



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2024 – 03:57 AM EST

PDB ID : 3SDA  
Title : Crystal structure of autoreactive-Valpha14-Vbeta6 NKT TCR in complex with CD1d-beta-galactosylceramide  
Authors : Clarke, A.J.; Rossjohn, J.  
Deposited on : 2011-06-08  
Resolution : 2.80 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

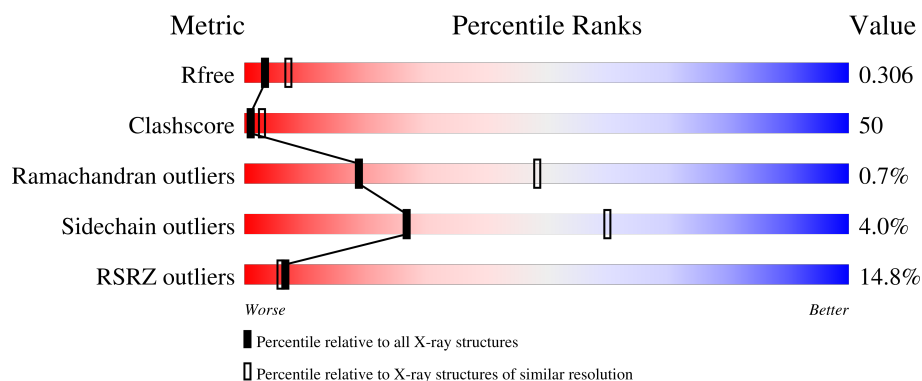
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	302	
2	B	99	
3	C	207	
4	D	245	
5	E	2	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6739 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	10	0	0
			2333	1486	406	427	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	expression tag	UNP P11609
A	281	SER	-	expression tag	UNP P11609
A	282	LEU	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	ILE	-	expression tag	UNP P11609
A	286	LEU	-	expression tag	UNP P11609
A	287	ASP	-	expression tag	UNP P11609
A	288	ALA	-	expression tag	UNP P11609
A	289	GLN	-	expression tag	UNP P11609
A	290	LYS	-	expression tag	UNP P11609
A	291	MET	-	expression tag	UNP P11609
A	292	VAL	-	expression tag	UNP P11609
A	293	TRP	-	expression tag	UNP P11609
A	294	ASN	-	expression tag	UNP P11609
A	295	HIS	-	expression tag	UNP P11609
A	296	ARG	-	expression tag	UNP P11609
A	297	HIS	-	expression tag	UNP P11609
A	298	HIS	-	expression tag	UNP P11609
A	299	HIS	-	expression tag	UNP P11609
A	300	HIS	-	expression tag	UNP P11609
A	301	HIS	-	expression tag	UNP P11609
A	302	HIS	-	expression tag	UNP P11609

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	3	0	0
			814	520	138	149	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887

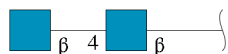
- Molecule 3 is a protein called NKT TCR Valpha14 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	196	Total	C	N	O	S	5	0	0
			1511	937	260	307	7			

- Molecule 4 is a protein called NKT TCR autoreactive-Vbeta6 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	7	0	0
			1900	1202	326	365	7			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



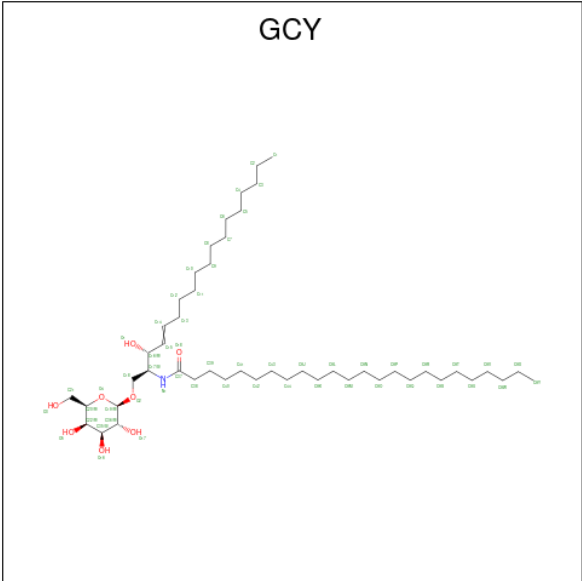
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is N-[(2S,3R)-1-(beta-D-galactopyranosyloxy)-3-hydroxyoctadec-4-en-2-yl]tetracosanamide (three-letter code: GCY) (formula: C<sub>48</sub>H<sub>93</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			57	48	1	8		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

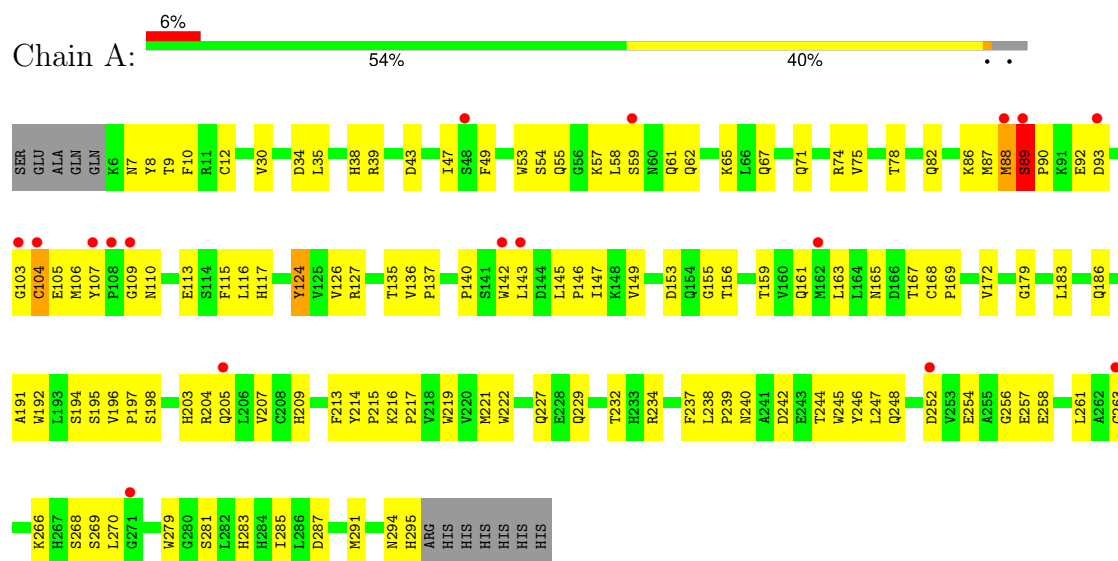
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	19	Total	O	0	0
			19	19		
9	B	12	Total	O	0	0
			12	12		
9	C	16	Total	O	0	0
			16	16		
9	D	15	Total	O	0	0
			15	15		

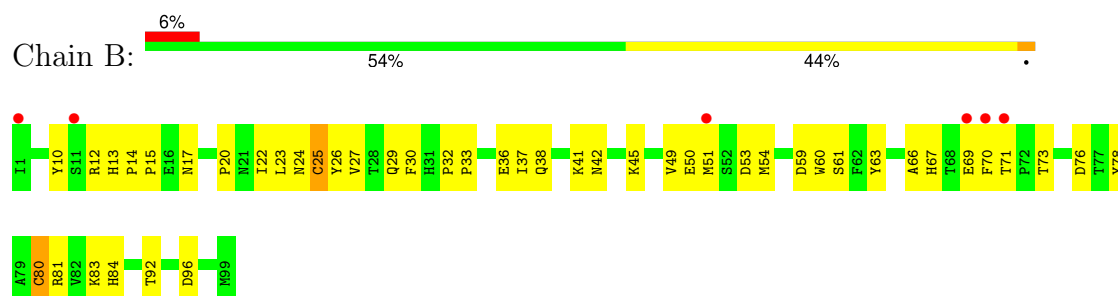
### 3 Residue-property plots [i](#)

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.

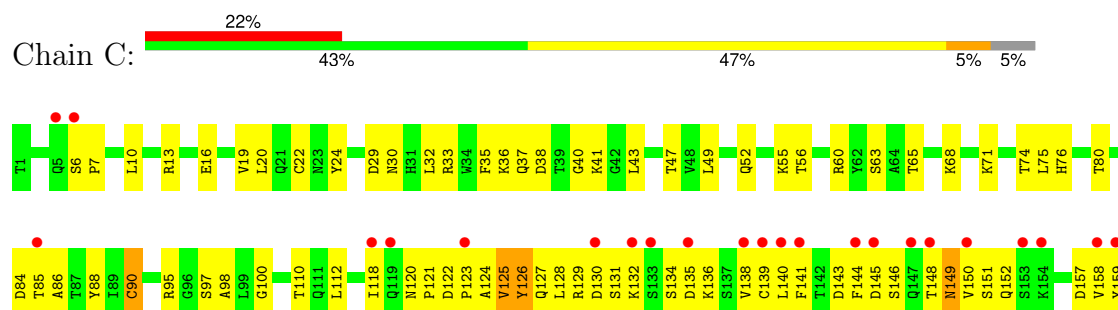
#### • Molecule 1: Antigen-presenting glycoprotein CD1d1

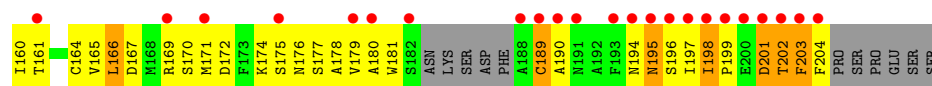


#### • Molecule 2: Beta-2-microglobulin

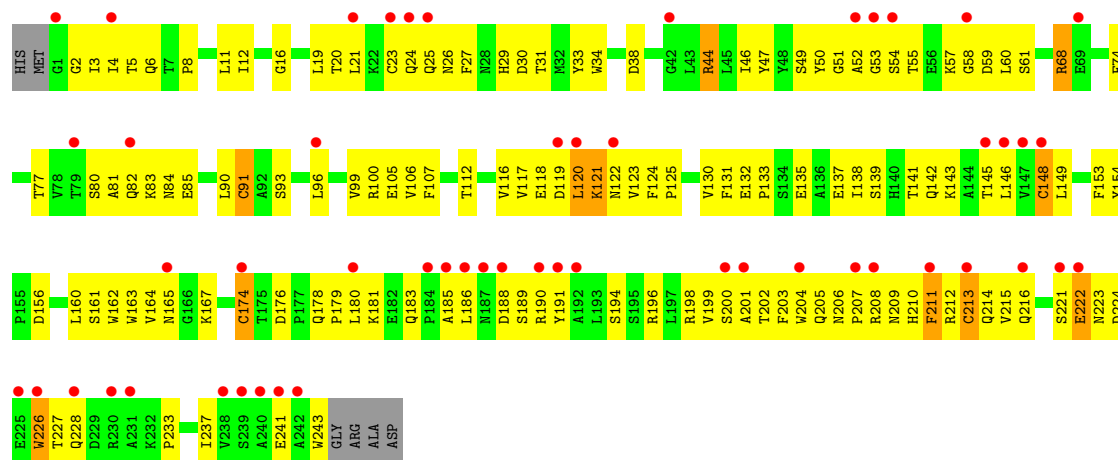


#### • Molecule 3: NKT TCR Valpha14 chain





• Molecule 4: NKT TCR autoreactive-Vbeta6 chain



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.75Å 94.75Å 287.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.25 – 2.80 65.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.25-2.80) 97.0 (65.25-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.272 , 0.312 0.272 , 0.306	Depositor DCC
$R_{free}$ test set	1634 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GCY, 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	1.51	2/2403 (0.1%)	0.72	0/3266
2	B	1.47	0/840	0.79	2/1140 (0.2%)
3	C	1.28	0/1536	0.78	1/2085 (0.0%)
4	D	1.26	2/1947 (0.1%)	0.75	1/2640 (0.0%)
All	All	1.39	4/6726 (0.1%)	0.75	4/9131 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	CYS	CB-SG	-6.61	1.71	1.82
1	A	124	TYR	CD2-CE2	-5.53	1.31	1.39
4	D	106	VAL	CB-CG2	-5.52	1.41	1.52
4	D	105	GLU	CD-OE1	-5.12	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	90	CYS	CA-CB-SG	7.63	127.74	114.00
4	D	91	CYS	CA-CB-SG	7.10	126.77	114.00
2	B	80	CYS	CA-CB-SG	7.08	126.75	114.00
2	B	25	CYS	CA-CB-SG	6.40	125.51	114.00

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	2333	0	2233	147	1
2	B	814	0	790	73	0
3	C	1511	0	1464	187	0
4	D	1900	0	1829	280	0
5	E	28	0	25	0	0
6	A	28	0	26	0	0
7	A	57	0	88	9	0
8	B	6	0	8	1	0
9	A	19	0	0	1	0
9	B	12	0	0	0	0
9	C	16	0	0	0	0
9	D	15	0	0	2	0
All	All	6739	0	6463	651	1

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 50.

All (651) 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)
3:C:140:LEU:CD1	3:C:178:ALA:O	1.67	1.43
4:D:8:PRO:HD2	4:D:21:LEU:CD2	1.49	1.42
2:B:25:CYS:SG	2:B:80:CYS:CB	2.11	1.39
1:A:89:SER:HB2	1:A:90:PRO:CD	1.45	1.38
3:C:130:ASP:CB	4:D:131:PHE:CD2	2.05	1.37
4:D:30:ASP:HB2	4:D:96:LEU:CD1	1.57	1.34
4:D:23:CYS:SG	4:D:34:TRP:CZ2	2.23	1.31
4:D:226:TRP:CZ2	4:D:228:GLN:HB2	1.65	1.31
4:D:131:PHE:CE1	4:D:149:LEU:HD12	1.70	1.25
3:C:131:SER:HB2	3:C:132:LYS:CA	1.67	1.24
3:C:131:SER:HB2	3:C:132:LYS:C	1.56	1.23
3:C:22:CYS:CB	3:C:90:CYS:SG	2.25	1.23
4:D:176:ASP:OD2	4:D:194:SER:OG	1.56	1.23
2:B:38:GLN:NE2	2:B:45:LYS:CD	2.01	1.22
4:D:4:ILE:CG1	4:D:27:PHE:HE1	1.53	1.22
4:D:4:ILE:HG13	4:D:27:PHE:CE1	1.77	1.20
4:D:131:PHE:CE1	4:D:149:LEU:CD1	2.24	1.20
3:C:22:CYS:SG	3:C:90:CYS:SG	1.36	1.17
2:B:51:MET:SD	2:B:66:ALA:HB2	1.86	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:PHE:HE1	4:D:149:LEU:CD1	1.58	1.16
1:A:104:CYS:SG	1:A:168:CYS:SG	1.36	1.15
2:B:38:GLN:HE21	2:B:45:LYS:CG	1.59	1.14
1:A:89:SER:CB	1:A:90:PRO:CD	2.25	1.13
4:D:176:ASP:CG	4:D:194:SER:OG	1.86	1.12
4:D:4:ILE:HG13	4:D:27:PHE:HE1	0.98	1.10
2:B:63:TYR:OH	8:B:100:GOL:O1	1.68	1.10
4:D:30:ASP:HB2	4:D:96:LEU:HD11	1.10	1.09
3:C:130:ASP:CB	3:C:136:LYS:O	1.99	1.09
3:C:157:ASP:OD1	3:C:158:VAL:HG23	1.51	1.09
4:D:181:LYS:HG2	4:D:191:TYR:CE1	1.87	1.09
4:D:216:GLN:OE1	4:D:237:ILE:HG12	1.52	1.09
2:B:23:LEU:HB2	2:B:70:PHE:CE2	1.86	1.08
1:A:104:CYS:CB	1:A:168:CYS:SG	2.41	1.08
2:B:38:GLN:HE21	2:B:45:LYS:CD	1.62	1.08
3:C:130:ASP:CB	4:D:131:PHE:CE2	2.36	1.08
4:D:8:PRO:HD2	4:D:21:LEU:HD23	1.21	1.08
3:C:22:CYS:SG	3:C:90:CYS:CB	2.40	1.08
1:A:135:THR:HG23	1:A:147:ILE:CD1	1.84	1.07
3:C:152:GLN:CA	3:C:160:ILE:HD11	1.83	1.07
2:B:38:GLN:NE2	2:B:45:LYS:HG2	1.67	1.07
3:C:16:GLU:O	3:C:80:THR:HG23	1.54	1.07
4:D:117:VAL:HG21	4:D:154:TYR:HE2	0.97	1.07
4:D:117:VAL:HG21	4:D:154:TYR:CE2	1.88	1.06
2:B:38:GLN:NE2	2:B:45:LYS:CG	2.17	1.06
4:D:30:ASP:CB	4:D:96:LEU:HD11	1.84	1.06
3:C:136:LYS:O	4:D:131:PHE:HE2	1.38	1.06
3:C:166:LEU:H	3:C:166:LEU:CD1	1.67	1.06
3:C:131:SER:HB2	3:C:132:LYS:HA	1.34	1.04
3:C:152:GLN:HA	3:C:160:ILE:CD1	1.87	1.04
2:B:25:CYS:SG	2:B:80:CYS:SG	1.03	1.03
4:D:206:ASN:HD22	4:D:208:ARG:HB2	1.20	1.03
4:D:117:VAL:CG2	4:D:154:TYR:HE2	1.71	1.02
3:C:136:LYS:O	4:D:131:PHE:CE2	2.14	1.01
4:D:8:PRO:HD2	4:D:21:LEU:HD22	1.33	1.01
4:D:21:LEU:CD1	4:D:112:THR:HG21	1.91	1.00
3:C:127:GLN:HG3	3:C:189:CYS:SG	2.00	1.00
3:C:140:LEU:HD12	3:C:178:ALA:O	0.85	1.00
2:B:51:MET:SD	2:B:66:ALA:CB	2.49	1.00
3:C:126:TYR:CE1	4:D:137:GLU:CA	2.45	1.00
3:C:135:ASP:HA	3:C:136:LYS:HB2	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PRO:CD	4:D:21:LEU:CD2	2.40	1.00
1:A:140:PRO:HB2	1:A:142:TRP:CD1	1.97	1.00
3:C:131:SER:HB2	3:C:132:LYS:O	1.62	0.99
2:B:38:GLN:HE21	2:B:45:LYS:HG2	1.19	0.99
4:D:137:GLU:O	4:D:141:THR:OG1	1.79	0.98
3:C:144:PHE:HD1	3:C:148:THR:OG1	1.45	0.98
1:A:89:SER:CB	1:A:90:PRO:HD3	1.86	0.98
1:A:142:TRP:CH2	1:A:143:LEU:HD13	1.98	0.98
2:B:29:GLN:HA	2:B:61:SER:OG	1.63	0.98
2:B:81:ARG:HG3	2:B:92:THR:OG1	1.64	0.98
1:A:205:GLN:HG2	1:A:252:ASP:OD1	1.64	0.98
4:D:185:ALA:H	4:D:186:LEU:HA	1.28	0.98
4:D:49:SER:OG	4:D:68:ARG:HD2	1.64	0.97
2:B:70:PHE:HD1	2:B:78:TYR:CZ	1.82	0.96
4:D:164:VAL:HG22	4:D:165:ASN:H	1.30	0.96
4:D:226:TRP:CE2	4:D:228:GLN:HB2	2.00	0.96
1:A:186:GLN:NE2	1:A:268:SER:OG	1.98	0.96
3:C:130:ASP:CB	4:D:131:PHE:HD2	1.77	0.96
3:C:55:LYS:HG2	3:C:65:THR:HG22	1.48	0.95
4:D:21:LEU:HD11	4:D:112:THR:HG21	1.46	0.95
4:D:30:ASP:HB2	4:D:96:LEU:HD13	1.47	0.95
3:C:60:ARG:NH2	3:C:84:ASP:OD2	1.99	0.94
4:D:160:LEU:HD13	4:D:215:VAL:HG22	1.48	0.94
4:D:164:VAL:HG22	4:D:165:ASN:N	1.79	0.94
3:C:126:TYR:HE1	4:D:137:GLU:CA	1.79	0.94
4:D:181:LYS:HG2	4:D:191:TYR:HE1	1.26	0.94
3:C:131:SER:CB	3:C:132:LYS:C	2.36	0.94
3:C:161:THR:OG1	3:C:179:VAL:N	2.00	0.93
4:D:6:GLN:NE2	4:D:91:CYS:H	1.67	0.93
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.49	0.93
3:C:131:SER:CB	3:C:132:LYS:HA	1.96	0.93
4:D:226:TRP:CZ2	4:D:228:GLN:CB	2.52	0.93
4:D:131:PHE:HE1	4:D:149:LEU:HD12	1.11	0.93
3:C:134:SER:O	3:C:136:LYS:HB2	1.69	0.91
3:C:166:LEU:H	3:C:166:LEU:HD12	1.33	0.91
4:D:131:PHE:CZ	4:D:149:LEU:HD12	2.04	0.91
4:D:4:ILE:CG1	4:D:27:PHE:CE1	2.45	0.90
2:B:25:CYS:SG	2:B:80:CYS:HB2	2.10	0.90
3:C:126:TYR:HE1	4:D:137:GLU:N	1.70	0.89
2:B:38:GLN:OE1	2:B:81:ARG:NH2	2.05	0.89
3:C:166:LEU:CD1	3:C:166:LEU:N	2.30	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:ASN:ND2	4:D:208:ARG:HB2	1.87	0.89
1:A:89:SER:HB2	1:A:90:PRO:HD3	0.91	0.89
4:D:226:TRP:HD1	4:D:226:TRP:O	1.56	0.89
4:D:117:VAL:CG2	4:D:154:TYR:CE2	2.51	0.88
3:C:166:LEU:HD12	3:C:166:LEU:N	1.89	0.88
3:C:196:SER:O	3:C:197:ILE:HG13	1.74	0.87
3:C:140:LEU:HD13	3:C:179:VAL:HG22	1.56	0.87
4:D:25:GLN:OE1	4:D:29:HIS:HB2	1.74	0.86
1:A:135:THR:CG2	1:A:147:ILE:CD1	2.52	0.86
3:C:140:LEU:HD12	3:C:178:ALA:C	1.95	0.86
3:C:203:PHE:HD1	3:C:204:PHE:N	1.72	0.86
4:D:226:TRP:CD1	4:D:226:TRP:C	2.48	0.86
3:C:128:LEU:HB3	4:D:132:GLU:O	1.76	0.85
3:C:140:LEU:HD13	3:C:179:VAL:CG2	2.07	0.85
2:B:70:PHE:CD1	2:B:78:TYR:CE2	2.64	0.85
3:C:145:ASP:OD1	3:C:146:SER:N	2.10	0.85
1:A:227:GLN:HG3	1:A:227:GLN:O	1.76	0.84
3:C:194:ASN:O	3:C:195:ASN:HB2	1.77	0.84
3:C:203:PHE:O	3:C:204:PHE:CD2	2.30	0.84
3:C:166:LEU:H	3:C:166:LEU:HD13	1.42	0.84
3:C:47:THR:OG1	3:C:56:THR:OG1	1.90	0.84
3:C:126:TYR:CE1	4:D:137:GLU:N	2.46	0.84
2:B:23:LEU:HB2	2:B:70:PHE:HE2	1.41	0.83
1:A:198:SER:HB3	1:A:205:GLN:HG3	1.60	0.83
4:D:131:PHE:CE1	4:D:149:LEU:HD11	2.12	0.83
3:C:202:THR:O	3:C:204:PHE:CE2	2.32	0.82
3:C:140:LEU:CD1	3:C:178:ALA:C	2.47	0.82
3:C:166:LEU:HD13	3:C:166:LEU:O	1.79	0.82
4:D:145:THR:HG22	4:D:198:ARG:HG3	1.61	0.82
4:D:186:LEU:HD12	4:D:186:LEU:O	1.79	0.82
4:D:185:ALA:N	4:D:186:LEU:HA	1.87	0.82
4:D:6:GLN:HE22	4:D:90:LEU:HA	1.44	0.82
3:C:126:TYR:CE1	4:D:137:GLU:HA	2.12	0.82
4:D:180:LEU:O	4:D:191:TYR:HA	1.78	0.82
4:D:51:GLY:O	4:D:68:ARG:HD3	1.79	0.82
3:C:144:PHE:CD1	3:C:148:THR:OG1	2.30	0.82
4:D:38:ASP:OD2	4:D:44:ARG:NH2	2.13	0.81
3:C:145:ASP:O	3:C:148:THR:OG1	1.98	0.81
3:C:203:PHE:HD1	3:C:204:PHE:H	1.28	0.81
4:D:216:GLN:OE1	4:D:237:ILE:CG1	2.28	0.81
4:D:226:TRP:NE1	4:D:228:GLN:O	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:CYS:HG	3:C:90:CYS:CB	1.91	0.81
1:A:142:TRP:HH2	7:A:601:GCY:H2	1.44	0.80
1:A:143:LEU:HD11	7:A:601:GCY:H4	1.60	0.80
4:D:138:ILE:HD12	4:D:138:ILE:H	1.46	0.80
3:C:165:VAL:N	4:D:174:CYS:SG	2.55	0.80
1:A:135:THR:CG2	1:A:147:ILE:HD11	2.11	0.80
2:B:70:PHE:CD1	2:B:78:TYR:CZ	2.69	0.80
3:C:55:LYS:CG	3:C:65:THR:HG22	2.11	0.80
4:D:145:THR:HG22	4:D:198:ARG:CG	2.12	0.80
3:C:161:THR:HG21	3:C:179:VAL:HB	1.64	0.80
4:D:4:ILE:CD1	4:D:27:PHE:HE1	1.94	0.79
2:B:30:PHE:CZ	2:B:54:MET:HE3	2.17	0.79
3:C:86:ALA:O	3:C:88:TYR:CE1	2.35	0.79
4:D:207:PRO:HA	4:D:243:TRP:O	1.82	0.79
4:D:207:PRO:HB3	4:D:243:TRP:O	1.82	0.79
3:C:118:ILE:HD12	3:C:145:ASP:HA	1.65	0.79
3:C:152:GLN:HA	3:C:160:ILE:HD11	0.91	0.79
3:C:194:ASN:O	3:C:195:ASN:CB	2.31	0.79
4:D:117:VAL:HG22	9:D:252:HOH:O	1.81	0.79
4:D:3:ILE:O	4:D:26:ASN:OD1	2.01	0.78
4:D:137:GLU:O	4:D:141:THR:N	2.15	0.78
4:D:226:TRP:O	4:D:226:TRP:CD1	2.36	0.78
4:D:160:LEU:HD13	4:D:215:VAL:CG2	2.14	0.78
1:A:59:SER:CB	1:A:62:GLN:OE1	2.31	0.77
3:C:203:PHE:C	3:C:204:PHE:HD2	1.86	0.77
4:D:47:TYR:CE1	4:D:57:LYS:HG2	2.19	0.77
3:C:198:ILE:HD11	3:C:202:THR:HG21	1.66	0.77
4:D:23:CYS:SG	4:D:34:TRP:CE2	2.77	0.77
1:A:55:GLN:NE2	1:A:58:LEU:O	2.16	0.77
2:B:70:PHE:HD1	2:B:78:TYR:CE2	2.00	0.77
3:C:126:TYR:CE1	4:D:137:GLU:HB2	2.19	0.76
1:A:186:GLN:HE22	1:A:268:SER:HG	1.32	0.76
3:C:177:SER:OG	4:D:196:ARG:HD3	1.83	0.76
2:B:22:ILE:HD13	2:B:69:GLU:HG3	1.67	0.76
3:C:126:TYR:CE1	4:D:137:GLU:CB	2.69	0.76
3:C:22:CYS:HB2	3:C:90:CYS:SG	2.25	0.76
3:C:177:SER:OG	4:D:196:ARG:CD	2.34	0.76
1:A:89:SER:CB	1:A:90:PRO:HD2	2.15	0.76
4:D:23:CYS:SG	4:D:34:TRP:CH2	2.78	0.75
3:C:135:ASP:CA	3:C:136:LYS:HB2	2.17	0.75
4:D:8:PRO:CD	4:D:21:LEU:HD23	2.09	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:O	1:A:57:LYS:HG2	1.87	0.74
3:C:203:PHE:C	3:C:204:PHE:CD2	2.61	0.74
7:A:601:GCY:O17	7:A:601:GCY:H18	1.89	0.73
3:C:198:ILE:HD12	3:C:199:PRO:HD2	1.70	0.73
4:D:6:GLN:HE21	4:D:91:CYS:H	1.36	0.73
4:D:199:VAL:HG21	4:D:203:PHE:CD1	2.23	0.73
2:B:30:PHE:CZ	2:B:54:MET:CE	2.71	0.73
4:D:8:PRO:CD	4:D:21:LEU:HD22	2.11	0.73
4:D:21:LEU:HD13	4:D:112:THR:HG21	1.68	0.73
3:C:130:ASP:HA	4:D:131:PHE:HA	1.70	0.72
3:C:22:CYS:SG	3:C:90:CYS:HB3	2.28	0.72
4:D:164:VAL:CG2	4:D:165:ASN:H	2.02	0.72
1:A:135:THR:HG23	1:A:147:ILE:HD13	1.72	0.72
4:D:210:HIS:NE2	4:D:241:GLU:HG3	2.05	0.72
4:D:141:THR:C	4:D:142:GLN:HG2	2.08	0.72
4:D:211:PHE:CD2	4:D:211:PHE:N	2.56	0.72
4:D:135:GLU:HA	4:D:138:ILE:HD13	1.72	0.72
1:A:227:GLN:O	1:A:227:GLN:CG	2.38	0.71
3:C:85:THR:O	3:C:112:LEU:O	2.08	0.71
4:D:3:ILE:HG22	4:D:4:ILE:N	2.05	0.71
4:D:131:PHE:CZ	4:D:149:LEU:CD1	2.70	0.71
1:A:140:PRO:CB	1:A:142:TRP:CD1	2.72	0.70
1:A:242:ASP:OD1	1:A:244:THR:OG1	2.08	0.70
1:A:281:SER:O	1:A:285:ILE:HG13	1.91	0.70
1:A:142:TRP:CH2	7:A:601:GCY:H2	2.27	0.70
2:B:73:THR:OG1	2:B:76:ASP:OD1	2.10	0.69
3:C:131:SER:CB	3:C:132:LYS:O	2.38	0.69
4:D:30:ASP:CB	4:D:96:LEU:CD1	2.51	0.69
4:D:206:ASN:CG	4:D:206:ASN:O	2.30	0.69
4:D:46:ILE:O	4:D:58:GLY:N	2.23	0.69
4:D:135:GLU:CA	4:D:138:ILE:HD13	2.22	0.69
1:A:110:ASN:OD1	1:A:110:ASN:O	2.10	0.69
3:C:203:PHE:CD1	3:C:204:PHE:N	2.58	0.69
3:C:24:TYR:CE1	3:C:71:LYS:HD3	2.27	0.69
4:D:4:ILE:CD1	4:D:27:PHE:CE1	2.74	0.68
4:D:131:PHE:HE1	4:D:149:LEU:CG	2.07	0.68
1:A:135:THR:HG22	1:A:147:ILE:HD11	1.76	0.68
3:C:202:THR:O	3:C:204:PHE:HE2	1.75	0.68
3:C:138:VAL:HG23	3:C:181:TRP:HB3	1.75	0.68
4:D:226:TRP:CD2	4:D:228:GLN:OE1	2.47	0.68
4:D:4:ILE:HA	4:D:24:GLN:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:207:PRO:CA	4:D:243:TRP:O	2.42	0.68
1:A:295:HIS:CD2	1:A:295:HIS:H	2.10	0.67
4:D:202:THR:O	4:D:205:GLN:HB2	1.94	0.67
1:A:74:ARG:NH1	9:A:312:HOH:O	2.25	0.67
3:C:202:THR:O	3:C:204:PHE:CD2	2.47	0.67
4:D:16:GLY:HA2	4:D:80:SER:OG	1.95	0.67
2:B:30:PHE:CE2	2:B:54:MET:HE3	2.28	0.67
4:D:216:GLN:CD	4:D:237:ILE:HG12	2.15	0.67
4:D:122:ASN:O	4:D:124:PHE:CD2	2.47	0.67
2:B:17:ASN:OD1	2:B:73:THR:CA	2.43	0.67
4:D:51:GLY:C	4:D:68:ARG:HD3	2.15	0.67
4:D:160:LEU:CD1	4:D:215:VAL:HG22	2.25	0.66
1:A:30:VAL:HB	1:A:38:HIS:HB2	1.76	0.66
4:D:138:ILE:HD12	4:D:138:ILE:N	2.11	0.66
4:D:11:LEU:HD12	4:D:12:ILE:N	2.11	0.66
1:A:227:GLN:HE21	1:A:229:GLN:HE22	1.43	0.66
4:D:25:GLN:NE2	4:D:29:HIS:O	2.29	0.66
3:C:141:PHE:CZ	3:C:144:PHE:HB3	2.31	0.66
3:C:43:LEU:N	3:C:43:LEU:HD12	2.09	0.66
3:C:118:ILE:CD1	3:C:145:ASP:HA	2.25	0.66
2:B:38:GLN:HE22	2:B:45:LYS:CD	1.89	0.66
1:A:205:GLN:HG2	1:A:252:ASP:CG	2.16	0.65
3:C:127:GLN:CG	3:C:189:CYS:SG	2.82	0.65
3:C:125:VAL:HA	3:C:140:LEU:O	1.97	0.65
4:D:25:GLN:OE1	4:D:93:SER:HB2	1.96	0.65
1:A:191:ALA:HA	1:A:209:HIS:O	1.96	0.65
1:A:78:THR:O	1:A:82:GLN:HG3	1.97	0.65
4:D:145:THR:HG22	4:D:198:ARG:CD	2.27	0.65
4:D:31:THR:HG21	4:D:33:TYR:OH	1.97	0.65
4:D:227:THR:HG23	4:D:228:GLN:N	2.11	0.65
4:D:207:PRO:CB	4:D:243:TRP:O	2.45	0.64
1:A:59:SER:HB2	1:A:62:GLN:OE1	1.95	0.64
2:B:81:ARG:HG3	2:B:92:THR:HG1	1.61	0.64
2:B:30:PHE:HZ	2:B:54:MET:HE3	1.63	0.64
2:B:30:PHE:CE2	2:B:54:MET:CE	2.81	0.64
4:D:4:ILE:HD11	4:D:27:PHE:CE1	2.33	0.64
1:A:116:LEU:C	1:A:116:LEU:HD23	2.18	0.64
3:C:125:VAL:O	3:C:125:VAL:HG22	1.96	0.64
2:B:17:ASN:OD1	2:B:73:THR:HA	1.98	0.63
4:D:209:ASN:HB3	4:D:211:PHE:CE2	2.33	0.63
4:D:221:SER:O	4:D:224:ASP:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LYS:C	4:D:131:PHE:HE2	2.02	0.63
1:A:59:SER:OG	1:A:62:GLN:OE1	2.16	0.63
2:B:96:ASP:OD1	2:B:96:ASP:C	2.34	0.62
3:C:161:THR:CG2	3:C:179:VAL:HB	2.29	0.62
4:D:221:SER:O	4:D:223:ASN:N	2.31	0.62
1:A:294:ASN:O	1:A:295:HIS:C	2.37	0.62
4:D:206:ASN:C	4:D:208:ARG:H	2.01	0.62
4:D:226:TRP:CH2	4:D:228:GLN:HB2	2.27	0.62
3:C:19:VAL:HG12	3:C:19:VAL:O	1.99	0.62
4:D:132:GLU:HB3	4:D:133:PRO:HD2	1.82	0.62
4:D:185:ALA:N	4:D:186:LEU:CA	2.60	0.62
1:A:49:PHE:CD2	1:A:54:SER:HB3	2.35	0.62
3:C:124:ALA:CB	3:C:126:TYR:CE2	2.83	0.62
3:C:196:SER:O	3:C:197:ILE:CG1	2.47	0.62
4:D:51:GLY:O	4:D:68:ARG:CD	2.47	0.62
4:D:164:VAL:O	4:D:165:ASN:C	2.37	0.62
1:A:143:LEU:C	1:A:146:PRO:HD2	2.19	0.61
4:D:145:THR:CG2	4:D:198:ARG:HG3	2.30	0.61
1:A:53:TRP:CD2	1:A:179:GLY:HA3	2.35	0.61
1:A:142:TRP:CZ3	1:A:143:LEU:HD13	2.35	0.61
1:A:143:LEU:O	1:A:146:PRO:HD2	2.01	0.61
3:C:43:LEU:N	3:C:43:LEU:CD1	2.62	0.61
1:A:142:TRP:CH2	1:A:143:LEU:CD1	2.78	0.61
4:D:146:LEU:HD12	4:D:146:LEU:N	2.16	0.61
3:C:166:LEU:N	3:C:166:LEU:HD13	2.07	0.61
4:D:137:GLU:O	4:D:141:THR:CB	2.49	0.60
7:A:601:GCY:O16	3:C:30:ASN:ND2	2.34	0.60
3:C:159:TYR:O	3:C:180:ALA:HA	2.01	0.60
3:C:124:ALA:HB1	3:C:126:TYR:CE2	2.37	0.60
1:A:196:VAL:HG13	1:A:197:PRO:N	2.16	0.60
3:C:166:LEU:HD11	3:C:175:SER:OG	2.02	0.60
4:D:25:GLN:O	4:D:25:GLN:HG3	2.00	0.60
1:A:145:LEU:O	1:A:149:VAL:HG23	2.01	0.60
4:D:213:CYS:O	4:D:213:CYS:SG	2.59	0.60
4:D:221:SER:O	4:D:222:GLU:C	2.39	0.59
1:A:142:TRP:CZ2	1:A:143:LEU:HD13	2.37	0.59
3:C:157:ASP:CG	3:C:158:VAL:HG23	2.23	0.59
3:C:126:TYR:HE1	4:D:137:GLU:HA	1.50	0.59
4:D:206:ASN:O	4:D:208:ARG:N	2.30	0.59
3:C:124:ALA:HB3	3:C:126:TYR:HE2	1.68	0.59
3:C:38:ASP:OD1	3:C:86:ALA:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ILE:CG2	4:D:4:ILE:N	2.65	0.59
3:C:85:THR:HG23	3:C:112:LEU:O	2.03	0.59
3:C:131:SER:CA	3:C:132:LYS:C	2.71	0.59
4:D:120:LEU:HD12	4:D:123:VAL:HG23	1.84	0.59
1:A:104:CYS:SG	1:A:168:CYS:CB	2.81	0.58
3:C:140:LEU:HD13	3:C:179:VAL:HG23	1.86	0.58
4:D:30:ASP:O	4:D:68:ARG:NH1	2.36	0.58
4:D:189:SER:O	4:D:191:TYR:CE2	2.56	0.58
4:D:117:VAL:CG1	4:D:119:ASP:O	2.51	0.58
4:D:141:THR:O	4:D:142:GLN:HG2	2.03	0.58
3:C:135:ASP:HA	3:C:136:LYS:CB	2.11	0.58
2:B:10:TYR:CE2	2:B:24:ASN:HB2	2.38	0.58
1:A:59:SER:N	1:A:62:GLN:OE1	2.32	0.57
4:D:138:ILE:H	4:D:138:ILE:CD1	2.13	0.57
1:A:57:LYS:O	1:A:57:LYS:CG	2.53	0.57
2:B:29:GLN:HA	2:B:61:SER:HG	1.69	0.57
2:B:51:MET:SD	2:B:66:ALA:CA	2.93	0.57
4:D:20:THR:HG23	4:D:77:THR:HG22	1.84	0.57
4:D:25:GLN:HE22	4:D:29:HIS:N	2.02	0.57
4:D:226:TRP:NE1	4:D:228:GLN:N	2.53	0.57
4:D:199:VAL:HG22	4:D:203:PHE:HB3	1.85	0.57
1:A:89:SER:HG	1:A:90:PRO:HD2	1.69	0.57
1:A:194:SER:OG	1:A:207:VAL:HB	2.05	0.57
4:D:202:THR:O	4:D:205:GLN:CB	2.53	0.57
4:D:120:LEU:HD12	4:D:123:VAL:CG2	2.34	0.57
4:D:120:LEU:CD1	4:D:123:VAL:HG21	2.35	0.57
4:D:137:GLU:CG	4:D:143:LYS:O	2.52	0.57
1:A:10:PHE:O	1:A:103:GLY:HA3	2.04	0.56
2:B:10:TYR:CE2	2:B:24:ASN:ND2	2.73	0.56
2:B:20:PRO:HA	2:B:71:THR:HG22	1.87	0.56
3:C:32:LEU:HD21	3:C:90:CYS:SG	2.46	0.56
4:D:137:GLU:HG3	4:D:141:THR:HG21	1.87	0.56
1:A:237:PHE:C	1:A:238:LEU:HD23	2.25	0.56
3:C:131:SER:CB	3:C:132:LYS:CA	2.40	0.56
4:D:119:ASP:O	4:D:122:ASN:OD1	2.24	0.56
4:D:132:GLU:HB3	4:D:133:PRO:CD	2.35	0.56
2:B:38:GLN:HE21	2:B:45:LYS:HD3	1.59	0.56
1:A:198:SER:CB	1:A:205:GLN:HG3	2.34	0.56
4:D:49:SER:OG	4:D:68:ARG:CD	2.48	0.56
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.39	0.56
4:D:6:GLN:NE2	4:D:91:CYS:N	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:GLU:HG2	4:D:143:LYS:O	2.05	0.56
3:C:136:LYS:O	4:D:131:PHE:CD2	2.60	0.55
4:D:145:THR:CG2	4:D:198:ARG:CD	2.84	0.55
4:D:23:CYS:SG	4:D:34:TRP:HZ2	2.15	0.55
1:A:145:LEU:HB3	1:A:146:PRO:CD	2.28	0.55
1:A:237:PHE:O	1:A:238:LEU:HD23	2.05	0.55
4:D:137:GLU:C	4:D:141:THR:HG1	1.99	0.55
3:C:190:ALA:HA	3:C:204:PHE:HE1	1.71	0.55
4:D:161:SER:OG	4:D:163:TRP:NE1	2.32	0.55
4:D:181:LYS:HE2	4:D:191:TYR:CE1	2.41	0.55
3:C:198:ILE:HD12	3:C:199:PRO:CD	2.36	0.55
4:D:6:GLN:NE2	4:D:90:LEU:HA	2.18	0.55
1:A:104:CYS:HB3	1:A:168:CYS:SG	2.42	0.54
1:A:186:GLN:HB3	1:A:269:SER:HB3	1.89	0.54
3:C:134:SER:O	3:C:136:LYS:HD2	2.07	0.54
4:D:25:GLN:CD	4:D:29:HIS:HB2	2.27	0.54
3:C:167:ASP:OD2	3:C:174:LYS:NZ	2.38	0.54
3:C:198:ILE:HG13	3:C:199:PRO:N	2.23	0.54
4:D:11:LEU:HD12	4:D:12:ILE:H	1.71	0.54
4:D:145:THR:HG22	4:D:198:ARG:HD2	1.90	0.54
4:D:211:PHE:N	4:D:211:PHE:HD2	2.02	0.54
3:C:196:SER:C	3:C:197:ILE:HG13	2.27	0.54
1:A:135:THR:HG23	1:A:147:ILE:HD12	1.84	0.54
2:B:12:ARG:HH11	2:B:12:ARG:HG3	1.72	0.54
1:A:140:PRO:HB2	1:A:142:TRP:NE1	2.22	0.54
4:D:163:TRP:O	4:D:212:ARG:N	2.30	0.54
3:C:126:TYR:N	3:C:126:TYR:CD2	2.75	0.54
1:A:240:ASN:HB2	1:A:244:THR:O	2.08	0.54
3:C:29:ASP:OD1	3:C:29:ASP:N	2.40	0.54
4:D:141:THR:O	4:D:142:GLN:CB	2.55	0.54
1:A:227:GLN:NE2	1:A:229:GLN:HE22	2.04	0.54
3:C:40:GLY:O	3:C:41:LYS:HG2	2.06	0.54
1:A:161:GLN:O	1:A:165:ASN:HB2	2.08	0.54
4:D:122:ASN:O	4:D:124:PHE:CE2	2.61	0.54
3:C:169:ARG:O	3:C:170:SER:CB	2.56	0.53
4:D:99:VAL:HG12	4:D:99:VAL:O	2.08	0.53
3:C:138:VAL:HG22	3:C:180:ALA:O	2.08	0.53
4:D:165:ASN:N	4:D:210:HIS:O	2.41	0.53
1:A:142:TRP:CZ3	1:A:143:LEU:CD1	2.92	0.53
4:D:120:LEU:HD12	4:D:120:LEU:O	2.09	0.53
4:D:185:ALA:HB3	4:D:186:LEU:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TRP:CE3	1:A:179:GLY:HA3	2.43	0.53
1:A:156:THR:HG23	7:A:601:GCY:H38A	1.91	0.53
1:A:294:ASN:OD1	1:A:294:ASN:C	2.48	0.53
1:A:295:HIS:CD2	1:A:295:HIS:N	2.76	0.53
3:C:36:LYS:HE2	3:C:86:ALA:HB3	1.91	0.53
3:C:128:LEU:CB	4:D:132:GLU:O	2.52	0.53
4:D:8:PRO:O	4:D:112:THR:OG1	2.20	0.53
1:A:283:HIS:O	1:A:287:ASP:HB2	2.08	0.53
3:C:52:GLN:HA	3:C:68:LYS:HD2	1.90	0.53
3:C:138:VAL:CG2	3:C:180:ALA:O	2.56	0.53
4:D:156:ASP:CG	4:D:156:ASP:O	2.46	0.53
2:B:51:MET:SD	2:B:66:ALA:HA	2.49	0.53
3:C:32:LEU:HD23	3:C:33:ARG:N	2.24	0.53
4:D:83:LYS:O	4:D:84:ASN:HB2	2.08	0.53
3:C:118:ILE:HG22	3:C:120:ASN:H	1.73	0.52
1:A:92:GLU:C	1:A:93:ASP:OD1	2.48	0.52
4:D:125:PRO:HD3	4:D:233:PRO:HB3	1.90	0.52
1:A:196:VAL:HG13	1:A:197:PRO:CD	2.39	0.52
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.91	0.52
2:B:81:ARG:CG	2:B:92:THR:OG1	2.49	0.52
4:D:216:GLN:OE1	4:D:237:ILE:CD1	2.57	0.52
1:A:104:CYS:SG	1:A:172:VAL:HG21	2.50	0.52
1:A:216:LYS:HD2	1:A:245:TRP:CE2	2.44	0.52
3:C:124:ALA:HB3	3:C:126:TYR:CE2	2.45	0.52
3:C:144:PHE:CZ	3:C:176:ASN:HB3	2.44	0.52
3:C:13:ARG:NH1	3:C:16:GLU:OE2	2.39	0.52
4:D:121:LYS:HG3	4:D:228:GLN:HG2	1.91	0.52
4:D:120:LEU:CD1	4:D:123:VAL:CG2	2.88	0.52
1:A:192:TRP:O	1:A:209:HIS:HD2	1.91	0.51
2:B:13:HIS:HB3	2:B:14:PRO:HD2	1.91	0.51
1:A:87:MET:HG3	4:D:50:TYR:CD2	2.45	0.51
4:D:31:THR:HG22	4:D:33:TYR:CE1	2.45	0.51
3:C:164:CYS:C	4:D:174:CYS:SG	2.88	0.51
1:A:246:TYR:C	1:A:246:TYR:CD2	2.84	0.51
3:C:38:ASP:OD1	3:C:86:ALA:CB	2.58	0.51
3:C:161:THR:HG1	3:C:179:VAL:H	1.46	0.51
3:C:138:VAL:HG21	3:C:179:VAL:CG1	2.41	0.51
3:C:149:ASN:ND2	3:C:149:ASN:N	2.59	0.51
3:C:13:ARG:HB3	3:C:16:GLU:CD	2.31	0.51
1:A:256:GLY:N	1:A:258:GLU:OE1	2.43	0.51
3:C:194:ASN:OD1	3:C:194:ASN:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:GLU:O	3:C:80:THR:CG2	2.42	0.50
3:C:151:SER:HB3	3:C:195:ASN:ND2	2.26	0.50
4:D:25:GLN:HE22	4:D:29:HIS:CA	2.23	0.50
3:C:128:LEU:HD12	3:C:128:LEU:N	2.26	0.50
3:C:172:ASP:O	3:C:172:ASP:OD2	2.30	0.50
4:D:57:LYS:HB3	4:D:61:SER:CB	2.42	0.50
4:D:212:ARG:HH21	4:D:212:ARG:HG2	1.76	0.50
1:A:196:VAL:HG22	1:A:197:PRO:HD2	1.92	0.50
4:D:156:ASP:O	4:D:156:ASP:OD1	2.30	0.50
1:A:294:ASN:O	1:A:294:ASN:OD1	2.29	0.50
4:D:181:LYS:HE2	4:D:191:TYR:HE1	1.77	0.49
2:B:13:HIS:HB3	2:B:14:PRO:CD	2.41	0.49
3:C:124:ALA:CB	3:C:126:TYR:HE2	2.21	0.49
4:D:185:ALA:H	4:D:186:LEU:CA	2.10	0.49
1:A:155:GLY:O	1:A:159:THR:HG23	2.12	0.49
4:D:3:ILE:HG22	4:D:5:THR:HG23	1.95	0.49
4:D:181:LYS:HE2	4:D:191:TYR:OH	2.12	0.49
1:A:49:PHE:HD2	1:A:54:SER:HB3	1.76	0.49
4:D:49:SER:CB	4:D:68:ARG:HD2	2.43	0.49
1:A:213:PHE:CE2	1:A:245:TRP:HB2	2.47	0.49
3:C:157:ASP:OD1	3:C:158:VAL:N	2.46	0.49
4:D:205:GLN:O	4:D:207:PRO:HD3	2.13	0.49
4:D:221:SER:C	4:D:223:ASN:N	2.62	0.49
4:D:227:THR:CG2	4:D:228:GLN:N	2.75	0.49
4:D:164:VAL:HG12	4:D:167:LYS:O	2.13	0.49
1:A:116:LEU:HD23	1:A:117:HIS:N	2.28	0.49
2:B:23:LEU:HD13	2:B:70:PHE:CZ	2.48	0.49
2:B:27:VAL:HG21	2:B:37:ILE:HD13	1.94	0.49
1:A:58:LEU:N	1:A:58:LEU:HD23	2.28	0.49
1:A:198:SER:OG	1:A:203:HIS:CB	2.60	0.49
4:D:145:THR:CG2	4:D:198:ARG:HD2	2.42	0.48
2:B:30:PHE:HZ	2:B:54:MET:CE	2.20	0.48
3:C:49:LEU:HD23	3:C:56:THR:HG23	1.95	0.48
4:D:4:ILE:CD1	4:D:107:PHE:HB2	2.42	0.48
1:A:205:GLN:CG	1:A:252:ASP:OD1	2.50	0.48
1:A:219:TRP:CH2	1:A:221:MET:HB2	2.48	0.48
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.94	0.48
1:A:49:PHE:HB3	1:A:54:SER:HB2	1.94	0.48
4:D:57:LYS:HB3	4:D:61:SER:HB3	1.95	0.48
4:D:137:GLU:O	4:D:141:THR:HG23	2.14	0.48
1:A:196:VAL:CG1	1:A:197:PRO:N	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG13	1:A:197:PRO:HD2	1.95	0.48
3:C:160:ILE:O	3:C:160:ILE:HG13	2.14	0.48
4:D:117:VAL:HG23	4:D:154:TYR:OH	2.14	0.48
4:D:58:GLY:C	4:D:60:LEU:H	2.16	0.48
4:D:206:ASN:C	4:D:208:ARG:N	2.65	0.48
1:A:216:LYS:N	1:A:217:PRO:HD2	2.28	0.48
4:D:2:GLY:HA2	4:D:26:ASN:ND2	2.29	0.48
3:C:171:MET:SD	4:D:143:LYS:NZ	2.86	0.47
3:C:37:GLN:O	3:C:86:ALA:HB1	2.13	0.47
3:C:10:LEU:HD23	3:C:112:LEU:HD13	1.97	0.47
4:D:26:ASN:OD1	4:D:26:ASN:N	2.48	0.47
1:A:254:GLU:O	1:A:257:GLU:HB2	2.14	0.47
4:D:186:LEU:HD12	4:D:186:LEU:C	2.35	0.47
1:A:294:ASN:O	1:A:294:ASN:CG	2.52	0.47
4:D:141:THR:O	4:D:142:GLN:CG	2.62	0.47
4:D:188:ASP:HB3	9:D:252:HOH:O	2.13	0.47
3:C:86:ALA:O	3:C:88:TYR:CD1	2.68	0.47
3:C:141:PHE:HZ	3:C:199:PRO:HG2	1.79	0.47
4:D:117:VAL:CG2	4:D:154:TYR:CZ	2.97	0.47
1:A:219:TRP:CE3	1:A:266:LYS:HG3	2.50	0.47
2:B:17:ASN:OD1	2:B:73:THR:C	2.52	0.47
3:C:63:SER:HB2	3:C:76:HIS:HB2	1.97	0.47
3:C:143:ASP:OD1	3:C:143:ASP:N	2.47	0.47
4:D:204:TRP:O	4:D:204:TRP:CD2	2.68	0.47
1:A:126:VAL:HG12	1:A:127:ARG:N	2.28	0.47
2:B:38:GLN:NE2	2:B:45:LYS:HD3	2.11	0.47
1:A:67:GLN:O	1:A:71:GLN:HG3	2.15	0.46
2:B:20:PRO:CA	2:B:71:THR:HG22	2.45	0.46
2:B:27:VAL:HG21	2:B:37:ILE:CD1	2.46	0.46
4:D:25:GLN:NE2	4:D:29:HIS:HB2	2.31	0.46
2:B:10:TYR:CZ	2:B:24:ASN:HB2	2.50	0.46
4:D:130:VAL:HG13	4:D:130:VAL:O	2.15	0.46
1:A:116:LEU:C	1:A:116:LEU:CD2	2.84	0.46
1:A:140:PRO:HG2	1:A:142:TRP:HE1	1.79	0.46
4:D:25:GLN:OE1	4:D:93:SER:CB	2.63	0.46
7:A:601:GCM:O17	7:A:601:GCM:C18	2.59	0.46
3:C:127:GLN:CG	3:C:139:CYS:SG	3.04	0.46
3:C:149:ASN:ND2	3:C:149:ASN:H	2.13	0.46
4:D:54:SER:O	4:D:55:THR:CG2	2.64	0.46
1:A:291:MET:HG2	2:B:15:PRO:O	2.16	0.46
1:A:9:THR:OG1	1:A:105:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TRP:CE3	2:B:14:PRO:HG3	2.51	0.46
1:A:234:ARG:HG3	1:A:247:LEU:HD11	1.97	0.46
1:A:198:SER:OG	1:A:203:HIS:HB3	2.16	0.46
2:B:41:LYS:O	2:B:42:ASN:HB2	2.15	0.46
3:C:134:SER:O	3:C:136:LYS:CB	2.54	0.46
2:B:70:PHE:CD1	2:B:78:TYR:CD2	3.04	0.46
1:A:88:MET:O	1:A:90:PRO:HD2	2.16	0.45
4:D:68:ARG:HG3	4:D:74:PHE:CD1	2.51	0.45
4:D:120:LEU:HD11	4:D:123:VAL:HG21	1.98	0.45
1:A:30:VAL:HG21	7:A:601:GCY:HAP	1.98	0.45
1:A:103:GLY:HA3	1:A:115:PHE:CZ	2.50	0.45
4:D:226:TRP:CE2	4:D:228:GLN:CB	2.85	0.45
4:D:201:ALA:O	4:D:202:THR:C	2.54	0.45
3:C:141:PHE:HZ	3:C:144:PHE:HB3	1.80	0.45
1:A:186:GLN:HB3	1:A:186:GLN:HE21	1.58	0.45
1:A:214:TYR:CG	1:A:215:PRO:HA	2.52	0.45
4:D:164:VAL:CG2	4:D:165:ASN:N	2.51	0.45
1:A:92:GLU:O	1:A:93:ASP:OD1	2.34	0.45
3:C:150:VAL:O	3:C:150:VAL:HG12	2.13	0.45
3:C:165:VAL:C	4:D:174:CYS:SG	2.95	0.45
3:C:141:PHE:CZ	3:C:199:PRO:HG2	2.51	0.45
4:D:243:TRP:CD1	4:D:243:TRP:N	2.84	0.45
1:A:109:GLY:HA2	1:A:110:ASN:HA	1.48	0.45
2:B:23:LEU:O	2:B:67:HIS:HA	2.16	0.45
3:C:177:SER:OG	4:D:196:ARG:NE	2.50	0.45
4:D:137:GLU:CD	4:D:143:LYS:O	2.55	0.45
2:B:32:PRO:CB	2:B:33:PRO:HD2	2.46	0.45
3:C:127:GLN:C	3:C:128:LEU:HD12	2.37	0.45
3:C:165:VAL:O	4:D:174:CYS:SG	2.75	0.45
4:D:3:ILE:H	4:D:26:ASN:HD21	1.65	0.45
1:A:143:LEU:HD11	7:A:601:GCY:C4	2.38	0.44
4:D:153:PHE:CE2	4:D:191:TYR:O	2.70	0.44
4:D:226:TRP:CE3	4:D:228:GLN:OE1	2.69	0.44
2:B:51:MET:CE	2:B:66:ALA:HB2	2.45	0.44
3:C:38:ASP:HA	3:C:86:ALA:HB1	1.98	0.44
3:C:84:ASP:O	3:C:112:LEU:HD23	2.17	0.44
1:A:136:VAL:HB	1:A:137:PRO:HD2	1.99	0.44
4:D:8:PRO:CG	4:D:21:LEU:CD2	2.94	0.44
4:D:3:ILE:N	4:D:26:ASN:OD1	2.50	0.44
4:D:54:SER:O	4:D:55:THR:HG23	2.17	0.44
4:D:137:GLU:C	4:D:141:THR:OG1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:ILE:CG1	3:C:199:PRO:N	2.80	0.44
1:A:247:LEU:HG	1:A:248:GLN:N	2.32	0.44
2:B:32:PRO:O	2:B:84:HIS:HE1	2.01	0.44
4:D:25:GLN:NE2	4:D:29:HIS:H	2.16	0.44
1:A:192:TRP:O	1:A:209:HIS:CD2	2.70	0.44
3:C:55:LYS:HG3	3:C:65:THR:HG22	1.99	0.44
1:A:10:PHE:HD2	1:A:104:CYS:SG	2.41	0.44
1:A:163:LEU:HA	1:A:167:THR:HB	2.00	0.44
3:C:135:ASP:OD1	3:C:135:ASP:O	2.36	0.44
3:C:201:ASP:N	3:C:201:ASP:OD1	2.50	0.44
1:A:34:ASP:OD1	1:A:34:ASP:N	2.42	0.43
1:A:61:GLN:O	1:A:65:LYS:HG3	2.18	0.43
2:B:10:TYR:OH	2:B:26:TYR:HB2	2.17	0.43
2:B:49:VAL:HG12	2:B:50:GLU:N	2.33	0.43
3:C:131:SER:OG	3:C:132:LYS:HA	2.16	0.43
4:D:25:GLN:HE22	4:D:29:HIS:H	1.65	0.43
3:C:97:SER:C	4:D:99:VAL:CG2	2.87	0.43
3:C:160:ILE:HG22	3:C:180:ALA:HB2	2.01	0.43
4:D:137:GLU:O	4:D:141:THR:CG2	2.66	0.43
4:D:137:GLU:HG3	4:D:141:THR:OG1	2.18	0.43
2:B:12:ARG:HG3	2:B:12:ARG:NH1	2.33	0.43
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.84	0.43
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.43
3:C:98:ALA:HA	4:D:99:VAL:HG22	2.00	0.43
4:D:185:ALA:CB	4:D:186:LEU:HA	2.41	0.43
4:D:204:TRP:O	4:D:204:TRP:CE3	2.72	0.43
1:A:53:TRP:CD2	1:A:179:GLY:CA	3.01	0.43
3:C:20:LEU:HD12	3:C:75:LEU:HD23	2.00	0.43
3:C:161:THR:HG23	3:C:179:VAL:O	2.18	0.43
1:A:10:PHE:CD2	1:A:104:CYS:SG	3.12	0.43
4:D:124:PHE:HE2	4:D:190:ARG:HH21	1.66	0.43
1:A:240:ASN:CG	2:B:12:ARG:HD2	2.39	0.43
4:D:52:ALA:HA	4:D:53:GLY:HA2	1.48	0.43
4:D:120:LEU:O	4:D:121:LYS:C	2.56	0.43
4:D:137:GLU:CG	4:D:141:THR:OG1	2.67	0.43
3:C:6:SER:HB2	3:C:7:PRO:HA	2.01	0.42
1:A:107:TYR:HE1	1:A:113:GLU:HG3	1.84	0.42
4:D:4:ILE:HD12	4:D:107:PHE:HB2	2.01	0.42
1:A:145:LEU:N	1:A:146:PRO:CD	2.82	0.42
4:D:209:ASN:O	4:D:243:TRP:HA	2.19	0.42
4:D:226:TRP:CD1	4:D:228:GLN:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:HG23	1:A:105:GLU:HG3	2.00	0.42
4:D:119:ASP:HB2	4:D:122:ASN:OD1	2.20	0.42
4:D:199:VAL:HG22	4:D:200:SER:N	2.34	0.42
4:D:202:THR:C	4:D:205:GLN:HB2	2.38	0.42
1:A:7:ASN:HB3	1:A:8:TYR:CD2	2.54	0.42
1:A:35:LEU:HD12	1:A:183:LEU:HD23	2.00	0.42
1:A:239:PRO:HD2	2:B:26:TYR:CE2	2.55	0.42
3:C:7:PRO:O	3:C:110:THR:HG23	2.20	0.42
4:D:117:VAL:CG2	4:D:154:TYR:OH	2.68	0.42
1:A:291:MET:HE3	1:A:291:MET:HB3	1.75	0.42
4:D:120:LEU:O	4:D:122:ASN:N	2.53	0.42
1:A:43:ASP:C	1:A:43:ASP:OD2	2.58	0.42
4:D:11:LEU:HD22	4:D:21:LEU:HD21	2.01	0.42
1:A:153:ASP:C	1:A:153:ASP:OD1	2.57	0.42
1:A:195:SER:HB3	1:A:279:TRP:HH2	1.84	0.42
2:B:22:ILE:CD1	2:B:69:GLU:HG3	2.44	0.42
3:C:118:ILE:HD13	3:C:144:PHE:O	2.19	0.42
4:D:176:ASP:OD2	4:D:194:SER:CB	2.60	0.42
3:C:95:ARG:HB2	3:C:100:GLY:HA3	2.02	0.41
3:C:128:LEU:N	3:C:128:LEU:CD1	2.83	0.41
4:D:165:ASN:O	4:D:165:ASN:OD1	2.37	0.41
3:C:126:TYR:CZ	4:D:137:GLU:HB2	2.52	0.41
4:D:82:GLN:O	4:D:85:GLU:HB2	2.20	0.41
1:A:240:ASN:ND2	2:B:12:ARG:HD2	2.35	0.41
3:C:122:ASP:N	3:C:123:PRO:CD	2.84	0.41
3:C:126:TYR:N	3:C:126:TYR:HD2	2.16	0.41
1:A:88:MET:C	1:A:89:SER:OG	2.59	0.41
4:D:178:GLN:HA	4:D:179:PRO:HD3	1.74	0.41
2:B:41:LYS:O	2:B:42:ASN:C	2.57	0.41
3:C:80:THR:O	3:C:80:THR:OG1	2.30	0.41
4:D:30:ASP:HB3	4:D:96:LEU:HD11	1.91	0.41
4:D:199:VAL:HG21	4:D:203:PHE:CG	2.55	0.41
3:C:35:PHE:CD1	3:C:43:LEU:HB3	2.56	0.41
4:D:135:GLU:C	4:D:138:ILE:HD13	2.40	0.41
1:A:47:ILE:H	1:A:67:GLN:HE21	1.68	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.80	0.41
3:C:120:ASN:N	3:C:121:PRO:CD	2.83	0.41
3:C:128:LEU:CG	4:D:132:GLU:O	2.69	0.41
4:D:3:ILE:H	4:D:26:ASN:ND2	2.19	0.41
4:D:54:SER:C	4:D:55:THR:HG23	2.42	0.41
4:D:139:SER:O	4:D:142:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:TRP:H	1:A:232:THR:HG21	1.86	0.41
4:D:131:PHE:HE1	4:D:149:LEU:HG	1.82	0.41
4:D:81:ALA:HB1	4:D:116:VAL:HG21	2.03	0.40
4:D:100:ARG:HH11	4:D:100:ARG:HD2	1.75	0.40
1:A:39:ARG:HD3	2:B:53:ASP:OD2	2.21	0.40
1:A:135:THR:CG2	1:A:147:ILE:HD12	2.45	0.40
2:B:10:TYR:CD1	2:B:10:TYR:N	2.89	0.40
4:D:25:GLN:HE22	4:D:29:HIS:C	2.24	0.40
4:D:185:ALA:HB3	4:D:186:LEU:CA	2.50	0.40
1:A:82:GLN:O	1:A:86:LYS:HG3	2.22	0.40
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.57	0.40
1:A:168:CYS:N	1:A:169:PRO:CD	2.85	0.40
3:C:74:THR:HG22	3:C:75:LEU:N	2.36	0.40
4:D:96:LEU:N	4:D:96:LEU:HD12	2.37	0.40
1:A:10:PHE:O	1:A:103:GLY:CA	2.69	0.40
4:D:132:GLU:CB	4:D:133:PRO:CD	2.96	0.40
4:D:199:VAL:CG2	4:D:203:PHE:HB3	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:OG	1:A:283:HIS:NE2[6_424]	2.06	0.14

## 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	288/302 (95%)	284 (99%)	3 (1%)	1 (0%)	37	67
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
3	C	192/207 (93%)	181 (94%)	9 (5%)	2 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	237/245 (97%)	229 (97%)	5 (2%)	3 (1%)	10	32
All	All	814/853 (95%)	789 (97%)	19 (2%)	6 (1%)	19	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	SER
3	C	195	ASN
3	C	202	THR
4	D	121	LYS
4	D	222	GLU
4	D	59	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/264 (96%)	245 (97%)	8 (3%)	34	68
2	B	92/93 (99%)	92 (100%)	0	100	100
3	C	174/186 (94%)	165 (95%)	9 (5%)	19	50
4	D	207/211 (98%)	195 (94%)	12 (6%)	17	45
All	All	726/754 (96%)	697 (96%)	29 (4%)	27	60

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	88	MET
1	A	89	SER
1	A	104	CYS
1	A	106	MET
1	A	204	ARG
1	A	263	CYS
1	A	270	LEU

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Mol	Chain	Res	Type
3	C	125	VAL
3	C	126	TYR
3	C	129	ARG
3	C	149	ASN
3	C	166	LEU
3	C	189	CYS
3	C	198	ILE
3	C	201	ASP
3	C	203	PHE
4	D	19	LEU
4	D	44	ARG
4	D	68	ARG
4	D	118	GLU
4	D	120	LEU
4	D	148	CYS
4	D	174	CYS
4	D	183	GLN
4	D	211	PHE
4	D	213	CYS
4	D	214	GLN
4	D	226	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	110	ASN
1	A	117	HIS
1	A	186	GLN
1	A	229	GLN
1	A	273	GLN
1	A	283	HIS
1	A	295	HIS
2	B	29	GLN
2	B	31	HIS
2	B	38	GLN
2	B	84	HIS
3	C	30	ASN
3	C	149	ASN
4	D	6	GLN
4	D	165	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 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
5	NAG	E	1	5,1	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
5	NAG	E	2	5	14,14,15	0.65	0	17,19,21	0.89	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
5	NAG	E	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	O4-C4-C3	-2.90	103.53	110.38
5	E	1	NAG	C1-O5-C5	2.35	115.33	112.19

There are no chirality outliers.

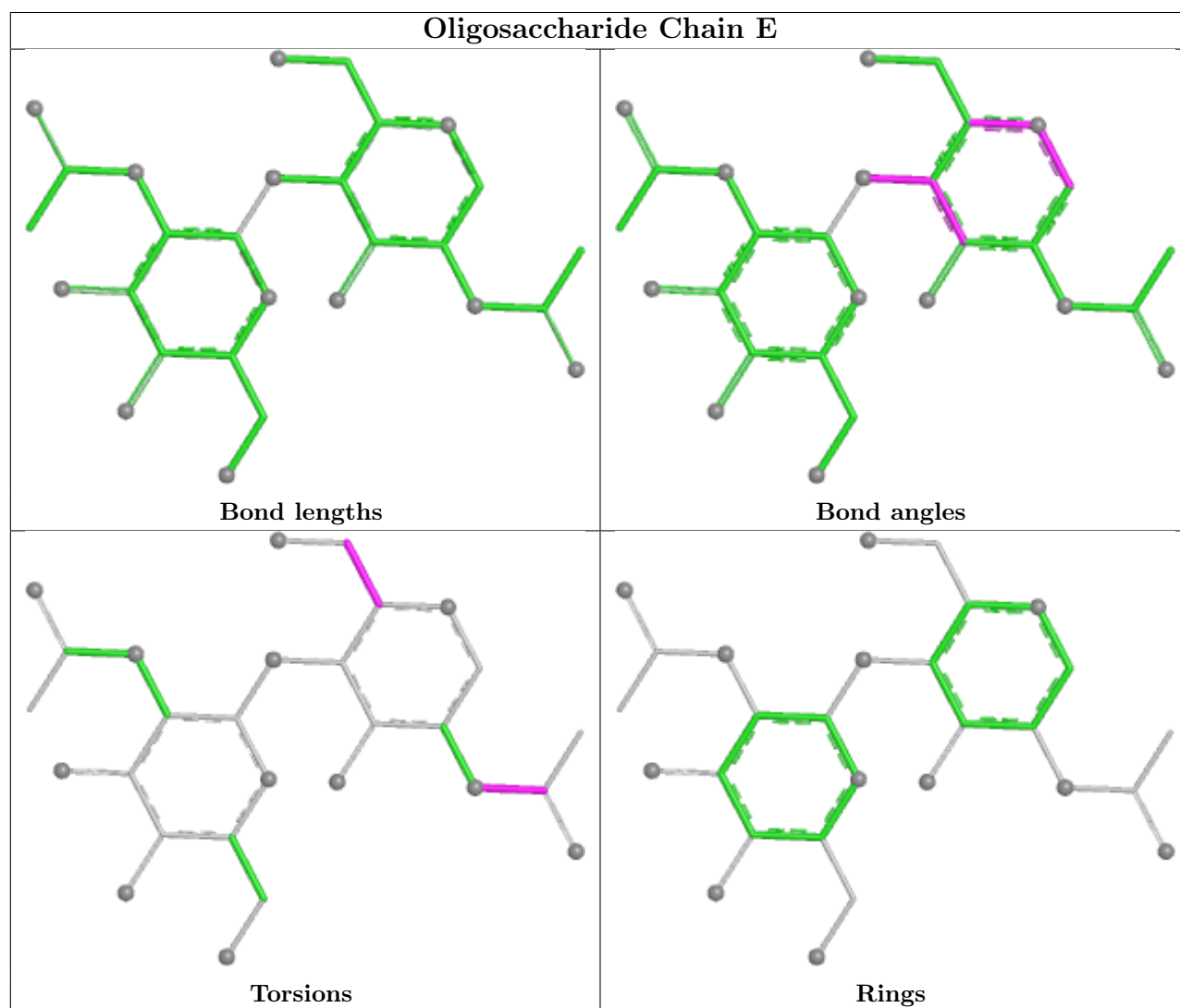
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

4 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	$\# Z  > 2$
6	NAG	A	303	1	14,14,15	0.48	0	17,19,21	0.91	0
7	GCY	A	601	-	56,57,57	2.28	12 (21%)	63,65,65	1.53	10 (15%)
8	GOL	B	100	-	5,5,5	0.52	0	5,5,5	0.64	0
6	NAG	A	304	1	14,14,15	0.53	0	17,19,21	1.35	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
6	NAG	A	303	1	-	0/6/23/26	0/1/1/1
7	GCY	A	601	-	-	28/53/73/73	0/1/1/1
8	GOL	B	100	-	-	0/4/4/4	-
6	NAG	A	304	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	601	GCY	O1-C16	-10.28	1.25	1.43
7	A	601	GCY	CAX-CAW	-7.70	1.04	1.51
7	A	601	GCY	C16-C15	-6.24	1.40	1.50
7	A	601	GCY	CAQ-CAP	-3.18	1.35	1.51
7	A	601	GCY	O2-C19	3.09	1.45	1.40
7	A	601	GCY	CAN-CAM	-2.88	1.37	1.51
7	A	601	GCY	CAY-CAX	-2.77	1.30	1.50
7	A	601	GCY	C22-C20	2.70	1.58	1.53
7	A	601	GCY	O4-C20	2.42	1.50	1.44
7	A	601	GCY	CAT-CAS	-2.27	1.40	1.51
7	A	601	GCY	CAR-CAQ	-2.22	1.40	1.51
7	A	601	GCY	CAP-CAO	2.15	1.62	1.51

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	GCY	CAY-CAX-CAW	4.85	146.13	113.36
7	A	601	GCY	CAO-CAN-CAM	4.67	137.97	114.37
7	A	601	GCY	C18-C17-C16	-3.87	104.26	112.90
6	A	304	NAG	O5-C1-C2	-3.48	105.90	111.29
7	A	601	GCY	C13-C14-C15	-3.39	110.35	125.47
7	A	601	GCY	CAV-CAU-CAT	3.22	130.64	114.37
7	A	601	GCY	O4-C19-O2	3.05	117.25	110.04
7	A	601	GCY	C18-O2-C19	-2.94	107.49	113.80
7	A	601	GCY	C18-C17-N1	2.59	113.34	109.66
6	A	304	NAG	C4-C3-C2	-2.44	107.44	111.02
7	A	601	GCY	O1-C16-C17	2.34	114.01	107.85
7	A	601	GCY	C19-O4-C20	-2.15	109.52	113.72

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	GCY	O4-C19-O2-C18
7	A	601	GCY	C13-C14-C15-C16
7	A	601	GCY	C14-C15-C16-O1
7	A	601	GCY	C14-C15-C16-C17
7	A	601	GCY	C15-C16-C17-N1
7	A	601	GCY	C15-C16-C17-C18
7	A	601	GCY	O4-C20-C21-O3
7	A	601	GCY	C22-C20-C21-O3
7	A	601	GCY	C36-C19-O2-C18
7	A	601	GCY	CAL-CAM-CAN-CAO
7	A	601	GCY	C43-C44-CAJ-CAK
7	A	601	GCY	C4-C5-C6-C7
7	A	601	GCY	C3-C4-C5-C6
7	A	601	GCY	CAQ-CAR-CAS-CAT
7	A	601	GCY	C2-C3-C4-C5
7	A	601	GCY	C6-C7-C8-C9
7	A	601	GCY	C7-C8-C9-C10
7	A	601	GCY	C10-C11-C12-C13
7	A	601	GCY	CAO-CAP-CAQ-CAR
7	A	601	GCY	C11-C12-C13-C14
7	A	601	GCY	CAP-CAQ-CAR-CAS
7	A	601	GCY	C41-C42-C43-C44
7	A	601	GCY	O1-C16-C17-N1
7	A	601	GCY	O1-C16-C17-C18
7	A	601	GCY	CAR-CAS-CAT-CAU
7	A	601	GCY	C37-C38-C39-C40

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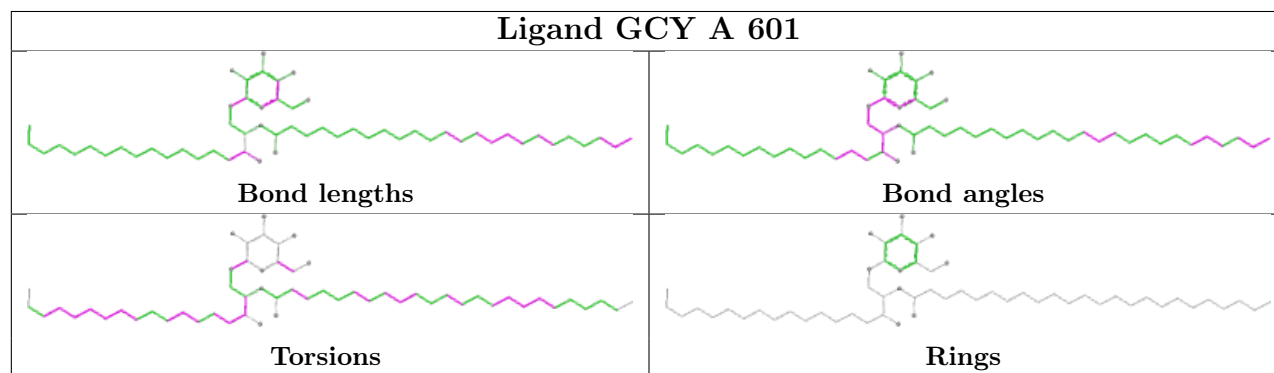
Mol	Chain	Res	Type	Atoms
7	A	601	GCY	C5-C6-C7-C8
7	A	601	GCY	C44-CAJ-CAK-CAL

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	GCY	9	0
8	B	100	GOL	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	290/302 (96%)	0.34	17 (5%)	29 22	39, 50, 62, 67	9 (3%)
2	B	99/99 (100%)	0.32	6 (6%)	28 21	42, 51, 60, 62	3 (3%)
3	C	196/207 (94%)	1.05	46 (23%)	2 3	38, 59, 113, 117	6 (3%)
4	D	239/245 (97%)	1.19	53 (22%)	3 3	38, 65, 85, 88	5 (2%)
All	All	824/853 (96%)	0.75	122 (14%)	7 6	38, 54, 97, 117	23 (2%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	202	THR	8.0
1	A	109	GLY	7.4
3	C	196	SER	6.8
4	D	213	CYS	6.8
3	C	197	ILE	5.8
4	D	1	GLY	5.7
4	D	191	TYR	5.2
1	A	104	CYS	5.2
4	D	119	ASP	5.1
4	D	186	LEU	4.7
1	A	107	TYR	4.6
3	C	140	LEU	4.5
3	C	191	ASN	4.5
4	D	146	LEU	4.5
4	D	228	GLN	4.5
3	C	188	ALA	4.4
4	D	120	LEU	4.4
4	D	240	ALA	4.4
4	D	226	TRP	4.4
4	D	23	CYS	4.3
3	C	204	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	51	MET	4.1
3	C	193	PHE	4.0
4	D	211	PHE	3.8
4	D	21	LEU	3.8
3	C	150	VAL	3.8
4	D	187	ASN	3.7
4	D	185	ALA	3.7
1	A	89	SER	3.7
3	C	180	ALA	3.7
3	C	189	CYS	3.5
3	C	199	PRO	3.5
3	C	201	ASP	3.5
3	C	195	ASN	3.5
2	B	70	PHE	3.4
3	C	132	LYS	3.4
4	D	53	GLY	3.3
1	A	205	GLN	3.3
3	C	6	SER	3.2
1	A	252	ASP	3.2
4	D	242	ALA	3.2
4	D	4	ILE	3.2
4	D	192	ALA	3.1
1	A	271	GLY	3.1
1	A	48	SER	3.1
4	D	200	SER	3.1
3	C	147	GLN	3.1
3	C	141	PHE	3.0
4	D	122	ASN	3.0
3	C	175	SER	3.0
4	D	241	GLU	3.0
1	A	142	TRP	3.0
3	C	139	CYS	3.0
3	C	154	LYS	3.0
3	C	203	PHE	3.0
4	D	25	GLN	3.0
4	D	207	PRO	3.0
4	D	96	LEU	3.0
4	D	188	ASP	3.0
4	D	180	LEU	3.0
1	A	88	MET	2.9
4	D	184	PRO	2.9
4	D	204	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	159	TYR	2.9
4	D	52	ALA	2.9
2	B	69	GLU	2.9
1	A	93	ASP	2.8
4	D	54	SER	2.8
4	D	148	CYS	2.8
3	C	119	GLN	2.7
3	C	5	GLN	2.6
3	C	198	ILE	2.6
1	A	103	GLY	2.6
3	C	145	ASP	2.6
3	C	123	PRO	2.6
3	C	182	SER	2.6
1	A	143	LEU	2.6
3	C	179	VAL	2.5
3	C	118	ILE	2.5
1	A	108	PRO	2.5
3	C	130	ASP	2.5
4	D	79	THR	2.5
3	C	133	SER	2.5
3	C	138	VAL	2.5
4	D	147	VAL	2.5
1	A	162	MET	2.5
3	C	171	MET	2.5
2	B	1	ILE	2.5
4	D	221	SER	2.4
3	C	158	VAL	2.4
4	D	201	ALA	2.4
1	A	263	CYS	2.4
4	D	230	ARG	2.4
4	D	82	GLN	2.4
4	D	190	ARG	2.4
3	C	190	ALA	2.4
4	D	174	CYS	2.4
3	C	85	THR	2.4
3	C	169	ARG	2.4
4	D	231	ALA	2.3
3	C	148	THR	2.3
3	C	194	ASN	2.3
4	D	24	GLN	2.3
4	D	58	GLY	2.3
4	D	69	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	59	SER	2.3
4	D	208	ARG	2.2
2	B	71	THR	2.2
4	D	145	THR	2.2
4	D	216	GLN	2.2
3	C	144	PHE	2.2
2	B	11	SER	2.2
3	C	200	GLU	2.1
4	D	239	SER	2.1
4	D	222	GLU	2.1
4	D	238	VAL	2.1
3	C	161	THR	2.1
3	C	153	SER	2.1
4	D	225	GLU	2.1
4	D	42	GLY	2.1
4	D	165	ASN	2.0
3	C	135	ASP	2.0

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

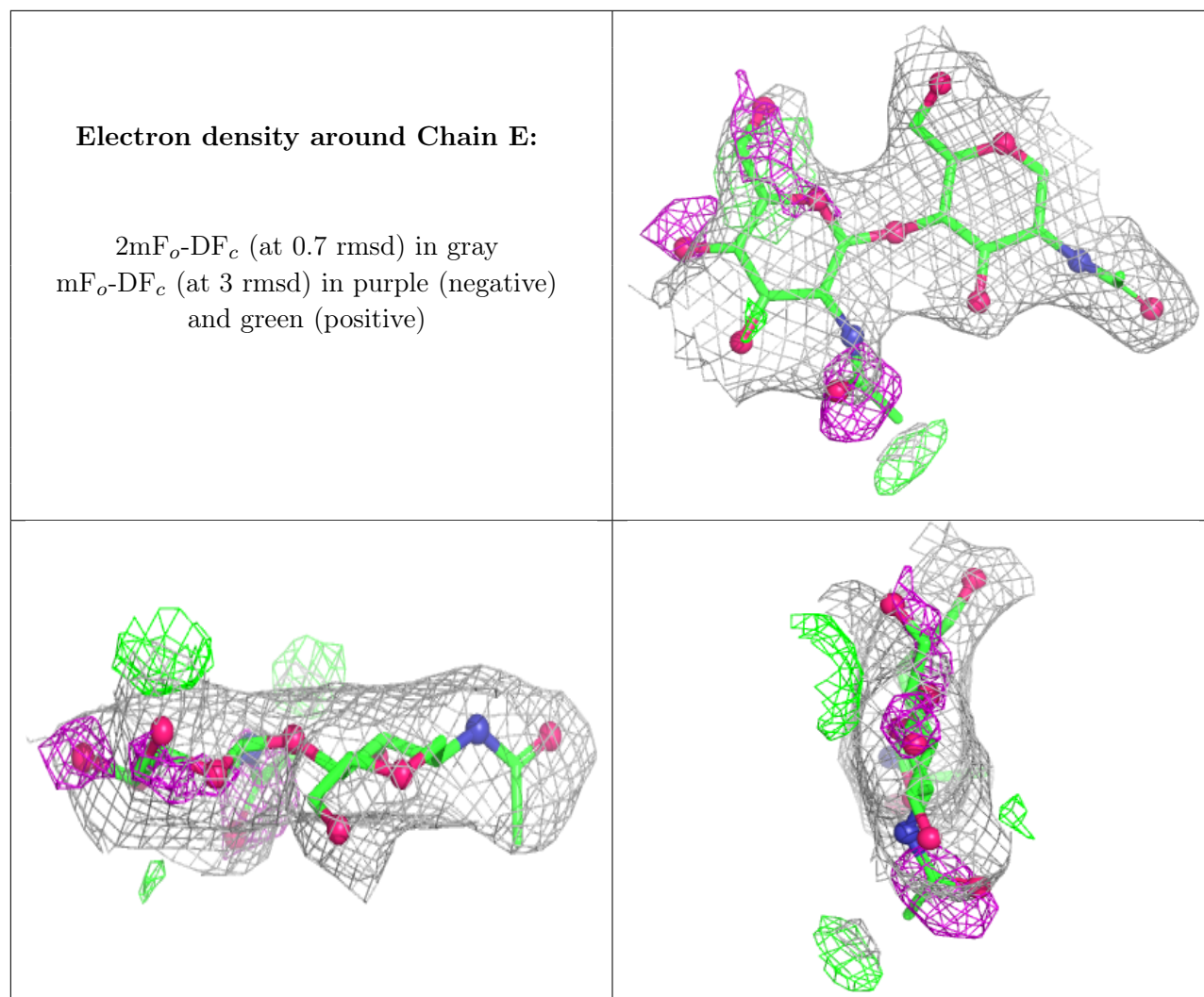
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	E	2	14/15	0.58	0.19	44,47,48,48	0
5	NAG	E	1	14/15	0.91	0.09	46,48,49,51	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.

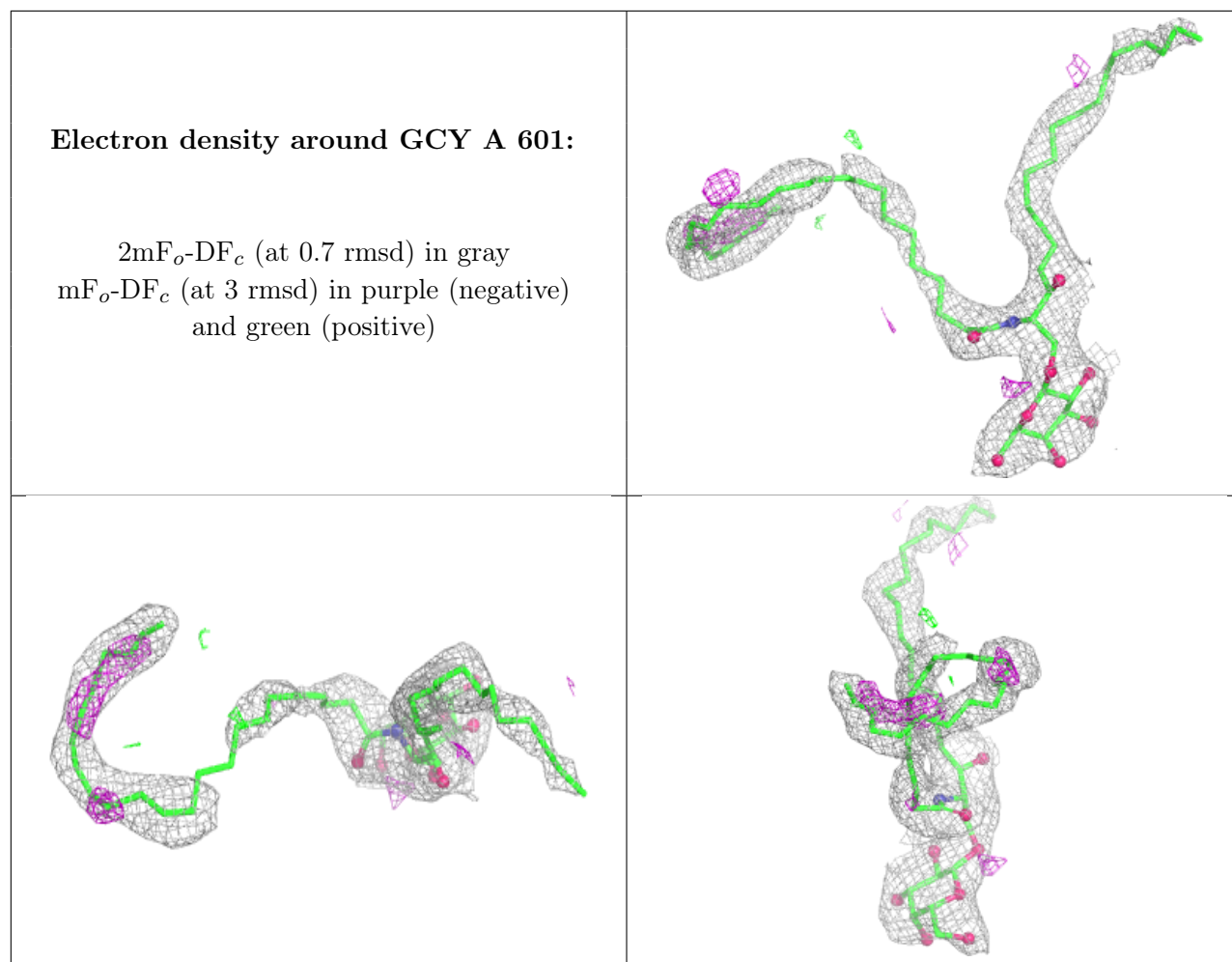


## 6.4 Ligands ⓘ

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	304	14/15	0.55	0.26	64,66,67,68	0
6	NAG	A	303	14/15	0.64	0.23	75,76,76,77	0
8	GOL	B	100	6/6	0.79	0.23	68,69,69,69	0
7	GCY	A	601	57/57	0.86	0.18	30,58,68,69	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.