.49	0.48
1:A:66:MET:CG	2:B:124:PHE:CZ	2.97	0.48
1:A:366:CYS:SG	1:A:367:GLU:N	2.87	0.48
1:A:387:GLU:HG3	1:A:388:PRO:HD2	1.94	0.48
1:C:46:HIS:C	1:C:46:HIS:HD2	2.18	0.48
1:C:244:ARG:CZ	1:C:244:ARG:HB2	2.42	0.48
1:C:338:VAL:HG12	1:C:340:MET:H	1.78	0.48
1:C:380:GLU:O	1:C:383:VAL:HG22	2.13	0.48
1:C:383:VAL:HG12	1:C:402:LEU:HD23	1.94	0.48
1:A:85:TRP:HD1	1:A:179:TYR:CE1	2.32	0.48
1:A:333:HIS:HB3	1:A:349:THR:HG22	1.96	0.48
1:A:385:TYR:CD2	1:A:399:VAL:HG22	2.49	0.48
1:C:124:ALA:HB2	1:C:139:PHE:CD2	2.48	0.48
2:D:54:ILE:HD12	2:D:54:ILE:HA	1.66	0.48
2:D:118:PHE:HD1	2:D:130:PHE:CE1	2.32	0.48
1:C:122:TYR:HB3	1:C:139:PHE:HB3	1.96	0.48
2:D:43:PHE:CE1	2:D:48:TYR:CD2	3.02	0.48
2:B:54:ILE:O	2:B:55:ASN:HB2	2.13	0.48
1:C:167:GLU:C	1:C:168:ARG:HG2	2.39	0.48
1:A:95:PHE:HB2	1:A:197:TYR:CE2	2.49	0.48
1:C:100:PHE:O	1:C:163:LEU:HD12	2.14	0.48
1:C:233:HIS:O	1:C:234:ALA:HB2	2.13	0.48
1:A:47:PRO:O	1:A:48:TYR:C	2.57	0.47
1:A:85:TRP:HD1	1:A:179:TYR:CZ	2.32	0.47
1:A:333:HIS:HB3	1:A:349:THR:HG21	1.96	0.47
1:A:411:THR:HB	1:A:429:THR:CG2	2.42	0.47
2:B:31:ARG:NH1	2:B:59:ASP:OD2	2.48	0.47
2:B:159:ARG:HD2	2:B:163:SER:O	2.15	0.47
2:B:161:THR:O	2:B:162:ASN:OD1	2.32	0.47
1:A:235:VAL:HG22	1:A:236:VAL:CG1	2.45	0.47
1:C:68:SER:HB3	2:D:124:PHE:CZ	2.47	0.47
1:C:335:LEU:HD22	1:C:412:VAL:HG12	1.95	0.47
2:D:32:TYR:N	2:D:57:TYR:O	2.47	0.47
1:A:119:PHE:HD2	1:A:189:VAL:HG11	1.77	0.47
2:B:59:ASP:OD1	2:B:113:LYS:HE3	2.15	0.47
1:C:211:PHE:O	1:C:212:PRO:O	2.31	0.47
1:A:56:GLN:NE2	2:B:114:PHE:HD2	2.13	0.47
1:A:391:GLY:O	1:A:392:LEU:HD12	2.15	0.47
2:D:47:ASP:O	2:D:48:TYR:C	2.56	0.47
1:A:99:LYS:HE3	1:A:165:VAL:CG1	2.45	0.47
1:A:115:CYS:O	1:A:116:LYS:NZ	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:O	1:A:212:PRO:O	2.32	0.47
1:A:255:VAL:HG23	1:A:255:VAL:O	2.13	0.47
1:A:346:LEU:HB3	1:A:348:TRP:CZ3	2.49	0.47
1:A:385:TYR:HD2	1:A:399:VAL:HG22	1.80	0.47
1:A:400:SER:O	1:A:401:ASP:HB3	2.15	0.47
2:B:109:ASN:C	1:C:137:ARG:NE	2.73	0.47
1:C:31:LEU:O	1:C:32:LEU:CB	2.59	0.47
1:C:108:PHE:HB3	1:C:111:GLY:H	1.79	0.47
2:B:66:GLU:C	2:B:68:SER:N	2.72	0.47
2:B:99:ARG:HB3	2:B:99:ARG:CZ	2.43	0.47
1:C:41:LEU:HD21	1:C:84:ASN:ND2	2.30	0.47
2:D:81:MET:HE1	2:D:128:PHE:CD2	2.49	0.47
1:A:86:VAL:HB	1:A:178:PHE:CE1	2.49	0.47
1:A:102:VAL:HG11	1:A:117:GLU:CB	2.45	0.47
1:A:350:PRO:HA	1:A:362:TYR:OH	2.15	0.47
2:B:89:ALA:O	2:B:90:CYS:C	2.57	0.47
2:B:144:PRO:HB2	2:B:146:ASN:ND2	2.24	0.47
1:C:229:THR:HG23	1:C:230:CYS:N	2.30	0.47
1:C:326:THR:HG21	1:C:357:ARG:CG	2.45	0.47
1:C:345:GLU:HG3	1:C:347:ARG:HG3	1.96	0.47
1:C:34:PHE:C	1:C:34:PHE:CD2	2.92	0.47
1:C:58:ILE:O	1:C:58:ILE:HG22	2.14	0.47
1:C:366:CYS:HB2	1:C:410:PHE:HE2	1.77	0.47
2:D:62:CYS:HB3	2:D:63:PRO:CD	2.45	0.47
1:A:62:MET:HA	1:A:63:PRO:HD3	1.72	0.46
2:B:100:TRP:HD1	2:B:114:PHE:CD2	2.33	0.46
1:C:137:ARG:HG3	1:C:138:LEU:CD2	2.45	0.46
1:C:296:HIS:O	1:C:325:CYS:SG	2.72	0.46
2:D:82:VAL:HG21	2:D:139:ILE:HD11	1.97	0.46
1:A:370:TRP:HD1	1:A:371:PRO:N	2.13	0.46
1:C:48:TYR:C	1:C:50:LYS:N	2.72	0.46
1:A:355:GLY:O	1:A:357:ARG:HG3	2.15	0.46
2:B:126:LEU:O	2:B:127:GLY:O	2.33	0.46
2:D:56:ASP:O	2:D:118:PHE:HB2	2.16	0.46
1:A:135:GLN:HG2	1:A:138:LEU:HD23	1.96	0.46
1:A:235:VAL:O	1:A:237:PRO:HD3	2.15	0.46
1:A:242:GLU:OE1	1:A:242:GLU:HA	2.15	0.46
1:C:100:PHE:N	1:C:100:PHE:CD2	2.83	0.46
2:D:82:VAL:CG2	2:D:139:ILE:HD11	2.46	0.46
2:D:122:THR:C	2:D:124:PHE:H	2.23	0.46
1:A:207:GLY:O	1:A:208:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:O	1:A:216:ALA:O	2.34	0.46
1:A:327:ARG:O	1:A:355:GLY:HA3	2.16	0.46
2:B:82:VAL:CG1	2:B:96:GLY:HA3	2.44	0.46
2:B:87:TYR:CE2	2:B:155:LYS:HG3	2.51	0.46
2:B:160:PRO:CD	2:B:163:SER:HB2	2.45	0.46
1:C:149:GLU:N	1:C:164:ASN:OD1	2.43	0.46
2:B:76:ARG:HB2	2:B:144:PRO:HD3	1.97	0.46
2:B:152:LEU:HD23	2:B:152:LEU:HA	1.49	0.46
1:C:370:TRP:O	1:C:373:SER:HB3	2.15	0.46
1:A:72:VAL:HG11	1:A:108:PHE:CZ	2.50	0.46
1:A:86:VAL:CG2	1:A:178:PHE:CE1	2.98	0.46
1:A:279:GLY:C	1:A:280:PHE:CD1	2.94	0.46
2:D:122:THR:HG22	2:D:124:PHE:N	2.31	0.46
2:D:161:THR:O	2:D:162:ASN:CB	2.63	0.46
1:A:233:HIS:O	1:A:273:CYS:SG	2.74	0.46
1:A:400:SER:O	1:A:401:ASP:CB	2.64	0.46
2:B:107:SER:HA	2:B:108:PRO:HD2	1.63	0.46
1:C:237:PRO:CB	1:C:238:PRO:HD3	2.44	0.46
1:C:362:TYR:O	1:C:392:LEU:HB2	2.15	0.46
1:C:392:LEU:HD12	1:C:392:LEU:HA	1.74	0.46
1:A:107:SER:CB	1:A:153:SER:HB3	2.46	0.46
2:B:35:TYR:N	2:B:35:TYR:CD1	2.84	0.46
2:B:66:GLU:O	2:B:68:SER:N	2.49	0.46
2:B:79:LEU:HD23	2:B:79:LEU:N	2.31	0.46
1:C:70:CYS:O	1:C:70:CYS:SG	2.74	0.46
1:C:103:ARG:NE	2:D:121:PHE:HZ	2.11	0.46
1:A:407:ASN:OD1	4:A:501:NAG:O5	2.32	0.45
1:C:100:PHE:CE1	1:C:119:PHE:CE2	3.04	0.45
1:C:103:ARG:NH2	2:D:121:PHE:HE1	2.13	0.45
1:A:80:TRP:NE1	1:A:136:LYS:HG2	2.32	0.45
1:C:56:GLN:OE1	2:D:114:PHE:HA	2.16	0.45
1:C:68:SER:CB	2:D:124:PHE:CZ	3.00	0.45
1:C:134:PHE:CD2	1:C:134:PHE:C	2.93	0.45
1:C:367:GLU:OE2	4:C:501:NAG:H82	2.16	0.45
1:A:332:PRO:HG2	1:A:412:VAL:CG1	2.46	0.45
1:A:357:ARG:HB3	1:A:359:ASP:OD1	2.17	0.45
1:A:145:ILE:HD13	1:A:145:ILE:H	1.81	0.45
2:B:43:PHE:CD1	2:B:48:TYR:CD2	3.04	0.45
1:C:73:MET:O	1:C:75:GLY:N	2.49	0.45
1:C:167:GLU:CG	1:C:168:ARG:N	2.79	0.45
1:A:120:ASN:HB3	1:A:122:TYR:CE1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:HH12	1:A:257:ILE:HD12	1.82	0.45
2:B:79:LEU:HB2	2:B:100:TRP:HB2	1.98	0.45
2:D:61:PHE:CD1	2:D:61:PHE:N	2.84	0.45
1:A:158:ALA:O	1:A:159:ARG:HB2	2.16	0.45
2:B:87:TYR:HB2	2:B:137:PHE:CB	2.46	0.45
2:B:122:THR:CG2	2:B:124:PHE:H	2.29	0.45
2:B:95:LYS:HG2	2:B:96:GLY:N	2.32	0.45
1:C:47:PRO:CD	1:C:79:ASN:HA	2.46	0.45
1:C:100:PHE:H	1:C:100:PHE:HD2	1.64	0.45
1:C:236:VAL:HA	1:C:237:PRO:HD3	1.67	0.45
1:C:276:CYS:O	1:C:277:SER:C	2.58	0.45
2:D:51:ASP:HB3	2:D:159:ARG:CD	2.40	0.45
2:D:128:PHE:CD2	2:D:130:PHE:CE2	3.05	0.45
1:A:350:PRO:HA	1:A:351:PRO:HD3	1.80	0.45
1:A:363:SER:HA	1:A:390:HIS:HA	1.99	0.45
1:C:316:ALA:HB3	1:C:319:ASP:CG	2.42	0.45
2:D:42:ARG:HH22	2:D:50:ILE:HG22	1.80	0.45
2:D:118:PHE:HA	2:D:130:PHE:HD1	1.81	0.45
1:A:139:PHE:N	1:A:139:PHE:CD2	2.85	0.45
1:A:313:PHE:CB	1:A:325:CYS:HB3	2.44	0.45
1:A:411:THR:OG1	1:A:427:PHE:CD1	2.69	0.45
2:B:100:TRP:CD1	2:B:114:PHE:CG	3.05	0.45
2:B:164:CYS:O	2:B:165:MET:CB	2.64	0.45
1:C:316:ALA:O	1:C:317:PRO:C	2.60	0.45
1:C:335:LEU:HD12	1:C:336:THR:N	2.32	0.45
1:C:369:CYS:C	1:C:371:PRO:HD3	2.41	0.45
2:D:75:GLU:HB3	2:D:77:TYR:CE2	2.52	0.45
1:A:180:LEU:O	1:A:181:ALA:HB2	2.17	0.44
1:A:300:SER:HB2	1:A:301:PRO:HD2	1.98	0.44
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.71	0.44
2:D:66:GLU:O	2:D:69:VAL:HG23	2.17	0.44
2:D:133:GLY:CA	2:D:160:PRO:HD3	2.47	0.44
1:A:88:ARG:HD2	1:A:173:LEU:HB3	1.99	0.44
1:A:163:LEU:HG	1:A:164:ASN:N	2.33	0.44
1:A:434:ILE:HG13	1:A:435:ASN:H	1.83	0.44
2:D:159:ARG:HA	2:D:160:PRO:HD2	1.64	0.44
1:A:85:TRP:CD1	1:A:179:TYR:CZ	3.06	0.44
1:A:266:TYR:CE1	1:A:275:ALA:HB2	2.52	0.44
1:A:349:THR:HA	1:A:350:PRO:HD3	1.78	0.44
1:A:406:MET:O	1:A:408:TYR:N	2.36	0.44
2:D:71:GLU:O	2:D:74:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:CG2	1:A:79:ASN:HD22	2.28	0.44
1:A:137:ARG:NE	2:D:109:ASN:O	2.50	0.44
2:B:122:THR:HG22	2:B:124:PHE:H	1.82	0.44
2:D:74:THR:O	2:D:74:THR:HG22	2.18	0.44
1:A:310:GLU:OE2	1:A:313:PHE:HE2	2.01	0.44
1:A:69:VAL:HG11	1:A:184:ASP:OD2	2.17	0.44
1:A:344:VAL:HG22	1:A:402:LEU:HD11	1.99	0.44
1:A:346:LEU:O	1:A:396:SER:CB	2.66	0.44
1:C:54:LEU:HA	1:C:66:MET:O	2.17	0.44
1:C:72:VAL:HG11	1:C:108:PHE:CZ	2.52	0.44
1:C:159:ARG:NH2	2:D:126:LEU:O	2.51	0.44
1:C:326:THR:CB	1:C:357:ARG:HD2	2.48	0.44
2:D:69:VAL:HA	2:D:70:PRO:HD3	1.76	0.44
1:A:99:LYS:HG3	1:A:193:SER:HB3	1.99	0.44
1:A:160:HIS:CE1	1:A:162:LYS:HZ2	2.36	0.44
2:B:43:PHE:CE1	2:B:48:TYR:CD2	3.06	0.44
1:C:31:LEU:HD21	1:C:198:TYR:CE2	2.52	0.44
1:C:100:PHE:N	1:C:100:PHE:HD2	2.15	0.44
1:C:232:ASP:O	1:C:273:CYS:HB2	2.18	0.44
1:C:282:LYS:HZ1	1:C:286:SER:H	1.64	0.44
1:A:43:TRP:CD1	1:A:84:ASN:N	2.80	0.44
1:A:392:LEU:HD12	1:A:392:LEU:HA	1.80	0.44
2:B:143:ILE:N	2:B:144:PRO:CD	2.81	0.43
1:C:44:LEU:C	1:C:44:LEU:HD23	2.43	0.43
1:C:101:THR:H	1:C:190:ALA:HB3	1.83	0.43
2:D:31:ARG:NH1	2:D:59:ASP:OD2	2.52	0.43
2:D:52:VAL:HG21	2:D:118:PHE:CD2	2.52	0.43
2:D:100:TRP:CG	2:D:114:PHE:CG	3.06	0.43
1:A:101:THR:HG22	1:A:162:LYS:C	2.43	0.43
1:A:151:THR:HG23	1:A:162:LYS:HB2	2.00	0.43
1:A:246:HIS:O	1:A:253:TRP:HA	2.18	0.43
1:C:39:GLY:C	1:C:41:LEU:H	2.26	0.43
1:C:221:PRO:HG2	1:C:222:SER:N	2.32	0.43
1:C:238:PRO:HG2	1:C:241:GLU:N	2.32	0.43
1:C:280:PHE:CD2	1:C:292:GLU:HA	2.54	0.43
1:C:147:PRO:HB3	1:C:164:ASN:ND2	2.33	0.43
1:A:188:CYS:SG	2:B:121:PHE:CE2	3.12	0.43
1:C:332:PRO:O	1:C:333:HIS:C	2.60	0.43
2:D:82:VAL:HG21	2:D:139:ILE:CD1	2.47	0.43
1:A:31:LEU:HD21	1:A:198:TYR:CE2	2.54	0.43
1:A:128:LEU:O	1:A:129:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:C	1:A:178:PHE:HD1	2.27	0.43
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.79	0.43
1:A:241:GLU:HG3	1:A:242:GLU:N	2.33	0.43
1:A:364:VAL:HG23	1:A:389:PRO:O	2.19	0.43
2:B:99:ARG:HH11	2:B:99:ARG:CG	2.31	0.43
2:D:146:ASN:O	2:D:147:GLY:C	2.62	0.43
1:A:43:TRP:CD2	1:A:83:THR:HA	2.53	0.43
1:C:86:VAL:O	1:C:177:GLY:HA2	2.18	0.43
1:C:102:VAL:HG11	1:C:147:PRO:HG2	2.00	0.43
1:A:156:PHE:O	1:A:159:ARG:N	2.47	0.43
2:B:126:LEU:H	2:B:126:LEU:HG	1.57	0.43
1:C:174:THR:C	1:C:175:ARG:HG2	2.43	0.43
1:A:72:VAL:HB	1:A:115:CYS:HB2	1.99	0.43
1:C:100:PHE:CD1	1:C:119:PHE:CE2	3.07	0.43
1:C:281:PHE:HD1	1:C:306:SER:HA	1.84	0.43
1:A:56:GLN:O	1:A:57:ASN:CB	2.64	0.43
1:C:255:VAL:HG23	1:C:255:VAL:O	2.18	0.43
1:C:257:ILE:O	1:C:257:ILE:HG22	2.18	0.43
2:B:98:LYS:HD3	2:B:98:LYS:C	2.44	0.43
2:B:66:GLU:H	2:B:66:GLU:HG3	1.57	0.42
2:B:77:TYR:CD1	2:B:142:ALA:HA	2.54	0.42
1:C:47:PRO:HG2	1:C:51:GLY:CA	2.49	0.42
1:A:238:PRO:HG2	1:A:241:GLU:N	2.34	0.42
1:A:370:TRP:O	1:A:373:SER:HB3	2.19	0.42
4:A:501:NAG:O7	4:A:501:NAG:H3	2.19	0.42
1:C:43:TRP:NE1	1:C:83:THR:HA	2.34	0.42
1:C:116:LYS:HD2	1:C:185:ILE:CG1	2.50	0.42
1:C:259:GLN:HE21	1:C:259:GLN:HB2	1.64	0.42
2:D:52:VAL:HA	2:D:159:ARG:HH21	1.83	0.42
1:A:72:VAL:HB	1:A:115:CYS:CB	2.49	0.42
1:A:323:MET:O	1:A:324:PRO:O	2.37	0.42
1:C:53:ASP:CB	1:C:55:MET:HE1	2.38	0.42
1:C:326:THR:CG2	1:C:357:ARG:HG3	2.49	0.42
2:D:43:PHE:C	2:D:45:ARG:N	2.75	0.42
2:D:122:THR:HG23	2:D:124:PHE:HD1	1.77	0.42
2:D:143:ILE:C	2:D:145:ASP:H	2.27	0.42
1:C:83:THR:CG2	1:C:180:LEU:HB2	2.49	0.42
1:C:326:THR:HB	1:C:357:ARG:HD2	2.01	0.42
1:C:335:LEU:HD12	1:C:336:THR:H	1.84	0.42
1:A:29:VAL:HG11	1:A:198:TYR:CZ	2.55	0.42
1:A:128:LEU:HD11	1:A:130:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HA	1:A:138:LEU:HD22	1.64	0.42
2:B:65:TYR:CE1	2:B:74:THR:HA	2.54	0.42
1:C:83:THR:HG21	1:C:180:LEU:HB2	2.02	0.42
1:C:142:ILE:HG22	1:C:143:ASP:N	2.34	0.42
1:A:72:VAL:CG1	1:A:108:PHE:HE1	2.30	0.42
1:A:121:LEU:C	1:A:122:TYR:CD1	2.97	0.42
1:A:190:ALA:HB1	2:B:124:PHE:CE1	2.43	0.42
1:A:235:VAL:HG22	1:A:236:VAL:HG13	2.00	0.42
1:A:422:VAL:HG13	1:A:422:VAL:O	2.18	0.42
1:C:100:PHE:C	1:C:163:LEU:HD12	2.44	0.42
1:C:313:PHE:C	1:C:314:PHE:CG	2.98	0.42
1:C:54:LEU:CD1	1:C:65:TYR:HB3	2.49	0.42
1:C:246:HIS:O	1:C:253:TRP:HA	2.20	0.42
1:C:47:PRO:HG2	1:C:51:GLY:N	2.35	0.42
1:C:211:PHE:HA	1:C:212:PRO:HD3	1.83	0.42
1:C:415:ARG:HH11	1:C:419:SER:HB3	1.81	0.42
2:D:80:TYR:CE1	2:D:92:HIS:HB2	2.54	0.42
2:D:152:LEU:O	2:D:153:LYS:HB3	2.19	0.42
1:A:305:THR:HG23	1:A:306:SER:H	1.83	0.42
1:C:87:TYR:CD2	1:C:88:ARG:N	2.88	0.42
1:A:120:ASN:O	1:A:182:PHE:HA	2.20	0.42
1:A:156:PHE:O	1:A:157:GLU:C	2.62	0.42
1:C:44:LEU:HD22	1:C:82:ARG:HB3	2.01	0.42
1:C:129:ASP:OD1	1:C:179:TYR:OH	2.36	0.42
1:C:221:PRO:CG	1:C:222:SER:N	2.83	0.42
1:C:283:PHE:O	1:C:283:PHE:CD1	2.72	0.42
2:D:43:PHE:CD1	2:D:48:TYR:HD2	2.38	0.42
1:C:85:TRP:HE1	1:C:126:SER:HB3	1.86	0.41
1:C:406:MET:C	1:C:408:TYR:N	2.78	0.41
2:D:93:THR:O	2:D:94:SER:C	2.63	0.41
1:A:117:GLU:O	1:A:147:PRO:HD3	2.20	0.41
1:A:154:SER:C	1:A:156:PHE:N	2.76	0.41
2:B:52:VAL:HG11	2:B:118:PHE:CE2	2.55	0.41
2:D:43:PHE:CZ	2:D:48:TYR:HD2	2.38	0.41
2:D:124:PHE:C	2:D:126:LEU:N	2.77	0.41
1:A:66:MET:HE2	1:A:192:LEU:CD1	2.49	0.41
2:B:122:THR:HG21	2:B:127:GLY:HA3	2.02	0.41
1:C:27:LYS:O	1:C:28:GLU:C	2.62	0.41
1:C:86:VAL:HG11	1:C:178:PHE:CZ	2.55	0.41
1:A:121:LEU:HB2	1:A:145:ILE:HD11	2.02	0.41
2:B:74:THR:HG23	2:B:105:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:O	1:C:50:LYS:N	2.53	0.41
1:C:225:THR:O	1:C:225:THR:HG22	2.20	0.41
2:B:47:ASP:O	2:B:48:TYR:C	2.63	0.41
2:B:47:ASP:OD1	2:B:47:ASP:N	2.54	0.41
1:C:71:ASN:CB	1:C:77:GLN:CD	2.93	0.41
1:C:167:GLU:HG3	1:C:168:ARG:N	2.36	0.41
1:C:199:LYS:O	1:C:216:ALA:N	2.52	0.41
1:C:236:VAL:O	1:C:236:VAL:CG2	2.66	0.41
2:D:118:PHE:HD1	2:D:130:PHE:CD1	2.38	0.41
1:A:146:ALA:HA	1:A:147:PRO:HD3	1.83	0.41
1:C:95:PHE:CB	1:C:197:TYR:CE1	3.00	0.41
1:C:349:THR:HA	1:C:350:PRO:HD3	1.89	0.41
2:D:107:SER:HA	2:D:108:PRO:HD2	1.80	0.41
1:C:146:ALA:HA	1:C:147:PRO:HD3	1.88	0.41
2:D:60:VAL:HG12	2:D:60:VAL:O	2.20	0.41
1:A:136:LYS:O	1:A:137:ARG:C	2.63	0.41
2:B:54:ILE:HA	2:B:54:ILE:HD12	1.63	0.41
2:B:160:PRO:CG	2:B:163:SER:HB2	2.51	0.41
1:C:128:LEU:CD1	1:C:130:TYR:CE2	3.04	0.41
1:A:133:ASN:ND2	1:C:40:GLU:HG3	2.35	0.41
1:A:226:VAL:CG2	1:A:253:TRP:HZ3	2.27	0.41
1:A:342:ALA:O	1:A:402:LEU:HD12	2.21	0.41
1:A:370:TRP:CD1	1:A:371:PRO:N	2.89	0.41
1:C:94:ILE:H	1:C:94:ILE:HG13	1.68	0.41
1:C:95:PHE:HB2	1:C:197:TYR:CD1	2.54	0.41
1:C:128:LEU:CD1	1:C:130:TYR:HE2	2.33	0.41
1:C:139:PHE:CD1	1:C:181:ALA:CB	3.03	0.41
1:C:302:GLU:O	1:C:303:GLY:C	2.63	0.41
2:D:37:ASN:O	2:D:38:SER:C	2.63	0.41
2:D:143:ILE:HB	2:D:144:PRO:HD3	2.02	0.41
1:A:41:LEU:HD13	1:A:43:TRP:CE2	2.56	0.41
1:A:120:ASN:CB	1:A:122:TYR:HE1	2.29	0.41
1:C:318:GLN:O	1:C:318:GLN:CG	2.69	0.41
1:C:326:THR:C	1:C:418:VAL:HG21	2.46	0.41
1:C:387:GLU:HG3	1:C:388:PRO:HD2	2.02	0.41
1:C:404:PRO:HB3	1:C:435:ASN:HA	2.02	0.41
2:D:52:VAL:HG22	2:D:156:VAL:HG12	2.03	0.41
2:D:99:ARG:HG3	2:D:99:ARG:NH1	2.34	0.41
2:D:144:PRO:HB2	2:D:146:ASN:HD21	1.86	0.41
1:A:34:PHE:CD1	1:A:43:TRP:CH2	3.09	0.40
1:A:129:ASP:C	1:A:131:GLY:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.65	0.40
1:C:34:PHE:O	1:C:35:ALA:C	2.64	0.40
1:C:88:ARG:CD	1:C:173:LEU:HB2	2.51	0.40
1:C:238:PRO:HD2	1:C:241:GLU:N	2.36	0.40
1:A:190:ALA:CB	2:B:124:PHE:CZ	2.74	0.40
1:A:191:LEU:HA	1:A:191:LEU:HD23	1.85	0.40
1:A:281:PHE:HB2	1:A:304:ALA:O	2.21	0.40
1:C:56:GLN:O	1:C:56:GLN:HG3	2.21	0.40
1:C:93:ARG:CD	1:C:95:PHE:CE2	3.01	0.40
2:D:37:ASN:HB2	2:D:75:GLU:OE1	2.21	0.40
2:D:159:ARG:O	2:D:164:CYS:SG	2.79	0.40
2:B:100:TRP:HZ2	2:B:115:SER:O	2.03	0.40
2:B:121:PHE:C	2:B:121:PHE:HD2	2.27	0.40
2:B:121:PHE:CD2	2:B:122:THR:N	2.90	0.40
1:C:386:SER:HB3	1:C:398:THR:HB	2.03	0.40
2:D:98:LYS:HZ3	2:D:100:TRP:C	2.29	0.40
1:A:339:GLY:HA2	1:A:344:VAL:HG12	2.02	0.40
1:C:41:LEU:CD2	1:C:84:ASN:ND2	2.85	0.40
1:C:46:HIS:CA	1:C:47:PRO:C	2.93	0.40
1:C:370:TRP:N	1:C:371:PRO:HD3	2.37	0.40
2:D:98:LYS:HE2	2:D:100:TRP:O	2.21	0.40
2:D:122:THR:C	2:D:124:PHE:N	2.79	0.40
1:A:86:VAL:HB	1:A:178:PHE:CZ	2.56	0.40
2:D:76:ARG:NH1	2:D:144:PRO:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	400/409 (98%)	291 (73%)	67 (17%)	42 (10%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	400/409 (98%)	309 (77%)	54 (14%)	37 (9%)	0	6
2	B	136/138 (99%)	103 (76%)	24 (18%)	9 (7%)	1	11
2	D	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	0	7
All	All	1072/1094 (98%)	800 (75%)	172 (16%)	100 (9%)	0	6

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	A	84	ASN
1	A	212	PRO
1	A	216	ALA
1	A	273	CYS
1	A	277	SER
1	A	299	PRO
1	A	324	PRO
1	A	408	TYR
2	B	94	SER
2	B	162	ASN
1	C	112	ALA
1	C	212	PRO
1	C	289	PRO
1	C	407	ASN
2	D	36	TRP
2	D	94	SER
2	D	108	PRO
1	A	42	GLY
1	A	48	TYR
1	A	57	ASN
1	A	74	SER
1	A	128	LEU
1	A	142	ILE
1	A	181	ALA
1	A	190	ALA
1	A	235	VAL
1	A	264	ALA
1	A	294	PRO
1	A	301	PRO
1	A	379	CYS
1	A	407	ASN
2	B	127	GLY

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Mol	Chain	Res	Type
2	B	161	THR
1	C	35	ALA
1	C	70	CYS
1	C	74	SER
1	C	131	GLY
1	C	170	VAL
1	C	219	ASP
1	C	221	PRO
1	C	222	SER
1	C	303	GLY
1	C	313	PHE
2	D	34	VAL
2	D	90	CYS
2	D	109	ASN
2	D	160	PRO
1	A	32	LEU
1	A	112	ALA
1	A	231	VAL
1	A	374	GLY
1	A	391	GLY
2	B	45	ARG
2	B	126	LEU
2	B	151	CYS
1	C	32	LEU
1	C	301	PRO
1	C	312	GLY
1	C	340	MET
1	C	351	PRO
1	C	392	LEU
2	D	44	GLN
2	D	55	ASN
2	D	162	ASN
1	A	70	CYS
1	A	131	GLY
1	A	234	ALA
1	A	289	PRO
1	A	401	ASP
2	B	145	ASP
1	C	49	GLY
1	C	85	TRP
1	C	114	SER
1	C	115	CYS

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Mol	Chain	Res	Type
1	C	132	THR
1	C	154	SER
1	C	234	ALA
1	C	294	PRO
1	C	332	PRO
2	D	39	SER
1	A	109	PRO
1	A	263	GLN
2	B	67	ASP
1	C	60	ASN
1	C	91	ALA
1	C	233	HIS
1	C	424	SER
1	A	233	HIS
1	A	305	THR
1	A	405	HIS
1	C	81	LEU
1	C	142	ILE
1	A	303	GLY
1	A	351	PRO
1	C	317	PRO
1	A	256	PRO
1	C	299	PRO
2	D	62	CYS
1	A	378	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	330/345 (96%)	261 (79%)	69 (21%)	1 6
1	C	330/345 (96%)	259 (78%)	71 (22%)	1 6
2	B	127/127 (100%)	113 (89%)	14 (11%)	6 26
2	D	127/127 (100%)	113 (89%)	14 (11%)	6 26
All	All	914/944 (97%)	746 (82%)	168 (18%)	1 9

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	41	LEU
1	A	44	LEU
1	A	54	LEU
1	A	66	MET
1	A	69	VAL
1	A	70	CYS
1	A	72	VAL
1	A	86	VAL
1	A	87	TYR
1	A	90	GLU
1	A	93	ARG
1	A	97	GLU
1	A	98	LEU
1	A	100	PHE
1	A	114	SER
1	A	115	CYS
1	A	116	LYS
1	A	118	THR
1	A	123	TYR
1	A	126	SER
1	A	128	LEU
1	A	138	LEU
1	A	140	THR
1	A	141	LYS
1	A	145	ILE
1	A	149	GLU
1	A	151	THR
1	A	152	VAL
1	A	161	VAL
1	A	165	VAL
1	A	174	THR
1	A	185	ILE
1	A	189	VAL
1	A	197	TYR
1	A	204	LEU
1	A	206	GLN
1	A	225	THR
1	A	226	VAL
1	A	229	THR
1	A	235	VAL
1	A	236	VAL

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Mol	Chain	Res	Type
1	A	249	VAL
1	A	257	ILE
1	A	261	LEU
1	A	262	CYS
1	A	273	CYS
1	A	280	PHE
1	A	284	GLU
1	A	291	LEU
1	A	297	THR
1	A	298	LEU
1	A	305	THR
1	A	306	SER
1	A	307	CYS
1	A	309	CYS
1	A	335	LEU
1	A	344	VAL
1	A	349	THR
1	A	364	VAL
1	A	365	THR
1	A	367	GLU
1	A	368	GLN
1	A	379	CYS
1	A	392	LEU
1	A	408	TYR
1	A	418	VAL
1	A	426	SER
1	A	432	VAL
2	B	47	ASP
2	B	52	VAL
2	B	54	ILE
2	B	74	THR
2	B	79	LEU
2	B	82	VAL
2	B	104	ARG
2	B	112	LEU
2	B	120	LEU
2	B	122	THR
2	B	145	ASP
2	B	155	LYS
2	B	161	THR
2	B	162	ASN
1	C	31	LEU

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Mol	Chain	Res	Type
1	C	32	LEU
1	C	41	LEU
1	C	44	LEU
1	C	46	HIS
1	C	48	TYR
1	C	54	LEU
1	C	55	MET
1	C	56	GLN
1	C	58	ILE
1	C	72	VAL
1	C	79	ASN
1	C	93	ARG
1	C	94	ILE
1	C	100	PHE
1	C	102	VAL
1	C	107	SER
1	C	114	SER
1	C	118	THR
1	C	121	LEU
1	C	123	TYR
1	C	128	LEU
1	C	132	THR
1	C	133	ASN
1	C	138	LEU
1	C	145	ILE
1	C	150	ILE
1	C	151	THR
1	C	152	VAL
1	C	153	SER
1	C	154	SER
1	C	157	GLU
1	C	161	VAL
1	C	169	SER
1	C	170	VAL
1	C	174	THR
1	C	183	GLN
1	C	185	ILE
1	C	188	CYS
1	C	189	VAL
1	C	191	LEU
1	C	214	THR
1	C	215	ILE

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Mol	Chain	Res	Type
1	C	225	THR
1	C	229	THR
1	C	235	VAL
1	C	236	VAL
1	C	249	VAL
1	C	259	GLN
1	C	260	CYS
1	C	281	PHE
1	C	287	GLU
1	C	290	CYS
1	C	293	CYS
1	C	297	THR
1	C	305	THR
1	C	309	CYS
1	C	313	PHE
1	C	325	CYS
1	C	364	VAL
1	C	366	CYS
1	C	367	GLU
1	C	379	CYS
1	C	392	LEU
1	C	403	GLU
1	C	406	MET
1	C	411	THR
1	C	422	VAL
1	C	427	PHE
1	C	429	THR
1	C	432	VAL
2	D	30	ASP
2	D	34	VAL
2	D	54	ILE
2	D	67	ASP
2	D	74	THR
2	D	79	LEU
2	D	107	SER
2	D	126	LEU
2	D	135	GLU
2	D	139	ILE
2	D	141	SER
2	D	149	ARG
2	D	162	ASN
2	D	164	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	79	ASN
1	A	259	GLN
1	A	274	GLN
1	A	318	GLN
1	A	368	GLN
2	B	106	HIS
2	B	109	ASN
2	B	146	ASN
2	B	162	ASN
1	C	46	HIS
1	C	60	ASN
1	C	71	ASN
1	C	77	GLN
1	C	133	ASN
1	C	135	GLN
1	C	183	GLN
1	C	259	GLN
1	C	274	GLN
1	C	368	GLN
1	C	416	ASN
2	D	146	ASN
2	D	162	ASN

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](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	2,3	14,14,15	0.51	0	17,19,21	1.21	3 (17%)
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	1.18	2 (11%)
3	NAG	E	3	3	14,14,15	0.73	0	17,19,21	1.50	2 (11%)
3	NAG	F	1	2,3	14,14,15	0.65	0	17,19,21	1.31	2 (11%)
3	NAG	F	2	3	14,14,15	0.68	0	17,19,21	1.32	3 (17%)
3	NAG	F	3	3	14,14,15	0.88	1 (7%)	17,19,21	1.62	2 (11%)

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	NAG	E	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	E	3	3	-	5/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	3	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	NAG	C1-C2	2.59	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	NAG	C2-N2-C7	5.54	130.32	122.90
3	E	3	NAG	C2-N2-C7	4.21	128.54	122.90
3	F	1	NAG	C3-C4-C5	-3.50	103.88	110.23
3	F	2	NAG	C4-C3-C2	2.87	115.22	111.02
3	E	2	NAG	C4-C3-C2	2.67	114.92	111.02
3	E	1	NAG	C1-O5-C5	2.46	115.49	112.19
3	E	3	NAG	C3-C4-C5	2.45	114.68	110.23
3	E	1	NAG	C1-C2-N2	-2.38	106.69	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O4-C4-C5	2.33	115.06	109.32
3	F	3	NAG	O7-C7-N2	2.23	125.93	121.98
3	E	2	NAG	O4-C4-C3	-2.12	105.37	110.38
3	F	2	NAG	C1-O5-C5	-2.08	109.39	112.19
3	F	2	NAG	O5-C5-C6	2.08	111.71	107.66
3	E	1	NAG	O5-C1-C2	2.06	114.48	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

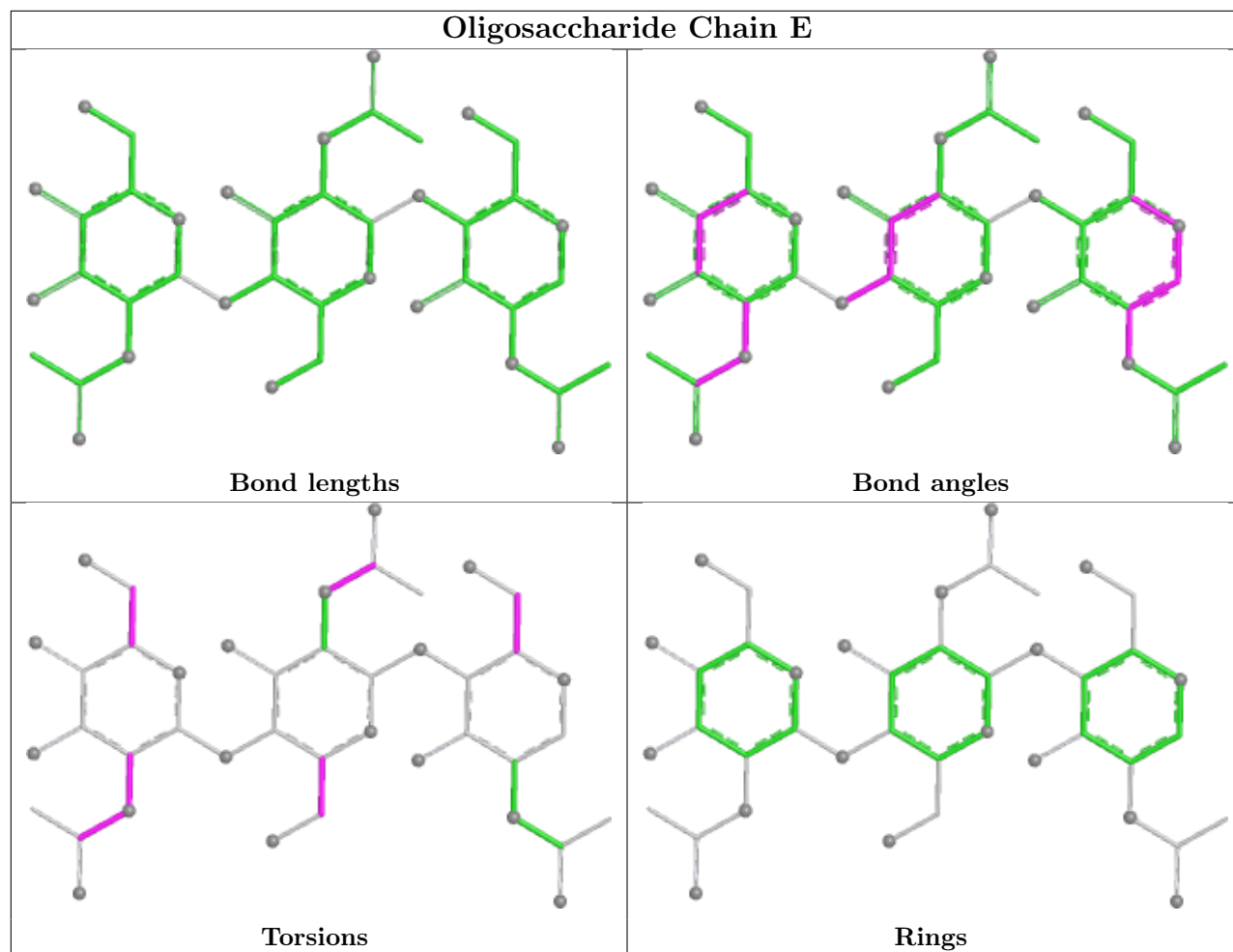
Mol	Chain	Res	Type	Atoms
3	E	3	NAG	C3-C2-N2-C7
3	F	3	NAG	C3-C2-N2-C7
3	E	3	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	3	NAG	C8-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	3	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	3	NAG	O5-C5-C6-O6
3	E	2	NAG	O7-C7-N2-C2
3	F	3	NAG	C8-C7-N2-C2
3	F	3	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

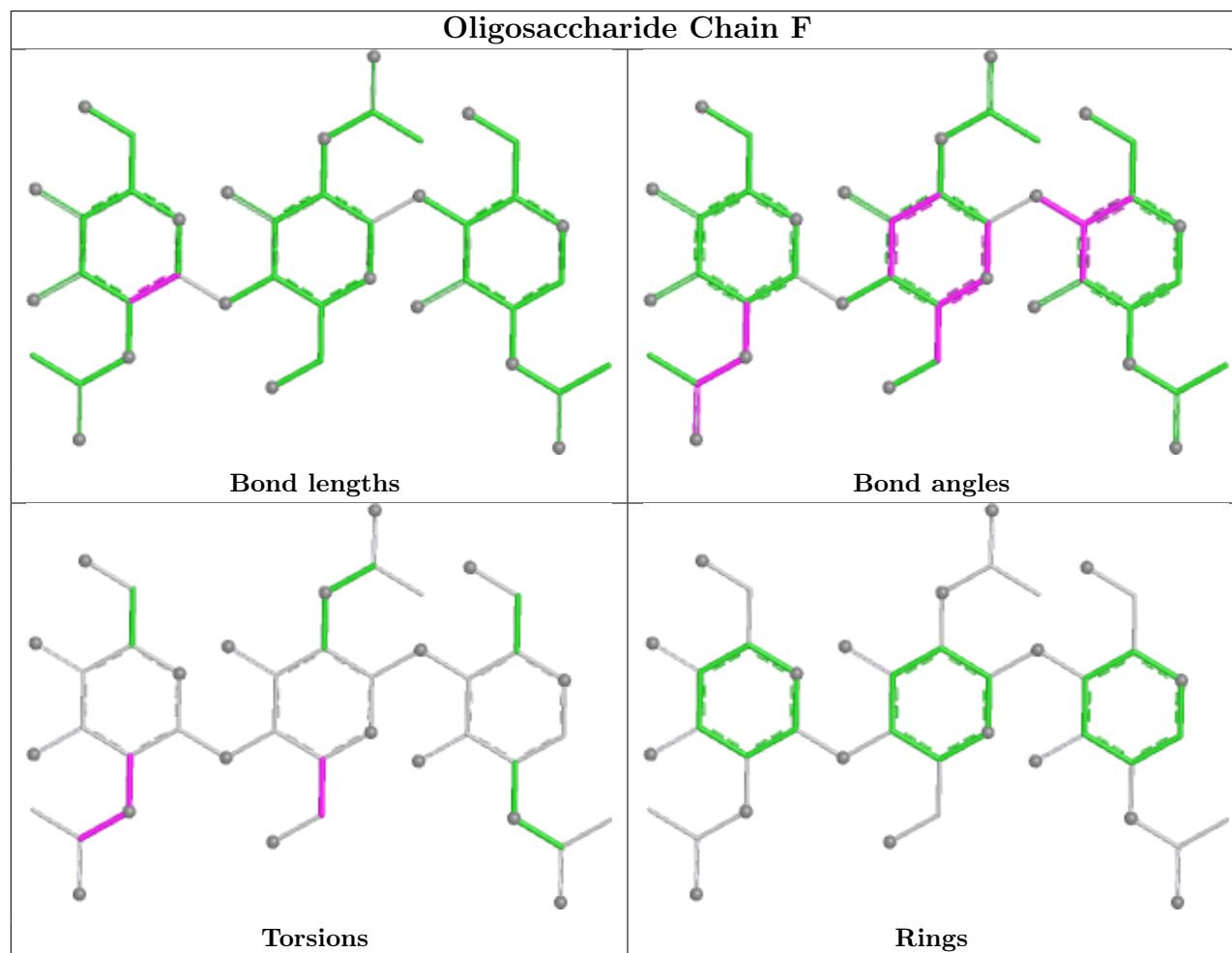
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
3	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	501	1	14,14,15	1.01	1 (7%)	17,19,21	1.54	3 (17%)
4	NAG	C	501	1	14,14,15	1.17	1 (7%)	17,19,21	1.87	3 (17%)

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
4	NAG	A	501	1	-	4/6/23/26	0/1/1/1
4	NAG	C	501	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	NAG	C1-C2	3.81	1.57	1.52
4	A	501	NAG	C1-C2	2.99	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAG	C1-O5-C5	4.67	118.45	112.19
4	A	501	NAG	C4-C3-C2	3.42	116.04	111.02
4	C	501	NAG	C2-N2-C7	3.14	127.10	122.90
4	A	501	NAG	O7-C7-C8	-2.51	117.58	122.05
4	A	501	NAG	O7-C7-N2	2.38	126.19	121.98
4	C	501	NAG	O7-C7-C8	-2.21	118.11	122.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C3-C2-N2-C7
4	A	501	NAG	O7-C7-N2-C2
4	C	501	NAG	C3-C2-N2-C7
4	A	501	NAG	C8-C7-N2-C2
4	C	501	NAG	C8-C7-N2-C2
4	C	501	NAG	O7-C7-N2-C2
4	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	2	0
4	C	501	NAG	1	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

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	406/409 (99%)	0.01	5 (1%) 76 52	52, 119, 209, 337	0
1	C	406/409 (99%)	-0.04	5 (1%) 76 52	52, 121, 208, 253	0
2	B	138/138 (100%)	0.14	3 (2%) 62 37	79, 161, 251, 284	0
2	D	138/138 (100%)	0.25	6 (4%) 40 21	78, 161, 255, 350	0
All	All	1088/1094 (99%)	0.04	19 (1%) 69 43	52, 130, 227, 350	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	124	PHE	4.9
2	D	124	PHE	4.9
1	A	27	LYS	4.4
1	C	27	LYS	4.4
1	A	271	ASP	3.2
1	C	73	MET	2.8
2	D	121	PHE	2.8
2	D	128	PHE	2.8
2	D	55	ASN	2.7
1	A	40	GLU	2.7
2	B	121	PHE	2.6
2	D	63	PRO	2.6
1	A	65	TYR	2.4
2	D	72	ASP	2.3
1	C	151	THR	2.3
1	A	272	ALA	2.3
1	C	72	VAL	2.1
1	C	421	LEU	2.1
2	B	125	SER	2.0

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

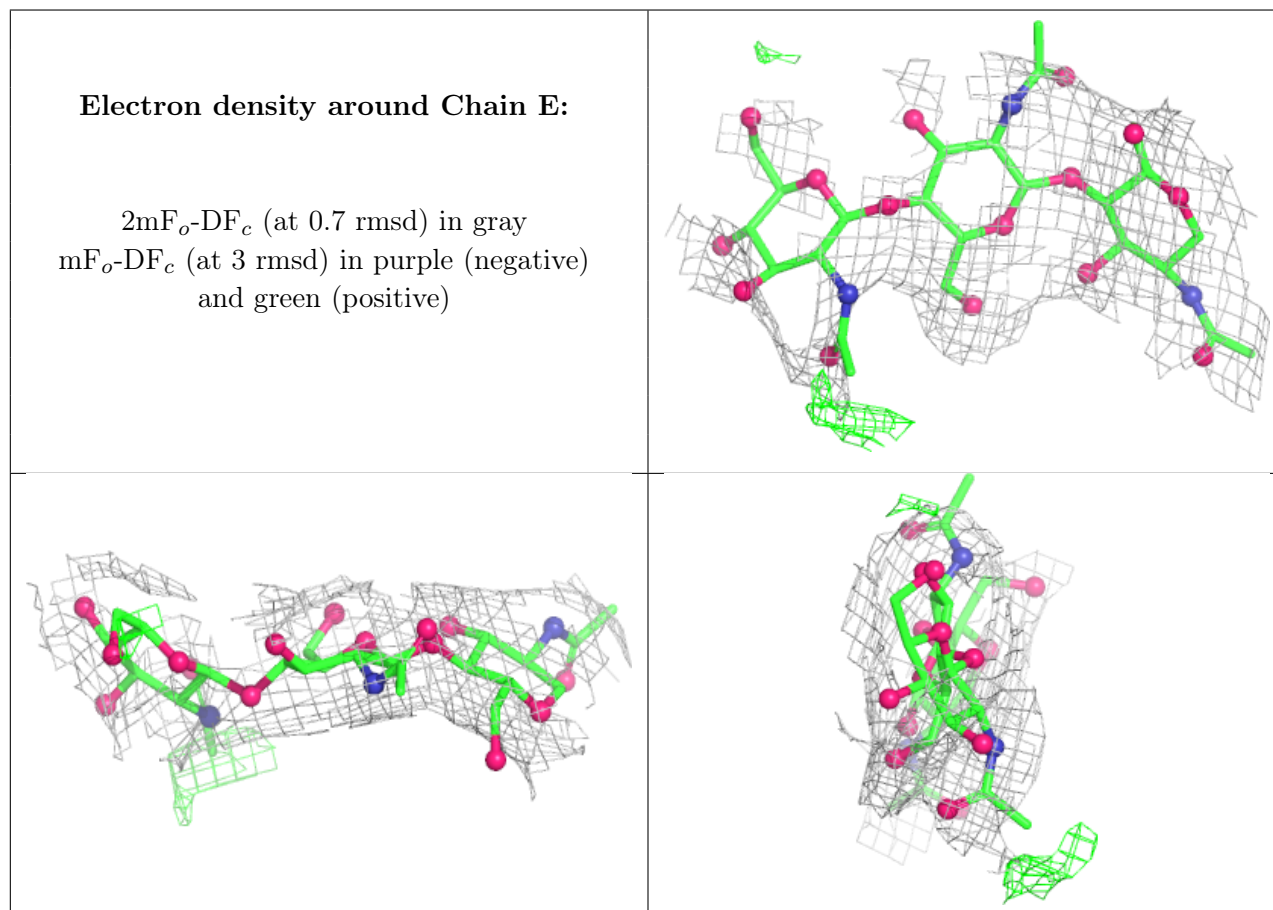
There are no non-standard protein/DNA/RNA residues in this entry.

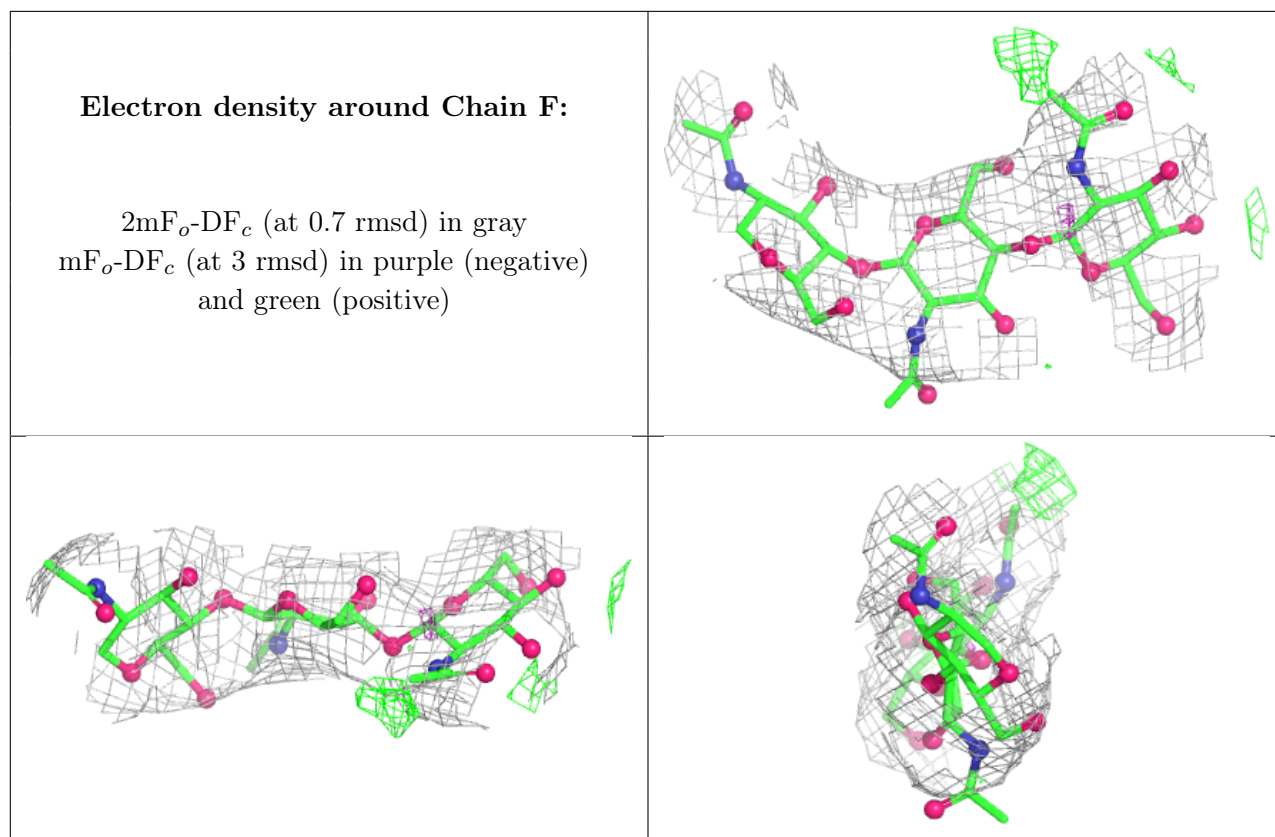
6.3 Carbohydrates [i](#)

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
3	NAG	F	3	14/15	0.44	0.17	184,184,184,184	0
3	NAG	E	3	14/15	0.52	0.18	205,205,205,205	0
3	NAG	E	2	14/15	0.79	0.10	146,146,146,146	0
3	NAG	E	1	14/15	0.82	0.10	146,146,146,146	0
3	NAG	F	2	14/15	0.90	0.10	149,149,149,149	0
3	NAG	F	1	14/15	0.93	0.07	135,135,135,135	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	501	14/15	0.69	0.13	155,155,155,155	0
4	NAG	C	501	14/15	0.71	0.11	153,153,153,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.