



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:01 pm GMT

PDB ID : 2J0Y
Title : L-FICOLIN COMPLEXED TO B-1,3-D-GLUCAN
Authors : Garlatti, V.; Gaboriaud, C.
Deposited on : 2006-08-08
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

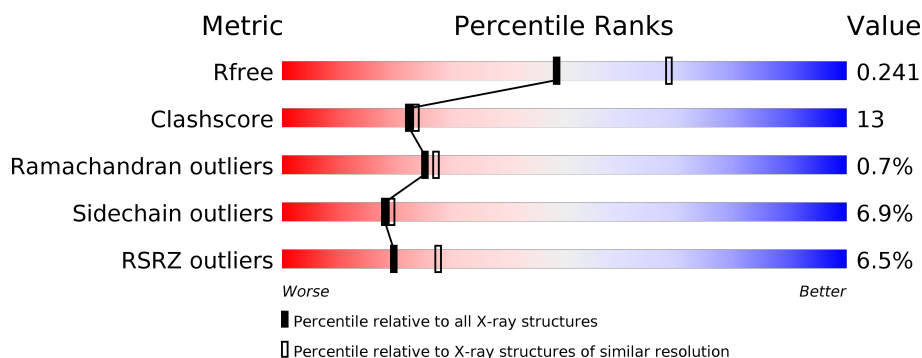
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	218	<div> <div>13%</div> <div>58%</div> <div>27%</div> <div>•</div> <div>11%</div> </div>
1	B	218	<div> <div>%</div> <div>78%</div> <div>19%</div> <div>•</div> </div>
1	C	218	<div> <div>74%</div> <div>22%</div> <div>••</div> </div>
1	D	218	<div> <div>22%</div> <div>61%</div> <div>27%</div> <div>5%</div> <div>7%</div> </div>
1	E	218	<div> <div>78%</div> <div>19%</div> <div>•</div> </div>
1	F	218	<div> <div>%</div> <div>76%</div> <div>18%</div> <div>5%</div> <div>•</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1291	-	-	-	X
5	BGC	C	1289	-	-	-	X
5	BGC	C	1291	-	-	-	X
5	BGC	F	1290	-	-	-	X
5	BGC	F	1292	-	-	-	X
7	BGC	F	1289	-	-	X	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10651 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 FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1566	988	273	297	8			
1	B	218	Total	C	N	O	S	0	0	0
			1744	1096	307	332	9			
1	C	215	Total	C	N	O	S	0	0	0
			1723	1084	303	328	8			
1	D	202	Total	C	N	O	S	0	1	0
			1631	1024	288	310	9			
1	E	218	Total	C	N	O	S	0	0	0
			1744	1096	307	332	9			
1	F	215	Total	C	N	O	S	0	1	0
			1734	1093	304	329	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	CONFLICT	UNP Q15485
A	247	THR	VAL	CONFLICT	UNP Q15485
B	168	THR	VAL	CONFLICT	UNP Q15485
B	247	THR	VAL	CONFLICT	UNP Q15485
C	168	THR	VAL	CONFLICT	UNP Q15485
C	247	THR	VAL	CONFLICT	UNP Q15485
D	168	THR	VAL	CONFLICT	UNP Q15485
D	247	THR	VAL	CONFLICT	UNP Q15485
E	168	THR	VAL	CONFLICT	UNP Q15485
E	247	THR	VAL	CONFLICT	UNP Q15485
F	168	THR	VAL	CONFLICT	UNP Q15485
F	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	C	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	E	1	Total	Ca	0	0
			1	1		

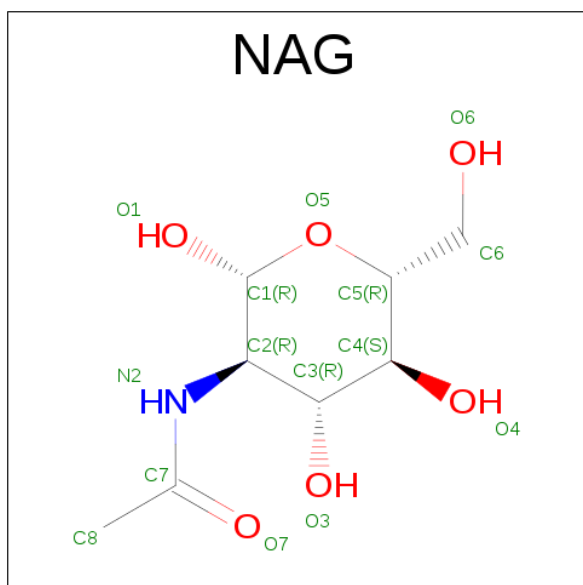
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

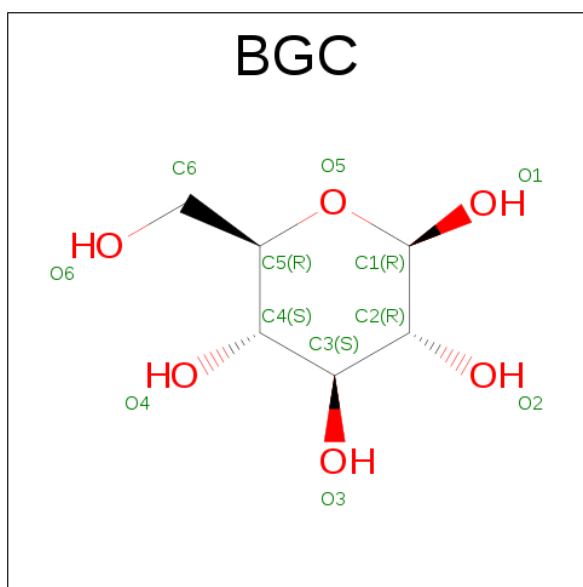
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	4	Total	C	O	0	0
			44	24	20		
5	F	4	Total	C	O	0	0
			44	24	20		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			11	6	5		

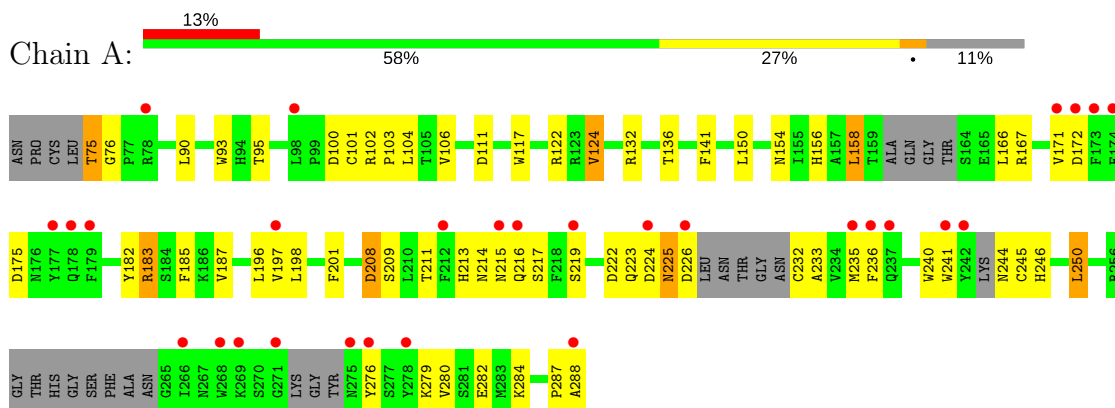
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	32	Total	O	0	0
			32	32		
8	B	61	Total	O	0	0
			61	61		
8	C	57	Total	O	0	0
			57	57		
8	D	24	Total	O	0	0
			24	24		
8	E	66	Total	O	0	0
			66	66		
8	F	54	Total	O	0	0
			54	54		

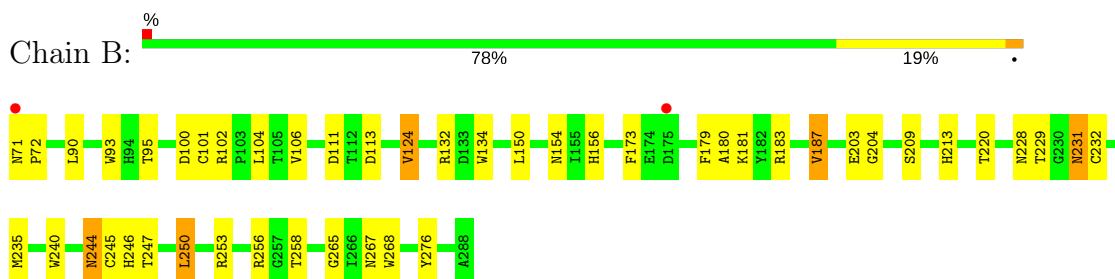
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

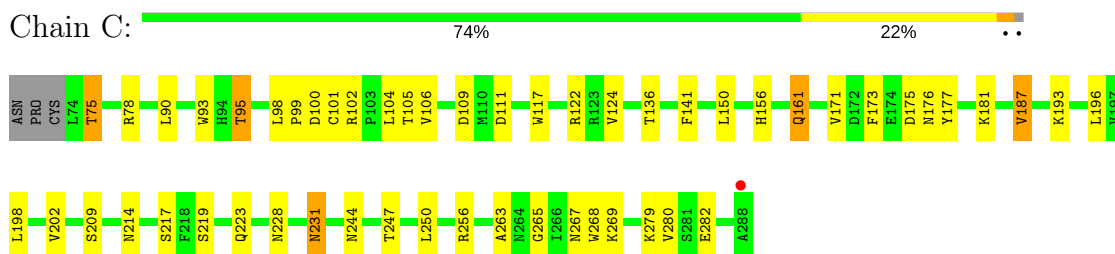
• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2

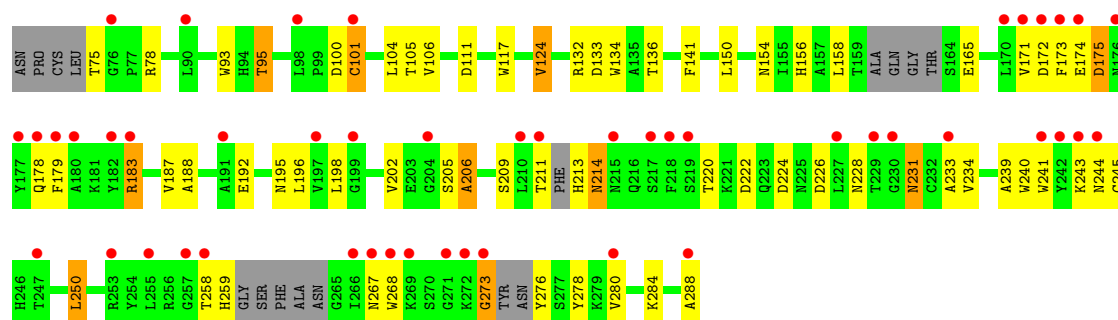


• Molecule 1: FICOLIN-2



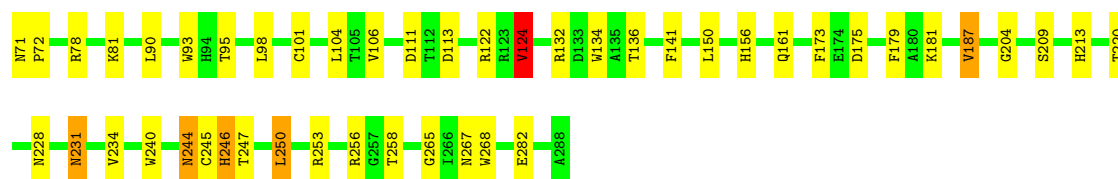
• Molecule 1: FICOLIN-2





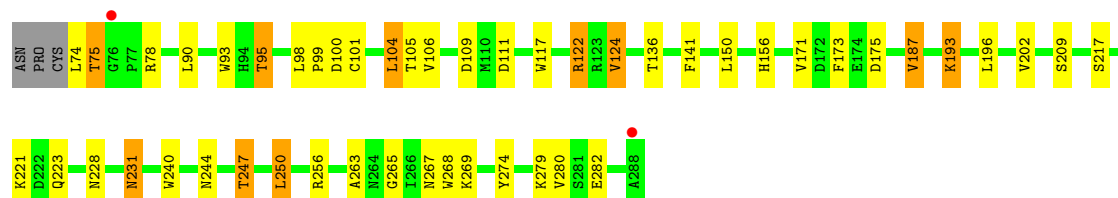
• Molecule 1: FICOLIN-2

Chain E: 78% 19% •



• Molecule 1: FICOLIN-2

Chain F: % 76% 18% 5% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.08Å 96.08Å 140.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.35 19.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.35) 98.8 (19.95-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.242 0.196 , 0.241	Depositor DCC
R_{free} test set	2990 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.470 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10651	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: BGC, CA, BMA, NAG, ACT

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	0.57	1/1605 (0.1%)	0.60	1/2164 (0.0%)
1	B	0.54	0/1792	0.66	0/2425
1	C	0.53	0/1770	0.65	0/2394
1	D	0.70	1/1671 (0.1%)	0.56	0/2253
1	E	0.52	0/1792	0.65	0/2425
1	F	0.54	0/1782	0.66	0/2410
All	All	0.57	2/10412 (0.0%)	0.63	1/14071 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	273	GLY	C-O	21.08	1.57	1.23
1	A	208	ASP	CG-OD1	8.77	1.45	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	CB-CG-OD2	-5.43	113.42	118.30

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	1566	0	1441	55	0
1	B	1744	0	1611	31	1
1	C	1723	0	1595	37	0
1	D	1631	0	1510	64	1
1	E	1744	0	1611	33	0
1	F	1734	0	1603	32	0
2	B	4	0	3	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
4	B	39	0	34	0	0
4	E	39	0	34	0	0
5	C	44	0	37	5	0
5	F	44	0	37	6	0
6	C	14	0	13	0	0
6	F	14	0	13	0	0
7	F	11	0	10	8	0
8	A	32	0	0	12	0
8	B	61	0	0	7	0
8	C	57	0	0	6	0
8	D	24	0	0	24	0
8	E	66	0	0	9	0
8	F	54	0	0	3	0
All	All	10651	0	9552	258	1

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 13.

All (258) 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:D:183:ARG:HG3	1:D:183:ARG:HH11	1.06	1.10
1:D:206:ALA:HB1	8:D:2022:HOH:O	1.57	1.05
7:F:1289:BGC:H6C1	7:F:1289:BGC:H2	1.45	0.98
1:D:220:THR:HG22	8:D:2018:HOH:O	1.63	0.98
1:B:71:ASN:N	1:B:72:PRO:HD3	1.83	0.94
1:D:183:ARG:CG	1:D:183:ARG:HH11	1.80	0.94
1:E:124:VAL:HB	8:E:2010:HOH:O	1.67	0.93
1:D:214:ASN:HB2	8:D:2017:HOH:O	1.67	0.92
1:E:253:ARG:HD3	8:E:2050:HOH:O	1.69	0.90
1:F:223:GLN:CD	5:F:1290:BGC:H6C2	1.93	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ASN:N	1:E:72:PRO:HD3	1.89	0.88
1:C:75:THR:HA	8:C:2002:HOH:O	1.70	0.88
1:A:240:TRP:HD1	8:A:2022:HOH:O	1.55	0.87
1:A:224:ASP:O	1:A:225:ASN:ND2	2.08	0.86
1:A:214:ASN:ND2	1:A:215:ASN:N	2.24	0.86
1:D:198:LEU:H	1:D:214:ASN:HD21	1.24	0.85
1:D:239:ALA:HB1	8:D:2018:HOH:O	1.76	0.85
1:D:211:THR:HA	8:D:2017:HOH:O	1.76	0.84
1:E:228:ASN:HD22	1:E:244:ASN:ND2	1.75	0.84
1:A:214:ASN:HD22	1:A:215:ASN:H	1.24	0.84
1:A:183:ARG:HB2	1:A:183:ARG:HH11	1.43	0.84
1:D:183:ARG:HG3	1:D:183:ARG:NH1	1.85	0.83
1:A:201:PHE:CD1	8:A:2019:HOH:O	2.32	0.83
1:A:214:ASN:HD22	1:A:215:ASN:N	1.77	0.81
1:B:228:ASN:HD22	1:B:244:ASN:ND2	1.77	0.81
1:D:239:ALA:CB	8:D:2018:HOH:O	2.31	0.78
1:F:221:LYS:NZ	7:F:1289:BGC:H6C2	1.97	0.78
1:D:198:LEU:HB3	1:D:214:ASN:ND2	1.99	0.78
1:A:219:SER:OG	1:A:225:ASN:HB2	1.83	0.77
1:A:211:THR:HG22	8:A:2020:HOH:O	1.85	0.77
1:B:228:ASN:HD22	1:B:244:ASN:HD22	1.33	0.76
7:F:1289:BGC:C6	7:F:1289:BGC:H2	2.15	0.76
1:C:223:GLN:CD	5:C:1289:BGC:H6C2	2.06	0.75
1:A:183:ARG:HB2	1:A:183:ARG:NH1	2.01	0.75
1:B:71:ASN:N	1:B:72:PRO:CD	2.49	0.75
1:E:228:ASN:HD22	1:E:244:ASN:HD22	1.34	0.74
1:B:101:CYS:SG	8:B:2005:HOH:O	2.46	0.73
1:A:240:TRP:CD1	8:A:2022:HOH:O	2.34	0.71
1:A:201:PHE:HD1	8:A:2019:HOH:O	1.73	0.71
1:D:213:HIS:N	1:D:243:LYS:HZ2	1.88	0.71
1:F:223:GLN:OE1	5:F:1290:BGC:H6C2	1.91	0.70
1:C:198:LEU:H	1:C:214:ASN:ND2	1.88	0.70
1:D:205:SER:O	1:D:206:ALA:HB2	1.91	0.70
1:D:172:ASP:HB3	8:D:2012:HOH:O	1.90	0.69
1:C:100:ASP:O	1:C:101:CYS:HB2	1.93	0.69
1:D:178:GLN:C	8:D:2014:HOH:O	2.30	0.69
1:C:175:ASP:OD2	1:C:279:LYS:NZ	2.23	0.68
1:D:278:TYR:HD2	8:D:2012:HOH:O	1.77	0.68
7:F:1289:BGC:H6C1	7:F:1289:BGC:C2	2.20	0.67
1:C:223:GLN:OE1	5:C:1289:BGC:H6C2	1.95	0.67
1:D:173:PHE:N	8:D:2013:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:TRP:HA	1:D:220:THR:HG21	1.77	0.66
1:A:214:ASN:ND2	1:A:215:ASN:H	1.92	0.65
1:D:209:SER:HB2	1:D:268:TRP:CE2	2.32	0.65
1:E:124:VAL:CG2	8:E:2010:HOH:O	2.45	0.64
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.32	0.64
1:A:224:ASP:O	1:A:225:ASN:CG	2.35	0.64
1:E:71:ASN:N	1:E:72:PRO:CD	2.60	0.64
7:F:1289:BGC:C6	7:F:1289:BGC:C2	2.76	0.64
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.33	0.63
1:D:211:THR:CA	8:D:2017:HOH:O	2.42	0.63
1:C:161:GLN:H	1:C:161:GLN:HE21	1.45	0.63
1:E:124:VAL:CB	8:E:2010:HOH:O	2.35	0.63
1:F:75:THR:HA	8:F:2003:HOH:O	1.99	0.62
1:C:231:ASN:C	1:C:231:ASN:HD22	2.03	0.62
1:A:111:ASP:HB2	8:A:2006:HOH:O	2.00	0.62
1:A:279:LYS:NZ	8:A:2032:HOH:O	2.32	0.62
1:A:214:ASN:HB2	8:A:2023:HOH:O	1.99	0.61
1:D:240:TRP:CH2	1:D:250:LEU:HB2	2.36	0.61
1:F:221:LYS:HZ1	7:F:1289:BGC:H6C2	1.64	0.61
1:D:244:ASN:N	1:D:245:CYS:HA	2.15	0.61
1:C:75:THR:HG23	8:C:2001:HOH:O	1.99	0.61
1:D:258:THR:HG23	1:D:276:TYR:HD2	1.65	0.61
1:F:231:ASN:HD22	1:F:231:ASN:C	2.04	0.61
1:C:102:ARG:HG2	8:C:2008:HOH:O	2.00	0.60
1:E:228:ASN:ND2	1:E:244:ASN:ND2	2.48	0.60
5:F:1292:BGC:O4	5:F:1293:BGC:O5	2.15	0.60
1:A:183:ARG:CB	1:A:183:ARG:HH11	2.13	0.60
1:B:228:ASN:ND2	1:B:244:ASN:ND2	2.49	0.60
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.37	0.59
1:F:228:ASN:ND2	1:F:244:ASN:OD1	2.31	0.59
1:C:198:LEU:H	1:C:214:ASN:HD21	1.49	0.59
1:D:198:LEU:N	1:D:214:ASN:HD21	1.98	0.59
1:E:78:ARG:NH2	1:E:98:LEU:O	2.35	0.59
1:D:132:ARG:NH2	1:E:111:ASP:OD1	2.35	0.58
1:D:258:THR:HA	1:D:276:TYR:HA	1.86	0.58
1:A:100:ASP:O	1:A:101:CYS:HB2	2.03	0.58
1:C:181:LYS:HE2	8:C:2027:HOH:O	2.03	0.58
1:D:211:THR:C	8:D:2015:HOH:O	2.41	0.58
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.86	0.57
1:E:101:CYS:HB2	8:E:2003:HOH:O	2.03	0.57
1:F:99:PRO:HG2	8:F:2025:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ASP:OD2	1:D:228:ASN:O	2.23	0.57
1:A:171:VAL:HB	1:A:280:VAL:HB	1.87	0.57
1:B:102:ARG:NH2	1:B:154:ASN:OD1	2.37	0.57
1:D:179:PHE:N	8:D:2014:HOH:O	2.38	0.57
1:A:222:ASP:O	1:A:223:GLN:HG2	2.04	0.56
1:D:273:GLY:HA2	8:D:2023:HOH:O	2.07	0.55
1:E:113:ASP:OD2	1:E:181:LYS:NZ	2.27	0.55
1:D:198:LEU:H	1:D:214:ASN:ND2	2.01	0.55
1:D:211:THR:O	1:D:213:HIS:N	2.40	0.55
1:B:244:ASN:N	1:B:245:CYS:HA	2.22	0.55
1:C:171:VAL:HB	1:C:280:VAL:HB	1.89	0.55
1:E:244:ASN:N	1:E:245:CYS:HA	2.22	0.55
1:C:263:ALA:HA	1:C:267:ASN:ND2	2.22	0.54
1:D:211:THR:C	8:D:2017:HOH:O	2.45	0.54
1:C:176:ASN:HB3	1:D:202:VAL:O	2.08	0.53
1:D:231:ASN:HD22	1:D:231:ASN:C	2.11	0.53
1:D:171:VAL:HB	1:D:280:VAL:HB	1.89	0.53
1:A:244:ASN:N	1:A:245:CYS:HA	2.23	0.53
1:E:81:LYS:HE3	8:E:2001:HOH:O	2.08	0.53
7:F:1289:BGC:H3	5:F:1293:BGC:H3	1.91	0.53
1:A:132:ARG:NH2	1:B:111:ASP:OD1	2.39	0.53
5:C:1290:BGC:HD	5:C:1291:BGC:C1	2.20	0.53
1:E:265:GLY:H	1:E:267:ASN:HD21	1.57	0.52
1:D:205:SER:O	1:D:206:ALA:CB	2.57	0.52
1:B:258:THR:HG22	1:B:276:TYR:HD2	1.74	0.52
1:B:229:THR:CG2	8:B:2042:HOH:O	2.58	0.52
5:F:1291:BGC:HD	5:F:1292:BGC:C1	2.22	0.52
1:B:240:TRP:CH2	1:B:250:LEU:HB2	2.45	0.52
1:F:175:ASP:OD2	1:F:279:LYS:NZ	2.34	0.52
1:B:229:THR:HG21	8:B:2042:HOH:O	2.10	0.52
1:C:193:LYS:HB3	1:C:217:SER:HB3	1.90	0.51
1:D:154:ASN:O	1:D:158:LEU:HB2	2.11	0.51
1:C:247:THR:HG23	1:C:269:LYS:HB3	1.93	0.51
1:E:231:ASN:ND2	1:E:234:VAL:H	2.09	0.51
1:A:111:ASP:CB	8:A:2006:HOH:O	2.56	0.51
1:A:222:ASP:O	1:A:223:GLN:CG	2.59	0.50
5:F:1291:BGC:O4	5:F:1292:BGC:C1	2.59	0.50
1:B:101:CYS:CB	8:B:2005:HOH:O	2.60	0.50
5:C:1290:BGC:O4	5:C:1291:BGC:C1	2.59	0.50
1:A:287:PRO:O	1:A:288:ALA:C	2.50	0.50
1:B:102:ARG:HD3	8:B:2004:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.46	0.49
1:D:259:HIS:HE1	1:D:267:ASN:HD21	1.60	0.49
1:F:263:ALA:HA	1:F:267:ASN:ND2	2.28	0.49
1:D:231:ASN:HD21	1:D:233:ALA:HB3	1.78	0.49
1:F:221:LYS:NZ	7:F:1289:BGC:C6	2.74	0.49
1:C:228:ASN:ND2	1:C:244:ASN:OD1	2.40	0.48
1:B:265:GLY:H	1:B:267:ASN:HD21	1.60	0.48
1:C:122:ARG:HD2	1:C:282:GLU:OE2	2.13	0.48
1:E:240:TRP:CH2	1:E:250:LEU:HB2	2.48	0.48
1:F:100:ASP:O	1:F:101:CYS:HB2	2.13	0.48
1:B:231:ASN:HD22	1:B:231:ASN:C	2.17	0.48
1:D:196:LEU:HB2	1:D:241:TRP:CD1	2.49	0.48
1:B:93:TRP:HA	1:B:106:VAL:O	2.13	0.48
1:B:156:HIS:HD2	1:B:187:VAL:O	1.96	0.48
1:E:231:ASN:HD22	1:E:231:ASN:C	2.17	0.48
1:F:240:TRP:CH2	1:F:250:LEU:HB2	2.49	0.48
1:E:93:TRP:HA	1:E:106:VAL:O	2.14	0.47
1:F:98:LEU:HB3	1:F:99:PRO:CD	2.44	0.47
1:B:101:CYS:HB2	8:B:2005:HOH:O	2.13	0.47
1:C:209:SER:HB2	1:C:268:TRP:CE2	2.49	0.47
1:D:156:HIS:HD2	1:D:187:VAL:O	1.97	0.47
1:A:214:ASN:CB	8:A:2023:HOH:O	2.61	0.47
1:C:247:THR:HG21	8:C:2029:HOH:O	2.14	0.47
1:D:231:ASN:N	8:D:2020:HOH:O	2.47	0.47
1:E:173:PHE:CE1	1:E:256:ARG:HA	2.50	0.47
1:F:269:LYS:HD2	1:F:274:TYR:CE2	2.49	0.47
1:A:93:TRP:HA	1:A:106:VAL:O	2.15	0.47
1:A:213:HIS:HE1	1:A:246:HIS:CB	2.27	0.47
1:D:165:GLU:HB3	1:D:288:ALA:HB2	1.95	0.47
1:D:93:TRP:HA	1:D:106:VAL:O	2.15	0.47
1:E:156:HIS:HD2	1:E:187:VAL:O	1.96	0.47
1:A:213:HIS:HE1	1:A:246:HIS:HB2	1.80	0.47
1:D:100:ASP:O	1:D:101[B]:CYS:HB2	2.14	0.47
1:C:78:ARG:NH2	1:C:98:LEU:O	2.49	0.46
1:D:174:GLU:O	1:D:175:ASP:HB2	2.15	0.46
1:F:171:VAL:HB	1:F:280:VAL:HB	1.97	0.46
1:A:154:ASN:O	1:A:158:LEU:HB2	2.15	0.46
1:C:95:THR:HA	1:C:105:THR:HA	1.96	0.46
1:C:209:SER:HB3	1:C:247:THR:HG22	1.98	0.46
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.97	0.46
1:B:113:ASP:OD2	1:B:181:LYS:NZ	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:HD2	1:A:187:VAL:O	1.99	0.46
1:B:173:PHE:CE1	1:B:256:ARG:HA	2.51	0.45
1:C:156:HIS:HD2	1:C:187:VAL:O	1.99	0.45
1:A:75:THR:CG2	1:A:76:GLY:N	2.80	0.45
1:A:226:ASP:CG	8:A:2025:HOH:O	2.53	0.45
1:C:93:TRP:HA	1:C:106:VAL:O	2.16	0.45
1:F:136:THR:HG22	1:F:141:PHE:CD1	2.52	0.45
1:F:109:ASP:HB3	1:F:117:TRP:HB2	1.97	0.45
1:F:93:TRP:HA	1:F:106:VAL:O	2.16	0.45
1:F:78:ARG:NH2	1:F:98:LEU:O	2.50	0.45
1:C:109:ASP:HB3	1:C:117:TRP:HB2	1.98	0.45
1:E:81:LYS:CE	8:E:2001:HOH:O	2.62	0.45
1:F:209:SER:HB3	1:F:247:THR:HG22	1.99	0.45
1:E:209:SER:HB2	1:E:268:TRP:CD2	2.52	0.44
1:A:201:PHE:HB2	1:A:208:ASP:OD1	2.17	0.44
1:A:222:ASP:N	1:A:222:ASP:OD1	2.47	0.44
1:B:179:PHE:CE2	1:B:204:GLY:HA2	2.53	0.44
1:A:211:THR:O	1:A:214:ASN:HB3	2.18	0.44
1:A:122:ARG:NH1	1:A:282:GLU:OE2	2.40	0.44
1:E:124:VAL:HG23	8:E:2010:HOH:O	2.14	0.44
1:C:247:THR:CG2	8:C:2029:HOH:O	2.66	0.44
1:E:134:TRP:HA	1:E:220:THR:HG21	1.98	0.44
1:E:161:GLN:NE2	8:E:2024:HOH:O	2.50	0.44
1:F:104:LEU:HD13	1:F:106:VAL:CG1	2.48	0.44
1:F:74:LEU:HB3	8:F:2002:HOH:O	2.18	0.44
1:F:156:HIS:HD2	1:F:187:VAL:O	2.01	0.43
1:B:253:ARG:HD2	8:B:2049:HOH:O	2.17	0.43
1:E:122:ARG:HD2	1:E:282:GLU:OE2	2.18	0.43
1:C:171:VAL:HG22	1:C:177:TYR:CD2	2.53	0.43
1:E:132:ARG:HH22	1:F:111:ASP:CG	2.21	0.43
1:F:173:PHE:CZ	1:F:256:ARG:HA	2.54	0.43
1:F:193:LYS:HB3	1:F:217:SER:HB3	1.99	0.43
1:F:95:THR:HA	1:F:105:THR:HA	1.99	0.43
1:D:133:ASP:HB2	1:D:222:ASP:CG	2.39	0.43
1:D:188:ALA:HB1	1:D:192:GLU:OE2	2.19	0.43
1:A:196:LEU:HB2	1:A:241:TRP:CD1	2.53	0.43
1:D:78:ARG:HE	1:D:78:ARG:HB2	1.39	0.43
1:A:214:ASN:ND2	1:A:214:ASN:C	2.69	0.43
1:E:179:PHE:CE2	1:E:204:GLY:HA2	2.54	0.43
1:A:136:THR:HG22	1:A:141:PHE:CD1	2.54	0.42
1:A:172:ASP:HB2	1:A:276:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:209:SER:HB2	1:F:268:TRP:CE2	2.54	0.42
1:F:122:ARG:HD2	1:F:282:GLU:OE2	2.19	0.42
1:A:102:ARG:HA	1:A:103:PRO:HD3	1.92	0.42
1:A:124:VAL:HG23	1:A:280:VAL:HG22	2.01	0.42
1:A:166:LEU:HB2	1:A:185:PHE:CB	2.48	0.42
1:B:134:TRP:HA	1:B:220:THR:HG21	2.02	0.42
1:D:172:ASP:N	8:D:2012:HOH:O	2.52	0.42
1:A:232:CYS:O	1:A:235:MET:N	2.53	0.42
1:A:117:TRP:HB3	1:A:284:LYS:HB2	2.02	0.42
1:C:193:LYS:HE2	1:C:217:SER:OG	2.19	0.42
1:D:239:ALA:HB2	8:D:2018:HOH:O	2.10	0.42
1:A:217:SER:O	1:A:241:TRP:HA	2.19	0.42
1:C:173:PHE:CZ	1:C:256:ARG:HA	2.55	0.42
1:F:265:GLY:H	1:F:267:ASN:HD21	1.68	0.42
1:D:136:THR:HG22	1:D:141:PHE:CD1	2.55	0.42
1:A:182:TYR:CE2	1:A:198:LEU:HD21	2.56	0.41
1:D:224:ASP:HA	8:D:2019:HOH:O	2.19	0.41
5:C:1290:BGC:O6	5:C:1290:BGC:O4	2.31	0.41
1:D:214:ASN:CB	8:D:2017:HOH:O	2.44	0.41
1:D:214:ASN:CG	8:D:2016:HOH:O	2.58	0.41
1:B:132:ARG:HH22	1:C:111:ASP:CG	2.23	0.41
1:D:111:ASP:HB2	8:D:2004:HOH:O	2.21	0.41
1:D:183:ARG:NH1	1:D:183:ARG:CG	2.51	0.41
1:C:173:PHE:CE1	1:C:256:ARG:HA	2.55	0.41
1:D:278:TYR:CD2	8:D:2012:HOH:O	2.56	0.41
1:B:100:ASP:O	1:B:101:CYS:HB2	2.19	0.41
1:B:213:HIS:CE1	1:B:246:HIS:HA	2.56	0.41
1:D:231:ASN:ND2	1:D:234:VAL:H	2.19	0.41
1:D:133:ASP:HB2	1:D:222:ASP:OD2	2.21	0.41
1:C:136:THR:HG22	1:C:141:PHE:CD1	2.56	0.41
1:B:232:CYS:HA	1:B:235:MET:HE3	2.03	0.41
1:C:161:GLN:N	1:C:161:GLN:HE21	2.15	0.41
1:C:265:GLY:H	1:C:267:ASN:HD21	1.69	0.41
1:D:117:TRP:HB3	1:D:284:LYS:HB2	2.03	0.41
1:D:171:VAL:C	8:D:2012:HOH:O	2.59	0.41
1:B:180:ALA:HA	1:B:204:GLY:HA3	2.03	0.41
1:E:136:THR:HG22	1:E:141:PHE:CD1	2.56	0.41
1:A:224:ASP:O	1:A:225:ASN:CB	2.69	0.40
1:A:236:PHE:CD1	1:A:246:HIS:NE2	2.76	0.40
1:A:232:CYS:O	1:A:233:ALA:C	2.59	0.40
1:A:167:ARG:NH1	8:A:2017:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:THR:HA	1:D:105:THR:HA	2.04	0.40
1:E:213:HIS:CE1	1:E:246:HIS:HA	2.56	0.40

All (1) 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:B:183:ARG:NH1	1:D:288:ALA:O[3_455]	2.12	0.08

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	181/218 (83%)	162 (90%)	17 (9%)	2 (1%)	17	16
1	B	216/218 (99%)	205 (95%)	10 (5%)	1 (0%)	32	37
1	C	213/218 (98%)	199 (93%)	13 (6%)	1 (0%)	32	37
1	D	193/218 (88%)	171 (89%)	19 (10%)	3 (2%)	11	9
1	E	216/218 (99%)	203 (94%)	12 (6%)	1 (0%)	32	37
1	F	214/218 (98%)	201 (94%)	12 (6%)	1 (0%)	32	37
All	All	1233/1308 (94%)	1141 (92%)	83 (7%)	9 (1%)	25	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	D	206	ALA
1	D	195	ASN
1	A	124	VAL
1	B	124	VAL
1	C	124	VAL

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Mol	Chain	Res	Type
1	D	124	VAL
1	E	124	VAL
1	F	124	VAL

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	165/183 (90%)	153 (93%)	12 (7%)	16	18
1	B	183/183 (100%)	172 (94%)	11 (6%)	22	26
1	C	180/183 (98%)	168 (93%)	12 (7%)	19	21
1	D	172/183 (94%)	160 (93%)	12 (7%)	18	19
1	E	183/183 (100%)	170 (93%)	13 (7%)	17	18
1	F	181/183 (99%)	167 (92%)	14 (8%)	15	16
All	All	1064/1098 (97%)	990 (93%)	74 (7%)	18	19

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
1	A	150	LEU
1	A	158	LEU
1	A	175	ASP
1	A	183	ARG
1	A	197	VAL
1	A	209	SER
1	A	216	GLN
1	A	250	LEU
1	B	90	LEU
1	B	95	THR
1	B	104	LEU

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Mol	Chain	Res	Type
1	B	124	VAL
1	B	150	LEU
1	B	187	VAL
1	B	203	GLU
1	B	231	ASN
1	B	244	ASN
1	B	247	THR
1	B	250	LEU
1	C	75	THR
1	C	90	LEU
1	C	95	THR
1	C	104	LEU
1	C	150	LEU
1	C	161	GLN
1	C	187	VAL
1	C	196	LEU
1	C	202	VAL
1	C	219	SER
1	C	231	ASN
1	C	250	LEU
1	D	75	THR
1	D	95	THR
1	D	101[A]	CYS
1	D	101[B]	CYS
1	D	104	LEU
1	D	124	VAL
1	D	150	LEU
1	D	175	ASP
1	D	183	ARG
1	D	214	ASN
1	D	231	ASN
1	D	250	LEU
1	E	90	LEU
1	E	95	THR
1	E	104	LEU
1	E	124	VAL
1	E	150	LEU
1	E	175	ASP
1	E	187	VAL
1	E	231	ASN
1	E	244	ASN
1	E	246	HIS

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Mol	Chain	Res	Type
1	E	247	THR
1	E	250	LEU
1	E	258	THR
1	F	75	THR
1	F	90	LEU
1	F	95	THR
1	F	104	LEU
1	F	122	ARG
1	F	124	VAL
1	F	150	LEU
1	F	187	VAL
1	F	193	LYS
1	F	196	LEU
1	F	202	VAL
1	F	231	ASN
1	F	247	THR
1	F	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	156	HIS
1	A	176	ASN
1	A	195	ASN
1	A	214	ASN
1	A	225	ASN
1	B	139	GLN
1	B	156	HIS
1	B	223	GLN
1	B	231	ASN
1	B	244	ASN
1	B	246	HIS
1	B	267	ASN
1	B	275	ASN
1	C	139	GLN
1	C	156	HIS
1	C	161	GLN
1	C	214	ASN
1	C	216	GLN
1	C	231	ASN
1	C	267	ASN

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Mol	Chain	Res	Type
1	D	139	GLN
1	D	156	HIS
1	D	195	ASN
1	D	214	ASN
1	D	228	ASN
1	D	231	ASN
1	D	267	ASN
1	E	139	GLN
1	E	156	HIS
1	E	161	GLN
1	E	231	ASN
1	E	244	ASN
1	E	246	HIS
1	E	267	ASN
1	E	275	ASN
1	F	139	GLN
1	F	156	HIS
1	F	195	ASN
1	F	216	GLN
1	F	231	ASN
1	F	267	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 ⓘ

14 carbohydrates 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	1291	1,4	14,14,15	0.82	0	15,19,21	1.04	0
4	NAG	B	1292	4	14,14,15	0.63	0	15,19,21	0.91	0
4	BMA	B	1293	4	11,11,12	0.78	0	13,15,17	1.26	2 (15%)
5	BGC	C	1289	5	11,11,12	0.84	0	13,15,17	1.52	4 (30%)
5	BGC	C	1290	5	11,11,12	0.69	0	13,15,17	2.55	5 (38%)
5	BGC	C	1291	5	11,11,12	0.61	0	13,15,17	1.66	3 (23%)
5	BGC	C	1292	5	11,11,12	0.61	0	13,15,17	2.01	6 (46%)
4	NAG	E	1290	1,4	14,14,15	0.76	0	15,19,21	1.35	2 (13%)
4	NAG	E	1291	4	14,14,15	0.55	0	15,19,21	1.04	1 (6%)
4	BMA	E	1292	4	11,11,12	0.43	0	13,15,17	2.07	2 (15%)
5	BGC	F	1290	5	11,11,12	0.76	0	13,15,17	1.64	4 (30%)
5	BGC	F	1291	5	11,11,12	0.69	0	13,15,17	2.44	5 (38%)
5	BGC	F	1292	5	11,11,12	0.60	0	13,15,17	1.23	1 (7%)
5	BGC	F	1293	5	11,11,12	0.64	0	13,15,17	1.74	3 (23%)

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	1291	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1292	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1293	4	-	0/2/19/22	0/1/1/1
5	BGC	C	1289	5	-	0/2/19/22	0/1/1/1
5	BGC	C	1290	5	-	0/2/19/22	0/1/1/1
5	BGC	C	1291	5	-	0/2/19/22	0/1/1/1
5	BGC	C	1292	5	-	0/2/19/22	0/1/1/1
4	NAG	E	1290	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1291	4	-	0/6/23/26	0/1/1/1
4	BMA	E	1292	4	-	0/2/19/22	0/1/1/1
5	BGC	F	1290	5	-	0/2/19/22	0/1/1/1
5	BGC	F	1291	5	-	0/2/19/22	0/1/1/1
5	BGC	F	1292	5	-	0/2/19/22	0/1/1/1
5	BGC	F	1293	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1290	BGC	C2-C3-C4	-5.19	101.82	110.88
5	F	1291	BGC	C2-C3-C4	-4.25	103.46	110.88
5	F	1293	BGC	C6-C5-C4	-3.19	105.53	113.00
5	F	1290	BGC	O3-C3-C2	-3.10	104.39	110.02
5	C	1292	BGC	O5-C1-C2	-2.91	106.23	110.79
4	E	1290	NAG	O5-C1-C2	-2.87	107.49	111.47
5	C	1291	BGC	C2-C3-C4	-2.86	105.88	110.88
5	C	1291	BGC	O3-C3-C2	-2.80	104.93	110.02
5	C	1290	BGC	C3-C4-C5	-2.77	105.34	110.22
5	F	1293	BGC	O5-C1-C2	-2.61	106.70	110.79
4	E	1291	NAG	O4-C4-C3	-2.30	105.35	110.36
5	F	1292	BGC	O3-C3-C2	-2.28	105.88	110.02
5	C	1292	BGC	C6-C5-C4	-2.27	107.69	113.00
5	F	1290	BGC	C2-C3-C4	-2.25	106.95	110.88
5	C	1289	BGC	O3-C3-C2	-2.23	105.96	110.02
4	B	1293	BMA	O5-C1-C2	-2.16	107.41	110.79
5	F	1291	BGC	C6-C5-C4	-2.14	107.99	113.00
5	C	1289	BGC	C2-C3-C4	-2.10	107.21	110.88
5	C	1290	BGC	C6-C5-C4	-2.10	108.09	113.00
5	C	1291	BGC	C6-C5-C4	-2.08	108.14	113.00
5	F	1291	BGC	C3-C4-C5	-2.05	106.61	110.22
5	C	1292	BGC	O3-C3-C4	-2.02	105.97	110.36
5	F	1290	BGC	C3-C4-C5	2.21	114.12	110.22
5	C	1289	BGC	C1-O5-C5	2.29	115.32	112.17
5	F	1290	BGC	C1-O5-C5	2.29	115.32	112.17
4	E	1290	NAG	C1-O5-C5	2.29	115.32	112.17
4	B	1293	BMA	C1-C2-C3	2.35	112.63	109.65
5	C	1289	BGC	O2-C2-C3	2.49	115.07	110.17
5	C	1292	BGC	C2-C3-C4	2.63	115.46	110.88
5	C	1292	BGC	C1-C2-C3	2.65	113.01	109.65
4	E	1292	BMA	C3-C4-C5	2.97	115.45	110.22
5	C	1290	BGC	O2-C2-C1	3.15	115.58	109.18
5	F	1293	BGC	C3-C4-C5	3.21	115.87	110.22
5	C	1292	BGC	C3-C4-C5	3.90	117.08	110.22
5	F	1291	BGC	O2-C2-C1	4.20	117.72	109.18
5	F	1291	BGC	C1-O5-C5	5.20	119.34	112.17
5	C	1290	BGC	C1-O5-C5	5.50	119.75	112.17
4	E	1292	BMA	C1-O5-C5	6.12	120.60	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1289	BGC	2	0
5	C	1290	BGC	3	0
5	C	1291	BGC	2	0
5	F	1290	BGC	2	0
5	F	1291	BGC	2	0
5	F	1292	BGC	3	0
5	F	1293	BGC	2	0

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	B	1289	-	1,3,3	1.36	0	0,3,3	0.00	-
6	NAG	C	1295	1	14,14,15	0.63	0	15,19,21	0.73	0
7	BGC	F	1289	-	11,11,12	0.53	0	13,15,17	1.30	2 (15%)
6	NAG	F	1296	1	14,14,15	0.62	0	15,19,21	1.07	1 (6%)

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	ACT	B	1289	-	-	0/0/0/0	0/0/0/0
6	NAG	C	1295	1	-	0/6/23/26	0/1/1/1
7	BGC	F	1289	-	-	0/2/19/22	0/1/1/1
6	NAG	F	1296	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	F	1289	BGC	C1-C2-C3	-2.09	107.00	109.65
7	F	1289	BGC	O4-C4-C5	2.16	114.73	109.28
6	F	1296	NAG	C4-C3-C2	2.31	114.40	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1289	BGC	8	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	193/218 (88%)	0.83	29 (15%) 3 4	42, 46, 56, 59	0
1	B	218/218 (100%)	-0.30	2 (0%) 84 91	38, 45, 54, 62	0
1	C	215/218 (98%)	-0.32	1 (0%) 90 95	39, 45, 56, 67	0
1	D	202/218 (92%)	1.03	48 (23%) 1 1	42, 45, 50, 53	0
1	E	218/218 (100%)	-0.31	0 100 100	38, 45, 54, 61	0
1	F	215/218 (98%)	-0.29	2 (0%) 84 91	39, 45, 55, 68	0
All	All	1261/1308 (96%)	0.08	82 (6%) 20 27	38, 45, 54, 68	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	4.9
1	D	268	TRP	4.8
1	D	227	LEU	4.8
1	D	174	GLU	4.7
1	D	229	THR	4.6
1	D	255	LEU	4.6
1	A	275	ASN	4.2
1	D	258	THR	4.1
1	A	268	TRP	4.1
1	A	173	PHE	3.9
1	D	171	VAL	3.7
1	D	178	GLN	3.6
1	D	271	GLY	3.6
1	D	191	ALA	3.5
1	A	78	ARG	3.4
1	D	273	GLY	3.3
1	D	197	VAL	3.3
1	D	218	PHE	3.3
1	D	211	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	215	ASN	3.2
1	D	230	GLY	3.2
1	D	199	GLY	3.2
1	D	241	TRP	3.1
1	D	288	ALA	3.1
1	A	172	ASP	3.1
1	D	176	ASN	3.1
1	A	269	LYS	3.1
1	A	226	ASP	3.0
1	A	278	TYR	2.9
1	D	242	TYR	2.9
1	D	210	LEU	2.9
1	A	271	GLY	2.8
1	D	269	LYS	2.8
1	A	242	TYR	2.8
1	C	288	ALA	2.8
1	D	233	ALA	2.8
1	A	224	ASP	2.8
1	A	177	TYR	2.7
1	A	288	ALA	2.7
1	F	76	GLY	2.7
1	A	235	MET	2.7
1	D	253	ARG	2.7
1	D	170	LEU	2.7
1	D	243	LYS	2.7
1	D	257	GLY	2.7
1	A	197	VAL	2.7
1	A	266	ILE	2.6
1	A	171	VAL	2.6
1	A	216	GLN	2.6
1	D	182	TYR	2.6
1	D	266	ILE	2.6
1	D	267	ASN	2.6
1	A	219	SER	2.6
1	D	98	LEU	2.5
1	D	219	SER	2.5
1	A	237	GLN	2.5
1	D	76	GLY	2.5
1	D	280	VAL	2.5
1	B	71	ASN	2.5
1	F	288	ALA	2.5
1	A	276	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	2.4
1	D	204	GLY	2.4
1	B	175	ASP	2.4
1	D	217	SER	2.3
1	A	236	PHE	2.3
1	D	173	PHE	2.3
1	D	90	LEU	2.2
1	D	180	ALA	2.2
1	D	183	ARG	2.2
1	D	244	ASN	2.2
1	A	215	ASN	2.2
1	D	247	THR	2.2
1	A	178	GLN	2.2
1	A	241	TRP	2.2
1	D	272	LYS	2.1
1	A	179	PHE	2.1
1	D	179	PHE	2.1
1	D	172	ASP	2.1
1	D	177	TYR	2.0
1	D	101[A]	CYS	2.0
1	A	174	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	1291	14/15	0.76	0.30	13.56	45,47,50,50	0
5	BGC	F	1292	11/12	0.93	0.20	10.82	50,52,54,55	0
5	BGC	C	1291	11/12	0.92	0.19	8.00	52,53,55,56	0
5	BGC	C	1289	11/12	0.82	0.16	3.61	47,51,52,55	0
5	BGC	F	1290	11/12	0.88	0.19	2.14	47,51,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	E	1290	14/15	0.95	0.12	0.75	36,38,40,41	0
4	BMA	E	1292	11/12	0.91	0.10	-	54,58,60,61	0
4	NAG	E	1291	14/15	0.97	0.09	-	40,41,44,49	0
4	BMA	B	1293	11/12	0.75	0.48	-	63,65,66,66	0
4	NAG	B	1292	14/15	0.88	0.32	-	52,53,55,59	0
5	BGC	F	1293	11/12	0.91	0.15	-	55,56,57,59	0
5	BGC	C	1292	11/12	0.90	0.19	-	54,57,59,61	0
5	BGC	C	1290	11/12	0.91	0.16	-	47,50,53,55	0
5	BGC	F	1291	11/12	0.91	0.25	-	50,52,54,55	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
7	BGC	F	1289	11/12	0.81	0.24	7.88	70,76,77,78	0
3	CA	C	1293	1/1	0.99	0.06	-1.79	42,42,42,42	0
3	CA	F	1294	1/1	0.98	0.04	-3.12	38,38,38,38	0
3	CA	E	1289	1/1	0.99	0.03	-4.93	28,28,28,28	0
3	CA	B	1290	1/1	0.99	0.05	-11.41	27,27,27,27	0
3	CA	C	1294	1/1	0.98	0.03	-	46,46,46,46	0
6	NAG	F	1296	14/15	0.89	0.24	-	62,65,68,68	0
2	ACT	B	1289	4/4	0.98	0.08	-	56,57,58,58	0
3	CA	F	1295	1/1	0.95	0.05	-	48,48,48,48	0
6	NAG	C	1295	14/15	0.85	0.20	-	61,65,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.