Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 04:00 PM EDT

PDB ID	:	3ULA
Title	:	Crystal structure of the TV3 mutant F63W-MD-2-Eritoran complex
Authors	:	Kim, H.J.; Cheong, H.K.; Jeon, Y.H.
Deposited on	:	2011-11-10
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

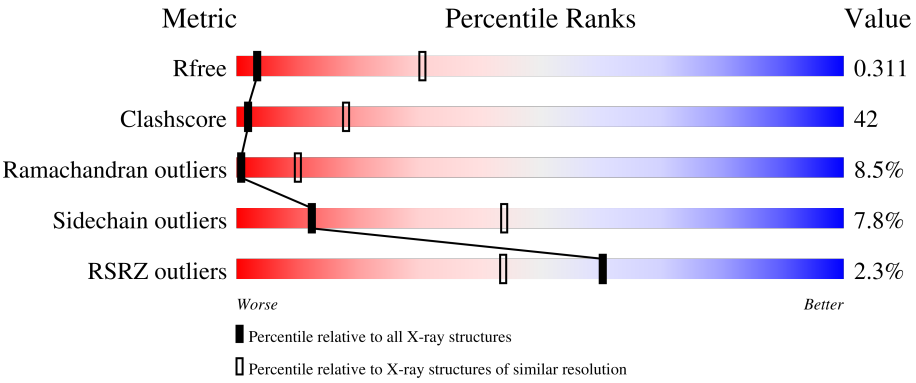
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	279	34% 56% 8% ·
1	C	279	% 37% 54% 8% ·
2	B	142	4% 35% 49% 14% ··
2	D	142	8% 35% 49% 14% ··
3	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	1	-	-	-	X
3	BMA	E	3	-	-	-	X
3	NAG	F	1	-	-	-	X
3	BMA	F	3	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6962 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 Toll-like receptor 4, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2191	1402	367	411	11			
1	C	276	Total	C	N	O	S	0	0	0
			2191	1402	367	411	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP O00206
A	26	SER	-	expression tag	UNP O00206
A	63	TRP	PHE	engineered mutation	UNP O00206
A	303	THR	-	expression tag	UNP Q4G1L2
C	25	GLY	-	expression tag	UNP O00206
C	26	SER	-	expression tag	UNP O00206
C	63	TRP	PHE	engineered mutation	UNP O00206
C	303	THR	-	expression tag	UNP Q4G1L2

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	S	0	0	0
			1134	730	186	208	10			
2	D	140	Total	C	N	O	S	0	0	0
			1134	730	186	208	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	GLY	-	expression tag	UNP Q9Y6Y9
B	18	SER	-	expression tag	UNP Q9Y6Y9
B	56	GLY	ARG	SEE REMARK 999	UNP Q9Y6Y9
D	17	GLY	-	expression tag	UNP Q9Y6Y9

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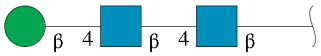
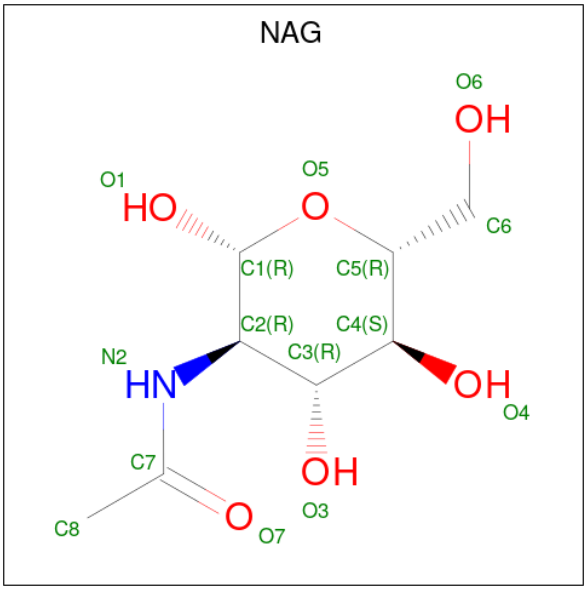
Chain	Residue	Modelled	Actual	Comment	Reference
D	18	SER	-	expression tag	UNP Q9Y6Y9
D	56	GLY	ARG	SEE REMARK 999	UNP Q9Y6Y9

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(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
3	E	3	Total C N O 39 22 2 15	0	0	0
3	F	3	Total C N O 39 22 2 15	0	0	0

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



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

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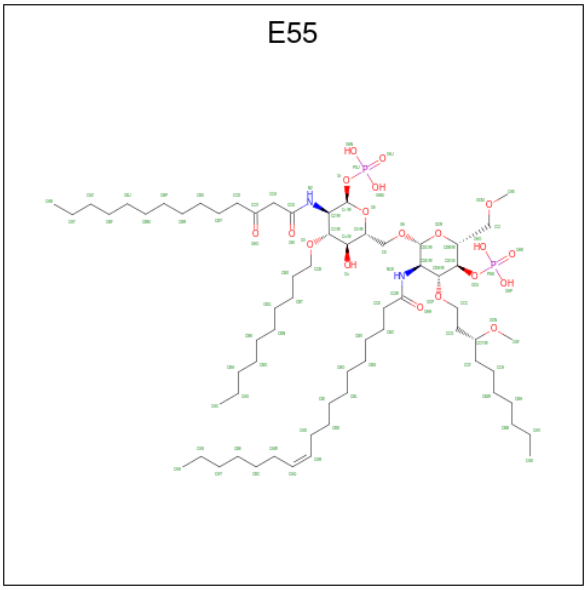
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 3-O-DECYL-2-DEOXY-6-O-{2-DEOXY-3-O-[(3R)-3-METHOXYDECYL]-6-O-METHYL-2-[(11Z)-OCTADEC-11-ENOYLAMINO]-4-O-PHOSPHONO-BETA-D-GLUCOPYRANOSYL}-2-[(3-OXOTETRADECANOYL)AMINO]-1-O-PHOSPHONO-ALPHA-D-GLUCOPYRANOSE (three-letter code: E55) (formula: $C_{66}H_{126}N_2O_{19}P_2$).



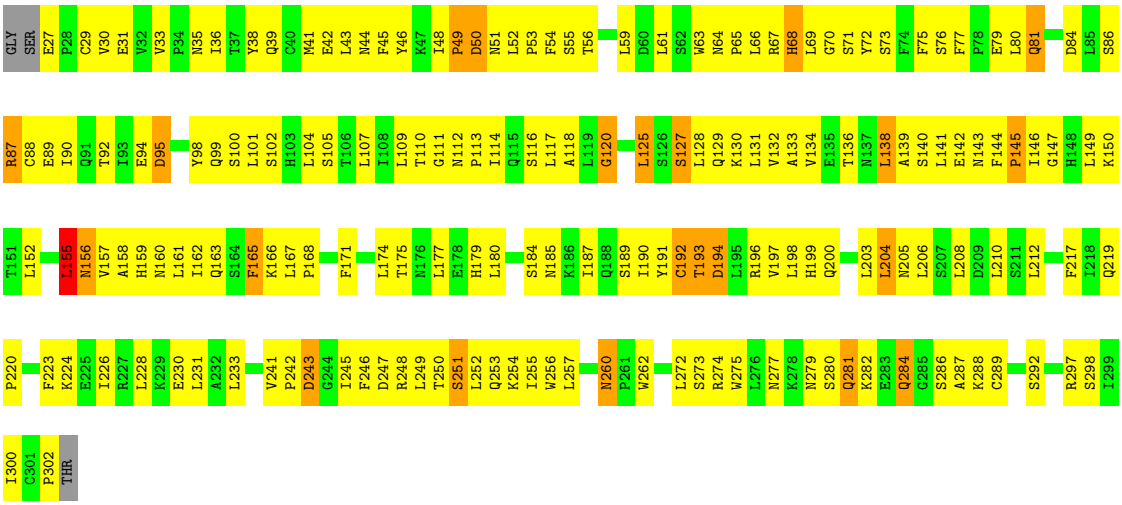
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			89	66	2	19	2		
5	C	1	Total	C	N	O	P	0	0
			89	66	2	19	2		

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.

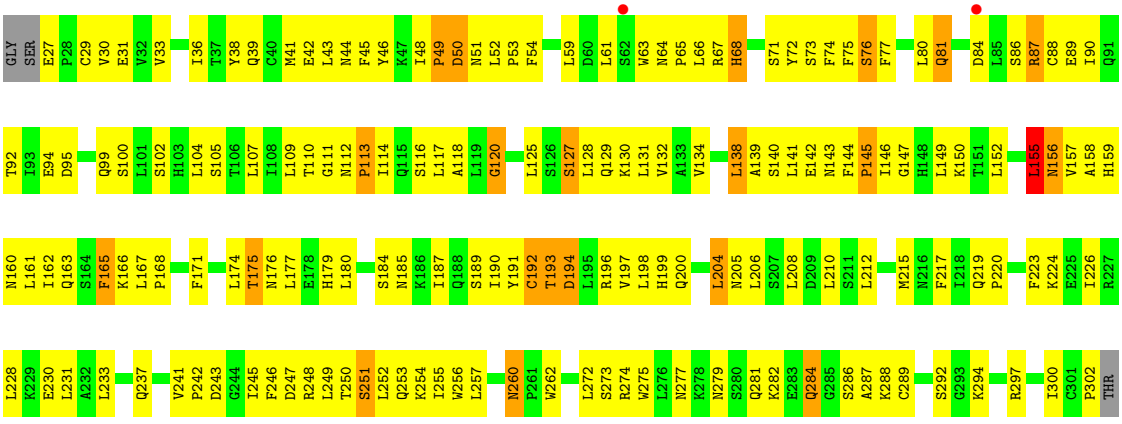
• Molecule 1: Toll-like receptor 4, Variable lymphocyte receptor B

Chain A:



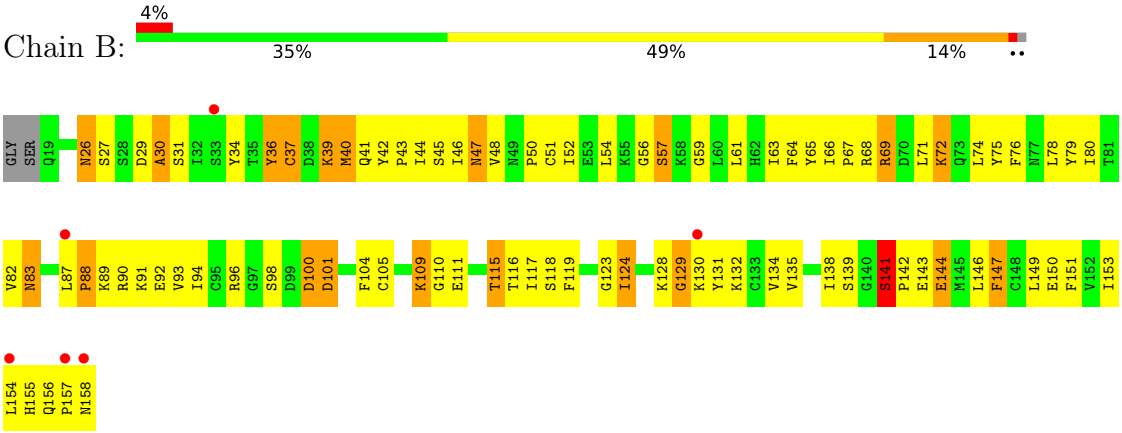
• Molecule 1: Toll-like receptor 4, Variable lymphocyte receptor B

Chain C:



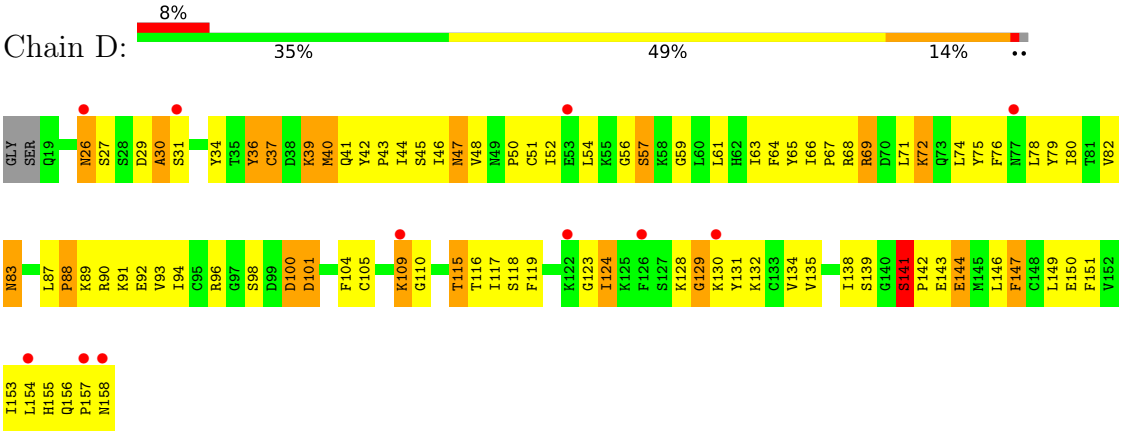
• Molecule 2: Lymphocyte antigen 96

Chain B:



• Molecule 2: Lymphocyte antigen 96

Chain D:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.21Å 126.94Å 129.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 90.65 – 3.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.60) 99.3 (90.65-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.306 , 0.341 0.304 , 0.311	Depositor DCC
R_{free} test set	789 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.040 for -h,l,k	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6962	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1344e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: E55, NAG, BMA

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	0.51	0/2241	0.75	1/3046 (0.0%)
1	C	0.51	0/2241	0.75	1/3046 (0.0%)
2	B	0.54	0/1160	0.80	1/1562 (0.1%)
2	D	0.55	0/1160	0.81	1/1562 (0.1%)
All	All	0.52	0/6802	0.77	4/9216 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	141	SER	C-N-CD	6.67	142.40	128.40
2	B	141	SER	C-N-CD	6.42	141.89	128.40
1	A	155	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	155	LEU	CA-CB-CG	5.32	127.53	115.30

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	2191	0	2194	183	0
1	C	2191	0	2194	172	0
2	B	1134	0	1130	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1134	0	1130	119	0
3	E	39	0	34	7	0
3	F	39	0	34	3	0
4	A	28	0	26	3	0
4	C	28	0	26	2	0
5	A	89	0	122	18	0
5	C	89	0	122	14	0
All	All	6962	0	7012	586	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 42.

All (586) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:LEU:HD22	2:D:124:ILE:HD11	1.43	1.01
1:A:102:SER:O	1:A:127:SER:HB2	1.62	1.00
1:A:204:LEU:HD13	1:A:206:LEU:HB2	1.45	0.98
1:C:204:LEU:HD13	1:C:206:LEU:HB2	1.44	0.97
1:C:94:GLU:HA	1:C:118:ALA:HB2	1.45	0.97
2:B:54:LEU:HD22	2:B:124:ILE:HD11	1.47	0.97
1:C:102:SER:O	1:C:127:SER:HB2	1.63	0.96
2:B:131:TYR:HB2	2:B:153:ILE:HG23	1.48	0.96
2:D:131:TYR:HB2	2:D:153:ILE:HG23	1.50	0.93
1:A:94:GLU:HA	1:A:118:ALA:HB2	1.48	0.93
1:C:230:GLU:HG2	1:C:254:LYS:HB2	1.53	0.91
2:B:131:TYR:HB2	2:B:153:ILE:CG2	2.02	0.90
1:A:132:VAL:HG12	1:A:134:VAL:HG23	1.54	0.89
1:A:230:GLU:HG2	1:A:254:LYS:HB2	1.56	0.88
2:D:131:TYR:HB2	2:D:153:ILE:CG2	2.04	0.87
1:C:223:PHE:HA	1:C:226:ILE:HD12	1.57	0.86
1:A:228:LEU:HD23	1:A:249:LEU:HD11	1.58	0.86
1:A:223:PHE:HA	1:A:226:ILE:HD12	1.57	0.85
1:C:132:VAL:HG12	1:C:134:VAL:HG23	1.56	0.85
1:C:228:LEU:HD23	1:C:249:LEU:HD11	1.60	0.83
1:C:252:LEU:O	1:C:282:LYS:HE3	1.79	0.82
1:A:132:VAL:CG1	1:A:134:VAL:HG23	2.10	0.82
4:C:402:NAG:H83	4:C:402:NAG:O3	1.80	0.80
1:A:252:LEU:O	1:A:282:LYS:HE3	1.81	0.80
1:C:132:VAL:CG1	1:C:134:VAL:HG23	2.12	0.80
2:B:90:ARG:HH12	1:C:300:ILE:HA	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:OD2	2:B:109:LYS:HE3	1.83	0.78
2:B:96:ARG:CZ	1:C:297:ARG:NH2	2.47	0.78
2:B:156:GLN:O	2:B:156:GLN:HG3	1.83	0.78
1:C:129:GLN:O	1:C:152:LEU:HD12	1.84	0.77
1:A:129:GLN:O	1:A:152:LEU:HD12	1.85	0.77
1:C:157:VAL:HG23	1:C:157:VAL:O	1.85	0.77
1:C:94:GLU:HA	1:C:118:ALA:CB	2.13	0.77
2:B:27:SER:HB3	2:B:51:CYS:SG	2.24	0.77
1:A:114:ILE:HG21	1:A:117:LEU:HD13	1.68	0.76
1:A:157:VAL:HG23	1:A:157:VAL:O	1.83	0.76
1:C:84:ASP:OD2	2:D:109:LYS:HE3	1.86	0.76
1:C:152:LEU:HD21	1:C:155:LEU:HB2	1.66	0.76
1:C:289:CYS:HB2	1:C:292:SER:HB3	1.68	0.76
1:A:45:PHE:HD1	1:A:49:PRO:HD3	1.51	0.76
1:C:45:PHE:HD1	1:C:49:PRO:HD3	1.52	0.75
2:D:27:SER:HB3	2:D:51:CYS:SG	2.26	0.75
1:C:114:ILE:HG21	1:C:117:LEU:HD13	1.69	0.74
3:E:2:NAG:H62	3:E:3:BMA:O2	1.86	0.74
1:A:289:CYS:HB2	1:A:292:SER:HB3	1.68	0.73
5:A:1206:E55:HCB1	5:A:1206:E55:OAG	1.88	0.73
2:D:156:GLN:O	2:D:156:GLN:HG3	1.87	0.73
1:C:289:CYS:CB	1:C:292:SER:HB3	2.18	0.73
1:C:87:ARG:NH1	1:C:111:GLY:HA3	2.04	0.73
1:A:152:LEU:HD21	1:A:155:LEU:HB2	1.70	0.72
1:A:87:ARG:NH1	1:A:111:GLY:HA3	2.03	0.72
1:A:156:ASN:C	1:A:156:ASN:HD22	1.91	0.72
1:A:289:CYS:CB	1:A:292:SER:HB3	2.20	0.72
1:A:92:THR:HG22	1:A:116:SER:OG	1.90	0.71
2:B:29:ASP:O	2:B:155:HIS:CD2	2.43	0.71
2:B:44:ILE:HG22	2:B:46:ILE:HG13	1.72	0.71
2:B:96:ARG:CZ	1:C:297:ARG:HH21	2.03	0.71
2:B:142:PRO:O	2:B:144:GLU:HG3	1.90	0.71
1:C:44:ASN:ND2	1:C:46:TYR:HE1	1.89	0.71
1:A:107:LEU:HD21	1:A:109:LEU:HD11	1.73	0.71
2:B:130:LYS:HG2	2:B:154:LEU:HD13	1.73	0.71
2:B:146:LEU:O	2:B:147:PHE:HB3	1.91	0.71
1:A:94:GLU:HA	1:A:118:ALA:CB	2.18	0.70
5:C:401:E55:HCI2	5:C:401:E55:OAK	1.91	0.70
1:A:44:ASN:ND2	1:A:46:TYR:HE1	1.90	0.70
1:C:44:ASN:HD21	1:C:46:TYR:HE1	1.38	0.70
1:C:59:LEU:HD11	1:C:61:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASN:C	1:C:156:ASN:HD22	1.93	0.70
2:D:135:VAL:HG23	2:D:135:VAL:O	1.92	0.70
2:D:146:LEU:O	2:D:147:PHE:HB3	1.90	0.70
5:A:1206:E55:HBG2	2:D:76:PHE:CE1	2.26	0.70
2:B:79:TYR:HB2	2:B:134:VAL:HB	1.72	0.70
1:A:302:PRO:HB3	5:A:1206:E55:HAF2	1.74	0.69
1:C:107:LEU:HD21	1:C:109:LEU:HD11	1.74	0.69
2:D:142:PRO:O	2:D:144:GLU:HG3	1.92	0.69
2:B:74:LEU:HD12	2:B:94:ILE:HB	1.74	0.69
2:B:90:ARG:NH1	1:C:300:ILE:HA	2.07	0.69
2:D:29:ASP:O	2:D:155:HIS:CD2	2.45	0.69
1:A:33:VAL:HG12	1:A:36:ILE:HB	1.74	0.69
5:A:1206:E55:HCI2	5:A:1206:E55:OAK	1.93	0.69
1:C:204:LEU:CD1	1:C:206:LEU:HB2	2.20	0.69
2:D:79:TYR:HB2	2:D:134:VAL:HB	1.73	0.69
3:F:2:NAG:H62	3:F:3:BMA:O2	1.93	0.69
5:C:401:E55:HCB1	5:C:401:E55:OAG	1.92	0.68
2:D:130:LYS:HG2	2:D:154:LEU:HD13	1.73	0.68
1:A:279:ASN:HB3	1:A:282:LYS:HD2	1.75	0.68
1:A:44:ASN:HD21	1:A:46:TYR:HE1	1.42	0.68
1:A:220:PRO:HG3	1:A:242:PRO:HB3	1.75	0.68
1:C:33:VAL:HG12	1:C:36:ILE:HB	1.74	0.68
1:C:59:LEU:HD11	1:C:61:LEU:CD2	2.24	0.68
2:B:135:VAL:HG23	2:B:135:VAL:O	1.92	0.68
1:C:262:TRP:NE1	1:C:287:ALA:HB1	2.09	0.68
2:D:115:THR:OG1	2:D:116:THR:N	2.24	0.67
1:A:297:ARG:NH2	2:D:96:ARG:CZ	2.58	0.67
4:A:1201:NAG:O3	4:A:1201:NAG:H83	1.94	0.67
2:D:54:LEU:HD22	2:D:124:ILE:CD1	2.21	0.67
2:D:74:LEU:HD12	2:D:94:ILE:HB	1.74	0.67
1:A:262:TRP:NE1	1:A:287:ALA:HB1	2.10	0.67
1:C:92:THR:HG22	1:C:116:SER:OG	1.93	0.67
2:D:44:ILE:HG22	2:D:46:ILE:HG13	1.76	0.67
1:A:204:LEU:CD1	1:A:206:LEU:HB2	2.20	0.67
1:A:59:LEU:HD11	1:A:61:LEU:HD21	1.77	0.67
2:B:52:ILE:HD11	5:C:401:E55:HBC2	1.77	0.67
1:C:171:PHE:CD2	1:C:174:LEU:HD12	2.31	0.66
1:C:220:PRO:HG3	1:C:242:PRO:HB3	1.77	0.66
2:D:93:VAL:O	2:D:94:ILE:HD13	1.95	0.66
2:D:80:ILE:HD12	2:D:80:ILE:N	2.10	0.66
1:A:146:ILE:HG22	1:A:149:LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ILE:HD12	2:B:80:ILE:N	2.11	0.65
1:C:146:ILE:HG22	1:C:149:LEU:HD12	1.77	0.65
1:C:279:ASN:HB3	1:C:282:LYS:HD2	1.77	0.65
2:B:115:THR:OG1	2:B:116:THR:N	2.26	0.65
1:A:171:PHE:CD2	1:A:174:LEU:HD12	2.31	0.65
1:A:27:GLU:HG2	1:A:52:LEU:HD23	1.78	0.65
1:C:43:LEU:HB3	1:C:45:PHE:HE2	1.63	0.64
2:D:130:LYS:HG2	2:D:154:LEU:CD1	2.27	0.64
2:B:93:VAL:O	2:B:94:ILE:HD13	1.96	0.64
2:D:83:ASN:HB2	2:D:129:GLY:HA3	1.79	0.64
1:A:141:LEU:H	1:A:141:LEU:HD12	1.63	0.64
1:C:302:PRO:HB3	5:C:401:E55:HAF2	1.78	0.64
1:A:64:ASN:O	1:A:66:LEU:N	2.30	0.64
1:A:156:ASN:HD22	1:A:157:VAL:N	1.95	0.64
2:B:54:LEU:HD22	2:B:124:ILE:CD1	2.25	0.64
2:B:83:ASN:HB2	2:B:129:GLY:HA3	1.80	0.64
1:C:141:LEU:HD12	1:C:141:LEU:H	1.63	0.64
1:C:27:GLU:HG2	1:C:52:LEU:HD23	1.80	0.63
1:C:64:ASN:O	1:C:66:LEU:N	2.30	0.63
1:C:150:LYS:NZ	4:C:406:NAG:O4	2.25	0.63
1:A:33:VAL:CG1	1:A:36:ILE:HB	2.29	0.63
2:B:130:LYS:HG2	2:B:154:LEU:CD1	2.28	0.62
1:A:59:LEU:HD11	1:A:61:LEU:CD2	2.28	0.62
2:D:44:ILE:HG12	2:D:65:TYR:CD1	2.35	0.62
1:A:43:LEU:HB3	1:A:45:PHE:HE2	1.63	0.62
1:A:110:THR:HG23	1:A:134:VAL:HB	1.81	0.62
2:D:141:SER:OG	2:D:142:PRO:HD3	2.00	0.61
1:A:66:LEU:O	1:A:68:HIS:N	2.31	0.61
1:C:156:ASN:HD22	1:C:157:VAL:N	1.98	0.61
1:C:141:LEU:HD12	1:C:141:LEU:N	2.16	0.61
2:B:141:SER:OG	2:B:142:PRO:HD3	2.01	0.61
1:A:141:LEU:HD12	1:A:141:LEU:N	2.16	0.61
1:C:110:THR:HG23	1:C:134:VAL:HB	1.81	0.61
1:C:138:LEU:HD11	1:C:144:PHE:CD1	2.37	0.60
1:A:43:LEU:CB	1:A:45:PHE:CE2	2.85	0.60
1:C:33:VAL:CG1	1:C:36:ILE:HB	2.31	0.60
1:C:43:LEU:CB	1:C:45:PHE:CE2	2.85	0.60
1:C:156:ASN:ND2	1:C:158:ALA:H	2.00	0.60
2:D:29:ASP:O	2:D:30:ALA:HB2	2.00	0.60
1:A:45:PHE:CD1	1:A:49:PRO:HD3	2.37	0.60
2:D:69:ARG:HG2	2:D:144:GLU:OE2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:VAL:HG12	2:B:50:PRO:O	2.02	0.59
2:D:48:VAL:HG12	2:D:50:PRO:O	2.02	0.59
2:B:69:ARG:HG2	2:B:144:GLU:OE2	2.02	0.59
1:C:66:LEU:O	1:C:68:HIS:N	2.33	0.59
1:A:112:ASN:O	1:A:114:ILE:N	2.32	0.59
1:A:138:LEU:HD11	1:A:144:PHE:CD1	2.37	0.59
2:B:29:ASP:O	2:B:30:ALA:HB2	2.02	0.59
5:A:1206:E55:HCH2	2:D:119:PHE:CB	2.33	0.59
2:B:36:TYR:HD1	2:B:36:TYR:H	1.51	0.59
2:B:39:LYS:O	2:B:41:GLN:HG3	2.02	0.59
2:B:40:MET:HG3	2:B:42:TYR:CE1	2.38	0.59
1:A:177:LEU:HD11	1:A:179:HIS:O	2.03	0.58
1:A:156:ASN:ND2	1:A:158:ALA:H	2.01	0.58
1:A:189:SER:HB3	1:A:217:PHE:HD2	1.68	0.58
1:A:155:LEU:HD13	1:A:157:VAL:HG13	1.84	0.58
2:B:76:PHE:CE1	5:C:401:E55:HBG2	2.39	0.58
2:B:44:ILE:HG12	2:B:65:TYR:CD1	2.38	0.58
2:D:36:TYR:HD1	2:D:36:TYR:H	1.51	0.58
2:D:54:LEU:O	2:D:124:ILE:HG13	2.03	0.58
1:C:118:ALA:C	1:C:120:GLY:H	2.06	0.58
1:A:43:LEU:HB2	1:A:45:PHE:CE2	2.39	0.58
1:C:189:SER:HB3	1:C:217:PHE:HD2	1.68	0.58
1:C:205:ASN:HD22	3:F:1:NAG:C7	2.16	0.58
1:A:231:LEU:HD11	1:A:233:LEU:HD11	1.86	0.57
2:D:40:MET:HG3	2:D:42:TYR:CE1	2.38	0.57
2:B:54:LEU:O	2:B:124:ILE:HG13	2.05	0.57
1:C:155:LEU:HD13	1:C:157:VAL:HG13	1.85	0.57
2:B:104:PHE:HE2	2:B:117:ILE:HD11	1.69	0.57
2:D:34:TYR:HA	2:D:150:GLU:O	2.04	0.57
2:D:98:SER:OG	2:D:100:ASP:OD1	2.23	0.57
5:C:401:E55:HBL1	5:C:401:E55:HAD3	1.87	0.57
2:B:34:TYR:HA	2:B:150:GLU:O	2.04	0.57
1:C:43:LEU:HB2	1:C:45:PHE:CE2	2.39	0.57
1:A:118:ALA:C	1:A:120:GLY:H	2.07	0.56
2:B:134:VAL:HG22	2:B:150:GLU:HG2	1.87	0.56
1:C:231:LEU:HD11	1:C:233:LEU:HD11	1.87	0.56
2:D:141:SER:OG	2:D:142:PRO:CD	2.53	0.56
2:D:135:VAL:O	2:D:135:VAL:CG2	2.54	0.56
1:A:155:LEU:HD12	1:A:180:LEU:HD13	1.86	0.56
2:B:98:SER:OG	2:B:100:ASP:OD1	2.22	0.56
1:A:71:SER:HB3	1:A:72:TYR:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1206:E55:CBG	2:D:76:PHE:CE1	2.89	0.56
1:C:141:LEU:HD11	1:C:162:ILE:HD13	1.88	0.56
3:E:2:NAG:O4	3:E:3:BMA:H61	2.06	0.56
1:C:112:ASN:O	1:C:114:ILE:N	2.32	0.56
1:A:43:LEU:HB3	1:A:45:PHE:CE2	2.42	0.55
1:A:302:PRO:HD3	5:A:1206:E55:HCC1	1.86	0.55
2:D:134:VAL:HG22	2:D:150:GLU:HG2	1.89	0.55
2:B:100:ASP:OD1	2:B:100:ASP:N	2.39	0.55
2:B:93:VAL:C	2:B:94:ILE:HD13	2.26	0.55
2:D:39:LYS:O	2:D:41:GLN:HG3	2.05	0.55
1:A:204:LEU:HD13	1:A:206:LEU:CB	2.28	0.55
5:A:1206:E55:HBC2	2:D:52:ILE:HD11	1.89	0.55
2:B:36:TYR:N	2:B:36:TYR:CD1	2.75	0.55
1:C:45:PHE:CD1	1:C:49:PRO:HD3	2.37	0.55
2:D:36:TYR:CD1	2:D:36:TYR:N	2.75	0.55
2:D:100:ASP:OD1	2:D:100:ASP:N	2.39	0.55
2:B:141:SER:OG	2:B:142:PRO:CD	2.54	0.55
1:C:155:LEU:HD12	1:C:180:LEU:HD13	1.87	0.55
1:C:72:TYR:CD1	1:C:72:TYR:N	2.75	0.55
2:D:93:VAL:C	2:D:94:ILE:HD13	2.27	0.55
1:A:72:TYR:N	1:A:72:TYR:CD1	2.75	0.55
2:B:36:TYR:CD2	2:B:41:GLN:HA	2.42	0.55
1:A:63:TRP:CE3	2:B:68:ARG:NH1	2.75	0.55
2:B:74:LEU:CD1	2:B:94:ILE:HB	2.36	0.55
2:D:104:PHE:HE2	2:D:117:ILE:HD11	1.71	0.55
1:C:162:ILE:HB	1:C:185:ASN:HD22	1.72	0.54
1:C:177:LEU:HD11	1:C:179:HIS:O	2.07	0.54
2:D:117:ILE:HG22	2:D:118:SER:O	2.07	0.54
2:B:117:ILE:HG22	2:B:118:SER:O	2.07	0.54
1:C:156:ASN:HD21	1:C:158:ALA:CB	2.20	0.54
1:C:204:LEU:HD13	1:C:206:LEU:CB	2.27	0.54
2:B:155:HIS:CD2	2:B:156:GLN:H	2.26	0.54
1:C:71:SER:HB3	1:C:72:TYR:HD1	1.72	0.54
1:C:231:LEU:HD11	1:C:233:LEU:CD1	2.38	0.54
1:C:156:ASN:HD21	1:C:158:ALA:HB2	1.73	0.54
3:F:2:NAG:O4	3:F:3:BMA:H61	2.06	0.54
2:D:155:HIS:CD2	2:D:156:GLN:H	2.26	0.54
1:C:43:LEU:HB3	1:C:45:PHE:CE2	2.42	0.54
1:C:289:CYS:HB3	1:C:292:SER:HB3	1.89	0.54
2:D:36:TYR:CD2	2:D:41:GLN:HA	2.43	0.54
2:B:36:TYR:HD2	2:B:41:GLN:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:O	2:B:155:HIS:HD2	1.91	0.54
1:A:300:ILE:HA	2:D:90:ARG:HH12	1.71	0.54
1:C:146:ILE:HG22	1:C:149:LEU:CD1	2.38	0.54
2:D:74:LEU:CD1	2:D:94:ILE:HB	2.38	0.54
1:A:114:ILE:CG2	1:A:117:LEU:HD13	2.36	0.53
2:D:56:GLY:O	2:D:57:SER:HB3	2.08	0.53
1:A:43:LEU:O	1:A:45:PHE:HD2	1.91	0.53
1:A:208:LEU:HD21	1:A:210:LEU:HD11	1.89	0.53
2:B:56:GLY:O	2:B:57:SER:HB3	2.07	0.53
1:A:156:ASN:HD21	1:A:158:ALA:HB2	1.74	0.53
1:A:155:LEU:CD1	1:A:157:VAL:HG13	2.39	0.53
1:A:302:PRO:HA	5:A:1206:E55:HAF1	1.89	0.53
2:B:101:ASP:HB3	2:B:105:CYS:SG	2.49	0.53
2:B:119:PHE:CD1	2:B:119:PHE:C	2.82	0.53
2:D:75:TYR:CE2	2:D:91:LYS:HE3	2.43	0.53
1:A:156:ASN:HD21	1:A:158:ALA:CB	2.21	0.53
1:C:31:GLU:OE1	1:C:38:TYR:HE2	1.92	0.53
1:C:165:PHE:CG	1:C:165:PHE:O	2.62	0.53
1:C:63:TRP:CE3	2:D:68:ARG:NH1	2.77	0.53
1:A:87:ARG:HH12	1:A:111:GLY:HA3	1.74	0.53
1:A:107:LEU:O	1:A:107:LEU:HG	2.08	0.52
1:A:141:LEU:HD11	1:A:162:ILE:HD13	1.89	0.52
2:B:65:TYR:CG	2:B:66:ILE:N	2.76	0.52
1:A:231:LEU:HD11	1:A:233:LEU:CD1	2.39	0.52
2:B:44:ILE:HG21	2:B:46:ILE:HD11	1.92	0.52
2:B:135:VAL:O	2:B:135:VAL:CG2	2.56	0.52
2:D:59:GLY:HA3	2:D:119:PHE:CZ	2.45	0.52
2:D:101:ASP:HB3	2:D:105:CYS:SG	2.50	0.52
1:A:165:PHE:CG	1:A:165:PHE:O	2.63	0.52
1:C:64:ASN:O	1:C:66:LEU:HG	2.10	0.52
1:A:142:GLU:HA	1:A:168:PRO:HG2	1.92	0.52
1:A:280:SER:OG	2:D:96:ARG:HD2	2.09	0.52
2:D:78:LEU:HB3	2:D:80:ILE:HD11	1.91	0.52
2:B:59:GLY:HA3	2:B:119:PHE:CZ	2.45	0.52
1:C:163:GLN:O	1:C:187:ILE:HA	2.10	0.52
1:C:165:PHE:HE1	1:C:190:ILE:HG23	1.75	0.52
1:A:71:SER:HB3	1:A:72:TYR:CD1	2.44	0.52
1:A:162:ILE:HB	1:A:185:ASN:HD22	1.74	0.52
1:C:142:GLU:HA	1:C:168:PRO:HG2	1.92	0.52
2:D:36:TYR:HD2	2:D:41:GLN:HA	1.74	0.52
1:C:166:LYS:O	1:C:167:LEU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:HD1	2:B:36:TYR:N	2.07	0.51
1:C:87:ARG:HH12	1:C:111:GLY:HA3	1.75	0.51
1:C:206:LEU:C	1:C:206:LEU:HD13	2.31	0.51
1:C:146:ILE:CG2	1:C:149:LEU:HD12	2.40	0.51
2:D:29:ASP:O	2:D:155:HIS:HD2	1.92	0.51
1:A:146:ILE:HG22	1:A:149:LEU:CD1	2.40	0.51
1:A:297:ARG:HH21	2:D:96:ARG:CZ	2.22	0.51
1:C:44:ASN:ND2	1:C:46:TYR:CE1	2.73	0.51
1:C:43:LEU:O	1:C:45:PHE:HD2	1.93	0.51
2:D:65:TYR:CG	2:D:66:ILE:N	2.79	0.51
2:D:74:LEU:HD13	2:D:74:LEU:C	2.31	0.51
2:B:96:ARG:C	2:B:98:SER:H	2.13	0.51
1:C:107:LEU:O	1:C:107:LEU:HG	2.11	0.51
2:D:119:PHE:CD1	2:D:119:PHE:C	2.84	0.51
1:A:146:ILE:CG2	1:A:149:LEU:HD12	2.41	0.51
2:D:128:LYS:O	2:D:129:GLY:O	2.29	0.51
1:A:274:ARG:O	1:A:277:ASN:N	2.44	0.51
1:A:289:CYS:HB3	1:A:292:SER:HB3	1.92	0.51
1:C:262:TRP:HE1	1:C:287:ALA:HB1	1.75	0.51
1:C:155:LEU:CD1	1:C:157:VAL:HG13	2.41	0.50
1:C:189:SER:HB2	1:C:191:TYR:CE2	2.45	0.50
1:C:31:GLU:OE1	1:C:38:TYR:CE2	2.65	0.50
1:C:294:LYS:HD3	5:C:401:E55:OAN	2.11	0.50
1:A:44:ASN:ND2	1:A:46:TYR:CE1	2.75	0.50
1:A:163:GLN:O	1:A:187:ILE:HA	2.11	0.50
1:A:165:PHE:HE1	1:A:190:ILE:HG23	1.75	0.50
1:C:71:SER:HB3	1:C:72:TYR:CD1	2.46	0.50
1:C:166:LYS:O	1:C:166:LYS:HG2	2.12	0.50
2:D:36:TYR:HD1	2:D:36:TYR:N	2.08	0.50
1:A:166:LYS:O	1:A:167:LEU:C	2.49	0.50
1:C:274:ARG:O	1:C:277:ASN:N	2.44	0.50
1:A:262:TRP:HE1	1:A:287:ALA:HB1	1.76	0.50
1:A:64:ASN:O	1:A:66:LEU:HG	2.12	0.50
1:A:206:LEU:HD11	1:A:208:LEU:HB2	1.93	0.50
2:B:78:LEU:HB3	2:B:80:ILE:HD11	1.93	0.50
1:A:112:ASN:O	1:A:114:ILE:HG13	2.11	0.50
5:A:1206:E55:CBG	2:D:76:PHE:HE1	2.24	0.50
1:C:88:CYS:O	1:C:90:ILE:N	2.45	0.50
1:C:112:ASN:O	1:C:114:ILE:HG13	2.12	0.49
5:C:401:E55:HBZ2	5:C:401:E55:HCA1	1.93	0.49
1:A:157:VAL:O	1:A:157:VAL:CG2	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:HD2	1:A:45:PHE:N	2.11	0.49
2:D:75:TYR:CD2	2:D:91:LYS:HE3	2.47	0.49
2:D:141:SER:CB	2:D:142:PRO:HD3	2.42	0.49
3:E:1:NAG:H61	3:E:2:NAG:H82	1.94	0.49
1:A:88:CYS:O	1:A:90:ILE:N	2.46	0.49
1:C:128:LEU:HD21	1:C:131:LEU:HB2	1.95	0.49
1:C:162:ILE:HD12	1:C:185:ASN:ND2	2.28	0.49
1:A:156:ASN:C	1:A:156:ASN:ND2	2.61	0.49
2:B:141:SER:CB	2:B:142:PRO:HD3	2.43	0.49
1:C:206:LEU:HD11	1:C:208:LEU:HB2	1.94	0.49
1:C:114:ILE:CG2	1:C:117:LEU:HD13	2.38	0.49
1:C:208:LEU:HD21	1:C:210:LEU:HD11	1.94	0.49
2:B:75:TYR:CE2	2:B:91:LYS:HE3	2.48	0.49
2:D:87:LEU:O	2:D:88:PRO:O	2.31	0.49
1:C:128:LEU:HD11	1:C:130:LYS:O	2.13	0.49
3:E:1:NAG:C6	3:E:2:NAG:H82	2.43	0.49
2:B:74:LEU:HD13	2:B:74:LEU:C	2.33	0.48
1:C:250:THR:O	1:C:252:LEU:N	2.46	0.48
1:A:45:PHE:N	1:A:45:PHE:CD2	2.81	0.48
1:A:206:LEU:HD13	1:A:206:LEU:C	2.33	0.48
1:C:159:HIS:HA	1:C:184:SER:O	2.12	0.48
1:A:139:ALA:O	1:A:162:ILE:HA	2.14	0.48
2:B:67:PRO:HB3	2:B:71:LEU:HD21	1.95	0.48
1:A:128:LEU:HD11	1:A:130:LYS:O	2.13	0.48
1:A:191:TYR:O	1:A:194:ASP:HB2	2.12	0.48
1:C:27:GLU:CD	1:C:27:GLU:N	2.67	0.48
1:C:156:ASN:C	1:C:156:ASN:ND2	2.63	0.48
2:D:96:ARG:C	2:D:98:SER:H	2.15	0.48
1:A:166:LYS:O	1:A:166:LYS:HG2	2.13	0.48
2:B:151:PHE:CE2	5:C:401:E55:HAR	2.49	0.48
1:A:162:ILE:HD12	1:A:185:ASN:ND2	2.28	0.48
1:C:81:GLN:O	1:C:104:LEU:HD12	2.13	0.48
1:A:31:GLU:OE1	1:A:38:TYR:HE2	1.96	0.48
1:A:159:HIS:HA	1:A:184:SER:O	2.14	0.48
2:D:45:SER:HB2	2:D:64:PHE:HB3	1.96	0.48
2:D:69:ARG:HG2	2:D:144:GLU:CD	2.34	0.48
2:D:74:LEU:HD22	2:D:75:TYR:N	2.29	0.48
1:A:260:ASN:HD22	1:A:260:ASN:HA	1.58	0.47
2:D:44:ILE:HG21	2:D:46:ILE:HD11	1.96	0.47
1:A:29:CYS:HA	1:A:43:LEU:HD11	1.95	0.47
2:B:69:ARG:HG2	2:B:144:GLU:CD	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:O	1:A:45:PHE:CD2	2.68	0.47
2:D:139:SER:O	2:D:143:GLU:HA	2.15	0.47
2:D:146:LEU:O	2:D:147:PHE:CB	2.62	0.47
1:A:250:THR:O	1:A:252:LEU:N	2.48	0.47
1:A:138:LEU:HB2	1:A:160:ASN:OD1	2.14	0.47
1:C:139:ALA:O	1:C:162:ILE:HA	2.14	0.47
1:C:29:CYS:HA	1:C:43:LEU:HD11	1.97	0.47
1:C:191:TYR:O	1:C:194:ASP:HB2	2.14	0.47
2:D:61:LEU:HD21	2:D:63:ILE:HD11	1.96	0.47
2:D:138:ILE:CG2	2:D:143:GLU:HB2	2.45	0.47
1:A:143:ASN:O	1:A:145:PRO:HD3	2.15	0.47
1:A:277:ASN:ND2	2:D:92:GLU:OE2	2.48	0.47
5:A:1206:E55:HBN2	2:D:76:PHE:CD1	2.49	0.47
1:C:198:LEU:CD2	1:C:204:LEU:HD12	2.45	0.47
2:D:44:ILE:HG12	2:D:65:TYR:HD1	1.77	0.47
2:D:82:VAL:HG13	2:D:131:TYR:CE2	2.50	0.47
2:B:74:LEU:HD22	2:B:75:TYR:N	2.30	0.47
1:C:262:TRP:CD1	1:C:287:ALA:HB1	2.50	0.47
1:A:50:ASP:C	1:A:52:LEU:H	2.16	0.46
1:A:198:LEU:CD2	1:A:204:LEU:HD12	2.45	0.46
1:A:199:HIS:HB2	1:A:200:GLN:NE2	2.29	0.46
2:D:74:LEU:HA	2:D:138:ILE:O	2.15	0.46
2:B:37:CYS:SG	2:B:150:GLU:HG3	2.55	0.46
2:B:96:ARG:NH1	1:C:297:ARG:HH21	2.14	0.46
1:C:45:PHE:HD2	1:C:45:PHE:N	2.13	0.46
1:C:184:SER:HA	1:C:212:LEU:O	2.15	0.46
2:D:47:ASN:OD1	2:D:47:ASN:N	2.47	0.46
1:A:104:LEU:O	1:A:128:LEU:HA	2.15	0.46
2:B:66:ILE:HG23	2:B:66:ILE:O	2.15	0.46
1:C:165:PHE:O	1:C:194:ASP:OD2	2.33	0.46
1:A:27:GLU:HG2	1:A:52:LEU:CD2	2.43	0.46
1:A:255:ILE:HD13	1:A:257:LEU:HD11	1.98	0.46
1:A:302:PRO:HB3	5:A:1206:E55:CAF	2.43	0.46
1:C:143:ASN:O	1:C:145:PRO:HD3	2.15	0.46
1:C:199:HIS:HB2	1:C:200:GLN:NE2	2.30	0.46
2:D:66:ILE:HG23	2:D:66:ILE:O	2.15	0.46
2:D:132:LYS:HB2	2:D:132:LYS:NZ	2.30	0.46
1:A:39:GLN:HE21	1:A:41:MET:HB3	1.80	0.46
1:A:165:PHE:O	1:A:194:ASP:OD2	2.34	0.46
1:A:245:ILE:HG23	1:A:246:PHE:CD2	2.51	0.46
2:D:71:LEU:O	2:D:72:LYS:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:O	1:A:273:SER:C	2.54	0.46
1:C:245:ILE:HG23	1:C:246:PHE:CD2	2.50	0.46
5:C:401:E55:HBB1	5:C:401:E55:HBS1	1.97	0.46
2:D:67:PRO:HB3	2:D:71:LEU:HD21	1.97	0.46
1:A:31:GLU:OE1	1:A:38:TYR:CE2	2.69	0.46
1:A:256:TRP:CE2	1:A:284:GLN:HG3	2.50	0.46
1:C:44:ASN:ND2	1:C:44:ASN:O	2.48	0.46
1:A:39:GLN:HE21	1:A:41:MET:CB	2.29	0.46
1:A:184:SER:HA	1:A:212:LEU:O	2.16	0.46
1:A:274:ARG:O	1:A:275:TRP:C	2.54	0.46
2:B:132:LYS:HB2	2:B:132:LYS:NZ	2.31	0.46
1:A:203:LEU:O	3:E:1:NAG:H82	2.16	0.45
2:D:79:TYR:OH	2:D:89:LYS:NZ	2.39	0.45
2:D:155:HIS:CD2	2:D:156:GLN:N	2.84	0.45
2:D:155:HIS:CE1	2:D:157:PRO:HD3	2.51	0.45
1:C:272:LEU:O	1:C:273:SER:C	2.54	0.45
1:C:274:ARG:O	1:C:275:TRP:C	2.53	0.45
2:D:156:GLN:O	2:D:158:ASN:N	2.48	0.45
1:A:27:GLU:CD	1:A:27:GLU:N	2.70	0.45
1:A:300:ILE:HA	2:D:90:ARG:NH1	2.32	0.45
5:A:1206:E55:HCH2	2:D:119:PHE:HB2	1.97	0.45
2:B:139:SER:O	2:B:143:GLU:HA	2.17	0.45
2:B:45:SER:HB2	2:B:64:PHE:HB3	1.98	0.45
2:B:135:VAL:HG22	2:B:149:LEU:HB2	1.98	0.45
2:B:61:LEU:HD21	2:B:63:ILE:HD11	1.98	0.45
1:C:27:GLU:HG2	1:C:52:LEU:CD2	2.46	0.45
1:C:104:LEU:O	1:C:128:LEU:HA	2.16	0.45
1:C:105:SER:O	1:C:128:LEU:HD12	2.17	0.45
1:C:192:CYS:O	1:C:193:THR:C	2.55	0.45
5:A:1206:E55:HBN2	2:D:76:PHE:HD1	1.82	0.45
2:B:71:LEU:O	2:B:72:LYS:C	2.54	0.45
2:B:75:TYR:CD2	2:B:91:LYS:HE3	2.52	0.45
1:C:45:PHE:N	1:C:45:PHE:CD2	2.84	0.45
1:C:286:SER:O	1:C:288:LYS:HG3	2.17	0.45
2:D:37:CYS:SG	2:D:150:GLU:HG3	2.57	0.45
1:A:192:CYS:O	1:A:193:THR:C	2.54	0.45
1:C:223:PHE:HB3	1:C:249:LEU:HD13	1.97	0.45
2:D:79:TYR:CE2	2:D:89:LYS:HG3	2.52	0.45
1:A:42:GLU:OE1	2:B:42:TYR:HE2	2.00	0.45
1:A:87:ARG:HH11	1:A:87:ARG:HB2	1.82	0.45
5:A:1206:E55:OAG	5:A:1206:E55:N2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:GLU:HG3	1:C:300:ILE:HD11	1.99	0.45
2:B:155:HIS:CE1	2:B:157:PRO:HD3	2.52	0.45
1:A:262:TRP:CD1	1:A:287:ALA:HB1	2.52	0.45
1:C:231:LEU:HD13	1:C:233:LEU:HG	1.99	0.45
2:D:26:ASN:OD1	2:D:31:SER:HB3	2.17	0.45
1:C:260:ASN:HD22	1:C:260:ASN:HA	1.58	0.44
2:D:149:LEU:HB3	2:D:151:PHE:CE1	2.52	0.44
2:B:128:LYS:O	2:B:129:GLY:O	2.34	0.44
1:A:223:PHE:HB3	1:A:249:LEU:HD13	1.98	0.44
2:B:74:LEU:HA	2:B:138:ILE:O	2.17	0.44
2:B:138:ILE:CG2	2:B:143:GLU:HB2	2.47	0.44
1:C:50:ASP:C	1:C:52:LEU:H	2.19	0.44
1:A:48:ILE:HD12	1:A:48:ILE:H	1.83	0.44
1:A:105:SER:O	1:A:128:LEU:HD12	2.17	0.44
1:A:128:LEU:HD21	1:A:131:LEU:HB2	1.99	0.44
1:A:241:VAL:HB	1:A:242:PRO:CD	2.48	0.44
2:B:44:ILE:HG22	2:B:46:ILE:CG1	2.45	0.44
2:B:82:VAL:HG13	2:B:131:TYR:CE2	2.52	0.44
1:C:165:PHE:HB3	1:C:187:ILE:CD1	2.48	0.44
1:A:81:GLN:O	1:A:104:LEU:HD12	2.17	0.44
1:A:165:PHE:HB3	1:A:187:ILE:CD1	2.48	0.44
1:A:251:SER:O	1:A:253:GLN:HG3	2.17	0.44
1:C:256:TRP:CE2	1:C:284:GLN:HG3	2.52	0.44
1:A:189:SER:HB2	1:A:191:TYR:CE2	2.52	0.44
1:A:286:SER:O	1:A:288:LYS:HG3	2.17	0.44
2:B:82:VAL:HG12	2:B:83:ASN:N	2.33	0.44
2:B:87:LEU:O	2:B:88:PRO:O	2.35	0.44
2:B:96:ARG:O	2:B:101:ASP:OD2	2.36	0.44
2:B:119:PHE:HA	5:C:401:E55:HCH2	1.99	0.44
5:C:401:E55:HCA1	5:C:401:E55:CBZ	2.47	0.44
1:A:281:GLN:CD	1:A:281:GLN:H	2.21	0.44
2:B:149:LEU:HB3	2:B:151:PHE:CE1	2.52	0.44
1:A:231:LEU:HD13	1:A:233:LEU:HG	2.00	0.44
2:B:79:TYR:CE2	2:B:89:LYS:HG3	2.53	0.44
1:A:77:PHE:HB3	1:A:80:LEU:HG	2.00	0.44
1:A:217:PHE:CZ	1:A:219:GLN:HB2	2.53	0.44
5:A:1206:E55:HCH2	2:D:119:PHE:HA	2.00	0.44
2:B:26:ASN:OD1	2:B:31:SER:HB3	2.18	0.44
2:B:96:ARG:NH2	1:C:297:ARG:NH2	2.66	0.44
2:D:44:ILE:HG22	2:D:46:ILE:CG1	2.47	0.44
2:D:135:VAL:HG22	2:D:149:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLN:HA	1:C:220:PRO:HD3	1.88	0.43
1:A:191:TYR:HB3	1:A:219:GLN:OE1	2.18	0.43
1:C:86:SER:O	1:C:87:ARG:C	2.56	0.43
1:C:118:ALA:C	1:C:120:GLY:N	2.72	0.43
1:C:255:ILE:HD13	1:C:257:LEU:HD11	2.00	0.43
1:A:160:ASN:HB3	1:A:161:LEU:H	1.70	0.43
2:B:71:LEU:O	2:B:74:LEU:HB2	2.19	0.43
2:B:155:HIS:CD2	2:B:156:GLN:N	2.85	0.43
1:C:77:PHE:HB3	1:C:80:LEU:HG	2.00	0.43
1:C:138:LEU:HB2	1:C:160:ASN:OD1	2.17	0.43
1:C:43:LEU:O	1:C:45:PHE:CD2	2.70	0.43
1:C:48:ILE:HD12	1:C:48:ILE:H	1.82	0.43
2:D:82:VAL:HG12	2:D:83:ASN:N	2.34	0.43
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.85	0.43
1:A:44:ASN:ND2	1:A:44:ASN:O	2.52	0.43
1:C:42:GLU:OE1	2:D:42:TYR:HE2	2.02	0.43
3:E:2:NAG:H62	3:E:3:BMA:C2	2.48	0.43
4:A:1201:NAG:O3	4:A:1201:NAG:C8	2.65	0.43
5:A:1206:E55:HAF1	2:D:87:LEU:HD11	2.01	0.43
1:C:112:ASN:HA	1:C:113:PRO:HD2	1.91	0.43
1:C:241:VAL:HB	1:C:242:PRO:CD	2.49	0.43
1:C:246:PHE:O	1:C:249:LEU:HB2	2.19	0.43
2:D:82:VAL:HG13	2:D:131:TYR:HE2	1.84	0.43
1:A:69:LEU:HD13	1:A:90:ILE:HD13	2.00	0.43
1:A:150:LYS:NZ	4:A:1205:NAG:O4	2.37	0.43
1:A:165:PHE:HB3	1:A:187:ILE:HD13	2.00	0.43
1:A:192:CYS:O	1:A:194:ASP:N	2.52	0.43
1:A:246:PHE:O	1:A:248:ARG:N	2.52	0.43
1:C:51:ASN:H	1:C:51:ASN:ND2	2.15	0.43
1:C:166:LYS:HG3	1:C:194:ASP:HA	2.00	0.43
1:C:217:PHE:CZ	1:C:219:GLN:HB2	2.54	0.43
1:A:55:SER:O	1:A:56:THR:C	2.58	0.42
1:C:144:PHE:O	1:C:146:ILE:HG12	2.19	0.42
1:C:246:PHE:O	1:C:248:ARG:N	2.52	0.42
5:C:401:E55:OAG	5:C:401:E55:N2	2.48	0.42
1:A:256:TRP:C	1:A:257:LEU:HG	2.39	0.42
1:C:165:PHE:HB3	1:C:187:ILE:HD13	2.01	0.42
1:A:133:ALA:O	1:A:136:THR:HG23	2.19	0.42
2:B:47:ASN:OD1	2:B:47:ASN:N	2.51	0.42
2:B:80:ILE:N	2:B:80:ILE:CD1	2.80	0.42
1:C:165:PHE:CE1	1:C:190:ILE:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:O	1:A:249:LEU:HB2	2.19	0.42
1:C:144:PHE:HA	1:C:145:PRO:HD2	1.85	0.42
1:A:118:ALA:C	1:A:120:GLY:N	2.72	0.42
1:A:166:LYS:HG3	1:A:194:ASP:HA	2.01	0.42
1:C:251:SER:O	1:C:253:GLN:HG3	2.19	0.42
1:A:110:THR:O	1:A:112:ASN:ND2	2.53	0.42
2:B:147:PHE:CD1	2:B:147:PHE:C	2.93	0.42
2:D:69:ARG:HD2	2:D:69:ARG:HA	1.86	0.42
2:D:96:ARG:O	2:D:101:ASP:OD2	2.38	0.42
1:A:177:LEU:HD21	1:A:180:LEU:HB2	2.02	0.42
2:B:149:LEU:HB3	2:B:151:PHE:HE1	1.85	0.42
2:D:149:LEU:HB3	2:D:151:PHE:HE1	1.85	0.42
1:C:157:VAL:O	1:C:157:VAL:CG2	2.57	0.41
1:A:98:TYR:OH	1:A:109:LEU:HD21	2.20	0.41
2:B:42:TYR:HA	2:B:43:PRO:HD3	1.83	0.41
1:C:87:ARG:HA	1:C:87:ARG:HD3	1.82	0.41
1:A:77:PHE:C	1:A:79:GLU:H	2.24	0.41
2:B:29:ASP:O	2:B:30:ALA:CB	2.68	0.41
1:C:39:GLN:HE21	1:C:41:MET:HB3	1.84	0.41
2:D:27:SER:N	2:D:30:ALA:O	2.53	0.41
2:D:42:TYR:HA	2:D:43:PRO:HD3	1.81	0.41
1:A:205:ASN:HD22	3:E:1:NAG:C7	2.29	0.41
2:B:82:VAL:HG13	2:B:131:TYR:HE2	1.86	0.41
2:B:156:GLN:O	2:B:158:ASN:N	2.54	0.41
1:C:39:GLN:HE21	1:C:41:MET:CB	2.33	0.41
5:A:1206:E55:HBL1	5:A:1206:E55:HAD3	2.03	0.41
2:D:29:ASP:O	2:D:30:ALA:CB	2.66	0.41
2:D:36:TYR:CD2	2:D:41:GLN:HB3	2.55	0.41
1:A:30:VAL:HG12	1:A:31:GLU:N	2.34	0.41
1:A:70:GLY:O	1:A:71:SER:C	2.59	0.41
1:A:86:SER:O	1:A:87:ARG:C	2.58	0.41
1:A:101:LEU:HB3	1:A:104:LEU:HB2	2.03	0.41
2:B:104:PHE:CD1	2:B:104:PHE:C	2.94	0.41
2:B:143:GLU:C	2:B:144:GLU:HG3	2.40	0.41
1:C:50:ASP:N	1:C:50:ASP:OD1	2.53	0.41
2:D:147:PHE:C	2:D:147:PHE:CD1	2.94	0.41
1:A:95:ASP:OD2	1:A:118:ALA:HB1	2.21	0.41
1:A:144:PHE:O	1:A:146:ILE:HG12	2.20	0.41
2:B:109:LYS:O	2:B:111:GLU:N	2.53	0.41
2:B:141:SER:CB	2:B:142:PRO:CD	2.99	0.41
1:C:74:PHE:O	1:C:76:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ILE:HG12	2:B:65:TYR:HD1	1.80	0.41
1:C:110:THR:O	1:C:112:ASN:ND2	2.54	0.41
1:C:215:MET:O	1:C:237:GLN:N	2.51	0.41
2:D:74:LEU:HA	2:D:139:SER:HB3	2.02	0.41
2:D:141:SER:CB	2:D:142:PRO:CD	2.98	0.41
1:A:51:ASN:ND2	1:A:51:ASN:H	2.19	0.41
1:A:87:ARG:CZ	2:B:66:ILE:HD11	2.51	0.41
1:A:141:LEU:H	1:A:141:LEU:CD1	2.31	0.41
1:A:297:ARG:HH21	2:D:96:ARG:NH1	2.19	0.41
1:C:160:ASN:HB3	1:C:161:LEU:H	1.72	0.41
1:C:175:THR:HG23	1:C:176:ASN:ND2	2.36	0.41
1:A:87:ARG:HA	1:A:87:ARG:HD3	1.78	0.40
1:A:125:LEU:HA	1:A:125:LEU:HD12	1.82	0.40
1:A:165:PHE:CE1	1:A:190:ILE:HG23	2.54	0.40
1:C:192:CYS:O	1:C:194:ASP:N	2.53	0.40
2:D:138:ILE:O	2:D:139:SER:HB3	2.21	0.40
2:B:36:TYR:CD2	2:B:41:GLN:CA	3.04	0.40
1:C:30:VAL:HG12	1:C:31:GLU:N	2.35	0.40
2:D:71:LEU:O	2:D:74:LEU:HB2	2.21	0.40
2:D:143:GLU:C	2:D:144:GLU:HG3	2.41	0.40
1:A:98:TYR:CD1	1:A:98:TYR:N	2.89	0.40
1:C:48:ILE:HG22	1:C:49:PRO:O	2.21	0.40
1:C:256:TRP:C	1:C:257:LEU:HG	2.41	0.40
5:C:401:E55:HBL1	5:C:401:E55:CAD	2.50	0.40
1:A:242:PRO:O	1:A:243:ASP:C	2.60	0.40
1:C:141:LEU:H	1:C:141:LEU:CD1	2.32	0.40
2:D:36:TYR:CD2	2:D:41:GLN:CA	3.04	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	274/279 (98%)	197 (72%)	55 (20%)	22 (8%)	1 11
1	C	274/279 (98%)	198 (72%)	54 (20%)	22 (8%)	1 11
2	B	138/142 (97%)	105 (76%)	20 (14%)	13 (9%)	0 8
2	D	138/142 (97%)	105 (76%)	20 (14%)	13 (9%)	0 8
All	All	824/842 (98%)	605 (73%)	149 (18%)	70 (8%)	1 10

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	89	GLU
1	A	99	GLN
1	A	175	THR
1	A	247	ASP
1	A	251	SER
2	B	72	LYS
2	B	109	LYS
2	B	141	SER
1	C	67	ARG
1	C	89	GLU
1	C	99	GLN
1	C	175	THR
1	C	247	ASP
1	C	251	SER
2	D	72	LYS
2	D	109	LYS
2	D	141	SER
1	A	50	ASP
1	A	73	SER
1	A	194	ASP
2	B	39	LYS
2	B	88	PRO
2	B	123	GLY
1	C	50	ASP
1	C	73	SER
1	C	194	ASP
2	D	39	LYS
2	D	88	PRO
2	D	123	GLY
2	D	129	GLY
1	A	53	PRO
1	A	65	PRO

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Mol	Chain	Res	Type
1	A	75	PHE
1	A	95	ASP
1	A	113	PRO
1	A	145	PRO
1	A	192	CYS
1	A	193	THR
2	B	129	GLY
2	B	147	PHE
1	C	53	PRO
1	C	65	PRO
1	C	75	PHE
1	C	95	ASP
1	C	113	PRO
1	C	192	CYS
1	C	193	THR
2	D	147	PHE
2	B	30	ALA
2	B	57	SER
1	C	145	PRO
1	C	147	GLY
2	D	30	ALA
2	D	83	ASN
2	D	101	ASP
1	A	49	PRO
1	A	147	GLY
1	A	197	VAL
2	B	83	ASN
2	B	101	ASP
2	B	110	GLY
1	C	49	PRO
1	C	196	ARG
1	C	197	VAL
2	D	57	SER
1	A	196	ARG
2	D	110	GLY
1	A	120	GLY
1	C	120	GLY

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	256/258 (99%)	235 (92%)	21 (8%)	11	42
1	C	256/258 (99%)	237 (93%)	19 (7%)	13	46
2	B	130/131 (99%)	120 (92%)	10 (8%)	13	45
2	D	130/131 (99%)	120 (92%)	10 (8%)	13	45
All	All	772/778 (99%)	712 (92%)	60 (8%)	12	44

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	54	PHE
1	A	68	HIS
1	A	76	SER
1	A	81	GLN
1	A	87	ARG
1	A	100	SER
1	A	125	LEU
1	A	127	SER
1	A	138	LEU
1	A	140	SER
1	A	155	LEU
1	A	156	ASN
1	A	165	PHE
1	A	204	LEU
1	A	224	LYS
1	A	243	ASP
1	A	260	ASN
1	A	281	GLN
1	A	284	GLN
1	A	298	SER
2	B	26	ASN
2	B	36	TYR
2	B	37	CYS
2	B	40	MET
2	B	47	ASN
2	B	69	ARG
2	B	100	ASP

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Mol	Chain	Res	Type
2	B	115	THR
2	B	124	ILE
2	B	144	GLU
1	C	54	PHE
1	C	68	HIS
1	C	76	SER
1	C	81	GLN
1	C	87	ARG
1	C	100	SER
1	C	125	LEU
1	C	127	SER
1	C	138	LEU
1	C	140	SER
1	C	155	LEU
1	C	156	ASN
1	C	165	PHE
1	C	204	LEU
1	C	224	LYS
1	C	243	ASP
1	C	260	ASN
1	C	281	GLN
1	C	284	GLN
2	D	26	ASN
2	D	36	TYR
2	D	37	CYS
2	D	40	MET
2	D	47	ASN
2	D	69	ARG
2	D	100	ASP
2	D	115	THR
2	D	124	ILE
2	D	144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	44	ASN
1	A	156	ASN
1	A	163	GLN
1	A	176	ASN
1	A	185	ASN

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Mol	Chain	Res	Type
1	A	200	GLN
1	A	237	GLN
1	A	260	ASN
2	B	155	HIS
1	C	39	GLN
1	C	44	ASN
1	C	156	ASN
1	C	163	GLN
1	C	173	ASN
1	C	176	ASN
1	C	185	ASN
1	C	200	GLN
1	C	237	GLN
1	C	260	ASN
2	D	155	HIS

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	1,3	14,14,15	1.02	1 (7%)	17,19,21	0.79	0
3	NAG	E	2	3	14,14,15	0.91	0	17,19,21	0.74	0
3	BMA	E	3	3	11,11,12	1.13	1 (9%)	15,15,17	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	1	1,3	14,14,15	1.15	1 (7%)	17,19,21	0.61	0
3	NAG	F	2	3	14,14,15	0.99	0	17,19,21	0.61	0
3	BMA	F	3	3	11,11,12	1.11	0	15,15,17	0.82	1 (6%)

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	1,3	-	6/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	1/1/1/1
3	NAG	F	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	2.78	1.56	1.52
3	E	1	NAG	C1-C2	2.14	1.55	1.52
3	E	3	BMA	O5-C5	2.09	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	BMA	C1-O5-C5	2.31	115.33	112.19
3	E	3	BMA	C1-O5-C5	2.02	114.94	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	3	BMA	O5-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	3	BMA	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	F	1	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	E	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

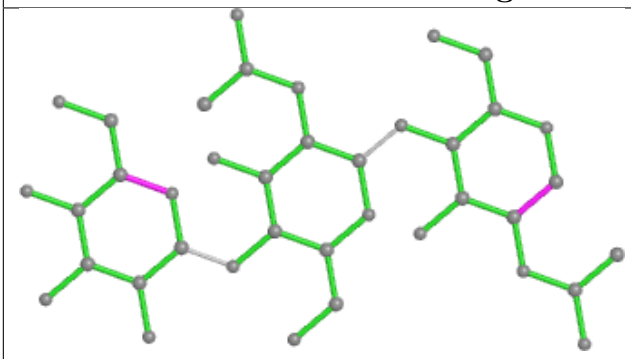
Mol	Chain	Res	Type	Atoms
3	F	3	BMA	C1-C2-C3-C4-C5-O5
3	E	3	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 10 short contacts:

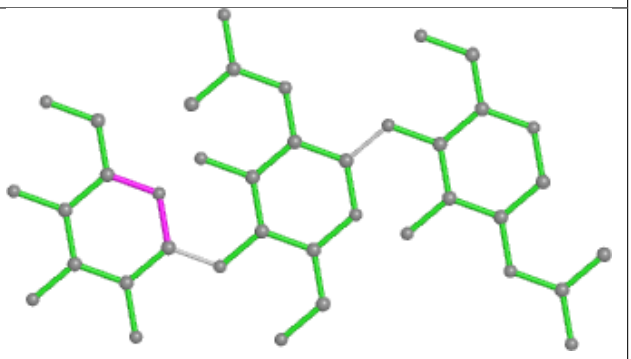
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	2	0
3	E	2	NAG	5	0
3	F	1	NAG	1	0
3	F	3	BMA	2	0
3	E	1	NAG	4	0
3	E	3	BMA	3	0

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

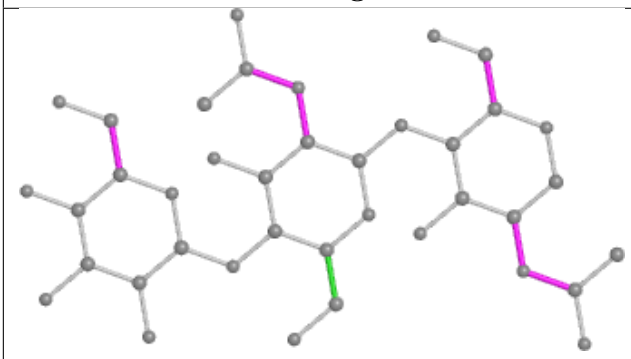
Oligosaccharide Chain E



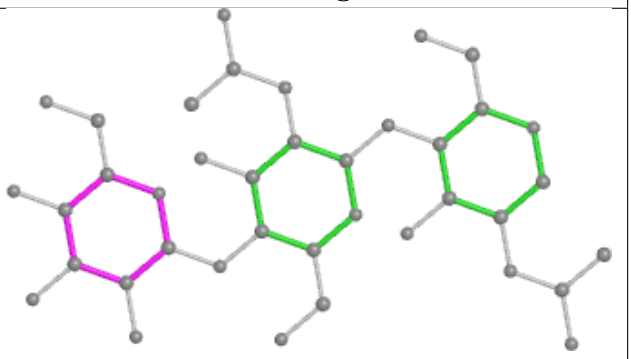
Bond lengths



Bond angles

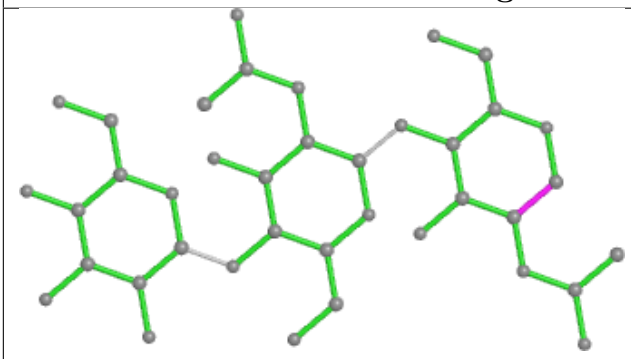


Torsions

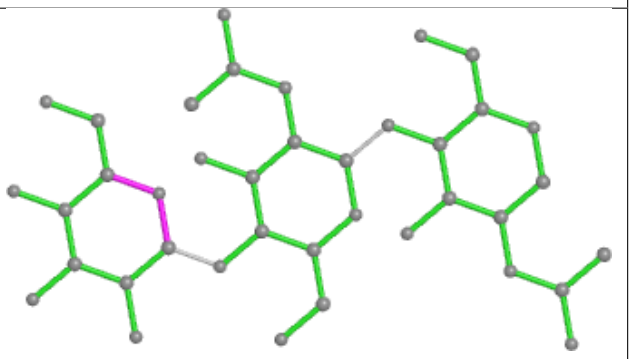


Rings

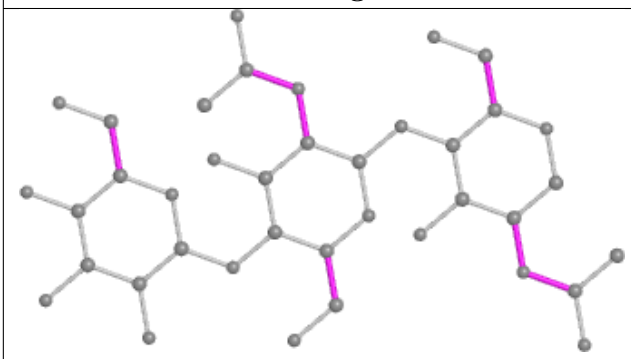
Oligosaccharide Chain F



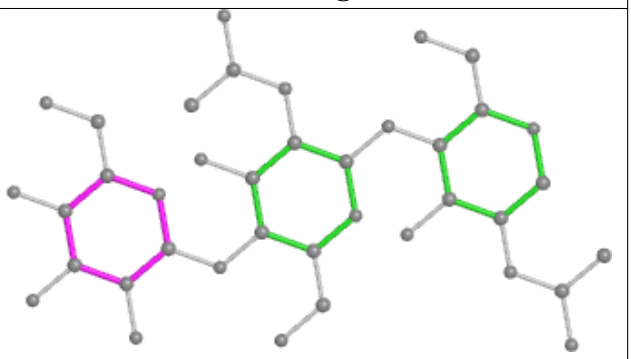
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1201	1	14,14,15	1.10	1 (7%)	17,19,21	1.14	1 (5%)
5	E55	A	1206	-	89,90,90	0.71	1 (1%)	106,111,111	0.84	3 (2%)
4	NAG	C	402	1	14,14,15	1.10	1 (7%)	17,19,21	0.96	0
5	E55	C	401	-	89,90,90	0.68	1 (1%)	106,111,111	0.87	2 (1%)
4	NAG	A	1205	-	14,14,15	1.12	1 (7%)	17,19,21	0.88	0
4	NAG	C	406	-	14,14,15	1.03	1 (7%)	17,19,21	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1201	1	-	6/6/23/26	0/1/1/1
5	E55	A	1206	-	-	6/83/124/124	0/2/2/2
4	NAG	C	402	1	-	3/6/23/26	0/1/1/1
5	E55	C	401	-	-	8/83/124/124	0/2/2/2
4	NAG	A	1205	-	-	4/6/23/26	0/1/1/1
4	NAG	C	406	-	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	NAG	C1-C2	2.83	1.56	1.52
4	A	1201	NAG	C1-C2	2.67	1.56	1.52
4	A	1205	NAG	C1-C2	2.38	1.55	1.52
5	A	1206	E55	O6-CDC	2.35	1.44	1.40
4	C	406	NAG	C1-C2	2.33	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	E55	O6-CDC	2.31	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	401	E55	C6-C5-C4	-3.27	105.26	112.09
5	A	1206	E55	C6-C5-C4	-2.64	106.57	112.09
5	C	401	E55	O3-C3-C4	-2.30	105.03	109.83
5	A	1206	E55	CDC-OCR-CDB	-2.12	109.54	113.69
5	A	1206	E55	CBY-CCD-CCV	-2.11	109.18	114.60
4	A	1201	NAG	C2-N2-C7	-2.06	119.97	122.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1201	NAG	C1-C2-N2-C7
4	A	1201	NAG	C8-C7-N2-C2
4	A	1201	NAG	O7-C7-N2-C2
4	A	1205	NAG	C8-C7-N2-C2
4	A	1205	NAG	O7-C7-N2-C2
4	C	402	NAG	C8-C7-N2-C2
4	C	402	NAG	O7-C7-N2-C2
4	C	406	NAG	O7-C7-N2-C2
5	A	1206	E55	CCV-CCH-CCX-OAI
5	A	1206	E55	CCV-CCH-CCX-N2
5	A	1206	E55	C1-O1-PDJ-OAN
5	A	1206	E55	CCF-CCY-OCN-CAF
5	C	401	E55	CCV-CCH-CCX-OAI
5	C	401	E55	CCV-CCH-CCX-N2
4	C	406	NAG	C8-C7-N2-C2
4	A	1201	NAG	C4-C5-C6-O6
4	A	1201	NAG	O5-C5-C6-O6
4	C	402	NAG	C1-C2-N2-C7
4	A	1205	NAG	C1-C2-N2-C7
5	C	401	E55	C1-O1-PDJ-OAN
5	C	401	E55	CCG-CCY-OCN-CAF
5	C	401	E55	CCF-CCY-OCN-CAF
4	A	1201	NAG	C3-C2-N2-C7
4	A	1205	NAG	C3-C2-N2-C7
5	A	1206	E55	CAW-CBC-CBE-CAY
5	C	401	E55	CAR-CAQ-CAW-CBC

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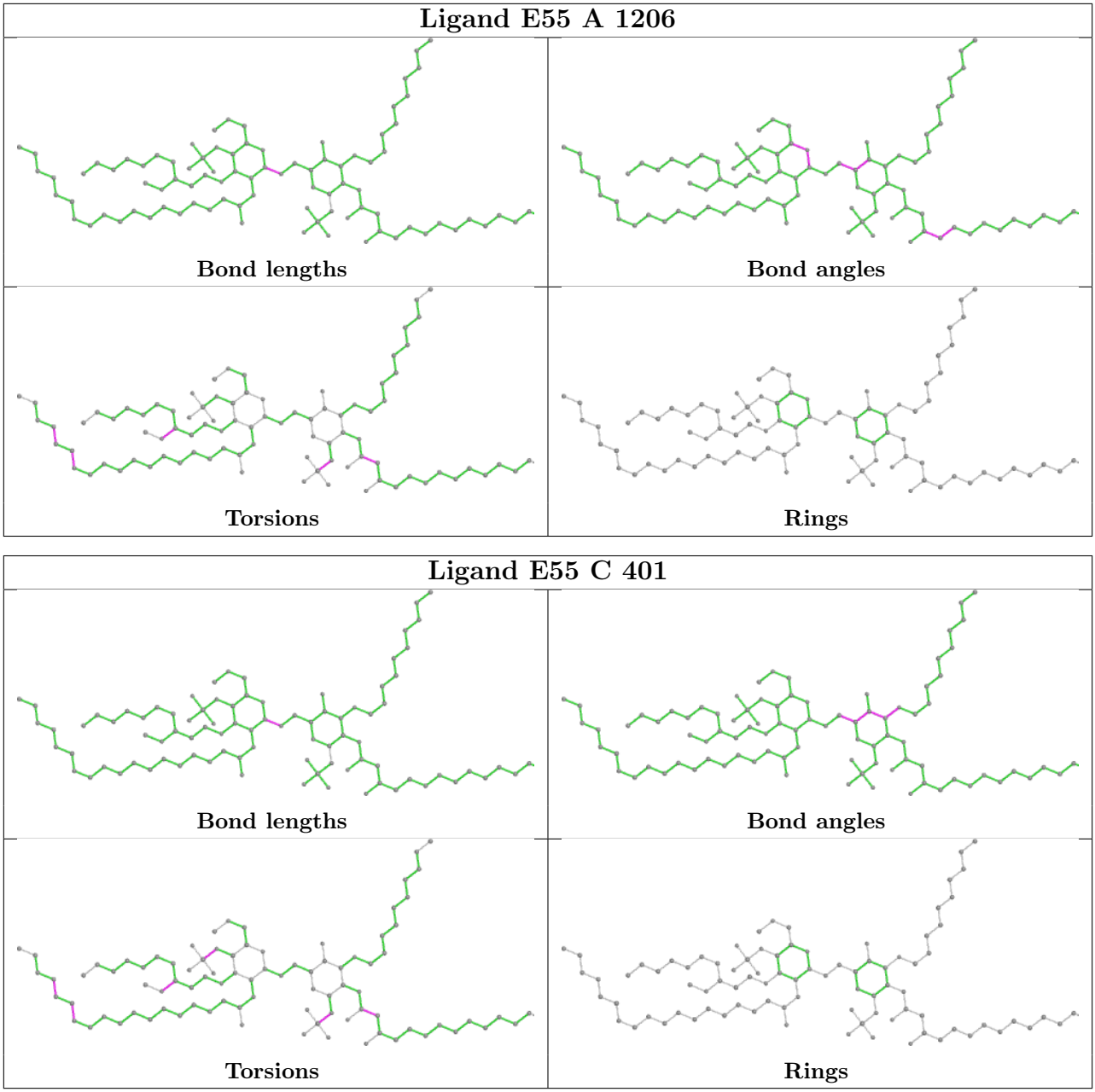
Mol	Chain	Res	Type	Atoms
5	C	401	E55	CAW-CBC-CBE-CAY
5	C	401	E55	CDI-OCU-PDK-OAO
5	A	1206	E55	CAR-CAQ-CAW-CBC
4	C	406	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1201	NAG	2	0
5	A	1206	E55	18	0
4	C	402	NAG	1	0
5	C	401	E55	14	0
4	A	1205	NAG	1	0
4	C	406	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	276/279 (98%)	0.22	0 100 100	51, 87, 100, 100	0
1	C	276/279 (98%)	0.21	2 (0%) 87 78	49, 87, 100, 100	0
2	B	140/142 (98%)	0.46	6 (4%) 35 22	72, 94, 100, 100	0
2	D	140/142 (98%)	0.49	11 (7%) 12 7	71, 94, 100, 100	0
All	All	832/842 (98%)	0.30	19 (2%) 60 44	49, 89, 100, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	158	ASN	6.9
2	D	31	SER	3.6
1	C	62	SER	3.4
2	B	154	LEU	3.3
2	B	157	PRO	3.3
2	D	157	PRO	3.3
2	D	53	GLU	3.0
2	B	130	LYS	2.6
1	C	84	ASP	2.5
2	B	158	ASN	2.5
2	D	126	PHE	2.4
2	D	26	ASN	2.3
2	D	154	LEU	2.3
2	B	33	SER	2.2
2	D	122	LYS	2.1
2	B	87	LEU	2.1
2	D	77	ASN	2.1
2	D	109	LYS	2.0
2	D	130	LYS	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)

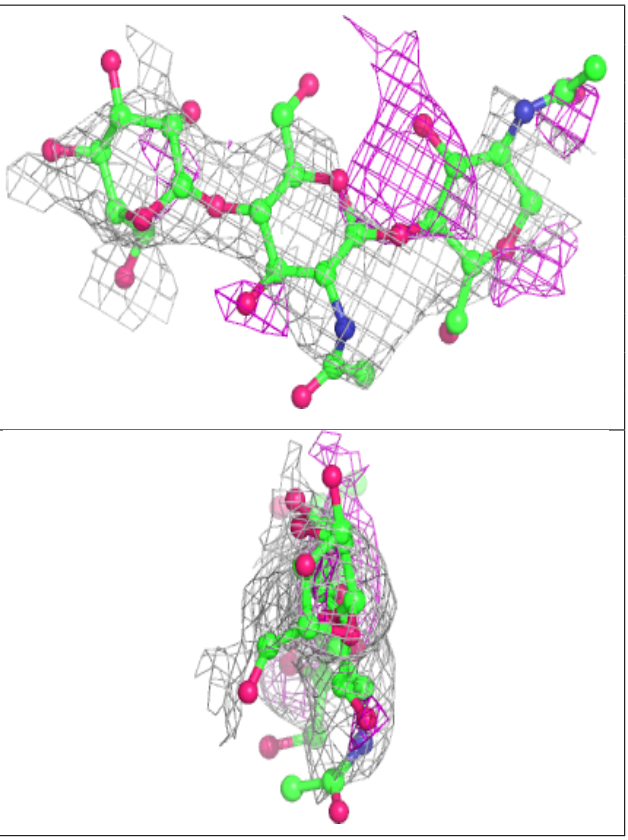
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	E	1	14/15	0.68	0.71	100,100,100,100	0
3	BMA	E	3	11/12	0.68	0.44	100,100,100,100	0
3	BMA	F	3	11/12	0.70	0.40	100,100,100,100	0
3	NAG	F	1	14/15	0.74	0.40	100,100,100,100	0
3	NAG	F	2	14/15	0.79	0.39	100,100,100,100	0
3	NAG	E	2	14/15	0.82	0.51	100,100,100,100	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.

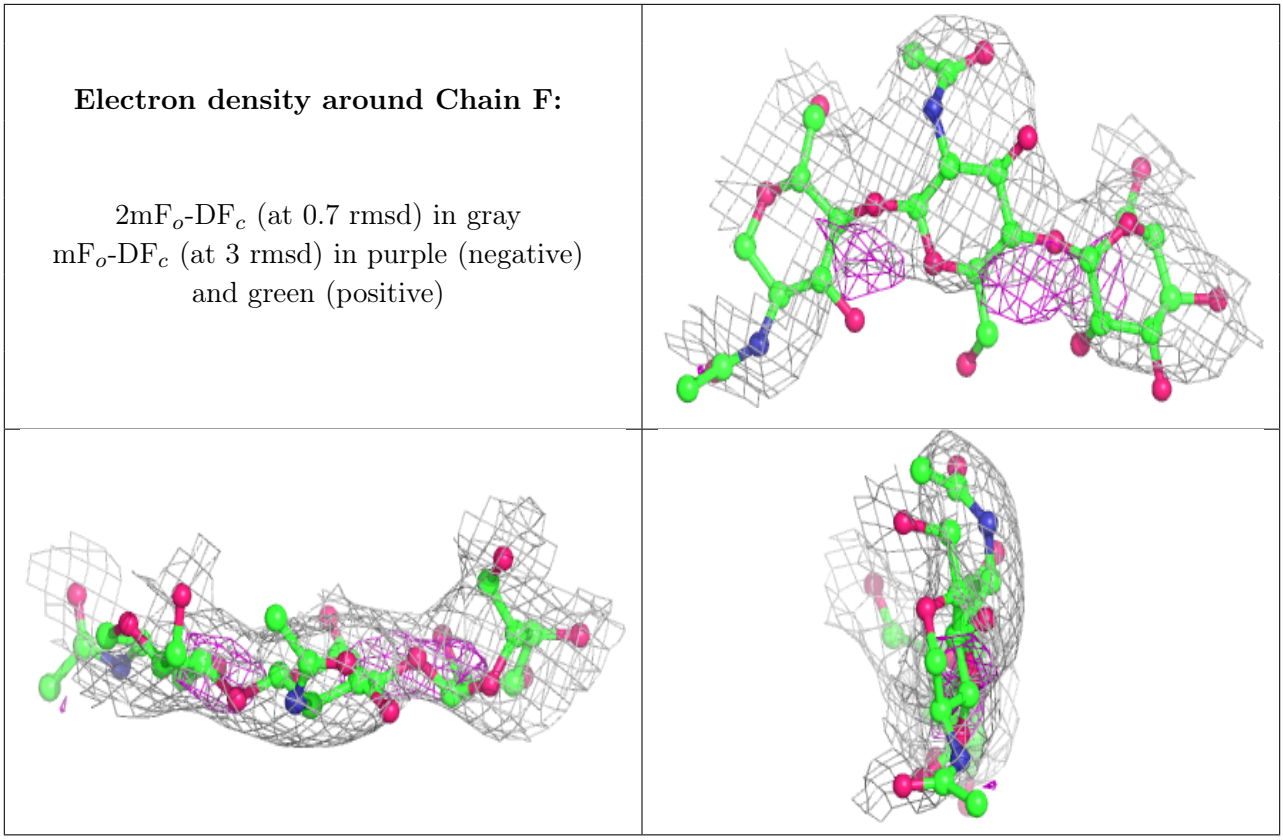
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands

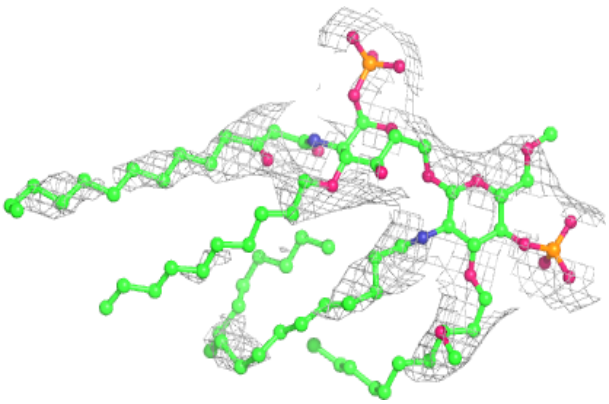
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

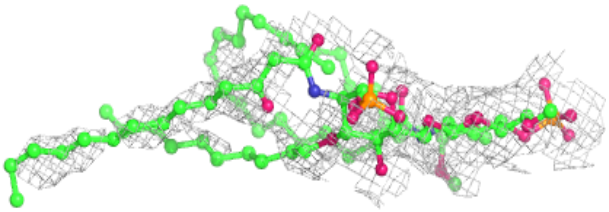
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	1205	14/15	0.52	0.33	100,100,100,100	0
4	NAG	C	406	14/15	0.66	0.35	100,100,100,100	0
4	NAG	C	402	14/15	0.68	0.26	98,100,100,100	0
4	NAG	A	1201	14/15	0.73	0.19	100,100,100,100	0
5	E55	C	401	89/89	0.91	0.51	66,100,100,100	0
5	E55	A	1206	89/89	0.92	0.48	44,94,100,100	0

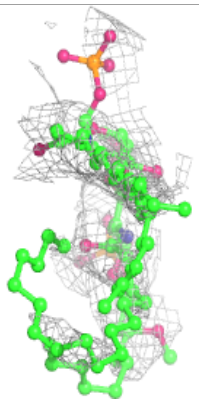
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around E55 C 401:

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

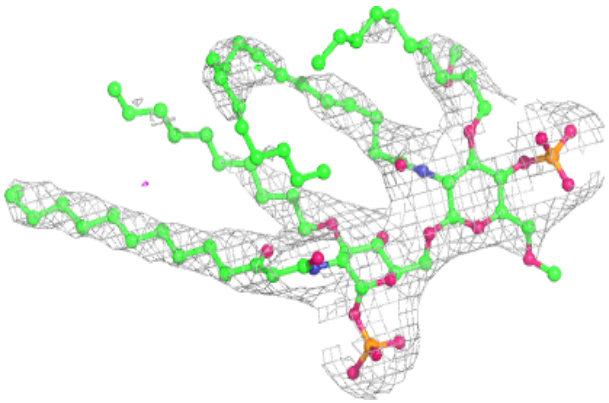


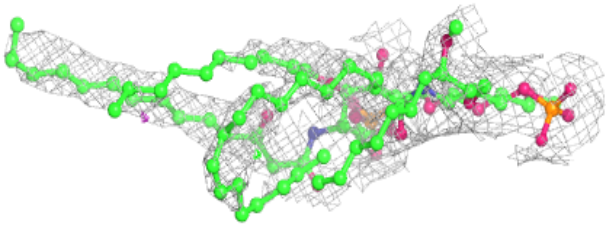


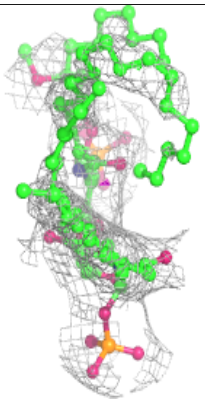


Electron density around E55 A 1206:

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







6.5 Other polymers (i)

There are no such residues in this entry.