



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 05:29 PM EST

PDB ID : 2WR2
Title : structure of influenza H2 avian hemagglutinin with avian receptor
Authors : Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2009-08-29
Resolution : 2.40 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:

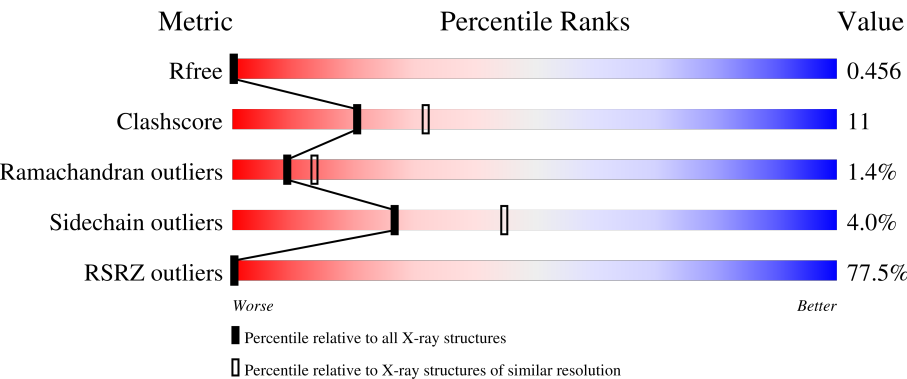
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	509	<div><div>83%</div><div>77%</div><div>18%</div><div>• •</div></div>
1	B	509	<div><div>59%</div><div>72%</div><div>22%</div><div>• • •</div></div>
1	C	509	<div><div>81%</div><div>76%</div><div>17%</div><div>• 5%</div></div>
2	D	3	<div><div>33%</div><div>33%</div><div>33%</div></div>
2	E	3	<div><div>100%</div></div>

2 Entry composition [i](#)

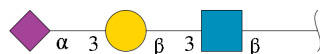
There are 4 unique types of molecules in this entry. The entry contains 12274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	4	0	0
			3882	2436	671	753	22			
1	B	490	Total	C	N	O	S	0	1	0
			3887	2438	672	755	22			
1	C	485	Total	C	N	O	S	0	0	0
			3844	2413	664	745	22			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	E	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			13	8	1	4		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

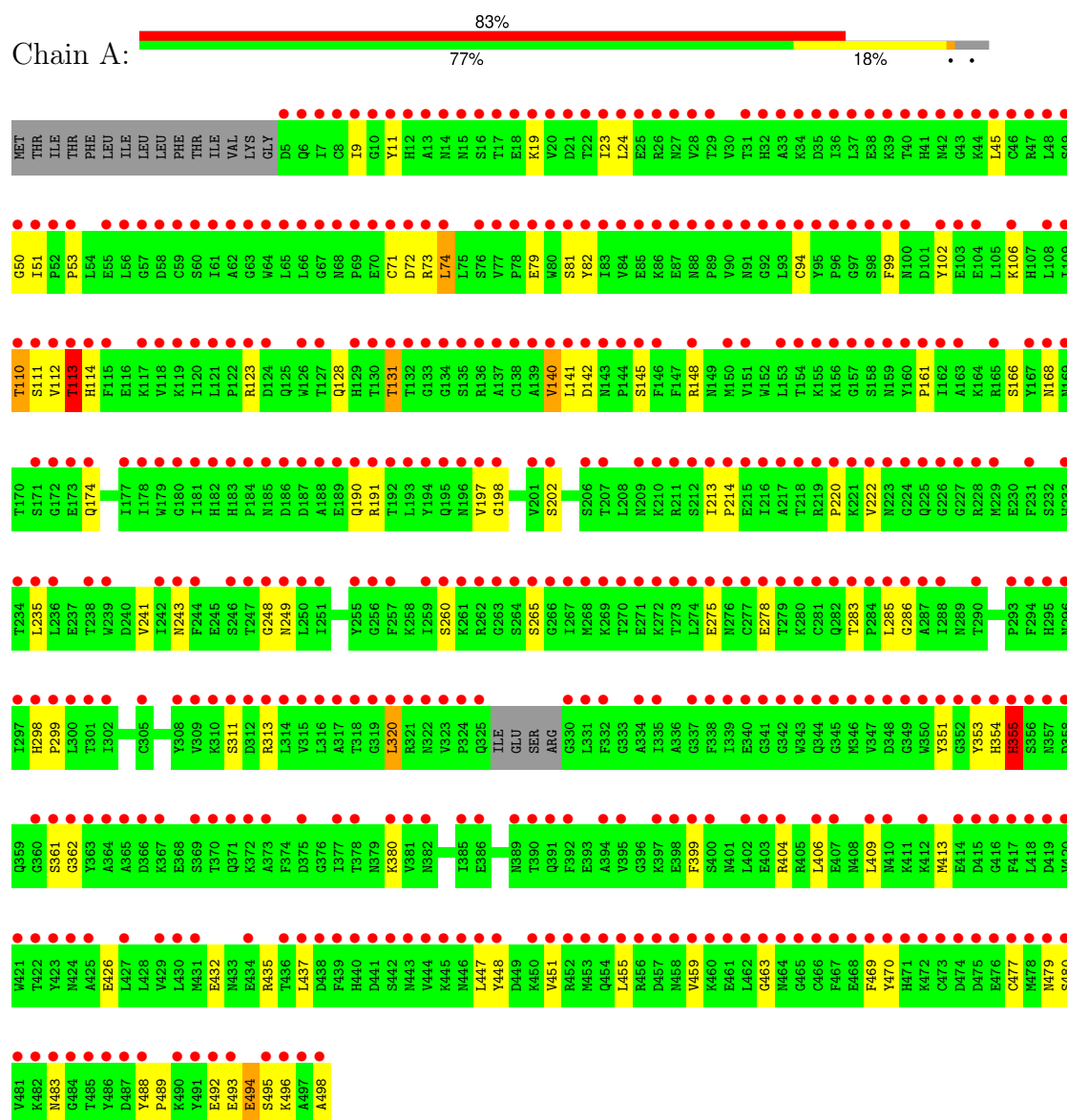
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	169	Total	O	0	0
			169	169		
4	C	174	Total	O	0	0
			174	174		

3 Residue-property plots

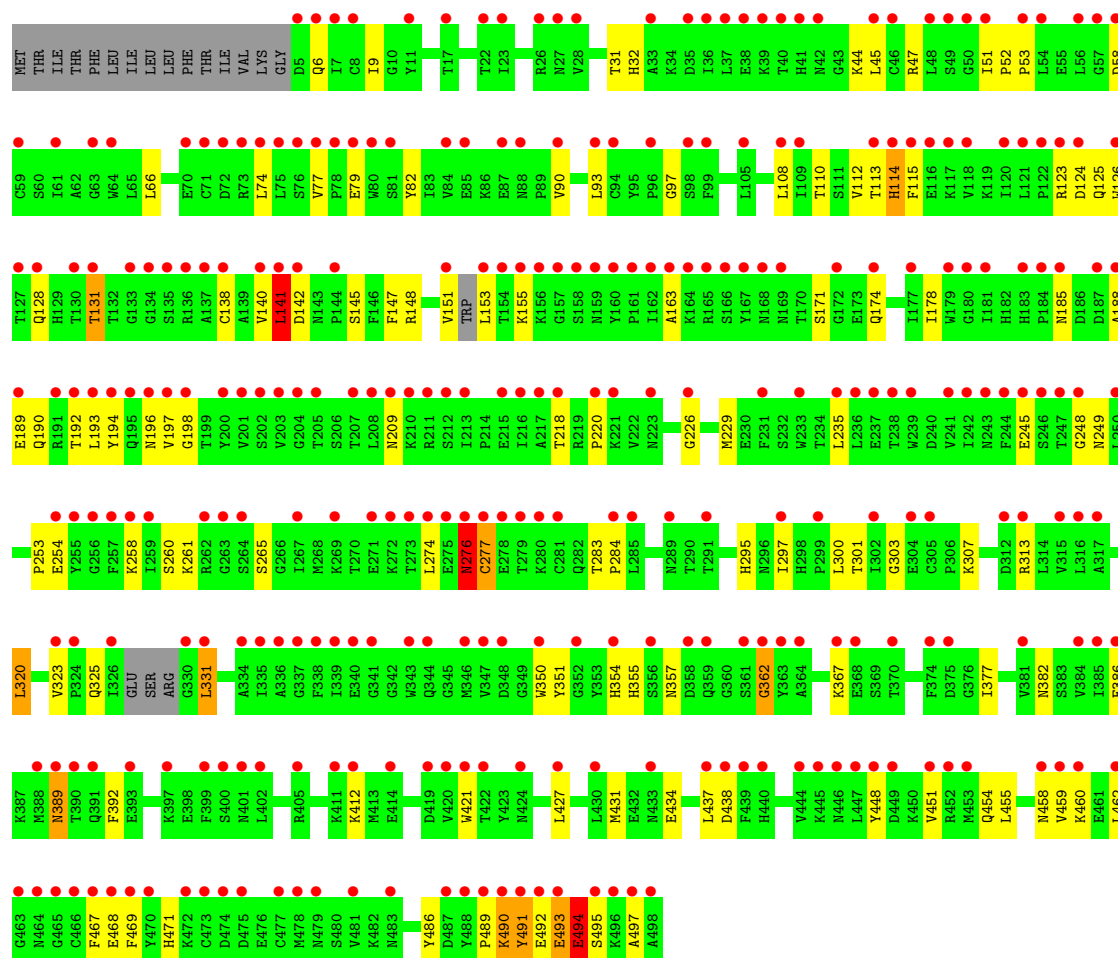
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: HEMAGGLUTININ

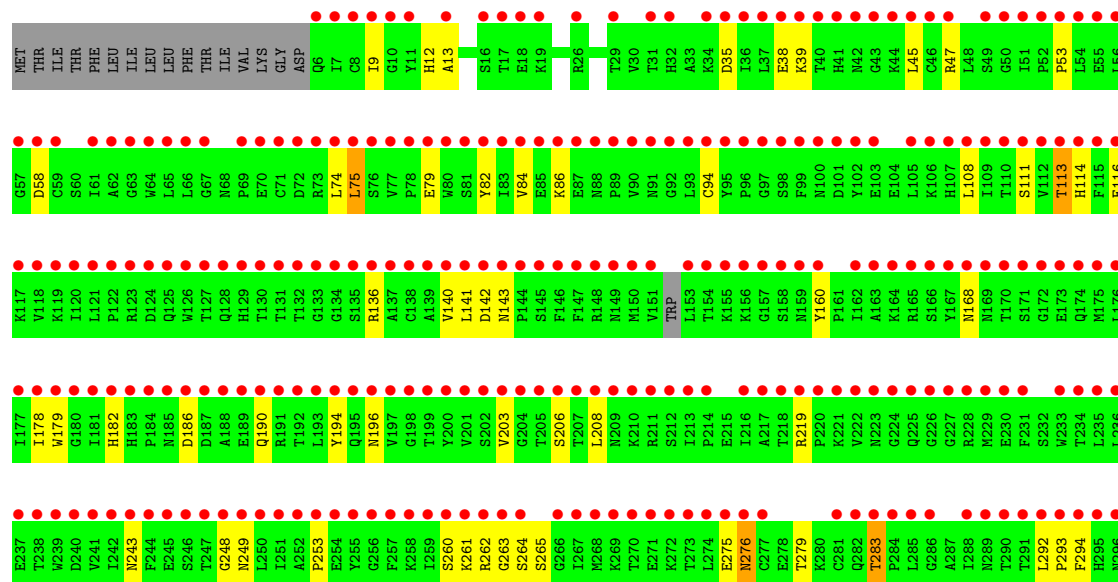
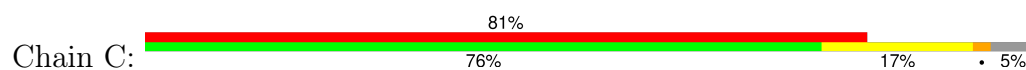


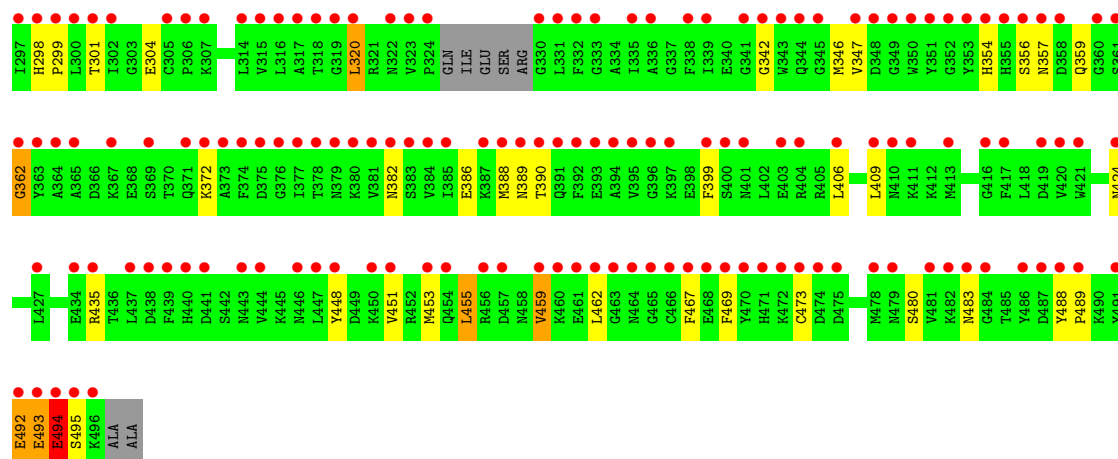
• Molecule 1: HEMAGGLUTININ





- Molecule 1: HEMAGGLUTININ





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 33%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.88Å 142.72Å 199.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.94-2.40) 99.8 (29.94-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.248 0.447 , 0.456	Depositor DCC
R_{free} test set	3956 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	12274	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.33	0/3968	0.51	0/5372
1	B	0.33	0/3970	0.53	0/5372
1	C	0.33	0/3927	0.51	0/5313
All	All	0.33	0/11865	0.52	0/16057

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

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	3882	0	3742	85	2
1	B	3887	0	3756	109	2
1	C	3844	0	3718	67	0
2	D	46	0	40	2	0
2	E	46	0	40	0	0
3	A	27	0	25	7	0
3	C	14	0	13	3	0
4	A	185	0	0	5	0
4	B	169	0	0	9	0
4	C	174	0	0	2	0
All	All	12274	0	11334	254	2

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 11.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLN:NE2	4:B:2109:HOH:O	1.62	1.27
1:A:283:THR:HG22	1:A:285:LEU:H	1.18	1.05
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.32	0.94
1:B:325:GLN:HB3	4:B:2110:HOH:O	1.65	0.93
1:A:361:SER:HB3	1:A:362:GLY:HA3	1.49	0.92
1:C:114:HIS:H	1:C:260:SER:HB2	1.35	0.91
1:B:140:VAL:O	1:B:141:LEU:HB2	1.72	0.89
1:B:459:VAL:HG22	1:B:469:PHE:HA	1.55	0.89
1:B:276:ASN:HA	1:B:277:CYS:O	1.73	0.89
1:A:110:THR:CG2	1:A:265:SER:H	1.86	0.88
1:B:459:VAL:HG11	1:B:467:PHE:HB3	1.54	0.88
1:C:168:ASN:HD21	3:C:1500:NAG:C1	1.89	0.84
1:B:47:ARG:HE	1:B:276:ASN:HB2	1.42	0.84
1:C:141:LEU:N	1:C:142:ASP:HA	1.95	0.82
1:A:110:THR:HG21	1:A:265:SER:H	1.44	0.82
1:B:141:LEU:N	1:B:142:ASP:HA	1.97	0.79
1:A:114:HIS:H	1:A:260:SER:HB2	1.45	0.79
1:B:32:HIS:CD2	4:B:2124:HOH:O	2.37	0.78
1:B:110:THR:CG2	1:B:265:SER:H	1.95	0.78
1:C:114:HIS:N	1:C:260:SER:HB2	1.98	0.77
1:A:479:ASN:HB3	3:A:1499:NAG:H81	1.64	0.77
1:A:168:ASN:HD21	3:A:1500:NAG:C5	1.97	0.77
1:B:113:THR:HB	1:B:114:HIS:HB3	1.66	0.77
1:A:190:GLN:HE22	1:A:249:ASN:HD21	1.33	0.77
1:A:174:GLN:HE21	1:A:235:LEU:HD13	1.51	0.76
1:B:455:LEU:HD13	1:B:459:VAL:HG21	1.66	0.75
1:B:458:ASN:OD1	1:B:494:GLU:HG2	1.86	0.74
1:A:493:GLU:O	1:A:494:GLU:HB3	1.88	0.73
1:A:174:GLN:NE2	1:A:235:LEU:HD13	2.04	0.73
1:C:190:GLN:HE22	1:C:249:ASN:HD21	1.36	0.73
1:A:283:THR:HG22	1:A:285:LEU:N	1.99	0.73
1:A:320:LEU:HD23	1:A:320:LEU:H	1.53	0.72
1:A:166:SER:HB3	1:A:243:ASN:ND2	2.05	0.72
1:A:283:THR:HB	1:A:286:GLY:O	1.89	0.72
1:B:354:HIS:HA	1:B:362:GLY:O	1.90	0.72
1:B:140:VAL:HG12	1:B:141:LEU:HD23	1.73	0.70
1:C:74:LEU:O	1:C:75:LEU:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HG23	1:B:265:SER:H	1.57	0.69
1:A:313:ARG:HA	4:A:2015:HOH:O	1.93	0.69
1:A:380:LYS:HE3	1:A:432:GLU:OE1	1.93	0.68
1:C:320:LEU:H	1:C:320:LEU:HD23	1.58	0.68
1:A:493:GLU:O	1:A:494:GLU:CB	2.43	0.67
1:A:168:ASN:ND2	3:A:1500:NAG:C1	2.58	0.66
1:B:490:LYS:O	1:B:490:LYS:HG2	1.93	0.66
1:B:188:ALA:O	1:B:192:THR:HG22	1.95	0.66
1:B:295:HIS:HD2	1:B:297:ILE:H	1.44	0.66
1:C:354:HIS:HA	1:C:362:GLY:O	1.94	0.66
1:A:114:HIS:N	1:A:260:SER:HB2	2.09	0.65
1:C:275:GLU:O	1:C:276:ASN:HB3	1.96	0.65
1:B:459:VAL:HG13	1:B:468:GLU:O	1.96	0.65
1:C:79:GLU:HG3	1:C:113:THR:HB	1.78	0.64
1:C:357:ASN:HB3	1:C:359:GLN:H	1.62	0.64
1:C:262:ARG:HG3	1:C:263:GLY:H	1.63	0.64
1:C:168:ASN:ND2	3:C:1500:NAG:C1	2.59	0.63
1:A:168:ASN:HD21	3:A:1500:NAG:C1	2.12	0.63
1:C:459:VAL:HG23	1:C:469:PHE:HA	1.80	0.62
1:A:283:THR:CG2	1:A:285:LEU:H	2.05	0.62
1:B:350:TRP:NE1	4:B:2124:HOH:O	2.27	0.62
1:B:113:THR:HB	1:B:114:HIS:CB	2.29	0.61
1:A:140:VAL:HG23	1:A:145:SER:HB2	1.81	0.61
1:A:455:LEU:HD23	1:A:459:VAL:HG21	1.81	0.61
1:A:50:GLY:HA2	1:A:278:GLU:OE2	2.00	0.61
1:C:111:SER:HB2	1:C:265:SER:HB2	1.83	0.61
1:A:191:ARG:HD2	4:A:2085:HOH:O	2.00	0.61
1:A:248:GLY:C	1:A:249:ASN:HD22	2.04	0.60
1:A:470:TYR:HB3	1:A:495:SER:HA	1.83	0.60
1:A:353:TYR:OH	1:A:447:LEU:HD11	2.01	0.60
1:B:320:LEU:HD23	1:B:320:LEU:H	1.66	0.60
1:A:435:ARG:NH1	1:C:435:ARG:NH1	2.49	0.60
1:C:459:VAL:HG21	1:C:467:PHE:HB3	1.84	0.59
1:B:190:GLN:HE22	1:B:249:ASN:HD21	1.49	0.59
1:B:454:GLN:NE2	1:B:486:TYR:H	2.00	0.58
1:A:72:ASP:OD1	1:A:73:ARG:N	2.36	0.58
1:B:123:ARG:HB2	1:B:254:GLU:OE2	2.03	0.58
1:B:171:SER:HB2	1:B:258:LYS:HD2	1.85	0.58
1:B:492:GLU:HA	1:B:493:GLU:C	2.23	0.58
1:B:325:GLN:CB	4:B:2110:HOH:O	2.38	0.57
1:C:58:ASP:HB3	1:C:86:LYS:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:THR:HG23	1:C:113:THR:O	2.03	0.57
1:B:110:THR:HG21	1:B:265:SER:H	1.68	0.57
1:A:111:SER:HB2	1:A:265:SER:HB2	1.85	0.57
1:A:148:ARG:HH11	1:A:148:ARG:CG	2.10	0.56
1:C:488:TYR:HB3	1:C:489:PRO:HD3	1.87	0.56
1:C:53:PRO:HG3	1:C:82:TYR:CZ	2.41	0.56
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.86	0.56
1:B:493:GLU:O	1:B:494:GLU:HB2	2.05	0.56
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.20	0.56
1:A:9:ILE:HD11	1:A:451:VAL:HG21	1.88	0.56
1:B:44:LYS:HD3	1:B:277:CYS:SG	2.46	0.56
1:B:140:VAL:C	1:B:142:ASP:HA	2.25	0.56
1:C:179:TRP:CE2	1:C:203:VAL:HG21	2.41	0.56
1:A:11:TYR:HB2	1:A:320:LEU:HD11	1.87	0.55
1:C:283:THR:HG22	1:C:301:THR:HG22	1.87	0.55
1:B:492:GLU:OE2	1:B:495:SER:N	2.39	0.55
1:C:47:ARG:O	1:C:279:THR:HG22	2.06	0.55
1:B:193:LEU:HD21	2:D:3:SIA:O10	2.06	0.55
1:C:493:GLU:C	1:C:494:GLU:HG3	2.27	0.55
1:C:114:HIS:H	1:C:260:SER:CB	2.14	0.55
1:C:45:LEU:HD21	1:C:84:VAL:HG21	1.88	0.54
1:A:72:ASP:OD2	1:A:148:ARG:HD2	2.07	0.54
1:B:283:THR:HG22	1:B:301:THR:HG22	1.89	0.54
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.89	0.54
1:B:382:ASN:O	1:B:386:GLU:HG2	2.07	0.54
1:A:148:ARG:HG2	1:A:148:ARG:NH1	2.11	0.54
1:A:110:THR:HG23	1:A:265:SER:HB3	1.90	0.54
1:B:138:CYS:O	1:B:145:SER:HB3	2.08	0.53
1:C:114:HIS:CE1	1:C:116:GLU:HB2	2.43	0.53
1:B:124:ASP:OD1	1:B:125:GLN:HG3	2.08	0.53
1:C:424:ASN:ND2	4:C:2149:HOH:O	2.42	0.53
1:B:492:GLU:CD	1:B:495:SER:H	2.12	0.52
1:A:110:THR:CG2	1:A:265:SER:N	2.66	0.52
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.45	0.52
1:B:355:HIS:CE1	1:B:362:GLY:HA2	2.44	0.52
1:C:357:ASN:OD1	1:C:473:CYS:O	2.28	0.52
1:B:490:LYS:HB2	4:B:2167:HOH:O	2.09	0.52
1:C:262:ARG:HG3	1:C:263:GLY:N	2.24	0.52
1:A:495:SER:HB2	4:A:2177:HOH:O	2.10	0.52
1:C:304:GLU:HB3	1:C:390:THR:HG22	1.90	0.51
1:B:490:LYS:C	1:B:492:GLU:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:SER:CB	1:A:362:GLY:HA3	2.29	0.51
1:B:491:TYR:O	1:B:494:GLU:HB2	2.09	0.51
1:A:19:LYS:O	1:A:313:ARG:NH2	2.44	0.51
1:B:126:TRP:HZ3	1:B:163:ALA:HB1	1.76	0.51
1:A:113:THR:HG23	1:A:113:THR:O	2.10	0.51
1:B:490:LYS:C	1:B:492:GLU:N	2.63	0.51
1:A:355:HIS:CE1	1:A:361:SER:HB2	2.46	0.50
1:B:492:GLU:HA	1:B:492:GLU:OE1	2.11	0.50
1:C:143:ASN:N	1:C:143:ASN:HD22	2.10	0.50
1:C:492:GLU:O	1:C:492:GLU:HG2	2.11	0.50
1:C:262:ARG:NH1	4:C:2029:HOH:O	2.44	0.50
1:A:213:ILE:HD12	1:A:214:PRO:O	2.12	0.50
1:A:141:LEU:HG	1:A:141:LEU:O	2.12	0.49
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.94	0.49
1:B:491:TYR:O	1:B:494:GLU:CB	2.61	0.49
1:B:357:ASN:HB2	4:B:2126:HOH:O	2.12	0.49
1:B:495:SER:C	1:B:497:ALA:N	2.65	0.49
1:A:140:VAL:HG12	1:A:141:LEU:HD22	1.93	0.49
1:A:413:MET:HE1	1:B:412:LYS:HE3	1.93	0.49
1:A:479:ASN:O	1:A:483:ASN:HB2	2.13	0.49
1:B:31:THR:C	1:B:32:HIS:CD2	2.86	0.49
1:B:126:TRP:CZ3	1:B:163:ALA:HB1	2.48	0.49
1:B:113:THR:HG22	1:B:114:HIS:HB2	1.96	0.48
1:C:248:GLY:O	1:C:249:ASN:HB2	2.13	0.48
1:B:123:ARG:HG2	1:B:131:THR:HG21	1.94	0.48
1:C:160:TYR:CZ	1:C:248:GLY:HA2	2.48	0.48
1:C:168:ASN:HD21	3:C:1500:NAG:C2	2.26	0.48
1:A:361:SER:HB3	1:A:362:GLY:CA	2.33	0.48
1:C:113:THR:C	1:C:260:SER:HB2	2.34	0.48
1:A:51:ILE:HB	1:A:81:SER:HB3	1.96	0.47
1:B:31:THR:OG1	1:B:32:HIS:HD2	1.98	0.47
1:A:354:HIS:O	1:A:355:HIS:CD2	2.67	0.47
1:B:471:HIS:HD2	1:B:494:GLU:OE2	1.98	0.47
1:A:102:TYR:CZ	1:A:106:LYS:HD3	2.50	0.47
1:B:331:LEU:HD22	1:B:438:ASP:OD2	2.14	0.47
1:B:459:VAL:CG1	1:B:460:LYS:N	2.77	0.47
1:B:218:THR:HA	4:B:2072:HOH:O	2.14	0.46
1:A:248:GLY:O	1:A:249:ASN:HB2	2.16	0.46
1:A:399:PHE:CE1	1:A:406:LEU:HG	2.51	0.46
1:B:189:GLU:HA	1:B:192:THR:HG22	1.97	0.46
1:B:459:VAL:HG12	1:B:460:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ALA:HB2	1:C:342:GLY:HA3	1.96	0.46
2:D:3:SIA:O1A	2:D:3:SIA:H6	2.16	0.46
1:B:491:TYR:C	1:B:494:GLU:HB2	2.36	0.46
1:C:480:SER:HA	1:C:483:ASN:OD1	2.16	0.46
1:B:155:LYS:HE2	1:B:192:THR:O	2.16	0.45
1:C:9:ILE:HG13	1:C:448:TYR:HA	1.98	0.45
3:A:1500:NAG:C5	3:A:1500:NAG:C1	2.95	0.45
1:A:220:PRO:HD3	1:C:243:ASN:HD22	1.81	0.45
1:C:12:HIS:HD2	1:C:346:MET:O	1.99	0.45
1:C:455:LEU:HD23	1:C:459:VAL:HG11	1.99	0.45
1:B:51:ILE:HG23	1:B:79:GLU:HG2	1.99	0.45
1:B:276:ASN:HA	1:B:277:CYS:C	2.35	0.45
1:A:9:ILE:HG13	1:A:448:TYR:HA	1.98	0.45
1:B:114:HIS:HB3	1:B:260:SER:HB2	1.98	0.45
1:A:498:ALA:C	4:A:2177:HOH:O	2.55	0.44
1:B:459:VAL:CG1	1:B:467:PHE:HB3	2.38	0.44
1:B:197:VAL:HG22	1:B:198:GLY:H	1.82	0.44
1:B:248:GLY:O	1:B:249:ASN:HB2	2.17	0.44
1:B:174:GLN:OE1	1:B:235:LEU:HD13	2.18	0.44
1:B:178:ILE:O	1:B:253:PRO:HG3	2.18	0.44
1:C:140:VAL:C	1:C:142:ASP:HA	2.38	0.44
1:C:182:HIS:CD2	1:C:194:TYR:OH	2.70	0.44
1:A:128:GLN:HB3	1:A:161:PRO:HG2	1.99	0.44
1:B:108:LEU:HD11	1:B:261:LYS:HE2	1.99	0.44
1:C:390:THR:HG22	1:C:390:THR:O	2.17	0.44
1:B:131:THR:HG23	1:B:131:THR:O	2.18	0.44
1:C:38:GLU:HB2	1:C:292:LEU:HD12	2.00	0.44
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.99	0.44
1:B:303:GLY:HA2	1:B:392:PHE:CE1	2.53	0.44
1:B:295:HIS:CD2	1:B:297:ILE:H	2.32	0.43
1:A:123:ARG:HG2	1:A:131:THR:HG21	2.00	0.43
1:A:220:PRO:HD3	1:C:243:ASN:ND2	2.34	0.43
1:B:66:LEU:O	1:B:147:PHE:HB3	2.18	0.43
1:B:113:THR:HB	1:B:260:SER:HB2	2.00	0.43
1:B:151:VAL:HG12	1:B:153:LEU:HD12	1.99	0.43
1:B:389:ASN:HD22	1:B:389:ASN:HA	1.68	0.43
1:A:71:CYS:O	1:A:74:LEU:HB2	2.18	0.43
1:B:9:ILE:HG13	1:B:448:TYR:HA	2.01	0.43
1:B:112:VAL:CG1	1:B:115:PHE:HB2	2.48	0.43
1:B:493:GLU:O	1:B:494:GLU:CB	2.66	0.43
1:C:9:ILE:HD11	1:C:451:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD13	1:A:74:LEU:O	2.18	0.43
1:A:480:SER:HA	1:A:483:ASN:HB3	2.01	0.43
1:B:458:ASN:OD1	1:B:491:TYR:HA	2.19	0.43
1:C:494:GLU:OE2	1:C:495:SER:N	2.42	0.43
1:A:23:ILE:HG23	1:A:24:LEU:HG	2.01	0.43
1:B:185[B]:ASN:OD1	1:B:226:GLY:C	2.56	0.43
1:B:194:TYR:O	1:B:196:ASN:N	2.47	0.43
1:A:112:VAL:C	1:A:113:THR:HG22	2.39	0.43
1:B:209:ASN:OD1	1:C:219:ARG:NH1	2.50	0.42
1:B:307:LYS:HD3	1:B:307:LYS:HA	1.90	0.42
1:C:320:LEU:HD23	1:C:320:LEU:N	2.30	0.42
1:A:110:THR:HG23	1:A:265:SER:H	1.77	0.42
1:A:197:VAL:HG12	1:A:198:GLY:N	2.33	0.42
1:B:189:GLU:HA	1:B:192:THR:CG2	2.48	0.42
1:A:492:GLU:O	4:A:2177:HOH:O	2.22	0.42
1:B:320:LEU:HD23	1:B:320:LEU:N	2.33	0.42
1:A:140:VAL:HG23	1:A:145:SER:CB	2.48	0.42
1:C:108:LEU:O	1:C:261:LYS:HD2	2.18	0.42
1:B:471:HIS:CD2	1:B:494:GLU:OE2	2.72	0.42
1:C:178:ILE:O	1:C:253:PRO:HG3	2.19	0.42
1:C:399:PHE:CE1	1:C:406:LEU:HG	2.55	0.42
1:A:311:SER:HB3	1:A:426:GLU:OE1	2.20	0.42
1:A:463:GLY:HA2	1:C:453:MET:CE	2.49	0.42
1:C:293:PRO:HG2	1:C:294:PHE:CD2	2.55	0.42
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.55	0.42
1:B:307:LYS:HE2	1:B:421:TRP:NE1	2.35	0.42
1:B:459:VAL:HG13	1:B:468:GLU:C	2.39	0.41
1:B:458:ASN:HA	1:B:494:GLU:CG	2.49	0.41
1:A:409:LEU:HD21	1:C:409:LEU:HD22	2.02	0.41
1:A:488:TYR:N	1:A:489:PRO:CD	2.83	0.41
1:C:388:MET:HB2	1:C:388:MET:HE2	1.85	0.41
1:B:367:LYS:HD3	1:B:367:LYS:HA	1.64	0.41
1:A:459:VAL:HG12	1:A:469:PHE:HA	2.02	0.41
1:B:52:PRO:HA	1:B:53:PRO:HD3	1.86	0.41
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.35	0.41
1:A:141:LEU:O	1:A:141:LEU:CG	2.68	0.41
1:B:163:ALA:O	1:B:245:GLU:HA	2.21	0.41
1:A:79:GLU:HG3	1:A:113:THR:HA	2.02	0.41
1:A:241:VAL:HG23	3:A:1500:NAG:H61	2.03	0.41
1:B:97:GLY:HA3	1:B:229:MET:O	2.21	0.41
1:B:113:THR:CB	1:B:114:HIS:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:HG12	4:B:2108:HOH:O	2.21	0.41
1:B:427:LEU:O	1:B:431:MET:HG3	2.20	0.41
1:C:143:ASN:N	1:C:143:ASN:ND2	2.69	0.41
1:C:382:ASN:O	1:C:386:GLU:HB2	2.21	0.41
1:A:222:VAL:HG22	1:C:206:SER:HB2	2.03	0.41
1:B:495:SER:C	1:B:497:ALA:H	2.24	0.40
1:C:35:ASP:OD2	1:C:39:LYS:NZ	2.54	0.40
1:A:241:VAL:HB	1:B:220:PRO:HG3	2.03	0.40
1:C:372:LYS:HA	1:C:372:LYS:HD2	1.91	0.40
1:A:168:ASN:ND2	3:A:1500:NAG:C5	2.75	0.40
1:B:6:GLN:HB2	1:B:467:PHE:O	2.22	0.40
1:B:284:PRO:HD3	1:B:300:LEU:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:CD2	1:B:128:GLN:OE1[1_655]	1.82	0.38
1:A:141:LEU:CD1	1:B:128:GLN:OE1[1_655]	2.03	0.17

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	486/509 (96%)	459 (94%)	21 (4%)	6 (1%)	11	16
1	B	485/509 (95%)	456 (94%)	20 (4%)	9 (2%)	6	8
1	C	479/509 (94%)	457 (95%)	16 (3%)	6 (1%)	10	15
All	All	1450/1527 (95%)	1372 (95%)	57 (4%)	21 (1%)	9	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	494	GLU
1	B	277	CYS
1	B	490	LYS
1	B	494	GLU
1	C	113	THR
1	B	114	HIS
1	B	141	LEU
1	B	276	ASN
1	C	276	ASN
1	B	362	GLY
1	C	362	GLY
1	C	492	GLU
1	C	494	GLU
1	A	496	LYS
1	B	489	PRO
1	C	75	LEU
1	A	140	VAL
1	B	313	ARG
1	A	74	LEU
1	A	355	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/447 (96%)	413 (97%)	14 (3%)	33	53
1	B	429/447 (96%)	408 (95%)	21 (5%)	21	36
1	C	425/447 (95%)	409 (96%)	16 (4%)	28	47
All	All	1281/1341 (96%)	1230 (96%)	51 (4%)	27	45

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	94	CYS

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Mol	Chain	Res	Type
1	A	110	THR
1	A	113	THR
1	A	131	THR
1	A	142	ASP
1	A	202	SER
1	A	275	GLU
1	A	320	LEU
1	A	351	TYR
1	A	355	HIS
1	A	404	ARG
1	A	437	LEU
1	A	477	CYS
1	B	45	LEU
1	B	58	ASP
1	B	74	LEU
1	B	77	VAL
1	B	90	VAL
1	B	93	LEU
1	B	131	THR
1	B	141	LEU
1	B	148	ARG
1	B	276	ASN
1	B	320	LEU
1	B	331	LEU
1	B	351	TYR
1	B	377	ILE
1	B	389	ASN
1	B	434	GLU
1	B	437	LEU
1	B	462	LEU
1	B	491	TYR
1	B	493	GLU
1	B	494	GLU
1	C	94	CYS
1	C	136	ARG
1	C	186	ASP
1	C	196	ASN
1	C	208	LEU
1	C	264	SER
1	C	283	THR
1	C	320	LEU
1	C	347	VAL

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Mol	Chain	Res	Type
1	C	356	SER
1	C	389	ASN
1	C	455	LEU
1	C	459	VAL
1	C	462	LEU
1	C	493	GLU
1	C	494	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	A	114	HIS
1	A	168	ASN
1	A	174	GLN
1	A	182	HIS
1	A	243	ASN
1	A	249	ASN
1	A	295	HIS
1	A	483	ASN
1	B	27	ASN
1	B	32	HIS
1	B	114	HIS
1	B	182	HIS
1	B	249	ASN
1	B	295	HIS
1	B	382	ASN
1	B	391	GLN
1	B	408	ASN
1	B	454	GLN
1	C	12	HIS
1	C	15	ASN
1	C	32	HIS
1	C	91	ASN
1	C	100	ASN
1	C	114	HIS
1	C	125	GLN
1	C	143	ASN
1	C	168	ASN
1	C	174	GLN
1	C	182	HIS
1	C	243	ASN

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Mol	Chain	Res	Type
1	C	249	ASN
1	C	389	ASN
1	C	408	ASN
1	C	454	GLN
1	C	479	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2	15,15,15	0.91	1 (6%)	21,21,21	0.74	0
2	GAL	D	2	2	11,11,12	0.74	0	15,15,17	0.67	0
2	SIA	D	3	2	20,20,21	0.90	0	21,28,31	0.92	1 (4%)
2	NAG	E	1	2	15,15,15	0.89	0	21,21,21	1.10	2 (9%)
2	GAL	E	2	2	11,11,12	0.60	0	15,15,17	0.99	1 (6%)
2	SIA	E	3	2	20,20,21	0.98	1 (5%)	21,28,31	0.90	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
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	NAG	E	1	2	-	1/6/26/26	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	SIA	E	3	2	-	0/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	SIA	C4-C5	2.17	1.55	1.53
2	D	1	NAG	C1-C2	2.04	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GAL	C1-C2-C3	3.02	114.05	109.64
2	E	1	NAG	C3-C4-C5	2.72	115.16	110.23
2	D	3	SIA	O1B-C1-C2	2.28	118.64	112.71
2	E	1	NAG	O5-C5-C4	2.06	113.41	109.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

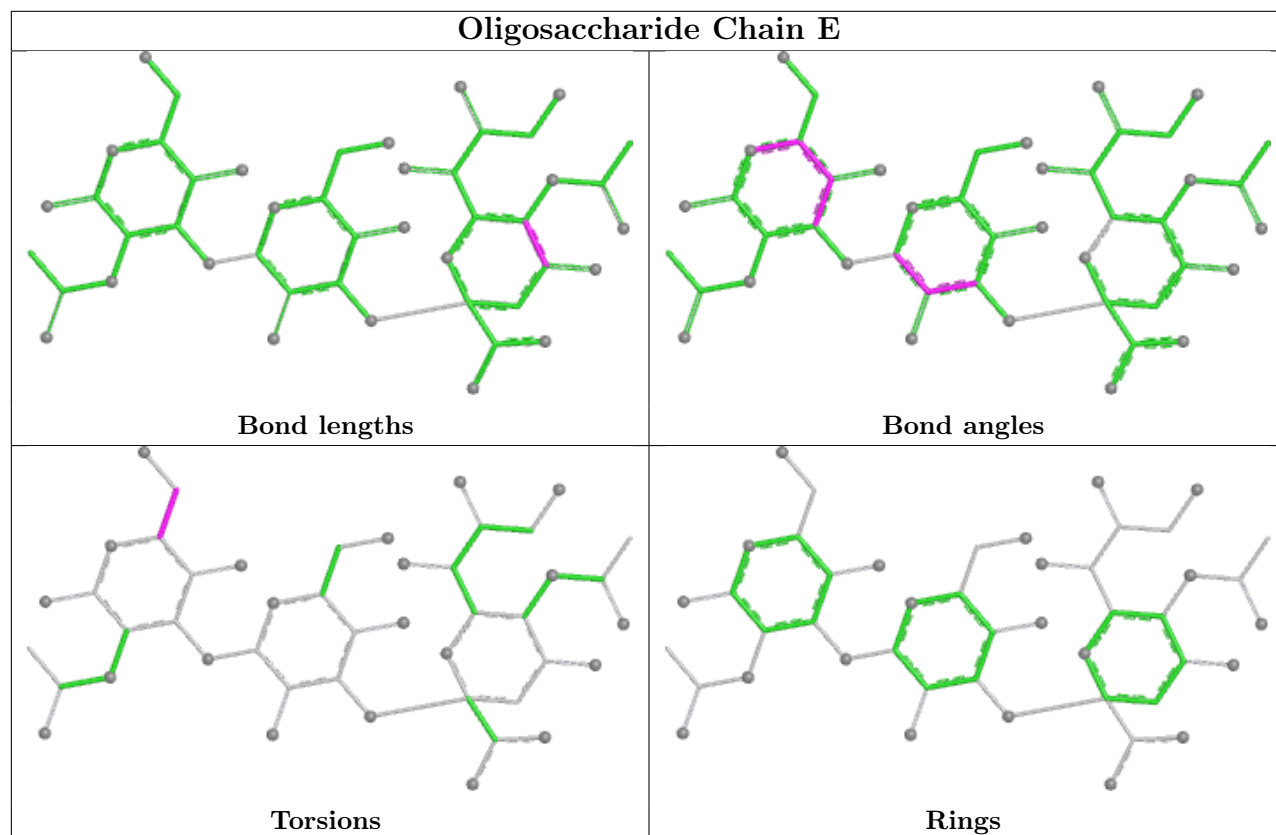
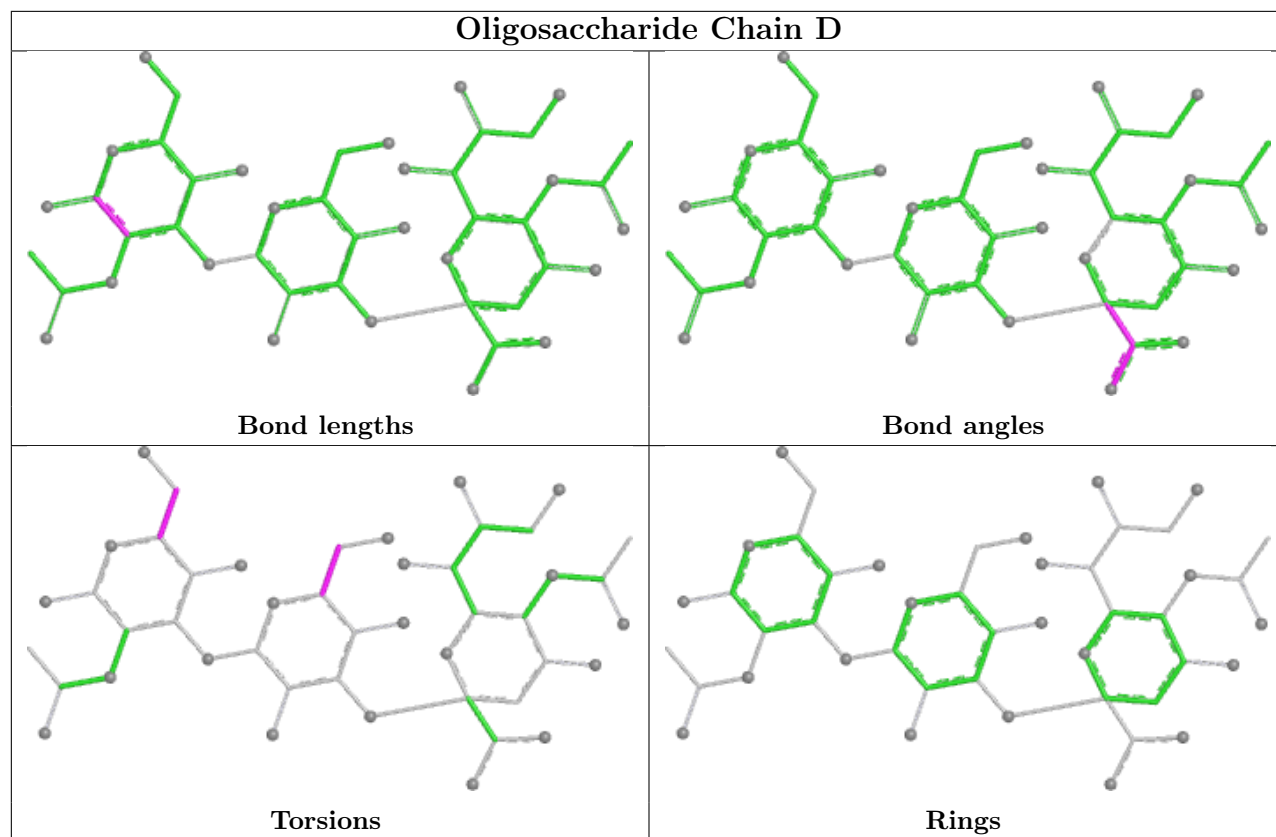
Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	SIA	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.



5.6 Ligand geometry

3 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	$\# Z > 2$
3	NAG	C	1500	-	14,14,15	0.56	0	17,19,21	0.90	0
3	NAG	A	1500	-	12,12,15	0.45	0	14,15,21	0.88	0
3	NAG	A	1499	-	14,14,15	0.46	0	17,19,21	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1500	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1500	-	-	6/15/15/26	-
3	NAG	A	1499	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1499	NAG	C1-C2-N2-C7
3	A	1500	NAG	C1-C2-N2-C7
3	A	1500	NAG	O4-C4-C5-C6
3	A	1500	NAG	C8-C7-N2-C2
3	A	1500	NAG	O7-C7-N2-C2
3	A	1499	NAG	C8-C7-N2-C2
3	A	1499	NAG	O7-C7-N2-C2
3	C	1500	NAG	O5-C5-C6-O6
3	A	1500	NAG	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	C	1500	NAG	C4-C5-C6-O6
3	A	1499	NAG	O5-C5-C6-O6
3	A	1500	NAG	C4-C5-C6-O6
3	C	1500	NAG	C8-C7-N2-C2
3	C	1500	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1500	NAG	3	0
3	A	1500	NAG	6	0
3	A	1499	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)









There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.4472, which does not match the depositor's R factor of 0.2101. Please interpret the results in this section carefully.

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	490/509 (96%)	3.32	424 (86%)  	29, 54, 94, 134	1 (0%)
1	B	490/509 (96%)	2.46	301 (61%)  	30, 55, 95, 159	1 (0%)
1	C	485/509 (95%)	3.31	411 (84%)  	36, 55, 87, 134	0
All	All	1465/1527 (95%)	3.03	1136 (77%)  	29, 55, 92, 159	2 (0%)

All (1136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	ASN	8.9
1	C	206	SER	7.9
1	A	9	ILE	7.7
1	C	66	LEU	7.5
1	C	120	ILE	7.4
1	C	198	GLY	7.4
1	C	197	VAL	7.2
1	B	213	ILE	7.1
1	C	253	PRO	6.9
1	A	153	LEU	6.9
1	C	151	VAL	6.8
1	A	463	GLY	6.7
1	C	141	LEU	6.6
1	C	157	GLY	6.5
1	A	90	VAL	6.5
1	C	166	SER	6.5
1	C	9	ILE	6.5
1	A	109	ILE	6.4
1	C	140	VAL	6.4
1	A	316	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	288	ILE	6.4
1	A	323	VAL	6.3
1	B	162	ILE	6.3
1	C	153	LEU	6.3
1	C	44	LYS	6.3
1	A	224	GLY	6.3
1	A	354	HIS	6.3
1	C	154	THR	6.2
1	C	194	TYR	6.2
1	C	85	GLU	6.2
1	B	277	CYS	6.2
1	A	42	ASN	6.1
1	B	498	ALA	6.1
1	A	350	TRP	6.1
1	C	222	VAL	6.0
1	A	364	ALA	6.0
1	C	147	PHE	6.0
1	A	219	ARG	6.0
1	A	247	THR	5.9
1	C	138	CYS	5.9
1	C	235	LEU	5.9
1	A	459	VAL	5.9
1	C	93	LEU	5.8
1	A	45	LEU	5.8
1	C	128	GLN	5.8
1	A	189	GLU	5.8
1	C	272	LYS	5.8
1	C	131	THR	5.7
1	C	126	TRP	5.7
1	A	95	TYR	5.7
1	A	89	PRO	5.6
1	C	180	GLY	5.6
1	C	463	GLY	5.6
1	A	451	VAL	5.6
1	A	302	ILE	5.6
1	A	8	CYS	5.6
1	A	49	SER	5.6
1	B	491	TYR	5.6
1	C	187	ASP	5.6
1	C	387	LYS	5.5
1	A	138	CYS	5.5
1	B	51	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	95	TYR	5.5
1	C	160	TYR	5.5
1	C	121	LEU	5.5
1	C	127	THR	5.5
1	B	120	ILE	5.5
1	B	167	TYR	5.5
1	C	376	GLY	5.4
1	A	287	ALA	5.4
1	A	80	TRP	5.4
1	A	210	LYS	5.4
1	B	140	VAL	5.4
1	A	56	LEU	5.4
1	A	356	SER	5.4
1	C	65	LEU	5.4
1	A	134	GLY	5.4
1	A	214	PRO	5.3
1	B	163	ALA	5.3
1	C	223	ASN	5.3
1	A	97	GLY	5.3
1	A	422	THR	5.3
1	C	274	LEU	5.3
1	B	159	ASN	5.3
1	A	74	LEU	5.3
1	B	204	GLY	5.3
1	C	118	VAL	5.3
1	A	137	ALA	5.3
1	C	191	ARG	5.2
1	B	235	LEU	5.2
1	B	462	LEU	5.2
1	C	352	GLY	5.2
1	C	258	LYS	5.2
1	C	184	PRO	5.2
1	C	113	THR	5.2
1	A	93	LEU	5.2
1	C	129	HIS	5.2
1	B	226	GLY	5.2
1	C	53	PRO	5.2
1	B	390	THR	5.2
1	A	181	ILE	5.2
1	A	362	GLY	5.2
1	A	469	PHE	5.1
1	A	91	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	51	ILE	5.1
1	C	57	GLY	5.1
1	A	353	TYR	5.1
1	A	157	GLY	5.1
1	C	363	TYR	5.1
1	A	462	LEU	5.1
1	C	130	THR	5.1
1	C	251	ILE	5.1
1	C	96	PRO	5.0
1	C	264	SER	5.0
1	A	61	ILE	5.0
1	A	324	PRO	5.0
1	C	89	PRO	5.0
1	A	140	VAL	5.0
1	C	64	TRP	5.0
1	C	109	ILE	5.0
1	A	225	GLN	5.0
1	A	78	PRO	5.0
1	A	414	GLU	5.0
1	A	142	ASP	4.9
1	A	296	ASN	4.9
1	A	85	GLU	4.9
1	A	177	ILE	4.9
1	A	335	ILE	4.9
1	C	243	ASN	4.9
1	A	347	VAL	4.9
1	A	265	SER	4.9
1	C	397	LYS	4.9
1	C	87	GLU	4.8
1	A	58	ASP	4.8
1	B	244	PHE	4.8
1	C	82	TYR	4.8
1	A	184	PRO	4.8
1	A	357	ASN	4.8
1	C	62	ALA	4.8
1	C	297	ILE	4.8
1	A	497	ALA	4.8
1	C	252	ALA	4.8
1	C	133	GLY	4.8
1	B	262	ARG	4.8
1	C	115	PHE	4.8
1	A	18	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	473	CYS	4.7
1	A	195	GLN	4.7
1	B	264	SER	4.7
1	A	229	MET	4.7
1	A	470	TYR	4.7
1	A	98	SER	4.7
1	A	14	ASN	4.7
1	B	157	GLY	4.7
1	B	495	SER	4.7
1	C	204	GLY	4.7
1	A	77	VAL	4.7
1	A	84	VAL	4.7
1	C	79	GLU	4.6
1	A	319	GLY	4.6
1	A	131	THR	4.6
1	B	118	VAL	4.6
1	A	346	MET	4.6
1	A	5	ASP	4.6
1	A	482	LYS	4.6
1	C	356	SER	4.6
1	A	417	PHE	4.6
1	C	302	ILE	4.6
1	C	262	ARG	4.6
1	B	242	ILE	4.6
1	A	299	PRO	4.6
1	C	144	PRO	4.6
1	C	434	GLU	4.6
1	C	256	GLY	4.6
1	B	203	VAL	4.5
1	A	136	ARG	4.5
1	A	36	ILE	4.5
1	B	326	ILE	4.5
1	C	178	ILE	4.5
1	B	121	LEU	4.5
1	C	324	PRO	4.5
1	C	237	GLU	4.5
1	C	263	GLY	4.5
1	A	301	THR	4.5
1	C	143	ASN	4.5
1	A	197	VAL	4.5
1	C	177	ILE	4.5
1	A	53	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	45	LEU	4.5
1	A	6	GLN	4.5
1	C	269	LYS	4.5
1	B	313	ARG	4.5
1	A	146	PHE	4.5
1	C	384	VAL	4.5
1	C	78	PRO	4.5
1	C	306	PRO	4.5
1	B	79	GLU	4.5
1	C	43	GLY	4.5
1	C	241	VAL	4.5
1	A	13	ALA	4.5
1	B	38	GLU	4.5
1	B	73	ARG	4.5
1	C	250	LEU	4.4
1	C	150	MET	4.4
1	A	481	VAL	4.4
1	B	126	TRP	4.4
1	C	244	PHE	4.4
1	C	257	PHE	4.4
1	A	55	GLU	4.4
1	A	256	GLY	4.4
1	C	465	GLY	4.4
1	A	277	CYS	4.4
1	A	218	THR	4.4
1	A	196	ASN	4.4
1	B	75	LEU	4.4
1	B	459	VAL	4.4
1	A	278	GLU	4.4
1	A	260	SER	4.4
1	B	76	SER	4.4
1	A	69	PRO	4.4
1	A	144	PRO	4.4
1	B	77	VAL	4.4
1	C	163	ALA	4.4
1	B	411	LYS	4.4
1	A	73	ARG	4.4
1	A	300	LEU	4.3
1	A	115	PHE	4.3
1	C	156	LYS	4.3
1	B	5	ASP	4.3
1	C	318	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	284	PRO	4.3
1	A	264	SER	4.3
1	A	394	ALA	4.3
1	A	67	GLY	4.3
1	B	160	TYR	4.3
1	C	193	LEU	4.3
1	A	213	ILE	4.3
1	B	216	ILE	4.3
1	A	59	CYS	4.3
1	B	142	ASP	4.3
1	A	92	GLY	4.3
1	A	360	GLY	4.3
1	A	72	ASP	4.2
1	C	155	LYS	4.2
1	C	236	LEU	4.2
1	A	297	ILE	4.2
1	A	222	VAL	4.2
1	B	451	VAL	4.2
1	C	171	SER	4.2
1	C	420	VAL	4.2
1	A	331	LEU	4.2
1	C	54	LEU	4.2
1	C	176	LEU	4.2
1	B	53	PRO	4.2
1	A	216	ILE	4.2
1	B	291	THR	4.2
1	A	94	CYS	4.2
1	A	389	ASN	4.2
1	A	455	LEU	4.2
1	C	116	GLU	4.2
1	A	29	THR	4.2
1	A	351	TYR	4.2
1	B	200	TYR	4.2
1	B	241	VAL	4.2
1	B	209	ASN	4.2
1	C	209	ASN	4.2
1	A	272	LYS	4.2
1	C	67	GLY	4.2
1	B	48	LEU	4.2
1	C	18	GLU	4.2
1	B	114	HIS	4.2
1	C	481	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	258	LYS	4.2
1	B	141	LEU	4.1
1	C	242	ILE	4.1
1	A	217	ALA	4.1
1	C	394	ALA	4.1
1	C	361	SER	4.1
1	A	71	CYS	4.1
1	C	459	VAL	4.1
1	A	425	ALA	4.1
1	A	454	GLN	4.1
1	C	139	ALA	4.1
1	A	68	ASN	4.1
1	A	133	GLY	4.1
1	C	91	ASN	4.1
1	A	70	GLU	4.1
1	A	124	ASP	4.1
1	C	438	ASP	4.1
1	C	40	THR	4.1
1	C	291	THR	4.1
1	A	295	HIS	4.1
1	C	367	LYS	4.1
1	A	112	VAL	4.1
1	A	201	VAL	4.1
1	A	483	ASN	4.0
1	C	108	LEU	4.0
1	A	280	LYS	4.0
1	A	309	VAL	4.0
1	A	315	VAL	4.0
1	B	315	VAL	4.0
1	A	373	ALA	4.0
1	A	361	SER	4.0
1	C	212	SER	4.0
1	C	32	HIS	4.0
1	C	173	GLU	4.0
1	C	245	GLU	4.0
1	C	496	LYS	4.0
1	A	40	THR	4.0
1	C	170	THR	4.0
1	A	465	GLY	4.0
1	B	42	ASN	4.0
1	B	137	ALA	4.0
1	A	121	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	105	LEU	4.0
1	A	76	SER	4.0
1	A	474	ASP	4.0
1	C	217	ALA	3.9
1	A	330	GLY	3.9
1	C	416	GLY	3.9
1	B	275	GLU	3.9
1	C	238	THR	3.9
1	C	270	THR	3.9
1	A	429	VAL	3.9
1	C	395	VAL	3.9
1	A	182	HIS	3.9
1	C	299	PRO	3.9
1	A	255	TYR	3.9
1	C	167	TYR	3.9
1	A	113	THR	3.9
1	B	211	ARG	3.9
1	A	41	HIS	3.9
1	C	417	PHE	3.9
1	C	29	THR	3.9
1	C	482	LYS	3.9
1	A	43	GLY	3.9
1	C	330	GLY	3.9
1	A	12	HIS	3.9
1	B	169	ASN	3.9
1	B	361	SER	3.9
1	C	179	TRP	3.9
1	C	488	TYR	3.9
1	C	450	LYS	3.9
1	B	257	PHE	3.8
1	B	381	VAL	3.8
1	C	59	CYS	3.8
1	B	259	ILE	3.8
1	A	126	TRP	3.8
1	A	194	TYR	3.8
1	C	74	LEU	3.8
1	B	362	GLY	3.8
1	C	7	ILE	3.8
1	A	111	SER	3.8
1	C	225	GLN	3.8
1	A	11	TYR	3.8
1	B	279	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	437	LEU	3.8
1	C	218	THR	3.8
1	A	298	HIS	3.8
1	C	61	ILE	3.8
1	C	216	ILE	3.8
1	A	228	ARG	3.8
1	A	262	ARG	3.8
1	C	255	TYR	3.8
1	A	320	LEU	3.8
1	A	38	GLU	3.8
1	A	186	ASP	3.8
1	B	475	ASP	3.8
1	C	364	ALA	3.8
1	A	477	CYS	3.8
1	A	464	ASN	3.8
1	B	250	LEU	3.7
1	C	231	PHE	3.7
1	C	175	MET	3.7
1	A	50	GLY	3.7
1	B	87	GLU	3.7
1	A	348	ASP	3.7
1	C	348	ASP	3.7
1	A	114	HIS	3.7
1	A	231	PHE	3.7
1	A	392	PHE	3.7
1	A	467	PHE	3.7
1	C	406	LEU	3.7
1	A	160	TYR	3.7
1	B	207	THR	3.7
1	A	10	GLY	3.7
1	C	172	GLY	3.7
1	C	224	GLY	3.7
1	C	317	ALA	3.7
1	B	124	ASP	3.7
1	B	358	ASP	3.7
1	B	138	CYS	3.7
1	A	480	SER	3.7
1	A	491	TYR	3.7
1	C	110	THR	3.7
1	A	172	GLY	3.7
1	B	198	GLY	3.7
1	B	256	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	162	ILE	3.7
1	B	27	ASN	3.7
1	C	159	ASN	3.7
1	B	324	PRO	3.7
1	A	423	TYR	3.7
1	B	239	TRP	3.7
1	C	86	LYS	3.7
1	C	444	VAL	3.7
1	C	219	ARG	3.7
1	C	83	ILE	3.7
1	B	305	CYS	3.6
1	C	300	LEU	3.6
1	A	407	GLU	3.6
1	A	486	TYR	3.6
1	A	325	GLN	3.6
1	C	92	GLY	3.6
1	C	207	THR	3.6
1	C	162	ILE	3.6
1	A	48	LEU	3.6
1	C	320	LEU	3.6
1	A	248	GLY	3.6
1	A	370	THR	3.6
1	A	420	VAL	3.6
1	C	165	ARG	3.6
1	A	363	TYR	3.6
1	B	343	TRP	3.6
1	A	156	LYS	3.6
1	A	221	LYS	3.6
1	A	158	SER	3.6
1	B	158	SER	3.6
1	C	49	SER	3.6
1	C	135	SER	3.6
1	B	336	ALA	3.6
1	A	51	ILE	3.6
1	B	80	TRP	3.6
1	A	487	ASP	3.6
1	C	58	ASP	3.6
1	C	56	LEU	3.5
1	A	215	GLU	3.5
1	B	215	GLU	3.5
1	C	374	PHE	3.5
1	C	158	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	CYS	3.5
1	C	94	CYS	3.5
1	A	444	VAL	3.5
1	A	132	THR	3.5
1	A	270	THR	3.5
1	A	436	THR	3.5
1	C	268	MET	3.5
1	A	308	TYR	3.5
1	A	310	LYS	3.5
1	C	117	LYS	3.5
1	C	119	LYS	3.5
1	A	159	ASN	3.5
1	C	69	PRO	3.5
1	C	483	ASN	3.5
1	A	311	SER	3.5
1	A	318	THR	3.5
1	A	391	GLN	3.5
1	B	6	GLN	3.5
1	C	6	GLN	3.5
1	A	7	ILE	3.5
1	C	213	ILE	3.5
1	C	385	ILE	3.5
1	C	41	HIS	3.5
1	C	124	ASP	3.5
1	B	115	PHE	3.5
1	A	400	SER	3.5
1	C	202	SER	3.5
1	A	478	MET	3.5
1	B	478	MET	3.5
1	B	481	VAL	3.5
1	A	120	ILE	3.5
1	C	354	HIS	3.5
1	A	448	TYR	3.5
1	A	64	TRP	3.5
1	A	421	TRP	3.5
1	B	161	PRO	3.5
1	C	493	GLU	3.5
1	A	338	PHE	3.5
1	C	345	GLY	3.5
1	A	460	LYS	3.5
1	C	190	GLN	3.5
1	C	221	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	3.4
1	A	88	ASN	3.4
1	C	169	ASN	3.4
1	C	332	PHE	3.4
1	A	86	LYS	3.4
1	B	127	THR	3.4
1	A	141	LEU	3.4
1	A	285	LEU	3.4
1	A	375	ASP	3.4
1	C	375	ASP	3.4
1	C	200	TYR	3.4
1	A	343	TRP	3.4
1	A	461	GLU	3.4
1	C	239	TRP	3.4
1	B	49	SER	3.4
1	C	90	VAL	3.4
1	C	347	VAL	3.4
1	C	383	SER	3.4
1	A	183	HIS	3.4
1	A	267	ILE	3.4
1	C	137	ALA	3.4
1	A	418	LEU	3.4
1	C	211	ARG	3.4
1	A	366	ASP	3.4
1	A	275	GLU	3.4
1	C	55	GLU	3.4
1	A	344	GLN	3.4
1	A	349	GLY	3.4
1	B	341	GLY	3.4
1	A	20	VAL	3.4
1	A	471	HIS	3.4
1	C	112	VAL	3.4
1	C	267	ILE	3.4
1	B	364	ALA	3.4
1	A	250	LEU	3.4
1	B	191	ARG	3.4
1	C	123	ARG	3.4
1	C	277	CYS	3.4
1	B	144	PRO	3.4
1	C	122	PRO	3.4
1	B	312	ASP	3.4
1	C	487	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	453	MET	3.4
1	A	82	TYR	3.4
1	B	467	PHE	3.4
1	A	168	ASN	3.4
1	C	125	GLN	3.4
1	A	37	LEU	3.3
1	B	153	LEU	3.3
1	A	468	GLU	3.3
1	A	475	ASP	3.3
1	B	58	ASP	3.3
1	A	198	GLY	3.3
1	A	263	GLY	3.3
1	C	80	TRP	3.3
1	A	334	ALA	3.3
1	B	202	SER	3.3
1	C	284	PRO	3.3
1	C	8	CYS	3.3
1	A	457	ASP	3.3
1	C	72	ASP	3.3
1	C	351	TYR	3.3
1	C	201	VAL	3.3
1	B	26	ARG	3.3
1	A	279	THR	3.3
1	B	331	LEU	3.3
1	A	106	LYS	3.3
1	A	450	LYS	3.3
1	B	453	MET	3.3
1	B	254	GLU	3.3
1	B	278	GLU	3.3
1	B	468	GLU	3.3
1	B	187	ASP	3.3
1	C	63	GLY	3.3
1	C	470	TYR	3.3
1	B	385	ILE	3.3
1	A	193	LEU	3.3
1	A	274	LEU	3.3
1	A	130	THR	3.3
1	B	217	ALA	3.3
1	B	430	LEU	3.3
1	C	336	ALA	3.3
1	C	229	MET	3.3
1	C	393	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	403	GLU	3.3
1	A	21	ASP	3.3
1	A	305	CYS	3.3
1	C	392	PHE	3.3
1	A	341	GLY	3.3
1	A	377	ILE	3.2
1	A	479	ASN	3.2
1	B	401	ASN	3.2
1	C	289	ASN	3.2
1	A	412	LYS	3.2
1	A	496	LYS	3.2
1	B	151	VAL	3.2
1	C	34	LYS	3.2
1	C	106	LYS	3.2
1	C	210	LYS	3.2
1	C	472	LYS	3.2
1	B	238	THR	3.2
1	B	246	SER	3.2
1	B	128	GLN	3.2
1	C	195	GLN	3.2
1	A	187	ASP	3.2
1	A	244	PHE	3.2
1	C	396	GLY	3.2
1	C	315	VAL	3.2
1	C	437	LEU	3.2
1	A	239	TRP	3.2
1	B	131	THR	3.2
1	C	273	THR	3.2
1	C	145	SER	3.2
1	A	340	GLU	3.2
1	A	386	GLU	3.2
1	B	304	GLU	3.2
1	B	340	GLU	3.2
1	C	469	PHE	3.2
1	A	226	GLY	3.2
1	B	134	GLY	3.2
1	C	100	ASN	3.2
1	A	268	MET	3.2
1	C	188	ALA	3.2
1	A	110	THR	3.2
1	A	16	SER	3.2
1	A	135	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	GLU	3.2
1	C	471	HIS	3.2
1	A	339	ILE	3.2
1	B	473	CYS	3.2
1	A	395	VAL	3.2
1	C	11	TYR	3.2
1	A	60	SER	3.2
1	A	313	ARG	3.2
1	A	332	PHE	3.2
1	B	35	ASP	3.1
1	C	335	ILE	3.1
1	C	453	MET	3.1
1	B	197	VAL	3.1
1	B	243	ASN	3.1
1	B	347	VAL	3.1
1	C	203	VAL	3.1
1	C	382	ASN	3.1
1	C	102	TYR	3.1
1	C	489	PRO	3.1
1	A	104	GLU	3.1
1	B	492	GLU	3.1
1	A	212	SER	3.1
1	A	119	LYS	3.1
1	B	99	PHE	3.1
1	B	263	GLY	3.1
1	B	346	MET	3.1
1	A	83	ILE	3.1
1	A	27	ASN	3.1
1	B	223	ASN	3.1
1	B	276	ASN	3.1
1	A	62	ALA	3.1
1	A	122	PRO	3.1
1	A	188	ALA	3.1
1	B	218	THR	3.1
1	C	271	GLU	3.1
1	B	280	LYS	3.1
1	A	437	LEU	3.1
1	B	57	GLY	3.1
1	C	77	VAL	3.1
1	C	220	PRO	3.1
1	B	393	GLU	3.1
1	C	230	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	275	GLU	3.1
1	A	273	THR	3.1
1	A	19	LYS	3.1
1	A	355	HIS	3.1
1	A	495	SER	3.1
1	C	76	SER	3.1
1	A	314	LEU	3.1
1	C	316	LEU	3.1
1	C	341	GLY	3.1
1	C	88	ASN	3.1
1	A	271	GLU	3.1
1	B	116	GLU	3.1
1	C	373	ALA	3.1
1	A	155	LYS	3.1
1	B	17	THR	3.1
1	C	372	LYS	3.1
1	C	174	GLN	3.1
1	C	448	TYR	3.1
1	C	285	LEU	3.0
1	A	28	VAL	3.0
1	B	472	LYS	3.0
1	C	254	GLU	3.0
1	C	461	GLU	3.0
1	C	479	ASN	3.0
1	A	321	ARG	3.0
1	C	390	THR	3.0
1	C	466	CYS	3.0
1	B	297	ILE	3.0
1	B	487	ASP	3.0
1	B	184	PRO	3.0
1	A	269	LYS	3.0
1	A	381	VAL	3.0
1	B	493	GLU	3.0
1	A	443	ASN	3.0
1	C	389	ASN	3.0
1	A	238	THR	3.0
1	B	71	CYS	3.0
1	B	212	SER	3.0
1	A	99	PHE	3.0
1	A	259	ILE	3.0
1	A	117	LYS	3.0
1	A	367	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	3.0
1	B	245	GLU	3.0
1	C	381	VAL	3.0
1	C	401	ASN	3.0
1	A	390	THR	3.0
1	B	247	THR	3.0
1	B	194	TYR	3.0
1	B	470	TYR	3.0
1	B	74	LEU	3.0
1	B	98	SER	3.0
1	C	331	LEU	3.0
1	A	352	GLY	3.0
1	C	146	PHE	3.0
1	C	475	ASP	3.0
1	C	84	VAL	3.0
1	B	40	THR	3.0
1	A	24	LEU	2.9
1	C	353	TYR	2.9
1	A	23	ILE	2.9
1	A	372	LYS	2.9
1	B	61	ILE	2.9
1	A	161	PRO	2.9
1	B	421	TRP	2.9
1	A	25	GLU	2.9
1	A	398	GLU	2.9
1	C	103	GLU	2.9
1	C	355	HIS	2.9
1	A	322	ASN	2.9
1	A	22	THR	2.9
1	A	31	THR	2.9
1	C	132	THR	2.9
1	A	402	LEU	2.9
1	B	45	LEU	2.9
1	C	380	LYS	2.9
1	A	227	GLY	2.9
1	A	288	ILE	2.9
1	A	294	PHE	2.9
1	B	374	PHE	2.9
1	C	349	GLY	2.9
1	C	136	ARG	2.9
1	C	114	HIS	2.9
1	C	240	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	479	ASN	2.9
1	A	485	THR	2.9
1	A	445	LYS	2.9
1	B	208	LEU	2.9
1	C	462	LEU	2.9
1	C	36	ILE	2.9
1	B	248	GLY	2.9
1	C	226	GLY	2.9
1	B	123	ARG	2.9
1	C	298	HIS	2.9
1	A	150	MET	2.9
1	A	151	VAL	2.9
1	C	186	ASP	2.9
1	A	209	ASN	2.9
1	A	382	ASN	2.9
1	C	149	ASN	2.9
1	A	154	THR	2.9
1	A	235	LEU	2.9
1	B	274	LEU	2.9
1	B	59	CYS	2.9
1	B	81	SER	2.9
1	C	293	PRO	2.9
1	A	431	MET	2.9
1	A	312	ASP	2.9
1	A	33	ALA	2.9
1	C	343	TRP	2.9
1	A	15	ASN	2.9
1	A	249	ASN	2.9
1	A	424	ASN	2.9
1	C	205	THR	2.9
1	C	410	ASN	2.9
1	A	66	LEU	2.8
1	C	427	LEU	2.8
1	A	211	ARG	2.8
1	B	177	ILE	2.8
1	C	181	ILE	2.8
1	A	399	PHE	2.8
1	A	281	CYS	2.8
1	B	466	CYS	2.8
1	A	358	ASP	2.8
1	C	261	LYS	2.8
1	A	290	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	247	THR	2.8
1	B	236	LEU	2.8
1	C	314	LEU	2.8
1	A	220	PRO	2.8
1	A	337	GLY	2.8
1	C	107	HIS	2.8
1	B	189	GLU	2.8
1	A	167	TYR	2.8
1	A	34	LYS	2.8
1	C	323	VAL	2.8
1	C	451	VAL	2.8
1	B	474	ASP	2.8
1	A	17	THR	2.8
1	A	406	LEU	2.8
1	A	410	ASN	2.8
1	A	430	LEU	2.8
1	B	154	THR	2.8
1	C	199	THR	2.8
1	C	409	LEU	2.8
1	C	464	ASN	2.8
1	B	181	ILE	2.8
1	A	180	GLY	2.8
1	C	260	SER	2.8
1	A	174	GLN	2.8
1	A	466	CYS	2.8
1	B	90	VAL	2.8
1	A	317	ALA	2.8
1	A	498	ALA	2.8
1	B	188	ALA	2.8
1	B	375	ASP	2.8
1	C	457	ASP	2.8
1	A	65	LEU	2.8
1	C	75	LEU	2.8
1	B	22	THR	2.8
1	A	123	ARG	2.8
1	C	413	MET	2.8
1	B	78	PRO	2.8
1	C	440	HIS	2.8
1	C	484	GLY	2.8
1	B	271	GLU	2.8
1	A	171	SER	2.8
1	C	307	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	2.8
1	C	474	ASP	2.7
1	B	289	ASN	2.7
1	B	483	ASN	2.7
1	A	178	ILE	2.7
1	A	63	GLY	2.7
1	C	10	GLY	2.7
1	A	44	LYS	2.7
1	C	19	LYS	2.7
1	B	391	GLN	2.7
1	C	344	GLN	2.7
1	B	166	SER	2.7
1	C	81	SER	2.7
1	C	495	SER	2.7
1	B	255	TYR	2.7
1	A	456	ARG	2.7
1	B	405	ARG	2.7
1	C	283	THR	2.7
1	A	96	PRO	2.7
1	A	242	ILE	2.7
1	A	385	ILE	2.7
1	B	465	GLY	2.7
1	C	338	PHE	2.7
1	A	190	GLN	2.7
1	A	371	GLN	2.7
1	A	202	SER	2.7
1	B	84	VAL	2.7
1	B	323	VAL	2.7
1	C	404	ARG	2.7
1	B	130	THR	2.7
1	A	143	ASN	2.7
1	B	168	ASN	2.7
1	C	379	ASN	2.7
1	C	286	GLY	2.7
1	C	350	TRP	2.7
1	C	492	GLU	2.7
1	C	391	GLN	2.7
1	C	439	PHE	2.7
1	C	246	SER	2.7
1	B	37	LEU	2.7
1	A	488	TYR	2.7
1	C	358	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	490	LYS	2.7
1	B	412	LYS	2.7
1	C	322	ASN	2.7
1	A	257	PHE	2.7
1	B	195	GLN	2.7
1	B	344	GLN	2.7
1	B	359	GLN	2.7
1	C	467	PHE	2.7
1	B	56	LEU	2.6
1	B	444	VAL	2.6
1	C	148	ARG	2.6
1	B	317	ALA	2.6
1	B	448	TYR	2.6
1	A	127	THR	2.6
1	B	196	ASN	2.6
1	C	214	PRO	2.6
1	B	368	GLU	2.6
1	B	231	PHE	2.6
1	A	191	ARG	2.6
1	A	442	SER	2.6
1	C	37	LEU	2.6
1	C	292	LEU	2.6
1	C	447	LEU	2.6
1	A	380	LYS	2.6
1	A	440	HIS	2.6
1	B	164	LYS	2.6
1	C	182	HIS	2.6
1	B	205	THR	2.6
1	B	185[A]	ASN	2.6
1	B	50	GLY	2.6
1	B	172	GLY	2.6
1	B	330	GLY	2.6
1	A	233	TRP	2.6
1	A	404	ARG	2.6
1	C	73	ARG	2.6
1	B	105	LEU	2.6
1	A	145	SER	2.6
1	B	201	VAL	2.6
1	C	16	SER	2.6
1	B	367	LYS	2.6
1	A	129	HIS	2.6
1	A	102	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	113	THR	2.6
1	B	192	THR	2.6
1	A	458	ASN	2.6
1	C	446	ASN	2.6
1	A	416	GLY	2.6
1	C	282	GLN	2.6
1	C	342	GLY	2.6
1	C	360	GLY	2.6
1	A	261	LYS	2.6
1	B	384	VAL	2.6
1	B	41	HIS	2.6
1	A	283	THR	2.6
1	B	23	ILE	2.6
1	C	419	ASP	2.6
1	A	243	ASN	2.6
1	B	8	CYS	2.6
1	B	463	GLY	2.6
1	C	249	ASN	2.6
1	C	371	GLN	2.6
1	A	108	LEU	2.5
1	B	193	LEU	2.5
1	B	210	LYS	2.5
1	B	445	LYS	2.5
1	B	496	LYS	2.5
1	B	354	HIS	2.5
1	B	420	VAL	2.5
1	B	440	HIS	2.5
1	C	295	HIS	2.5
1	A	173	GLU	2.5
1	B	302	ILE	2.5
1	C	17	THR	2.5
1	A	57	GLY	2.5
1	B	180	GLY	2.5
1	A	46	CYS	2.5
1	B	165	ARG	2.5
1	B	469	PHE	2.5
1	C	228	ARG	2.5
1	A	472	LYS	2.5
1	B	221	LYS	2.5
1	A	81	SER	2.5
1	C	400	SER	2.5
1	C	35	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	227	GLY	2.5
1	A	26	ARG	2.5
1	A	169	ASN	2.5
1	A	223	ASN	2.5
1	C	47	ARG	2.5
1	B	285	LEU	2.5
1	B	183	HIS	2.5
1	B	28	VAL	2.5
1	A	246	SER	2.5
1	A	476	GLU	2.5
1	A	192	THR	2.5
1	A	286	GLY	2.5
1	B	133	GLY	2.5
1	C	50	GLY	2.5
1	A	100	ASN	2.5
1	C	208	LEU	2.5
1	B	11	TYR	2.5
1	C	357	ASN	2.5
1	C	99	PHE	2.5
1	A	427	LEU	2.4
1	B	93	LEU	2.4
1	B	402	LEU	2.4
1	B	497	ALA	2.4
1	C	478	MET	2.4
1	C	378	THR	2.4
1	B	352	GLY	2.4
1	C	134	GLY	2.4
1	C	296	ASN	2.4
1	B	108	LEU	2.4
1	B	85	GLU	2.4
1	B	334	ALA	2.4
1	B	174	GLN	2.4
1	B	64	TRP	2.4
1	B	135	SER	2.4
1	B	269	LYS	2.4
1	B	233	TRP	2.4
1	C	31	THR	2.4
1	C	142	ASP	2.4
1	A	409	LEU	2.4
1	B	54	LEU	2.4
1	C	185	ASN	2.4
1	C	294	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	32	HIS	2.4
1	B	299	PRO	2.4
1	B	70	GLU	2.4
1	B	490	LYS	2.4
1	C	494	GLU	2.4
1	B	7	ILE	2.4
1	C	435	ARG	2.4
1	C	111	SER	2.4
1	B	179	TRP	2.4
1	C	421	TRP	2.4
1	A	207	THR	2.4
1	B	72	ASP	2.4
1	C	441	ASP	2.4
1	B	156	LYS	2.4
1	A	403	GLU	2.4
1	C	339	ILE	2.4
1	C	369	SER	2.4
1	B	449	ASP	2.3
1	B	464	ASN	2.3
1	B	363	TYR	2.3
1	B	397	LYS	2.3
1	B	46	CYS	2.3
1	A	365	ALA	2.3
1	B	109	ILE	2.3
1	C	13	ALA	2.3
1	B	337	GLY	2.3
1	B	338	PHE	2.3
1	A	185	ASN	2.3
1	B	117	LYS	2.3
1	B	284	PRO	2.3
1	C	70	GLU	2.3
1	C	454	GLN	2.3
1	B	356	SER	2.3
1	C	333	GLY	2.3
1	B	427	LEU	2.3
1	C	192	THR	2.3
1	C	234	THR	2.3
1	B	350	TRP	2.3
1	A	397	LYS	2.3
1	C	276	ASN	2.3
1	C	52	PRO	2.3
1	C	486	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	ALA	2.3
1	C	281	CYS	2.3
1	A	206	SER	2.3
1	A	35	ASP	2.3
1	A	415	ASP	2.3
1	A	419	ASP	2.3
1	B	389	ASN	2.3
1	A	148	ARG	2.3
1	A	452	ARG	2.3
1	B	136	ARG	2.3
1	C	26	ARG	2.3
1	B	122	PRO	2.3
1	A	434	GLU	2.3
1	B	414	GLU	2.3
1	A	118	VAL	2.3
1	A	251	ILE	2.3
1	A	39	LYS	2.2
1	B	155	LYS	2.2
1	C	168	ASN	2.2
1	B	386	GLU	2.2
1	C	491	TYR	2.2
1	C	365	ALA	2.2
1	B	39	LYS	2.2
1	C	46	CYS	2.2
1	C	362	GLY	2.2
1	A	165	ARG	2.2
1	A	293	PRO	2.2
1	B	220	PRO	2.2
1	C	42	ASN	2.2
1	C	233	TRP	2.2
1	A	103	GLU	2.2
1	B	36	ILE	2.2
1	A	236	LEU	2.2
1	B	272	LYS	2.2
1	B	460	LYS	2.2
1	A	342	GLY	2.2
1	B	63	GLY	2.2
1	C	248	GLY	2.2
1	B	400	SER	2.2
1	C	290	THR	2.2
1	B	439	PHE	2.2
1	B	489	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	493	GLU	2.2
1	B	88	ASN	2.2
1	B	237	GLU	2.2
1	A	179	TRP	2.2
1	C	259	ILE	2.2
1	B	33	ALA	2.2
1	C	164	LYS	2.2
1	C	183	HIS	2.2
1	A	447	LEU	2.2
1	B	447	LEU	2.2
1	C	266	GLY	2.2
1	C	319	GLY	2.2
1	C	71	CYS	2.2
1	C	305	CYS	2.2
1	C	399	PHE	2.2
1	B	348	ASP	2.2
1	B	433	ASN	2.2
1	B	438	ASP	2.2
1	B	446	ASN	2.2
1	C	39	LYS	2.2
1	A	234	THR	2.1
1	A	378	THR	2.1
1	B	370	THR	2.1
1	C	301	THR	2.1
1	A	439	PHE	2.1
1	A	282	GLN	2.1
1	B	458	ASN	2.1
1	B	316	LEU	2.1
1	A	484	GLY	2.1
1	B	94	CYS	2.1
1	C	411	LYS	2.1
1	B	335	ILE	2.1
1	C	388	MET	2.1
1	A	345	GLY	2.1
1	B	422	THR	2.1
1	C	189	GLU	2.1
1	A	438	ASP	2.1
1	A	441	ASP	2.1
1	A	47	ARG	2.1
1	A	266	GLY	2.1
1	C	97	GLY	2.1
1	B	488	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	273	THR	2.1
1	B	399	PHE	2.1
1	C	38	GLU	2.1
1	C	98	SER	2.1
1	A	446	ASN	2.1
1	B	419	ASP	2.1
1	C	377	ILE	2.1
1	B	388	MET	2.1
1	C	443	ASN	2.1
1	B	452	ARG	2.0
1	C	456	ARG	2.0
1	A	79	GLU	2.0
1	C	468	GLU	2.0
1	A	369	SER	2.0
1	B	281	CYS	2.0
1	B	477	CYS	2.0
1	B	424	ASN	2.0
1	C	101	ASP	2.0
1	C	460	LYS	2.0
1	B	96	PRO	2.0
1	B	267	ILE	2.0
1	B	339	ILE	2.0
1	A	276	ASN	2.0
1	C	424	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

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

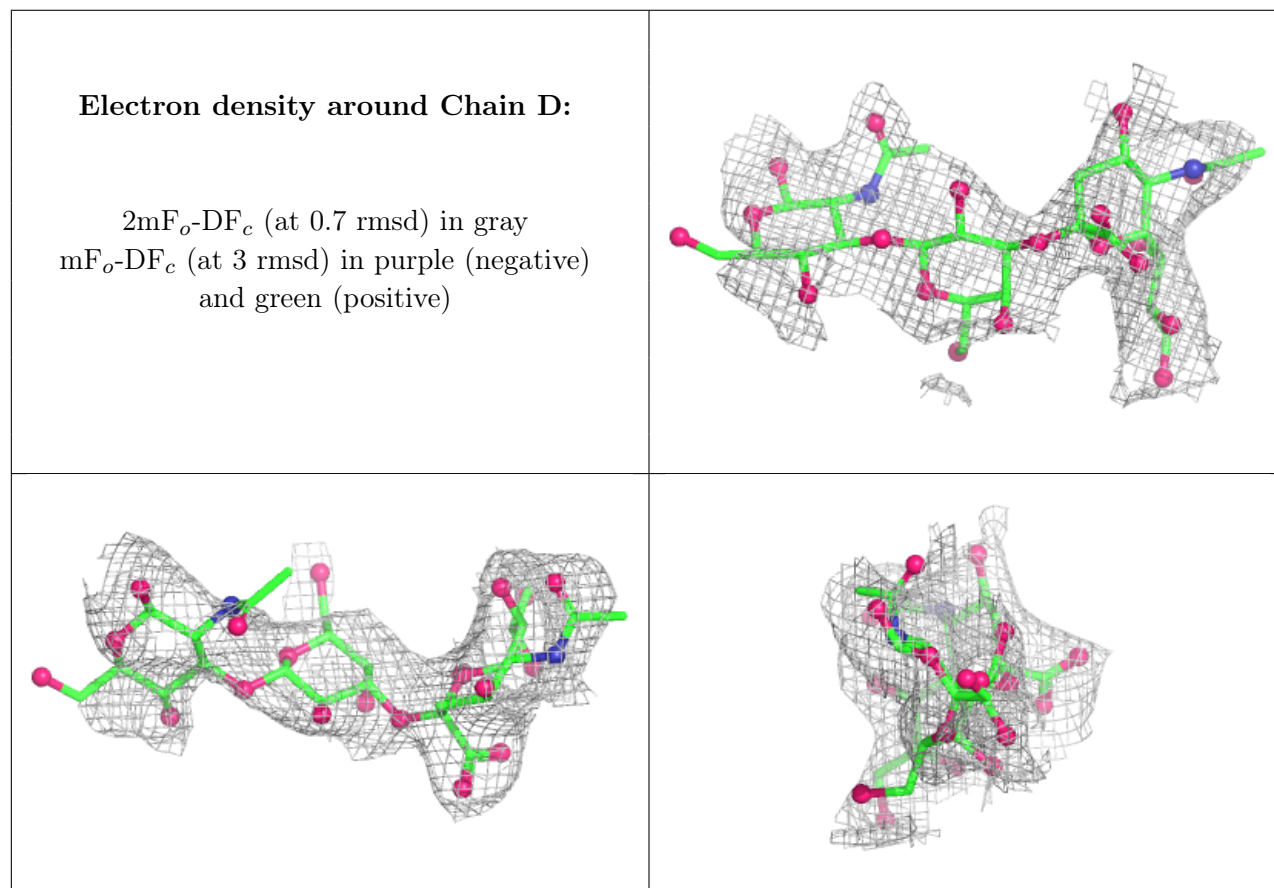
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	D	2	11/12	0.55	0.18	82,84,85,85	0
2	NAG	E	1	15/15	0.56	0.20	70,74,74,75	0
2	NAG	D	1	15/15	0.60	0.19	86,89,89,90	0
2	SIA	E	3	20/21	0.63	0.24	54,58,60,61	0

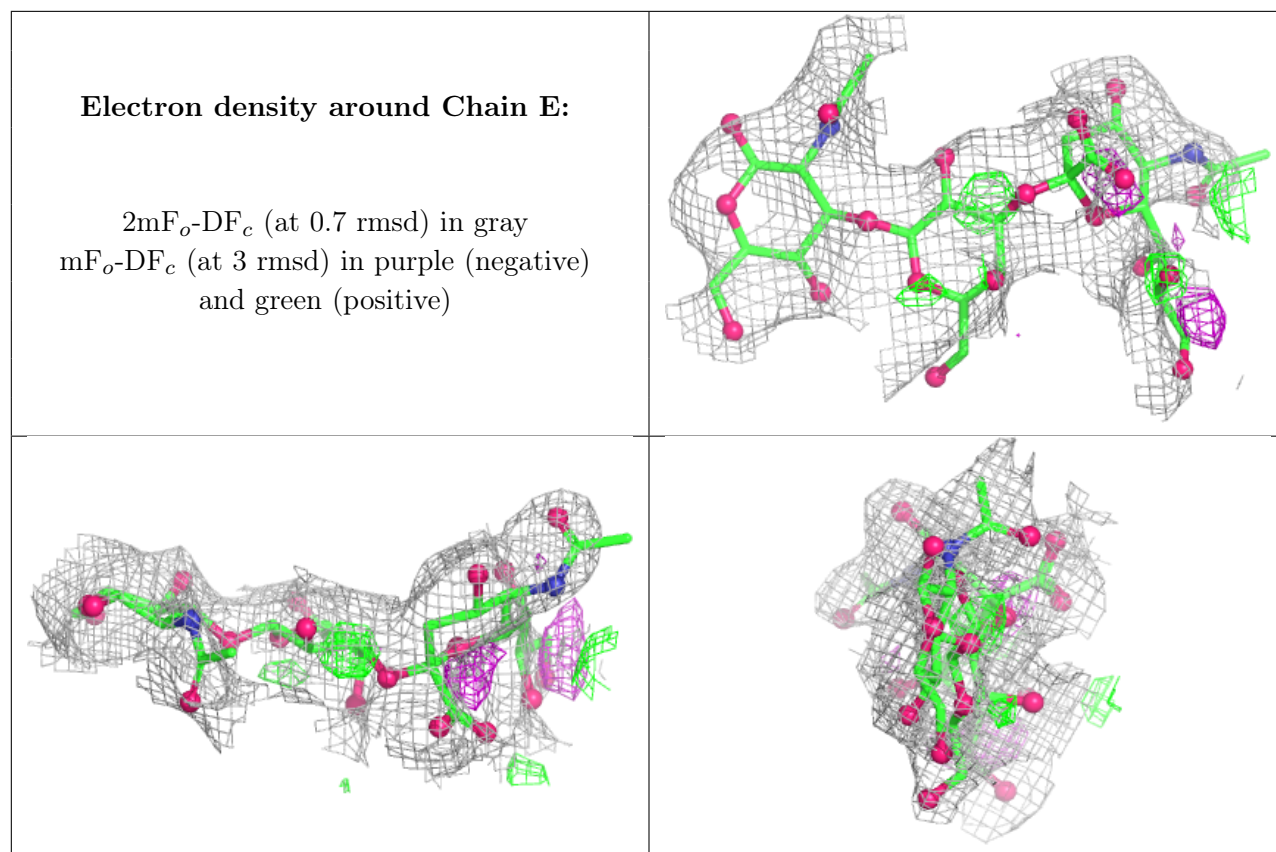
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GAL	E	2	11/12	0.73	0.25	63,66,67,68	0
2	SIA	D	3	20/21	0.76	0.15	77,79,81,81	0

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.





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(\AA^2)	Q<0.9
3	NAG	A	1499	14/15	0.43	0.26	111,114,114,115	0
3	NAG	C	1500	14/15	0.47	0.26	78,79,80,80	0
3	NAG	A	1500	13/15	0.68	0.19	69,70,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.