Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 06:35 AM EDT

PDB ID	:	3O4O
Title	:	Crystal structure of an Interleukin-1 receptor complex
Authors	:	Wang, X.Q.; Wang, D.L.; Zhang, S.Y.; Li, L.; Liu, X.; Mei, K.R.
Deposited on	:	2010-07-27
Resolution	:	3.30 Å(reported)

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

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

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

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

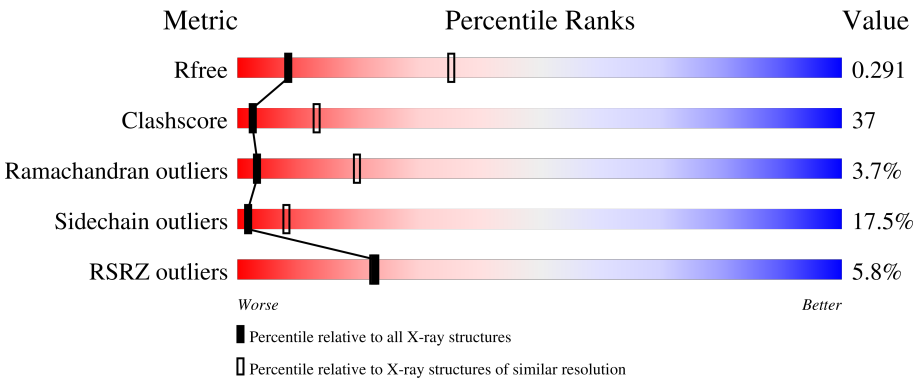
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	158	.%, 47%, 38%, 11%, .
2	C	339	7%, 29%, 48%, 14%, ., 7%
3	B	339	6%, 44%, 40%, 11%, 5%
4	D	2	100%
4	E	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6506 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 Interleukin-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1212	770	200	234	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01584
A	-3	PRO	-	expression tag	UNP P01584
A	-2	LEU	-	expression tag	UNP P01584
A	-1	GLY	-	expression tag	UNP P01584
A	0	SER	-	expression tag	UNP P01584

- Molecule 2 is a protein called Interleukin-1 receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	316	2562	1631	439	480	12	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P27930
C	-1	ASP	-	expression tag	UNP P27930
C	0	PRO	-	expression tag	UNP P27930
C	331	HIS	-	expression tag	UNP P27930
C	332	HIS	-	expression tag	UNP P27930
C	333	HIS	-	expression tag	UNP P27930
C	334	HIS	-	expression tag	UNP P27930
C	335	HIS	-	expression tag	UNP P27930
C	336	HIS	-	expression tag	UNP P27930

- Molecule 3 is a protein called Interleukin-1 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	323	2620	1673	442	489	16	0	0	0

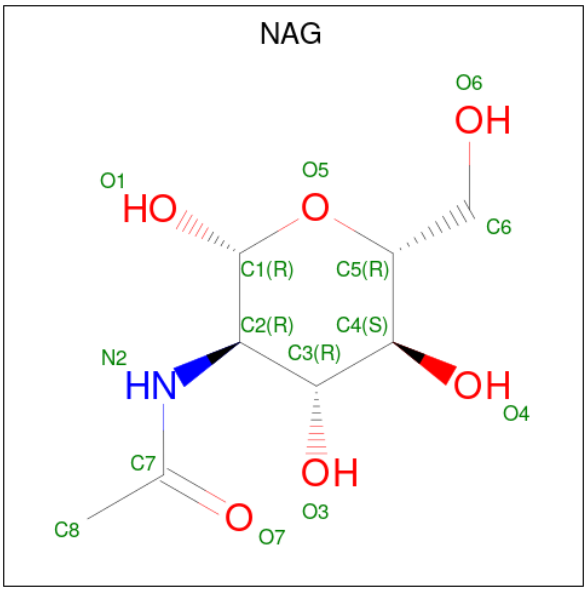
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP Q9NPH3
B	-1	ASP	-	expression tag	UNP Q9NPH3
B	0	PRO	-	expression tag	UNP Q9NPH3
B	331	HIS	-	expression tag	UNP Q9NPH3
B	332	HIS	-	expression tag	UNP Q9NPH3
B	333	HIS	-	expression tag	UNP Q9NPH3
B	334	HIS	-	expression tag	UNP Q9NPH3
B	335	HIS	-	expression tag	UNP Q9NPH3
B	336	HIS	-	expression tag	UNP Q9NPH3

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



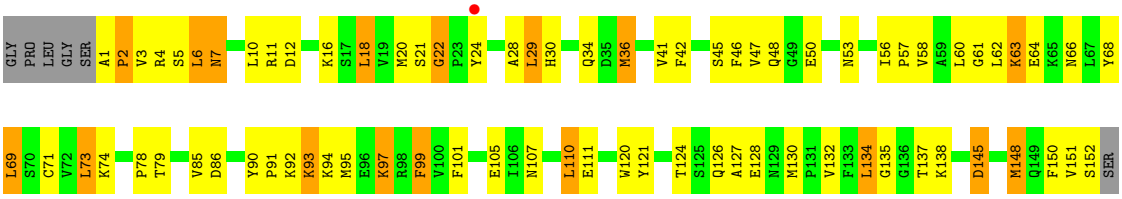
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	C	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

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.

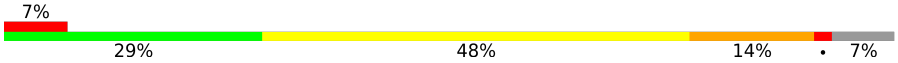
• Molecule 1: Interleukin-1 beta

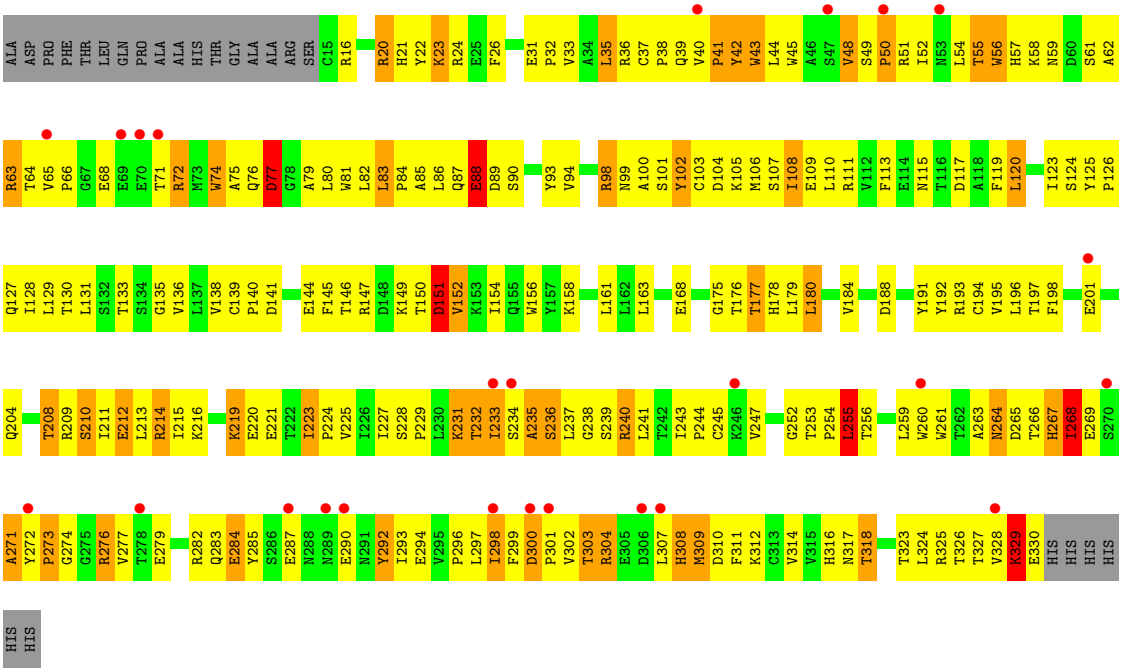
Chain A:



• Molecule 2: Interleukin-1 receptor type 2

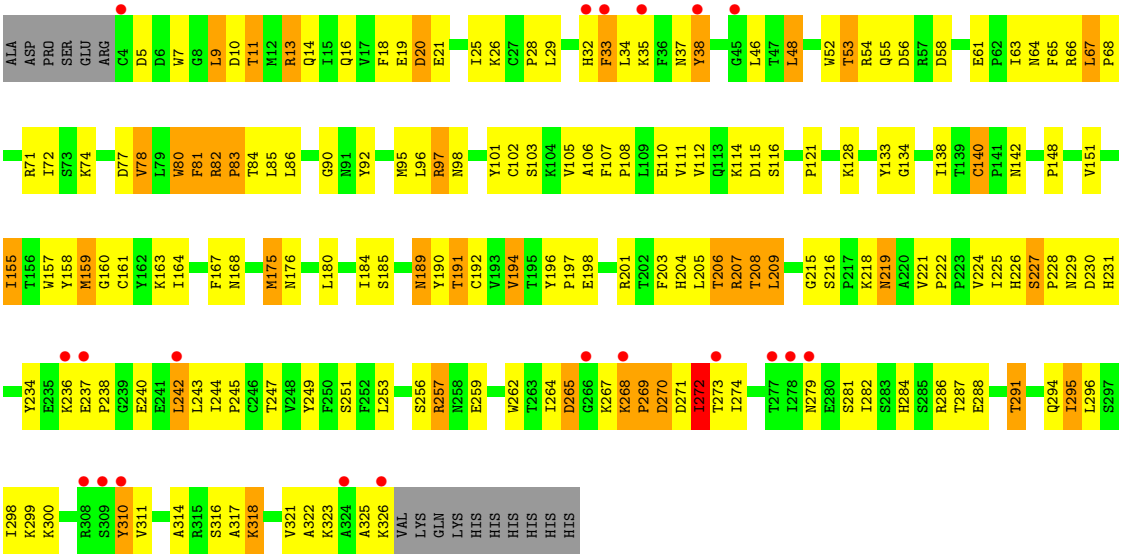
Chain C:





• Molecule 3: Interleukin-1 receptor accessory protein

Chain B:



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

Chain D: 100%

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

Chain E: 100%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.83Å 177.47Å 180.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.59 – 3.30 36.58 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (36.59-3.30) 94.8 (36.58-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.252 , 0.289 0.247 , 0.291	Depositor DCC
R_{free} test set	1101 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 71.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.42	0/1235	0.54	0/1662
2	C	0.29	0/2626	0.53	0/3573
3	B	0.33	0/2689	0.52	0/3659
All	All	0.34	0/6550	0.53	0/8894

There are no bond length outliers.

There are no bond angle outliers.

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	1212	0	1213	77	0
2	C	2562	0	2520	254	0
3	B	2620	0	2564	157	0
4	D	28	0	25	5	0
4	E	28	0	25	1	0
5	B	28	0	26	0	0
5	C	28	0	26	0	0
All	All	6506	0	6399	478	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 37.

All (478) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:234:TYR:O	3:B:326:LYS:HA	1.52	1.06
2:C:214:ARG:HH11	2:C:214:ARG:HG3	1.19	1.05
2:C:74:TRP:HZ3	2:C:83:LEU:HD11	1.24	1.01
3:B:55:GLN:HA	4:D:1:NAG:O7	1.59	1.01
2:C:127:GLN:HG3	2:C:211:ILE:HG23	1.44	0.99
2:C:38:PRO:HG3	2:C:108:ILE:HD13	1.49	0.94
2:C:99:ASN:O	2:C:102:TYR:N	1.99	0.93
3:B:191:THR:HB	3:B:208:THR:HB	1.49	0.93
2:C:243:ILE:HG21	2:C:298:ILE:CG2	2.02	0.90
1:A:105:GLU:HG3	1:A:110:LEU:HB3	1.53	0.88
2:C:243:ILE:HG21	2:C:298:ILE:HG22	1.53	0.88
3:B:236:LYS:HG3	3:B:242:LEU:HB2	1.53	0.88
2:C:147:ARG:HG2	2:C:147:ARG:HH11	1.35	0.88
2:C:312:LYS:HA	2:C:324:LEU:O	1.74	0.87
1:A:5:SER:HB3	1:A:45:SER:HB3	1.57	0.87
1:A:69:LEU:H	1:A:69:LEU:HD23	1.38	0.86
2:C:16:ARG:HG2	2:C:104:ASP:HB3	1.57	0.86
2:C:274:GLY:N	2:C:276:ARG:HH11	1.75	0.84
2:C:285:TYR:HB3	2:C:287:GLU:HG2	1.61	0.83
2:C:274:GLY:H	2:C:276:ARG:HD3	1.43	0.82
2:C:193:ARG:HH21	2:C:208:THR:HG21	1.43	0.82
3:B:311:VAL:HG22	3:B:323:LYS:HA	1.61	0.82
1:A:36:MET:HE3	1:A:36:MET:HA	1.61	0.81
2:C:131:LEU:HA	2:C:184:VAL:HG13	1.61	0.81
2:C:152:VAL:HG12	2:C:154:ILE:HG13	1.63	0.81
2:C:231:LYS:HB3	2:C:327:THR:HB	1.63	0.81
3:B:67:LEU:N	3:B:68:PRO:HA	1.97	0.80
3:B:98:ASN:HB3	3:B:101:TYR:H	1.48	0.79
2:C:231:LYS:HE3	2:C:233:ILE:HD12	1.66	0.78
2:C:193:ARG:NH2	2:C:208:THR:HG21	1.99	0.77
2:C:64:THR:HB	2:C:66:PRO:HA	1.64	0.77
1:A:92:LYS:HG2	1:A:95:MET:HE2	1.66	0.77
3:B:279:ASN:HB3	3:B:295:ILE:HG13	1.65	0.77
3:B:46:LEU:HA	3:B:97:ARG:O	1.83	0.77
2:C:176:THR:HG22	2:C:177:THR:H	1.50	0.76
2:C:133:THR:O	2:C:184:VAL:HG12	1.86	0.76
3:B:5:ASP:O	3:B:103:SER:HA	1.86	0.76
3:B:26:LYS:HA	3:B:78:VAL:HG22	1.69	0.75
1:A:7:ASN:HA	1:A:42:PHE:O	1.88	0.74
2:C:49:SER:HB3	2:C:50:PRO:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:CYS:HB3	2:C:177:THR:HG22	1.70	0.73
2:C:24:ARG:HG2	2:C:109:GLU:HB3	1.68	0.73
2:C:219:LYS:HE3	2:C:219:LYS:HA	1.70	0.73
3:B:64:ASN:HA	3:B:67:LEU:HD23	1.70	0.73
1:A:3:VAL:HG12	1:A:93:LYS:HG2	1.70	0.72
2:C:93:TYR:O	2:C:107:SER:HA	1.89	0.72
2:C:238:GLY:HA3	2:C:240:ARG:NH1	2.04	0.72
3:B:221:VAL:HG22	3:B:222:PRO:HD2	1.72	0.72
3:B:10:ASP:HB3	3:B:13:ARG:HB3	1.71	0.71
1:A:94:LYS:HD3	1:A:94:LYS:N	2.05	0.71
2:C:48:VAL:O	2:C:51:ARG:HG2	1.90	0.71
3:B:259:GLU:O	3:B:314:ALA:HA	1.91	0.70
2:C:214:ARG:HG3	2:C:214:ARG:NH1	1.97	0.70
2:C:237:LEU:HD13	2:C:237:LEU:O	1.89	0.70
1:A:120:TRP:HB3	1:A:134:LEU:CD1	2.22	0.70
2:C:74:TRP:CZ3	2:C:83:LEU:HD11	2.16	0.70
2:C:26:PHE:HB3	2:C:113:PHE:HE1	1.56	0.70
2:C:145:PHE:HB3	2:C:198:PHE:CE2	2.26	0.70
2:C:263:ALA:HB1	2:C:310:ASP:O	1.91	0.70
2:C:131:LEU:HB3	2:C:215:ILE:CG2	2.22	0.69
2:C:227:ILE:HG22	2:C:227:ILE:O	1.92	0.69
2:C:109:GLU:HG3	2:C:110:LEU:N	2.08	0.69
3:B:274:ILE:O	3:B:274:ILE:HG23	1.93	0.69
1:A:4:ARG:HG3	2:C:282:ARG:HE	1.58	0.69
3:B:224:VAL:HG12	3:B:249:TYR:HB3	1.73	0.69
2:C:231:LYS:CB	2:C:327:THR:HB	2.22	0.68
2:C:140:PRO:HD3	2:C:211:ILE:HD11	1.75	0.68
2:C:87:GLN:O	2:C:88:GLU:HB3	1.92	0.68
2:C:255:LEU:HG	2:C:256:THR:H	1.59	0.68
2:C:52:ILE:CG2	2:C:98:ARG:H	2.06	0.68
1:A:41:VAL:HG21	1:A:151:VAL:HG11	1.75	0.68
3:B:55:GLN:CA	4:D:1:NAG:O7	2.38	0.68
3:B:95:MET:HA	3:B:103:SER:O	1.93	0.68
3:B:77:ASP:O	3:B:78:VAL:HG23	1.94	0.67
2:C:127:GLN:HG3	2:C:211:ILE:CG2	2.22	0.67
2:C:273:PRO:HA	2:C:276:ARG:HG2	1.75	0.67
1:A:46:PHE:HD1	1:A:58:VAL:HG12	1.58	0.67
3:B:9:LEU:HD13	3:B:11:THR:HG23	1.76	0.67
1:A:126:GLN:OE1	3:B:168:ASN:HA	1.94	0.67
3:B:46:LEU:HD22	3:B:98:ASN:HB2	1.77	0.67
3:B:237:GLU:HB3	3:B:238:PRO:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TRP:HB3	1:A:134:LEU:HD11	1.76	0.66
2:C:312:LYS:HG3	2:C:325:ARG:HG3	1.77	0.66
2:C:274:GLY:H	2:C:276:ARG:HH11	1.44	0.66
3:B:21:GLU:O	3:B:84:THR:HG22	1.96	0.66
2:C:40:VAL:HB	2:C:41:PRO:HD3	1.77	0.66
1:A:3:VAL:CG1	1:A:93:LYS:HG2	2.26	0.66
2:C:223:ILE:HD13	2:C:223:ILE:H	1.61	0.66
2:C:208:THR:O	2:C:209:ARG:HD2	1.96	0.66
3:B:14:GLN:HG2	3:B:108:PRO:HG2	1.78	0.66
2:C:110:LEU:HD23	2:C:111:ARG:N	2.12	0.65
3:B:225:ILE:HG22	3:B:228:PRO:HD2	1.79	0.65
2:C:215:ILE:O	2:C:216:LYS:HD3	1.95	0.65
2:C:243:ILE:HG21	2:C:298:ILE:HG23	1.79	0.65
2:C:214:ARG:HH11	2:C:214:ARG:CG	2.04	0.64
2:C:219:LYS:HE3	2:C:220:GLU:H	1.62	0.64
3:B:299:LYS:HB2	3:B:299:LYS:NZ	2.13	0.64
2:C:299:PHE:O	2:C:301:PRO:HD3	1.97	0.64
2:C:235:ALA:HB3	2:C:330:GLU:HB3	1.79	0.64
2:C:256:THR:HG21	2:C:318:THR:HG22	1.80	0.64
2:C:263:ALA:HA	2:C:311:PHE:HA	1.78	0.64
3:B:11:THR:O	3:B:14:GLN:HG3	1.97	0.64
4:D:1:NAG:H61	4:D:2:NAG:N2	2.12	0.64
2:C:136:VAL:CG2	2:C:178:HIS:HB3	2.28	0.64
2:C:327:THR:HG22	2:C:328:VAL:N	2.13	0.64
2:C:253:THR:N	2:C:254:PRO:HD3	2.13	0.63
1:A:58:VAL:N	1:A:101:PHE:O	2.24	0.63
3:B:92:TYR:O	3:B:106:ALA:HA	1.98	0.63
2:C:82:LEU:O	2:C:85:ALA:N	2.32	0.63
1:A:6:LEU:HD11	1:A:150:PHE:CD2	2.34	0.63
2:C:147:ARG:HG2	2:C:147:ARG:NH1	2.10	0.63
2:C:125:TYR:CD2	2:C:140:PRO:HG2	2.33	0.63
2:C:327:THR:CG2	2:C:328:VAL:H	2.11	0.63
3:B:234:TYR:O	3:B:325:ALA:O	2.17	0.62
2:C:240:ARG:H	2:C:240:ARG:HD3	1.63	0.62
1:A:22:GLY:HA3	1:A:24:TYR:N	2.15	0.62
2:C:37:CYS:O	2:C:41:PRO:HD2	1.99	0.62
3:B:229:ASN:O	3:B:230:ASP:HB2	1.99	0.62
3:B:52:TRP:CZ3	3:B:54:ARG:HB2	2.35	0.62
2:C:45:TRP:CG	2:C:48:VAL:HG21	2.35	0.61
3:B:287:THR:O	3:B:288:GLU:HB2	1.99	0.61
3:B:19:GLU:HG2	3:B:20:ASP:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:299:LYS:HG2	3:B:300:LYS:H	1.64	0.61
2:C:102:TYR:C	2:C:102:TYR:CD2	2.73	0.61
3:B:21:GLU:HB2	3:B:204:HIS:O	1.99	0.61
3:B:221:VAL:CG2	3:B:222:PRO:HD2	2.31	0.61
2:C:58:LYS:HB3	2:C:61:SER:HB2	1.83	0.60
3:B:234:TYR:HB2	3:B:325:ALA:O	2.01	0.60
1:A:73:LEU:HD12	1:A:73:LEU:H	1.66	0.60
2:C:237:LEU:H	2:C:304:ARG:HH22	1.48	0.60
2:C:255:LEU:CG	2:C:256:THR:H	2.13	0.60
3:B:67:LEU:N	3:B:68:PRO:CA	2.64	0.60
3:B:85:LEU:HD12	3:B:86:LEU:H	1.67	0.59
3:B:37:ASN:O	3:B:38:TYR:HB2	2.00	0.59
2:C:228:SER:N	2:C:229:PRO:HD3	2.17	0.59
2:C:61:SER:C	2:C:63:ARG:HH12	2.06	0.59
2:C:128:ILE:O	2:C:129:LEU:HD12	2.03	0.59
2:C:263:ALA:O	2:C:264:ASN:HB2	2.03	0.59
2:C:109:GLU:HG3	2:C:110:LEU:H	1.66	0.59
3:B:74:LYS:HG3	3:B:74:LYS:O	2.03	0.59
2:C:327:THR:CG2	2:C:328:VAL:N	2.66	0.59
3:B:9:LEU:HA	3:B:106:ALA:O	2.03	0.59
3:B:221:VAL:HG12	3:B:251:SER:OG	2.03	0.59
3:B:310:TYR:OH	3:B:326:LYS:HE3	2.02	0.58
2:C:271:ALA:H	2:C:273:PRO:HD2	1.67	0.58
3:B:81:PHE:CD1	3:B:81:PHE:N	2.71	0.58
2:C:247:VAL:O	2:C:293:ILE:HG23	2.04	0.58
2:C:223:ILE:HG13	3:B:226:HIS:CD2	2.38	0.58
3:B:55:GLN:HB2	4:D:1:NAG:H81	1.86	0.58
1:A:30:HIS:CG	2:C:140:PRO:HB3	2.39	0.58
2:C:86:LEU:O	2:C:89:ASP:HB2	2.04	0.58
1:A:6:LEU:HD22	1:A:7:ASN:N	2.18	0.58
1:A:69:LEU:HD23	1:A:69:LEU:N	2.16	0.58
1:A:18:LEU:HD11	1:A:132:VAL:HG21	1.86	0.58
2:C:76:GLN:CB	2:C:81:TRP:HE1	2.17	0.58
2:C:139:CYS:CB	2:C:177:THR:HG22	2.33	0.58
2:C:239:SER:HB3	2:C:302:VAL:O	2.04	0.58
1:A:138:LYS:HE3	3:B:185:SER:HA	1.85	0.57
2:C:102:TYR:C	2:C:102:TYR:HD2	2.07	0.57
1:A:22:GLY:HA3	1:A:24:TYR:H	1.69	0.57
2:C:20:ARG:HD3	2:C:21:HIS:O	2.03	0.57
3:B:316:SER:C	3:B:318:LYS:H	2.08	0.57
1:A:86:ASP:O	1:A:90:TYR:HD1	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:267:LYS:O	3:B:268:LYS:C	2.43	0.57
2:C:98:ARG:HB3	2:C:98:ARG:NH1	2.20	0.57
3:B:264:ILE:O	3:B:265:ASP:HB2	2.03	0.57
2:C:65:VAL:N	2:C:66:PRO:CA	2.68	0.57
2:C:180:LEU:HD11	3:B:134:GLY:O	2.05	0.56
2:C:234:SER:O	2:C:235:ALA:HB2	2.06	0.56
3:B:54:ARG:HA	3:B:90:GLY:HA3	1.86	0.56
2:C:229:PRO:HA	2:C:324:LEU:HD21	1.87	0.56
2:C:129:LEU:CD2	2:C:135:GLY:HA3	2.36	0.56
2:C:238:GLY:HA3	2:C:240:ARG:HH11	1.71	0.56
3:B:224:VAL:CG1	3:B:249:TYR:HB3	2.34	0.56
1:A:28:ALA:O	1:A:128:GLU:O	2.24	0.56
3:B:164:ILE:HA	3:B:167:PHE:CE1	2.41	0.56
2:C:64:THR:CB	2:C:66:PRO:HA	2.35	0.56
2:C:74:TRP:CD1	2:C:75:ALA:N	2.74	0.55
3:B:227:SER:HB2	3:B:247:THR:H	1.71	0.55
2:C:131:LEU:HA	2:C:184:VAL:CG1	2.35	0.55
2:C:64:THR:HB	2:C:66:PRO:CA	2.35	0.55
2:C:72:ARG:NH1	2:C:84:PRO:HD2	2.21	0.55
2:C:42:TYR:HB2	2:C:44:LEU:HD13	1.88	0.55
3:B:80:TRP:CE3	3:B:82:ARG:HD2	2.42	0.55
3:B:197:PRO:HA	3:B:201:ARG:O	2.06	0.55
2:C:98:ARG:HB3	2:C:98:ARG:HH11	1.71	0.55
3:B:298:ILE:HG22	3:B:299:LYS:O	2.07	0.55
2:C:58:LYS:HG3	2:C:59:ASN:N	2.19	0.55
2:C:214:ARG:NH1	2:C:214:ARG:CG	2.68	0.55
2:C:260:TRP:HE3	2:C:314:VAL:HG11	1.71	0.55
2:C:236:SER:O	2:C:237:LEU:HB3	2.07	0.54
1:A:99:PHE:N	1:A:99:PHE:HD2	2.06	0.54
2:C:87:GLN:O	2:C:88:GLU:CB	2.56	0.54
2:C:302:VAL:O	2:C:303:THR:HG23	2.08	0.54
2:C:327:THR:HG22	2:C:328:VAL:H	1.72	0.54
1:A:56:ILE:HG12	2:C:316:HIS:NE2	2.23	0.54
2:C:129:LEU:HD23	2:C:135:GLY:HA3	1.89	0.54
3:B:268:LYS:O	3:B:269:PRO:O	2.25	0.54
3:B:316:SER:O	3:B:318:LYS:HD2	2.08	0.54
2:C:219:LYS:HA	2:C:219:LYS:CE	2.37	0.54
2:C:128:ILE:C	2:C:129:LEU:HD12	2.28	0.54
2:C:123:ILE:HD12	2:C:123:ILE:N	2.23	0.53
3:B:86:LEU:HA	3:B:111:VAL:HG11	1.89	0.53
3:B:311:VAL:HG13	3:B:322:ALA:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:96:LEU:O	3:B:102:CYS:HA	2.08	0.53
1:A:20:MET:HG2	1:A:21:SER:N	2.23	0.53
2:C:16:ARG:CG	2:C:104:ASP:HB3	2.33	0.53
2:C:65:VAL:N	2:C:66:PRO:HA	2.23	0.53
2:C:225:VAL:HG11	3:B:229:ASN:ND2	2.24	0.53
2:C:124:SER:HG	2:C:191:TYR:HE1	1.57	0.52
1:A:99:PHE:N	1:A:99:PHE:CD2	2.77	0.52
2:C:76:GLN:HB2	2:C:81:TRP:NE1	2.23	0.52
2:C:253:THR:O	2:C:255:LEU:HD22	2.09	0.52
2:C:196:LEU:HD12	2:C:197:THR:N	2.23	0.52
2:C:283:GLN:O	2:C:294:GLU:HA	2.09	0.52
1:A:63:LYS:HD2	1:A:64:GLU:HB3	1.92	0.52
3:B:114:LYS:NZ	3:B:206:THR:HG21	2.25	0.52
2:C:308:HIS:O	2:C:309:MET:HG2	2.10	0.51
3:B:317:ALA:O	3:B:318:LYS:HG3	2.11	0.51
3:B:219:ASN:N	3:B:219:ASN:OD1	2.44	0.51
3:B:299:LYS:HB2	3:B:299:LYS:HZ2	1.76	0.51
2:C:227:ILE:C	2:C:229:PRO:HD3	2.31	0.51
2:C:268:ILE:HG23	2:C:268:ILE:O	2.11	0.51
3:B:194:VAL:HG13	3:B:205:LEU:HB2	1.91	0.51
3:B:295:ILE:O	3:B:296:LEU:HD23	2.11	0.51
3:B:63:ILE:HG22	3:B:67:LEU:HD22	1.93	0.51
1:A:41:VAL:CG2	1:A:151:VAL:HG11	2.41	0.51
2:C:176:THR:HG22	2:C:177:THR:N	2.21	0.51
3:B:175:MET:HA	3:B:175:MET:HE2	1.93	0.51
2:C:123:ILE:O	2:C:123:ILE:HG22	2.11	0.51
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.25	0.50
2:C:99:ASN:O	2:C:102:TYR:O	2.28	0.50
3:B:29:LEU:O	3:B:33:PHE:HA	2.11	0.50
1:A:6:LEU:HD22	1:A:7:ASN:H	1.75	0.50
1:A:10:LEU:HD23	1:A:148:MET:HB2	1.93	0.50
1:A:85:VAL:HB	1:A:90:TYR:CE1	2.46	0.50
2:C:266:THR:O	2:C:267:HIS:CB	2.60	0.50
1:A:12:ASP:OD2	1:A:16:LYS:HE3	2.11	0.50
3:B:281:SER:O	3:B:282:ILE:HG13	2.11	0.50
2:C:49:SER:O	2:C:50:PRO:C	2.50	0.50
2:C:81:TRP:CD1	2:C:81:TRP:N	2.79	0.50
3:B:9:LEU:CD1	3:B:11:THR:HG23	2.41	0.50
3:B:16:GLN:HG2	3:B:112:VAL:HG21	1.92	0.50
3:B:53:THR:O	3:B:54:ARG:HB3	2.10	0.50
3:B:18:PHE:CD1	3:B:114:LYS:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:SER:CA	2:C:63:ARG:HH12	2.25	0.49
3:B:204:HIS:O	3:B:205:LEU:HD12	2.12	0.49
1:A:50:GLU:H	1:A:57:PRO:HG2	1.77	0.49
2:C:38:PRO:O	2:C:40:VAL:N	2.45	0.49
2:C:147:ARG:NH1	2:C:147:ARG:CG	2.74	0.49
2:C:254:PRO:HB3	2:C:284:GLU:OE2	2.12	0.49
2:C:328:VAL:O	2:C:329:LYS:HB3	2.13	0.49
2:C:328:VAL:O	2:C:329:LYS:HD3	2.12	0.49
2:C:36:ARG:HH12	2:C:43:TRP:H	1.60	0.49
2:C:120:LEU:HD21	2:C:193:ARG:NH1	2.28	0.49
2:C:223:ILE:H	2:C:223:ILE:CD1	2.25	0.49
2:C:272:TYR:CE2	2:C:277:VAL:HG21	2.48	0.49
2:C:42:TYR:HB2	2:C:44:LEU:CD1	2.43	0.49
2:C:212:GLU:O	2:C:212:GLU:HG3	2.10	0.49
3:B:209:LEU:N	3:B:209:LEU:HD13	2.28	0.49
2:C:328:VAL:O	2:C:329:LYS:CB	2.60	0.49
3:B:114:LYS:HZ2	3:B:206:THR:HG21	1.78	0.49
2:C:23:LYS:NZ	2:C:23:LYS:HB2	2.28	0.49
3:B:46:LEU:N	3:B:46:LEU:HD23	2.27	0.49
3:B:142:ASN:HB3	3:B:207:ARG:NH1	2.28	0.49
2:C:256:THR:HG23	2:C:317:ASN:HB2	1.94	0.48
3:B:245:PRO:HA	3:B:295:ILE:HG23	1.94	0.48
1:A:127:ALA:HB3	1:A:130:MET:HG2	1.95	0.48
2:C:45:TRP:CD2	2:C:48:VAL:HG21	2.47	0.48
2:C:223:ILE:HD13	2:C:223:ILE:N	2.27	0.48
3:B:71:ARG:HH12	3:B:85:LEU:HB3	1.79	0.48
3:B:216:SER:HB3	3:B:218:LYS:HB3	1.96	0.48
2:C:76:GLN:HB3	2:C:81:TRP:HE1	1.76	0.48
2:C:298:ILE:O	2:C:299:PHE:HD1	1.97	0.48
1:A:22:GLY:CA	1:A:24:TYR:H	2.26	0.48
2:C:129:LEU:HD13	2:C:213:LEU:HD13	1.95	0.48
1:A:66:ASN:O	1:A:85:VAL:HG22	2.12	0.48
3:B:54:ARG:HG2	3:B:55:GLN:N	2.29	0.48
1:A:29:LEU:HD11	2:C:22:TYR:CE1	2.49	0.48
2:C:22:TYR:HD1	2:C:23:LYS:N	2.12	0.48
2:C:48:VAL:HG13	2:C:51:ARG:HG2	1.95	0.48
3:B:112:VAL:CG1	3:B:121:PRO:HD2	2.44	0.48
2:C:33:VAL:O	2:C:81:TRP:HA	2.13	0.48
2:C:40:VAL:CB	2:C:41:PRO:HD3	2.44	0.48
2:C:86:LEU:HB2	2:C:89:ASP:OD2	2.14	0.48
2:C:312:LYS:HE2	2:C:323:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:ILE:HG12	2:C:223:ILE:O	2.13	0.48
2:C:131:LEU:HB3	2:C:215:ILE:HG21	1.95	0.47
3:B:215:GLY:N	3:B:287:THR:HG23	2.29	0.47
2:C:22:TYR:CD1	2:C:23:LYS:N	2.82	0.47
2:C:125:TYR:CG	2:C:140:PRO:HG2	2.49	0.47
1:A:20:MET:CE	1:A:62:LEU:HD13	2.43	0.47
2:C:99:ASN:O	2:C:100:ALA:C	2.53	0.47
2:C:108:ILE:H	2:C:108:ILE:HG12	1.62	0.47
3:B:28:PRO:O	3:B:29:LEU:HD23	2.15	0.47
3:B:271:ASP:O	3:B:272:ILE:HG12	2.13	0.47
2:C:245:CYS:H	2:C:296:PRO:HD2	1.79	0.47
2:C:188:ASP:O	2:C:213:LEU:HD23	2.14	0.47
2:C:237:LEU:N	2:C:304:ARG:HH22	2.11	0.47
2:C:154:ILE:HG23	2:C:195:VAL:H	1.79	0.47
3:B:66:ARG:C	3:B:68:PRO:HA	2.34	0.47
3:B:112:VAL:HG13	3:B:121:PRO:HD2	1.96	0.47
1:A:151:VAL:HG22	1:A:152:SER:H	1.79	0.47
2:C:99:ASN:O	2:C:101:SER:N	2.47	0.47
3:B:198:GLU:HB3	3:B:203:PHE:HE2	1.79	0.47
3:B:270:ASP:HA	3:B:274:ILE:CG2	2.45	0.47
1:A:18:LEU:HD11	1:A:132:VAL:CG2	2.45	0.47
2:C:56:TRP:CH2	2:C:79:ALA:HA	2.50	0.47
3:B:196:TYR:HE2	3:B:205:LEU:HD13	1.77	0.47
1:A:6:LEU:C	1:A:6:LEU:HD13	2.35	0.47
3:B:97:ARG:HD3	3:B:98:ASN:N	2.30	0.47
1:A:36:MET:HA	1:A:36:MET:CE	2.39	0.47
1:A:78:PRO:HG2	1:A:120:TRP:CD2	2.50	0.47
2:C:241:LEU:HD23	2:C:300:ASP:OD2	2.15	0.47
3:B:26:LYS:HA	3:B:78:VAL:CG2	2.43	0.47
3:B:115:ASP:OD1	3:B:116:SER:N	2.48	0.47
2:C:161:LEU:O	2:C:163:LEU:HD12	2.15	0.46
2:C:279:GLU:O	2:C:279:GLU:HG2	2.15	0.46
3:B:138:ILE:O	3:B:176:ASN:HA	2.16	0.46
3:B:262:TRP:CD1	3:B:296:LEU:HD21	2.50	0.46
1:A:90:TYR:HB3	1:A:91:PRO:HA	1.96	0.46
2:C:23:LYS:HG3	2:C:23:LYS:O	2.15	0.46
3:B:242:LEU:HD23	3:B:298:ILE:HG13	1.97	0.46
1:A:3:VAL:CG2	1:A:91:PRO:HB2	2.46	0.46
2:C:272:TYR:N	2:C:273:PRO:CD	2.79	0.46
3:B:291:THR:O	3:B:291:THR:OG1	2.34	0.46
3:B:311:VAL:HG11	3:B:321:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:ARG:NH1	2:C:41:PRO:HG2	2.30	0.46
2:C:76:GLN:HB2	2:C:81:TRP:HE1	1.81	0.46
3:B:159:MET:HE2	3:B:190:TYR:CZ	2.51	0.46
3:B:209:LEU:O	3:B:209:LEU:HD22	2.15	0.46
2:C:21:HIS:ND1	2:C:38:PRO:HB3	2.31	0.45
2:C:76:GLN:HG3	2:C:77:ASP:H	1.81	0.45
2:C:237:LEU:H	2:C:304:ARG:NH2	2.14	0.45
1:A:94:LYS:N	1:A:94:LYS:CD	2.75	0.45
1:A:110:LEU:HD12	1:A:110:LEU:O	2.16	0.45
3:B:228:PRO:HB2	3:B:322:ALA:HB1	1.99	0.45
1:A:78:PRO:HG2	1:A:120:TRP:CE2	2.51	0.45
2:C:146:THR:HG22	2:C:146:THR:O	2.17	0.45
2:C:263:ALA:HA	2:C:311:PHE:CD1	2.51	0.45
2:C:64:THR:C	2:C:66:PRO:HA	2.36	0.45
3:B:25:ILE:O	3:B:78:VAL:HG13	2.16	0.45
2:C:42:TYR:N	2:C:42:TYR:CD2	2.84	0.45
2:C:94:VAL:HA	2:C:106:MET:O	2.15	0.45
3:B:64:ASN:C	3:B:64:ASN:OD1	2.55	0.45
3:B:142:ASN:HB3	3:B:207:ARG:HH11	1.82	0.45
1:A:29:LEU:H	1:A:29:LEU:HD23	1.81	0.45
3:B:310:TYR:N	3:B:310:TYR:CD2	2.84	0.45
3:B:189:ASN:N	3:B:189:ASN:ND2	2.64	0.45
3:B:236:LYS:NZ	3:B:242:LEU:HA	2.32	0.45
2:C:225:VAL:HG11	3:B:229:ASN:HD21	1.82	0.44
3:B:37:ASN:O	3:B:38:TYR:CB	2.64	0.44
2:C:136:VAL:HG21	2:C:178:HIS:HB3	1.99	0.44
3:B:140:CYS:HB2	3:B:175:MET:HG3	1.99	0.44
2:C:129:LEU:O	2:C:215:ILE:HA	2.17	0.44
2:C:58:LYS:HG2	2:C:61:SER:H	1.82	0.44
2:C:93:TYR:N	2:C:93:TYR:CD1	2.86	0.44
2:C:35:LEU:HD11	2:C:110:LEU:HD12	1.99	0.44
2:C:194:CYS:HB2	2:C:209:ARG:HB2	1.99	0.44
2:C:231:LYS:HE3	2:C:233:ILE:CD1	2.44	0.44
3:B:157:TRP:HZ2	3:B:175:MET:O	2.01	0.44
3:B:243:LEU:HD12	3:B:243:LEU:O	2.18	0.44
3:B:107:PHE:HA	3:B:108:PRO:HD2	1.85	0.44
3:B:224:VAL:HG13	3:B:224:VAL:O	2.17	0.44
1:A:29:LEU:N	1:A:29:LEU:CD2	2.81	0.44
2:C:99:ASN:ND2	2:C:101:SER:HB2	2.33	0.44
3:B:253:LEU:HB2	3:B:256:SER:HB2	2.00	0.44
3:B:316:SER:C	3:B:318:LYS:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:TYR:C	2:C:44:LEU:H	2.21	0.44
2:C:236:SER:O	2:C:237:LEU:CB	2.66	0.44
3:B:7:TRP:HZ2	3:B:32:HIS:CD2	2.36	0.44
3:B:54:ARG:CG	3:B:55:GLN:N	2.81	0.44
1:A:74:LYS:HB2	1:A:79:THR:OG1	2.18	0.43
2:C:124:SER:HA	2:C:210:SER:O	2.18	0.43
2:C:139:CYS:HA	2:C:140:PRO:HD3	1.78	0.43
3:B:198:GLU:HB3	3:B:203:PHE:CE2	2.53	0.43
2:C:268:ILE:O	2:C:268:ILE:CG2	2.65	0.43
2:C:99:ASN:C	2:C:101:SER:N	2.69	0.43
2:C:80:LEU:C	2:C:80:LEU:HD12	2.39	0.43
4:E:1:NAG:H61	4:E:2:NAG:N2	2.34	0.43
2:C:113:PHE:CD2	2:C:119:PHE:CD1	3.07	0.43
3:B:323:LYS:H	3:B:323:LYS:HG2	1.54	0.43
1:A:121:TYR:O	1:A:135:GLY:N	2.50	0.43
2:C:268:ILE:HD11	2:C:298:ILE:CD1	2.48	0.43
3:B:157:TRP:CZ3	3:B:192:CYS:HB3	2.54	0.43
1:A:36:MET:HG3	2:C:126:PRO:HG2	1.99	0.43
2:C:149:LYS:HD2	2:C:149:LYS:HA	1.71	0.43
2:C:314:VAL:O	2:C:314:VAL:HG12	2.19	0.43
1:A:69:LEU:H	1:A:69:LEU:CD2	2.18	0.43
2:C:123:ILE:O	2:C:123:ILE:CG2	2.67	0.43
2:C:151:ASP:O	2:C:175:GLY:HA2	2.19	0.43
2:C:272:TYR:N	2:C:273:PRO:HD3	2.33	0.43
2:C:31:GLU:HB2	2:C:32:PRO:HD2	2.00	0.43
2:C:240:ARG:O	2:C:240:ARG:HG2	2.18	0.43
1:A:18:LEU:HD13	1:A:18:LEU:HA	1.74	0.42
3:B:48:LEU:HA	3:B:96:LEU:HD23	2.01	0.42
3:B:82:ARG:HA	3:B:83:PRO:HA	1.83	0.42
3:B:222:PRO:HG3	3:B:318:LYS:HG2	2.01	0.42
3:B:229:ASN:ND2	3:B:231:HIS:HB2	2.33	0.42
1:A:63:LYS:O	1:A:64:GLU:HG2	2.19	0.42
2:C:227:ILE:O	2:C:227:ILE:CG2	2.63	0.42
2:C:260:TRP:O	2:C:314:VAL:HB	2.18	0.42
2:C:312:LYS:HG2	2:C:323:THR:OG1	2.20	0.42
2:C:38:PRO:C	2:C:40:VAL:H	2.22	0.42
3:B:225:ILE:HG21	3:B:322:ALA:HB3	2.00	0.42
2:C:65:VAL:HG12	2:C:65:VAL:O	2.19	0.42
2:C:252:GLY:HA2	2:C:292:TYR:HB2	2.01	0.42
3:B:7:TRP:CZ2	3:B:32:HIS:CD2	3.07	0.42
3:B:25:ILE:HG21	3:B:107:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:148:PRO:HG2	3:B:151:VAL:HG13	2.00	0.42
3:B:244:ILE:O	3:B:295:ILE:HA	2.19	0.42
1:A:120:TRP:HB3	1:A:134:LEU:HD12	1.99	0.42
2:C:158:LYS:HG2	2:C:192:TYR:CE2	2.54	0.42
2:C:245:CYS:HB2	2:C:261:TRP:CZ3	2.54	0.42
3:B:67:LEU:HG	3:B:72:ILE:HG13	2.00	0.42
3:B:274:ILE:O	3:B:274:ILE:CG2	2.64	0.42
1:A:34:GLN:O	2:C:24:ARG:NH2	2.53	0.42
2:C:62:ALA:N	2:C:63:ARG:HH12	2.17	0.42
3:B:158:TYR:CD2	3:B:163:LYS:HA	2.54	0.42
1:A:74:LYS:HD2	1:A:74:LYS:HA	1.73	0.42
2:C:139:CYS:HB3	2:C:177:THR:CG2	2.47	0.42
3:B:257:ARG:H	3:B:257:ARG:HD2	1.85	0.42
1:A:20:MET:HE2	1:A:62:LEU:HD13	2.02	0.42
2:C:54:LEU:O	2:C:55:THR:HG23	2.20	0.42
2:C:266:THR:O	2:C:267:HIS:HB2	2.20	0.42
2:C:109:GLU:CG	2:C:110:LEU:N	2.82	0.41
1:A:1:ALA:HA	1:A:2:PRO:HD3	1.83	0.41
1:A:47:VAL:HG13	1:A:95:MET:H	1.86	0.41
3:B:105:VAL:HG22	3:B:106:ALA:N	2.35	0.41
2:C:37:CYS:HA	2:C:38:PRO:HD3	1.89	0.41
2:C:64:THR:HB	2:C:66:PRO:O	2.20	0.41
2:C:83:LEU:HA	2:C:84:PRO:HA	1.77	0.41
2:C:168:GLU:H	2:C:168:GLU:HG2	1.66	0.41
1:A:16:LYS:HZ3	1:A:126:GLN:HA	1.85	0.41
3:B:98:ASN:HB3	3:B:101:TYR:HB2	2.03	0.41
1:A:60:LEU:H	1:A:60:LEU:HD23	1.86	0.41
1:A:73:LEU:HD12	1:A:73:LEU:N	2.33	0.41
3:B:245:PRO:HA	3:B:294:GLN:O	2.20	0.41
1:A:46:PHE:CD1	1:A:58:VAL:HG12	2.47	0.41
2:C:38:PRO:HB2	2:C:106:MET:CE	2.50	0.41
2:C:68:GLU:OE2	2:C:71:THR:HA	2.21	0.41
2:C:156:TRP:HZ2	2:C:177:THR:O	2.04	0.41
2:C:158:LYS:HB2	2:C:163:LEU:HD11	2.03	0.41
2:C:219:LYS:HE3	2:C:219:LYS:CA	2.46	0.41
2:C:231:LYS:O	2:C:233:ILE:N	2.54	0.41
3:B:114:LYS:HB3	3:B:114:LYS:HE2	1.61	0.41
3:B:134:GLY:O	3:B:180:LEU:O	2.38	0.41
3:B:155:ILE:HD13	3:B:175:MET:HA	2.01	0.41
1:A:90:TYR:CD1	1:A:90:TYR:N	2.89	0.41
2:C:16:ARG:O	2:C:104:ASP:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:ASP:OD2	2:C:300:ASP:N	2.54	0.41
3:B:95:MET:CA	3:B:103:SER:O	2.67	0.41
3:B:236:LYS:HD2	3:B:240:GLU:CB	2.51	0.41
2:C:22:TYR:HD1	2:C:23:LYS:H	1.67	0.41
2:C:58:LYS:HB3	2:C:61:SER:O	2.20	0.41
2:C:102:TYR:HD2	2:C:103:CYS:N	2.18	0.41
1:A:61:GLY:HA3	1:A:68:TYR:CD2	2.56	0.41
2:C:117:ASP:OD2	2:C:120:LEU:HD22	2.21	0.41
2:C:223:ILE:HA	2:C:224:PRO:HD3	1.89	0.41
2:C:243:ILE:O	2:C:243:ILE:CG2	2.69	0.41
2:C:265:ASP:OD2	2:C:265:ASP:N	2.53	0.41
3:B:158:TYR:HB2	3:B:191:THR:HG23	2.01	0.41
3:B:287:THR:O	3:B:287:THR:HG22	2.21	0.41
1:A:30:HIS:CB	2:C:140:PRO:HB3	2.51	0.41
1:A:111:GLU:HG2	1:A:145:ASP:HB3	2.03	0.41
2:C:234:SER:O	2:C:235:ALA:CB	2.69	0.41
3:B:72:ILE:HG22	3:B:72:ILE:O	2.21	0.41
2:C:36:ARG:NH1	2:C:43:TRP:H	2.19	0.40
2:C:123:ILE:N	2:C:123:ILE:CD1	2.83	0.40
1:A:93:LYS:HB2	1:A:94:LYS:HD3	2.03	0.40
2:C:198:PHE:O	2:C:204:GLN:HA	2.21	0.40
4:D:1:NAG:H61	4:D:2:NAG:C7	2.51	0.40
3:B:184:ILE:HD13	3:B:286:ARG:HD3	2.03	0.40
3:B:236:LYS:HD2	3:B:240:GLU:HB2	2.04	0.40
2:C:104:ASP:C	2:C:105:LYS:HG3	2.41	0.40
2:C:231:LYS:HB3	2:C:327:THR:H	1.87	0.40
2:C:238:GLY:O	2:C:239:SER:HB2	2.22	0.40
3:B:287:THR:O	3:B:288:GLU:CB	2.69	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	150/158 (95%)	134 (89%)	14 (9%)	2 (1%)	12 40
2	C	314/339 (93%)	254 (81%)	41 (13%)	19 (6%)	1 10
3	B	321/339 (95%)	271 (84%)	42 (13%)	8 (2%)	5 27
All	All	785/836 (94%)	659 (84%)	97 (12%)	29 (4%)	3 20

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
2	C	50	PRO
2	C	236	SER
2	C	244	PRO
2	C	264	ASN
2	C	268	ILE
2	C	329	LYS
3	B	38	TYR
3	B	265	ASP
3	B	269	PRO
2	C	151	ASP
2	C	152	VAL
2	C	232	THR
2	C	235	ALA
3	B	272	ILE
2	C	39	GLN
2	C	77	ASP
2	C	88	GLU
2	C	150	THR
2	C	255	LEU
2	C	271	ALA
3	B	273	THR
2	C	273	PRO
3	B	159	MET
3	B	268	LYS
2	C	141	ASP
1	A	22	GLY
2	C	41	PRO
3	B	160	GLY

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	139/143 (97%)	117 (84%)	22 (16%)	2 11
2	C	287/304 (94%)	227 (79%)	60 (21%)	1 4
3	B	299/314 (95%)	254 (85%)	45 (15%)	3 13
All	All	725/761 (95%)	598 (82%)	127 (18%)	2 8

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	7	ASN
1	A	11	ARG
1	A	18	LEU
1	A	29	LEU
1	A	36	MET
1	A	48	GLN
1	A	53	ASN
1	A	63	LYS
1	A	69	LEU
1	A	71	CYS
1	A	73	LEU
1	A	93	LYS
1	A	97	LYS
1	A	99	PHE
1	A	107	ASN
1	A	110	LEU
1	A	124	THR
1	A	134	LEU
1	A	137	THR
1	A	145	ASP
1	A	148	MET
2	C	20	ARG
2	C	23	LYS
2	C	35	LEU
2	C	42	TYR
2	C	43	TRP
2	C	48	VAL
2	C	55	THR
2	C	56	TRP

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Mol	Chain	Res	Type
2	C	57	HIS
2	C	63	ARG
2	C	72	ARG
2	C	74	TRP
2	C	77	ASP
2	C	83	LEU
2	C	88	GLU
2	C	90	SER
2	C	98	ARG
2	C	102	TYR
2	C	108	ILE
2	C	115	ASN
2	C	120	LEU
2	C	130	THR
2	C	138	VAL
2	C	144	GLU
2	C	151	ASP
2	C	177	THR
2	C	179	LEU
2	C	180	LEU
2	C	201	GLU
2	C	208	THR
2	C	210	SER
2	C	212	GLU
2	C	214	ARG
2	C	219	LYS
2	C	221	GLU
2	C	223	ILE
2	C	231	LYS
2	C	232	THR
2	C	233	ILE
2	C	240	ARG
2	C	255	LEU
2	C	259	LEU
2	C	267	HIS
2	C	268	ILE
2	C	269	GLU
2	C	276	ARG
2	C	284	GLU
2	C	290	GLU
2	C	292	TYR
2	C	297	LEU

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Mol	Chain	Res	Type
2	C	298	ILE
2	C	300	ASP
2	C	303	THR
2	C	304	ARG
2	C	307	LEU
2	C	308	HIS
2	C	309	MET
2	C	318	THR
2	C	326	THR
2	C	329	LYS
3	B	9	LEU
3	B	11	THR
3	B	13	ARG
3	B	20	ASP
3	B	33	PHE
3	B	34	LEU
3	B	35	LYS
3	B	48	LEU
3	B	53	THR
3	B	56	ASP
3	B	58	ASP
3	B	61	GLU
3	B	65	PHE
3	B	67	LEU
3	B	78	VAL
3	B	80	TRP
3	B	81	PHE
3	B	82	ARG
3	B	83	PRO
3	B	97	ARG
3	B	110	GLU
3	B	128	LYS
3	B	133	TYR
3	B	140	CYS
3	B	155	ILE
3	B	161	CYS
3	B	175	MET
3	B	189	ASN
3	B	191	THR
3	B	194	VAL
3	B	206	THR
3	B	207	ARG

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Mol	Chain	Res	Type
3	B	208	THR
3	B	209	LEU
3	B	219	ASN
3	B	227	SER
3	B	242	LEU
3	B	257	ARG
3	B	270	ASP
3	B	272	ILE
3	B	284	HIS
3	B	291	THR
3	B	295	ILE
3	B	310	TYR
3	B	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\#\|Z\| > 2$
4	NAG	D	1	3,4	14,14,15	0.69	0	17,19,21	1.78	4 (23%)
4	NAG	D	2	4	14,14,15	0.55	0	17,19,21	1.51	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	1	3,4	14,14,15	0.59	0	17,19,21	0.91	1 (5%)
4	NAG	E	2	4	14,14,15	0.54	0	17,19,21	1.29	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	NAG	C2-N2-C7	-4.65	116.29	122.90
4	E	2	NAG	C1-O5-C5	3.60	117.08	112.19
4	D	2	NAG	C2-N2-C7	-3.53	117.87	122.90
4	D	2	NAG	C1-O5-C5	3.47	116.90	112.19
4	D	1	NAG	C4-C3-C2	2.89	115.26	111.02
4	D	1	NAG	O4-C4-C5	2.66	115.90	109.30
4	D	2	NAG	O5-C1-C2	2.33	114.97	111.29
4	E	1	NAG	C4-C3-C2	2.26	114.33	111.02
4	D	1	NAG	C1-C2-N2	-2.25	106.64	110.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

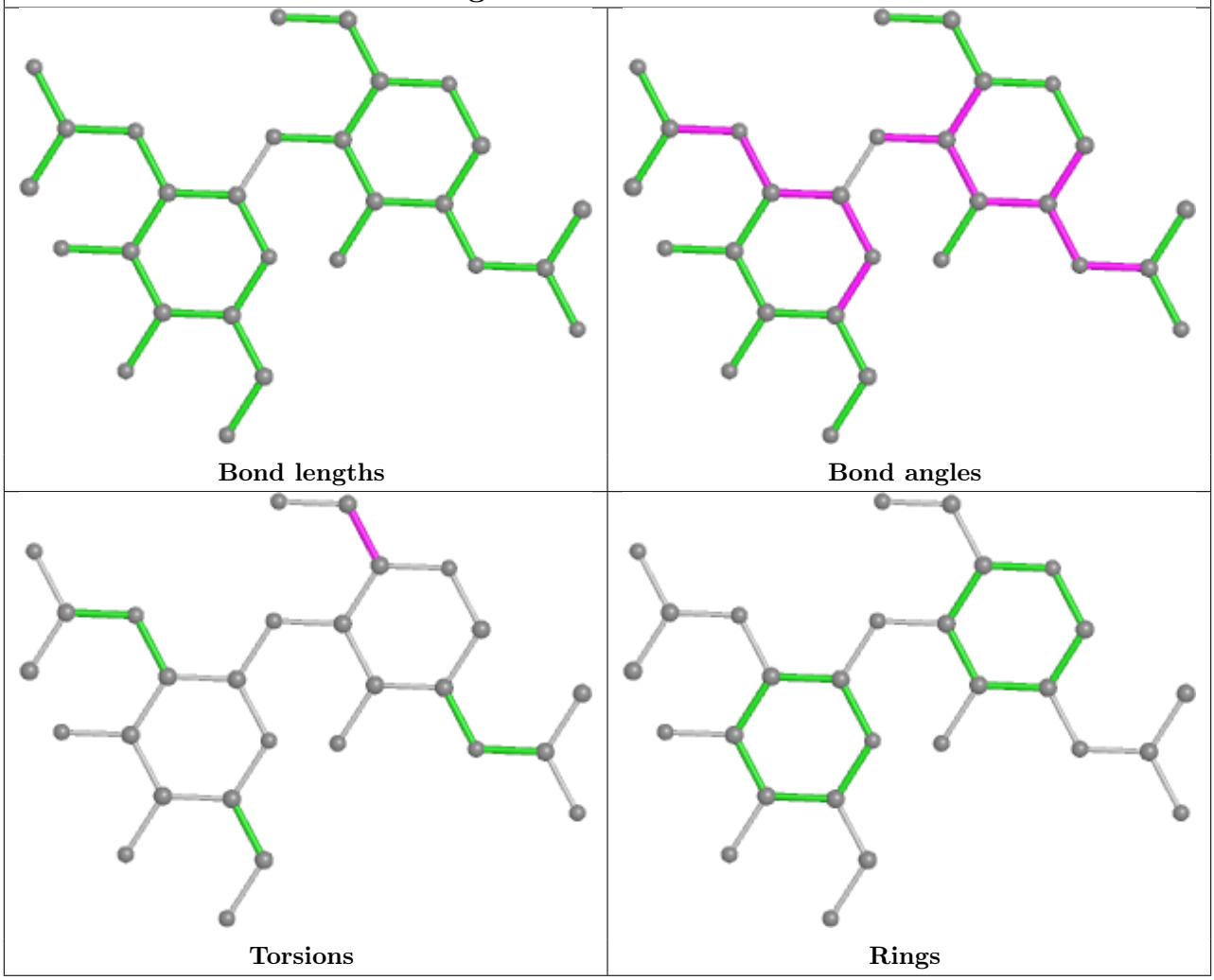
There are no ring outliers.

4 monomers are involved in 6 short contacts:

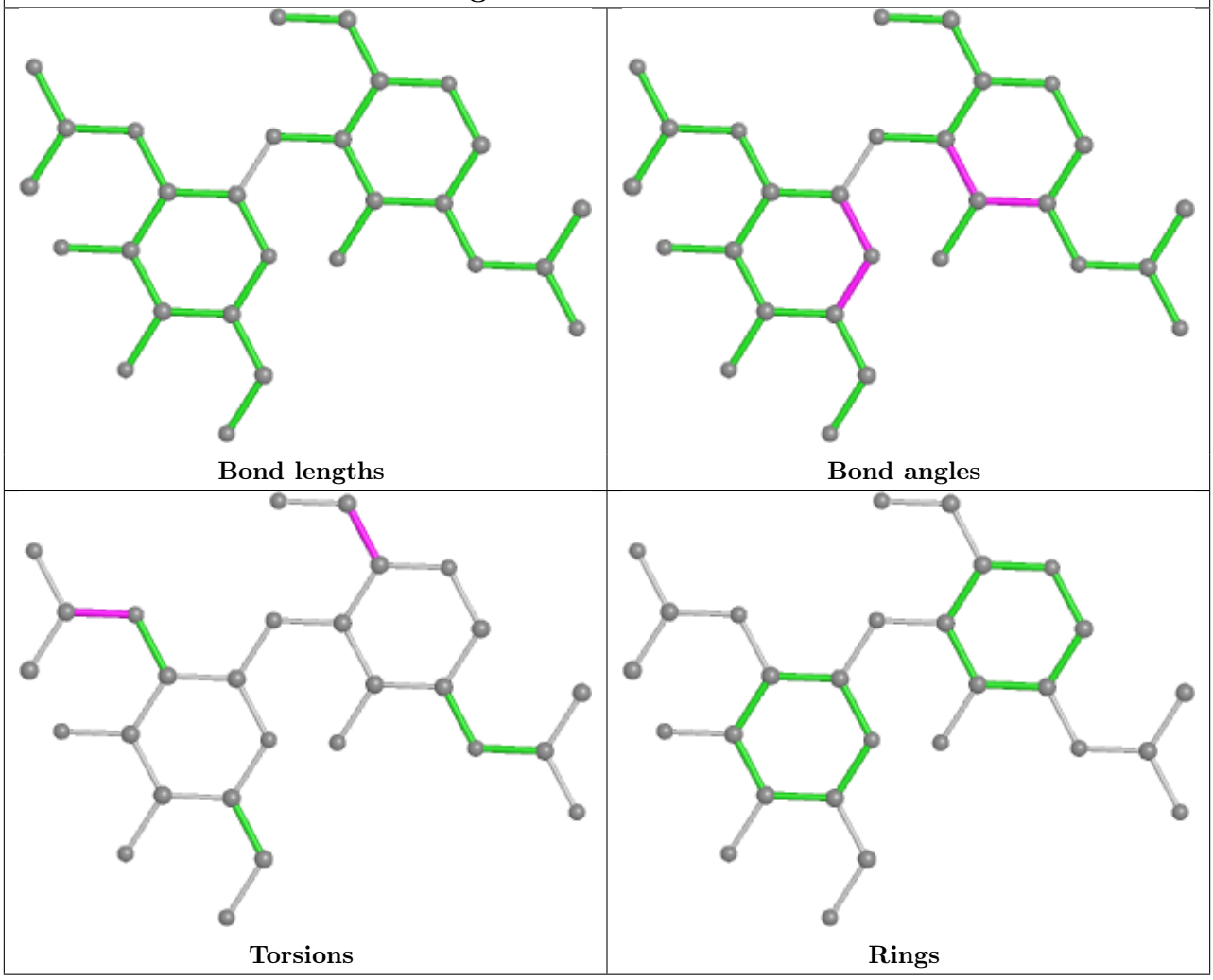
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
4	D	2	NAG	2	0
4	D	1	NAG	5	0
4	E	2	NAG	1	0

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

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	340	3	14,14,15	0.55	0	17,19,21	1.43	2 (11%)
5	NAG	B	337	3	14,14,15	0.53	0	17,19,21	0.82	0
5	NAG	C	337	2	14,14,15	0.58	0	17,19,21	1.18	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	338	2	14,14,15	0.50	0	17,19,21	1.18	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	340	3	-	4/6/23/26	0/1/1/1
5	NAG	B	337	3	-	0/6/23/26	0/1/1/1
5	NAG	C	337	2	-	1/6/23/26	0/1/1/1
5	NAG	C	338	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	340	NAG	C1-O5-C5	3.69	117.19	112.19
5	B	340	NAG	C2-N2-C7	-3.48	117.94	122.90
5	C	338	NAG	C1-O5-C5	3.24	116.58	112.19
5	C	337	NAG	C1-O5-C5	2.59	115.69	112.19
5	C	337	NAG	C2-N2-C7	-2.42	119.45	122.90
5	C	337	NAG	O5-C5-C6	2.34	110.87	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	340	NAG	C8-C7-N2-C2
5	B	340	NAG	O7-C7-N2-C2
5	B	340	NAG	C4-C5-C6-O6
5	B	340	NAG	O5-C5-C6-O6
5	C	337	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	152/158 (96%)	0.01	1 (0%)	87	88	53, 99, 166, 210	0
2	C	316/339 (93%)	0.41	25 (7%)	12	12	54, 139, 207, 253	0
3	B	323/339 (95%)	0.24	20 (6%)	20	20	46, 118, 199, 231	0
All	All	791/836 (94%)	0.27	46 (5%)	23	22	46, 122, 202, 253	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	50	PRO	5.2
3	B	268	LYS	4.8
2	C	70	GLU	4.5
2	C	328	VAL	4.5
3	B	277	THR	4.4
2	C	234	SER	4.0
2	C	71	THR	3.8
3	B	278	ILE	3.8
2	C	47	SER	3.7
2	C	306	ASP	3.7
1	A	24	TYR	3.7
2	C	307	LEU	3.7
2	C	301	PRO	3.6
2	C	246	LYS	3.4
2	C	69	GLU	3.4
2	C	278	THR	3.4
3	B	33	PHE	3.3
2	C	270	SER	3.3
3	B	38	TYR	3.3
3	B	273	THR	3.2
2	C	287	GLU	3.0
3	B	326	LYS	3.0
2	C	201	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	289	ASN	2.9
2	C	65	VAL	2.8
3	B	32	HIS	2.8
3	B	4	CYS	2.8
3	B	309	SER	2.7
3	B	308	ARG	2.7
2	C	53	ASN	2.6
2	C	290	GLU	2.6
2	C	40	VAL	2.5
3	B	35	LYS	2.5
3	B	242	LEU	2.4
2	C	298	ILE	2.4
3	B	279	ASN	2.3
2	C	233	ILE	2.3
3	B	310	TYR	2.3
3	B	266	GLY	2.3
2	C	300	ASP	2.2
3	B	324	ALA	2.2
3	B	236	LYS	2.1
2	C	272	TYR	2.1
3	B	237	GLU	2.1
3	B	45	GLY	2.1
2	C	260	TRP	2.1

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

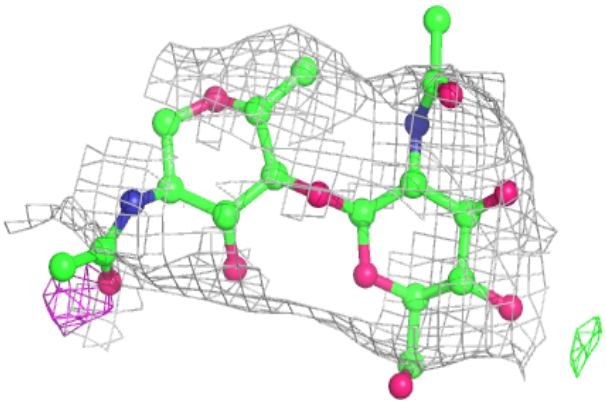
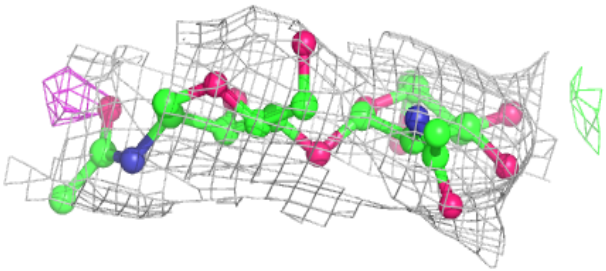
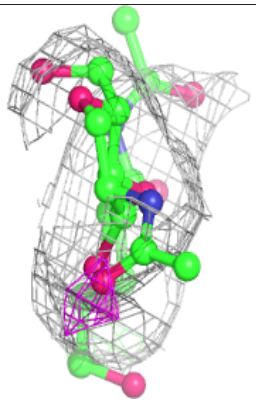
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

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

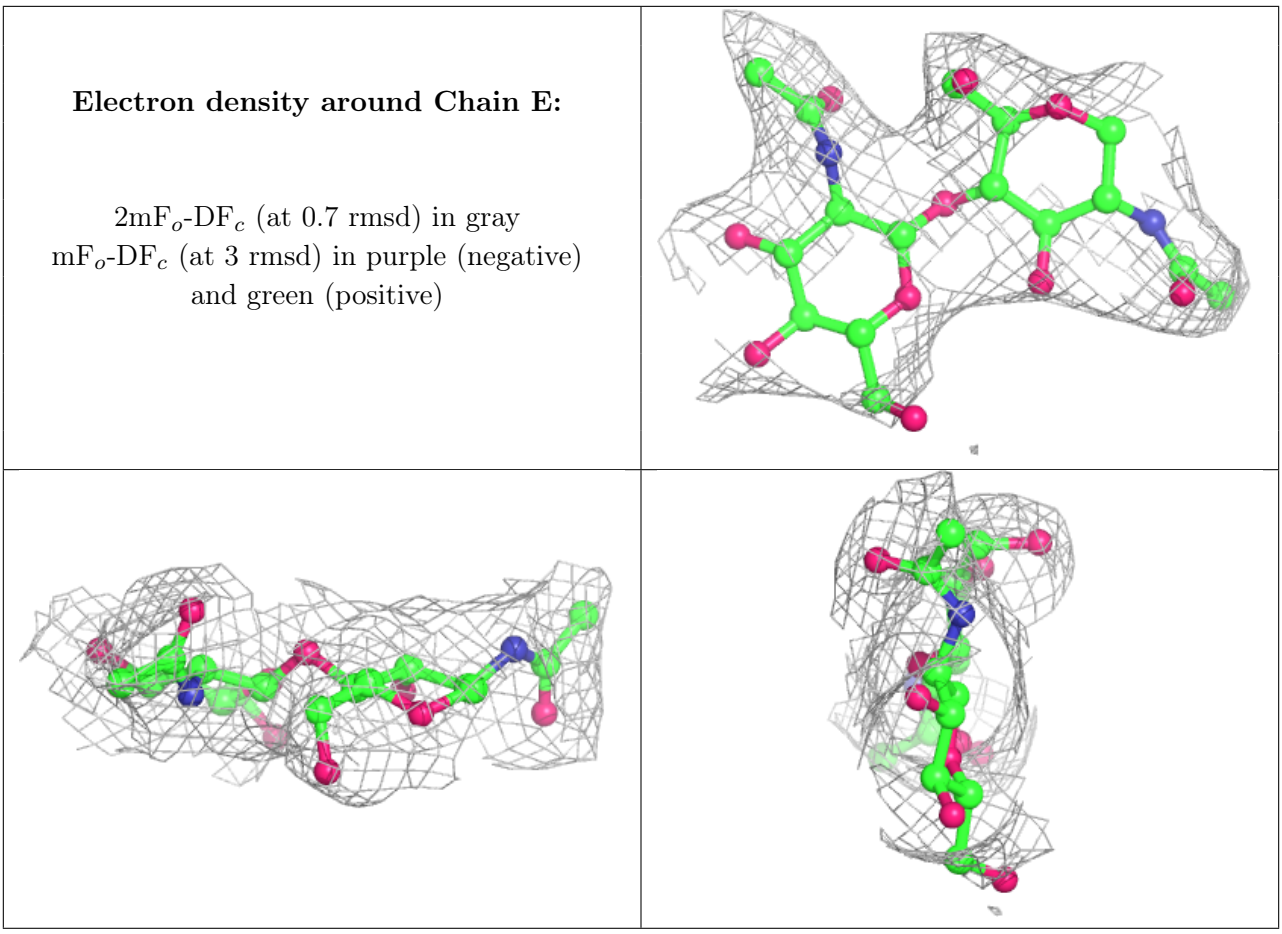
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	2	14/15	0.85	0.27	114,118,119,121	0
4	NAG	D	2	14/15	0.86	0.24	142,148,154,155	0
4	NAG	D	1	14/15	0.87	0.18	148,154,159,161	0
4	NAG	E	1	14/15	0.91	0.22	116,118,120,122	0

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 D: $2mF_o$-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 E:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	337	14/15	0.64	0.26	182,187,191,192	0
5	NAG	C	337	14/15	0.76	0.19	151,160,169,169	0
5	NAG	C	338	14/15	0.82	0.15	127,136,142,145	0
5	NAG	B	340	14/15	0.82	0.21	154,162,170,173	0

6.5 Other polymers (i)

There are no such residues in this entry.