



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:26 PM EDT

PDB ID : 9OFR / pdb_00009ofr
Title : CRYSTAL STRUCTURE OF THE HUMAN IGA1 FC FRAGMENT-FC-
ALPHA RECEPTOR (CD89) COMPLEX
Authors : Korzeniowski, M.; Tolbert, W.D.; Pazgier, M.
Deposited on : 2025-04-30
Resolution : 2.65 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

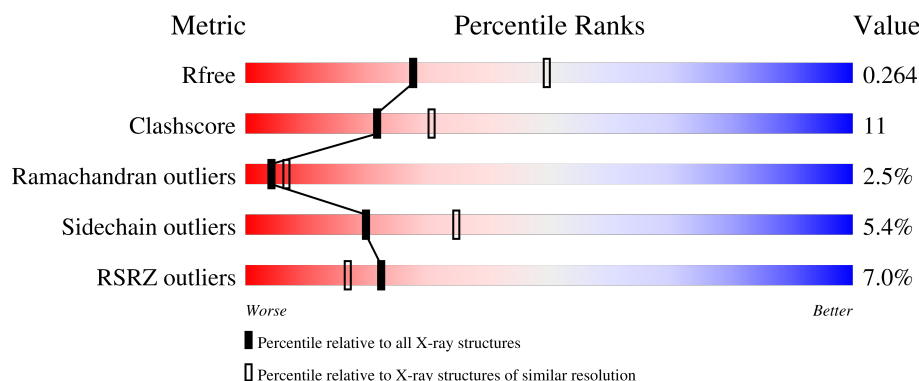
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 $\leq 5\%$. 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	214	<div> <div>7%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>
1	B	214	<div> <div>7%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	E	214	<div> <div>7%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	G	214	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>...</div> </div>
2	C	207	<div> <div>11%</div> <div>60%</div> <div>29%</div> <div>5%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	207	<div><div></div><div>3%63%29%6%</div></div>
2	F	207	<div><div></div><div>10%63%29%5%</div></div>
2	H	207	<div><div></div><div>6%64%27%6%</div></div>
3	I	2	<div><div></div><div>50%50%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13022 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 Isoform 1 of Immunoglobulin heavy constant alpha 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1605	1013	277	307	8			
1	B	212	Total	C	N	O	S	0	0	0
			1613	1018	278	308	9			
1	E	211	Total	C	N	O	S	0	0	0
			1611	1016	278	308	9			
1	G	211	Total	C	N	O	S	0	0	0
			1608	1015	277	307	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ALA	-	expression tag	UNP P01876
B	241	ALA	-	expression tag	UNP P01876
E	241	ALA	-	expression tag	UNP P01876
G	241	ALA	-	expression tag	UNP P01876

- Molecule 2 is a protein called Immunoglobulin alpha Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	195	Total	C	N	O	S	0	0	0
			1564	1002	267	287	8			
2	D	195	Total	C	N	O	S	0	0	0
			1564	1002	267	287	8			
2	F	196	Total	C	N	O	S	0	0	0
			1564	1003	267	287	7			
2	H	194	Total	C	N	O	S	0	0	0
			1555	997	265	285	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	196	ALA	-	expression tag	UNP P24071
C	197	ILE	-	expression tag	UNP P24071
C	198	ASP	-	expression tag	UNP P24071
C	199	GLY	-	expression tag	UNP P24071
C	200	ARG	-	expression tag	UNP P24071
C	201	ALA	-	expression tag	UNP P24071
C	202	HIS	-	expression tag	UNP P24071
C	203	HIS	-	expression tag	UNP P24071
C	204	HIS	-	expression tag	UNP P24071
C	205	HIS	-	expression tag	UNP P24071
C	206	HIS	-	expression tag	UNP P24071
C	207	HIS	-	expression tag	UNP P24071
D	196	ALA	-	expression tag	UNP P24071
D	197	ILE	-	expression tag	UNP P24071
D	198	ASP	-	expression tag	UNP P24071
D	199	GLY	-	expression tag	UNP P24071
D	200	ARG	-	expression tag	UNP P24071
D	201	ALA	-	expression tag	UNP P24071
D	202	HIS	-	expression tag	UNP P24071
D	203	HIS	-	expression tag	UNP P24071
D	204	HIS	-	expression tag	UNP P24071
D	205	HIS	-	expression tag	UNP P24071
D	206	HIS	-	expression tag	UNP P24071
D	207	HIS	-	expression tag	UNP P24071
F	196	ALA	-	expression tag	UNP P24071
F	197	ILE	-	expression tag	UNP P24071
F	198	ASP	-	expression tag	UNP P24071
F	199	GLY	-	expression tag	UNP P24071
F	200	ARG	-	expression tag	UNP P24071
F	201	ALA	-	expression tag	UNP P24071
F	202	HIS	-	expression tag	UNP P24071
F	203	HIS	-	expression tag	UNP P24071
F	204	HIS	-	expression tag	UNP P24071
F	205	HIS	-	expression tag	UNP P24071
F	206	HIS	-	expression tag	UNP P24071
F	207	HIS	-	expression tag	UNP P24071
H	196	ALA	-	expression tag	UNP P24071
H	197	ILE	-	expression tag	UNP P24071
H	198	ASP	-	expression tag	UNP P24071
H	199	GLY	-	expression tag	UNP P24071
H	200	ARG	-	expression tag	UNP P24071
H	201	ALA	-	expression tag	UNP P24071
H	202	HIS	-	expression tag	UNP P24071

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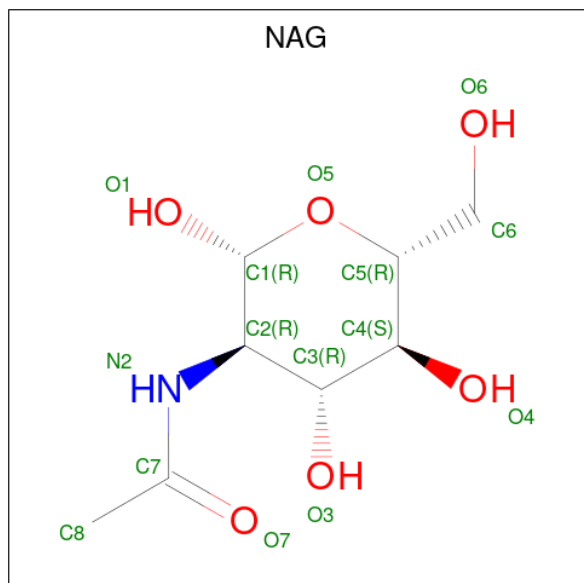
Chain	Residue	Modelled	Actual	Comment	Reference
H	203	HIS	-	expression tag	UNP P24071
H	204	HIS	-	expression tag	UNP P24071
H	205	HIS	-	expression tag	UNP P24071
H	206	HIS	-	expression tag	UNP P24071
H	207	HIS	-	expression tag	UNP P24071

- Molecule 3 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
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total	O	0	0
			18	18		
5	C	4	Total	O	0	0
			4	4		
5	B	25	Total	O	0	0
			25	25		
5	D	10	Total	O	0	0
			10	10		
5	E	16	Total	O	0	0
			16	16		
5	F	3	Total	O	0	0
			3	3		
5	G	25	Total	O	0	0
			25	25		

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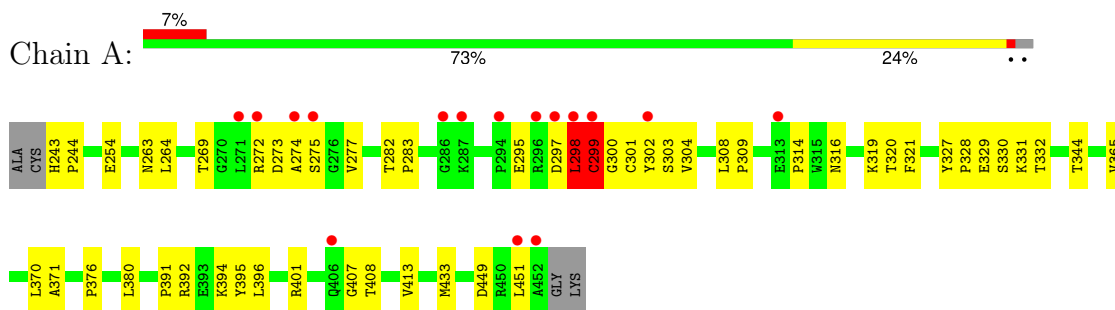
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	13	Total	O	0	0
			13	13		

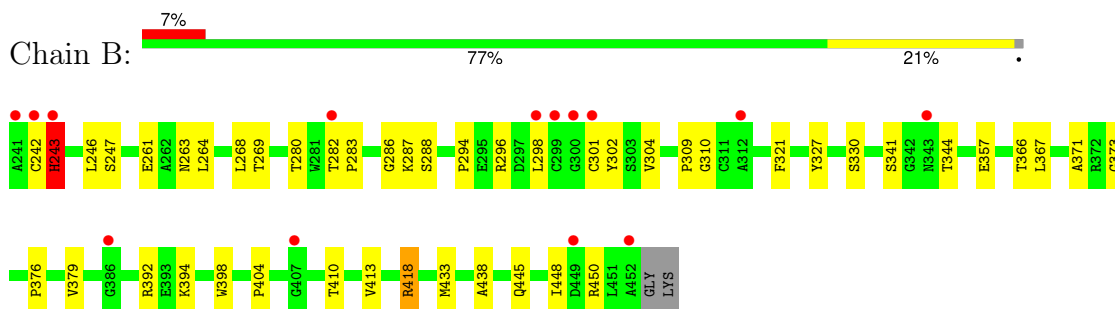
3 Residue-property plots [i](#)

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.

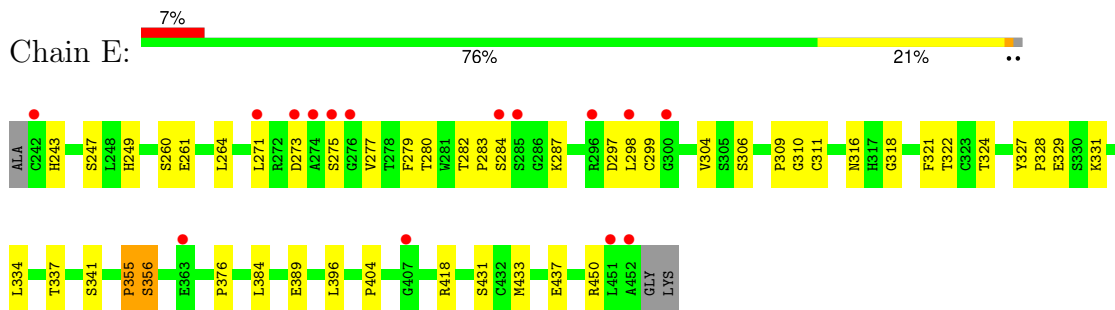
- Molecule 1: Isoform 1 of Immunoglobulin heavy constant alpha 1



- Molecule 1: Isoform 1 of Immunoglobulin heavy constant alpha 1

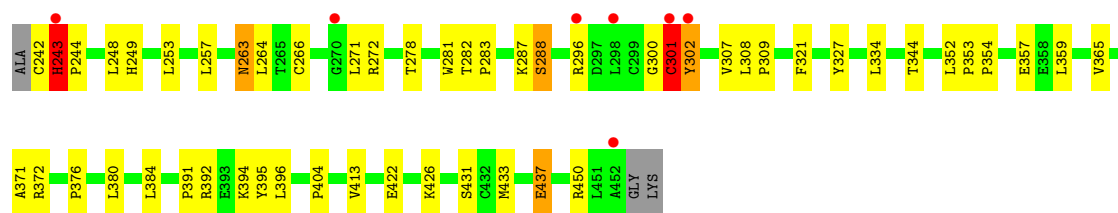


- Molecule 1: Isoform 1 of Immunoglobulin heavy constant alpha 1

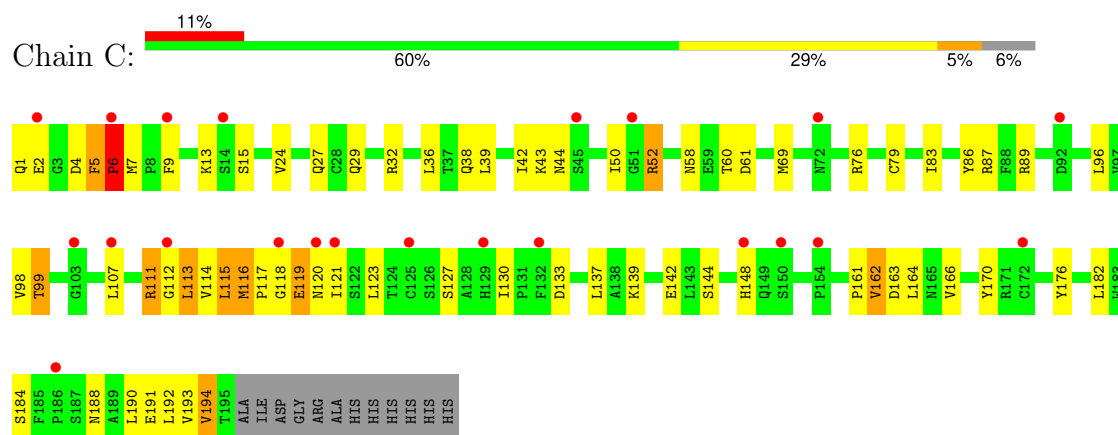


- Molecule 1: Isoform 1 of Immunoglobulin heavy constant alpha 1

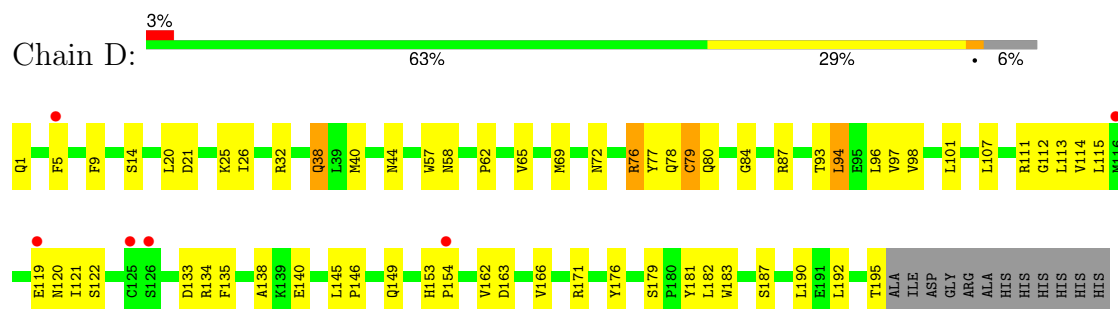




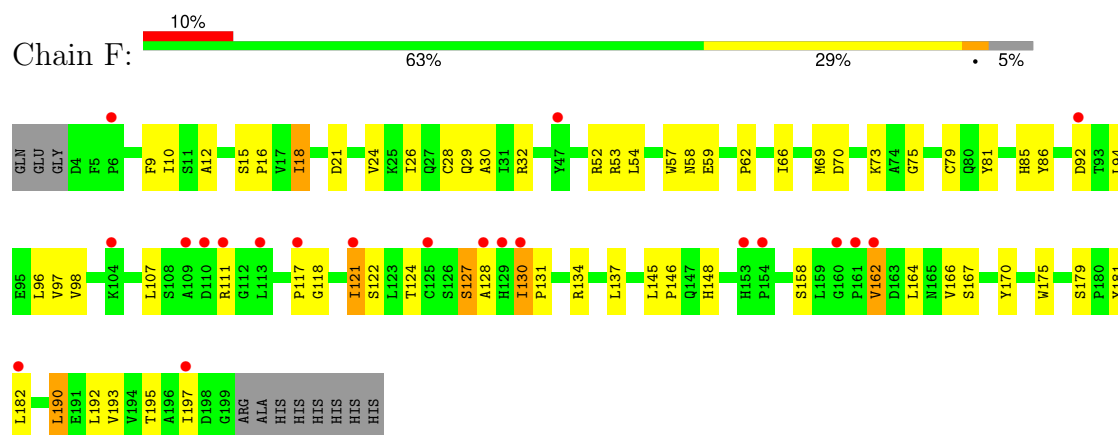
• Molecule 2: Immunoglobulin alpha Fc receptor



• Molecule 2: Immunoglobulin alpha Fc receptor

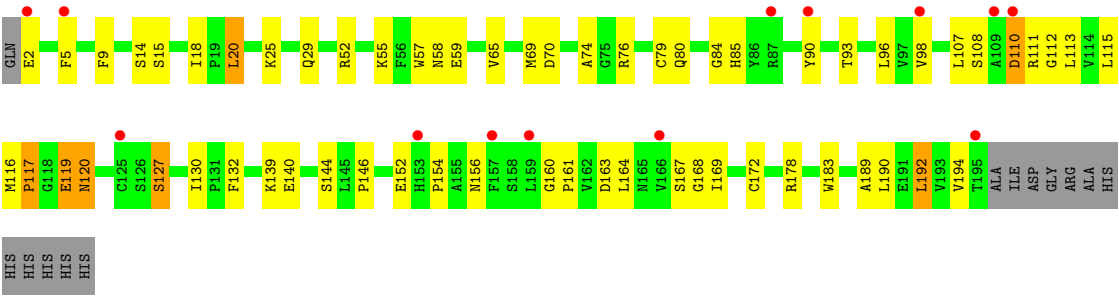


• Molecule 2: Immunoglobulin alpha Fc receptor



• Molecule 2: Immunoglobulin alpha Fc receptor





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.30Å 176.78Å 100.02Å 90.00° 96.10° 90.00°	Depositor
Resolution (Å)	40.39 – 2.65 40.39 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.39-2.65) 94.8 (40.39-2.65)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.213 , 0.264 0.214 , 0.264	Depositor DCC
R_{free} test set	2995 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13022	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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

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	0.20	0/1646	0.45	3/2248 (0.1%)
1	B	0.17	0/1654	0.46	0/2259
1	E	0.16	0/1652	0.40	0/2256
1	G	0.16	0/1649	0.41	0/2252
2	C	0.25	0/1608	0.50	1/2182 (0.0%)
2	D	0.18	0/1608	0.40	0/2182
2	F	0.16	0/1608	0.39	0/2184
2	H	0.22	0/1599	0.42	0/2170
All	All	0.19	0/13024	0.43	4/17733 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	CYS	N-CA-C	-5.73	98.60	110.80
2	C	6	PRO	N-CA-CB	-5.43	97.55	103.25
1	A	298	LEU	CA-C-N	5.37	131.80	121.54
1	A	298	LEU	C-N-CA	5.37	131.80	121.54

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	1605	0	1585	42	0
1	B	1613	0	1592	29	0
1	E	1611	0	1591	29	0
1	G	1608	0	1587	35	0
2	C	1564	0	1520	49	0
2	D	1564	0	1518	33	0
2	F	1564	0	1517	38	0
2	H	1555	0	1507	38	0
3	I	28	0	25	2	0
4	B	14	0	13	1	0
4	C	28	0	26	1	0
4	D	56	0	52	1	0
4	E	14	0	13	2	0
4	F	14	0	13	0	0
4	G	14	0	13	0	0
4	H	56	0	52	2	0
5	A	18	0	0	0	0
5	B	25	0	0	0	0
5	C	4	0	0	0	0
5	D	10	0	0	0	0
5	E	16	0	0	0	0
5	F	3	0	0	0	0
5	G	25	0	0	0	0
5	H	13	0	0	0	0
All	All	13022	0	12624	276	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 11.

All (276) 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)
2:D:115:LEU:HD22	2:D:121:ILE:HD11	1.44	0.97
1:B:418:ARG:HG3	1:B:418:ARG:HH11	1.31	0.96
1:A:298:LEU:HD12	1:A:298:LEU:H	1.32	0.94
2:C:115:LEU:HB2	2:C:121:ILE:HG13	1.54	0.87
2:C:119:GLU:HG3	2:C:120:ASN:H	1.48	0.79
2:C:5:PHE:CB	2:C:6:PRO:HD2	2.12	0.78
2:F:111:ARG:HH21	2:F:121:ILE:HA	1.51	0.76
2:H:116:MET:HG2	2:H:117:PRO:HD2	1.65	0.75
2:H:107:LEU:HD13	2:H:172:CYS:HB2	1.71	0.73
1:A:277:VAL:HG21	1:A:304:VAL:HG21	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:ASP:HB2	2:C:176:TYR:HA	1.73	0.70
2:D:101:LEU:HD12	2:D:182:LEU:HB3	1.74	0.70
1:B:287:LYS:HE3	1:B:310:GLY:HA3	1.73	0.69
2:C:69:MET:HG3	2:C:98:VAL:HG12	1.73	0.69
2:C:5:PHE:HB3	2:C:6:PRO:CD	2.24	0.68
2:C:5:PHE:O	2:C:6:PRO:C	2.36	0.67
2:D:76:ARG:HD3	2:D:93:THR:HG21	1.77	0.66
2:D:32:ARG:HD2	2:D:58:ASN:HA	1.78	0.66
2:F:118:GLY:H	2:F:162:VAL:HG12	1.61	0.66
1:E:309:PRO:HB3	4:E:701:NAG:H61	1.76	0.66
1:A:396:LEU:HB2	1:B:404:PRO:HD3	1.79	0.65
2:F:32:ARG:HH11	2:F:58:ASN:HB2	1.62	0.64
1:A:297:ASP:H	1:A:300:GLY:HA2	1.61	0.64
2:F:10:ILE:HG22	2:F:92:ASP:HB2	1.79	0.64
2:C:5:PHE:HB2	2:C:6:PRO:HD2	1.79	0.63
1:B:263:ASN:HB3	1:B:309:PRO:HA	1.80	0.63
2:C:5:PHE:CB	2:C:6:PRO:CD	2.76	0.63
2:H:127:SER:OG	2:H:130:ILE:HG12	1.99	0.62
2:C:115:LEU:HG	2:C:162:VAL:HG21	1.82	0.62
2:D:111:ARG:HH21	2:D:115:LEU:HD12	1.66	0.61
1:E:299:CYS:HA	1:G:243:HIS:CE1	2.36	0.61
2:H:80:GLN:HE21	2:H:90:TYR:HE1	1.48	0.61
1:G:422:GLU:HG2	1:G:426:LYS:HD3	1.83	0.60
1:G:263:ASN:HB3	1:G:309:PRO:HA	1.83	0.60
2:C:5:PHE:HB3	2:C:6:PRO:HD2	1.81	0.60
1:E:322:THR:HG23	1:E:337:THR:HG22	1.84	0.59
2:H:115:LEU:HB2	2:H:119:GLU:OE2	2.02	0.59
2:H:139:LYS:HE3	2:H:168:GLY:HA3	1.83	0.59
2:D:69:MET:HE3	2:D:98:VAL:HG22	1.83	0.59
2:H:117:PRO:HG3	2:H:164:LEU:HD11	1.85	0.59
1:G:371:ALA:HB3	1:G:413:VAL:HG12	1.85	0.59
1:A:297:ASP:C	1:A:299:CYS:H	2.11	0.58
2:F:179:SER:HB3	2:F:182:LEU:HD13	1.84	0.58
1:A:408:THR:HG22	1:E:318:GLY:HA3	1.85	0.58
2:C:118:GLY:H	2:C:162:VAL:HG13	1.68	0.58
2:H:18:ILE:HD11	2:H:96:LEU:HD22	1.85	0.58
2:C:32:ARG:HD2	2:C:58:ASN:HA	1.85	0.57
2:C:115:LEU:HD23	2:C:193:VAL:O	2.04	0.57
1:E:437:GLU:HA	2:F:85:HIS:CE1	2.39	0.57
2:C:139:LYS:O	2:C:142:GLU:HB2	2.06	0.56
1:A:298:LEU:H	1:A:298:LEU:CD1	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ALA:HB3	1:A:413:VAL:HG12	1.88	0.56
2:H:167:SER:HB2	2:H:194:VAL:HG23	1.87	0.55
1:A:327:TYR:CD2	1:A:329:GLU:HB3	2.41	0.55
1:B:344:THR:HB	1:B:438:ALA:HB2	1.89	0.55
1:A:297:ASP:HB3	1:A:298:LEU:HD12	1.89	0.55
1:B:371:ALA:HB3	1:B:413:VAL:HG12	1.89	0.55
1:G:357:GLU:CD	1:G:357:GLU:H	2.15	0.54
1:G:344:THR:HG22	1:G:376:PRO:HD3	1.88	0.54
2:D:115:LEU:HD23	2:D:162:VAL:HG11	1.90	0.54
2:H:55:LYS:HD3	2:H:57:TRP:CD2	2.43	0.54
2:D:138:ALA:HB2	2:D:146:PRO:HG3	1.90	0.53
1:A:282:THR:OG1	1:A:283:PRO:HD3	2.09	0.53
2:F:167:SER:HA	2:F:192:LEU:O	2.07	0.53
1:A:344:THR:HG22	1:A:376:PRO:HD3	1.90	0.53
2:F:166:VAL:HG12	2:F:192:LEU:HD22	1.91	0.53
2:F:9:PHE:HB2	2:F:29:GLN:HG3	1.91	0.52
1:G:296:ARG:H	1:G:296:ARG:HE	1.57	0.52
1:E:384:LEU:HB2	1:E:431:SER:HB2	1.90	0.52
2:F:107:LEU:HG	2:F:190:LEU:HD23	1.91	0.52
1:B:367:LEU:HD22	1:B:448:ILE:HD11	1.91	0.52
1:A:327:TYR:HD2	1:A:329:GLU:HB3	1.75	0.52
1:E:282:THR:OG1	1:E:283:PRO:HD3	2.10	0.52
1:G:282:THR:OG1	1:G:283:PRO:HD3	2.10	0.51
2:F:137:LEU:HD11	2:F:170:TYR:HD1	1.75	0.51
1:G:243:HIS:CE1	1:G:272:ARG:NH2	2.79	0.51
1:G:249:HIS:O	1:G:264:LEU:HD23	2.10	0.51
2:H:76:ARG:HD2	2:H:93:THR:HG21	1.91	0.51
2:C:5:PHE:O	2:C:7:MET:N	2.44	0.51
2:C:119:GLU:HG3	2:C:120:ASN:N	2.20	0.51
1:A:243:HIS:HB3	1:A:244:PRO:HD3	1.92	0.50
2:H:146:PRO:HG2	2:H:183:TRP:HH2	1.75	0.50
1:A:254:GLU:HA	1:A:380:LEU:HD11	1.93	0.50
2:D:113:LEU:HD12	2:D:192:LEU:HD12	1.93	0.50
1:E:433:MET:HE1	2:F:54:LEU:HG	1.93	0.50
2:D:133:ASP:HB2	2:D:176:TYR:HA	1.94	0.50
2:H:140:GLU:HG3	2:H:169:ILE:HB	1.94	0.50
1:B:282:THR:OG1	1:B:283:PRO:HD3	2.11	0.50
1:E:396:LEU:HB2	1:G:404:PRO:HD3	1.94	0.50
1:G:392:ARG:HA	1:G:395:TYR:CZ	2.46	0.50
2:D:25:LYS:HG2	2:D:65:VAL:HG22	1.93	0.49
1:A:316:ASN:HB3	2:C:86:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ASP:OD2	2:D:166:VAL:HG23	2.13	0.49
2:H:74:ALA:HB2	2:H:98:VAL:HG23	1.94	0.49
1:B:261:GLU:HG3	4:B:701:NAG:H4	1.94	0.49
2:C:43:LYS:HE3	4:C:701:NAG:H2	1.93	0.49
2:D:57:TRP:CD1	2:D:62:PRO:HG3	2.47	0.49
2:D:119:GLU:HA	4:D:703:NAG:H83	1.95	0.49
1:E:433:MET:CE	2:F:54:LEU:HG	2.42	0.49
2:H:152:GLU:HG3	2:H:156:ASN:OD1	2.12	0.49
2:D:121:ILE:HG22	2:D:122:SER:H	1.78	0.49
2:C:1:GLN:HB3	2:C:2:GLU:H	1.42	0.48
2:C:24:VAL:HG11	2:C:96:LEU:HD13	1.94	0.48
2:C:98:VAL:HG23	2:C:182:LEU:HA	1.95	0.48
2:H:25:LYS:HG2	2:H:65:VAL:HG22	1.94	0.48
1:A:314:PRO:HB2	1:A:321:PHE:HZ	1.77	0.48
2:F:30:ALA:HB2	2:F:62:PRO:HD3	1.96	0.48
1:G:253:LEU:HD23	1:G:380:LEU:HG	1.96	0.48
2:C:111:ARG:HD3	2:C:112:GLY:H	1.78	0.48
1:B:341:SER:HB2	1:B:376:PRO:HG3	1.94	0.48
2:D:97:VAL:HG12	2:D:181:TYR:HA	1.94	0.48
2:F:69:MET:HG3	2:F:98:VAL:HG22	1.95	0.48
2:H:146:PRO:HG2	2:H:183:TRP:CH2	2.49	0.48
2:C:191:GLU:O	2:C:192:LEU:HD23	2.13	0.48
1:B:392:ARG:HG3	1:B:392:ARG:HH11	1.78	0.48
1:E:418:ARG:HD3	1:G:372:ARG:HD2	1.94	0.48
1:E:277:VAL:HG12	1:E:328:PRO:HD3	1.96	0.48
2:F:57:TRP:CD1	2:F:62:PRO:HG3	2.48	0.48
1:B:394:LYS:O	1:B:394:LYS:HD3	2.14	0.48
2:D:26:ILE:HD11	2:D:96:LEU:HD11	1.96	0.48
2:H:163:ASP:O	2:H:194:VAL:HG11	2.13	0.48
2:C:5:PHE:C	2:C:7:MET:N	2.72	0.48
1:A:297:ASP:HB2	1:A:301:CYS:H	1.78	0.47
2:C:60:THR:HG22	2:C:61:ASP:H	1.78	0.47
1:A:298:LEU:HD12	1:A:298:LEU:N	2.14	0.47
1:A:396:LEU:HB2	1:B:404:PRO:CD	2.45	0.47
2:C:9:PHE:HE1	2:C:27:GLN:HG2	1.78	0.47
2:F:26:ILE:HD11	2:F:96:LEU:HD11	1.96	0.47
2:F:53:ARG:HG2	2:F:57:TRP:HZ2	1.78	0.47
1:B:373:GLY:HA2	1:B:410:THR:HB	1.96	0.47
2:F:127:SER:OG	2:F:130:ILE:HB	2.15	0.47
1:E:273:ASP:HB2	1:E:329:GLU:HG2	1.97	0.47
1:E:316:ASN:HB3	2:F:86:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:CYS:O	2:F:62:PRO:HD2	2.15	0.47
1:G:283:PRO:HG2	1:G:321:PHE:CD2	2.50	0.47
1:A:391:PRO:HD2	1:A:394:LYS:HG3	1.97	0.47
1:E:247:SER:HB2	1:E:249:HIS:HE1	1.80	0.46
1:E:287:LYS:HE3	1:E:310:GLY:O	2.14	0.46
2:C:142:GLU:HG3	2:C:144:SER:O	2.15	0.46
2:F:70:ASP:OD1	2:F:73:LYS:HG2	2.15	0.46
2:F:193:VAL:HG12	2:F:195:THR:HG23	1.97	0.46
1:B:294:PRO:HA	1:B:304:VAL:HG12	1.96	0.46
1:A:298:LEU:O	1:B:243:HIS:CE1	2.68	0.46
1:E:261:GLU:HG3	4:E:701:NAG:H3	1.97	0.46
1:E:327:TYR:CE1	1:E:334:LEU:HG	2.50	0.46
1:E:341:SER:HB2	1:E:376:PRO:HG3	1.97	0.46
2:H:111:ARG:HG2	2:H:112:GLY:H	1.80	0.46
1:A:297:ASP:HB2	1:A:301:CYS:N	2.30	0.46
1:A:331:LYS:HD2	1:A:331:LYS:HA	1.58	0.46
2:D:134:ARG:HH11	2:D:149:GLN:HG2	1.80	0.46
2:F:134:ARG:HD3	2:F:175:TRP:CH2	2.50	0.46
2:D:140:GLU:HG3	2:D:171:ARG:HH12	1.81	0.46
1:G:391:PRO:HD2	1:G:394:LYS:HD2	1.97	0.46
2:C:39:LEU:HG	2:C:50:ILE:HD11	1.97	0.46
1:B:327:TYR:CE2	1:B:330:SER:HB3	2.51	0.46
2:C:137:LEU:HD21	2:C:170:TYR:HB3	1.97	0.46
2:H:130:ILE:HG21	2:H:132:PHE:CZ	2.50	0.46
2:C:164:LEU:HA	2:C:194:VAL:HG21	1.98	0.46
1:A:263:ASN:HB3	3:I:1:NAG:H2	1.98	0.45
2:F:111:ARG:HH11	2:F:111:ARG:HB3	1.81	0.45
2:F:179:SER:HB3	2:F:182:LEU:HB2	1.98	0.45
2:D:40:MET:HE3	2:D:40:MET:HB2	1.82	0.45
2:F:145:LEU:HG	2:F:146:PRO:HD2	1.99	0.45
2:H:120:ASN:HB3	2:H:160:GLY:O	2.16	0.45
2:D:179:SER:HB2	2:D:182:LEU:HD12	1.99	0.45
1:E:277:VAL:HG12	1:E:327:TYR:HA	1.99	0.45
1:E:280:THR:HB	1:E:324:THR:OG1	2.16	0.45
2:C:4:ASP:HA	2:C:89:ARG:HH11	1.82	0.45
2:F:12:ALA:HB2	2:F:94:LEU:HD11	1.99	0.45
2:C:115:LEU:O	2:C:116:MET:C	2.60	0.45
1:B:433:MET:HE2	1:B:433:MET:HB3	1.72	0.45
1:A:273:ASP:OD1	1:A:328:PRO:HB2	2.17	0.45
1:G:327:TYR:HE1	1:G:334:LEU:HG	1.81	0.45
2:F:137:LEU:HB3	2:F:148:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD12	1:A:309:PRO:HD2	1.98	0.45
1:E:384:LEU:HD12	1:E:389:GLU:HA	1.99	0.45
2:F:30:ALA:HB1	2:F:57:TRP:HB2	1.98	0.44
1:G:243:HIS:HE1	1:G:272:ARG:NH2	2.16	0.44
1:A:274:ALA:HB3	1:A:328:PRO:HG2	1.98	0.44
1:A:392:ARG:HA	1:A:395:TYR:CE2	2.52	0.44
2:D:107:LEU:HG	2:D:190:LEU:HD12	1.99	0.44
1:E:279:PHE:CZ	1:E:304:VAL:HG12	2.52	0.44
2:D:134:ARG:NH1	2:D:149:GLN:HG2	2.33	0.44
2:F:18:ILE:HD11	2:F:96:LEU:HD22	1.98	0.44
2:C:42:ILE:HB	2:C:76:ARG:HB3	1.99	0.44
1:E:279:PHE:CD1	1:E:306:SER:HB2	2.53	0.44
2:C:15:SER:HA	2:C:142:GLU:O	2.18	0.44
1:G:354:PRO:HB3	1:G:365:VAL:HB	1.99	0.44
1:G:242:CYS:O	1:G:243:HIS:HB2	2.18	0.44
3:I:1:NAG:H82	3:I:1:NAG:H3	2.00	0.44
2:C:36:LEU:HD11	2:C:52:ARG:HG3	1.99	0.43
1:B:283:PRO:HG2	1:B:321:PHE:HA	2.00	0.43
1:B:392:ARG:HD2	1:B:392:ARG:HA	1.85	0.43
2:D:111:ARG:HG3	2:D:112:GLY:N	2.33	0.43
1:A:392:ARG:HA	1:A:395:TYR:CZ	2.53	0.43
1:A:433:MET:HE2	1:A:433:MET:HB3	1.93	0.43
2:C:127:SER:O	2:C:130:ILE:HD12	2.18	0.43
2:D:9:PHE:CD1	2:D:9:PHE:C	2.97	0.43
1:A:401:ARG:HD2	1:B:398:TRP:CD1	2.54	0.43
1:G:281:TRP:CE3	1:G:308:LEU:HD22	2.54	0.43
1:B:246:LEU:HD13	1:B:268:LEU:HD13	2.01	0.43
2:C:116:MET:SD	2:C:116:MET:N	2.85	0.43
1:A:319:LYS:NZ	1:A:320:THR:H	2.16	0.43
2:C:43:LYS:HD3	2:C:44:ASN:HB2	2.00	0.43
2:F:52:ARG:O	2:F:53:ARG:HD2	2.19	0.43
1:G:300:GLY:O	1:G:301:CYS:C	2.61	0.43
1:A:297:ASP:HB3	1:A:298:LEU:H	1.67	0.42
1:A:451:LEU:HD13	1:A:451:LEU:HA	1.83	0.42
1:E:331:LYS:HE3	1:E:331:LYS:HB3	1.66	0.42
1:E:355:PRO:HB2	1:E:356:SER:H	1.65	0.42
2:F:122:SER:HA	2:F:158:SER:HA	2.01	0.42
2:H:70:ASP:O	2:H:98:VAL:HG21	2.18	0.42
2:H:178:ARG:H	2:H:178:ARG:HG2	1.45	0.42
2:C:113:LEU:HD11	2:C:191:GLU:HG3	2.01	0.42
1:B:418:ARG:HG3	1:B:418:ARG:NH1	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:HIS:HB3	1:G:244:PRO:HD3	2.01	0.42
2:C:7:MET:HB3	2:C:7:MET:HE3	1.62	0.42
1:G:257:LEU:HD21	2:H:85:HIS:ND1	2.34	0.42
2:H:69:MET:HE3	2:H:98:VAL:HG22	2.02	0.42
2:H:113:LEU:HD22	2:H:192:LEU:HD12	2.01	0.42
1:B:357:GLU:CD	1:B:357:GLU:H	2.27	0.42
2:D:38:GLN:HG3	2:D:80:GLN:HB3	2.01	0.42
1:G:248:LEU:HD13	1:G:266:CYS:HB2	2.01	0.42
2:H:156:ASN:OD1	2:H:156:ASN:N	2.53	0.42
2:H:189:ALA:O	2:H:190:LEU:HD23	2.19	0.42
2:F:28:CYS:HB3	2:F:81:TYR:OH	2.19	0.42
1:G:359:LEU:HD23	1:G:365:VAL:HG11	2.02	0.42
2:H:9:PHE:CD2	2:H:29:GLN:HB2	2.55	0.42
2:H:110:ASP:OD1	2:H:110:ASP:N	2.52	0.42
2:C:60:THR:HG22	2:C:61:ASP:N	2.35	0.42
1:E:273:ASP:OD2	1:E:328:PRO:HB2	2.19	0.42
1:A:295:GLU:O	1:A:302:TYR:HA	2.19	0.42
2:D:146:PRO:HG2	2:D:183:TRP:CH2	2.55	0.42
1:G:287:LYS:HD2	1:G:309:PRO:HB2	2.02	0.42
1:G:296:ARG:H	1:G:296:ARG:NE	2.17	0.42
1:G:352:LEU:HA	1:G:353:PRO:HD3	1.89	0.42
2:D:135:PHE:HE2	2:D:153:HIS:HA	1.85	0.42
1:A:370:LEU:HD21	1:B:366:THR:HG21	2.02	0.42
1:A:449:ASP:C	1:A:451:LEU:N	2.78	0.41
1:A:395:TYR:C	1:B:404:PRO:HG2	2.46	0.41
1:E:283:PRO:HG2	1:E:321:PHE:CD2	2.55	0.41
2:H:55:LYS:HD3	2:H:57:TRP:CE2	2.55	0.41
1:G:437:GLU:HA	2:H:85:HIS:CE1	2.55	0.41
2:H:59:GLU:CG	4:H:702:NAG:H83	2.50	0.41
2:C:99:THR:HG23	2:C:184:SER:O	2.21	0.41
1:B:296:ARG:HD3	1:B:302:TYR:CE2	2.55	0.41
1:G:271:LEU:O	1:G:302:TYR:N	2.54	0.41
1:A:330:SER:O	1:A:332:THR:HG22	2.20	0.41
2:C:13:LYS:HA	2:C:13:LYS:HD2	1.96	0.41
2:C:107:LEU:HD21	2:C:123:LEU:HD23	2.02	0.41
2:D:114:VAL:O	2:D:114:VAL:HG23	2.21	0.41
2:F:75:GLY:HA2	2:F:181:TYR:CG	2.56	0.41
1:B:344:THR:HG22	1:B:376:PRO:HD3	2.03	0.41
1:G:334:LEU:HD23	1:G:334:LEU:HA	1.90	0.41
2:H:80:GLN:HG3	2:H:90:TYR:CE1	2.56	0.41
2:D:77:TYR:HB2	2:D:94:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LEU:HD22	2:D:113:LEU:H	1.85	0.41
2:D:145:LEU:HD23	2:D:145:LEU:HA	1.89	0.41
1:E:404:PRO:HD3	1:G:396:LEU:HB2	2.02	0.41
2:F:24:VAL:HG23	2:F:66:ILE:HB	2.03	0.41
1:G:384:LEU:HB2	1:G:431:SER:HB2	2.02	0.41
2:C:83:ILE:O	2:C:87:ARG:HB2	2.21	0.41
1:G:433:MET:HE2	1:G:433:MET:HB3	1.86	0.41
1:A:331:LYS:O	1:A:332:THR:C	2.64	0.40
2:C:9:PHE:CD1	2:C:9:PHE:C	2.99	0.40
2:F:97:VAL:HG13	2:F:145:LEU:HD11	2.03	0.40
2:H:14:SER:OG	2:H:15:SER:N	2.54	0.40
2:H:20:LEU:HD12	2:H:98:VAL:HG11	2.03	0.40
1:A:269:THR:HG22	1:A:303:SER:OG	2.21	0.40
2:H:113:LEU:O	2:H:115:LEU:HG	2.21	0.40
2:F:15:SER:HA	2:F:16:PRO:HD3	1.93	0.40
2:C:9:PHE:CE2	2:C:29:GLN:HG3	2.56	0.40
2:C:163:ASP:O	2:C:166:VAL:HG22	2.21	0.40
1:B:433:MET:HG2	1:B:445:GLN:HG3	2.03	0.40
2:D:78:GLN:HG2	2:D:79:CYS:H	1.86	0.40
2:H:58:ASN:CG	4:H:702:NAG:HN2	2.29	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	208/214 (97%)	184 (88%)	21 (10%)	3 (1%)	9 14
1	B	210/214 (98%)	190 (90%)	14 (7%)	6 (3%)	3 5
1	E	209/214 (98%)	185 (88%)	18 (9%)	6 (3%)	3 5
1	G	209/214 (98%)	191 (91%)	13 (6%)	5 (2%)	4 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	193/207 (93%)	166 (86%)	20 (10%)	7 (4%)	2	4
2	D	193/207 (93%)	173 (90%)	17 (9%)	3 (2%)	7	12
2	F	194/207 (94%)	175 (90%)	14 (7%)	5 (3%)	4	6
2	H	192/207 (93%)	165 (86%)	22 (12%)	5 (3%)	4	6
All	All	1608/1684 (96%)	1429 (89%)	139 (9%)	40 (2%)	4	7

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	CYS
2	C	5	PHE
2	C	6	PRO
1	B	242	CYS
1	B	243	HIS
1	B	288	SER
1	E	355	PRO
1	G	243	HIS
2	H	119	GLU
2	C	148	HIS
1	B	450	ARG
1	E	243	HIS
1	E	356	SER
1	G	288	SER
1	G	302	TYR
1	G	450	ARG
1	A	407	GLY
1	B	286	GLY
1	B	298	LEU
1	E	275	SER
2	F	131	PRO
2	C	116	MET
1	E	260	SER
1	E	297	ASP
2	F	59	GLU
2	F	117	PRO
2	F	128	ALA
1	G	301	CYS
1	A	298	LEU
2	C	119	GLU
2	D	84	GLY
2	D	187	SER

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Mol	Chain	Res	Type
2	H	154	PRO
2	F	197	ILE
2	H	117	PRO
2	H	161	PRO
2	C	161	PRO
2	C	117	PRO
2	D	154	PRO
2	H	84	GLY

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	179/181 (99%)	173 (97%)	6 (3%)	32	53
1	B	179/181 (99%)	171 (96%)	8 (4%)	24	42
1	E	180/181 (99%)	174 (97%)	6 (3%)	33	55
1	G	179/181 (99%)	172 (96%)	7 (4%)	28	48
2	C	171/180 (95%)	158 (92%)	13 (8%)	12	21
2	D	171/180 (95%)	157 (92%)	14 (8%)	10	18
2	F	170/180 (94%)	160 (94%)	10 (6%)	18	30
2	H	170/180 (94%)	159 (94%)	11 (6%)	15	27
All	All	1399/1444 (97%)	1324 (95%)	75 (5%)	20	35

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	LEU
1	A	272	ARG
1	A	275	SER
1	A	298	LEU
1	A	299	CYS
1	A	365	VAL
2	C	6	PRO

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Mol	Chain	Res	Type
2	C	38	GLN
2	C	52	ARG
2	C	79	CYS
2	C	99	THR
2	C	111	ARG
2	C	113	LEU
2	C	114	VAL
2	C	115	LEU
2	C	162	VAL
2	C	188	ASN
2	C	190	LEU
2	C	194	VAL
1	B	243	HIS
1	B	247	SER
1	B	264	LEU
1	B	269	THR
1	B	280	THR
1	B	301	CYS
1	B	379	VAL
1	B	418	ARG
2	D	1	GLN
2	D	5	PHE
2	D	14	SER
2	D	20	LEU
2	D	21	ASP
2	D	38	GLN
2	D	44	ASN
2	D	72	ASN
2	D	76	ARG
2	D	79	CYS
2	D	87	ARG
2	D	94	LEU
2	D	120	ASN
2	D	195	THR
1	E	264	LEU
1	E	271	LEU
1	E	284	SER
1	E	298	LEU
1	E	311	CYS
1	E	450	ARG
2	F	18	ILE
2	F	21	ASP

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Mol	Chain	Res	Type
2	F	79	CYS
2	F	121	ILE
2	F	124	THR
2	F	127	SER
2	F	130	ILE
2	F	162	VAL
2	F	164	LEU
2	F	190	LEU
1	G	243	HIS
1	G	263	ASN
1	G	278	THR
1	G	288	SER
1	G	301	CYS
1	G	307	VAL
1	G	437	GLU
2	H	2	GLU
2	H	5	PHE
2	H	20	LEU
2	H	52	ARG
2	H	79	CYS
2	H	108	SER
2	H	110	ASP
2	H	120	ASN
2	H	127	SER
2	H	144	SER
2	H	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	A	350	HIS
2	C	177	ASN
1	B	343	ASN
2	D	129	HIS
2	D	147	GLN
2	D	148	HIS
2	D	153	HIS
2	D	177	ASN
1	E	249	HIS
1	G	317	HIS
2	H	38	GLN

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Mol	Chain	Res	Type
2	H	80	GLN

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 ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.70	0	17,19,21	1.96	2 (11%)
3	NAG	I	2	3	14,14,15	0.75	0	17,19,21	0.83	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	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C2-N2-C7	6.38	131.45	122.90
3	I	1	NAG	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

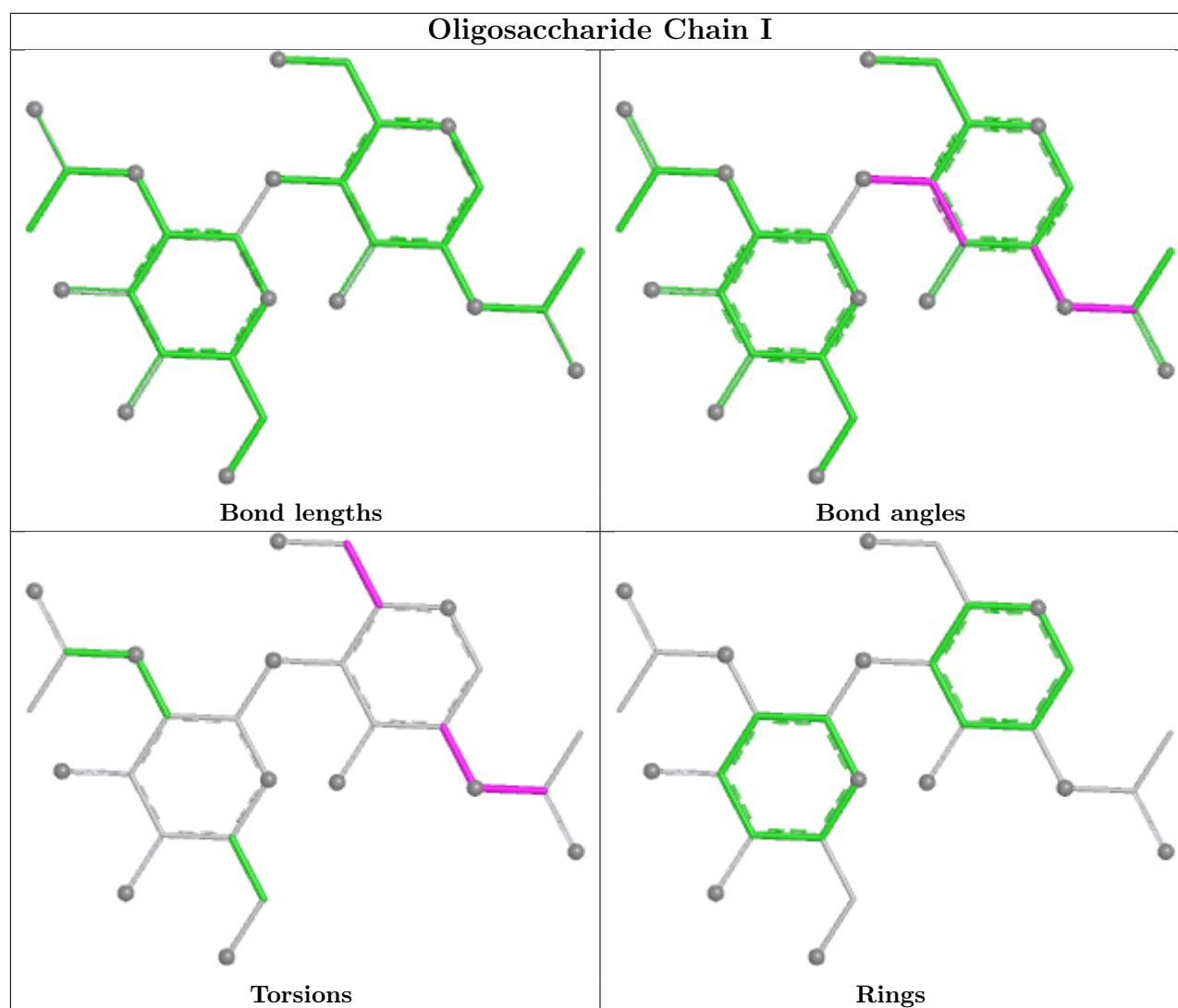
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	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 [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	701	1	14,14,15	0.64	0	17,19,21	0.82	0
4	NAG	H	701	2	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
4	NAG	E	701	1	14,14,15	0.64	0	17,19,21	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	702	2	14,14,15	0.71	0	17,19,21	1.63	3 (17%)
4	NAG	D	704	2	14,14,15	0.66	0	17,19,21	0.83	0
4	NAG	C	702	2	14,14,15	0.66	0	17,19,21	1.67	2 (11%)
4	NAG	H	704	2	14,14,15	0.68	0	17,19,21	0.92	1 (5%)
4	NAG	C	701	2	14,14,15	0.75	0	17,19,21	1.14	1 (5%)
4	NAG	F	301	2	14,14,15	0.64	0	17,19,21	0.94	1 (5%)
4	NAG	H	703	2	14,14,15	0.66	0	17,19,21	0.88	1 (5%)
4	NAG	D	703	2	14,14,15	0.72	0	17,19,21	1.45	3 (17%)
4	NAG	G	701	1	14,14,15	0.70	0	17,19,21	1.18	2 (11%)
4	NAG	D	702	2	14,14,15	0.66	0	17,19,21	0.78	0
4	NAG	D	701	2	14,14,15	0.75	0	17,19,21	0.95	2 (11%)

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	B	701	1	-	3/6/23/26	0/1/1/1
4	NAG	H	701	2	-	2/6/23/26	0/1/1/1
4	NAG	E	701	1	-	2/6/23/26	0/1/1/1
4	NAG	H	702	2	-	2/6/23/26	0/1/1/1
4	NAG	D	704	2	-	4/6/23/26	0/1/1/1
4	NAG	C	702	2	-	0/6/23/26	0/1/1/1
4	NAG	H	704	2	-	2/6/23/26	0/1/1/1
4	NAG	C	701	2	-	2/6/23/26	0/1/1/1
4	NAG	F	301	2	-	1/6/23/26	0/1/1/1
4	NAG	H	703	2	-	4/6/23/26	0/1/1/1
4	NAG	D	703	2	-	4/6/23/26	0/1/1/1
4	NAG	G	701	1	-	2/6/23/26	0/1/1/1
4	NAG	D	702	2	-	0/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	NAG	C1-O5-C5	5.78	119.93	112.19
4	H	702	NAG	C2-N2-C7	5.10	129.73	122.90
4	D	703	NAG	C1-O5-C5	3.88	117.38	112.19
4	H	701	NAG	C1-O5-C5	3.75	117.22	112.19
4	C	701	NAG	C1-O5-C5	3.62	117.04	112.19
4	E	701	NAG	C1-O5-C5	3.38	116.72	112.19
4	D	703	NAG	C2-N2-C7	2.73	126.55	122.90
4	H	704	NAG	C1-O5-C5	2.69	115.79	112.19
4	G	701	NAG	O5-C1-C2	-2.59	107.28	111.29
4	H	702	NAG	O5-C1-C2	-2.30	107.74	111.29
4	C	702	NAG	C2-N2-C7	2.26	125.92	122.90
4	E	701	NAG	O5-C1-C2	-2.20	107.88	111.29
4	F	301	NAG	C2-N2-C7	2.18	125.82	122.90
4	G	701	NAG	C2-N2-C7	2.18	125.82	122.90
4	D	701	NAG	O5-C1-C2	-2.15	107.97	111.29
4	D	701	NAG	C2-N2-C7	2.06	125.66	122.90
4	H	703	NAG	O5-C1-C2	-2.02	108.17	111.29
4	D	703	NAG	C3-C4-C5	-2.01	106.58	110.23
4	H	702	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	703	NAG	C4-C5-C6-O6
4	H	703	NAG	C4-C5-C6-O6
4	C	701	NAG	O5-C5-C6-O6
4	D	703	NAG	O5-C5-C6-O6
4	D	704	NAG	O5-C5-C6-O6
4	H	703	NAG	O5-C5-C6-O6
4	C	701	NAG	C4-C5-C6-O6
4	H	701	NAG	O5-C5-C6-O6
4	E	701	NAG	O5-C5-C6-O6
4	D	704	NAG	C4-C5-C6-O6
4	B	701	NAG	C8-C7-N2-C2
4	B	701	NAG	O7-C7-N2-C2
4	D	703	NAG	C8-C7-N2-C2
4	D	703	NAG	O7-C7-N2-C2
4	D	704	NAG	C8-C7-N2-C2
4	D	704	NAG	O7-C7-N2-C2
4	G	701	NAG	C8-C7-N2-C2
4	G	701	NAG	O7-C7-N2-C2
4	H	703	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	H	703	NAG	O7-C7-N2-C2
4	D	701	NAG	O5-C5-C6-O6
4	H	701	NAG	C4-C5-C6-O6
4	D	701	NAG	C4-C5-C6-O6
4	H	704	NAG	C4-C5-C6-O6
4	B	701	NAG	O5-C5-C6-O6
4	F	301	NAG	O5-C5-C6-O6
4	H	704	NAG	O5-C5-C6-O6
4	H	702	NAG	C1-C2-N2-C7
4	E	701	NAG	C4-C5-C6-O6
4	H	702	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	NAG	1	0
4	E	701	NAG	2	0
4	H	702	NAG	2	0
4	C	701	NAG	1	0
4	D	703	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

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	210/214 (98%)	0.35	16 (7%)	20	15	33, 64, 147, 190	0
1	B	212/214 (99%)	0.25	14 (6%)	24	18	31, 63, 108, 148	0
1	E	211/214 (98%)	0.47	15 (7%)	22	16	34, 64, 142, 183	0
1	G	211/214 (98%)	0.13	7 (3%)	49	40	34, 56, 112, 167	0
2	C	195/207 (94%)	0.95	22 (11%)	10	8	38, 102, 186, 235	0
2	D	195/207 (94%)	0.36	6 (3%)	51	43	36, 68, 128, 159	0
2	F	196/207 (94%)	0.90	21 (10%)	11	9	45, 86, 151, 192	0
2	H	194/207 (93%)	0.54	13 (6%)	24	18	38, 65, 146, 182	0
All	All	1624/1684 (96%)	0.49	114 (7%)	22	17	31, 69, 146, 235	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	109	ALA	4.9
2	C	132	PHE	4.8
1	E	452	ALA	4.5
1	A	452	ALA	4.5
1	B	452	ALA	4.5
1	B	301	CYS	4.4
2	D	119	GLU	4.2
2	F	113	LEU	4.0
2	F	110	ASP	3.9
1	E	285	SER	3.7
1	E	271	LEU	3.6
2	C	129	HIS	3.6
2	C	107	LEU	3.5
1	E	274	ALA	3.5
2	F	129	HIS	3.5
2	F	153	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	128	ALA	3.4
2	C	118	GLY	3.3
1	A	299	CYS	3.3
2	C	14	SER	3.3
2	H	153	HIS	3.2
2	F	121	ILE	3.2
1	E	300	GLY	3.2
2	D	5	PHE	3.2
1	G	243	HIS	3.2
1	B	241	ALA	3.1
1	A	302	TYR	3.0
2	H	109	ALA	3.0
1	A	287	LYS	3.0
1	B	343	ASN	3.0
2	D	154	PRO	3.0
1	E	242	CYS	2.9
2	H	110	ASP	2.9
1	E	407	GLY	2.9
1	A	274	ALA	2.9
2	C	150	SER	2.9
2	F	111	ARG	2.9
1	A	296	ARG	2.8
1	A	286	GLY	2.8
1	B	300	GLY	2.8
2	F	47	TYR	2.8
1	A	275	SER	2.7
2	C	125	CYS	2.7
1	A	298	LEU	2.7
2	C	121	ILE	2.7
1	A	451	LEU	2.7
2	C	103	GLY	2.6
1	A	297	ASP	2.6
1	A	272	ARG	2.6
2	H	125	CYS	2.6
1	E	284	SER	2.6
2	F	130	ILE	2.6
1	G	301	CYS	2.6
1	A	294	PRO	2.6
1	G	302	TYR	2.5
1	B	407	GLY	2.5
1	E	276	GLY	2.5
2	H	157	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	87	ARG	2.4
2	D	125	CYS	2.4
1	A	406	GLN	2.4
2	H	159	LEU	2.4
2	C	2	GLU	2.4
1	B	386	GLY	2.4
1	E	296	ARG	2.4
1	G	298	LEU	2.3
2	H	90	TYR	2.3
2	D	116	MET	2.3
2	F	6	PRO	2.3
2	F	162	VAL	2.3
1	E	363	GLU	2.3
1	G	452	ALA	2.3
1	B	282	THR	2.3
2	H	195	THR	2.3
1	G	296	ARG	2.3
2	C	72	ASN	2.3
1	E	451	LEU	2.3
2	H	98	VAL	2.3
1	E	275	SER	2.2
2	C	148	HIS	2.2
2	F	117	PRO	2.2
2	C	9	PHE	2.2
2	H	5	PHE	2.2
2	F	125	CYS	2.2
2	C	6	PRO	2.2
2	F	92	ASP	2.2
2	F	160	GLY	2.2
2	F	154	PRO	2.2
1	A	271	LEU	2.2
2	H	2	GLU	2.1
1	B	299	CYS	2.1
2	C	172	CYS	2.1
2	C	154	PRO	2.1
2	F	104	LYS	2.1
1	B	243	HIS	2.1
2	C	45	SER	2.1
2	H	166	VAL	2.1
1	A	313	GLU	2.1
1	B	298	LEU	2.1
2	C	120	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	449	ASP	2.1
2	C	51	GLY	2.1
2	F	197	ILE	2.1
1	E	273	ASP	2.1
2	C	92	ASP	2.1
1	B	312	ALA	2.1
1	E	298	LEU	2.1
2	F	182	LEU	2.1
2	D	126	SER	2.0
2	C	186	PRO	2.0
1	B	242	CYS	2.0
2	F	161	PRO	2.0
1	G	270	GLY	2.0
2	C	112	GLY	2.0

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

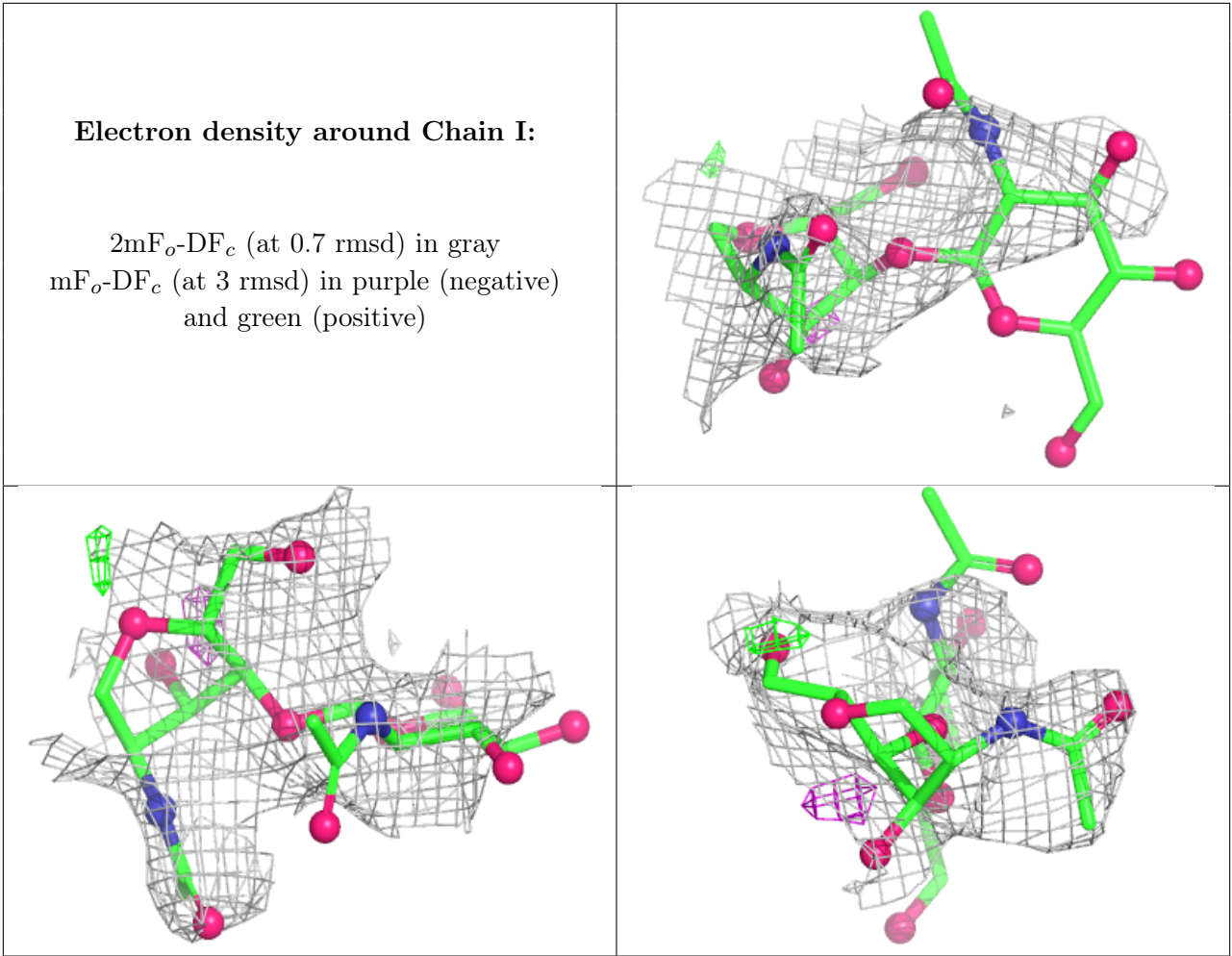
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	I	2	14/15	0.52	0.15	166,180,204,212	0
3	NAG	I	1	14/15	0.64	0.16	112,141,151,159	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 ⓘ

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	D	701	14/15	0.18	0.21	147,182,196,203	0
4	NAG	H	703	14/15	0.21	0.19	181,196,200,203	0
4	NAG	F	301	14/15	0.26	0.23	97,151,165,169	0
4	NAG	H	701	14/15	0.29	0.17	173,188,207,210	0
4	NAG	H	704	14/15	0.34	0.21	142,170,184,186	0
4	NAG	D	704	14/15	0.39	0.18	137,155,167,169	0
4	NAG	G	701	14/15	0.45	0.22	100,121,156,162	0
4	NAG	H	702	14/15	0.54	0.23	110,139,149,158	0
4	NAG	C	702	14/15	0.56	0.21	132,149,159,166	0
4	NAG	D	703	14/15	0.58	0.21	164,174,187,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	C	701	14/15	0.59	0.16	176,195,214,215	0
4	NAG	B	701	14/15	0.65	0.14	89,101,110,113	0
4	NAG	D	702	14/15	0.76	0.16	98,121,134,135	0
4	NAG	E	701	14/15	0.76	0.12	95,101,109,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.