



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:52 AM UTC

PDB ID : 2BE2 / pdb\_00002be2  
Title : Crystal structure of HIV-1 reverse transcriptase (RT) in complex with R221239  
Authors : Himmel, D.M.; Das, K.; Clark Jr., A.D.; Hughes, S.H.; Benjahad, A.; Oumouch, S.; Guillemont, J.; Coupa, S.; Poncelet, A.; Csoka, I.; Meyer, C.; Andries, K.; Nguyen, C.H.; Grierson, D.S.; Arnold, E.  
Deposited on : 2005-10-21  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

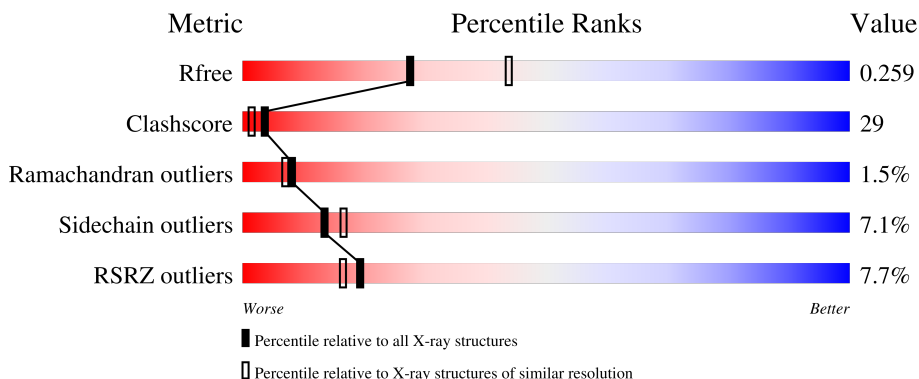
# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	 5% (red), 53% (green), 37% (yellow), 7% (orange), .. (grey)
2	B	430	 10% (red), 57% (green), 33% (yellow), 7% (orange), .. (grey)
3	C	2	 50% (yellow), 50% (orange)
3	D	2	 50% (green), 50% (yellow)

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	GOL	A	3001	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8262 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 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4498	2913	748	830	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

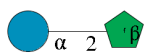
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	426	3525	2297	584	637	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	C	2	23	12	11	0	0	0
3	D	2	23	12	11	0	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

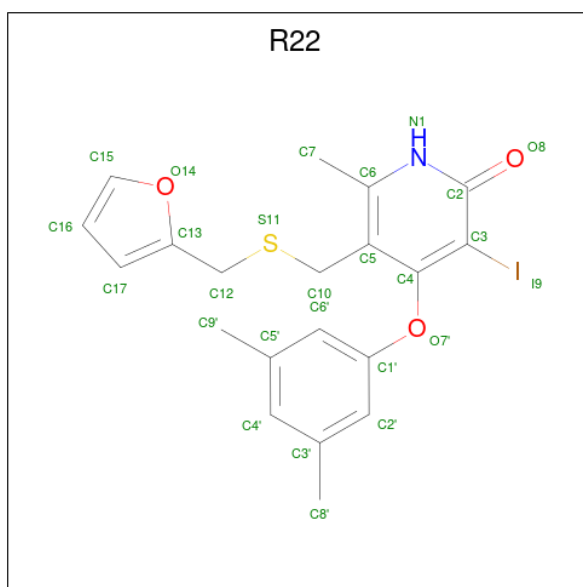


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0

- Molecule 6 is 4-(3,5-DIMETHYLPHENOXY)-5-(FURAN-2-YLMETHYLSULFANYLMETHYL)-3-IODO-6-METHYLPYRIDIN-2(1H)-ONE (CCD ID: R22) (formula: C<sub>20</sub>H<sub>20</sub>INO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	I	N	O			S
6	A	1	26	20	1	1	3	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 94 94	0	0
7	B	60	Total O 60 60	0	0

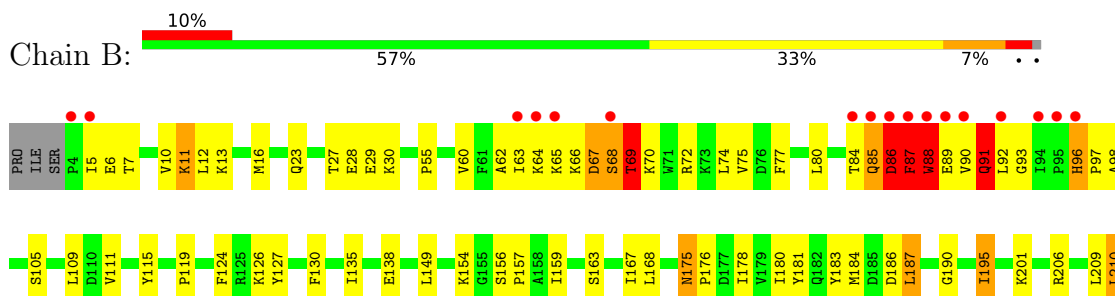
### 3 Residue-property plots

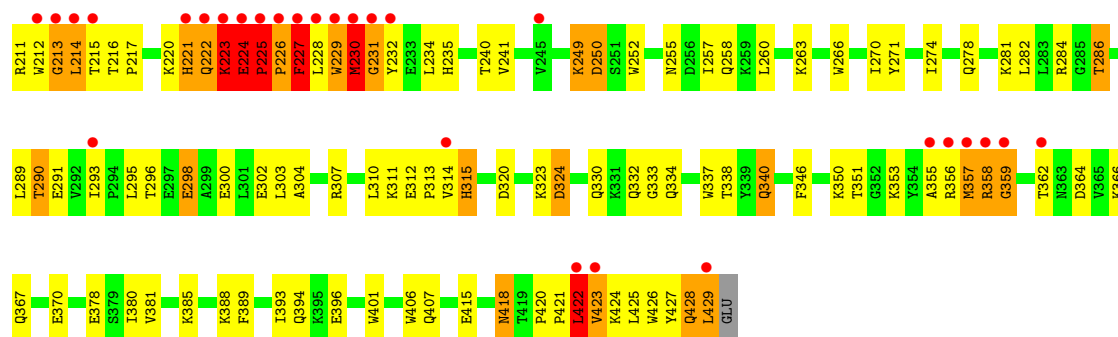
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: REVERSE TRANSCRIPTASE P66 SUBUNIT



- Molecule 2: REVERSE TRANSCRIPTASE P51 SUBUNIT





- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.85Å 68.80Å 104.43Å 90.00° 107.22° 90.00°	Depositor
Resolution (Å)	22.95 – 2.43 22.95 – 2.43	Depositor EDS
% Data completeness (in resolution range)	88.4 (22.95-2.43) 88.3 (22.95-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.44Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.265 0.224 , 0.259	Depositor DCC
$R_{free}$ test set	2554 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, GOL, GLC, R22, MN

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	0.58	1/4616 (0.0%)	1.17	50/6271 (0.8%)
2	B	0.65	1/3629 (0.0%)	1.33	59/4932 (1.2%)
All	All	0.61	2/8245 (0.0%)	1.24	109/11203 (1.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	LEU	CA-C	-7.84	1.48	1.52
2	B	225	PRO	CA-C	5.66	1.57	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	214	LEU	N-CA-C	-15.98	93.09	112.58
2	B	86	ASP	N-CA-C	-13.91	94.33	112.41
2	B	67	ASP	N-CA-C	12.05	136.46	110.80
2	B	89	GLU	N-CA-C	-11.24	86.86	110.80
2	B	85	GLN	N-CA-C	10.12	128.51	108.18
1	A	336	GLN	OE1-CD-NE2	-9.83	112.77	122.60
2	B	91	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	A	334	GLN	OE1-CD-NE2	-9.81	112.79	122.60
2	B	407	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	68	SER	N-CA-C	9.78	124.75	113.02
1	A	332	GLN	OE1-CD-NE2	-9.77	112.83	122.60
2	B	225	PRO	N-CA-C	-9.61	98.98	110.70
2	B	224	GLU	CA-C-N	9.53	130.19	120.38
2	B	224	GLU	C-N-CA	9.53	130.19	120.38
2	B	359	GLY	N-CA-C	-9.51	90.64	113.18
2	B	401	TRP	N-CA-C	9.21	125.69	113.72
2	B	214	LEU	CB-CA-C	9.12	125.53	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225	PRO	CA-C-N	9.01	131.10	119.84
2	B	225	PRO	C-N-CA	9.01	131.10	119.84
2	B	68	SER	N-CA-C	-8.58	102.81	113.20
1	A	435	VAL	N-CA-C	8.48	120.57	111.58
2	B	249	LYS	N-CA-C	8.48	123.22	109.40
1	A	349	LEU	N-CA-C	-8.44	101.31	111.69
1	A	285	GLY	N-CA-C	-8.40	93.28	113.18
1	A	222	GLN	N-CA-C	-8.19	93.36	110.80
2	B	229	TRP	N-CA-C	8.15	125.10	107.49
2	B	85	GLN	CA-C-N	-8.15	109.70	122.49
2	B	85	GLN	C-N-CA	-8.15	109.70	122.49
1	A	113	ASP	N-CA-C	-8.13	100.76	111.74
2	B	222	GLN	N-CA-C	8.06	120.72	110.33
2	B	226	PRO	N-CA-C	8.02	128.98	112.47
1	A	218	ASP	N-CA-C	7.96	119.59	111.07
2	B	423	VAL	N-CA-C	-7.66	101.47	111.05
2	B	87	PHE	CA-C-N	-7.63	106.97	121.54
2	B	87	PHE	C-N-CA	-7.63	106.97	121.54
1	A	287	LYS	N-CA-C	7.60	121.96	111.55
2	B	98	ALA	N-CA-C	7.20	121.82	112.89
2	B	86	ASP	CB-CA-C	7.19	122.67	111.02
2	B	223	LYS	N-CA-C	7.06	125.83	110.80
1	A	217	PRO	CA-C-N	7.02	129.57	120.44
1	A	217	PRO	C-N-CA	7.02	129.57	120.44
2	B	88	TRP	N-CA-C	-6.97	95.96	110.80
1	A	68	SER	CA-C-N	-6.75	109.09	121.52
1	A	68	SER	C-N-CA	-6.75	109.09	121.52
1	A	219	LYS	N-CA-C	-6.72	105.15	113.15
2	B	89	GLU	CB-CA-C	6.71	123.78	110.42
1	A	336	GLN	CG-CD-NE2	6.67	126.41	116.40
2	B	91	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	332	GLN	CG-CD-NE2	6.66	126.39	116.40
2	B	407	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	334	GLN	CG-CD-NE2	6.66	126.38	116.40
2	B	422	LEU	N-CA-C	-6.64	103.58	112.94
1	A	67	ASP	N-CA-C	-6.61	97.47	108.32
2	B	227	PHE	N-CA-C	6.60	124.85	110.80
1	A	139	THR	CA-C-N	6.59	127.11	119.47
1	A	139	THR	C-N-CA	6.59	127.11	119.47
1	A	132	ILE	CA-C-N	6.56	128.04	119.84
1	A	132	ILE	C-N-CA	6.56	128.04	119.84
1	A	26	LEU	N-CA-C	6.53	116.61	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	CA-C-N	-6.49	111.39	122.56
1	A	67	ASP	C-N-CA	-6.49	111.39	122.56
1	A	382	ILE	N-CA-C	6.43	117.21	110.72
2	B	357	MET	N-CA-C	6.38	121.73	113.88
2	B	85	GLN	CB-CA-C	-6.34	101.28	111.86
2	B	67	ASP	CB-CA-C	-6.32	97.85	110.42
1	A	113	ASP	CB-CA-C	-6.23	102.89	111.73
2	B	235	HIS	CA-C-N	6.23	126.69	119.47
2	B	235	HIS	C-N-CA	6.23	126.69	119.47
1	A	282	LEU	CA-C-N	-6.17	113.65	121.98
1	A	282	LEU	C-N-CA	-6.17	113.65	121.98
2	B	96	HIS	CA-C-N	6.12	125.88	119.76
2	B	96	HIS	C-N-CA	6.12	125.88	119.76
2	B	355	ALA	N-CA-C	6.06	118.37	108.55
2	B	69	THR	N-CA-C	-6.05	103.82	111.92
2	B	231	GLY	N-CA-C	-5.98	99.02	113.18
1	A	63	ILE	N-CA-C	5.96	118.58	108.86
2	B	93	GLY	N-CA-C	-5.96	99.06	113.18
2	B	186	ASP	N-CA-C	5.92	119.21	109.85
1	A	134	SER	N-CA-C	5.74	118.75	109.86
2	B	184	MET	CB-CA-C	-5.73	109.98	116.63
1	A	493	VAL	N-CA-C	5.64	116.49	108.42
1	A	54	ASN	CA-C-N	-5.58	112.86	119.84
1	A	54	ASN	C-N-CA	-5.58	112.86	119.84
2	B	216	THR	N-CA-C	5.57	120.75	108.73
1	A	391	LEU	CA-C-N	5.57	126.80	119.84
1	A	391	LEU	C-N-CA	5.57	126.80	119.84
1	A	73	LYS	CB-CA-C	5.55	119.75	109.54
2	B	214	LEU	CA-C-O	5.45	127.11	120.57
2	B	230	MET	N-CA-C	-5.41	99.28	110.80
1	A	132	ILE	CA-C-O	5.40	122.34	119.15
1	A	73	LYS	N-CA-C	-5.39	102.89	110.50
1	A	54	ASN	N-CA-C	5.35	121.64	109.81
1	A	346	PHE	N-CA-C	5.31	120.94	113.56
1	A	224	GLU	CA-C-N	5.27	125.81	120.38
1	A	224	GLU	C-N-CA	5.27	125.81	120.38
1	A	217	PRO	N-CA-C	5.25	119.12	111.03
1	A	151	GLN	N-CA-C	5.25	119.16	112.34
2	B	175	ASN	CA-C-N	5.24	126.39	119.84
2	B	175	ASN	C-N-CA	5.24	126.39	119.84
2	B	213	GLY	N-CA-C	-5.24	100.75	113.18
1	A	12	LEU	N-CA-C	-5.24	103.47	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	389	PHE	N-CA-C	5.16	118.63	109.96
2	B	68	SER	CB-CA-C	5.10	119.81	110.11
1	A	88	TRP	N-CA-C	-5.10	102.37	109.96
2	B	211	ARG	CA-C-N	-5.06	114.65	122.49
2	B	211	ARG	C-N-CA	-5.06	114.65	122.49
2	B	241	VAL	N-CA-C	-5.04	100.95	108.46
1	A	4	PRO	N-CA-C	-5.03	108.94	114.92
2	B	358	ARG	N-CA-C	5.02	118.80	109.56

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4498	0	4560	284	0
2	B	3525	0	3562	202	0
3	C	23	0	21	3	0
3	D	23	0	21	0	0
4	A	12	0	16	5	0
5	A	1	0	0	0	0
6	A	26	0	20	2	0
7	A	94	0	0	5	0
7	B	60	0	0	3	0
All	All	8262	0	8200	476	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 29.

All (476) 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:A:333:GLY:O	1:A:334:GLN:HG2	1.20	1.31
2:B:88:TRP:H	2:B:90:VAL:HG23	1.08	1.13
1:A:296:THR:HG23	1:A:299:ALA:H	1.09	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:OD1	1:A:259:LYS:HE3	1.52	1.09
1:A:26:LEU:HG	1:A:27:THR:H	1.10	1.08
1:A:330:GLN:HE21	1:A:338:THR:HG23	1.17	1.08
2:B:224:GLU:HB3	2:B:225:PRO:HD3	1.20	1.08
1:A:134:SER:OG	1:A:139:THR:HG22	1.53	1.05
1:A:134:SER:HB2	1:A:139:THR:O	1.55	1.05
2:B:11:LYS:HE2	2:B:11:LYS:H	1.12	1.05
2:B:257:ILE:HD12	2:B:293:ILE:HD11	1.41	1.01
1:A:296:THR:HG22	1:A:299:ALA:CB	1.90	1.01
2:B:90:VAL:HG12	2:B:90:VAL:O	1.58	1.01
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.41	0.99
1:A:253:THR:HG23	1:A:256:ASP:H	1.28	0.98
1:A:333:GLY:O	1:A:334:GLN:CG	2.11	0.97
2:B:63:ILE:HG21	2:B:406:TRP:O	1.64	0.97
2:B:85:GLN:CD	2:B:85:GLN:O	2.09	0.96
2:B:68:SER:HB3	2:B:70:LYS:HE2	1.46	0.96
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.46	0.95
1:A:195:ILE:HD12	1:A:195:ILE:H	1.29	0.95
2:B:224:GLU:CB	2:B:225:PRO:HD3	1.96	0.93
1:A:333:GLY:C	1:A:334:GLN:HG2	1.93	0.93
2:B:65:LYS:HE3	2:B:70:LYS:HD2	1.49	0.93
1:A:50:ILE:HD12	1:A:55:PRO:HG2	1.49	0.92
2:B:418:ASN:H	2:B:418:ASN:HD22	1.14	0.91
1:A:139:THR:OG1	1:A:140:PRO:HD2	1.69	0.91
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.50	0.91
2:B:206:ARG:HE	2:B:217:PRO:HG2	1.36	0.90
1:A:131:THR:CG2	1:A:143:ARG:HE	1.86	0.89
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.08	0.89
2:B:63:ILE:HG22	2:B:64:LYS:N	1.86	0.89
1:A:56:TYR:HD1	1:A:56:TYR:H	1.20	0.88
1:A:362:THR:HG22	1:A:363:ASN:H	1.39	0.87
2:B:11:LYS:HE2	2:B:11:LYS:N	1.90	0.86
1:A:500:GLN:H	4:A:3001:GOL:H12	1.39	0.85
2:B:84:THR:O	2:B:87:PHE:HE2	1.59	0.85
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.54	0.85
1:A:296:THR:CG2	1:A:299:ALA:H	1.89	0.85
2:B:429:LEU:HD23	2:B:429:LEU:H	1.41	0.85
2:B:270:ILE:HG22	2:B:314:VAL:HG21	1.58	0.85
2:B:13:LYS:NZ	2:B:86:ASP:HB2	1.92	0.85
2:B:63:ILE:HG22	2:B:64:LYS:H	1.42	0.85
1:A:54:ASN:ND2	1:A:54:ASN:O	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:THR:HG22	1:A:299:ALA:HB3	1.59	0.84
1:A:109:LEU:HB3	1:A:216:THR:CG2	2.06	0.84
1:A:296:THR:HG23	1:A:299:ALA:N	1.91	0.84
1:A:26:LEU:CG	1:A:27:THR:H	1.91	0.84
1:A:131:THR:HG23	1:A:143:ARG:HE	1.42	0.83
1:A:362:THR:HG22	1:A:363:ASN:N	1.92	0.83
1:A:296:THR:CG2	1:A:299:ALA:CB	2.56	0.83
2:B:87:PHE:CG	2:B:87:PHE:O	2.31	0.82
1:A:26:LEU:HG	1:A:27:THR:N	1.92	0.82
1:A:240:THR:HG22	1:A:241:VAL:H	1.44	0.82
1:A:282:LEU:O	1:A:282:LEU:HG	1.77	0.82
1:A:478:GLU:HG2	1:A:499:SER:CB	2.09	0.82
1:A:500:GLN:N	4:A:3001:GOL:H12	1.93	0.82
2:B:67:ASP:C	2:B:69:THR:H	1.85	0.82
1:A:134:SER:CB	1:A:139:THR:O	2.28	0.81
1:A:218:ASP:C	1:A:220:LYS:H	1.87	0.81
1:A:478:GLU:CG	1:A:499:SER:HB2	2.10	0.80
1:A:22:LYS:HE3	1:A:23:GLN:O	1.81	0.80
1:A:109:LEU:HB3	1:A:216:THR:HG22	1.64	0.79
1:A:56:TYR:N	1:A:56:TYR:CD1	2.47	0.79
2:B:13:LYS:HZ2	2:B:86:ASP:HB2	1.47	0.79
2:B:252:TRP:NE1	2:B:295:LEU:HD11	1.96	0.79
2:B:27:THR:HG22	2:B:29:GLU:H	1.46	0.78
2:B:66:LYS:O	2:B:66:LYS:HD3	1.83	0.78
1:A:19:PRO:O	1:A:56:TYR:HB3	1.84	0.78
1:A:343:GLN:HG3	1:A:349:LEU:HD21	1.63	0.78
1:A:308:GLU:OE1	1:A:311:LYS:HD2	1.83	0.78
2:B:88:TRP:N	2:B:90:VAL:HG23	1.94	0.78
2:B:257:ILE:CD1	2:B:293:ILE:HD11	2.13	0.78
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.65	0.78
2:B:68:SER:O	2:B:69:THR:OG1	2.02	0.77
1:A:253:THR:HG22	1:A:256:ASP:OD2	1.84	0.77
1:A:296:THR:CG2	1:A:299:ALA:HB2	2.14	0.76
1:A:330:GLN:NE2	1:A:338:THR:HG23	1.97	0.76
2:B:90:VAL:O	2:B:90:VAL:CG1	2.30	0.76
1:A:63:ILE:HG23	1:A:64:LYS:HE2	1.68	0.75
1:A:195:ILE:O	1:A:199:ARG:HG3	1.87	0.75
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.67	0.75
2:B:63:ILE:CG2	2:B:64:LYS:H	2.00	0.74
1:A:88:TRP:HD1	7:A:1154:HOH:O	1.69	0.74
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:256:ASP:CG	2.14	0.73
1:A:257:ILE:CG2	1:A:283:LEU:HD13	2.18	0.73
1:A:344:GLU:OE1	1:A:347:LYS:HD2	1.88	0.73
2:B:227:PHE:HD2	2:B:228:LEU:HG	1.52	0.73
1:A:50:ILE:HD12	1:A:55:PRO:CG	2.18	0.73
1:A:240:THR:HG22	1:A:241:VAL:N	2.01	0.73
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.54	0.72
1:A:217:PRO:HB3	1:A:222:GLN:HG2	1.72	0.72
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.37	0.72
2:B:63:ILE:CG2	2:B:64:LYS:N	2.53	0.71
2:B:388:LYS:HE2	2:B:415:GLU:OE1	1.92	0.70
2:B:12:LEU:CD2	2:B:84:THR:HG22	2.22	0.70
1:A:348:ASN:OD1	3:C:1:GLC:H61	1.91	0.70
1:A:547:GLN:HG3	2:B:286:THR:HG22	1.74	0.70
2:B:250:ASP:OD2	2:B:250:ASP:N	2.25	0.70
2:B:91:GLN:O	2:B:92:LEU:HG	1.92	0.69
2:B:85:GLN:O	2:B:85:GLN:CG	2.38	0.69
1:A:254:VAL:HB	1:A:288:ALA:O	1.91	0.69
1:A:366:LYS:O	1:A:370:GLU:HG3	1.91	0.69
1:A:254:VAL:CG2	1:A:293:ILE:HD11	2.20	0.69
2:B:282:LEU:HB3	2:B:293:ILE:HD12	1.73	0.69
1:A:132:ILE:HG12	1:A:142:ILE:HG12	1.75	0.69
1:A:197:GLN:O	1:A:200:THR:HB	1.93	0.69
2:B:67:ASP:C	2:B:69:THR:N	2.51	0.68
1:A:362:THR:CG2	1:A:363:ASN:H	2.06	0.68
2:B:84:THR:O	2:B:87:PHE:CE2	2.45	0.68
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.23	0.68
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.76	0.68
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.76	0.68
2:B:65:LYS:HE3	2:B:70:LYS:CD	2.23	0.67
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.29	0.67
1:A:139:THR:CB	1:A:140:PRO:HD2	2.25	0.67
1:A:92:LEU:HD12	1:A:93:GLY:N	2.09	0.67
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.31	0.66
2:B:223:LYS:N	2:B:229:TRP:O	2.29	0.66
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.11	0.66
2:B:420:PRO:HD2	2:B:422:LEU:HD23	1.77	0.66
2:B:249:LYS:HB2	2:B:252:TRP:NE1	2.11	0.65
2:B:314:VAL:HG12	2:B:315:HIS:N	2.12	0.65
1:A:109:LEU:HB3	1:A:216:THR:HG21	1.78	0.65
2:B:223:LYS:HA	2:B:229:TRP:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:HB2	4:A:3001:GOL:O2	1.95	0.65
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.61	0.65
2:B:96:HIS:HE1	2:B:381:VAL:O	1.80	0.65
2:B:87:PHE:O	2:B:87:PHE:CD2	2.49	0.65
1:A:22:LYS:HD2	1:A:23:GLN:H	1.62	0.64
2:B:222:GLN:HA	2:B:229:TRP:O	1.97	0.64
2:B:84:THR:HG21	2:B:124:PHE:HZ	1.62	0.64
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
1:A:65:LYS:HE2	1:A:67:ASP:HB3	1.78	0.64
1:A:362:THR:CG2	1:A:363:ASN:N	2.61	0.64
2:B:418:ASN:HD22	2:B:418:ASN:N	1.85	0.64
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.27	0.64
2:B:281:LYS:HA	2:B:284:ARG:NH1	2.13	0.64
2:B:6:GLU:O	2:B:6:GLU:HG3	1.98	0.64
1:A:503:LEU:HD12	1:A:533:LEU:CD1	2.28	0.64
1:A:19:PRO:O	1:A:56:TYR:CB	2.47	0.63
1:A:88:TRP:CD1	7:A:1154:HOH:O	2.46	0.63
1:A:317:VAL:HG12	1:A:348:ASN:O	1.99	0.63
1:A:265:ASN:O	1:A:268:SER:HB3	1.98	0.63
1:A:17:ASP:O	1:A:83:ARG:HD3	1.99	0.63
1:A:348:ASN:OD1	3:C:1:GLC:C6	2.47	0.63
1:A:134:SER:OG	1:A:135:ILE:N	2.32	0.63
1:A:54:ASN:O	1:A:55:PRO:C	2.36	0.63
1:A:257:ILE:HD12	1:A:293:ILE:HD12	1.81	0.62
1:A:218:ASP:C	1:A:220:LYS:N	2.56	0.62
2:B:296:THR:HB	2:B:298:GLU:OE2	1.99	0.62
1:A:330:GLN:HE21	1:A:338:THR:CG2	2.04	0.62
2:B:314:VAL:HG12	2:B:315:HIS:H	1.64	0.62
1:A:63:ILE:HG22	1:A:64:LYS:N	2.15	0.62
2:B:13:LYS:HE3	2:B:86:ASP:H	1.64	0.61
2:B:227:PHE:O	2:B:228:LEU:HD23	2.01	0.61
2:B:63:ILE:CG2	2:B:406:TRP:O	2.46	0.61
2:B:85:GLN:O	2:B:85:GLN:NE2	2.32	0.61
1:A:317:VAL:HG22	1:A:318:TYR:N	2.15	0.61
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.67	0.61
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.82	0.61
1:A:342:TYR:HA	1:A:349:LEU:CD2	2.30	0.61
1:A:51:GLY:HA3	1:A:53:GLU:OE1	2.01	0.61
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.35	0.61
2:B:126:LYS:HG2	2:B:127:TYR:N	2.15	0.61
1:A:460:ASN:H	1:A:460:ASN:HD22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:H	1:A:55:PRO:HD3	1.65	0.60
1:A:112:GLY:O	1:A:113:ASP:HB2	1.99	0.60
1:A:255:ASN:OD1	1:A:259:LYS:CE	2.40	0.60
2:B:220:LYS:HD2	2:B:231:GLY:O	2.02	0.60
2:B:324:ASP:OD1	2:B:324:ASP:N	2.26	0.60
1:A:253:THR:OG1	1:A:290:THR:HA	2.00	0.60
2:B:5:ILE:HG23	2:B:119:PRO:HG3	1.82	0.60
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.16	0.60
1:A:547:GLN:HG3	2:B:286:THR:CG2	2.31	0.60
1:A:55:PRO:HB3	1:A:129:ALA:HB2	1.82	0.60
1:A:439:THR:H	1:A:460:ASN:ND2	2.00	0.59
2:B:5:ILE:HG22	2:B:7:THR:HG23	1.84	0.59
2:B:63:ILE:HD13	2:B:406:TRP:HB3	1.84	0.59
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.83	0.59
2:B:210:LEU:HD13	2:B:217:PRO:HD2	1.83	0.59
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.85	0.59
2:B:68:SER:CB	2:B:70:LYS:HE2	2.28	0.59
2:B:224:GLU:HB3	2:B:225:PRO:CD	2.14	0.59
1:A:134:SER:CB	1:A:139:THR:HG22	2.33	0.59
1:A:518:VAL:O	1:A:522:ILE:HG13	2.02	0.59
1:A:50:ILE:CD1	1:A:55:PRO:HG2	2.27	0.59
1:A:63:ILE:CG2	1:A:64:LYS:N	2.66	0.59
1:A:181:TYR:CZ	2:B:138:GLU:HG3	2.38	0.59
1:A:253:THR:HG23	1:A:256:ASP:N	2.10	0.58
2:B:249:LYS:CB	2:B:252:TRP:CE2	2.84	0.58
2:B:266:TRP:CG	2:B:425:LEU:HD13	2.38	0.58
2:B:88:TRP:CH2	2:B:159:ILE:CG1	2.86	0.58
1:A:132:ILE:CG1	1:A:142:ILE:HG12	2.34	0.57
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.85	0.57
2:B:266:TRP:CE3	2:B:425:LEU:HB3	2.39	0.57
1:A:411:ILE:HG22	1:A:412:PRO:O	2.04	0.57
1:A:240:THR:CG2	1:A:241:VAL:H	2.15	0.57
1:A:253:THR:CG2	1:A:256:ASP:H	2.09	0.57
1:A:478:GLU:CG	1:A:499:SER:CB	2.79	0.57
1:A:376:THR:HG23	1:A:386:THR:HG22	1.85	0.57
1:A:94:ILE:HD12	1:A:230:MET:HE2	1.87	0.56
2:B:68:SER:C	2:B:69:THR:HG1	2.10	0.56
2:B:263:LYS:HA	2:B:425:LEU:HD22	1.86	0.56
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.87	0.56
2:B:12:LEU:HD22	2:B:84:THR:HG22	1.87	0.56
2:B:88:TRP:CH2	2:B:159:ILE:HG13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:GLU:CD	2:B:298:GLU:H	2.14	0.56
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.87	0.56
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.41	0.56
1:A:34:LEU:HD13	1:A:132:ILE:HG22	1.87	0.56
1:A:65:LYS:HB3	1:A:70:LYS:O	2.06	0.56
1:A:132:ILE:HD11	1:A:142:ILE:CD1	2.36	0.56
2:B:307:ARG:O	2:B:311:LYS:HG3	2.05	0.55
2:B:258:GLN:NE2	7:B:1061:HOH:O	2.30	0.55
2:B:210:LEU:CD1	2:B:217:PRO:HD2	2.37	0.55
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.37	0.55
1:A:223:LYS:HD2	1:A:225:PRO:HD3	1.88	0.55
2:B:11:LYS:HE3	2:B:87:PHE:CZ	2.42	0.55
2:B:284:ARG:HG3	2:B:284:ARG:NH1	2.22	0.54
1:A:139:THR:OG1	1:A:140:PRO:CD	2.49	0.54
1:A:3:SER:HB2	1:A:117:SER:O	2.06	0.54
1:A:194:GLU:OE1	1:A:197:GLN:NE2	2.40	0.54
1:A:195:ILE:H	1:A:195:ILE:CD1	2.06	0.54
2:B:420:PRO:HD2	2:B:422:LEU:CD2	2.37	0.54
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.89	0.54
1:A:5:ILE:HD13	1:A:163:SER:HB3	1.89	0.54
2:B:65:LYS:HB3	2:B:72:ARG:HH11	1.73	0.54
1:A:257:ILE:HG21	1:A:283:LEU:HD13	1.89	0.53
1:A:279:LEU:HD21	1:A:299:ALA:O	2.07	0.53
1:A:317:VAL:CG2	1:A:318:TYR:N	2.72	0.53
1:A:516:GLU:CD	1:A:516:GLU:H	2.15	0.53
1:A:194:GLU:CD	1:A:194:GLU:H	2.16	0.53
1:A:221:HIS:HB2	1:A:223:LYS:CG	2.38	0.53
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.55	0.53
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.39	0.53
1:A:94:ILE:HD11	1:A:183:TYR:CZ	2.44	0.53
1:A:201:LYS:O	1:A:204:GLU:HB2	2.09	0.52
1:A:254:VAL:CB	1:A:288:ALA:O	2.56	0.52
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.91	0.52
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.52
1:A:418:ASN:C	1:A:418:ASN:HD22	2.17	0.52
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.09	0.52
2:B:420:PRO:O	2:B:422:LEU:N	2.40	0.52
1:A:22:LYS:HD2	1:A:23:GLN:N	2.23	0.52
2:B:230:MET:O	2:B:231:GLY:C	2.50	0.52
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.43	0.52
1:A:102:LYS:O	1:A:103:LYS:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD11	1:A:507:GLN:OE1	2.09	0.52
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.74	0.52
2:B:10:VAL:HG22	2:B:88:TRP:CZ2	2.45	0.52
2:B:230:MET:O	2:B:232:TYR:N	2.43	0.52
1:A:177:ASP:OD1	1:A:178:ILE:HG12	2.10	0.51
1:A:134:SER:O	1:A:135:ILE:C	2.53	0.51
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.93	0.51
2:B:206:ARG:HE	2:B:217:PRO:CG	2.17	0.51
2:B:88:TRP:CZ3	2:B:159:ILE:HG13	2.46	0.51
2:B:249:LYS:HG3	2:B:252:TRP:CD2	2.46	0.51
2:B:88:TRP:HH2	2:B:159:ILE:HD11	1.75	0.51
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.93	0.51
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.46	0.51
2:B:393:ILE:HG12	2:B:394:GLN:N	2.26	0.51
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.92	0.50
2:B:333:GLY:O	2:B:334:GLN:HB2	2.10	0.50
1:A:1:PRO:C	1:A:2:ILE:HG12	2.36	0.50
1:A:54:ASN:O	1:A:54:ASN:CG	2.53	0.50
1:A:151:GLN:NE2	7:A:1066:HOH:O	2.44	0.50
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.11	0.50
1:A:50:ILE:HG21	1:A:145:GLN:HB3	1.93	0.50
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.11	0.50
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.93	0.50
1:A:55:PRO:CB	1:A:129:ALA:HB2	2.41	0.50
1:A:65:LYS:C	1:A:67:ASP:H	2.20	0.50
1:A:295:LEU:HD23	1:A:300:GLU:HG2	1.93	0.50
1:A:257:ILE:HD12	1:A:293:ILE:CD1	2.41	0.49
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.42	0.49
2:B:13:LYS:HZ1	2:B:86:ASP:HB2	1.74	0.49
1:A:544:GLY:HA2	2:B:286:THR:HB	1.94	0.49
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.42	0.49
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.48	0.49
2:B:220:LYS:HB2	2:B:231:GLY:H	1.77	0.49
2:B:80:LEU:HD11	2:B:84:THR:HG21	1.94	0.49
2:B:252:TRP:CG	2:B:295:LEU:HD21	2.48	0.49
1:A:296:THR:CG2	1:A:299:ALA:HB3	2.31	0.49
1:A:378:GLU:HG2	1:A:382:ILE:HD12	1.93	0.49
2:B:212:TRP:HA	2:B:212:TRP:CE3	2.47	0.49
2:B:358:ARG:C	2:B:359:GLY:O	2.49	0.49
1:A:457:TYR:C	1:A:457:TYR:CD2	2.91	0.49
2:B:6:GLU:O	2:B:6:GLU:CG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:HG12	2:B:394:GLN:H	1.76	0.49
1:A:447:ASN:O	1:A:451:LYS:HA	2.12	0.49
2:B:175:ASN:OD1	2:B:201:LYS:HD2	2.13	0.49
1:A:55:PRO:CB	1:A:129:ALA:CB	2.90	0.48
2:B:88:TRP:CH2	2:B:159:ILE:HD11	2.48	0.48
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.94	0.48
2:B:350:LYS:NZ	2:B:378:GLU:OE1	2.46	0.48
1:A:298:GLU:H	1:A:298:GLU:CD	2.21	0.48
2:B:65:LYS:CE	2:B:70:LYS:HD2	2.33	0.48
1:A:103:LYS:HE2	1:A:179:VAL:HG21	1.94	0.48
1:A:129:ALA:HA	1:A:144:TYR:O	2.14	0.48
1:A:142:ILE:HD11	1:A:144:TYR:HE1	1.78	0.48
1:A:470:THR:O	1:A:471:ASN:C	2.55	0.48
1:A:324:ASP:HA	7:A:1014:HOH:O	2.13	0.48
1:A:516:GLU:O	1:A:520:GLN:HG3	2.12	0.48
1:A:94:ILE:HD11	1:A:183:TYR:CE1	2.48	0.48
1:A:126:LYS:HE2	1:A:127:TYR:CZ	2.48	0.48
1:A:142:ILE:HD11	1:A:144:TYR:CE1	2.48	0.48
1:A:516:GLU:HG2	1:A:517:LEU:N	2.29	0.48
1:A:542:ILE:N	1:A:542:ILE:HD12	2.29	0.48
1:A:139:THR:HG23	1:A:141:GLY:H	1.78	0.47
1:A:55:PRO:HB3	1:A:129:ALA:CB	2.45	0.47
1:A:131:THR:HG21	1:A:143:ARG:HE	1.73	0.47
2:B:97:PRO:HD2	2:B:181:TYR:CD1	2.50	0.47
2:B:346:PHE:N	2:B:346:PHE:CD2	2.79	0.47
2:B:418:ASN:N	2:B:418:ASN:ND2	2.57	0.47
1:A:63:ILE:HG22	1:A:64:LYS:O	2.15	0.47
1:A:194:GLU:O	1:A:197:GLN:N	2.47	0.47
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.97	0.47
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.49	0.47
2:B:252:TRP:HE1	2:B:295:LEU:HD11	1.76	0.47
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.96	0.47
1:A:255:ASN:HB2	1:A:289:LEU:O	2.15	0.47
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.12	0.47
2:B:87:PHE:CD2	2:B:87:PHE:C	2.93	0.47
2:B:366:LYS:O	2:B:370:GLU:HG3	2.15	0.47
1:A:66:LYS:O	1:A:66:LYS:HG2	2.15	0.47
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.50	0.47
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.96	0.47
1:A:3:SER:HA	1:A:4:PRO:HD3	1.67	0.47
2:B:222:GLN:C	2:B:229:TRP:O	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:NE2	2:B:154:LYS:HD3	2.30	0.46
2:B:92:LEU:HD23	2:B:92:LEU:HA	1.80	0.46
1:A:254:VAL:HA	1:A:293:ILE:CD1	2.45	0.46
1:A:282:LEU:O	1:A:282:LEU:CG	2.54	0.46
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.45	0.46
2:B:320:ASP:OD1	2:B:320:ASP:C	2.57	0.46
1:A:23:GLN:OE1	1:A:60:VAL:HG23	2.14	0.46
1:A:132:ILE:HD11	1:A:142:ILE:HD11	1.97	0.46
1:A:216:THR:HG22	1:A:217:PRO:HD3	1.97	0.46
1:A:320:ASP:O	1:A:343:GLN:NE2	2.48	0.46
2:B:11:LYS:H	2:B:11:LYS:CE	2.04	0.46
2:B:91:GLN:O	2:B:91:GLN:HG3	2.15	0.46
1:A:72:ARG:HD2	1:A:72:ARG:HA	1.74	0.46
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.98	0.46
2:B:290:THR:O	2:B:291:GLU:C	2.58	0.46
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.46
1:A:223:LYS:HD2	1:A:223:LYS:C	2.40	0.46
1:A:454:LYS:HD2	1:A:552:VAL:O	2.16	0.46
1:A:50:ILE:CG2	1:A:145:GLN:HB3	2.46	0.45
1:A:546:GLU:OE1	1:A:546:GLU:HA	2.15	0.45
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.97	0.45
2:B:175:ASN:HB3	2:B:178:ILE:HD12	1.98	0.45
1:A:169:GLU:N	1:A:170:PRO:HD2	2.31	0.45
1:A:407:GLN:NE2	7:A:1033:HOH:O	2.49	0.45
2:B:337:TRP:O	2:B:353:LYS:HA	2.15	0.45
2:B:427:TYR:CD1	2:B:428:GLN:O	2.68	0.45
1:A:308:GLU:O	1:A:311:LYS:HB2	2.16	0.45
1:A:500:GLN:H	4:A:3001:GOL:C1	2.21	0.45
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.96	0.45
1:A:36:GLU:O	1:A:39:THR:HG22	2.15	0.45
1:A:229:TRP:O	1:A:232:TYR:HB2	2.16	0.45
1:A:103:LYS:HE2	1:A:179:VAL:CG2	2.46	0.45
2:B:63:ILE:HD12	2:B:74:LEU:HD22	1.99	0.45
2:B:332:GLN:HE22	2:B:423:VAL:HB	1.81	0.45
1:A:236:PRO:HA	6:A:4002:R22:C15	2.47	0.45
2:B:206:ARG:NE	2:B:217:PRO:HG2	2.17	0.45
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.52	0.45
1:A:221:HIS:C	1:A:223:LYS:H	2.24	0.45
1:A:408:ALA:O	2:B:393:ILE:HG13	2.16	0.45
1:A:55:PRO:HB2	1:A:129:ALA:CB	2.46	0.45
1:A:65:LYS:HG2	1:A:67:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:O	1:A:305:GLU:HG3	2.17	0.45
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.97	0.45
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.98	0.45
2:B:300:GLU:OE1	2:B:304:ALA:HB2	2.17	0.45
2:B:314:VAL:CG1	2:B:315:HIS:N	2.80	0.45
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.81	0.44
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.17	0.44
1:A:447:ASN:O	1:A:451:LYS:N	2.51	0.44
1:A:35:VAL:HG22	1:A:132:ILE:HD12	2.00	0.44
1:A:51:GLY:C	1:A:53:GLU:H	2.26	0.44
1:A:255:ASN:O	1:A:259:LYS:HG3	2.18	0.44
1:A:454:LYS:CB	1:A:552:VAL:HG13	2.46	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.53	0.44
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.99	0.44
2:B:282:LEU:N	2:B:282:LEU:HD12	2.33	0.44
1:A:206:ARG:NH1	1:A:217:PRO:O	2.50	0.44
1:A:218:ASP:C	1:A:218:ASP:OD1	2.59	0.44
1:A:368:LEU:O	1:A:372:VAL:HG23	2.18	0.44
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.99	0.44
1:A:77:PHE:O	1:A:80:LEU:N	2.51	0.44
1:A:357:MET:O	1:A:358:ARG:HB2	2.17	0.43
2:B:65:LYS:HE3	2:B:70:LYS:CE	2.48	0.43
2:B:340:GLN:NE2	7:B:1043:HOH:O	2.51	0.43
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.53	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
2:B:12:LEU:HD23	2:B:124:PHE:HE1	1.84	0.43
2:B:80:LEU:CD1	2:B:84:THR:CG2	2.97	0.43
2:B:156:SER:N	2:B:157:PRO:HD2	2.32	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
2:B:213:GLY:CA	2:B:215:THR:HG23	2.49	0.43
1:A:113:ASP:O	1:A:114:ALA:C	2.58	0.43
2:B:252:TRP:CE2	2:B:295:LEU:HD11	2.53	0.43
1:A:77:PHE:O	1:A:78:ARG:C	2.61	0.43
1:A:148:VAL:O	1:A:150:PRO:HD3	2.18	0.43
1:A:314:VAL:HG12	1:A:315:HIS:N	2.34	0.43
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.00	0.43
1:A:503:LEU:HD12	1:A:533:LEU:HD12	2.00	0.43
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.54	0.43
2:B:220:LYS:O	2:B:230:MET:HA	2.19	0.43
2:B:224:GLU:CB	2:B:225:PRO:CD	2.82	0.43
2:B:424:LYS:NZ	7:B:1082:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLN:HB2	4:A:3001:GOL:C1	2.49	0.43
2:B:212:TRP:HA	2:B:212:TRP:HE3	1.84	0.43
1:A:547:GLN:H	1:A:547:GLN:HG2	1.60	0.42
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.46	0.42
1:A:31:ILE:O	1:A:35:VAL:HG23	2.19	0.42
1:A:175:ASN:C	1:A:177:ASP:N	2.77	0.42
2:B:300:GLU:C	2:B:302:GLU:N	2.76	0.42
2:B:312:GLU:O	2:B:313:PRO:C	2.61	0.42
1:A:227:PHE:CD2	6:A:4002:R22:H122	2.54	0.42
1:A:451:LYS:HB3	1:A:451:LYS:HE2	1.82	0.42
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.54	0.42
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.50	0.42
1:A:94:ILE:HD11	1:A:230:MET:HE2	2.00	0.42
1:A:317:VAL:CG2	1:A:318:TYR:H	2.31	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.42
2:B:220:LYS:HB2	2:B:231:GLY:N	2.34	0.42
2:B:323:LYS:O	2:B:385:LYS:NZ	2.53	0.42
1:A:65:LYS:CE	1:A:67:ASP:HB3	2.47	0.42
1:A:406:TRP:CH2	1:A:407:GLN:OE1	2.73	0.42
1:A:503:LEU:HD12	1:A:533:LEU:HD11	2.01	0.42
2:B:11:LYS:N	2:B:11:LYS:CE	2.71	0.42
2:B:85:GLN:HA	2:B:87:PHE:HD2	1.84	0.42
1:A:257:ILE:HB	1:A:283:LEU:CD1	2.50	0.42
2:B:257:ILE:HD12	2:B:293:ILE:CD1	2.30	0.42
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.84	0.42
1:A:194:GLU:CD	1:A:194:GLU:N	2.78	0.42
2:B:213:GLY:HA3	2:B:215:THR:HG23	2.02	0.42
2:B:96:HIS:CE1	2:B:381:VAL:O	2.68	0.41
2:B:300:GLU:HA	2:B:303:LEU:HB3	2.00	0.41
2:B:350:LYS:HG2	2:B:351:THR:N	2.34	0.41
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.50	0.41
2:B:84:THR:CG2	2:B:124:PHE:HZ	2.32	0.41
2:B:422:LEU:HD12	2:B:426:TRP:CD1	2.56	0.41
2:B:423:VAL:HG23	2:B:424:LYS:N	2.36	0.41
1:A:142:ILE:CD1	1:A:144:TYR:CE1	3.03	0.41
2:B:424:LYS:HA	2:B:427:TYR:HD2	1.85	0.41
1:A:348:ASN:CG	3:C:1:GLC:H61	2.45	0.41
1:A:131:THR:HG22	1:A:143:ARG:HG2	2.03	0.41
2:B:80:LEU:HD12	2:B:84:THR:HG23	2.02	0.41
1:A:21:VAL:HB	1:A:59:PRO:HD3	2.01	0.41
2:B:209:LEU:HB3	2:B:215:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:GLU:C	2:B:302:GLU:H	2.28	0.41
1:A:291:GLU:OE1	1:A:292:VAL:O	2.39	0.41
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.77	0.41
2:B:68:SER:C	2:B:69:THR:OG1	2.58	0.41
2:B:13:LYS:O	2:B:16:MET:HB2	2.21	0.41
1:A:254:VAL:HA	1:A:293:ILE:HD12	2.03	0.41
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.56	0.41
1:A:439:THR:H	1:A:460:ASN:HD21	1.66	0.41
1:A:10:VAL:HG12	1:A:11:LYS:N	2.36	0.40
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.56	0.40
1:A:198:HIS:C	1:A:200:THR:N	2.77	0.40
1:A:360:ALA:HB3	1:A:361:HIS:NE2	2.36	0.40
1:A:406:TRP:CH2	2:B:418:ASN:CA	3.01	0.40
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.55	0.40
1:A:1:PRO:HB2	1:A:46:LYS:CE	2.52	0.40
1:A:240:THR:CG2	1:A:241:VAL:N	2.70	0.40
1:A:470:THR:CG2	1:A:471:ASN:N	2.83	0.40
2:B:195:ILE:H	2:B:195:ILE:HG13	1.58	0.40
2:B:278:GLN:HA	2:B:278:GLN:OE1	2.21	0.40
1:A:35:VAL:O	1:A:39:THR:HG22	2.22	0.40
1:A:194:GLU:O	1:A:196:GLY:N	2.55	0.40
2:B:30:LYS:HB3	2:B:62:ALA:HB3	2.03	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	550/560 (98%)	497 (90%)	45 (8%)	8 (2%)	8	7
2	B	424/430 (99%)	371 (88%)	46 (11%)	7 (2%)	7	6
All	All	974/990 (98%)	868 (89%)	91 (9%)	15 (2%)	8	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	54	ASN
1	A	2	ILE
1	A	195	ILE
2	B	221	HIS
1	A	56	TYR
2	B	226	PRO
1	A	27	THR
1	A	243	PRO
1	A	471	ASN
2	B	421	PRO
2	B	223	LYS
2	B	224	GLU
2	B	176	PRO
2	B	225	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/500 (99%)	459 (93%)	35 (7%)	13	16
2	B	388/392 (99%)	360 (93%)	28 (7%)	13	16
All	All	882/892 (99%)	819 (93%)	63 (7%)	13	16

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	40	GLU
1	A	56	TYR
1	A	64	LYS
1	A	68	SER
1	A	73	LYS
1	A	94	ILE
1	A	105	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	122	GLU
1	A	139	THR
1	A	142	ILE
1	A	162	SER
1	A	189	VAL
1	A	195	ILE
1	A	216	THR
1	A	221	HIS
1	A	223	LYS
1	A	224	GLU
1	A	243	PRO
1	A	244	ILE
1	A	263	LYS
1	A	281	LYS
1	A	282	LEU
1	A	287	LYS
1	A	291	GLU
1	A	295	LEU
1	A	357	MET
1	A	361	HIS
1	A	414	TRP
1	A	460	ASN
1	A	465	LYS
1	A	470	THR
1	A	529	GLU
1	A	547	GLN
1	A	551	LEU
2	B	11	LYS
2	B	55	PRO
2	B	69	THR
2	B	86	ASP
2	B	87	PHE
2	B	88	TRP
2	B	91	GLN
2	B	109	LEU
2	B	187	LEU
2	B	195	ILE
2	B	210	LEU
2	B	221	HIS
2	B	227	PHE
2	B	230	MET
2	B	240	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	250	ASP
2	B	286	THR
2	B	290	THR
2	B	298	GLU
2	B	315	HIS
2	B	324	ASP
2	B	340	GLN
2	B	356	ARG
2	B	357	MET
2	B	418	ASN
2	B	422	LEU
2	B	428	GLN
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	54	ASN
1	A	137	ASN
1	A	182	GLN
1	A	197	GLN
1	A	208	HIS
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	336	GLN
1	A	340	GLN
1	A	418	ASN
1	A	428	GLN
1	A	460	ASN
1	A	487	GLN
1	A	509	GLN
2	B	85	GLN
2	B	91	GLN
2	B	96	HIS
2	B	182	GLN
2	B	258	GLN
2	B	269	GLN
2	B	330	GLN
2	B	332	GLN
2	B	340	GLN
2	B	348	ASN

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Mol	Chain	Res	Type
2	B	394	GLN
2	B	418	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	GLC	C	1	3	11,11,12	2.28	5 (45%)	15,15,17	0.81	0
3	FRU	C	2	3	11,12,12	1.77	2 (18%)	10,18,18	0.83	0
3	GLC	D	1	3	11,11,12	1.88	2 (18%)	15,15,17	1.77	2 (13%)
3	FRU	D	2	3	11,12,12	0.61	0	10,18,18	0.58	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	GLC	C	1	3	-	2/2/19/22	0/1/1/1
3	FRU	C	2	3	-	2/5/24/24	0/1/1/1
3	GLC	D	1	3	-	0/2/19/22	0/1/1/1
3	FRU	D	2	3	-	0/5/24/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	GLC	O5-C5	4.66	1.52	1.43
3	C	2	FRU	O2-C2	4.26	1.48	1.40
3	C	1	GLC	O5-C5	4.24	1.51	1.43
3	C	1	GLC	O5-C1	4.04	1.50	1.43
3	D	1	GLC	O5-C1	3.54	1.49	1.43
3	C	1	GLC	C2-C3	3.02	1.57	1.52
3	C	2	FRU	O5-C5	2.92	1.50	1.43
3	C	1	GLC	C1-C2	2.79	1.58	1.52
3	C	1	GLC	C4-C5	2.23	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	GLC	C1-O5-C5	-5.51	104.80	112.19
3	D	1	GLC	O5-C5-C6	-2.86	102.09	107.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

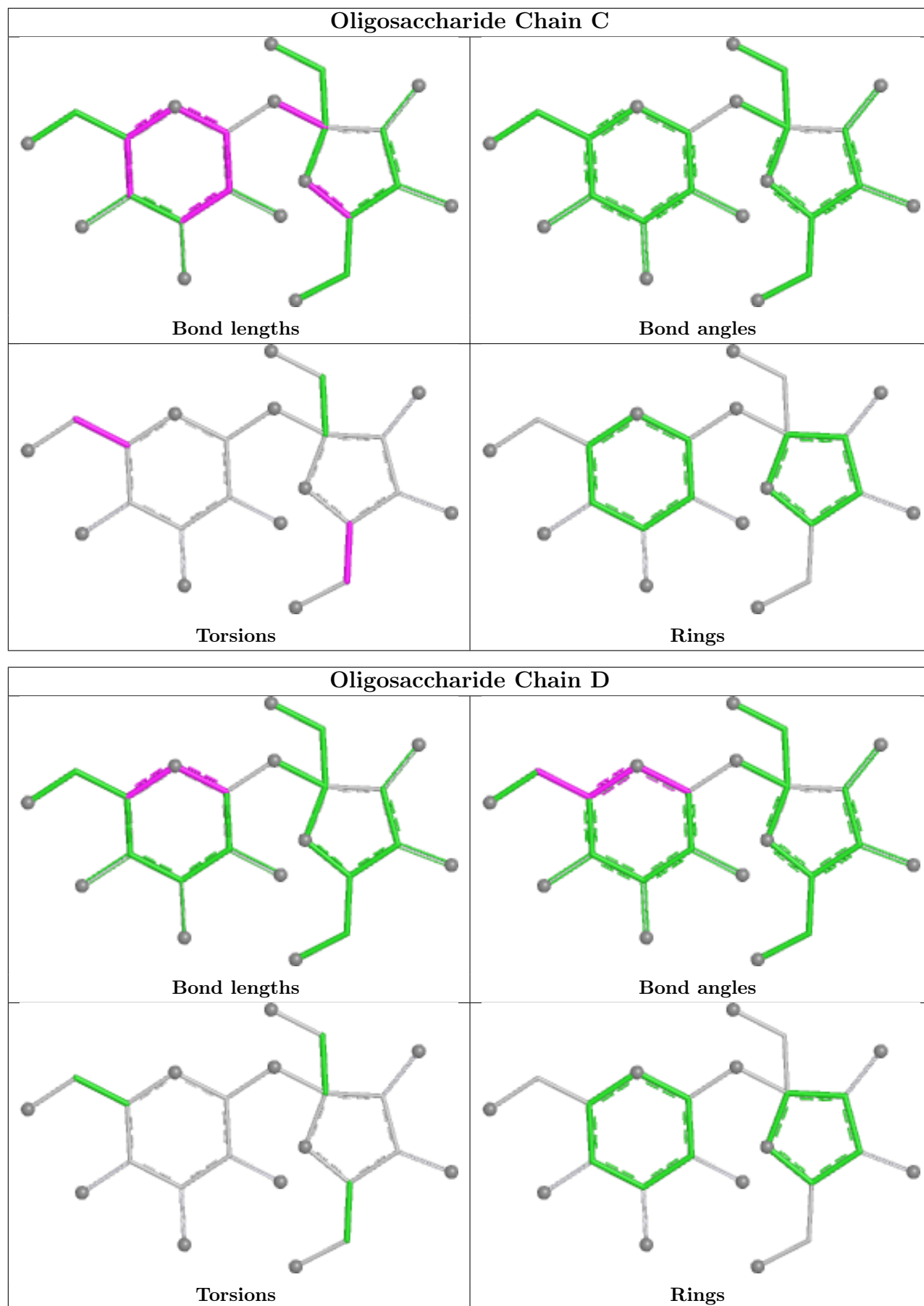
Mol	Chain	Res	Type	Atoms
3	C	2	FRU	O5-C5-C6-O6
3	C	2	FRU	C4-C5-C6-O6
3	C	1	GLC	O5-C5-C6-O6
3	C	1	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	GLC	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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
6	R22	A	4002	-	28,28,28	1.68	8 (28%)	32,39,39	1.44	5 (15%)
4	GOL	A	3001	-	5,5,5	0.60	0	5,5,5	0.38	0
4	GOL	A	3000	-	5,5,5	0.60	0	5,5,5	0.38	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
6	R22	A	4002	-	-	5/10/10/10	0/3/3/3
4	GOL	A	3001	-	-	0/4/4/4	-
4	GOL	A	3000	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4002	R22	C6'-C1'	3.61	1.44	1.39
6	A	4002	R22	C2'-C1'	2.87	1.43	1.39
6	A	4002	R22	C4'-C3'	2.83	1.43	1.39
6	A	4002	R22	C4'-C5'	2.65	1.43	1.39
6	A	4002	R22	C6-N1	2.61	1.41	1.38
6	A	4002	R22	C2'-C3'	2.31	1.42	1.39
6	A	4002	R22	C3-I9	-2.27	2.02	2.08
6	A	4002	R22	C2-C3	2.26	1.50	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4002	R22	C2-N1-C6	-3.74	123.53	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4002	R22	C4-C3-C2	-2.64	118.63	121.38
6	A	4002	R22	O14-C13-C12	-2.43	113.30	116.55
6	A	4002	R22	C12-S11-C10	2.40	106.22	100.69
6	A	4002	R22	O7'-C1'-C6'	2.28	124.99	118.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

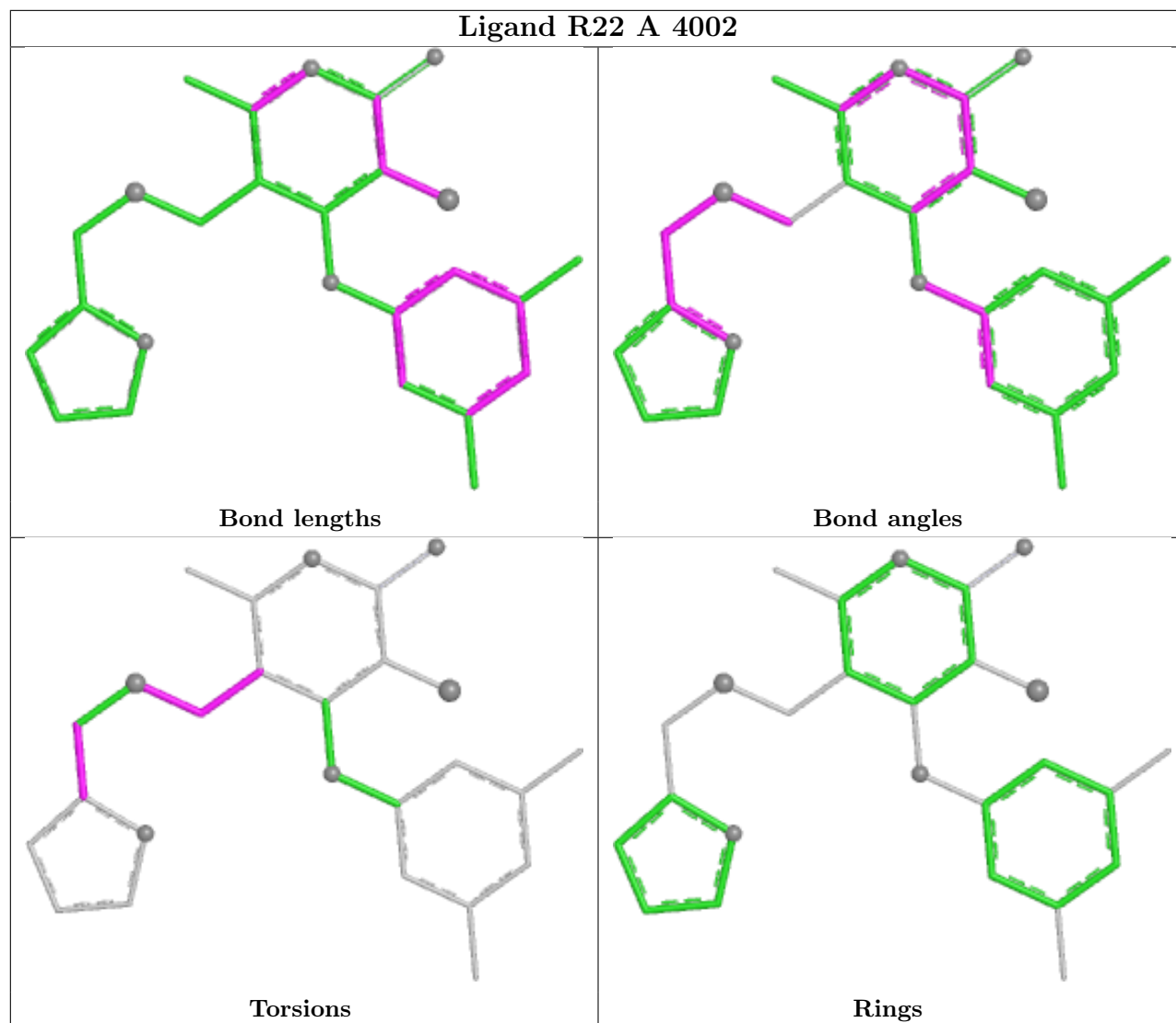
Mol	Chain	Res	Type	Atoms
6	A	4002	R22	S11-C10-C5-C4
6	A	4002	R22	S11-C10-C5-C6
6	A	4002	R22	S11-C12-C13-O14
6	A	4002	R22	S11-C12-C13-C17
4	A	3000	GOL	C1-C2-C3-O3
6	A	4002	R22	C5-C10-S11-C12
4	A	3000	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4002	R22	2	0
4	A	3001	GOL	5	0

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/560 (98%)	0.26	30 (5%) 31 28	28, 58, 106, 141	0
2	B	426/430 (99%)	0.33	45 (10%) 11 8	24, 55, 124, 150	0
All	All	978/990 (98%)	0.29	75 (7%) 19 16	24, 57, 118, 150	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	87	PHE	7.1
2	B	230	MET	5.9
2	B	88	TRP	5.3
2	B	85	GLN	5.1
2	B	226	PRO	4.3
1	A	357	MET	4.2
2	B	228	LEU	4.2
1	A	288	ALA	4.1
2	B	229	TRP	4.1
2	B	92	LEU	4.0
2	B	429	LEU	4.0
2	B	231	GLY	4.0
2	B	227	PHE	3.9
2	B	213	GLY	3.9
1	A	135	ILE	3.5
1	A	132	ILE	3.5
2	B	225	PRO	3.4
1	A	1	PRO	3.4
2	B	232	TYR	3.3
1	A	67	ASP	3.3
2	B	221	HIS	3.2
1	A	24	TRP	3.2
2	B	95	PRO	3.2
1	A	69	THR	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	94	ILE	3.2
1	A	355	ALA	3.1
1	A	52	PRO	3.1
1	A	2	ILE	3.1
2	B	84	THR	3.0
1	A	54	ASN	3.0
2	B	359	GLY	2.9
2	B	362	THR	2.9
2	B	64	LYS	2.9
2	B	357	MET	2.8
2	B	212	TRP	2.8
2	B	358	ARG	2.8
1	A	448	ARG	2.7
2	B	5	ILE	2.7
1	A	219	LYS	2.7
1	A	282	LEU	2.7
2	B	90	VAL	2.7
2	B	215	THR	2.6
2	B	422	LEU	2.6
1	A	142	ILE	2.6
2	B	68	SER	2.6
2	B	86	ASP	2.5
2	B	224	GLU	2.5
2	B	314	VAL	2.5
2	B	4	PRO	2.5
1	A	552	VAL	2.5
2	B	245	VAL	2.5
1	A	136	ASN	2.4
1	A	133	PRO	2.4
2	B	222	GLN	2.4
1	A	221	HIS	2.4
2	B	223	LYS	2.4
2	B	355	ALA	2.4
1	A	25	PRO	2.4
2	B	96	HIS	2.4
1	A	410	TRP	2.4
2	B	356	ARG	2.3
2	B	214	LEU	2.3
1	A	223	LYS	2.3
1	A	285	GLY	2.2
2	B	65	LYS	2.2
1	A	68	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	2.1
1	A	134	SER	2.1
1	A	435	VAL	2.1
2	B	63	ILE	2.1
2	B	423	VAL	2.0
2	B	89	GLU	2.0
1	A	296	THR	2.0
2	B	293	ILE	2.0
1	A	55	PRO	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

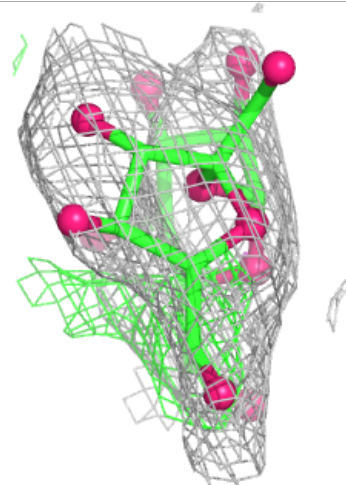
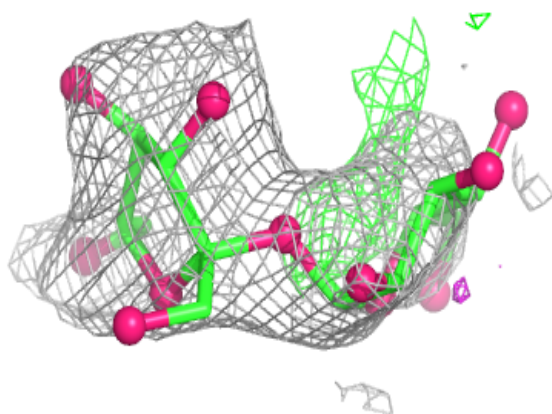
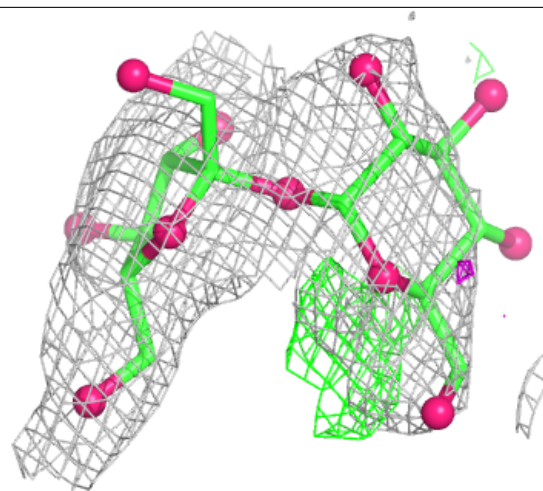
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

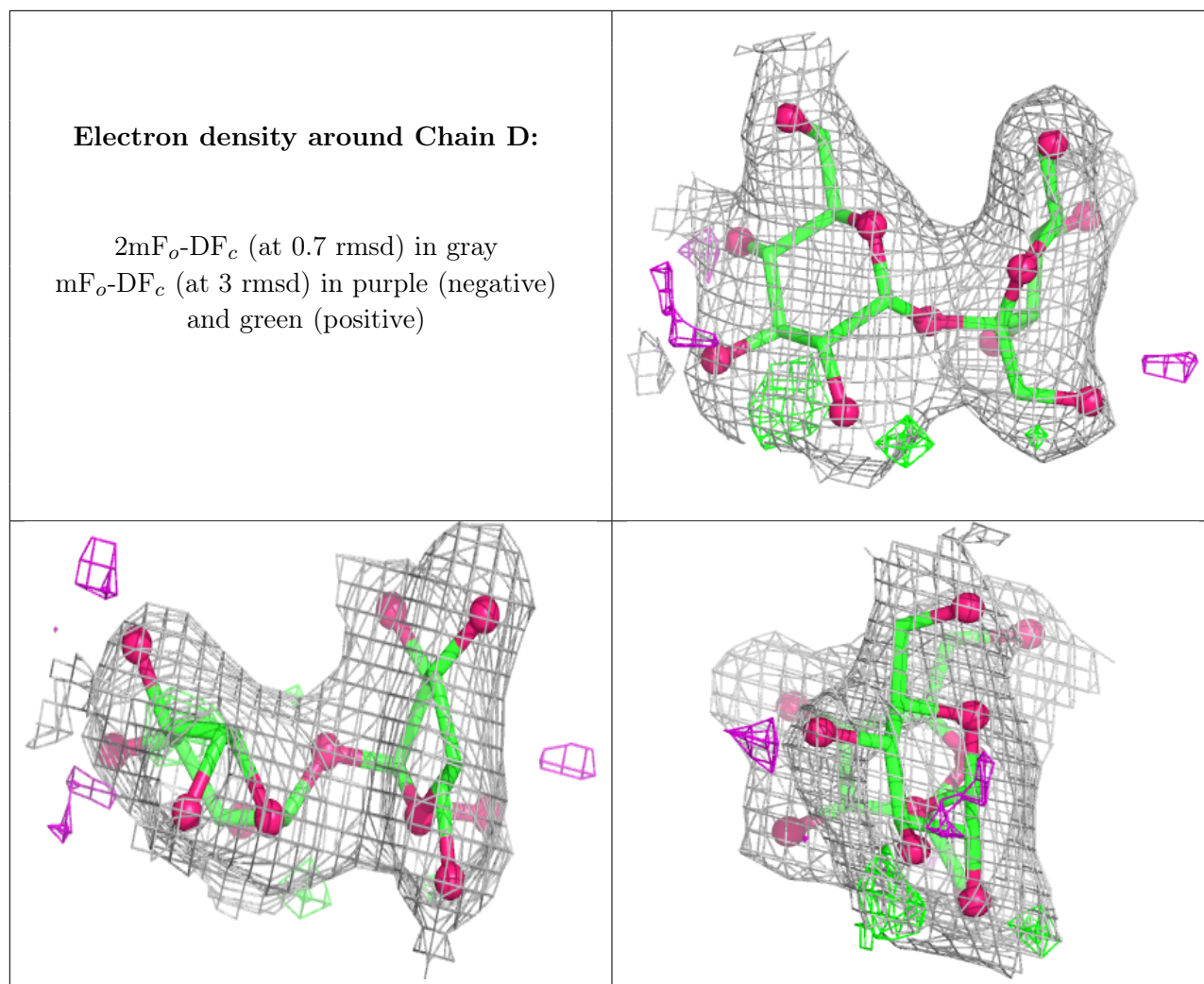
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GLC	C	1	11/12	0.78	0.21	92,102,107,114	0
3	FRU	C	2	12/12	0.85	0.15	93,102,106,106	0
3	FRU	D	2	12/12	0.91	0.09	36,51,63,68	0
3	GLC	D	1	11/12	0.92	0.11	29,42,50,51	0

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

**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)



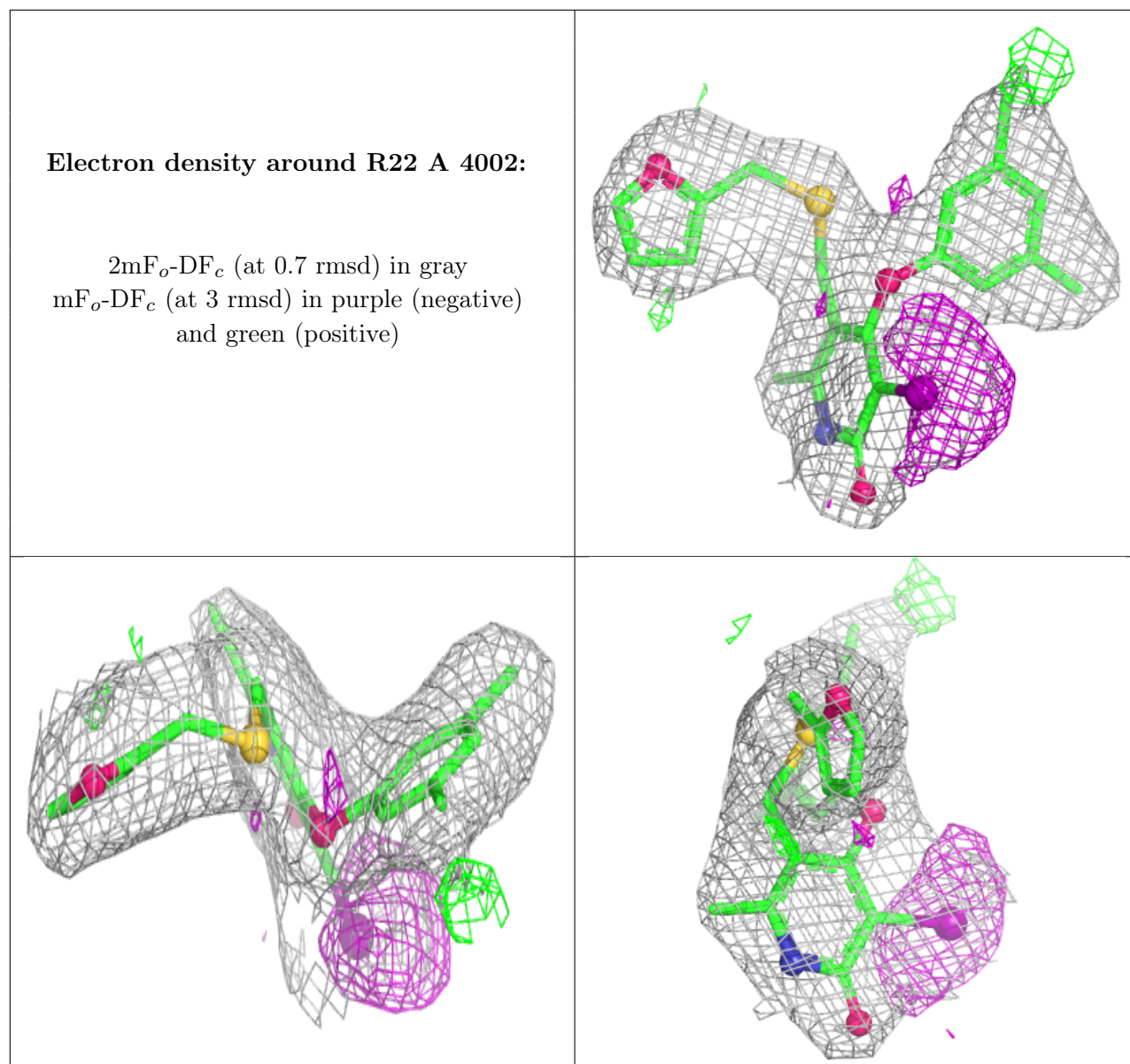


## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q < 0.9
4	GOL	A	3000	6/6	0.62	0.18	76,80,88,90	0
4	GOL	A	3001	6/6	0.75	0.19	80,88,96,97	0
6	R22	A	4002	26/26	0.95	0.11	33,45,81,88	0
5	MN	A	4001	1/1	0.99	0.03	40,40,40,40	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.