Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 09:02 PM BST

PDB ID	:	3F8S
Title	:	Crystal structure of dipeptidyl peptidase IV in complex with inhibitor
Authors	:	Ammirati, M.J.; Liu, S.; Piotrowski, D.W.
Deposited on	:	2008-11-13
Resolution	:	2.43 Å(reported)

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

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

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.43 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	Percentile Ranks	Value
Rfree		0.290
Clashscore		14
Ramachandran outliers		1.1%
Sidechain outliers		8.7%
RSRZ outliers		6.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
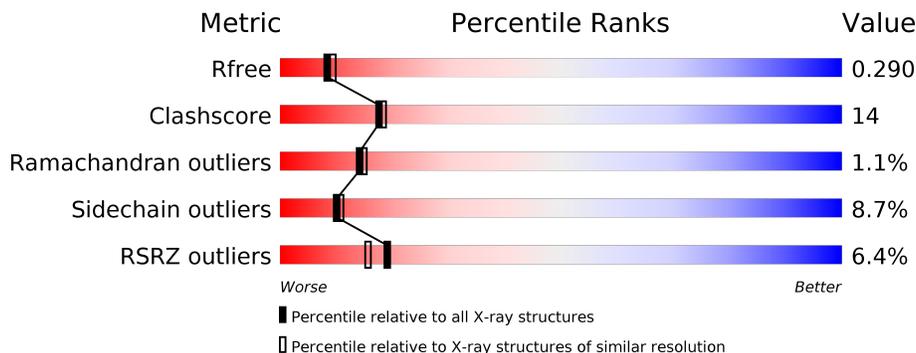
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	748	7% 66% 26% 5% · ·
1	B	748	6% 66% 27% · · ·
2	C	2	100%
2	D	2	100%
2	E	2	100%
2	F	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	799	X	-	-	-
4	PF2	B	900	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12132 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0
1	B	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	expression tag	UNP P27487
A	768	VAL	-	expression tag	UNP P27487
A	769	PRO	-	expression tag	UNP P27487
A	770	ARG	-	expression tag	UNP P27487
A	771	GLY	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	HIS	-	expression tag	UNP P27487
A	775	HIS	-	expression tag	UNP P27487
A	776	HIS	-	expression tag	UNP P27487
A	777	HIS	-	expression tag	UNP P27487
A	778	HIS	-	expression tag	UNP P27487
B	767	LEU	-	expression tag	UNP P27487
B	768	VAL	-	expression tag	UNP P27487
B	769	PRO	-	expression tag	UNP P27487
B	770	ARG	-	expression tag	UNP P27487
B	771	GLY	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	HIS	-	expression tag	UNP P27487
B	775	HIS	-	expression tag	UNP P27487
B	776	HIS	-	expression tag	UNP P27487
B	777	HIS	-	expression tag	UNP P27487
B	778	HIS	-	expression tag	UNP P27487

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
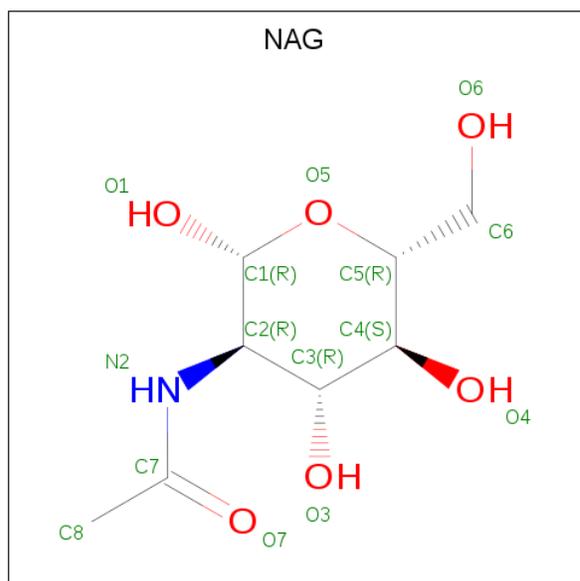
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-(4-{(3S,5S)-5-[(3,3-difluoropyrrolidin-1-yl)carbonyl]pyrrolidin-3-yl}piperazin

-1-yl)pyrimidine (three-letter code: PF2) (formula: $C_{17}H_{24}F_2N_6O$).
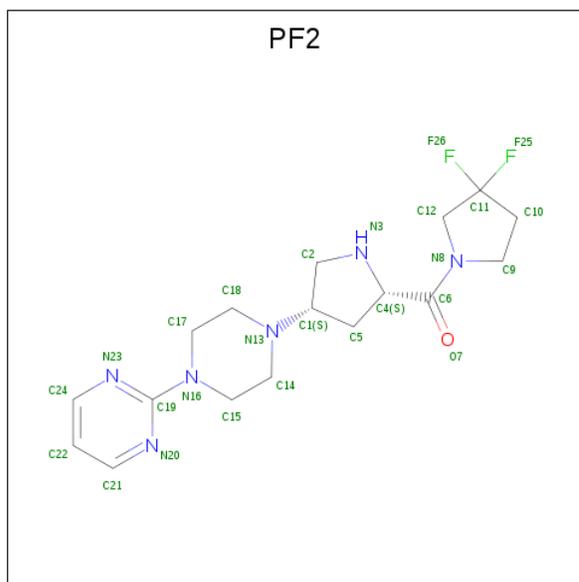
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	17	2	6	1		
4	B	1	Total	C	F	N	O	0	0
			26	17	2	6	1		

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: Dipeptidyl peptidase 4
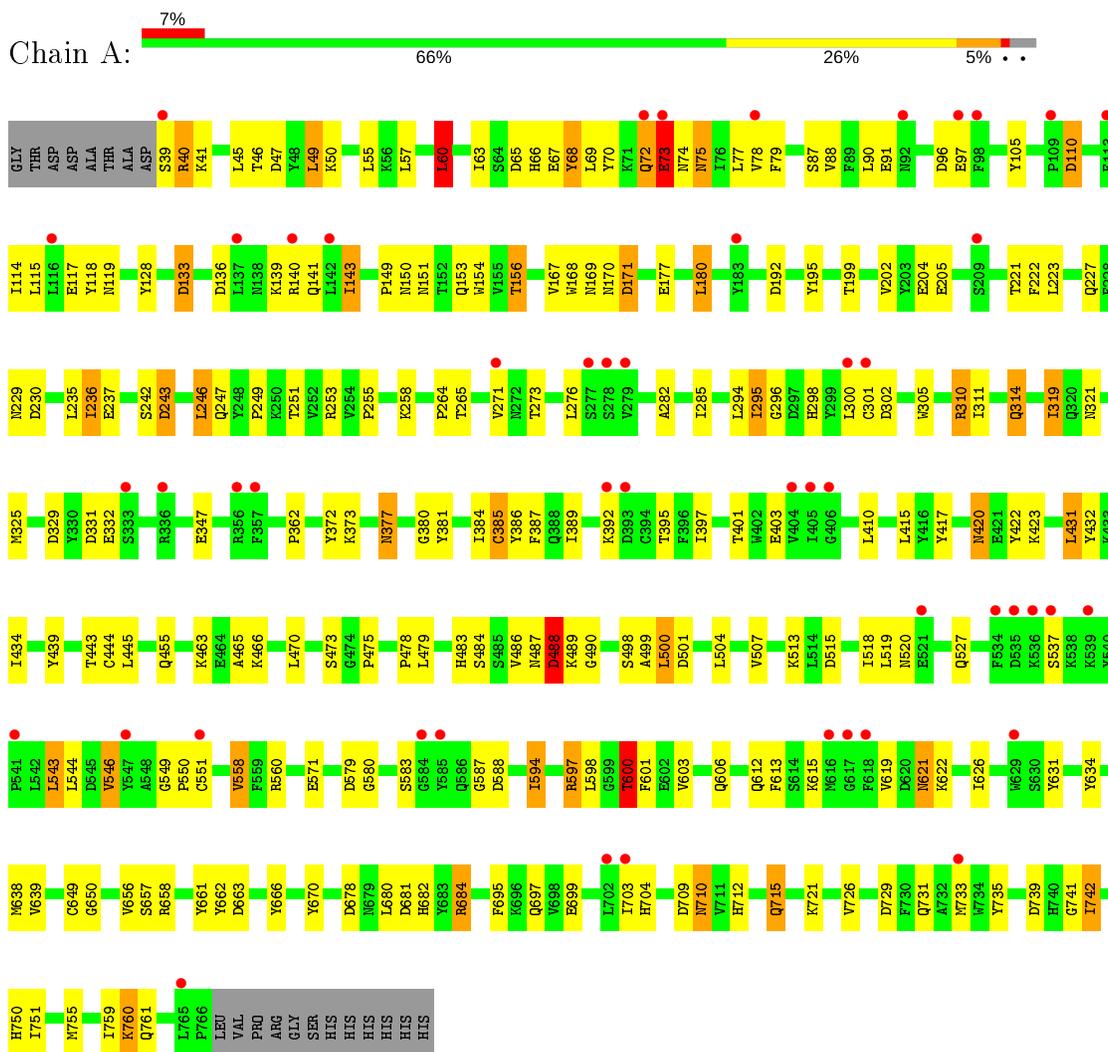
- Molecule 1: Dipeptidyl peptidase 4
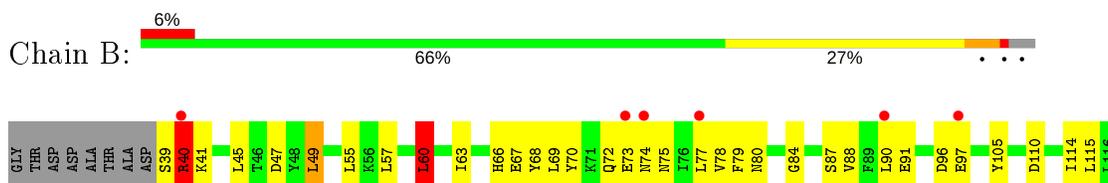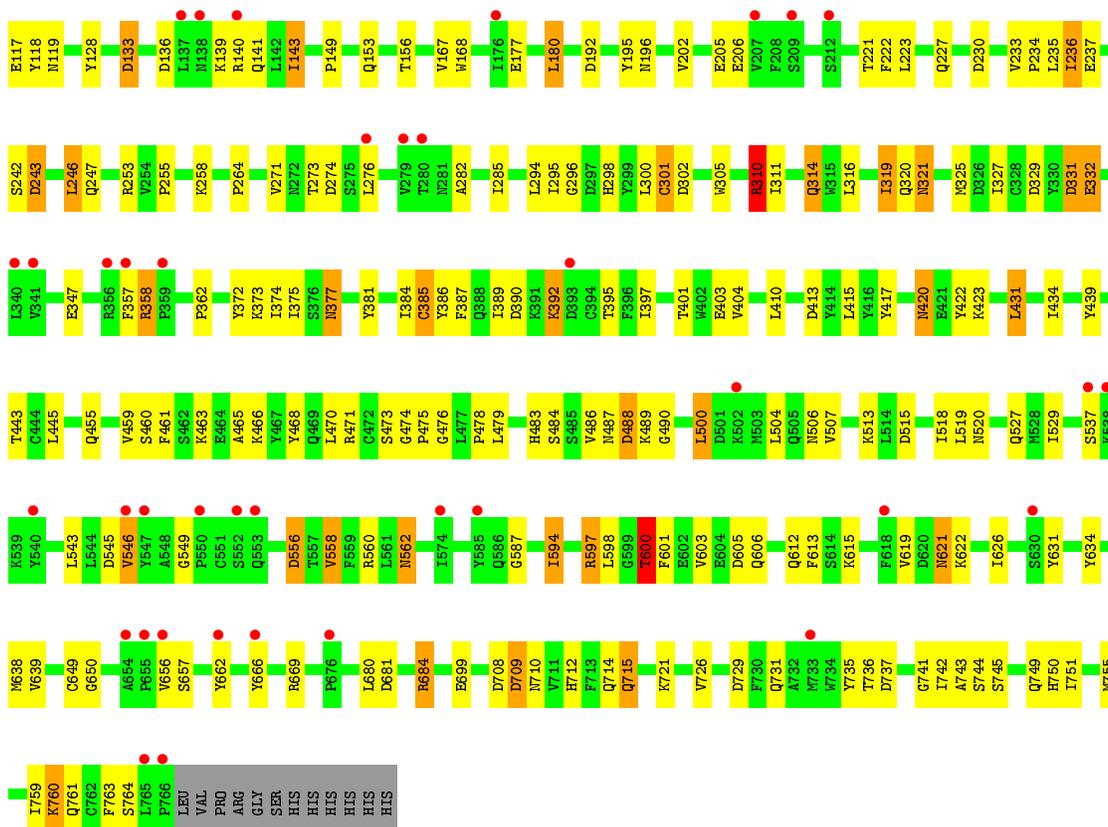
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain C:

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

Chain D:

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

Chain E:

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

Chain F:

100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.43Å 67.14Å 421.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.43 46.57 – 2.43	Depositor EDS
% Data completeness (in resolution range)	47.8 (50.00-2.43) 47.8 (46.57-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.84 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.243 , 0.295 0.248 , 0.290	Depositor DCC
R_{free} test set	1685 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	1.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 81.3	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12132	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PF2, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.57	0/6135	0.82	25/8344 (0.3%)
1	B	0.59	0/6135	0.84	22/8344 (0.3%)
All	All	0.58	0/12270	0.83	47/16688 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	310	ARG	NE-CZ-NH1	-20.39	110.11	120.30
1	A	310	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	B	310	ARG	NE-CZ-NH2	15.96	128.28	120.30
1	A	310	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	B	310	ARG	CD-NE-CZ	9.78	137.29	123.60
1	A	310	ARG	CD-NE-CZ	9.11	136.36	123.60
1	A	729	ASP	CB-CG-OD2	7.47	125.02	118.30
1	A	515	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	96	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	243	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	709	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	556	ASP	CB-CG-OD2	6.44	124.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	243	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	729	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	329	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	681	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	579	ASP	CB-CG-OD2	6.12	123.80	118.30
1	A	192	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	274	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	605	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	96	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	678	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	192	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	739	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	501	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	515	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	413	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	331	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	110	ASP	CB-CG-OD2	5.39	123.16	118.30
1	A	663	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	60	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	329	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	545	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	708	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	47	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	331	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	60	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	65	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	588	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	390	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	709	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	133	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	488	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	681	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	133	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	171	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	47	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	ARG	Sidechain
1	B	310	ARG	Sidechain

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	5963	0	5682	157	0
1	B	5963	0	5682	166	1
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	14	0	13	0	0
3	B	28	0	26	10	0
4	A	26	0	24	4	0
4	B	26	0	24	12	0
All	All	12132	0	11551	324	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 14.

All (324) 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:321:ASN:OD1	3:B:800:NAG:C1	2.04	1.06
3:B:799:NAG:H3	3:B:799:NAG:H83	1.41	1.01
1:B:321:ASN:CG	3:B:800:NAG:C1	2.33	0.97
1:A:470:LEU:HD12	1:A:483:HIS:HE1	1.30	0.96
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.04	0.93
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.02	0.93
1:B:470:LEU:HD12	1:B:483:HIS:HE1	1.33	0.92
1:A:558:VAL:HG12	1:A:560:ARG:NH1	1.83	0.91
1:B:321:ASN:ND2	3:B:800:NAG:C1	2.33	0.91
1:A:253:ARG:HH12	1:B:253:ARG:HH12	0.96	0.90
1:B:558:VAL:HG12	1:B:560:ARG:NH1	1.86	0.90
1:B:662:TYR:CE2	4:B:900:PF2:H9	2.08	0.89
1:B:39:SER:O	1:B:40:ARG:HD3	1.71	0.89
1:A:253:ARG:NH1	1:B:253:ARG:HH12	1.73	0.87
1:A:39:SER:O	1:A:40:ARG:HD3	1.76	0.86
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.58	0.85
1:A:445:LEU:HD22	1:A:488:ASP:OD2	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:O	1:B:139:LYS:O	1.99	0.80
1:A:347:GLU:OE2	1:A:373:LYS:NZ	2.14	0.79
1:A:253:ARG:HH12	1:B:253:ARG:NH1	1.80	0.78
1:A:558:VAL:CG1	1:A:560:ARG:CZ	2.61	0.77
1:B:39:SER:C	1:B:40:ARG:HD3	2.05	0.76
1:B:372:TYR:CE2	1:B:397:ILE:HD11	2.21	0.76
3:B:799:NAG:O6	3:B:799:NAG:O4	1.90	0.76
1:A:397:ILE:CG2	1:A:434:ILE:HG21	2.17	0.75
1:B:487:ASN:O	1:B:489:LYS:N	2.20	0.74
1:B:397:ILE:CG2	1:B:434:ILE:HG21	2.17	0.74
1:A:558:VAL:HG11	1:A:560:ARG:CZ	2.18	0.74
1:B:558:VAL:CG1	1:B:560:ARG:CZ	2.65	0.74
1:A:39:SER:C	1:A:40:ARG:HD3	2.08	0.73
1:A:558:VAL:CG1	1:A:560:ARG:NH1	2.51	0.73
1:B:662:TYR:HE2	4:B:900:PF2:H9	1.52	0.73
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.72	0.73
1:A:372:TYR:CE2	1:A:397:ILE:HD11	2.23	0.72
1:A:597:ARG:HD3	1:A:600:THR:HG21	1.70	0.72
1:B:321:ASN:HD21	3:B:800:NAG:C1	2.00	0.72
1:B:445:LEU:HD22	1:B:488:ASP:OD2	1.90	0.71
1:A:136:ASP:O	1:A:139:LYS:O	2.07	0.71
1:B:39:SER:O	1:B:40:ARG:CD	2.38	0.71
1:B:657:SER:H	1:B:715:GLN:NE2	1.89	0.70
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.27	0.70
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.57	0.70
1:B:666:TYR:CE1	4:B:900:PF2:H10	2.27	0.69
1:A:558:VAL:HG11	1:A:560:ARG:NH2	2.07	0.69
1:B:558:VAL:CG1	1:B:560:ARG:NH1	2.54	0.69
1:B:597:ARG:HD3	1:B:600:THR:HG21	1.75	0.69
1:B:518:ILE:O	1:B:519:LEU:HD23	1.93	0.69
1:B:666:TYR:CZ	4:B:900:PF2:C10	2.77	0.68
4:A:900:PF2:H9A	4:A:900:PF2:H5	1.74	0.68
1:A:518:ILE:O	1:A:519:LEU:HD23	1.95	0.67
1:B:487:ASN:O	1:B:488:ASP:C	2.32	0.67
1:B:558:VAL:HG11	1:B:560:ARG:CZ	2.23	0.67
1:A:657:SER:H	1:A:715:GLN:NE2	1.92	0.67
1:A:118:TYR:O	1:A:119:ASN:HB2	1.93	0.67
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.24	0.66
3:B:799:NAG:H3	3:B:799:NAG:C8	2.19	0.66
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.61	0.66
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:OE1	1:B:128:TYR:CE1	2.48	0.65
1:A:39:SER:O	1:A:40:ARG:CD	2.44	0.65
1:B:236:ILE:HG13	1:B:712:HIS:CE1	2.31	0.65
1:A:249:PRO:HD3	1:B:714:GLN:NE2	2.12	0.64
1:B:117:GLU:OE1	1:B:128:TYR:HE1	1.79	0.64
1:B:558:VAL:HG11	1:B:560:ARG:NH2	2.13	0.64
1:A:139:LYS:O	1:A:141:GLN:N	2.30	0.64
1:A:401:THR:HG22	1:A:401:THR:O	1.97	0.64
1:A:39:SER:O	1:A:40:ARG:HB2	1.98	0.64
1:A:397:ILE:HG21	1:A:434:ILE:HG21	1.80	0.64
1:A:680:LEU:HD11	1:A:684:ARG:NE	2.13	0.63
1:B:562:ASN:N	1:B:562:ASN:HD22	1.95	0.63
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.80	0.63
1:B:347:GLU:OE2	1:B:373:LYS:NZ	2.32	0.63
1:A:487:ASN:O	1:A:489:LYS:N	2.32	0.63
4:A:900:PF2:H9A	4:A:900:PF2:C5	2.28	0.62
1:B:321:ASN:OD1	3:B:800:NAG:N2	2.32	0.62
1:B:377:ASN:HD21	1:B:381:TYR:H	1.48	0.62
1:B:666:TYR:CE2	4:B:900:PF2:H9A	2.34	0.62
1:B:666:TYR:CZ	4:B:900:PF2:H10	2.35	0.62
1:B:403:GLU:OE2	1:B:587:GLY:HA2	1.99	0.62
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.81	0.61
1:B:403:GLU:H	1:B:420:ASN:HD21	1.48	0.61
1:B:310:ARG:HD3	1:B:327:ILE:HG23	1.81	0.61
1:A:372:TYR:HE2	1:A:397:ILE:HD11	1.65	0.60
1:B:546:VAL:HG23	1:B:606:GLN:OE1	2.01	0.60
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.83	0.60
4:B:900:PF2:C5	4:B:900:PF2:H9A	2.32	0.60
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.83	0.59
1:A:417:TYR:HE1	1:A:434:ILE:HG13	1.67	0.59
1:B:372:TYR:HE2	1:B:397:ILE:HD11	1.63	0.59
1:B:39:SER:O	1:B:40:ARG:HB2	2.03	0.59
1:B:431:LEU:HD13	1:B:445:LEU:HD12	1.84	0.59
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.85	0.59
1:B:483:HIS:HD2	1:B:490:GLY:HA2	1.67	0.58
1:B:473:SER:HB2	1:B:558:VAL:HG23	1.84	0.58
1:B:626:ILE:O	1:B:650:GLY:HA2	2.04	0.58
1:A:649:CYS:HB3	1:A:699:GLU:HB2	1.86	0.58
1:B:417:TYR:HE1	1:B:434:ILE:HG13	1.69	0.58
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.04	0.58
1:B:397:ILE:HG21	1:B:434:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLY:O	1:B:298:HIS:HD2	1.87	0.57
1:B:357:PHE:O	1:B:358:ARG:HB3	2.04	0.57
1:B:680:LEU:HD11	1:B:684:ARG:NE	2.19	0.57
1:A:710:ASN:C	1:A:710:ASN:HD22	2.06	0.57
1:B:206:GLU:OE2	4:B:900:PF2:N3	2.38	0.57
1:B:735:TYR:OH	1:B:750:HIS:CD2	2.50	0.57
1:B:242:SER:OG	1:B:243:ASP:N	2.38	0.56
1:B:377:ASN:ND2	1:B:381:TYR:H	2.03	0.56
4:B:900:PF2:H5	4:B:900:PF2:H9A	1.88	0.56
1:A:487:ASN:O	1:A:488:ASP:C	2.42	0.56
1:B:55:LEU:HD22	1:B:478:PRO:HG2	1.87	0.56
1:A:377:ASN:C	1:A:377:ASN:HD22	2.08	0.56
1:B:139:LYS:O	1:B:141:GLN:N	2.34	0.56
1:A:236:ILE:HG13	1:A:712:HIS:CE1	2.41	0.56
1:A:621:ASN:HD22	1:A:622:LYS:N	2.04	0.56
1:A:621:ASN:C	1:A:621:ASN:HD22	2.09	0.55
1:B:562:ASN:H	1:B:562:ASN:HD22	1.53	0.55
1:A:403:GLU:OE2	1:A:587:GLY:HA2	2.07	0.55
1:A:594:ILE:HG23	1:A:598:LEU:HD23	1.88	0.55
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.36	0.55
1:A:73:GLU:O	1:A:74:ASN:HB2	2.07	0.55
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.89	0.55
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.89	0.55
1:A:237:GLU:OE2	1:A:253:ARG:HD3	2.07	0.54
1:B:285:ILE:N	1:B:285:ILE:HD12	2.22	0.54
1:B:401:THR:O	1:B:401:THR:HG22	2.07	0.54
1:A:296:GLY:O	1:A:298:HIS:HD2	1.91	0.54
1:A:445:LEU:CD2	1:A:488:ASP:OD2	2.53	0.54
1:A:319:ILE:HD12	1:A:319:ILE:H	1.71	0.54
1:A:68:TYR:O	1:A:68:TYR:CD1	2.61	0.54
1:B:666:TYR:CD2	4:B:900:PF2:H9A	2.43	0.54
1:B:69:LEU:HD23	1:B:78:VAL:HG22	1.89	0.54
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.89	0.54
1:A:39:SER:O	1:A:40:ARG:CB	2.54	0.54
1:A:117:GLU:OE1	1:A:128:TYR:CE1	2.61	0.54
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.90	0.53
1:A:69:LEU:HD23	1:A:78:VAL:HG22	1.90	0.53
1:B:319:ILE:HD12	1:B:319:ILE:H	1.74	0.53
1:A:384:ILE:CG2	1:A:397:ILE:HD12	2.39	0.53
1:B:662:TYR:OH	4:B:900:PF2:C6	2.57	0.53
1:A:242:SER:OG	1:A:243:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ILE:O	1:A:650:GLY:HA2	2.08	0.53
1:A:69:LEU:CD2	1:A:78:VAL:HG22	2.39	0.53
1:B:594:ILE:HG23	1:B:594:ILE:O	2.09	0.52
1:B:463:LYS:C	1:B:465:ALA:H	2.13	0.52
1:A:403:GLU:H	1:A:420:ASN:HD21	1.58	0.52
1:B:483:HIS:CD2	1:B:490:GLY:HA2	2.45	0.52
1:A:432:TYR:CE2	1:A:444:CYS:SG	3.02	0.52
1:B:66:HIS:ND1	1:B:67:GLU:HG3	2.25	0.52
1:A:626:ILE:O	1:A:650:GLY:CA	2.58	0.52
1:B:39:SER:O	1:B:40:ARG:CB	2.57	0.51
1:A:473:SER:HB2	1:A:558:VAL:HG23	1.92	0.51
1:A:68:TYR:CD1	1:A:68:TYR:C	2.84	0.51
1:A:221:THR:O	1:A:273:THR:OG1	2.26	0.51
1:B:634:TYR:O	1:B:638:MET:HG2	2.10	0.51
1:B:301:CYS:SG	1:B:316:LEU:HB2	2.51	0.51
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.93	0.51
1:B:143:ILE:CG1	1:B:143:ILE:O	2.60	0.50
1:B:195:TYR:O	1:B:227:GLN:HA	2.11	0.50
1:B:221:THR:O	1:B:273:THR:OG1	2.26	0.50
1:A:150:ASN:O	1:A:151:ASN:HB2	2.11	0.50
1:A:247:GLN:HG2	1:B:258:LYS:HD2	1.94	0.50
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.12	0.50
1:A:463:LYS:C	1:A:465:ALA:H	2.13	0.50
1:A:253:ARG:NH1	1:B:253:ARG:NH1	2.51	0.50
1:A:377:ASN:HD21	1:A:381:TYR:H	1.58	0.50
1:B:513:LYS:O	1:B:527:GLN:HA	2.12	0.50
1:B:118:TYR:O	1:B:119:ASN:HB2	2.12	0.50
1:B:397:ILE:HG22	1:B:434:ILE:HG21	1.92	0.50
1:A:285:ILE:N	1:A:285:ILE:HD12	2.26	0.50
1:B:597:ARG:O	1:B:600:THR:OG1	2.15	0.50
1:B:626:ILE:O	1:B:650:GLY:CA	2.60	0.50
1:B:594:ILE:HG23	1:B:598:LEU:HD23	1.94	0.50
1:A:258:LYS:HD2	1:B:247:GLN:HG2	1.94	0.49
1:B:656:VAL:HG13	1:B:715:GLN:HE22	1.77	0.49
1:A:597:ARG:O	1:A:600:THR:OG1	2.23	0.49
1:A:410:LEU:HD12	1:A:415:LEU:HD12	1.95	0.49
1:B:621:ASN:C	1:B:621:ASN:HD22	2.15	0.49
1:A:377:ASN:ND2	1:A:381:TYR:H	2.09	0.49
1:A:543:LEU:HD22	1:A:544:LEU:N	2.28	0.49
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.47	0.49
1:A:735:TYR:OH	1:A:750:HIS:CD2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.95	0.49
1:B:666:TYR:CE2	4:B:900:PF2:H5	2.47	0.49
1:B:205:GLU:HA	1:B:205:GLU:OE1	2.12	0.49
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.94	0.49
1:A:612:GLN:HA	1:A:615:LYS:HE2	1.95	0.49
1:A:710:ASN:ND2	1:A:710:ASN:C	2.65	0.49
1:A:55:LEU:HD22	1:A:478:PRO:HG2	1.93	0.49
1:A:751:ILE:O	1:A:755:MET:HG3	2.13	0.49
1:B:484:SER:O	1:B:488:ASP:HA	2.12	0.48
1:B:612:GLN:HA	1:B:615:LYS:HE2	1.95	0.48
1:A:154:TRP:NE1	1:A:156:THR:HG22	2.29	0.48
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.43	0.48
1:B:235:LEU:HD23	1:B:255:PRO:HA	1.95	0.48
1:B:763:PHE:O	1:B:764:SER:HB2	2.13	0.48
1:A:484:SER:O	1:A:488:ASP:HA	2.13	0.48
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.14	0.48
1:A:60:LEU:HB2	1:A:68:TYR:CD1	2.49	0.47
1:B:613:PHE:O	1:B:619:VAL:HG21	2.15	0.47
1:B:743:ALA:O	1:B:744:SER:C	2.52	0.47
1:A:149:PRO:HB2	1:A:168:TRP:CD1	2.48	0.47
1:A:546:VAL:HG23	1:A:606:GLN:OE1	2.15	0.47
1:B:397:ILE:HG23	1:B:439:TYR:CD1	2.49	0.47
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.96	0.47
1:A:384:ILE:HG21	1:A:397:ILE:HD12	1.97	0.47
1:A:422:TYR:CE2	1:A:423:LYS:HD2	2.50	0.47
1:A:386:TYR:N	1:A:395:THR:O	2.46	0.47
1:A:695:PHE:C	1:A:697:GLN:H	2.18	0.47
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.14	0.47
1:A:251:THR:HG21	1:A:253:ARG:NH1	2.30	0.47
3:B:799:NAG:C3	3:B:799:NAG:H83	2.29	0.47
1:A:550:PRO:O	1:A:551:CYS:CB	2.64	0.46
1:B:60:LEU:HB2	1:B:68:TYR:CD1	2.50	0.46
1:A:167:VAL:HA	1:A:171:ASP:O	2.16	0.46
1:A:372:TYR:CE1	1:A:410:LEU:HD11	2.51	0.46
1:A:703:ILE:HA	1:A:733:MET:O	2.15	0.46
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.97	0.46
1:A:662:TYR:HE1	1:A:710:ASN:ND2	2.14	0.46
1:B:60:LEU:C	1:B:60:LEU:CD2	2.84	0.46
1:A:483:HIS:CD2	1:A:490:GLY:HA2	2.51	0.46
1:B:422:TYR:CE2	1:B:423:LYS:HD2	2.51	0.46
1:A:594:ILE:HG23	1:A:594:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:ND1	1:A:67:GLU:HG3	2.30	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.51	0.46
1:A:658:ARG:HB3	1:A:661:TYR:CD2	2.51	0.45
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.50	0.45
1:A:45:LEU:HG	1:A:49:LEU:HD22	1.97	0.45
1:A:199:THR:OG1	1:A:204:GLU:HB2	2.17	0.45
1:B:751:ILE:O	1:B:755:MET:HG3	2.17	0.45
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.46	0.45
1:A:325:MET:CE	1:A:362:PRO:HG3	2.47	0.45
1:B:600:THR:HB	1:B:601:PHE:H	1.51	0.45
1:A:549:GLY:HA2	1:A:631:TYR:CE1	2.51	0.45
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.99	0.45
1:A:55:LEU:HD23	1:A:500:LEU:HD12	1.99	0.44
1:B:657:SER:H	1:B:715:GLN:HE21	1.62	0.44
1:A:544:LEU:HD21	1:A:606:GLN:OE1	2.17	0.44
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.53	0.44
1:A:513:LYS:O	1:A:527:GLN:HA	2.17	0.44
1:B:325:MET:CE	1:B:362:PRO:HG3	2.47	0.44
1:B:759:ILE:HG22	1:B:760:LYS:N	2.32	0.44
1:A:377:ASN:ND2	1:A:377:ASN:C	2.71	0.44
1:A:499:ALA:O	1:A:500:LEU:C	2.57	0.44
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.99	0.44
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.99	0.44
1:A:153:GLN:OE1	1:A:167:VAL:HG12	2.17	0.43
1:B:372:TYR:CE1	1:B:410:LEU:HD11	2.53	0.43
1:B:562:ASN:N	1:B:562:ASN:ND2	2.65	0.43
1:B:621:ASN:HD22	1:B:622:LYS:N	2.16	0.43
1:B:73:GLU:O	1:B:74:ASN:HB2	2.17	0.43
1:A:603:VAL:HG13	1:A:639:VAL:HG23	2.00	0.43
1:A:656:VAL:HG13	1:A:715:GLN:HE22	1.83	0.43
1:B:276:LEU:CD2	1:B:282:ALA:HB2	2.48	0.43
1:B:55:LEU:HD23	1:B:500:LEU:HD12	2.00	0.43
1:B:90:LEU:HD23	1:B:91:GLU:N	2.34	0.43
1:B:384:ILE:CG2	1:B:397:ILE:HD12	2.48	0.43
1:A:558:VAL:HG12	1:A:560:ARG:HH12	1.71	0.43
1:B:445:LEU:CD2	1:B:488:ASP:OD2	2.63	0.43
1:A:143:ILE:CG1	1:A:143:ILE:O	2.66	0.43
1:A:634:TYR:O	1:A:638:MET:HG2	2.19	0.43
1:B:372:TYR:CD2	1:B:397:ILE:HD11	2.53	0.43
1:B:410:LEU:HD12	1:B:415:LEU:HD12	1.99	0.43
1:B:745:SER:O	1:B:749:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:ILE:CG2	1:B:760:LYS:N	2.81	0.43
1:A:222:PHE:HA	1:A:271:VAL:O	2.19	0.43
1:A:74:ASN:O	1:A:75:ASN:O	2.36	0.43
1:A:74:ASN:O	1:A:75:ASN:C	2.57	0.43
1:B:471:ARG:HG3	1:B:471:ARG:O	2.19	0.43
1:A:276:LEU:CD2	1:A:282:ALA:HB2	2.48	0.42
1:A:72:GLN:O	1:A:73:GLU:HB2	2.17	0.42
1:A:580:GLY:O	1:A:583:SER:OG	2.23	0.42
1:B:386:TYR:N	1:B:395:THR:O	2.49	0.42
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.53	0.42
1:B:474:GLY:HA2	1:B:476:GLY:N	2.34	0.42
1:A:666:TYR:O	1:A:670:TYR:CD2	2.73	0.42
1:B:77:LEU:HD23	1:B:88:VAL:HA	2.01	0.42
1:A:695:PHE:C	1:A:697:GLN:N	2.73	0.42
1:A:600:THR:HB	1:A:601:PHE:H	1.59	0.42
1:B:153:GLN:OE1	1:B:167:VAL:HG12	2.19	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.58	0.42
1:A:658:ARG:HD2	1:A:661:TYR:CZ	2.55	0.42
1:B:222:PHE:HA	1:B:271:VAL:O	2.20	0.42
1:A:662:TYR:CE1	1:A:710:ASN:ND2	2.88	0.42
1:B:347:GLU:OE1	1:B:375:ILE:HD13	2.19	0.42
1:A:295:ILE:HG12	1:A:295:ILE:O	2.19	0.42
1:B:377:ASN:HD22	1:B:377:ASN:C	2.23	0.42
1:B:321:ASN:OD1	3:B:800:NAG:C2	2.65	0.41
1:B:374:ILE:HD11	1:B:404:VAL:HG12	2.01	0.41
1:A:483:HIS:HD2	1:A:490:GLY:HA2	1.86	0.41
1:A:662:TYR:OH	4:A:900:PF2:C6	2.68	0.41
1:B:556:ASP:C	1:B:556:ASP:OD1	2.58	0.41
1:B:558:VAL:HG12	1:B:560:ARG:HH12	1.75	0.41
1:B:709:ASP:O	1:B:712:HIS:NE2	2.53	0.41
1:A:169:ASN:O	1:A:170:ASN:HB2	2.21	0.41
1:A:90:LEU:HD23	1:A:91:GLU:N	2.35	0.41
1:B:233:VAL:HA	1:B:234:PRO:HD3	1.94	0.41
1:A:377:ASN:HD22	1:A:380:GLY:H	1.68	0.41
1:A:613:PHE:O	1:A:619:VAL:HG21	2.19	0.41
1:A:759:ILE:HG22	1:A:760:LYS:N	2.35	0.41
1:A:372:TYR:CD2	1:A:397:ILE:HD11	2.56	0.41
1:A:397:ILE:HG23	1:A:439:TYR:CD1	2.55	0.41
1:B:372:TYR:CD1	1:B:410:LEU:HD11	2.55	0.41
1:A:455:GLN:HB2	1:A:475:PRO:HD3	2.02	0.41
1:A:195:TYR:O	1:A:227:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:TRP:CZ3	1:A:311:ILE:CG1	3.03	0.41
1:B:403:GLU:OE2	1:B:587:GLY:CA	2.66	0.41
1:A:46:THR:O	1:A:50:LYS:HB2	2.20	0.41
1:A:571:GLU:CD	1:A:760:LYS:HD3	2.40	0.41
1:B:549:GLY:HA2	1:B:631:TYR:CE1	2.55	0.41
1:A:205:GLU:OE2	4:A:900:PF2:N3	2.52	0.41
1:A:235:LEU:HD23	1:A:255:PRO:HA	2.01	0.41
1:A:377:ASN:ND2	1:A:380:GLY:N	2.68	0.40
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.21	0.40
1:A:543:LEU:CD2	1:A:544:LEU:N	2.84	0.40
1:B:459:VAL:HG22	1:B:460:SER:N	2.36	0.40
1:B:90:LEU:HD23	1:B:91:GLU:O	2.21	0.40
1:B:149:PRO:HB2	1:B:168:TRP:CD1	2.55	0.40
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.22	0.40
1:B:331:ASP:O	1:B:332:GLU:C	2.59	0.40
1:B:80:ASN:O	1:B:84:GLY:N	2.54	0.40
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.56	0.40
1:A:741:GLY:O	1:A:742:ILE:C	2.59	0.40
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.87	0.40
1:B:736:THR:O	1:B:737:ASP:HB2	2.21	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:B:392:LYS:CE	1:B:506:ASN:OD1[1_545]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/748 (97%)	667 (92%)	51 (7%)	8 (1%)	14	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	726/748 (97%)	669 (92%)	49 (7%)	8 (1%)	14	15
All	All	1452/1496 (97%)	1336 (92%)	100 (7%)	16 (1%)	14	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	140	ARG
1	A	488	ASP
1	B	140	ARG
1	B	488	ASP
1	A	332	GLU
1	B	75	ASN
1	B	332	GLU
1	A	486	VAL
1	B	486	VAL
1	B	600	THR
1	A	73	GLU
1	A	600	THR
1	B	40	ARG
1	B	358	ARG
1	A	742	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	653/669 (98%)	595 (91%)	58 (9%)	9	10
1	B	653/669 (98%)	597 (91%)	56 (9%)	10	11
All	All	1306/1338 (98%)	1192 (91%)	114 (9%)	10	11

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	41	LYS
1	A	49	LEU
1	A	57	LEU
1	A	60	LEU
1	A	63	ILE
1	A	68	TYR
1	A	72	GLN
1	A	73	GLU
1	A	87	SER
1	A	97	GLU
1	A	110	ASP
1	A	115	LEU
1	A	133	ASP
1	A	143	ILE
1	A	156	THR
1	A	180	LEU
1	A	202	VAL
1	A	223	LEU
1	A	236	ILE
1	A	246	LEU
1	A	294	LEU
1	A	295	ILE
1	A	300	LEU
1	A	301	CYS
1	A	314	GLN
1	A	319	ILE
1	A	321	ASN
1	A	377	ASN
1	A	385	CYS
1	A	389	ILE
1	A	392	LYS
1	A	420	ASN
1	A	431	LEU
1	A	443	THR
1	A	466	LYS
1	A	479	LEU
1	A	498	SER
1	A	500	LEU
1	A	507	VAL
1	A	520	ASN
1	A	537	SER
1	A	543	LEU

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Mol	Chain	Res	Type
1	A	546	VAL
1	A	558	VAL
1	A	594	ILE
1	A	597	ARG
1	A	600	THR
1	A	621	ASN
1	A	684	ARG
1	A	704	HIS
1	A	710	ASN
1	A	715	GLN
1	A	721	LYS
1	A	726	VAL
1	A	731	GLN
1	A	760	LYS
1	A	761	GLN
1	B	40	ARG
1	B	41	LYS
1	B	49	LEU
1	B	57	LEU
1	B	60	LEU
1	B	63	ILE
1	B	72	GLN
1	B	87	SER
1	B	97	GLU
1	B	110	ASP
1	B	115	LEU
1	B	133	ASP
1	B	143	ILE
1	B	156	THR
1	B	180	LEU
1	B	202	VAL
1	B	223	LEU
1	B	236	ILE
1	B	246	LEU
1	B	294	LEU
1	B	295	ILE
1	B	300	LEU
1	B	301	CYS
1	B	314	GLN
1	B	319	ILE
1	B	321	ASN
1	B	377	ASN

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Mol	Chain	Res	Type
1	B	385	CYS
1	B	389	ILE
1	B	392	LYS
1	B	420	ASN
1	B	431	LEU
1	B	443	THR
1	B	466	LYS
1	B	479	LEU
1	B	500	LEU
1	B	507	VAL
1	B	520	ASN
1	B	529	ILE
1	B	537	SER
1	B	543	LEU
1	B	546	VAL
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	597	ARG
1	B	600	THR
1	B	621	ASN
1	B	684	ARG
1	B	710	ASN
1	B	715	GLN
1	B	721	LYS
1	B	726	VAL
1	B	731	GLN
1	B	760	LYS
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	123	GLN
1	A	169	ASN
1	A	263	ASN
1	A	298	HIS
1	A	377	ASN
1	A	383	HIS
1	A	420	ASN
1	A	435	GLN

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Mol	Chain	Res	Type
1	A	483	HIS
1	A	487	ASN
1	A	621	ASN
1	A	679	ASN
1	A	710	ASN
1	A	715	GLN
1	A	750	HIS
1	B	72	GLN
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	483	HIS
1	B	487	ASN
1	B	562	ASN
1	B	592	HIS
1	B	621	ASN
1	B	679	ASN
1	B	710	ASN
1	B	715	GLN
1	B	750	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 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	$\#|Z| > 2$
2	NAG	C	1	1,2	14,14,15	0.59	0	17,19,21	1.17	3 (17%)
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	1.97	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.80	1 (7%)	17,19,21	2.42	6 (35%)
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	1.35	2 (11%)
2	NAG	E	1	1,2	14,14,15	0.82	1 (7%)	17,19,21	1.46	2 (11%)
2	NAG	E	2	2	14,14,15	0.64	0	17,19,21	1.19	3 (17%)
2	NAG	F	1	1,2	14,14,15	0.63	0	17,19,21	1.65	4 (23%)
2	NAG	F	2	2	14,14,15	0.50	0	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-2.59	1.39	1.43
2	D	1	NAG	C1-C2	2.58	1.56	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	7.24	122.00	112.19
2	C	2	NAG	C1-O5-C5	5.77	120.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	O5-C1-C2	-4.70	103.86	111.29
2	F	1	NAG	O5-C5-C6	4.11	113.64	107.20
2	D	1	NAG	C4-C3-C2	3.90	116.73	111.02
2	D	2	NAG	C1-O5-C5	3.69	117.19	112.19
2	C	2	NAG	O5-C5-C4	3.33	118.93	110.83
2	C	2	NAG	C3-C4-C5	2.86	115.34	110.24
2	F	1	NAG	O5-C1-C2	-2.78	106.89	111.29
2	C	1	NAG	C6-C5-C4	-2.52	107.11	113.00
2	D	1	NAG	O7-C7-N2	2.51	126.57	121.95
2	F	1	NAG	C6-C5-C4	-2.46	107.25	113.00
2	E	2	NAG	C1-O5-C5	2.45	115.51	112.19
2	F	2	NAG	C2-N2-C7	-2.39	119.50	122.90
2	E	2	NAG	C2-N2-C7	-2.38	119.52	122.90
2	D	1	NAG	C1-C2-N2	2.30	114.42	110.49
2	D	1	NAG	C6-C5-C4	-2.29	107.64	113.00
2	D	1	NAG	C2-N2-C7	2.28	126.14	122.90
2	C	1	NAG	C2-N2-C7	-2.24	119.71	122.90
2	D	2	NAG	O5-C1-C2	-2.22	107.79	111.29
2	E	1	NAG	C1-O5-C5	2.20	115.17	112.19
2	F	1	NAG	C2-N2-C7	-2.16	119.83	122.90
2	C	1	NAG	C3-C4-C5	2.06	113.91	110.24
2	E	2	NAG	C6-C5-C4	-2.00	108.31	113.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
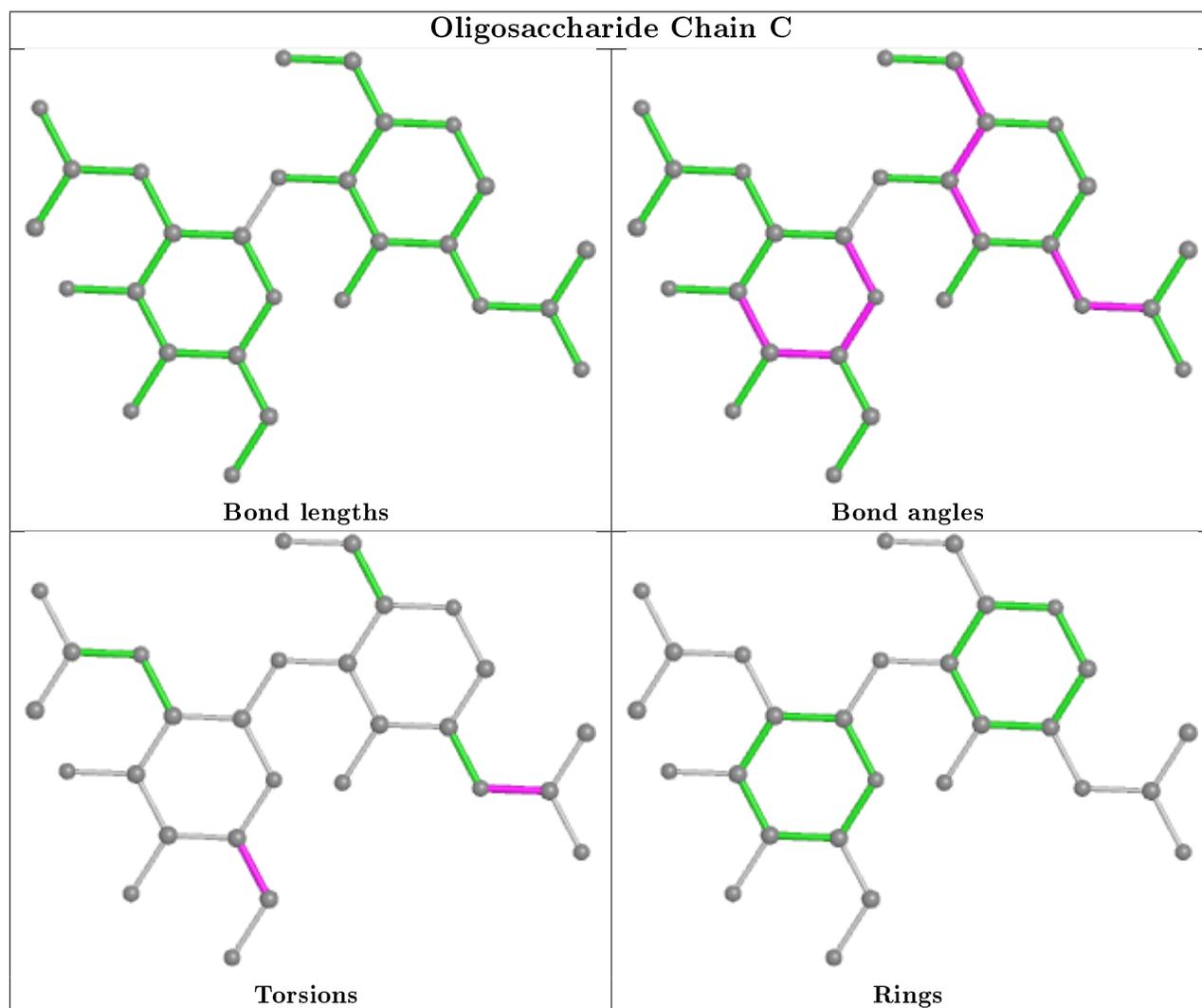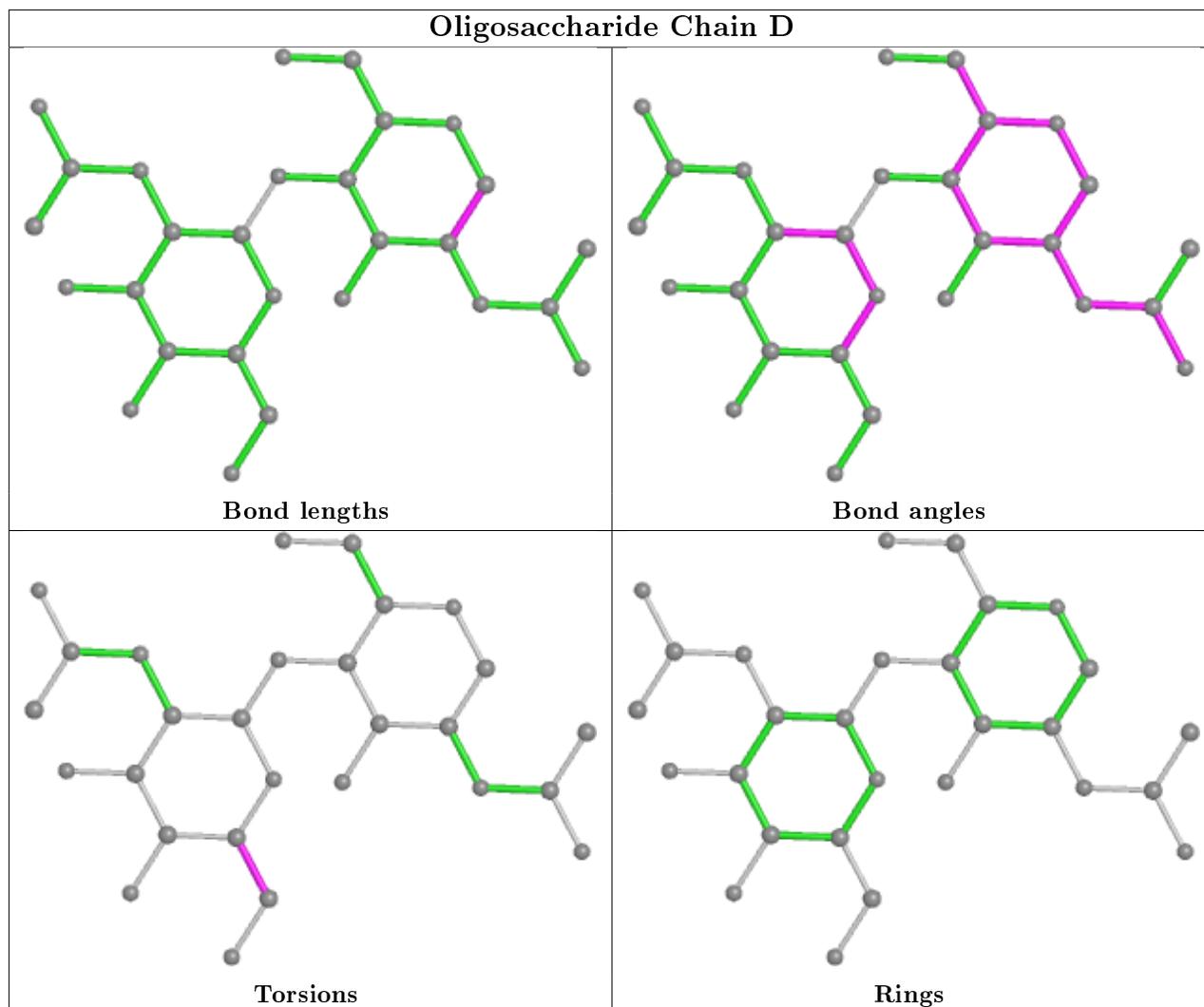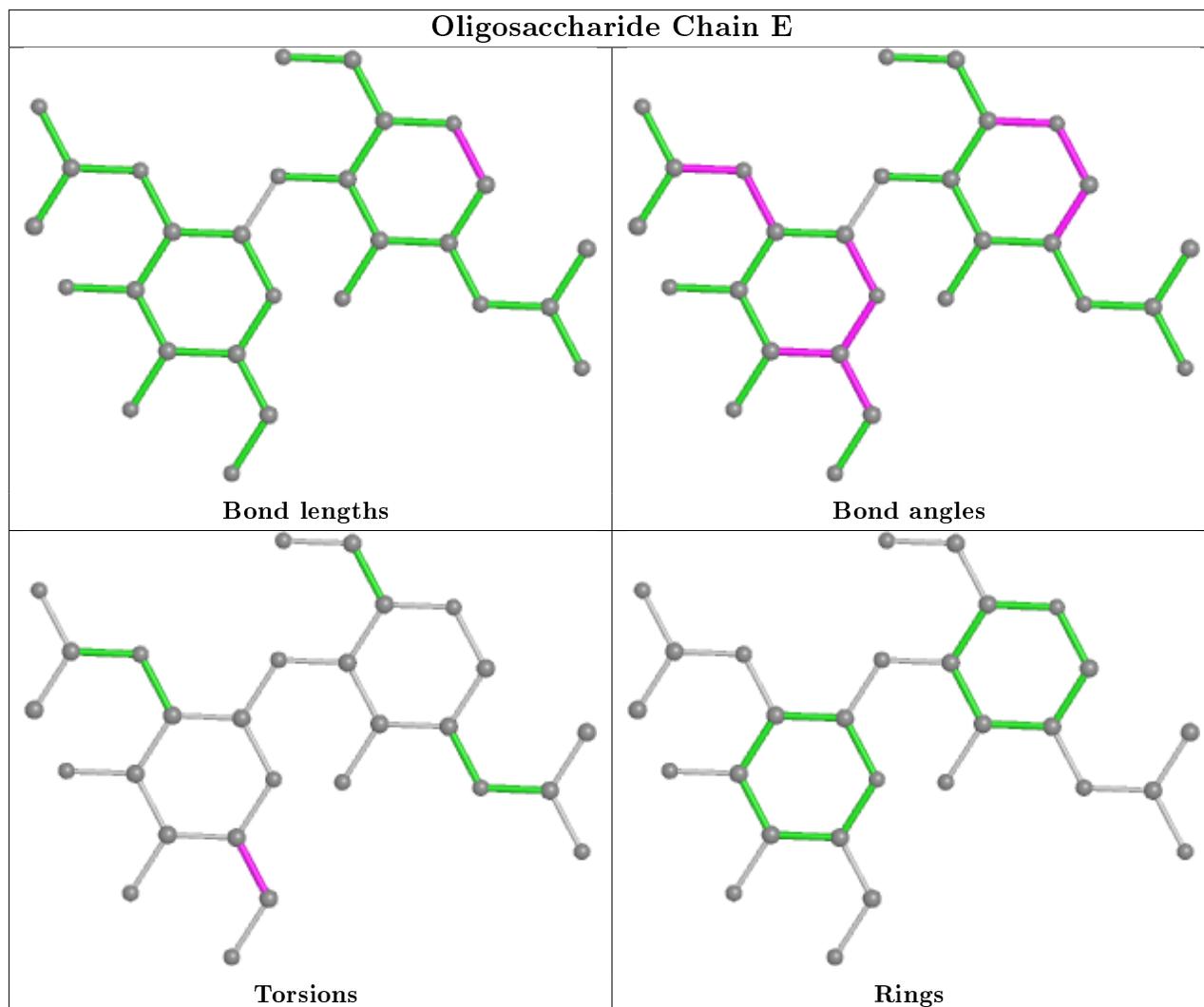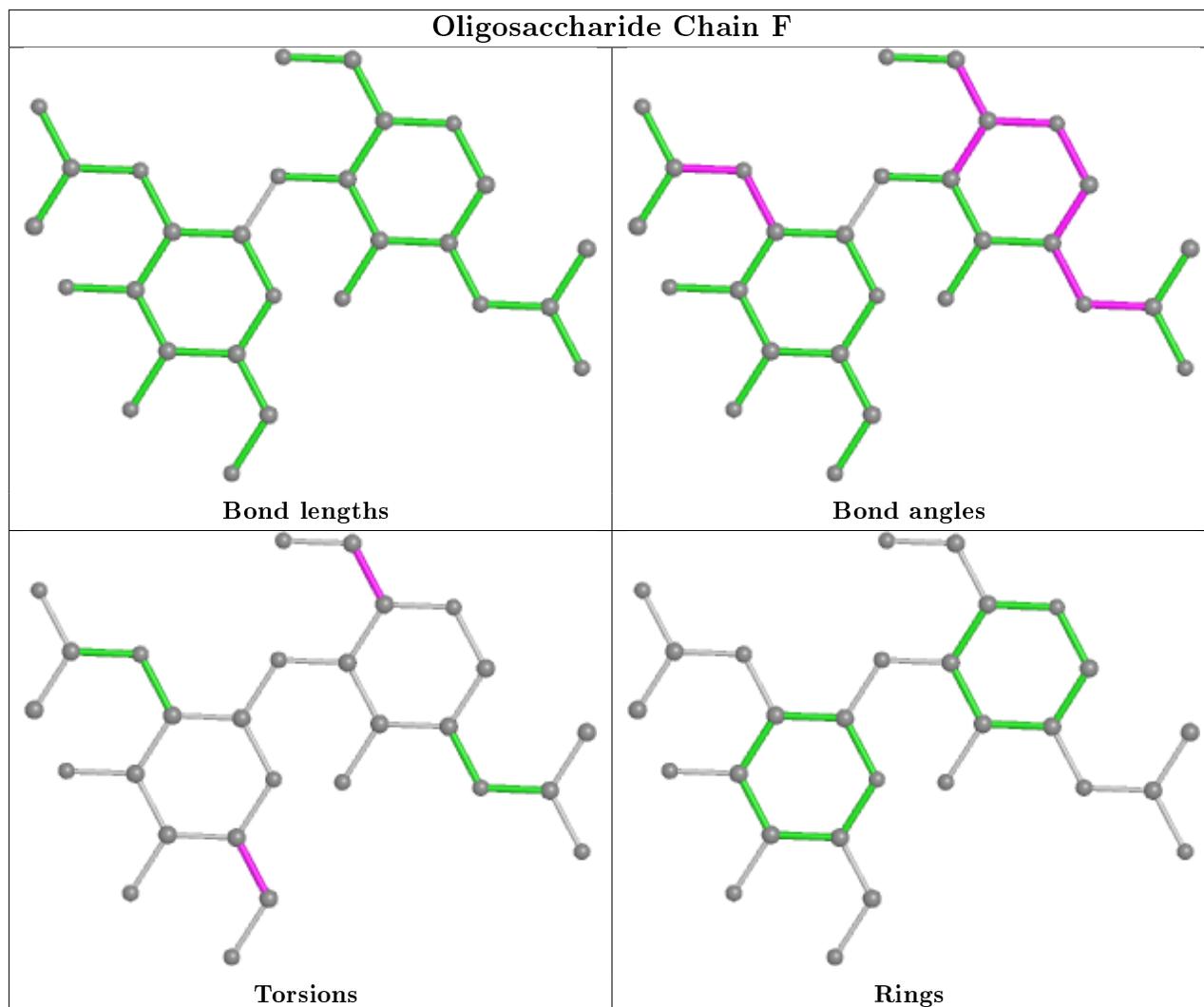
5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	PF2	B	900	-	26,29,29	1.22	2 (7%)	34,42,42	2.30	14 (41%)
3	NAG	A	796	1	14,14,15	0.63	0	17,19,21	1.02	1 (5%)
3	NAG	B	800	-	14,14,15	0.62	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	B	799	1	14,14,15	0.70	0	17,19,21	1.93	3 (17%)
4	PF2	A	900	-	26,29,29	1.35	2 (7%)	34,42,42	2.56	14 (41%)

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	PF2	B	900	-	-	0/16/46/46	1/4/4/4
3	NAG	A	796	1	-	4/6/23/26	0/1/1/1
3	NAG	B	800	-	-	2/6/23/26	0/1/1/1
3	NAG	B	799	1	1/1/5/7	4/6/23/26	0/1/1/1
4	PF2	A	900	-	-	0/16/46/46	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	PF2	F25-C11	-4.46	1.30	1.38
4	A	900	PF2	F25-C11	-3.80	1.31	1.38
4	A	900	PF2	F26-C11	-3.75	1.31	1.38
4	B	900	PF2	F26-C11	-2.43	1.34	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	900	PF2	C24-N23-C19	6.13	121.85	115.08
4	A	900	PF2	C15-N16-C17	5.33	123.28	111.52
4	B	900	PF2	O7-C6-N8	4.97	127.48	121.67
4	B	900	PF2	C15-N16-C17	4.96	122.47	111.52
4	A	900	PF2	F25-C11-C10	-4.60	100.92	111.44
3	B	799	NAG	O5-C5-C6	4.46	114.19	107.20
3	B	799	NAG	C6-C5-C4	-4.42	102.66	113.00
4	B	900	PF2	C4-C6-N8	-4.35	112.29	118.87
4	A	900	PF2	N20-C19-N23	-4.01	120.29	127.06
4	A	900	PF2	C10-C9-N8	-3.95	100.05	103.62
4	B	900	PF2	C24-N23-C19	3.68	119.15	115.08
4	A	900	PF2	C21-N20-C19	3.60	119.06	115.08
4	A	900	PF2	N20-C19-N16	3.34	120.51	116.90
4	A	900	PF2	C4-C6-N8	-3.34	113.83	118.87
4	A	900	PF2	C17-N16-C19	-3.25	116.30	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	PF2	C21-N20-C19	3.15	118.56	115.08
4	A	900	PF2	C22-C24-N23	-2.87	118.74	123.43
4	A	900	PF2	F26-C11-C10	-2.82	104.97	111.44
4	B	900	PF2	F25-C11-C10	-2.77	105.10	111.44
4	B	900	PF2	C14-C15-N16	-2.70	105.45	110.70
4	B	900	PF2	C18-C17-N16	-2.65	105.56	110.70
4	B	900	PF2	C22-C24-N23	-2.58	119.21	123.43
4	B	900	PF2	C21-C22-C24	2.55	120.33	116.67
4	B	900	PF2	C22-C21-N20	-2.42	119.47	123.43
4	B	900	PF2	N20-C19-N23	-2.24	123.27	127.06
4	A	900	PF2	O7-C6-N8	2.24	124.29	121.67
4	A	900	PF2	C12-N8-C6	2.19	131.52	124.02
4	B	900	PF2	C14-N13-C1	-2.19	106.47	112.64
3	B	799	NAG	C2-N2-C7	2.13	125.94	122.90
4	A	900	PF2	N23-C19-N16	2.13	119.20	116.90
4	B	900	PF2	C5-C1-N13	-2.12	108.70	113.54
3	A	796	NAG	C2-N2-C7	-2.11	119.89	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	799	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	799	NAG	C3-C2-N2-C7
3	B	799	NAG	C8-C7-N2-C2
3	B	799	NAG	O7-C7-N2-C2
3	A	796	NAG	O5-C5-C6-O6
3	A	796	NAG	C4-C5-C6-O6
3	B	799	NAG	O5-C5-C6-O6
3	A	796	NAG	C8-C7-N2-C2
3	A	796	NAG	O7-C7-N2-C2
3	B	800	NAG	C8-C7-N2-C2
3	B	800	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	900	PF2	C14-C15-C17-C18-N13-N16

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	900	PF2	12	0
3	B	800	NAG	6	0
3	B	799	NAG	4	0
4	A	900	PF2	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
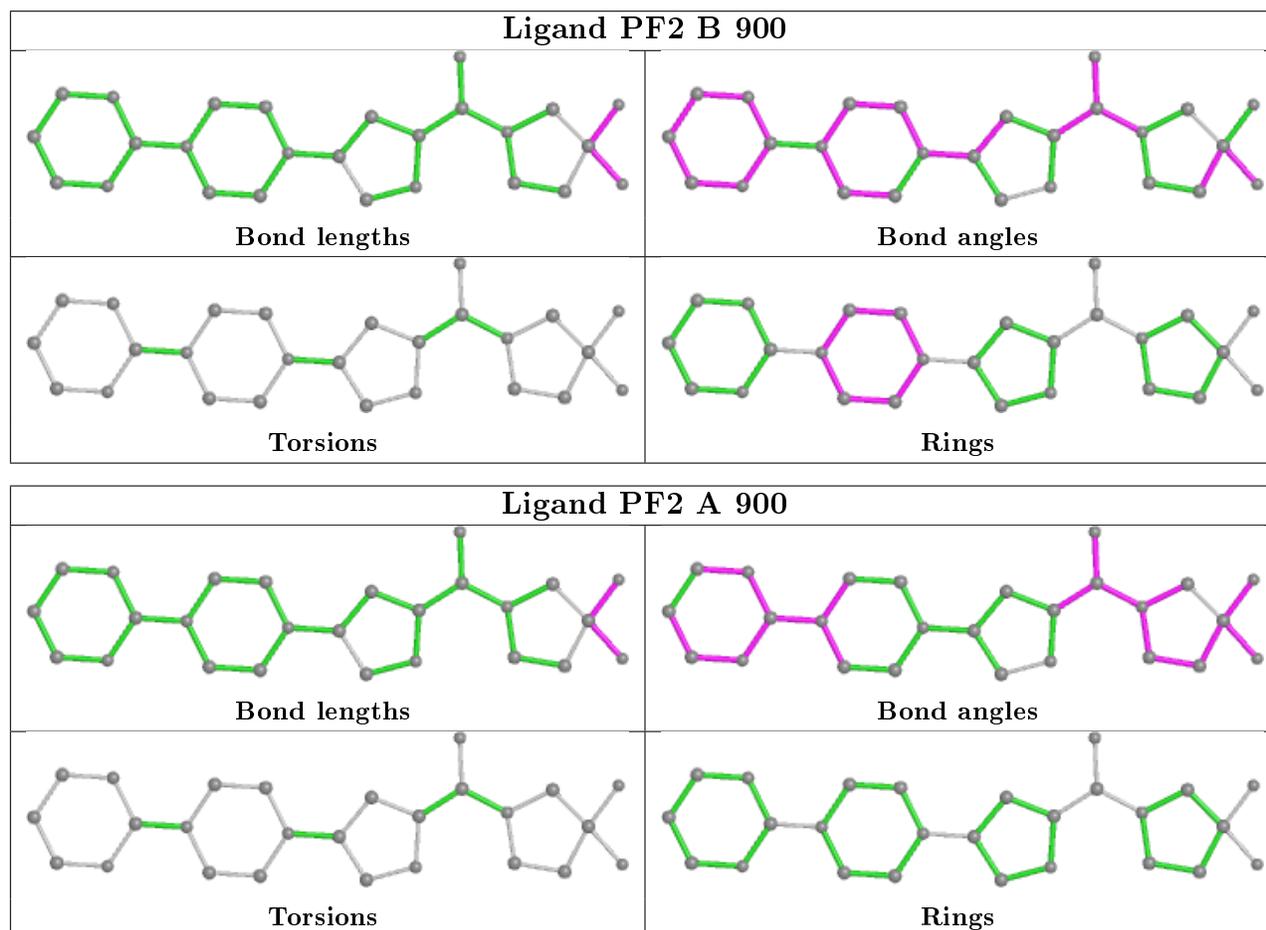
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	728/748 (97%)	0.54	49 (6%)	17	14	72, 84, 97, 104	0
1	B	728/748 (97%)	0.51	44 (6%)	21	18	72, 84, 97, 104	0
All	All	1456/1496 (97%)	0.52	93 (6%)	19	16	72, 84, 97, 104	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	LEU	6.0
1	B	279	VAL	6.0
1	A	39	SER	5.4
1	A	278	SER	4.9
1	A	279	VAL	4.7
1	A	142	LEU	4.7
1	A	618	PHE	4.5
1	A	536	LYS	4.4
1	B	280	THR	4.0
1	A	183	TYR	3.7
1	B	73	GLU	3.7
1	A	209	SER	3.6
1	A	140	ARG	3.5
1	B	357	PHE	3.5
1	B	630	SER	3.5
1	A	72	GLN	3.5
1	B	77	LEU	3.4
1	A	301	CYS	3.4
1	A	333	SER	3.4
1	B	538	LYS	3.3
1	A	539	LYS	3.0
1	A	617	GLY	3.0
1	B	655	PRO	3.0
1	A	392	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	537	SER	3.0
1	A	535	ASP	2.9
1	A	585	TYR	2.9
1	A	277	SER	2.9
1	A	73	GLU	2.8
1	A	271	VAL	2.8
1	A	97	GLU	2.8
1	B	176	ILE	2.8
1	B	585	TYR	2.8
1	B	618	PHE	2.7
1	B	74	ASN	2.7
1	A	393	ASP	2.7
1	B	340	LEU	2.7
1	A	702	LEU	2.7
1	B	137	LEU	2.7
1	B	552	SER	2.6
1	A	300	LEU	2.6
1	B	574	ILE	2.6
1	B	537	SER	2.6
1	A	98	PHE	2.6
1	B	138	ASN	2.6
1	A	405	ILE	2.6
1	B	766	PRO	2.6
1	A	765	LEU	2.6
1	A	116	LEU	2.6
1	B	97	GLU	2.6
1	A	584	GLY	2.6
1	A	534	PHE	2.5
1	B	90	LEU	2.5
1	A	406	GLY	2.5
1	B	765	LEU	2.5
1	A	521	GLU	2.5
1	A	551	CYS	2.5
1	B	540	TYR	2.4
1	A	109	PRO	2.4
1	B	656	VAL	2.4
1	B	666	TYR	2.4
1	A	357	PHE	2.4
1	B	546	VAL	2.3
1	A	92	ASN	2.3
1	B	393	ASP	2.3
1	A	616	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	733	MET	2.3
1	B	550	PRO	2.3
1	A	547	TYR	2.3
1	B	676	PRO	2.2
1	B	341	VAL	2.2
1	B	209	SER	2.2
1	B	276	LEU	2.2
1	B	212	SER	2.2
1	B	359	PRO	2.2
1	B	547	TYR	2.2
1	A	404	VAL	2.2
1	A	541	PRO	2.2
1	B	356	ARG	2.2
1	B	502	LYS	2.1
1	B	553	GLN	2.1
1	A	733	MET	2.1
1	A	703	ILE	2.1
1	A	356	ARG	2.1
1	B	40	ARG	2.1
1	A	336	ARG	2.1
1	A	629	TRP	2.1
1	B	140	ARG	2.1
1	B	207	VAL	2.1
1	A	113	PHE	2.0
1	B	654	ALA	2.0
1	A	78	VAL	2.0
1	B	662	TYR	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.82	0.29	113,115,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	1	14/15	0.83	0.17	103,106,110,113	0
2	NAG	D	2	14/15	0.84	0.31	117,120,121,122	0
2	NAG	F	2	14/15	0.86	0.41	114,117,119,119	0
2	NAG	F	1	14/15	0.87	0.18	89,93,100,108	0
2	NAG	E	2	14/15	0.92	0.17	91,93,96,96	0
2	NAG	E	1	14/15	0.93	0.11	78,83,89,89	0
2	NAG	C	1	14/15	0.93	0.14	97,101,104,109	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 C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
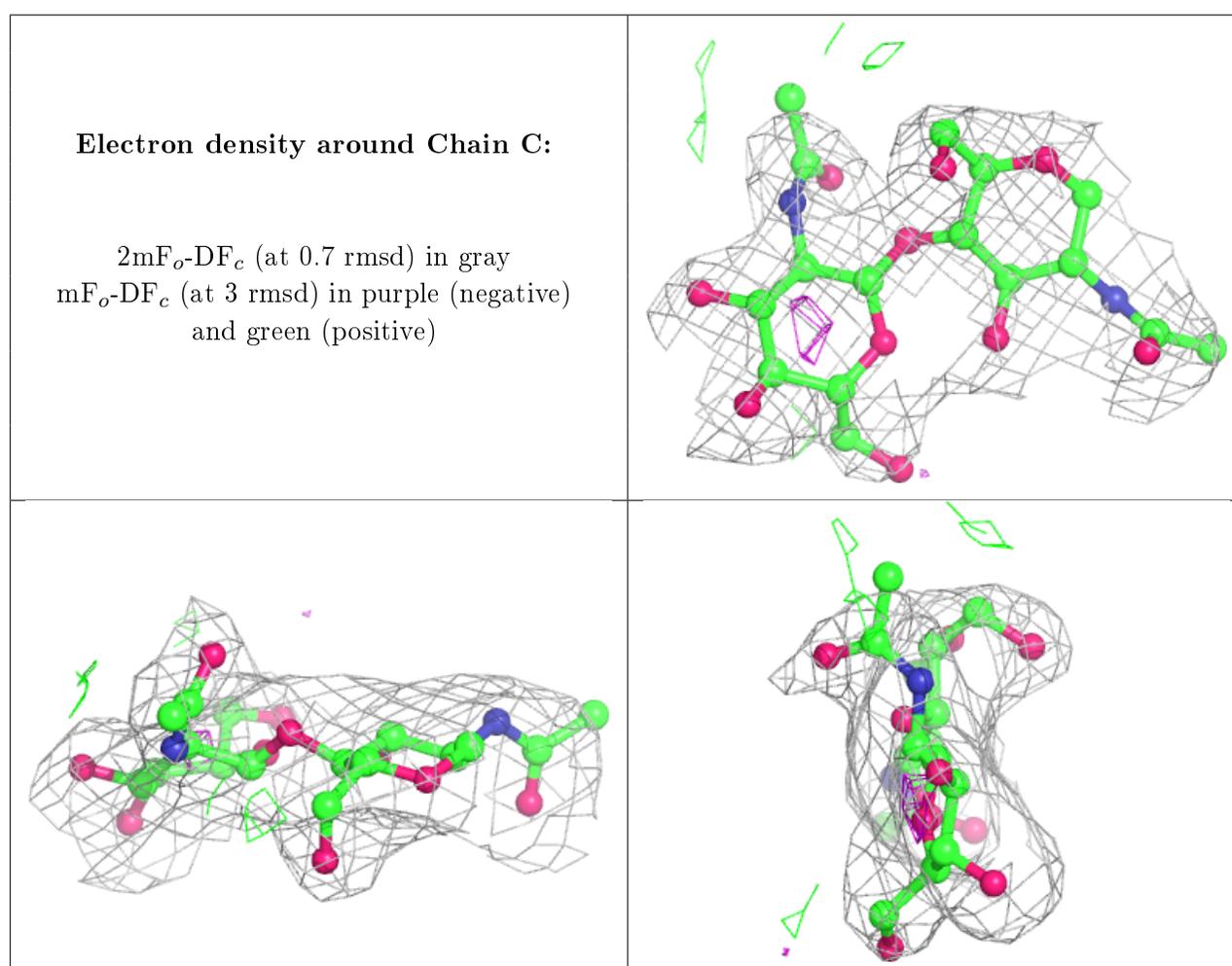
Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
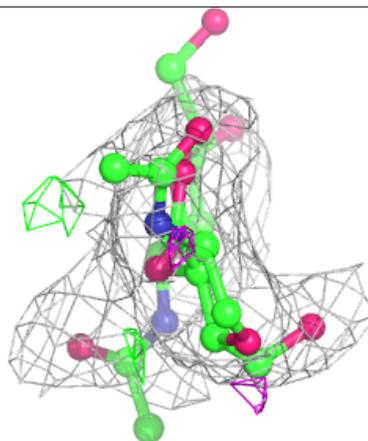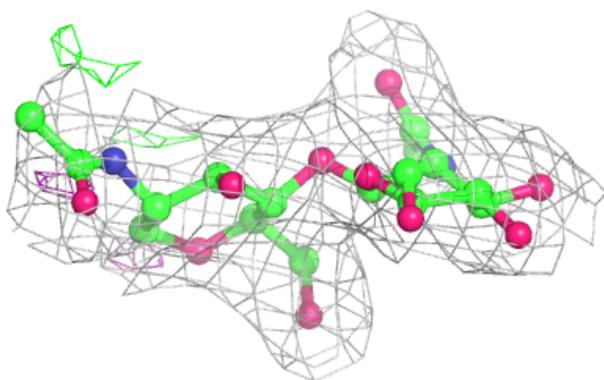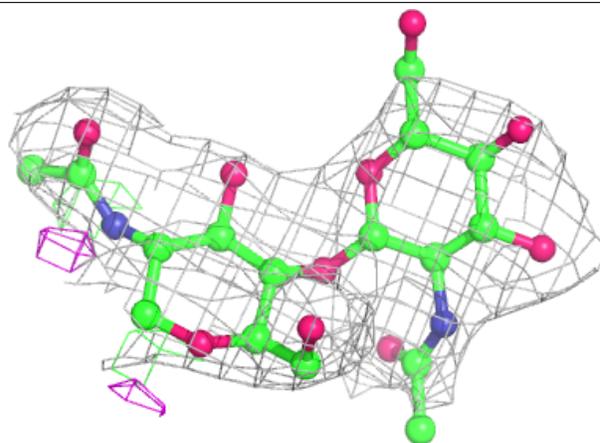
Electron density around Chain E:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
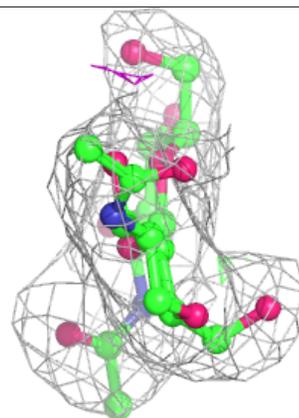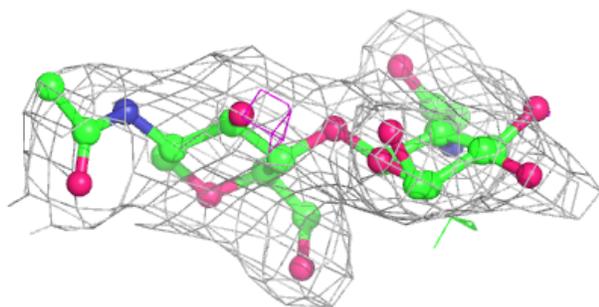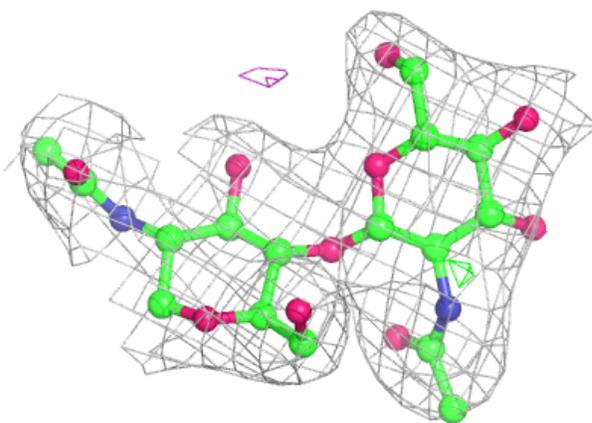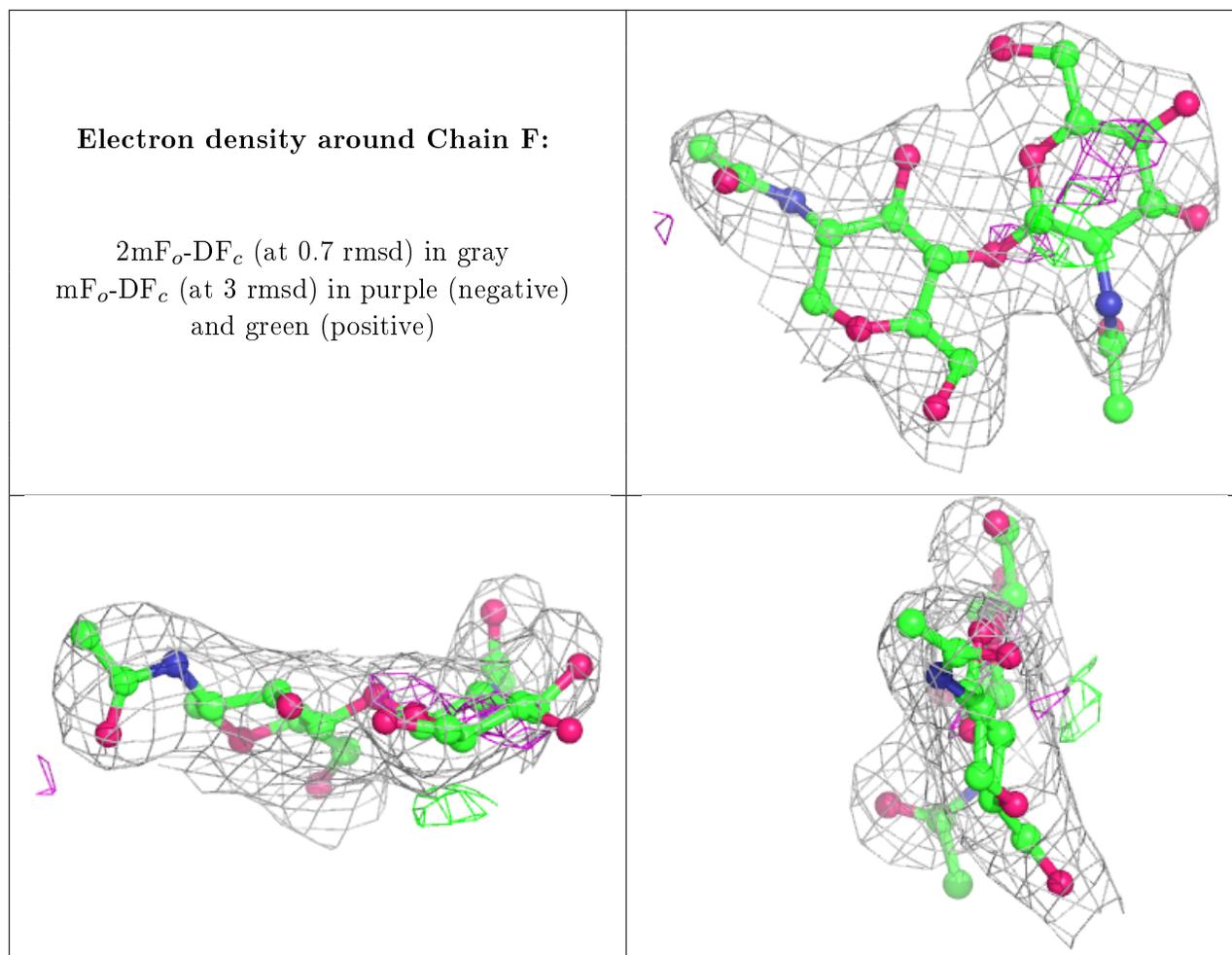
Electron density around Chain F:

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

6.4 Ligands ⓘ

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

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	NAG	B	799	14/15	0.86	0.17	100,104,105,106	0
3	NAG	A	796	14/15	0.89	0.18	85,89,92,92	0
3	NAG	B	800	14/15	0.93	0.19	108,109,110,111	0
4	PF2	B	900	26/26	0.93	0.27	71,73,78,78	0
4	PF2	A	900	26/26	0.94	0.25	73,77,79,81	0

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

Electron density around PF2 B 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
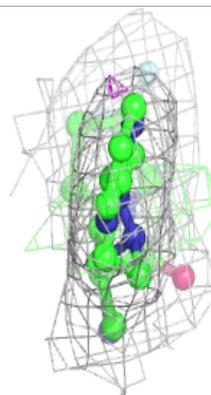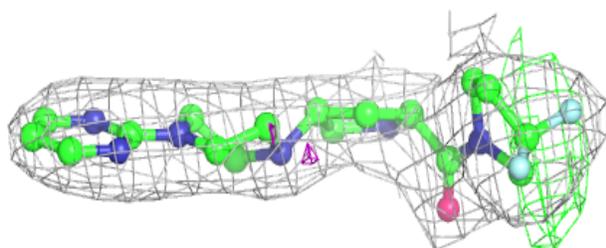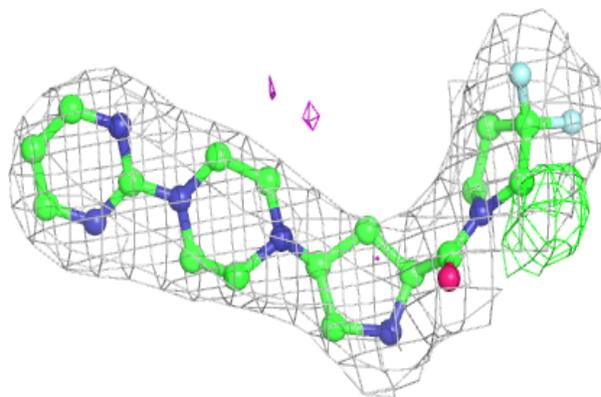
Electron density around PF2 A 900:

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

6.5 Other polymers (i)

There are no such residues in this entry.