



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:55 AM EDT

PDB ID : 2QEJ / pdb_00002qeJ
Title : Crystal structure of a Staphylococcus aureus protein (SSL7) in complex with Fc of human IgA1
Authors : Ramsland, P.A.; Willoughby, N.; Trist, H.M.; Farrugia, W.; Hogarth, P.M.; Fraser, J.D.; Wines, B.D.
Deposited on : 2007-06-26
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

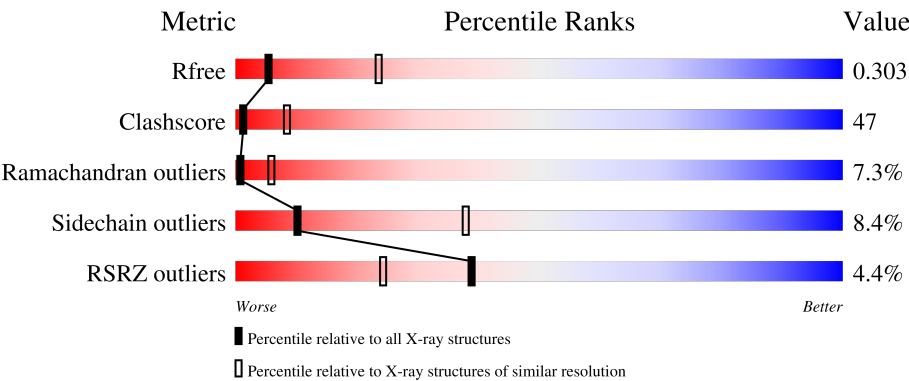
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	216	7% 35% 47% 13% • •
1	B	216	7% 35% 46% 15% • •
2	C	201	% 31% 54% 9% • 5%
2	D	201	% 31% 55% 7% • •
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	600	-	X	-	-
4	GOL	B	601	-	X	-	-
4	GOL	B	604	-	X	-	-
4	GOL	D	602	-	X	-	-
4	GOL	D	603	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6418 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 IG ALPHA-1 C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1613	1015	278	311	9			
1	B	209	Total	C	N	O	S	0	0	0
			1598	1007	276	306	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	expression tag	UNP P01876
A	241	SER	-	expression tag	UNP P01876
B	240	GLU	-	expression tag	UNP P01876
B	241	SER	-	expression tag	UNP P01876

- Molecule 2 is a protein called SUPERANTIGEN-LIKE MOLECULE 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	191	Total	C	N	O	S	0	0	0
			1534	966	264	303	1			
2	D	192	Total	C	N	O	S	0	0	0
			1542	972	265	304	1			

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		

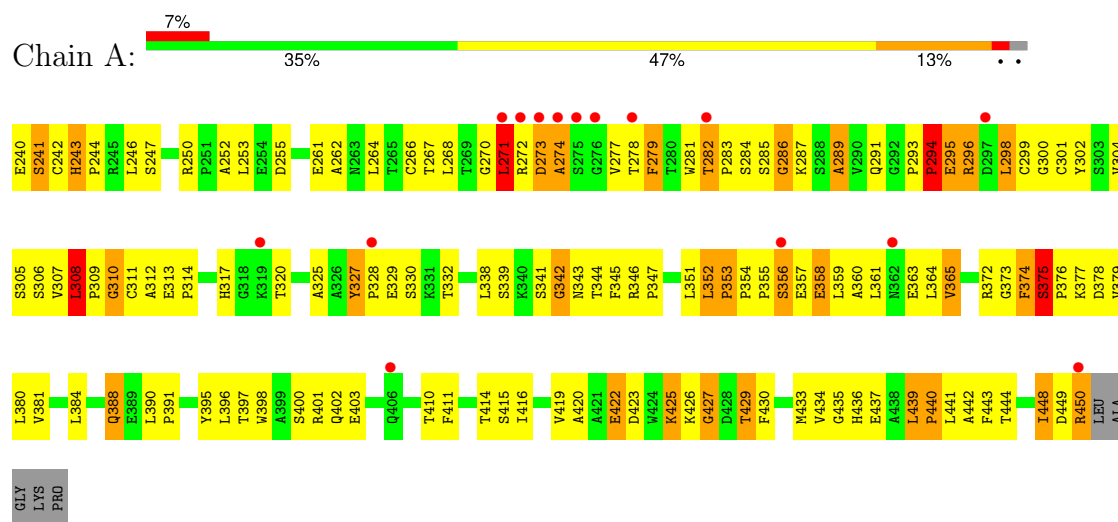
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total 14	O 14	0	0
6	B	11	Total 11	O 11	0	0
6	C	9	Total 9	O 9	0	0
6	D	9	Total 9	O 9	0	0
6	E	1	Total 1	O 1	0	0

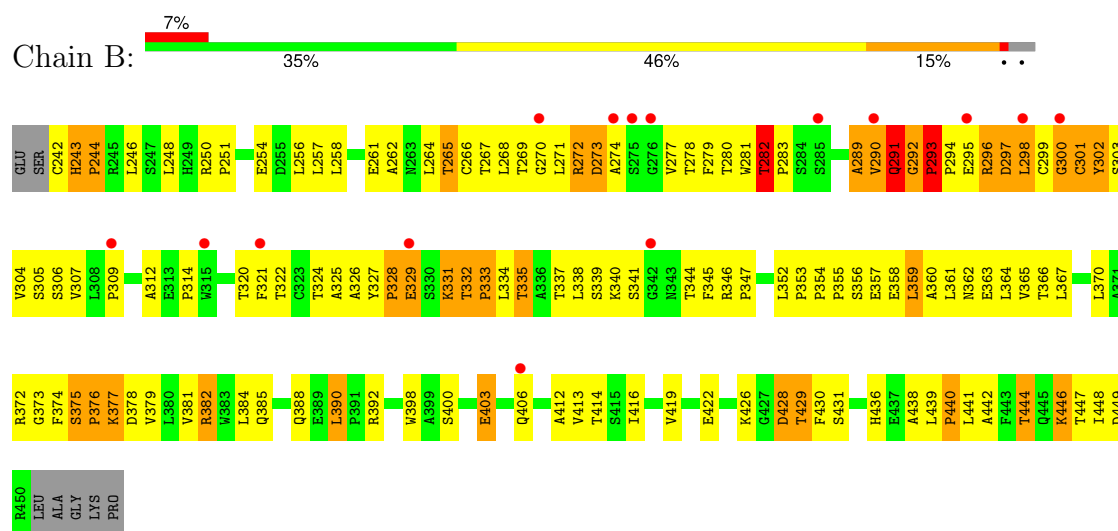
3 Residue-property plots

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: IG ALPHA-1 C REGION

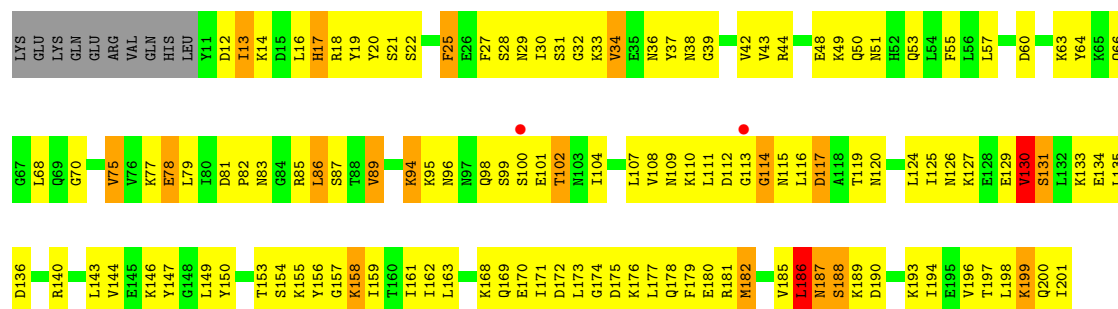


• Molecule 1: IG ALPHA-1 C REGION

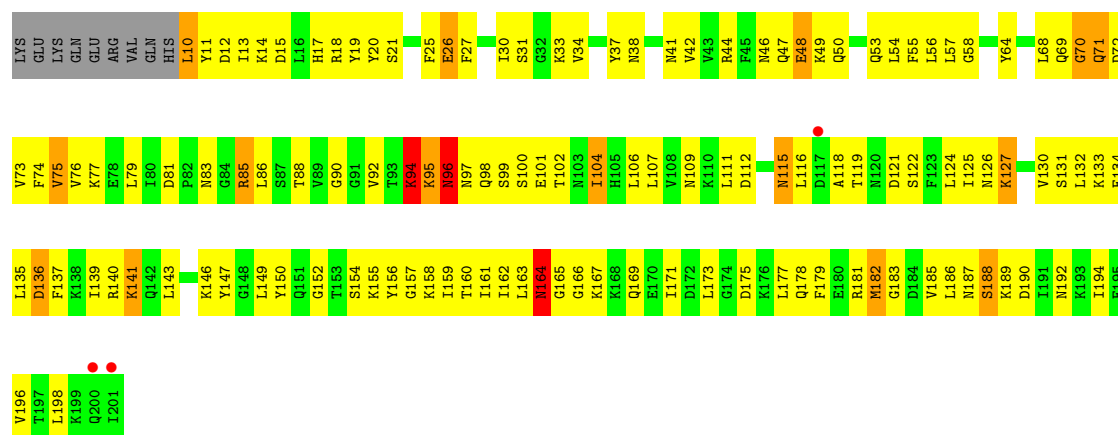


• Molecule 2: SUPERANTIGEN-LIKE MOLECULE 7





• Molecule 2: SUPERANTIGEN-LIKE MOLECULE 7



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



• Molecule 3: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.31Å 109.26Å 170.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.82 – 3.20 30.82 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.82-3.20) 92.5 (30.82-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 3.18Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.312 0.219 , 0.303	Depositor DCC
R_{free} test set	2220 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6418	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	0/1654	1.20	20/2258 (0.9%)
1	B	0.50	0/1639	1.05	13/2238 (0.6%)
2	C	0.51	0/1553	1.01	9/2078 (0.4%)
2	D	0.47	0/1561	0.95	4/2089 (0.2%)
All	All	0.51	0/6407	1.06	46/8663 (0.5%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	PRO	CA-C-N	8.70	126.01	119.66
1	A	353	PRO	C-N-CA	8.70	126.01	119.66
2	C	78	GLU	N-CA-C	-8.36	101.41	111.69
1	A	308	LEU	CA-C-N	8.28	128.33	119.89
1	A	308	LEU	C-N-CA	8.28	128.33	119.89
1	B	272	ARG	N-CA-C	-8.00	103.66	113.41
2	D	96	ASN	N-CA-C	-7.80	102.59	113.20
1	B	292	GLY	CA-C-N	6.97	127.56	120.38
1	B	292	GLY	C-N-CA	6.97	127.56	120.38
1	A	375	SER	CA-C-N	-6.85	113.45	120.85
1	A	375	SER	C-N-CA	-6.85	113.45	120.85
1	A	374	PHE	N-CA-C	6.84	120.83	109.95
2	C	17	HIS	N-CA-C	-6.76	103.60	110.97
2	D	58	GLY	N-CA-C	6.52	119.47	111.45
1	A	342	GLY	N-CA-C	-6.41	100.43	112.10
1	B	298	LEU	N-CA-C	-6.31	106.00	113.38
1	B	297	ASP	N-CA-C	-6.27	104.72	113.37
1	A	427	GLY	N-CA-C	6.26	123.34	115.21
1	B	444	THR	N-CA-C	-6.21	100.52	110.14
1	B	293	PRO	N-CA-C	6.19	118.25	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	SER	N-CA-C	6.01	118.72	110.24
1	A	352	LEU	CA-C-N	5.89	126.44	120.38
1	A	352	LEU	C-N-CA	5.89	126.44	120.38
1	A	243	HIS	CA-C-N	5.80	125.81	119.89
1	A	243	HIS	C-N-CA	5.80	125.81	119.89
2	C	130	VAL	N-CA-C	5.79	118.18	109.20
2	C	126	ASN	N-CA-C	5.73	118.30	111.71
1	A	439	LEU	CA-C-N	5.57	126.80	119.84
1	A	439	LEU	C-N-CA	5.57	126.80	119.84
1	B	390	LEU	CA-C-N	5.53	125.47	119.78
1	B	390	LEU	C-N-CA	5.53	125.47	119.78
1	B	429	THR	N-CA-C	5.46	117.57	110.53
2	C	186	LEU	N-CA-C	-5.40	101.55	109.81
1	A	395	TYR	N-CA-C	5.39	116.33	108.14
2	C	89	VAL	N-CA-C	5.38	115.61	107.75
2	C	189	LYS	N-CA-C	5.38	119.34	112.34
2	C	96	ASN	N-CA-C	-5.24	104.01	111.24
1	A	429	THR	N-CA-C	5.20	117.76	109.81
2	D	118	ALA	N-CA-C	5.16	117.18	110.53
1	B	265	THR	N-CA-C	5.14	117.45	108.76
1	B	335	THR	N-CA-C	5.09	116.46	107.61
2	D	94	LYS	N-CA-C	5.07	121.60	110.80
1	B	244	PRO	N-CA-C	5.07	118.45	110.80
1	A	298	LEU	N-CA-C	-5.05	103.82	110.33
1	A	296	ARG	N-CA-C	5.03	116.59	108.34
2	C	114	GLY	N-CA-C	-5.01	108.20	115.27

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	1613	0	1585	171	0
1	B	1598	0	1573	158	0
2	C	1534	0	1544	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1542	0	1555	138	0
3	E	28	0	25	2	0
3	F	28	0	25	3	0
4	B	18	0	12	1	0
4	D	12	0	8	2	0
5	C	1	0	0	0	0
6	A	14	0	0	3	0
6	B	11	0	0	0	0
6	C	9	0	0	0	0
6	D	9	0	0	1	0
6	E	1	0	0	0	0
All	All	6418	0	6327	600	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 47.

All (600) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:HA	1:B:302:TYR:HB3	1.24	1.12
1:A:345:PHE:H	1:A:375:SER:HB2	1.14	1.11
1:B:353:PRO:HG3	1:B:448:ILE:HD11	1.38	1.04
1:A:277:VAL:HG11	1:A:328:PRO:HD3	1.41	0.99
1:B:290:VAL:HG12	1:B:291:GLN:H	1.27	0.99
2:D:101:GLU:HG3	2:D:124:LEU:HD11	1.46	0.98
1:A:240:GLU:N	1:A:243:HIS:HE1	1.62	0.97
1:B:278:THR:HB	1:B:326:ALA:HB3	1.44	0.97
2:C:199:LYS:HE3	2:C:201:ILE:HD13	1.46	0.97
1:A:308:LEU:HD22	1:A:311:CYS:SG	2.05	0.97
1:A:240:GLU:HG2	1:A:241:SER:H	1.30	0.96
2:C:157:GLY:HA3	2:C:173:LEU:HD12	1.47	0.96
1:B:268:LEU:HG	1:B:271:LEU:HD21	1.48	0.95
1:A:365:VAL:HG23	1:A:419:VAL:HG23	1.46	0.95
1:A:345:PHE:N	1:A:375:SER:HB2	1.87	0.89
2:C:187:ASN:HD22	2:C:187:ASN:H	1.23	0.86
2:D:166:GLY:O	2:D:167:LYS:HG2	1.75	0.86
1:B:429:THR:HG22	1:B:449:ASP:HB3	1.56	0.85
1:A:375:SER:HB3	1:A:376:PRO:HD3	1.58	0.85
1:A:375:SER:CB	1:A:376:PRO:HD3	2.07	0.84
1:B:282:THR:OG1	1:B:283:PRO:HD3	1.77	0.84
1:A:274:ALA:HB1	1:A:277:VAL:HG13	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:LEU:HD12	2:D:150:TYR:H	1.43	0.83
1:A:240:GLU:N	1:A:243:HIS:CE1	2.47	0.82
1:B:297:ASP:HB2	1:B:302:TYR:HA	1.60	0.82
1:A:360:ALA:O	1:A:361:LEU:HD12	1.80	0.81
1:A:420:ALA:HB1	1:A:422:GLU:HG2	1.62	0.81
1:B:293:PRO:HA	1:B:304:VAL:HG12	1.64	0.80
3:F:1:NAG:H61	3:F:2:NAG:HN2	1.47	0.79
2:D:133:LYS:HZ3	2:D:182:MET:HE2	1.48	0.79
2:D:187:ASN:HB2	2:D:190:ASP:OD2	1.83	0.78
2:D:44:ARG:HH11	2:D:44:ARG:HG3	1.49	0.78
1:A:416:ILE:HD11	1:B:370:LEU:HD21	1.65	0.78
1:B:375:SER:HB3	1:B:376:PRO:HD3	1.64	0.77
2:D:143:LEU:HD21	2:D:196:VAL:HG21	1.67	0.77
1:B:353:PRO:HG3	1:B:448:ILE:CD1	2.13	0.76
1:B:269:THR:HA	1:B:303:SER:CB	2.16	0.76
2:D:49:LYS:HE2	2:D:49:LYS:HA	1.68	0.76
1:B:441:LEU:N	1:B:441:LEU:HD12	2.01	0.75
2:C:107:LEU:HD13	2:C:120:ASN:ND2	2.02	0.75
3:F:1:NAG:H61	3:F:2:NAG:N2	2.01	0.74
1:A:359:LEU:HD12	1:A:360:ALA:N	2.02	0.74
1:B:295:GLU:HA	1:B:302:TYR:CB	2.12	0.74
2:C:13:ILE:HD11	2:C:155:LYS:HB2	1.68	0.74
2:D:171:ILE:HG12	2:D:181:ARG:NH2	2.03	0.74
1:B:385:GLN:HB2	1:B:390:LEU:HD21	1.70	0.74
2:D:95:LYS:C	2:D:97:ASN:H	1.93	0.74
2:C:116:LEU:HG	2:C:117:ASP:H	1.53	0.73
2:C:104:ILE:HD13	2:C:194:ILE:HG12	1.68	0.73
2:C:187:ASN:HD22	2:C:187:ASN:N	1.84	0.73
2:D:116:LEU:O	2:D:116:LEU:HD23	1.88	0.73
2:D:158:LYS:N	2:D:173:LEU:HD12	2.04	0.73
1:A:282:THR:OG1	1:A:283:PRO:HD3	1.89	0.73
1:B:419:VAL:HG21	1:B:430:PHE:CZ	2.23	0.73
1:A:365:VAL:CG2	1:A:419:VAL:HG23	2.19	0.73
1:B:290:VAL:HG12	1:B:291:GLN:N	2.03	0.73
1:B:322:THR:HA	1:B:337:THR:HG22	1.70	0.73
1:B:440:PRO:HB2	1:B:441:LEU:HD12	1.71	0.72
2:D:169:GLN:NE2	2:D:186:LEU:HD11	2.04	0.72
1:A:422:GLU:CD	1:A:422:GLU:H	1.96	0.72
2:D:25:PHE:HB2	2:D:75:VAL:HG22	1.72	0.72
1:A:429:THR:HG22	1:A:449:ASP:HB3	1.71	0.71
2:D:21:SER:HA	2:D:141:LYS:HD2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:VAL:HG23	1:B:307:VAL:HG22	1.74	0.70
2:D:104:ILE:HD12	2:D:104:ILE:N	2.07	0.70
2:D:155:LYS:HD3	2:D:156:TYR:CE1	2.26	0.70
1:A:308:LEU:HD22	1:A:311:CYS:HG	1.55	0.70
1:B:374:PHE:HZ	1:B:413:VAL:HG23	1.56	0.70
2:D:161:ILE:HG13	2:D:194:ILE:HD12	1.74	0.70
1:A:375:SER:HB3	1:A:376:PRO:CD	2.21	0.70
2:C:86:LEU:HD12	2:C:86:LEU:C	2.17	0.69
2:C:158:LYS:HE2	2:C:170:GLU:CD	2.17	0.69
1:B:400:SER:HA	1:B:413:VAL:HG22	1.75	0.69
1:B:325:ALA:O	1:B:333:PRO:HB3	1.94	0.68
2:C:104:ILE:HD12	2:C:104:ILE:C	2.19	0.68
2:C:144:VAL:HA	2:C:149:LEU:H	1.59	0.67
1:A:365:VAL:HG23	1:A:419:VAL:CG2	2.22	0.67
1:A:360:ALA:C	1:A:361:LEU:HD12	2.20	0.67
2:C:89:VAL:HG11	2:C:179:PHE:HB3	1.77	0.67
2:C:110:LYS:HG2	2:C:200:GLN:NE2	2.10	0.67
2:D:11:TYR:C	2:D:13:ILE:H	2.03	0.67
1:B:268:LEU:O	1:B:303:SER:HB2	1.95	0.66
2:C:161:ILE:HG12	2:C:194:ILE:HD12	1.78	0.66
2:C:179:PHE:HA	2:C:182:MET:HG3	1.77	0.66
2:D:76:VAL:HG21	2:D:133:LYS:HZ2	1.60	0.66
1:A:375:SER:CB	1:A:376:PRO:CD	2.74	0.66
1:A:376:PRO:HD2	1:A:436:HIS:CE1	2.31	0.66
1:B:296:ARG:C	1:B:298:LEU:H	2.03	0.66
1:A:278:THR:HG22	1:A:279:PHE:H	1.59	0.65
2:C:81:ASP:OD2	2:C:82:PRO:HD2	1.96	0.65
1:B:361:LEU:HD12	1:B:363:GLU:H	1.61	0.65
1:A:279:PHE:HD2	1:A:325:ALA:HB2	1.62	0.65
1:B:321:PHE:O	1:B:337:THR:HB	1.97	0.65
2:C:116:LEU:O	2:C:117:ASP:HB2	1.97	0.64
1:A:281:TRP:CE3	1:A:308:LEU:HD12	2.32	0.64
2:C:25:PHE:HB2	2:C:75:VAL:HG22	1.78	0.64
2:C:33:LYS:O	2:C:34:VAL:HG12	1.98	0.64
1:B:392:ARG:HG2	1:B:392:ARG:HH21	1.60	0.64
1:A:296:ARG:HD2	1:A:300:GLY:HA2	1.79	0.64
2:C:50:GLN:HE21	2:C:51:ASN:N	1.95	0.64
1:B:264:LEU:HD23	1:B:265:THR:N	2.13	0.63
1:B:262:ALA:HB3	1:B:312:ALA:CB	2.28	0.63
1:A:433:MET:HE2	2:D:79:LEU:HD13	1.78	0.63
1:B:261:GLU:HG2	3:F:1:NAG:H5	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:THR:O	1:B:324:THR:HG22	1.97	0.63
2:D:44:ARG:HD3	2:D:53:GLN:HG3	1.80	0.63
1:A:375:SER:OG	1:A:376:PRO:HD3	1.98	0.63
2:D:161:ILE:HG13	2:D:194:ILE:CD1	2.29	0.63
1:A:327:TYR:H	1:A:327:TYR:HD2	1.47	0.63
2:D:126:ASN:HB2	2:D:127:LYS:NZ	2.14	0.63
2:C:108:VAL:HG11	2:C:147:TYR:CD2	2.34	0.63
2:C:110:LYS:HE2	2:C:200:GLN:NE2	2.14	0.63
1:A:353:PRO:HG3	1:A:448:ILE:HD11	1.79	0.62
1:A:439:LEU:HD13	1:A:444:THR:OG1	1.99	0.62
1:A:444:THR:HG23	4:D:602:GOL:O3	1.98	0.62
2:C:150:TYR:N	2:C:154:SER:O	2.33	0.62
1:A:372:ARG:HG2	1:A:373:GLY:N	2.14	0.62
1:A:240:GLU:N	6:A:502:HOH:O	2.31	0.62
2:D:98:GLN:HG3	2:D:99:SER:H	1.64	0.62
2:C:89:VAL:HG21	2:C:179:PHE:HD2	1.65	0.62
1:A:293:PRO:O	1:A:294:PRO:C	2.43	0.62
1:A:344:THR:HA	1:A:375:SER:OG	1.99	0.62
1:A:279:PHE:CD1	1:A:279:PHE:N	2.66	0.61
1:A:246:LEU:HD12	1:A:267:THR:O	2.00	0.61
2:D:101:GLU:HG3	2:D:124:LEU:CD1	2.27	0.61
2:D:164:ASN:HD22	2:D:192:ASN:HB2	1.64	0.61
1:A:267:THR:HG22	1:A:305:SER:HB3	1.82	0.61
1:B:244:PRO:HA	1:B:269:THR:O	2.01	0.61
1:A:359:LEU:HD12	1:A:360:ALA:H	1.66	0.61
1:A:267:THR:HG22	1:A:305:SER:CB	2.31	0.61
1:B:375:SER:O	1:B:377:LYS:N	2.34	0.61
2:C:120:ASN:N	2:C:120:ASN:HD22	1.98	0.61
2:D:94:LYS:O	2:D:95:LYS:HB3	2.00	0.61
2:D:133:LYS:NZ	2:D:182:MET:HE2	2.16	0.61
2:D:162:ILE:HG22	2:D:192:ASN:HB3	1.83	0.61
2:D:162:ILE:CG2	2:D:192:ASN:HB3	2.30	0.61
1:A:278:THR:HG22	1:A:279:PHE:N	2.15	0.61
1:A:271:LEU:HD22	1:A:272:ARG:N	2.16	0.60
1:B:297:ASP:CB	1:B:302:TYR:HA	2.29	0.60
1:A:279:PHE:CE1	1:A:306:SER:HB2	2.35	0.60
2:D:44:ARG:HG3	2:D:44:ARG:NH1	2.13	0.60
1:A:244:PRO:HA	1:A:270:GLY:H	1.66	0.60
1:A:262:ALA:HB3	1:A:312:ALA:HB2	1.82	0.60
1:A:376:PRO:HG2	1:A:437:GLU:OE1	2.00	0.60
1:B:322:THR:HA	1:B:337:THR:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ARG:CD	2:D:53:GLN:HG3	2.32	0.60
1:B:375:SER:CB	1:B:376:PRO:HD3	2.30	0.60
2:C:178:GLN:HE22	2:C:181:ARG:HH11	1.50	0.60
2:C:101:GLU:O	2:C:102:THR:HB	2.01	0.59
2:C:25:PHE:N	2:C:25:PHE:CD1	2.71	0.59
2:D:133:LYS:HZ3	2:D:182:MET:CE	2.14	0.59
1:B:376:PRO:O	1:B:377:LYS:C	2.45	0.59
1:A:402:GLN:HA	1:A:411:PHE:CD2	2.38	0.59
1:A:450:ARG:C	1:A:450:ARG:NE	2.61	0.59
1:B:300:GLY:O	1:B:301:CYS:HB3	2.02	0.59
2:D:136:ASP:HB2	2:D:171:ILE:HD13	1.85	0.58
1:A:246:LEU:HD11	1:A:266:CYS:SG	2.44	0.58
2:D:57:LEU:HD12	2:D:179:PHE:HB3	1.84	0.58
2:C:104:ILE:CD1	2:C:194:ILE:HG12	2.33	0.58
2:C:129:GLU:HG2	2:C:185:VAL:CG1	2.34	0.58
1:A:425:LYS:HE2	1:A:425:LYS:HA	1.85	0.58
1:B:354:PRO:HG3	1:B:367:LEU:HD23	1.86	0.58
1:B:269:THR:HA	1:B:303:SER:HB2	1.86	0.58
1:B:374:PHE:CZ	1:B:413:VAL:HG23	2.38	0.58
2:D:76:VAL:CG2	2:D:133:LYS:HZ2	2.16	0.58
1:A:441:LEU:O	1:A:442:ALA:HB3	2.03	0.58
1:B:273:ASP:CG	1:B:328:PRO:HG3	2.28	0.58
2:C:104:ILE:HD12	2:C:104:ILE:O	2.04	0.58
2:D:10:LEU:N	2:D:10:LEU:HD12	2.19	0.58
2:C:53:GLN:HG2	2:C:55:PHE:CE1	2.38	0.57
2:C:127:LYS:HG3	2:C:129:GLU:O	2.04	0.57
1:A:396:LEU:HB3	1:A:416:ILE:HG22	1.84	0.57
2:C:112:ASP:CG	2:C:113:GLY:N	2.60	0.57
2:C:178:GLN:NE2	2:C:181:ARG:HH11	2.02	0.57
1:B:294:PRO:HD2	1:B:303:SER:O	2.04	0.57
1:B:322:THR:HG22	1:B:337:THR:HG21	1.85	0.57
1:A:267:THR:C	1:A:268:LEU:HD12	2.29	0.57
1:B:331:LYS:O	1:B:332:THR:C	2.46	0.57
1:A:277:VAL:O	1:A:277:VAL:HG23	2.05	0.57
2:D:71:GLN:CD	2:D:71:GLN:H	2.13	0.57
1:B:291:GLN:HB3	1:B:293:PRO:HD3	1.87	0.57
2:D:100:SER:O	2:D:102:THR:HG23	2.05	0.57
2:D:79:LEU:HD12	2:D:79:LEU:C	2.29	0.57
1:A:338:LEU:HD12	1:A:339:SER:H	1.70	0.57
2:C:112:ASP:C	2:C:114:GLY:H	2.13	0.57
2:D:94:LYS:O	2:D:95:LYS:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLY:C	1:A:312:ALA:H	2.13	0.56
2:C:196:VAL:HG12	2:C:197:THR:N	2.17	0.56
1:B:441:LEU:N	1:B:441:LEU:CD1	2.69	0.56
2:C:178:GLN:HE22	2:C:181:ARG:NH1	2.03	0.56
2:D:95:LYS:C	2:D:97:ASN:N	2.60	0.56
2:C:157:GLY:O	2:C:158:LYS:HB2	2.04	0.56
1:A:271:LEU:HD13	1:A:271:LEU:C	2.31	0.56
1:B:361:LEU:HD12	1:B:361:LEU:C	2.31	0.56
2:C:144:VAL:HG22	2:C:149:LEU:HB3	1.88	0.56
1:A:282:THR:CB	1:A:283:PRO:HD3	2.35	0.55
1:B:244:PRO:HA	1:B:270:GLY:HA3	1.87	0.55
1:A:274:ALA:HB1	1:A:277:VAL:CG1	2.32	0.55
2:D:31:SER:HA	2:D:68:LEU:O	2.05	0.55
2:D:74:PHE:CE2	2:D:134:GLU:HA	2.41	0.55
2:D:161:ILE:C	2:D:162:ILE:HD12	2.31	0.55
2:D:163:LEU:O	2:D:164:ASN:C	2.50	0.55
1:B:344:THR:C	1:B:345:PHE:CD1	2.84	0.55
1:B:365:VAL:HG23	1:B:419:VAL:HG12	1.89	0.55
2:D:26:GLU:HG3	2:D:74:PHE:HD1	1.71	0.55
1:B:297:ASP:C	1:B:299:CYS:N	2.63	0.55
1:A:272:ARG:HD3	6:A:511:HOH:O	2.05	0.55
1:B:248:LEU:HD12	1:B:337:THR:HA	1.87	0.55
1:B:261:GLU:OE1	1:B:309:PRO:HB3	2.07	0.55
2:C:143:LEU:HD11	2:C:196:VAL:HG11	1.88	0.55
1:A:307:VAL:HG21	3:E:1:NAG:H82	1.89	0.55
2:D:72:ASP:O	2:D:92:VAL:HA	2.06	0.55
2:D:97:ASN:HD21	2:D:127:LYS:HB3	1.71	0.55
1:A:293:PRO:O	1:A:295:GLU:N	2.40	0.54
2:C:143:LEU:O	2:C:147:TYR:HB2	2.07	0.54
1:A:363:GLU:HG3	1:A:364:LEU:HD13	1.89	0.54
2:C:33:LYS:O	2:C:34:VAL:CB	2.56	0.54
1:A:240:GLU:HG2	1:A:241:SER:N	2.12	0.54
2:D:135:LEU:O	2:D:139:ILE:HG13	2.07	0.54
1:A:264:LEU:HD12	1:A:311:CYS:HB2	1.90	0.54
1:A:309:PRO:O	1:A:311:CYS:N	2.41	0.54
1:A:344:THR:O	1:A:345:PHE:CD2	2.61	0.54
1:A:346:ARG:NH2	6:A:509:HOH:O	2.41	0.54
2:D:130:VAL:HG11	2:D:135:LEU:HD21	1.90	0.54
1:B:347:PRO:HD2	1:B:439:LEU:HD21	1.90	0.54
1:B:357:GLU:HG3	2:D:11:TYR:CZ	2.43	0.53
2:C:120:ASN:HD22	2:C:120:ASN:H	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:140:ARG:NH1	2:C:150:TYR:OH	2.41	0.53
1:B:250:ARG:HH21	1:B:256:LEU:HD12	1.73	0.53
2:D:178:GLN:N	2:D:178:GLN:OE1	2.39	0.53
2:C:79:LEU:C	2:C:79:LEU:HD12	2.32	0.53
1:B:248:LEU:HD13	1:B:338:LEU:CD2	2.38	0.53
1:B:340:LYS:HG2	1:B:341:SER:N	2.24	0.53
1:B:361:LEU:HD12	1:B:363:GLU:N	2.22	0.53
2:C:94:LYS:HG2	2:C:129:GLU:OE1	2.07	0.53
2:C:169:GLN:NE2	2:C:186:LEU:HD11	2.24	0.53
2:D:106:LEU:HD11	2:D:196:VAL:HG23	1.91	0.53
2:C:159:ILE:HG13	2:C:173:LEU:HD21	1.90	0.53
1:A:289:ALA:HB1	1:A:306:SER:OG	2.09	0.53
1:A:296:ARG:HD3	1:A:302:TYR:CZ	2.43	0.53
1:A:298:LEU:HD12	1:A:299:CYS:H	1.73	0.53
1:A:327:TYR:N	1:A:327:TYR:CD2	2.77	0.53
1:B:281:TRP:O	1:B:282:THR:HG23	2.08	0.53
1:B:290:VAL:CG1	1:B:291:GLN:H	2.11	0.53
1:B:436:HIS:CD2	1:B:438:ALA:HB3	2.43	0.53
2:C:199:LYS:HG2	2:C:201:ILE:HG23	1.90	0.52
2:D:146:LYS:C	2:D:147:TYR:CD1	2.87	0.52
1:A:376:PRO:HD2	1:A:436:HIS:HE1	1.73	0.52
2:D:149:LEU:HD21	2:D:173:LEU:HD22	1.92	0.52
2:D:171:ILE:O	2:D:171:ILE:HG22	2.09	0.52
1:A:279:PHE:CD2	1:A:325:ALA:HB2	2.44	0.52
1:A:281:TRP:HZ2	1:A:306:SER:O	1.92	0.52
1:B:269:THR:HB	1:B:297:ASP:OD1	2.08	0.52
1:A:240:GLU:CA	1:A:243:HIS:CE1	2.92	0.52
1:B:242:CYS:O	1:B:243:HIS:HB2	2.09	0.52
1:B:267:THR:OG1	1:B:305:SER:HB3	2.09	0.52
1:B:320:THR:HA	1:B:339:SER:HB3	1.90	0.52
1:B:344:THR:C	1:B:345:PHE:HD1	2.18	0.52
2:C:37:TYR:HD2	2:C:38:ASN:N	2.07	0.52
1:A:291:GLN:OE1	1:A:304:VAL:HG11	2.09	0.52
1:B:440:PRO:HB2	1:B:441:LEU:CD1	2.38	0.52
2:C:81:ASP:C	2:C:83:ASN:H	2.17	0.52
1:A:416:ILE:HD11	1:B:370:LEU:CD2	2.38	0.52
2:C:187:ASN:N	2:C:187:ASN:ND2	2.50	0.52
1:B:398:TRP:CZ3	1:B:416:ILE:HG12	2.44	0.52
1:A:271:LEU:HD22	1:A:272:ARG:H	1.75	0.51
2:D:13:ILE:HG23	2:D:14:LYS:N	2.26	0.51
1:A:351:LEU:HD23	1:A:448:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASP:C	1:B:299:CYS:H	2.16	0.51
1:B:376:PRO:O	1:B:378:ASP:N	2.43	0.51
2:D:185:VAL:C	2:D:186:LEU:HD22	2.36	0.51
1:A:347:PRO:HD2	1:A:439:LEU:HG	1.93	0.51
2:C:119:THR:O	2:C:119:THR:HG22	2.09	0.51
1:A:377:LYS:HE3	1:A:400:SER:HB3	1.93	0.51
2:C:86:LEU:HD12	2:C:87:SER:N	2.25	0.51
2:C:94:LYS:NZ	2:C:95:LYS:O	2.43	0.51
1:B:278:THR:HB	1:B:326:ALA:CB	2.30	0.51
2:D:64:TYR:CD2	2:D:68:LEU:HD23	2.45	0.51
1:B:248:LEU:HD13	1:B:338:LEU:HD22	1.92	0.51
2:C:109:ASN:HD22	2:C:116:LEU:HD11	1.76	0.51
2:C:130:VAL:O	2:C:185:VAL:HA	2.10	0.51
2:D:11:TYR:O	2:D:13:ILE:HG22	2.11	0.51
2:D:139:ILE:HG21	2:D:159:ILE:HD13	1.92	0.51
2:D:161:ILE:N	2:D:161:ILE:HD12	2.26	0.51
1:A:372:ARG:HG2	1:A:373:GLY:H	1.76	0.50
1:A:373:GLY:HA2	1:A:410:THR:HB	1.93	0.50
2:C:130:VAL:HG12	2:C:131:SER:N	2.27	0.50
1:A:372:ARG:HG3	1:A:403:GLU:OE2	2.12	0.50
2:C:14:LYS:O	2:C:18:ARG:HB2	2.11	0.50
2:D:131:SER:O	2:D:134:GLU:N	2.44	0.50
2:C:171:ILE:HD12	2:C:177:LEU:HD13	1.93	0.50
2:D:56:LEU:O	2:D:57:LEU:HD23	2.10	0.50
1:B:372:ARG:HH11	1:B:403:GLU:CD	2.20	0.50
2:C:107:LEU:HD13	2:C:120:ASN:HD21	1.74	0.50
1:B:358:GLU:HA	1:B:361:LEU:HG	1.92	0.50
1:A:272:ARG:HB2	1:A:273:ASP:OD1	2.11	0.50
2:D:131:SER:C	2:D:133:LYS:N	2.67	0.50
2:C:101:GLU:O	2:C:102:THR:CB	2.59	0.50
1:B:436:HIS:HD2	1:B:438:ALA:HB3	1.76	0.50
2:D:130:VAL:HG22	2:D:131:SER:N	2.26	0.50
2:C:36:ASN:HD21	2:C:39:GLY:C	2.20	0.49
2:D:107:LEU:HG	2:D:109:ASN:OD1	2.11	0.49
1:B:282:THR:CB	1:B:283:PRO:HD3	2.41	0.49
2:C:33:LYS:O	2:C:34:VAL:CG1	2.60	0.49
2:C:110:LYS:HE2	2:C:200:GLN:CD	2.37	0.49
1:B:375:SER:O	1:B:376:PRO:C	2.55	0.49
1:B:426:LYS:HD2	1:B:428:ASP:OD2	2.11	0.49
2:D:42:VAL:HG12	2:D:55:PHE:HA	1.94	0.49
1:A:252:ALA:O	1:A:253:LEU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PHE:CE1	1:A:411:PHE:HB2	2.48	0.49
2:C:77:LYS:HA	2:C:86:LEU:HD11	1.94	0.49
2:C:153:THR:CG2	2:C:153:THR:O	2.59	0.49
2:D:124:LEU:HD12	2:D:125:ILE:H	1.76	0.49
2:C:119:THR:O	2:C:120:ASN:C	2.56	0.49
1:A:357:GLU:HG2	1:A:358:GLU:N	2.27	0.49
1:A:374:PHE:CZ	1:A:379:VAL:HG11	2.47	0.49
1:B:279:PHE:CD1	1:B:306:SER:HB2	2.48	0.49
1:B:398:TRP:HZ3	1:B:416:ILE:HG12	1.78	0.49
1:A:287:LYS:HD3	1:A:309:PRO:HB2	1.94	0.49
2:C:149:LEU:HD12	2:C:150:TYR:H	1.76	0.49
2:D:164:ASN:ND2	2:D:192:ASN:HB2	2.27	0.49
1:A:313:GLU:HB3	1:A:314:PRO:HD3	1.94	0.49
1:A:347:PRO:HD2	1:A:439:LEU:HD21	1.95	0.49
2:C:86:LEU:C	2:C:86:LEU:CD1	2.86	0.49
2:C:143:LEU:HD13	2:C:198:LEU:HD21	1.95	0.49
2:D:126:ASN:HB2	2:D:127:LYS:HZ2	1.77	0.49
1:A:363:GLU:HG3	1:A:364:LEU:CD1	2.42	0.48
1:A:429:THR:HG22	1:A:449:ASP:CB	2.42	0.48
1:B:257:LEU:HD22	1:B:442:ALA:HB1	1.94	0.48
1:B:294:PRO:C	1:B:296:ARG:N	2.71	0.48
1:B:327:TYR:HB2	1:B:328:PRO:HD2	1.94	0.48
1:B:361:LEU:CD1	1:B:363:GLU:H	2.25	0.48
2:C:34:VAL:O	2:C:34:VAL:HG13	2.13	0.48
2:C:146:LYS:C	2:C:147:TYR:CD1	2.91	0.48
1:A:363:GLU:OE2	1:A:363:GLU:HA	2.13	0.48
2:C:161:ILE:O	2:C:168:LYS:HB2	2.14	0.48
1:A:384:LEU:HA	1:A:388:GLN:O	2.13	0.48
2:C:99:SER:O	2:C:100:SER:HB3	2.13	0.48
2:D:77:LYS:HG3	2:D:86:LEU:HG	1.96	0.48
1:B:296:ARG:C	1:B:298:LEU:N	2.67	0.48
1:B:372:ARG:HG2	1:B:373:GLY:N	2.28	0.48
2:C:127:LYS:NZ	2:C:134:GLU:OE1	2.43	0.48
2:D:157:GLY:C	2:D:173:LEU:HD12	2.37	0.48
1:A:240:GLU:CG	1:A:241:SER:H	2.06	0.48
1:A:272:ARG:N	1:A:272:ARG:HD3	2.29	0.48
1:B:327:TYR:HE2	1:B:334:LEU:HG	1.79	0.48
1:B:346:ARG:HH21	4:B:601:GOL:H11	1.78	0.48
2:D:11:TYR:C	2:D:13:ILE:N	2.71	0.48
2:D:17:HIS:O	2:D:18:ARG:C	2.56	0.48
1:A:250:ARG:HD3	1:A:378:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TYR:HB2	1:A:328:PRO:HD2	1.95	0.48
1:A:351:LEU:CD2	1:A:448:ILE:HB	2.44	0.48
1:B:251:PRO:HB2	1:B:256:LEU:HD21	1.96	0.48
1:B:297:ASP:OD2	1:B:299:CYS:HB2	2.14	0.48
1:B:375:SER:CB	1:B:376:PRO:CD	2.91	0.48
1:B:446:LYS:NZ	1:B:446:LYS:HB3	2.27	0.48
2:D:49:LYS:HE2	2:D:49:LYS:CA	2.42	0.48
2:D:149:LEU:CD1	2:D:150:TYR:H	2.23	0.48
1:A:419:VAL:HG11	1:A:430:PHE:CE2	2.49	0.48
2:D:181:ARG:HD2	6:D:517:HOH:O	2.14	0.48
2:C:112:ASP:CG	2:C:113:GLY:H	2.22	0.47
2:D:94:LYS:HE3	2:D:96:ASN:ND2	2.29	0.47
2:D:111:LEU:HD23	2:D:198:LEU:O	2.14	0.47
1:A:264:LEU:CD1	1:A:311:CYS:HB2	2.44	0.47
1:A:308:LEU:HD23	1:A:309:PRO:HD2	1.95	0.47
1:B:258:LEU:HD21	2:C:82:PRO:HG2	1.95	0.47
2:C:163:LEU:HD12	2:C:190:ASP:O	2.14	0.47
1:A:355:PRO:HD2	1:A:358:GLU:HB2	1.96	0.47
1:B:360:ALA:C	1:B:362:ASN:N	2.71	0.47
1:B:372:ARG:NH1	1:B:403:GLU:OE1	2.48	0.47
1:B:392:ARG:HH21	1:B:392:ARG:CG	2.27	0.47
2:D:19:TYR:C	2:D:21:SER:H	2.23	0.47
2:D:143:LEU:HD22	2:D:196:VAL:HG11	1.97	0.47
1:B:374:PHE:CE1	1:B:379:VAL:HG11	2.50	0.47
2:D:106:LEU:HD11	2:D:196:VAL:CG2	2.45	0.47
1:A:355:PRO:HG2	1:A:358:GLU:HG3	1.95	0.47
1:B:299:CYS:O	1:B:301:CYS:N	2.41	0.47
2:C:27:PHE:HB3	2:C:30:ILE:HD11	1.95	0.47
2:C:33:LYS:O	2:C:34:VAL:HB	2.14	0.47
1:A:401:ARG:O	1:A:411:PHE:HB3	2.14	0.47
2:D:169:GLN:HE22	2:D:186:LEU:HD11	1.75	0.47
1:A:381:VAL:HG11	1:A:415:SER:HB2	1.97	0.47
1:B:379:VAL:HG21	1:B:413:VAL:HG21	1.97	0.47
1:B:436:HIS:HB3	1:B:439:LEU:HG	1.97	0.47
2:C:32:GLY:HA3	2:C:43:VAL:HG13	1.97	0.47
2:C:179:PHE:HA	2:C:182:MET:CG	2.44	0.47
2:D:104:ILE:N	2:D:104:ILE:CD1	2.77	0.47
1:A:272:ARG:C	1:A:273:ASP:OD1	2.58	0.47
1:A:347:PRO:HD2	1:A:439:LEU:CG	2.45	0.47
1:A:347:PRO:HD3	1:A:436:HIS:CD2	2.49	0.47
1:B:361:LEU:HD13	1:B:363:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:ASP:O	2:C:14:LYS:N	2.48	0.47
2:C:77:LYS:HA	2:C:86:LEU:CD1	2.45	0.47
1:A:327:TYR:CD1	1:A:329:GLU:HB2	2.50	0.46
1:A:416:ILE:O	1:A:416:ILE:CG2	2.63	0.46
1:B:366:THR:CG2	1:B:416:ILE:HG23	2.45	0.46
1:B:385:GLN:HG3	1:B:430:PHE:CE2	2.50	0.46
2:D:133:LYS:HD2	2:D:182:MET:HE2	1.97	0.46
1:A:272:ARG:O	1:A:273:ASP:HB2	2.16	0.46
1:A:274:ALA:HB2	1:A:328:PRO:HG3	1.97	0.46
1:A:313:GLU:HG2	1:A:317:HIS:HD2	1.80	0.46
2:C:13:ILE:CD1	2:C:150:TYR:HA	2.45	0.46
2:C:20:TYR:CZ	2:C:140:ARG:HD2	2.51	0.46
1:A:253:LEU:HD22	1:A:378:ASP:O	2.16	0.46
1:B:347:PRO:HD2	1:B:439:LEU:CD2	2.45	0.46
2:D:37:TYR:O	2:D:38:ASN:C	2.58	0.46
1:A:380:LEU:O	1:A:434:VAL:HG13	2.16	0.46
1:A:279:PHE:H	1:A:279:PHE:HD1	1.58	0.46
1:A:416:ILE:O	1:A:416:ILE:HG23	2.13	0.46
1:B:364:LEU:HD23	1:B:419:VAL:C	2.41	0.46
2:D:30:ILE:O	2:D:70:GLY:HA2	2.15	0.46
2:C:16:LEU:HD13	2:C:150:TYR:CE1	2.51	0.46
2:D:116:LEU:O	2:D:116:LEU:CD2	2.62	0.46
2:D:143:LEU:CD2	2:D:196:VAL:HG11	2.45	0.46
2:D:181:ARG:C	2:D:183:GLY:H	2.23	0.46
1:B:248:LEU:HB3	1:B:338:LEU:HD22	1.98	0.46
1:B:357:GLU:HG3	2:D:11:TYR:OH	2.16	0.45
2:C:129:GLU:HG2	2:C:185:VAL:HG11	1.97	0.45
2:C:130:VAL:HG12	2:C:131:SER:H	1.81	0.45
2:C:178:GLN:CD	2:C:181:ARG:HH11	2.23	0.45
1:A:298:LEU:HG	1:A:299:CYS:N	2.31	0.45
1:B:406:GLN:N	1:B:406:GLN:OE1	2.49	0.45
2:D:26:GLU:HG2	2:D:127:LYS:HE2	1.97	0.45
1:A:294:PRO:O	1:A:295:GLU:O	2.34	0.45
1:A:310:GLY:O	1:A:312:ALA:N	2.48	0.45
1:B:294:PRO:C	1:B:296:ARG:H	2.24	0.45
2:C:78:GLU:O	2:C:79:LEU:HB3	2.17	0.45
2:C:162:ILE:HD12	2:C:193:LYS:HG3	1.98	0.45
2:D:149:LEU:HD12	2:D:154:SER:O	2.16	0.45
2:D:189:LYS:HG3	2:D:190:ASP:N	2.31	0.45
1:B:291:GLN:O	1:B:292:GLY:C	2.59	0.45
1:B:360:ALA:C	1:B:362:ASN:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:THR:HG23	1:B:416:ILE:HG23	1.98	0.45
2:D:15:ASP:HB3	4:D:603:GOL:H12	1.99	0.45
2:D:112:ASP:OD1	2:D:112:ASP:C	2.59	0.45
2:D:115:ASN:N	2:D:115:ASN:ND2	2.61	0.45
1:A:279:PHE:HE1	1:A:291:GLN:HG2	1.81	0.45
2:D:54:LEU:HA	2:D:88:THR:HG23	1.99	0.45
2:C:19:TYR:C	2:C:21:SER:H	2.25	0.45
2:D:164:ASN:O	2:D:166:GLY:N	2.50	0.45
1:B:328:PRO:O	1:B:329:GLU:C	2.59	0.45
2:C:187:ASN:O	2:C:188:SER:C	2.58	0.45
1:A:347:PRO:HD2	1:A:439:LEU:CD2	2.47	0.45
1:B:269:THR:HA	1:B:303:SER:HB3	1.94	0.45
2:C:50:GLN:NE2	2:C:51:ASN:N	2.65	0.45
2:D:10:LEU:N	2:D:155:LYS:HZ2	2.15	0.45
2:D:149:LEU:HD12	2:D:150:TYR:N	2.22	0.45
1:A:414:THR:HG23	1:B:398:TRP:CZ2	2.53	0.44
1:A:448:ILE:HG23	1:A:449:ASP:N	2.30	0.44
1:B:431:SER:OG	1:B:447:THR:HG23	2.17	0.44
1:B:293:PRO:CA	1:B:304:VAL:HG12	2.42	0.44
2:C:155:LYS:HD3	2:C:156:TYR:CE1	2.52	0.44
2:C:161:ILE:HG23	2:C:194:ILE:CD1	2.48	0.44
2:D:131:SER:O	2:D:132:LEU:C	2.61	0.44
1:A:425:LYS:C	1:A:427:GLY:H	2.25	0.44
2:C:89:VAL:HG21	2:C:179:PHE:CD2	2.48	0.44
2:C:124:LEU:HG	2:C:125:ILE:N	2.32	0.44
1:A:271:LEU:HD23	1:A:327:TYR:HD1	1.82	0.44
1:B:352:LEU:HA	1:B:353:PRO:HD3	1.78	0.44
2:C:37:TYR:C	2:C:37:TYR:CD2	2.96	0.44
1:A:307:VAL:CG2	3:E:1:NAG:H82	2.47	0.44
1:B:289:ALA:C	1:B:290:VAL:HG23	2.43	0.44
1:B:381:VAL:C	1:B:382:ARG:HG2	2.42	0.44
2:C:201:ILE:OXT	2:C:201:ILE:HG13	2.17	0.44
1:A:355:PRO:O	1:A:357:GLU:N	2.50	0.44
1:B:327:TYR:CE2	1:B:334:LEU:HG	2.53	0.44
2:C:12:ASP:O	2:C:13:ILE:C	2.60	0.44
2:C:198:LEU:O	2:C:200:GLN:N	2.51	0.44
2:C:199:LYS:NZ	2:C:201:ILE:HG21	2.32	0.44
2:D:44:ARG:NE	2:D:53:GLN:HG3	2.33	0.44
1:A:351:LEU:HG	1:A:448:ILE:HB	1.99	0.44
1:B:372:ARG:HG3	1:B:412:ALA:HB2	1.99	0.44
2:D:10:LEU:N	2:D:156:TYR:HH	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ASP:OD2	2:D:85:ARG:HD3	2.17	0.44
2:D:133:LYS:NZ	2:D:182:MET:CE	2.78	0.44
1:B:358:GLU:OE1	1:B:366:THR:N	2.50	0.44
2:C:37:TYR:CD1	2:C:44:ARG:NH2	2.86	0.44
2:C:135:LEU:HD12	2:C:135:LEU:HA	1.78	0.44
2:D:27:PHE:HB3	2:D:30:ILE:HD11	2.00	0.44
2:D:149:LEU:O	2:D:150:TYR:C	2.58	0.44
1:A:243:HIS:HA	1:A:244:PRO:HD2	1.83	0.44
1:A:307:VAL:O	1:A:309:PRO:HD3	2.17	0.44
1:A:355:PRO:C	1:A:357:GLU:N	2.76	0.44
1:A:388:GLN:HA	1:A:388:GLN:OE1	2.17	0.44
2:C:20:TYR:CE2	2:C:140:ARG:HD2	2.53	0.44
2:C:101:GLU:O	2:C:125:ILE:O	2.36	0.43
2:D:83:ASN:CB	2:D:85:ARG:HD2	2.47	0.43
1:B:314:PRO:HB2	1:B:321:PHE:HZ	1.82	0.43
2:D:71:GLN:HA	2:D:95:LYS:HB2	2.00	0.43
1:A:401:ARG:HA	1:A:401:ARG:HD3	1.72	0.43
2:D:77:LYS:HA	2:D:86:LEU:HD21	2.00	0.43
1:B:250:ARG:HH21	1:B:256:LEU:CD1	2.31	0.43
2:D:19:TYR:O	2:D:21:SER:N	2.51	0.43
2:C:111:LEU:N	2:C:111:LEU:CD1	2.81	0.43
1:A:434:VAL:HG12	1:A:435:GLY:N	2.34	0.43
1:B:246:LEU:HD12	1:B:267:THR:O	2.18	0.43
2:C:19:TYR:CD2	2:C:176:LYS:HE2	2.53	0.43
2:C:112:ASP:C	2:C:114:GLY:N	2.77	0.43
2:D:136:ASP:O	2:D:140:ARG:HG3	2.19	0.43
1:A:296:ARG:CD	1:A:300:GLY:HA2	2.48	0.43
1:B:359:LEU:HD13	1:B:359:LEU:HA	1.84	0.43
2:C:42:VAL:HG12	2:C:55:PHE:HA	2.01	0.43
2:C:64:TYR:C	2:C:66:GLN:H	2.27	0.43
2:D:48:GLU:C	2:D:50:GLN:H	2.27	0.43
2:D:121:ASP:OD1	2:D:122:SER:N	2.43	0.43
2:D:187:ASN:O	2:D:188:SER:C	2.60	0.43
1:A:246:LEU:HD12	1:A:247:SER:H	1.84	0.43
1:B:335:THR:O	1:B:335:THR:HG22	2.17	0.43
2:C:81:ASP:C	2:C:83:ASN:N	2.76	0.43
2:C:115:ASN:N	2:C:115:ASN:ND2	2.65	0.43
2:C:179:PHE:O	2:C:180:GLU:C	2.62	0.43
2:C:196:VAL:HG12	2:C:197:THR:H	1.84	0.43
2:D:133:LYS:CD	2:D:182:MET:HE2	2.49	0.43
1:A:423:ASP:OD1	1:A:426:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:HIS:O	2:C:18:ARG:C	2.61	0.43
1:A:344:THR:O	1:A:345:PHE:CG	2.72	0.42
1:A:433:MET:HA	1:A:444:THR:O	2.19	0.42
1:A:298:LEU:CD1	1:A:299:CYS:H	2.32	0.42
1:B:248:LEU:CD1	1:B:337:THR:HA	2.49	0.42
1:B:281:TRP:HA	1:B:322:THR:O	2.18	0.42
2:D:73:VAL:HG12	2:D:75:VAL:HG12	2.00	0.42
2:D:155:LYS:HD3	2:D:156:TYR:CZ	2.54	0.42
2:C:29:ASN:HA	2:C:70:GLY:O	2.19	0.42
2:C:37:TYR:HD2	2:C:37:TYR:C	2.26	0.42
2:C:153:THR:O	2:C:153:THR:HG22	2.18	0.42
1:A:282:THR:O	1:A:284:SER:N	2.52	0.42
1:A:330:SER:C	1:A:332:THR:N	2.77	0.42
2:C:159:ILE:HB	2:C:171:ILE:HB	2.00	0.42
2:D:163:LEU:HD11	2:D:186:LEU:HD12	2.00	0.42
1:A:351:LEU:C	1:A:352:LEU:HD23	2.44	0.42
1:A:398:TRP:CH2	1:B:414:THR:HG23	2.55	0.42
2:C:44:ARG:HE	2:C:85:ARG:NH1	2.17	0.42
2:D:177:LEU:HD11	2:D:181:ARG:HE	1.83	0.42
1:B:293:PRO:HG3	1:B:304:VAL:HG11	2.02	0.42
2:D:46:ASN:O	2:D:47:GLN:HG2	2.19	0.42
1:B:262:ALA:HB3	1:B:312:ALA:HB2	2.01	0.42
1:A:397:THR:HA	1:A:415:SER:HA	2.02	0.42
2:D:163:LEU:N	2:D:163:LEU:HD22	2.35	0.42
1:A:272:ARG:HB3	1:A:302:TYR:CD2	2.54	0.42
1:A:330:SER:C	1:A:332:THR:H	2.27	0.42
2:D:115:ASN:N	2:D:115:ASN:HD22	2.18	0.42
1:B:295:GLU:OE1	1:B:302:TYR:HD1	2.03	0.42
1:B:364:LEU:HD23	1:B:419:VAL:O	2.19	0.42
1:A:242:CYS:HB3	1:A:270:GLY:O	2.20	0.41
1:A:373:GLY:HA2	1:A:410:THR:CB	2.50	0.41
1:B:347:PRO:HG3	1:B:374:PHE:HB3	2.02	0.41
1:B:354:PRO:HG3	1:B:367:LEU:CD2	2.48	0.41
1:B:370:LEU:HD13	1:B:414:THR:HG22	2.02	0.41
2:C:28:SER:O	2:C:30:ILE:HD12	2.20	0.41
1:A:252:ALA:HB3	1:A:255:ASP:OD2	2.20	0.41
1:A:310:GLY:C	1:A:312:ALA:N	2.75	0.41
2:D:98:GLN:O	2:D:99:SER:OG	2.32	0.41
1:A:307:VAL:O	1:A:307:VAL:HG23	2.19	0.41
1:B:277:VAL:HG23	1:B:277:VAL:O	2.20	0.41
2:D:64:TYR:CE2	2:D:71:GLN:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ASN:HB3	2:D:85:ARG:HD2	2.02	0.41
2:D:94:LYS:HE2	2:D:96:ASN:O	2.19	0.41
2:C:131:SER:C	2:C:133:LYS:N	2.75	0.41
2:C:143:LEU:CD1	2:C:196:VAL:HG11	2.49	0.41
1:A:286:GLY:O	1:A:287:LYS:C	2.62	0.41
1:B:279:PHE:CG	1:B:306:SER:HB2	2.54	0.41
1:A:285:SER:O	1:A:287:LYS:N	2.54	0.41
1:A:354:PRO:HA	1:A:355:PRO:HD3	1.95	0.41
1:B:257:LEU:O	1:B:258:LEU:HD23	2.21	0.41
1:B:290:VAL:O	1:B:291:GLN:NE2	2.54	0.41
2:C:60:ASP:HA	2:C:63:LYS:HB3	2.03	0.41
2:C:196:VAL:CG1	2:C:197:THR:N	2.83	0.41
2:D:44:ARG:NH1	2:D:44:ARG:CG	2.82	0.41
1:A:390:LEU:HA	1:A:391:PRO:HD3	1.94	0.41
1:A:441:LEU:C	1:A:443:PHE:H	2.28	0.41
1:B:266:CYS:HB2	1:B:281:TRP:CH2	2.55	0.41
1:B:372:ARG:HG2	1:B:372:ARG:NH1	2.36	0.41
2:C:48:GLU:O	2:C:49:LYS:HB2	2.21	0.41
2:D:26:GLU:HG2	2:D:127:LYS:CE	2.51	0.41
2:D:71:GLN:CD	2:D:71:GLN:N	2.79	0.41
2:D:177:LEU:CD1	2:D:181:ARG:HE	2.34	0.41
1:A:244:PRO:HA	1:A:270:GLY:N	2.35	0.41
1:A:298:LEU:CG	1:A:299:CYS:N	2.84	0.41
1:B:345:PHE:CD1	1:B:345:PHE:N	2.89	0.41
1:B:416:ILE:HD13	1:B:416:ILE:HA	1.90	0.41
1:B:298:LEU:O	1:B:299:CYS:SG	2.79	0.40
1:B:392:ARG:CG	1:B:392:ARG:NH2	2.84	0.40
2:C:120:ASN:ND2	2:C:120:ASN:N	2.68	0.40
2:D:171:ILE:HA	2:D:181:ARG:HH22	1.86	0.40
1:B:295:GLU:C	1:B:297:ASP:H	2.28	0.40
1:B:302:TYR:HB2	1:B:303:SER:H	1.71	0.40
2:C:31:SER:HA	2:C:68:LEU:O	2.21	0.40
2:C:120:ASN:ND2	2:C:120:ASN:H	2.19	0.40
2:D:64:TYR:HE2	2:D:71:GLN:HG2	1.87	0.40
1:A:342:GLY:O	1:A:343:ASN:HB3	2.20	0.40
1:A:356:SER:O	1:A:359:LEU:HD11	2.21	0.40
1:B:344:THR:HA	1:B:375:SER:CB	2.52	0.40
1:A:359:LEU:C	1:A:361:LEU:H	2.30	0.40
1:B:281:TRP:CD1	1:B:281:TRP:N	2.90	0.40
1:B:355:PRO:O	1:B:356:SER:C	2.63	0.40
2:C:53:GLN:HG2	2:C:55:PHE:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:LYS:C	2:C:111:LEU:HD12	2.47	0.40
2:C:172:ASP:OD1	2:C:174:GLY:N	2.46	0.40
2:C:178:GLN:NE2	2:C:181:ARG:HD3	2.36	0.40
2:D:13:ILE:HG23	2:D:14:LYS:H	1.86	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	209/216 (97%)	170 (81%)	25 (12%)	14 (7%)	1	7
1	B	207/216 (96%)	155 (75%)	30 (14%)	22 (11%)	0	2
2	C	189/201 (94%)	138 (73%)	42 (22%)	9 (5%)	2	14
2	D	190/201 (94%)	144 (76%)	33 (17%)	13 (7%)	1	7
All	All	795/834 (95%)	607 (76%)	130 (16%)	58 (7%)	1	6

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	ALA
1	A	295	GLU
1	A	310	GLY
1	A	375	SER
1	B	273	ASP
1	B	289	ALA
1	B	293	PRO
1	B	301	CYS
1	B	302	TYR
1	B	328	PRO
1	B	329	GLU

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Mol	Chain	Res	Type
2	C	13	ILE
2	C	34	VAL
2	C	94	LYS
2	C	117	ASP
2	C	158	LYS
2	D	94	LYS
1	A	241	SER
1	B	274	ALA
1	B	282	THR
1	B	290	VAL
1	B	377	LYS
2	C	199	LYS
2	D	20	TYR
2	D	71	GLN
2	D	95	LYS
2	D	164	ASN
2	D	165	GLY
2	D	182	MET
1	A	271	LEU
1	A	294	PRO
1	A	356	SER
1	B	331	LYS
1	B	375	SER
1	B	376	PRO
2	C	22	SER
2	C	102	THR
2	C	188	SER
2	D	12	ASP
2	D	70	GLY
1	A	273	ASP
1	A	289	ALA
1	A	301	CYS
1	A	358	GLU
1	B	291	GLN
1	B	422	GLU
2	D	90	GLY
2	D	188	SER
1	B	296	ARG
1	B	440	PRO
2	D	137	PHE
1	B	243	HIS
1	B	300	GLY

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Mol	Chain	Res	Type
1	B	333	PRO
1	A	286	GLY
1	A	440	PRO
1	B	332	THR
2	D	152	GLY

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	181/184 (98%)	166 (92%)	15 (8%)	10	38
1	B	179/184 (97%)	166 (93%)	13 (7%)	13	43
2	C	172/182 (94%)	160 (93%)	12 (7%)	14	45
2	D	173/182 (95%)	154 (89%)	19 (11%)	6	26
All	All	705/732 (96%)	646 (92%)	59 (8%)	10	38

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLU
1	A	271	LEU
1	A	279	PHE
1	A	282	THR
1	A	294	PRO
1	A	308	LEU
1	A	320	THR
1	A	327	TYR
1	A	365	VAL
1	A	388	GLN
1	A	422	GLU
1	A	425	LYS
1	A	440	PRO
1	A	448	ILE
1	A	450	ARG
1	B	254	GLU

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Mol	Chain	Res	Type
1	B	272	ARG
1	B	282	THR
1	B	291	GLN
1	B	293	PRO
1	B	359	LEU
1	B	382	ARG
1	B	384	LEU
1	B	388	GLN
1	B	403	GLU
1	B	428	ASP
1	B	444	THR
1	B	446	LYS
2	C	25	PHE
2	C	57	LEU
2	C	75	VAL
2	C	86	LEU
2	C	98	GLN
2	C	130	VAL
2	C	131	SER
2	C	136	ASP
2	C	175	ASP
2	C	182	MET
2	C	186	LEU
2	C	187	ASN
2	D	10	LEU
2	D	26	GLU
2	D	33	LYS
2	D	34	VAL
2	D	41	ASN
2	D	48	GLU
2	D	69	GLN
2	D	75	VAL
2	D	85	ARG
2	D	96	ASN
2	D	104	ILE
2	D	115	ASN
2	D	119	THR
2	D	127	LYS
2	D	136	ASP
2	D	141	LYS
2	D	160	THR
2	D	164	ASN

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Mol	Chain	Res	Type
2	D	175	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	316	ASN
1	A	317	HIS
1	A	350	HIS
1	A	385	GLN
1	A	436	HIS
1	B	385	GLN
1	B	436	HIS
2	C	17	HIS
2	C	36	ASN
2	C	46	ASN
2	C	50	GLN
2	C	105	HIS
2	C	115	ASN
2	C	120	ASN
2	C	142	GLN
2	C	151	GLN
2	C	169	GLN
2	C	187	ASN
2	C	200	GLN
2	D	29	ASN
2	D	41	ASN
2	D	46	ASN
2	D	51	ASN
2	D	98	GLN
2	D	115	ASN
2	D	120	ASN
2	D	151	GLN
2	D	164	ASN
2	D	169	GLN
2	D	192	ASN
2	D	200	GLN

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 ⓘ

4 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	0.61	0	17,19,21	0.70	0
3	NAG	E	2	3	14,14,15	0.56	0	17,19,21	0.90	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.58	0	17,19,21	0.93	1 (5%)
3	NAG	F	2	3	14,14,15	0.59	0	17,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	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(°)
3	E	2	NAG	C2-N2-C7	-2.62	119.39	122.90
3	F	1	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

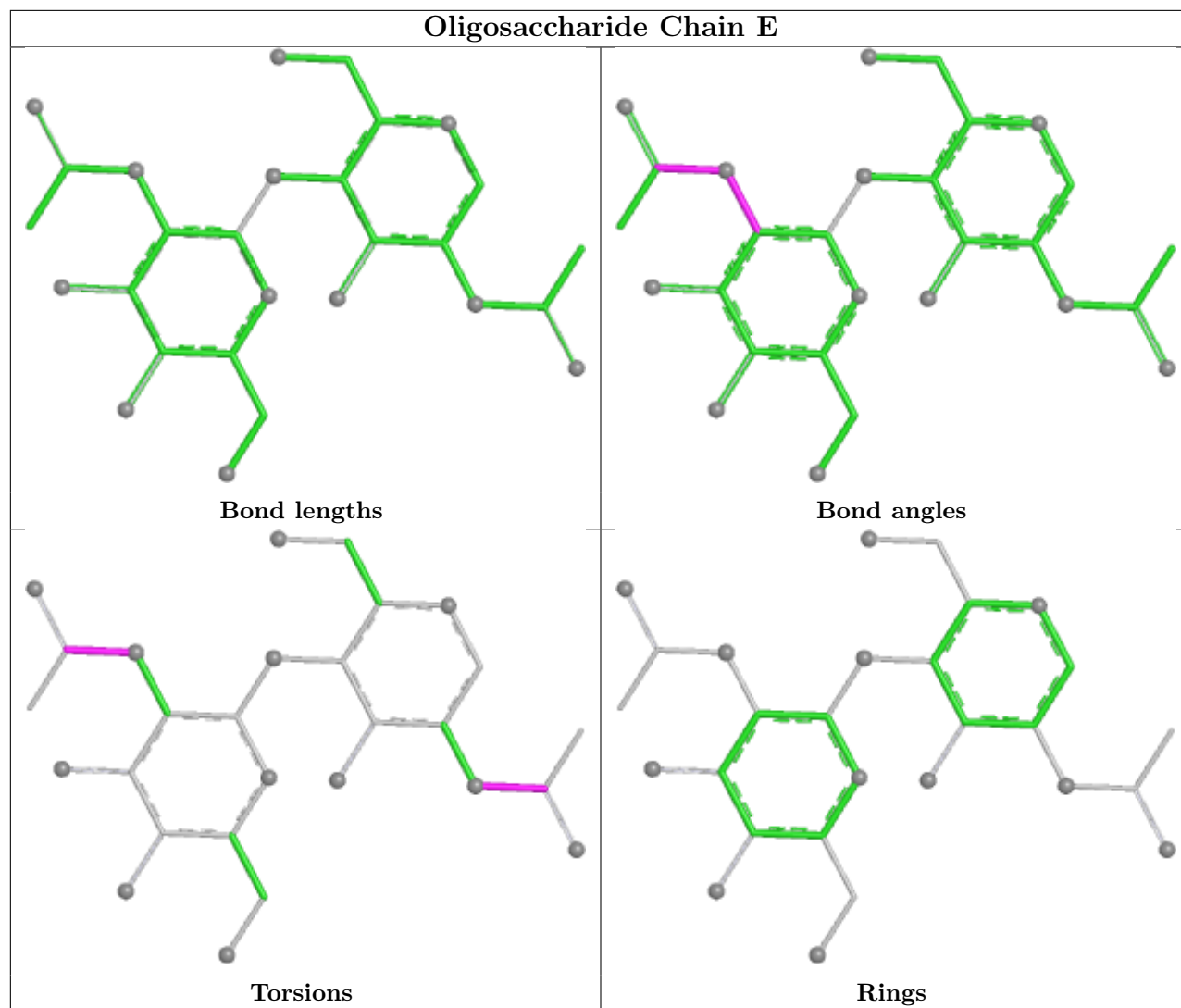
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O7-C7-N2-C2

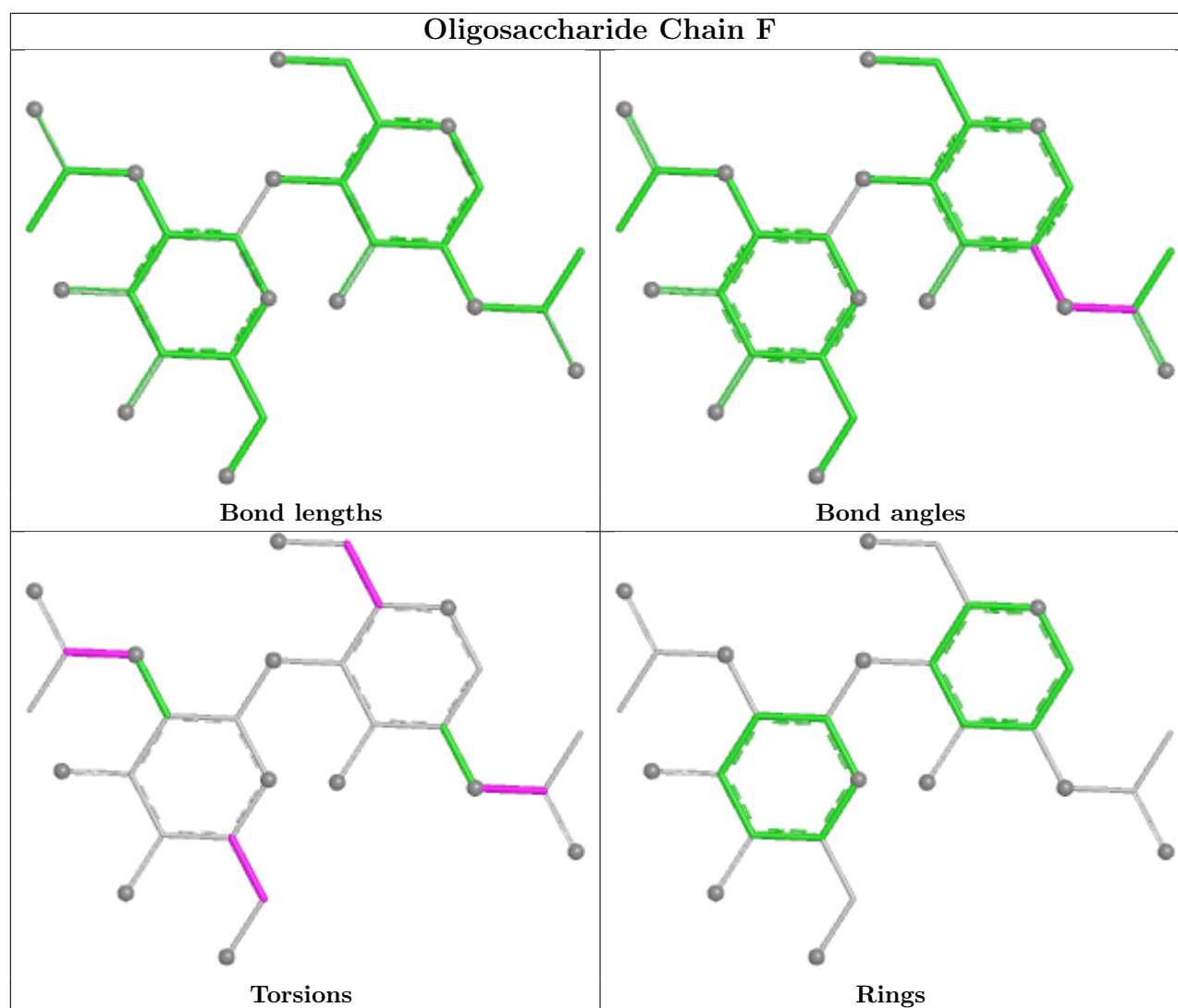
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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





5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	601	-	5,5,5	4.56	5 (100%)	5,5,5	4.61	3 (60%)
4	GOL	B	600	-	5,5,5	4.59	5 (100%)	5,5,5	4.62	3 (60%)
4	GOL	D	602	-	5,5,5	4.68	5 (100%)	5,5,5	4.62	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	604	-	5,5,5	4.69	5 (100%)	5,5,5	4.62	3 (60%)
4	GOL	D	603	-	5,5,5	4.66	5 (100%)	5,5,5	4.60	3 (60%)

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	GOL	B	601	-	-	2/4/4/4	-
4	GOL	B	600	-	-	3/4/4/4	-
4	GOL	D	602	-	-	2/4/4/4	-
4	GOL	B	604	-	-	2/4/4/4	-
4	GOL	D	603	-	-	3/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	GOL	C3-C2	-7.73	1.22	1.51
4	B	604	GOL	C3-C2	-7.68	1.22	1.51
4	D	603	GOL	C3-C2	-7.66	1.22	1.51
4	B	600	GOL	C3-C2	-7.44	1.23	1.51
4	B	601	GOL	C3-C2	-7.39	1.23	1.51
4	D	603	GOL	O1-C1	4.85	1.62	1.42
4	B	604	GOL	O1-C1	4.81	1.62	1.42
4	B	600	GOL	O1-C1	4.79	1.62	1.42
4	B	601	GOL	O1-C1	4.66	1.62	1.42
4	D	602	GOL	O1-C1	4.63	1.61	1.42
4	B	601	GOL	O3-C3	3.72	1.58	1.42
4	B	600	GOL	O3-C3	3.70	1.58	1.42
4	D	602	GOL	O3-C3	3.62	1.57	1.42
4	B	604	GOL	O3-C3	3.55	1.57	1.42
4	D	603	GOL	O3-C3	3.54	1.57	1.42
4	B	604	GOL	O2-C2	-2.87	1.35	1.43
4	D	602	GOL	O2-C2	-2.84	1.35	1.43
4	D	603	GOL	O2-C2	-2.73	1.35	1.43
4	D	602	GOL	C1-C2	-2.69	1.41	1.51
4	B	601	GOL	O2-C2	-2.65	1.35	1.43
4	B	604	GOL	C1-C2	-2.63	1.41	1.51
4	B	601	GOL	C1-C2	-2.61	1.41	1.51
4	B	600	GOL	C1-C2	-2.60	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	GOL	O2-C2	-2.53	1.36	1.43
4	D	603	GOL	C1-C2	-2.52	1.42	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	GOL	O3-C3-C2	7.31	143.29	110.38
4	B	600	GOL	O3-C3-C2	7.25	143.02	110.38
4	B	604	GOL	O3-C3-C2	7.21	142.83	110.38
4	D	603	GOL	O3-C3-C2	7.20	142.79	110.38
4	D	602	GOL	O3-C3-C2	7.14	142.50	110.38
4	D	602	GOL	O2-C2-C3	6.71	136.94	109.18
4	B	600	GOL	O2-C2-C3	6.63	136.65	109.18
4	B	604	GOL	O2-C2-C3	6.63	136.64	109.18
4	B	601	GOL	O2-C2-C3	6.62	136.58	109.18
4	D	603	GOL	O2-C2-C3	6.60	136.51	109.18
4	D	602	GOL	O1-C1-C2	2.88	123.36	110.38
4	B	604	GOL	O1-C1-C2	2.87	123.31	110.38
4	D	603	GOL	O1-C1-C2	2.85	123.21	110.38
4	B	600	GOL	O1-C1-C2	2.79	122.94	110.38
4	B	601	GOL	O1-C1-C2	2.65	122.33	110.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	GOL	O1-C1-C2-C3
4	B	600	GOL	C1-C2-C3-O3
4	B	601	GOL	C1-C2-C3-O3
4	B	604	GOL	C1-C2-C3-O3
4	D	602	GOL	O1-C1-C2-C3
4	D	602	GOL	C1-C2-C3-O3
4	D	603	GOL	C1-C2-C3-O3
4	D	603	GOL	O1-C1-C2-C3
4	B	600	GOL	O1-C1-C2-O2
4	B	601	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
4	D	603	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	GOL	1	0
4	D	602	GOL	1	0
4	D	603	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/216 (97%)	0.16	15 (7%) 22 14	1, 24, 83, 99	0
1	B	209/216 (96%)	0.43	15 (7%) 21 14	1, 44, 98, 99	0
2	C	191/201 (95%)	-0.17	2 (1%) 79 63	1, 20, 64, 99	0
2	D	192/201 (95%)	-0.06	3 (1%) 70 51	1, 27, 72, 89	0
All	All	803/834 (96%)	0.10	35 (4%) 39 24	1, 26, 86, 99	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	SER	4.8
1	B	274	ALA	4.8
1	A	278	THR	4.4
1	B	300	GLY	4.2
1	B	270	GLY	3.5
1	B	295	GLU	3.3
1	A	271	LEU	3.3
2	D	200	GLN	3.2
1	B	275	SER	3.0
1	A	276	GLY	3.0
1	A	356	SER	3.0
1	A	273	ASP	2.8
1	A	362	ASN	2.8
2	D	117	ASP	2.7
1	B	290	VAL	2.7
1	B	321	PHE	2.6
1	B	276	GLY	2.6
1	A	282	THR	2.6
1	B	285	SER	2.5
1	B	342	GLY	2.5
1	A	319	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	2.4
1	B	309	PRO	2.4
1	A	297	ASP	2.4
2	D	201	ILE	2.4
1	B	315	TRP	2.4
1	B	406	GLN	2.3
1	B	329	GLU	2.2
1	A	450	ARG	2.1
1	A	328	PRO	2.1
1	A	274	ALA	2.1
2	C	100	SER	2.0
1	A	272	ARG	2.0
1	A	406	GLN	2.0
2	C	113	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

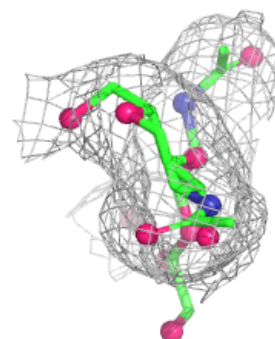
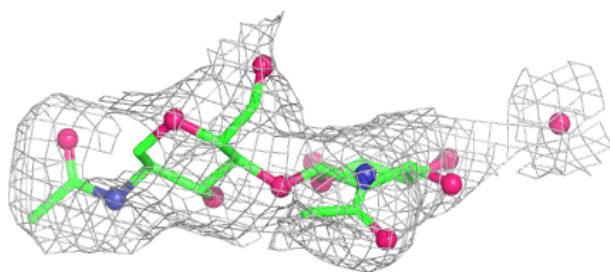
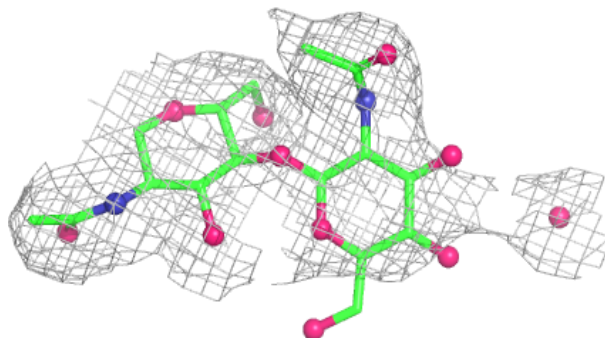
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

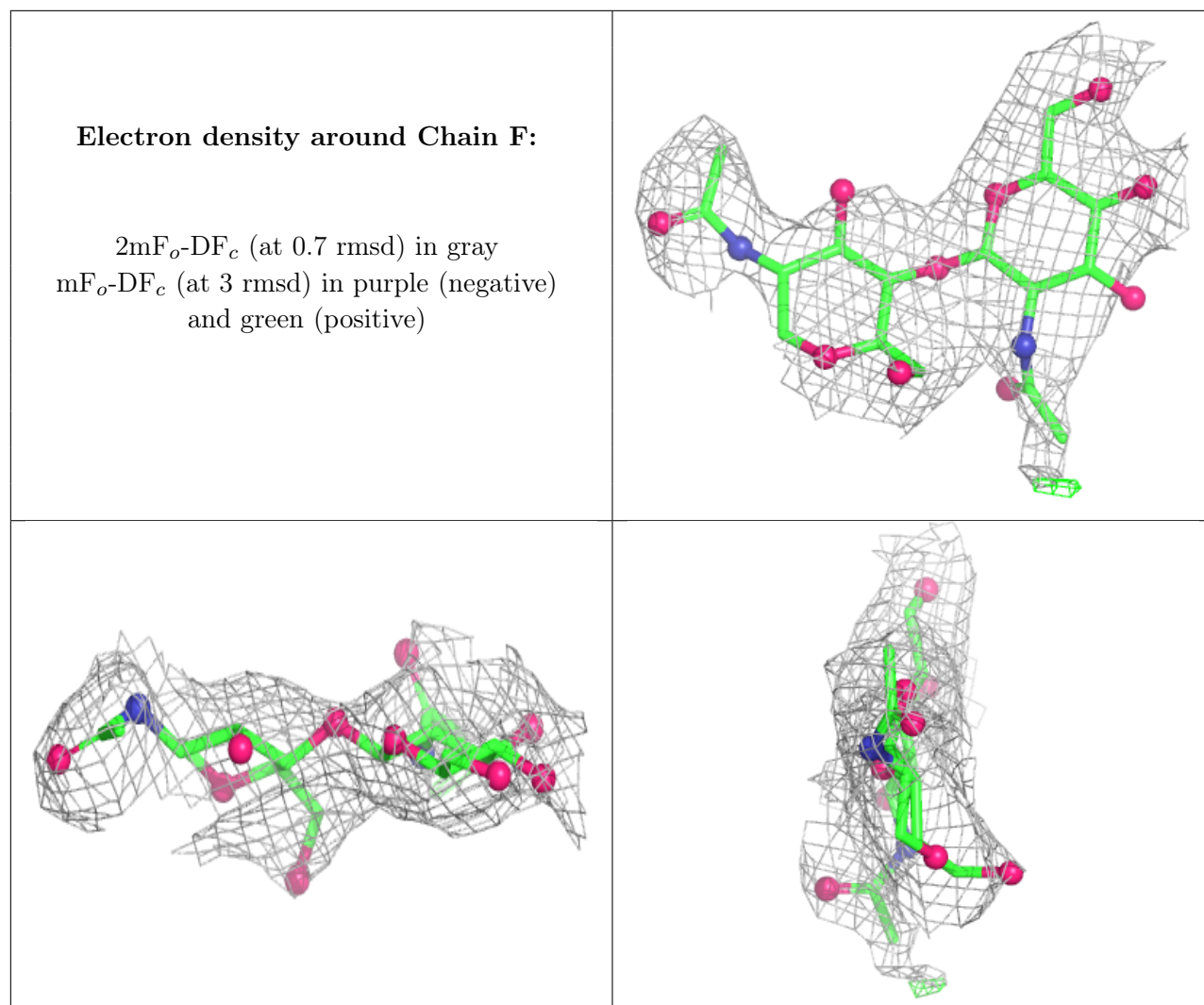
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.37	0.18	77,99,99,99	0
3	NAG	F	1	14/15	0.61	0.15	73,73,98,98	0
3	NAG	E	2	14/15	0.74	0.14	57,97,97,97	0
3	NAG	E	1	14/15	0.89	0.10	44,44,75,76	0

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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	D	603	6/6	0.79	0.19	43,46,47,51	0
4	GOL	D	602	6/6	0.80	0.20	43,46,47,51	0
4	GOL	B	601	6/6	0.80	0.11	43,46,47,51	0
4	GOL	B	600	6/6	0.83	0.16	43,46,47,51	0
4	GOL	B	604	6/6	0.86	0.16	34,37,38,43	0
5	CA	C	554	1/1	0.90	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.