Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 06:37 PM EDT

PDB ID	:	2BE2
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

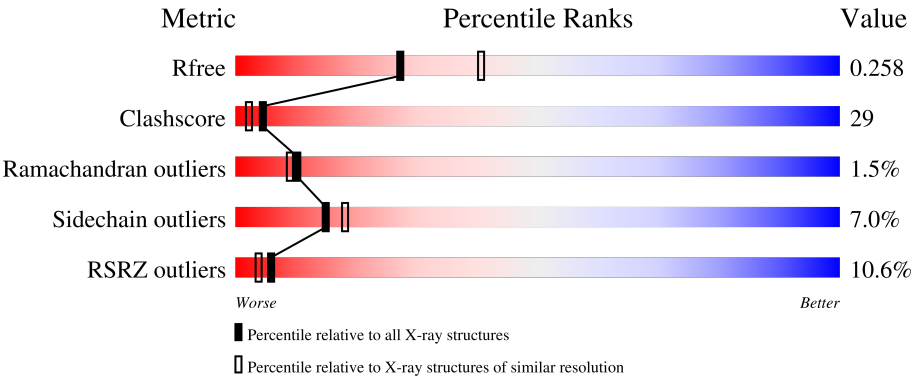
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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

Mol	Chain	Length	Quality of chain
1	A	560	9% 55% 38% 5%
2	B	430	12% 59% 33% 6%
3	C	2	50% 50%
3	D	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	3001	-	-	X	-

2 Entry composition (i)

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
1	A	552	Total	C	N	O	S	0	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

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

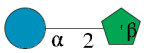
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE P51 SUBUNIT.

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

There is a discrepancy between the modelled and reference sequences:

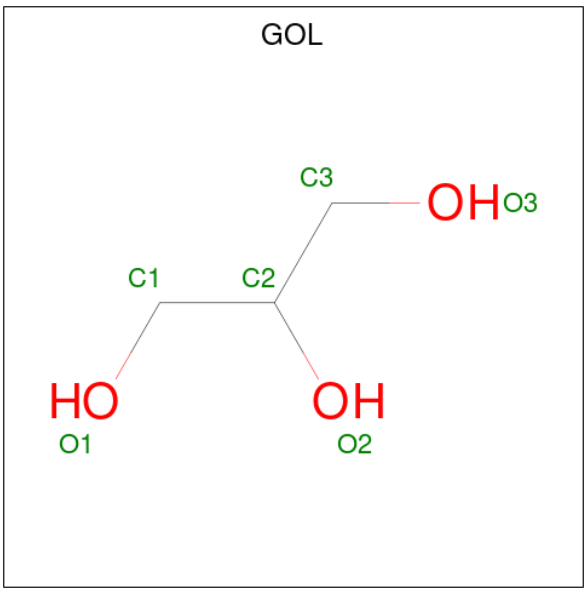
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

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



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

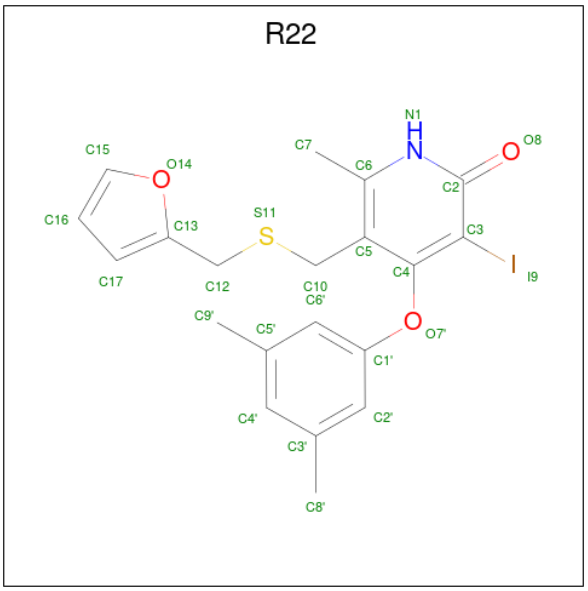


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: 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-YLMETHYLSULFANYLM ETHYL)-3-IODO-6-METHYLPYRIDIN-2(1H)-ONE (three-letter code: R22) (formula: $C_{20}H_{20}INO_3S$).



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

- Molecule 7 is water.

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

3 Residue-property plots (i)

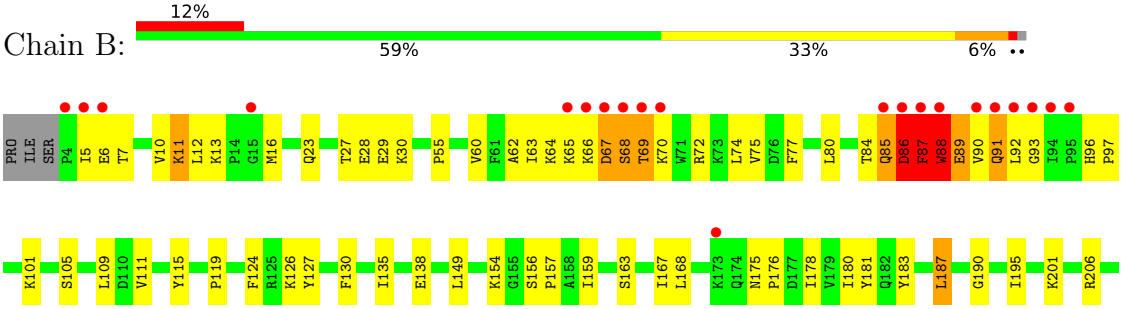
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

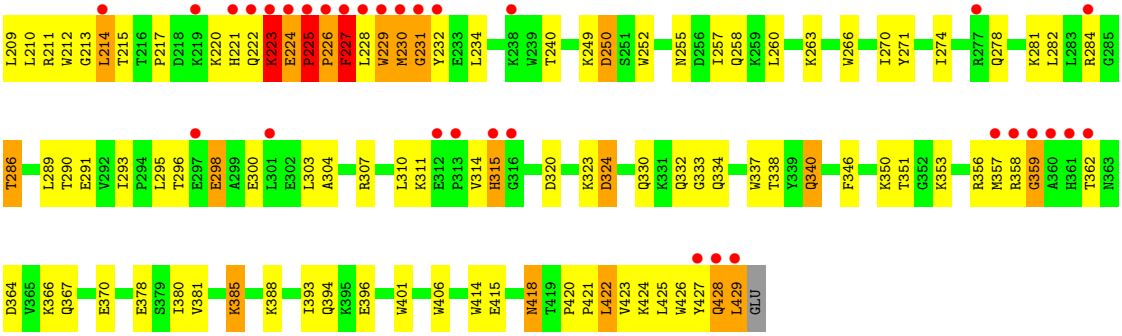
• Molecule 1: REVERSE TRANSCRIPTASE P66 SUBUNIT

Chain A:

• Molecule 2: REVERSE TRANSCRIPTASE P51 SUBUNIT

Chain B:





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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.85Å 68.80Å 104.43Å 90.00° 107.22° 90.00°	Depositor
Resolution (Å)	22.95 – 2.43 22.94 – 2.43	Depositor EDS
% Data completeness (in resolution range)	88.4 (22.95-2.43) 88.4 (22.94-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.44Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.265 0.223 , 0.258	Depositor DCC
R_{free} test set	2554 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 69.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage'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.*

[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: FRU, R22, GLC, MN, GOL

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	0.44	0/4616	0.75	5/6271 (0.1%)
2	B	0.48	0/3629	0.89	21/4932 (0.4%)
All	All	0.46	0/8245	0.81	26/11203 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	67	ASP	N-CA-C	9.43	136.46	111.00
2	B	359	GLY	N-CA-C	-8.98	90.64	113.10
2	B	89	GLU	N-CA-C	-8.94	86.86	111.00
2	B	214	LEU	CB-CA-C	8.07	125.53	110.20
1	A	285	GLY	N-CA-C	-7.93	93.28	113.10
2	B	89	GLU	CB-CA-C	6.69	123.78	110.40
2	B	214	LEU	N-CA-C	-6.63	93.09	111.00
1	A	222	GLN	N-CA-C	-6.53	93.36	111.00
2	B	226	PRO	N-CA-C	6.49	128.98	112.10
2	B	85	GLN	N-CA-C	6.49	128.51	111.00
2	B	67	ASP	CB-CA-C	-6.27	97.85	110.40
2	B	86	ASP	N-CA-C	-6.17	94.33	111.00
2	B	86	ASP	CB-CA-C	6.14	122.67	110.40
2	B	87	PHE	C-N-CA	-5.89	106.97	121.70
2	B	231	GLY	N-CA-C	-5.63	99.02	113.10
2	B	93	GLY	N-CA-C	-5.61	99.06	113.10
2	B	88	TRP	N-CA-C	-5.57	95.96	111.00
2	B	223	LYS	N-CA-C	5.49	125.83	111.00
2	B	401	TRP	N-CA-C	5.44	125.69	111.00
2	B	229	TRP	N-CA-C	5.22	125.10	111.00
2	B	227	PHE	N-CA-C	5.13	124.85	111.00
2	B	68	SER	CB-CA-C	5.11	119.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	SER	N-CA-C	5.09	124.75	111.00
2	B	225	PRO	N-CA-C	-5.05	98.98	112.10
1	A	68	SER	C-N-CA	-5.04	109.09	121.70
1	A	67	ASP	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4498	0	4560	277	0
2	B	3525	0	3562	198	0
3	C	23	0	21	2	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	3	0
7	A	94	0	0	5	0
7	B	60	0	0	3	0
All	All	8262	0	8200	465	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 (465) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:85:GLN:CD	2:B:85:GLN:O	2.09	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:333:GLY:C	1:A:334:GLN:HG2	1.93	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
1:A:362:THR:HG22	1:A:363:ASN:N	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:134:SER:CB	1:A:139:THR:O	2.28	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: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:218:ASP:C	1:A:220:LYS:H	1.87	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
2:B:67:ASP:C	2:B:69:THR:H	1.85	0.75
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:240:THR:HG22	1:A:241:VAL:N	2.01	0.73
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:253:THR:HG22	1:A:256:ASP:CG	2.14	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: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:13:LYS:HZ2	2:B:86:ASP:HB2	1.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:ILE:HD12	1:A:293:ILE:HD12	1.81	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:54:ASN:O	1:A:55:PRO:C	2.36	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:67:ASP:C	2:B:69:THR:N	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:13:LYS:HZ1	2:B:86:ASP:HB2	1.64	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:139:THR:HG1	1:A:140:PRO:HD2	1.73	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: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
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
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
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:68:SER:C	2:B:69:THR:HG1	2.10	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
2:B:298:GLU:CD	2:B:298:GLU:H	2.14	0.51
2:B:333:GLY:O	2:B:334:GLN:HB2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:6:GLU:O	2:B:6:GLU:CG	2.61	0.49
1:A:218:ASP:C	1:A:220:LYS:N	2.56	0.49
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:516:GLU:CD	1:A:516:GLU:H	2.15	0.48
2:B:65:LYS:CE	2:B:70:LYS:HD2	2.33	0.48
1:A:194:GLU:CD	1:A:194:GLU:H	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:ASN:C	1:A:418:ASN:HD22	2.17	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
2:B:230:MET:O	2:B:231:GLY:C	2.50	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: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:134:SER:O	1:A:135:ILE:C	2.53	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:358:ARG:C	2:B:359:GLY:O	2.49	0.47
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
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:224:GLU:CB	2:B:225:PRO:CD	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.46
1:A:54:ASN:O	1:A:54:ASN:CG	2.53	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:1:PRO:C	1:A:2:ILE:HG12	2.36	0.45
1:A:65:LYS:C	1:A:67:ASP:H	2.20	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: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
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:470:THR:O	1:A:471:ASN:C	2.55	0.44
2:B:388:LYS:NZ	7:B:1132:HOH:O	2.50	0.44
1:A:457:TYR:C	1:A:457:TYR:CD2	2.91	0.44
1:A:35:VAL:HG22	1:A:132:ILE:HD12	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.53	0.44
1:A:183:TYR:OH	1:A:230:MET:HE1	2.17	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: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:298:GLU:H	1:A:298:GLU:CD	2.21	0.43
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
2:B:252:TRP:CE2	2:B:295:LEU:HD11	2.53	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
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:227:PHE:CD2	6:A:4002:R22:H122	2.54	0.42
2:B:87:PHE:CD2	2:B:87:PHE:C	2.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:OD2	1:A:512:LYS:NZ	2.45	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
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:320:ASP:OD1	2:B:320:ASP:C	2.57	0.41
2:B:84:THR:CG2	2:B:124:PHE:HZ	2.32	0.41
2:B:222:GLN:C	2:B:229:TRP:O	2.58	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:470:THR:CG2	1:A:471:ASN:N	2.83	0.41
2:B:290:THR:O	2:B:291:GLU:C	2.58	0.41
1:A:113:ASP:O	1:A:114:ALA:C	2.58	0.41
1:A:131:THR:HG22	1:A:143:ARG:HG2	2.03	0.41
1:A:223:LYS:HD2	1:A:223:LYS:C	2.40	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
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: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:360:ALA:HB3	1:A:361:HIS:NE2	2.36	0.40
1:A:100:LEU:HD21	6:A:4002:R22:H9'1	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:C	1:A:223:LYS:H	2.24	0.40
1:A:240:THR:CG2	1:A:241:VAL:N	2.70	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%)	10 9
2	B	424/430 (99%)	371 (88%)	46 (11%)	7 (2%)	9 7
All	All	974/990 (98%)	868 (89%)	91 (9%)	15 (2%)	10 9

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

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Mol	Chain	Res	Type
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%)	461 (93%)	33 (7%)	16	20
2	B	388/392 (99%)	359 (92%)	29 (8%)	13	16
All	All	882/892 (99%)	820 (93%)	62 (7%)	15	18

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	46	LYS
1	A	56	TYR
1	A	64	LYS
1	A	68	SER
1	A	73	LYS
1	A	94	ILE
1	A	105	SER
1	A	110	ASP
1	A	122	GLU
1	A	137	ASN
1	A	139	THR
1	A	142	ILE
1	A	162	SER
1	A	216	THR
1	A	221	HIS
1	A	223	LYS
1	A	224	GLU
1	A	244	ILE

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Mol	Chain	Res	Type
1	A	277	ARG
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	418	ASN
1	A	460	ASN
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	89	GLU
2	B	91	GLN
2	B	101	LYS
2	B	109	LEU
2	B	187	LEU
2	B	211	ARG
2	B	227	PHE
2	B	230	MET
2	B	240	THR
2	B	250	ASP
2	B	286	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	385	LYS
2	B	414	TRP
2	B	418	ASN
2	B	422	LEU
2	B	428	GLN

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Mol	Chain	Res	Type
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	91	GLN
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	340	GLN
1	A	407	GLN
1	A	418	ASN
1	A	428	GLN
1	A	460	ASN
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	330	GLN
2	B	332	GLN
2	B	340	GLN
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	2.32	5 (45%)	15,15,17	0.91	0
3	FRU	C	2	3	11,12,12	1.85	3 (27%)	10,18,18	0.81	0
3	GLC	D	1	3	11,11,12	1.87	2 (18%)	15,15,17	1.84	2 (13%)
3	FRU	D	2	3	11,12,12	0.66	0	10,18,18	0.55	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	GLC	O5-C5	4.47	1.52	1.43
3	C	2	FRU	O2-C2	4.31	1.48	1.40
3	C	1	GLC	O5-C1	4.23	1.50	1.43
3	C	1	GLC	O5-C5	4.07	1.51	1.43
3	D	1	GLC	O5-C1	3.71	1.49	1.43
3	C	1	GLC	C2-C3	3.12	1.57	1.52
3	C	2	FRU	O5-C5	2.94	1.50	1.43
3	C	1	GLC	C1-C2	2.92	1.58	1.52
3	C	1	GLC	C4-C5	2.25	1.57	1.53
3	C	2	FRU	O5-C2	2.07	1.46	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	GLC	C1-O5-C5	-5.45	104.80	112.19
3	D	1	GLC	O5-C5-C6	-3.26	102.09	107.20

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

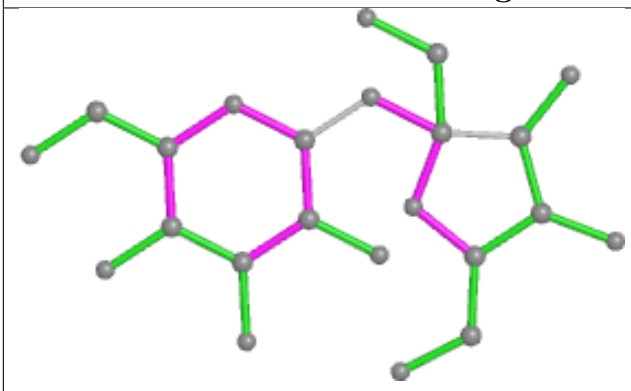
There are no ring outliers.

1 monomer is involved in 2 short contacts:

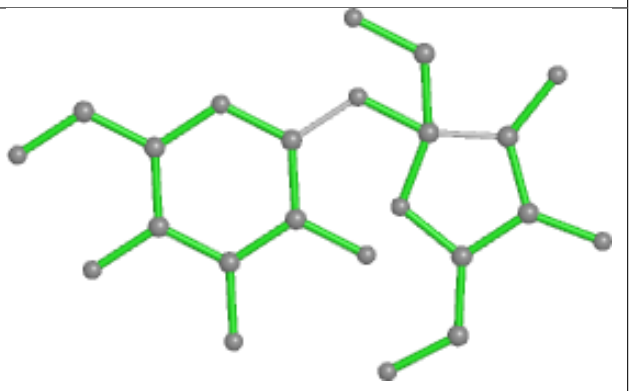
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	GLC	2	0

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

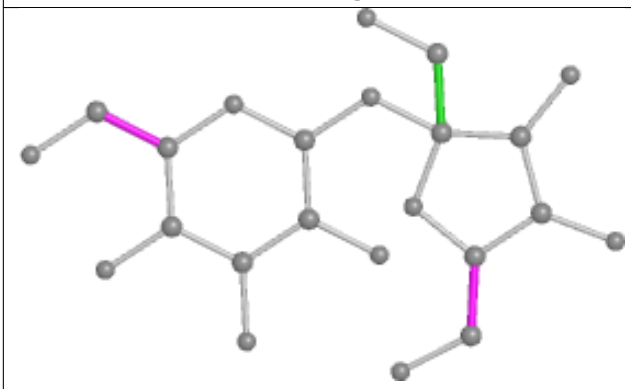
Oligosaccharide Chain C



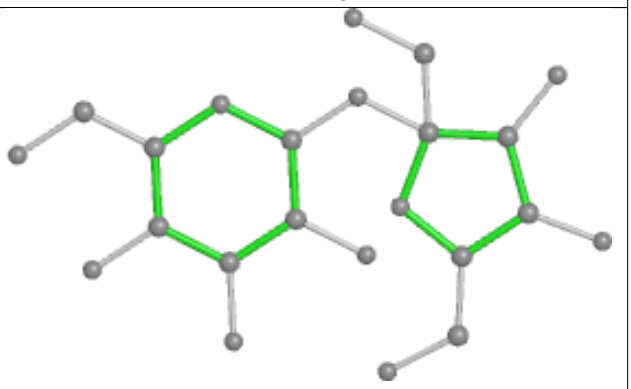
Bond lengths



Bond angles

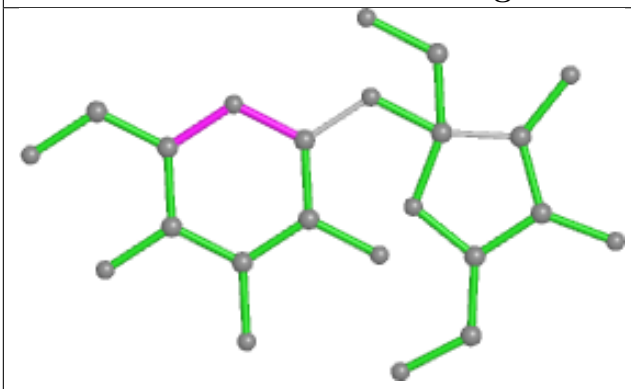


Torsions

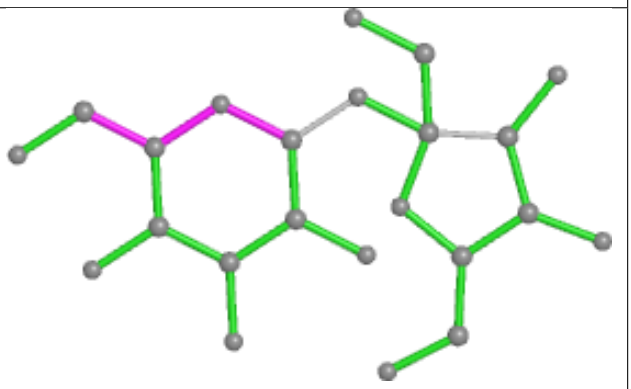


Rings

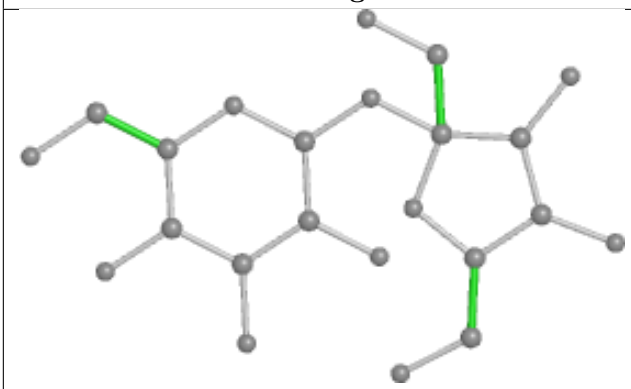
Oligosaccharide Chain D



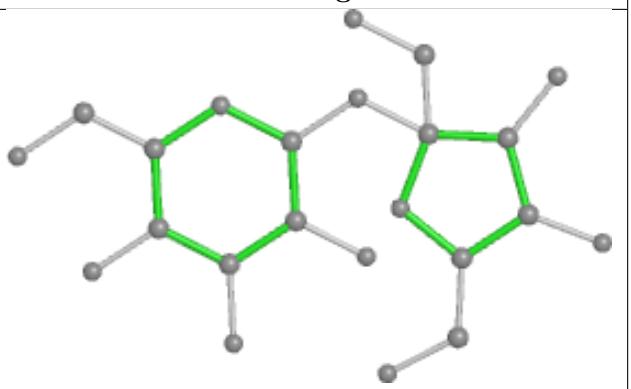
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	GOL	A	3000	-	5,5,5	0.58	0	5,5,5	0.36	0
6	R22	A	4002	-	24,28,28	2.20	10 (41%)	30,39,39	1.79	6 (20%)
4	GOL	A	3001	-	5,5,5	0.57	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	3000	-	-	2/4/4/4	-
6	R22	A	4002	-	-	4/9/10/10	0/3/3/3
4	GOL	A	3001	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4002	R22	C6-N1	5.05	1.41	1.34
6	A	4002	R22	C3-I9	-4.66	2.02	2.10
6	A	4002	R22	C6'-C1'	3.44	1.44	1.38
6	A	4002	R22	C2'-C1'	2.73	1.43	1.38
6	A	4002	R22	C4'-C3'	2.65	1.43	1.39
6	A	4002	R22	C4'-C5'	2.48	1.43	1.39
6	A	4002	R22	C12-S11	-2.46	1.78	1.82
6	A	4002	R22	C2-N1	2.38	1.37	1.33
6	A	4002	R22	C5-C6	-2.30	1.35	1.39
6	A	4002	R22	C2'-C3'	2.17	1.42	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4002	R22	C6-N1-C2	4.48	123.53	117.92
6	A	4002	R22	C7-C6-C5	3.46	127.23	122.32
6	A	4002	R22	C5-C10-S11	3.07	121.60	112.91
6	A	4002	R22	C7-C6-N1	-2.95	111.92	116.49
6	A	4002	R22	C12-C13-C17	2.30	135.06	129.15
6	A	4002	R22	C17-C16-C15	-2.03	105.70	112.92

There are no chirality outliers.

All (6) 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-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

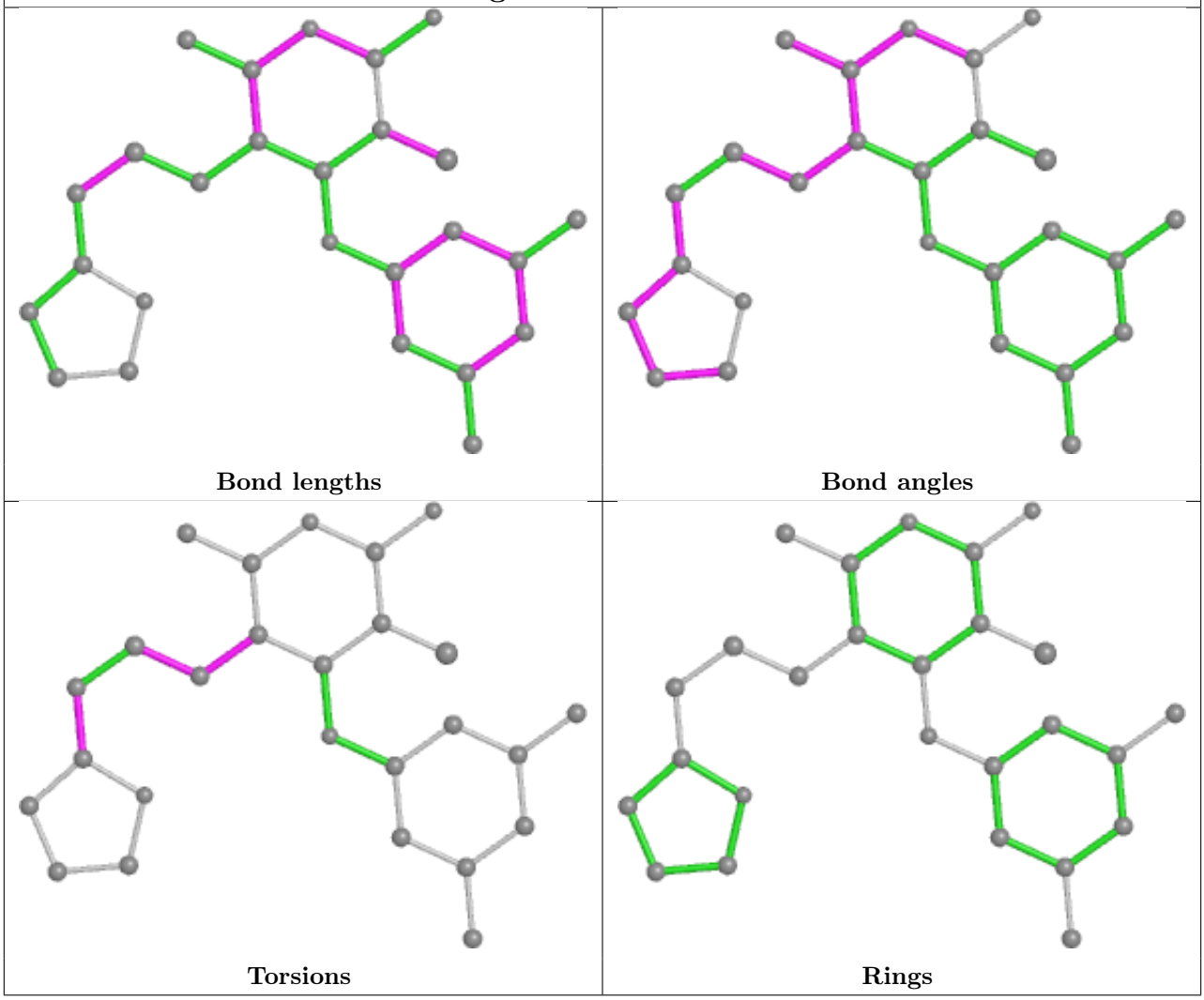
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4002	R22	3	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 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.

Ligand R22 A 4002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	552/560 (98%)	0.43	51 (9%) 9 6	28, 58, 106, 141	0
2	B	426/430 (99%)	0.66	53 (12%) 4 2	24, 55, 124, 150	0
All	All	978/990 (98%)	0.53	104 (10%) 6 4	24, 57, 118, 150	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	15.8
2	B	230	MET	11.7
2	B	358	ARG	9.6
2	B	4	PRO	9.3
2	B	229	TRP	9.2
2	B	359	GLY	8.5
2	B	5	ILE	8.2
2	B	224	GLU	7.6
2	B	66	LYS	7.4
2	B	92	LEU	7.1
2	B	226	PRO	7.1
2	B	361	HIS	7.1
2	B	90	VAL	6.7
2	B	357	MET	6.6
2	B	221	HIS	6.6
2	B	225	PRO	6.5
2	B	223	LYS	6.4
2	B	228	LEU	6.1
1	A	67	ASP	6.1
1	A	24	TRP	6.1
2	B	360	ALA	5.5
1	A	221	HIS	5.2
2	B	67	ASP	5.2
1	A	68	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	5.1
2	B	222	GLN	5.0
2	B	94	ILE	5.0
2	B	68	SER	4.9
2	B	91	GLN	4.9
2	B	429	LEU	4.6
1	A	136	ASN	4.5
1	A	135	ILE	4.5
1	A	92	LEU	4.3
1	A	66	LYS	4.2
2	B	362	THR	4.2
2	B	93	GLY	4.2
2	B	87	PHE	4.2
1	A	52	PRO	4.2
2	B	69	THR	4.2
1	A	65	LYS	4.1
1	A	25	PRO	4.0
1	A	360	ALA	3.9
2	B	85	GLN	3.9
1	A	139	THR	3.9
2	B	231	GLY	3.8
1	A	359	GLY	3.6
2	B	6	GLU	3.6
1	A	134	SER	3.5
2	B	301	LEU	3.5
2	B	219	LYS	3.5
2	B	316	GLY	3.4
1	A	284	ARG	3.4
1	A	358	ARG	3.4
2	B	86	ASP	3.4
1	A	495	ILE	3.3
2	B	232	TYR	3.1
2	B	95	PRO	3.1
2	B	88	TRP	3.1
2	B	312	GLU	3.0
2	B	297	GLU	3.0
2	B	427	TYR	3.0
1	A	69	THR	3.0
1	A	286	THR	2.9
2	B	238	LYS	2.9
2	B	313	PRO	2.8
1	A	173	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	496	VAL	2.7
2	B	15	GLY	2.7
1	A	32	LYS	2.7
1	A	2	ILE	2.7
1	A	312	GLU	2.7
2	B	70	LYS	2.7
1	A	26	LEU	2.7
1	A	72	ARG	2.6
1	A	435	VAL	2.6
2	B	315	HIS	2.6
1	A	357	MET	2.6
1	A	137	ASN	2.6
1	A	514	GLU	2.6
2	B	284	ARG	2.6
1	A	368	LEU	2.5
1	A	355	ALA	2.5
2	B	428	GLN	2.5
1	A	54	ASN	2.5
1	A	290	THR	2.5
1	A	356	ARG	2.5
2	B	277	ARG	2.4
2	B	173	LYS	2.4
2	B	214	LEU	2.4
1	A	194	GLU	2.3
1	A	138	GLU	2.3
1	A	224	GLU	2.3
1	A	282	LEU	2.3
1	A	177	ASP	2.3
1	A	334	GLN	2.2
2	B	65	LYS	2.2
1	A	287	LYS	2.2
1	A	448	ARG	2.2
1	A	251	SER	2.1
1	A	369	THR	2.1
1	A	133	PRO	2.0
1	A	146	TYR	2.0
1	A	482	ILE	2.0
1	A	197	GLN	2.0

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

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

6.3 Carbohydrates (i)

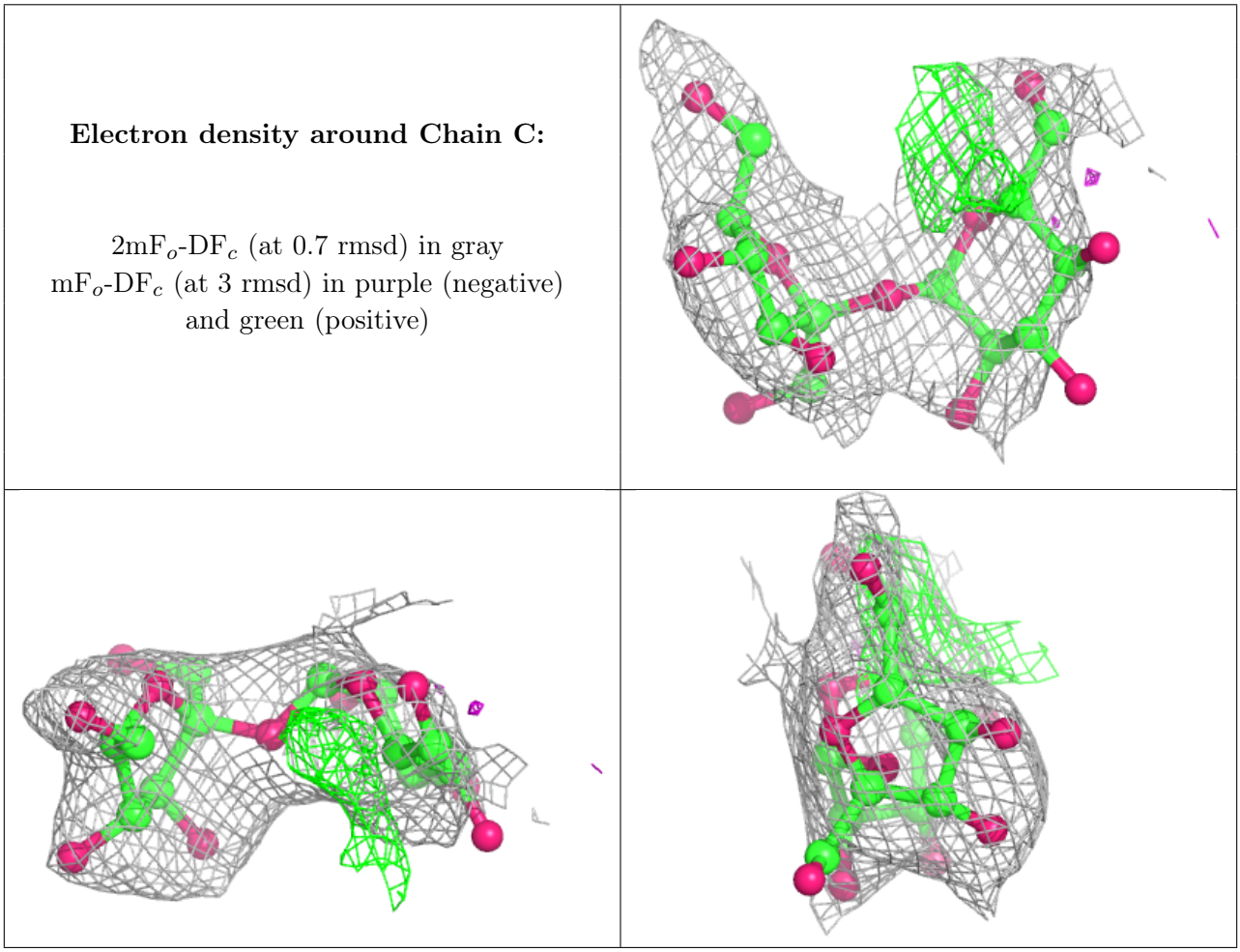
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	C	1	11/12	0.72	0.33	92,102,107,114	0
3	FRU	C	2	12/12	0.82	0.24	93,102,106,106	0
3	GLC	D	1	11/12	0.94	0.17	29,42,50,51	0
3	FRU	D	2	12/12	0.95	0.12	36,51,63,68	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.

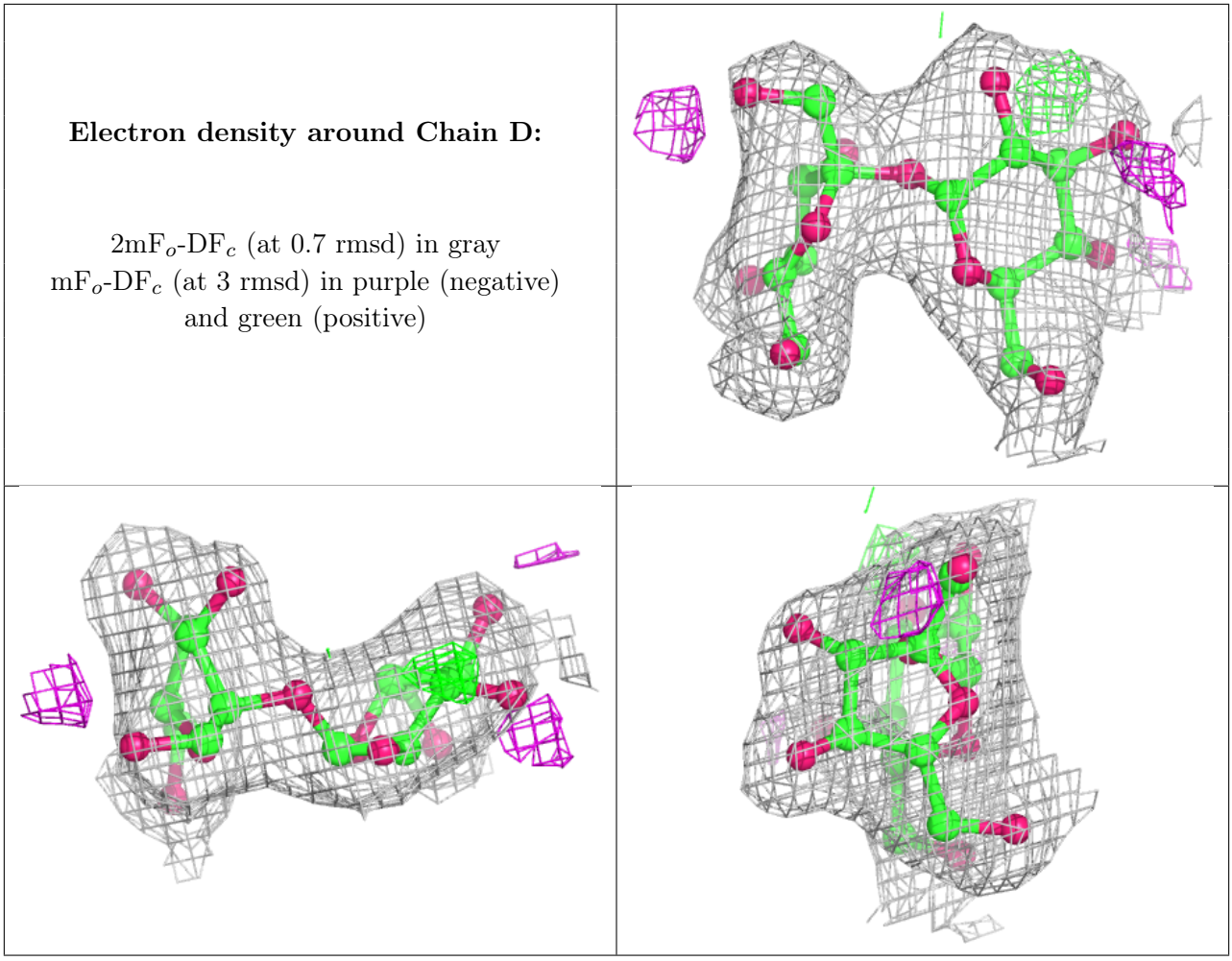
Electron density around Chain C:

$2mF_o$-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:

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



6.4 Ligands

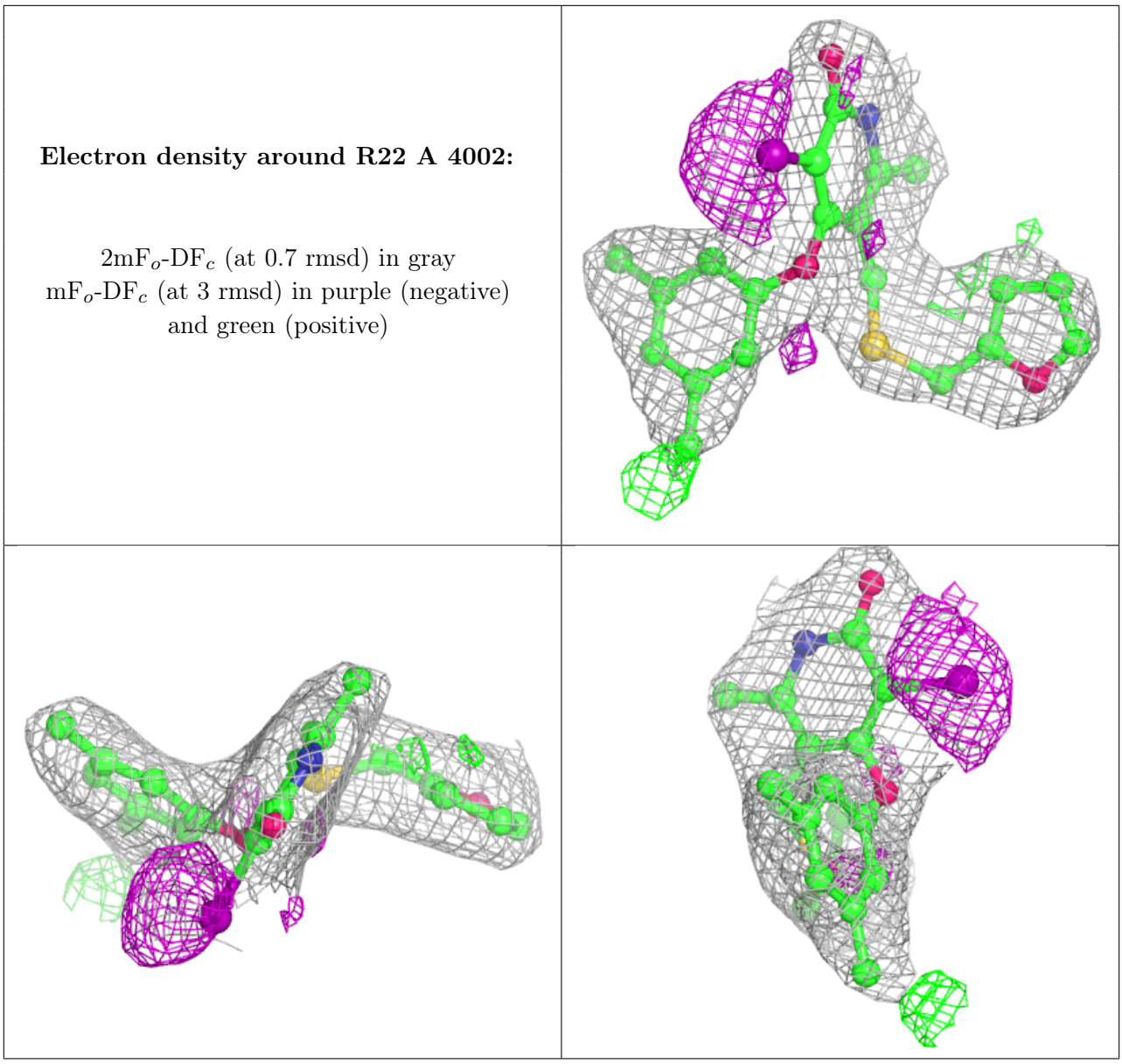
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	3000	6/6	0.65	0.20	76,80,88,90	0
4	GOL	A	3001	6/6	0.79	0.31	80,88,96,97	0
6	R22	A	4002	26/26	0.96	0.17	33,45,81,88	0
5	MN	A	4001	1/1	0.97	0.12	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.

Electron density around R22 A 4002:

$2mF_o$-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

There are no such residues in this entry.