



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2020 – 11:52 PM EST

PDB ID : 6O1J
Title : Alpha-L-fucosidase AlfC fucosyltransferase mutant N243A
Authors : Klontz, E.H.; Sundberg, E.J.
Deposited on : 2019-02-20
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

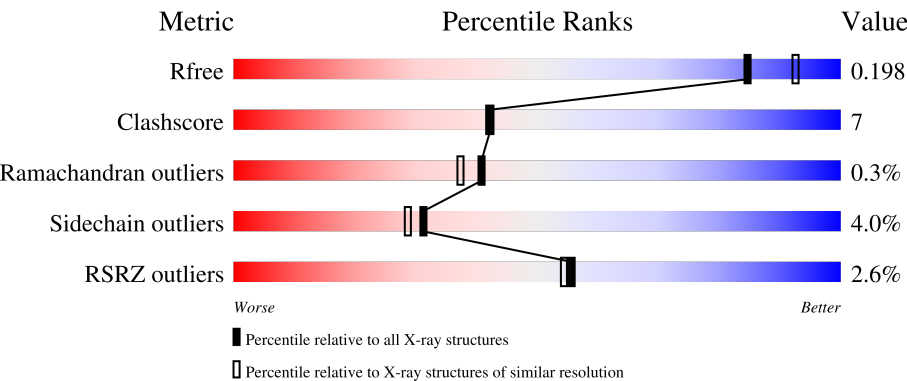
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.15.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.15.1

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	345	<div><div>81%13%• 5%</div></div>
1	B	345	<div><div>81%12%• 6%</div></div>
1	C	345	<div><div>4%78%15%• 6%</div></div>
1	D	345	<div><div>3%78%15%• 6%</div></div>
1	E	345	<div><div>2%81%12%• 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	345	<div><div>%</div><div><div></div><div>78%</div><div>14%</div><div>• 6%</div></div></div>
1	G	345	<div><div>3%</div><div><div></div><div>78%</div><div>12%</div><div>• 8%</div></div></div>
1	H	345	<div><div>4%</div><div><div></div><div>77%</div><div>16%</div><div>• 6%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21640 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 AlfC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2636	1685	433	505	13			
1	B	324	Total	C	N	O	S	0	0	0
			2600	1660	427	500	13			
1	C	323	Total	C	N	O	S	0	0	0
			2592	1655	426	499	12			
1	D	324	Total	C	N	O	S	0	0	0
			2602	1663	427	499	13			
1	E	327	Total	C	N	O	S	0	0	0
			2624	1678	431	503	12			
1	F	323	Total	C	N	O	S	0	0	0
			2593	1655	426	499	13			
1	G	317	Total	C	N	O	S	0	0	0
			2548	1628	419	489	12			
1	H	323	Total	C	N	O	S	0	0	0
			2596	1658	426	499	13			

There are 16 discrepancies between the modelled and reference sequences:

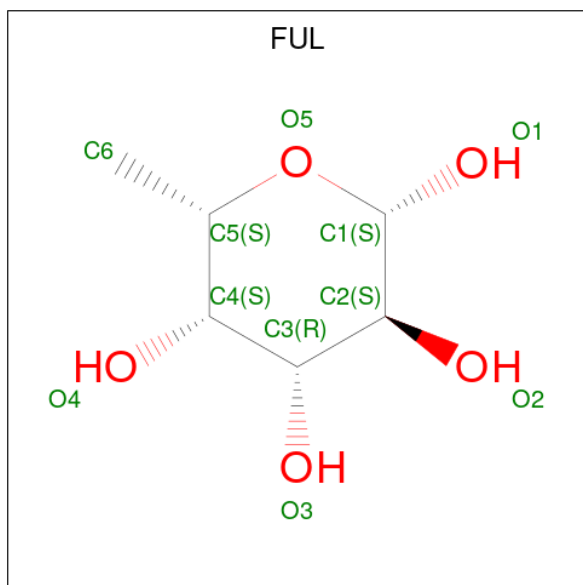
Chain	Residue	Modelled	Actual	Comment	Reference
A	243	ALA	ASN	engineered mutation	UNP K0NB39
A	345	LEU	-	expression tag	UNP K0NB39
B	243	ALA	ASN	engineered mutation	UNP K0NB39
B	345	LEU	-	expression tag	UNP K0NB39
C	243	ALA	ASN	engineered mutation	UNP K0NB39
C	345	LEU	-	expression tag	UNP K0NB39
D	243	ALA	ASN	engineered mutation	UNP K0NB39
D	345	LEU	-	expression tag	UNP K0NB39
E	243	ALA	ASN	engineered mutation	UNP K0NB39
E	345	LEU	-	expression tag	UNP K0NB39
F	243	ALA	ASN	engineered mutation	UNP K0NB39
F	345	LEU	-	expression tag	UNP K0NB39
G	243	ALA	ASN	engineered mutation	UNP K0NB39

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Chain	Residue	Modelled	Actual	Comment	Reference
G	345	LEU	-	expression tag	UNP K0NB39
H	243	ALA	ASN	engineered mutation	UNP K0NB39
H	345	LEU	-	expression tag	UNP K0NB39

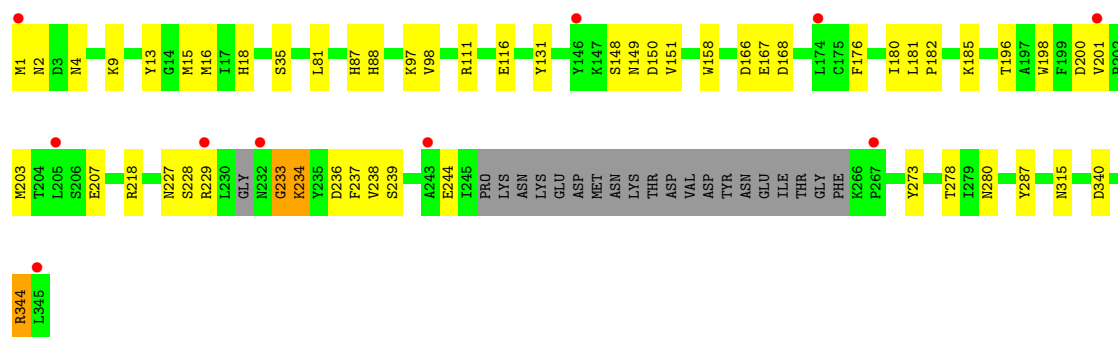
- Molecule 2 is beta-L-fucopyranose (three-letter code: FUL) (formula: C₆H₁₂O₅).



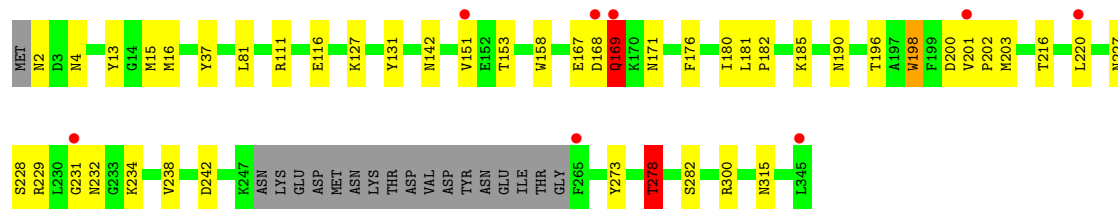
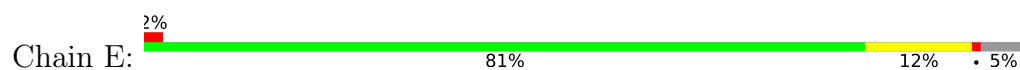
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 6 5	0	0
2	B	1	Total C O 11 6 5	0	0
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0
2	E	1	Total C O 11 6 5	0	0
2	F	1	Total C O 11 6 5	0	0
2	G	1	Total C O 11 6 5	0	0
2	H	1	Total C O 11 6 5	0	0

- Molecule 3 is water.

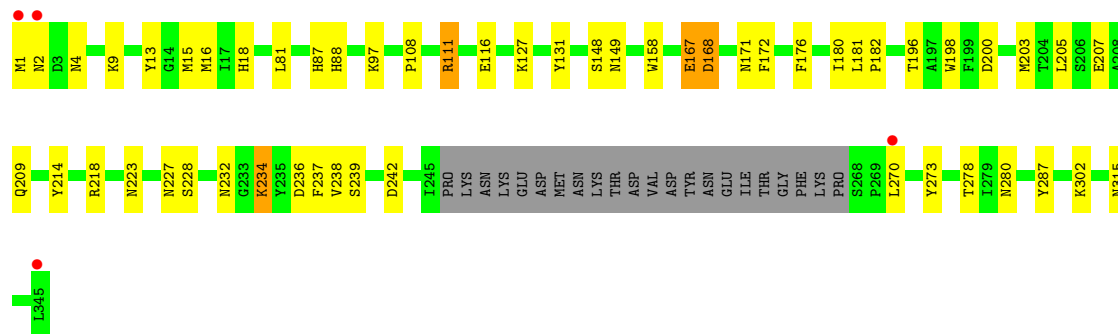
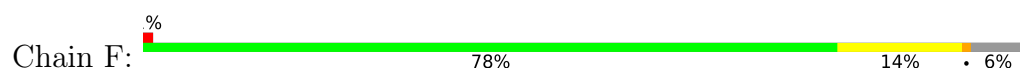
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0
3	B	120	Total 120	O 120	0	0
3	C	96	Total 96	O 96	0	0
3	D	95	Total 95	O 95	0	0
3	E	92	Total 92	O 92	0	0
3	F	99	Total 99	O 99	0	0
3	G	83	Total 83	O 83	0	0
3	H	60	Total 60	O 60	0	0



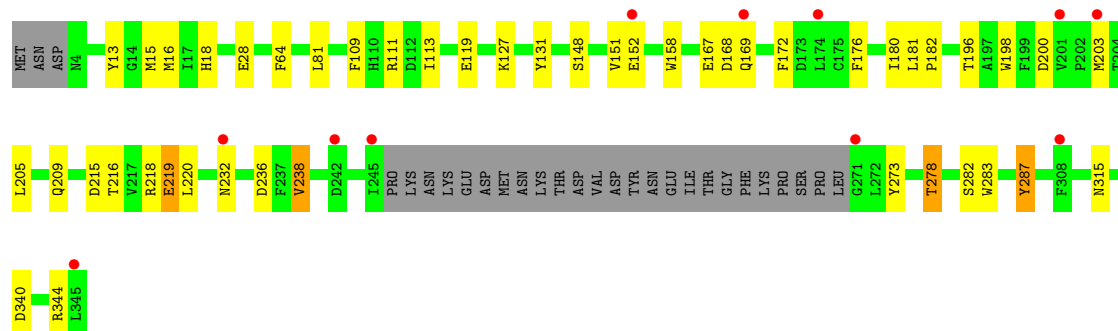
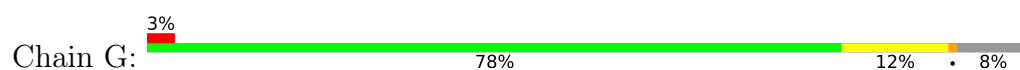
• Molecule 1: AlFC



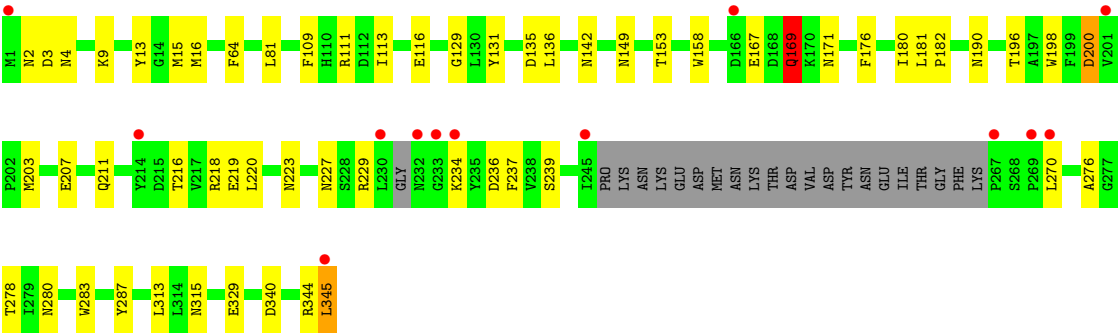
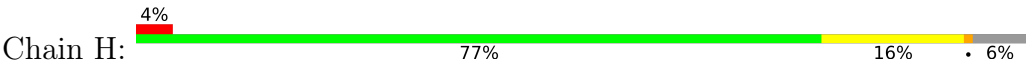
• Molecule 1: AlFC



• Molecule 1: AlFC



● Molecule 1: AlfC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.30Å 259.92Å 80.35Å 90.00° 118.81° 90.00°	Depositor
Resolution (Å)	47.75 – 2.00 47.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.3 (47.75-2.00) 91.3 (47.75-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.230 , 0.243 0.181 , 0.198	Depositor DCC
R_{free} test set	9045 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.088 for -h-l,k,h 0.088 for l,k,-h-l 0.088 for h,-k,-h-l 0.087 for -h-l,-k,l 0.356 for l,-k,h	Xtriage
Reported twinning fraction	0.645 for H, K, L 0.355 for -L, -K, -H	Depositor
Outliers	0 of 176954 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21640	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: FUL

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	0.75	2/2710 (0.1%)	0.84	2/3679 (0.1%)
1	B	0.74	1/2672 (0.0%)	0.86	2/3627 (0.1%)
1	C	0.70	1/2664 (0.0%)	0.81	1/3617 (0.0%)
1	D	0.74	0/2673	0.82	0/3627
1	E	0.71	0/2698	0.83	4/3664 (0.1%)
1	F	0.70	0/2664	0.81	1/3616 (0.0%)
1	G	0.69	1/2618 (0.0%)	0.82	3/3553 (0.1%)
1	H	0.70	1/2667 (0.0%)	0.79	1/3619 (0.0%)
All	All	0.72	6/21366 (0.0%)	0.82	14/29002 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	H	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	28	GLU	CD-OE1	6.24	1.32	1.25
1	B	3	ASP	CG-OD2	5.72	1.38	1.25
1	A	329	GLU	CD-OE1	-5.68	1.19	1.25
1	A	330	GLU	CD-OE1	-5.29	1.19	1.25
1	C	28	GLU	CD-OE2	5.25	1.31	1.25
1	H	329	GLU	CD-OE2	-5.21	1.20	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	G	287	TYR	CB-CA-C	6.09	122.58	110.40
1	A	218	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	F	111	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	G	111	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	E	190	ASN	N-CA-C	-5.49	96.18	111.00
1	E	278	THR	CA-CB-OG1	5.44	120.42	109.00
1	G	111	ARG	CB-CG-CD	5.34	125.49	111.60
1	E	300	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	287	TYR	CB-CA-C	5.13	120.67	110.40
1	A	312	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	H	190	ASN	N-CA-C	-5.07	97.30	111.00
1	B	312	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	E	37	TYR	CB-CG-CD1	5.04	124.03	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	169	GLN	Peptide
1	H	169	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2636	0	2481	26	1
1	B	2600	0	2448	33	1
1	C	2592	0	2436	38	0
1	D	2602	0	2452	34	1
1	E	2624	0	2466	33	1
1	F	2593	0	2440	44	1
1	G	2548	0	2395	31	0
1	H	2596	0	2444	46	1
2	A	11	0	11	1	0
2	B	11	0	11	0	0
2	C	11	0	12	1	0
2	D	11	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	11	0	11	0	0
2	F	11	0	11	3	0
2	G	11	0	11	0	0
2	H	11	0	11	0	0
3	A	116	0	0	0	0
3	B	120	0	0	1	0
3	C	96	0	0	6	0
3	D	95	0	0	3	0
3	E	92	0	0	1	0
3	F	99	0	0	9	1
3	G	83	0	0	0	0
3	H	60	0	0	0	1
All	All	21640	0	19652	280	4

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 7.

All (280) 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:C:341:GLU:HA	3:C:516:HOH:O	1.39	1.18
1:F:108:PRO:O	3:F:501:HOH:O	1.71	1.05
1:H:169:GLN:HE21	1:H:169:GLN:HA	1.36	0.89
1:G:215:ASP:O	1:G:219:GLU:HG2	1.74	0.88
1:G:278:THR:HG23	1:G:315:ASN:HB3	1.57	0.87
1:F:227:ASN:OD1	1:F:239:SER:HB2	1.74	0.86
1:H:211:GLN:OE1	1:H:234:LYS:NZ	2.12	0.82
1:H:200:ASP:OD1	1:H:229:ARG:NH1	2.13	0.82
1:B:278:THR:HG21	1:B:282:SER:O	1.81	0.80
1:E:278:THR:HG21	1:E:282:SER:O	1.82	0.80
1:F:218:ARG:HG2	3:F:553:HOH:O	1.81	0.79
1:A:325:PRO:HB3	1:C:287:TYR:OH	1.82	0.78
1:F:214:TYR:CE1	3:F:553:HOH:O	2.37	0.77
1:E:278:THR:HG23	1:E:315:ASN:HD22	1.50	0.76
1:E:242:ASP:OD1	3:E:501:HOH:O	2.02	0.76
1:B:186:GLU:CD	3:B:509:HOH:O	2.24	0.75
1:A:166:ASP:OD2	1:A:169:GLN:NE2	2.21	0.73
1:F:214:TYR:CD1	3:F:553:HOH:O	2.42	0.73
1:D:244:GLU:OE1	3:D:501:HOH:O	2.08	0.70
1:C:203:MET:SD	3:C:532:HOH:O	2.49	0.70
1:F:218:ARG:CG	3:F:553:HOH:O	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:GLN:NE2	1:H:169:GLN:HA	2.06	0.70
1:C:203:MET:HG2	3:C:532:HOH:O	1.92	0.69
1:F:149:ASN:HD21	1:F:158:TRP:H	1.40	0.68
1:B:219:GLU:OE2	1:B:220:LEU:CD2	2.42	0.68
1:C:149:ASN:HD21	1:C:158:TRP:H	1.40	0.68
1:D:166:ASP:OD1	1:D:168:ASP:OD1	2.11	0.68
1:D:149:ASN:HD21	1:D:158:TRP:H	1.41	0.67
1:H:149:ASN:HD21	1:H:158:TRP:H	1.41	0.67
1:B:278:THR:HG23	1:B:315:ASN:HD22	1.59	0.67
1:F:172:PHE:CE2	1:F:205:LEU:HD23	2.30	0.67
1:C:215:ASP:O	1:C:219:GLU:HG3	1.96	0.66
1:B:219:GLU:OE2	1:B:220:LEU:HD21	1.94	0.66
1:C:172:PHE:CE2	1:C:205:LEU:HD23	2.30	0.66
1:A:215:ASP:O	1:A:219:GLU:HG3	1.95	0.65
1:G:64:PHE:CE2	1:G:113:ILE:HD12	2.32	0.64
1:H:64:PHE:CE2	1:H:113:ILE:HD12	2.33	0.64
1:B:158:TRP:CG	1:B:203:MET:HE1	2.33	0.64
1:C:158:TRP:CG	1:C:203:MET:HE1	2.33	0.64
1:G:278:THR:HG23	1:G:315:ASN:CB	2.28	0.63
1:G:172:PHE:CE2	1:G:205:LEU:HD23	2.33	0.63
1:A:200:ASP:OD2	2:A:401:FUL:H2	1.99	0.63
1:E:278:THR:HG23	1:E:315:ASN:HB3	1.81	0.63
1:G:215:ASP:O	1:G:219:GLU:CG	2.46	0.63
1:G:278:THR:CG2	1:G:315:ASN:HB3	2.28	0.63
1:A:109:PHE:HE2	1:A:113:ILE:HD11	1.65	0.62
1:G:109:PHE:HE2	1:G:113:ILE:HD11	1.64	0.62
1:A:64:PHE:CE2	1:A:113:ILE:HD12	2.35	0.61
1:H:109:PHE:HE2	1:H:113:ILE:HD11	1.65	0.61
1:C:166:ASP:OD1	1:C:168:ASP:OD1	2.18	0.61
1:F:227:ASN:HB2	1:F:237:PHE:CZ	2.36	0.60
1:D:229:ARG:NH1	1:D:239:SER:OG	2.34	0.60
1:B:88:HIS:HE1	1:B:200:ASP:OD2	1.84	0.60
1:C:200:ASP:OD2	2:C:401:FUL:O1	2.19	0.60
1:E:278:THR:CG2	1:E:315:ASN:HD22	2.14	0.60
1:F:18:HIS:HE2	2:F:401:FUL:C6	2.14	0.59
1:D:340:ASP:O	1:D:344:ARG:HD3	2.02	0.59
1:G:158:TRP:CG	1:G:203:MET:HE1	2.38	0.58
1:B:278:THR:HG23	1:B:315:ASN:HB3	1.86	0.57
1:E:238:VAL:HG22	1:E:273:TYR:CD1	2.38	0.57
1:F:214:TYR:CZ	3:F:553:HOH:O	2.56	0.57
1:B:278:THR:CG2	1:B:315:ASN:HD22	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:ASN:HB2	1:H:237:PHE:CZ	2.40	0.57
1:A:118:ALA:O	1:A:122:GLN:HG3	2.04	0.57
1:G:278:THR:HG21	1:G:283:TRP:HA	1.88	0.56
1:H:200:ASP:OD1	1:H:229:ARG:NH2	2.38	0.56
1:F:172:PHE:HE2	1:F:205:LEU:HD23	1.71	0.56
1:C:227:ASN:HB2	1:C:237:PHE:CZ	2.41	0.56
1:C:205:LEU:HD22	1:C:209:GLN:HB3	1.86	0.56
1:D:238:VAL:CG2	1:D:273:TYR:CD1	2.89	0.56
1:D:238:VAL:HG22	1:D:273:TYR:CD1	2.39	0.56
1:G:238:VAL:HG12	1:G:273:TYR:CD1	2.40	0.56
1:A:118:ALA:O	1:A:122:GLN:CG	2.53	0.56
1:B:238:VAL:HG22	1:B:273:TYR:CD1	2.41	0.56
1:E:200:ASP:OD1	1:E:229:ARG:NH1	2.38	0.56
1:D:201:VAL:HG22	1:D:229:ARG:HD2	1.87	0.56
1:B:238:VAL:CG2	1:B:273:TYR:CD1	2.89	0.55
1:E:238:VAL:CG2	1:E:273:TYR:CD1	2.88	0.55
1:B:227:ASN:HB2	1:B:237:PHE:CZ	2.42	0.55
1:C:238:VAL:CG2	1:C:273:TYR:CD1	2.90	0.55
1:D:227:ASN:HB2	1:D:237:PHE:CZ	2.40	0.55
1:F:205:LEU:HD22	1:F:209:GLN:HB3	1.89	0.55
1:F:302:LYS:NZ	3:F:504:HOH:O	2.40	0.54
1:C:238:VAL:HG22	1:C:273:TYR:CD1	2.43	0.54
1:E:200:ASP:HA	1:E:229:ARG:NH1	2.22	0.54
1:C:203:MET:CG	3:C:532:HOH:O	2.51	0.54
1:G:205:LEU:HD22	1:G:209:GLN:HB3	1.88	0.54
1:D:158:TRP:CG	1:D:203:MET:HE1	2.42	0.54
1:B:270:LEU:HD12	1:B:270:LEU:N	2.23	0.54
1:C:172:PHE:HE2	1:C:205:LEU:HD23	1.71	0.54
1:F:158:TRP:CG	1:F:203:MET:HE1	2.42	0.54
1:A:275:THR:HG22	1:A:305:LEU:HD13	1.89	0.53
1:E:181:LEU:HD13	1:E:181:LEU:C	2.29	0.53
1:D:181:LEU:C	1:D:181:LEU:HD13	2.28	0.53
1:B:67:LYS:NZ	1:G:168:ASP:OD2	2.42	0.53
1:H:109:PHE:CE2	1:H:113:ILE:HD11	2.43	0.53
1:F:238:VAL:HG22	1:F:273:TYR:CD1	2.44	0.52
1:F:238:VAL:CG2	1:F:273:TYR:CD1	2.92	0.52
1:E:111:ARG:HD2	1:E:116:GLU:OE2	2.10	0.52
1:F:214:TYR:CG	3:F:553:HOH:O	2.60	0.52
1:H:136:LEU:N	1:H:136:LEU:HD12	2.24	0.52
1:H:16:MET:HE1	1:H:283:TRP:HZ3	1.75	0.52
1:C:111:ARG:HD2	1:C:116:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:PHE:CE2	1:G:113:ILE:HD11	2.44	0.52
1:H:2:ASN:CG	1:H:223:ASN:HD22	2.13	0.52
1:F:18:HIS:HE2	2:F:401:FUL:H62	1.74	0.51
1:A:109:PHE:CE2	1:A:113:ILE:HD11	2.43	0.51
1:E:200:ASP:OD1	1:E:229:ARG:NH2	2.43	0.51
1:F:18:HIS:ND1	1:F:315:ASN:ND2	2.59	0.51
1:B:67:LYS:HE2	1:G:168:ASP:OD1	2.10	0.51
1:H:16:MET:HE1	1:H:276:ALA:HB1	1.91	0.51
1:H:270:LEU:HD12	1:H:270:LEU:N	2.26	0.51
1:G:172:PHE:HE2	1:G:205:LEU:HD23	1.75	0.51
1:E:201:VAL:HG23	1:E:229:ARG:NH2	2.25	0.51
1:E:278:THR:HG23	1:E:315:ASN:ND2	2.23	0.50
1:F:2:ASN:CG	1:F:223:ASN:HD22	2.14	0.50
1:G:18:HIS:ND1	1:G:315:ASN:ND2	2.59	0.50
1:F:149:ASN:ND2	1:F:158:TRP:H	2.08	0.50
1:G:278:THR:CG2	1:G:315:ASN:OD1	2.58	0.50
1:H:111:ARG:HD2	1:H:116:GLU:OE2	2.12	0.50
1:C:149:ASN:ND2	1:C:158:TRP:H	2.08	0.50
1:D:18:HIS:ND1	1:D:315:ASN:ND2	2.60	0.50
1:A:111:ARG:HD2	1:A:116:GLU:OE2	2.12	0.50
1:C:341:GLU:CA	3:C:516:HOH:O	2.22	0.50
1:F:87:HIS:HD1	1:F:88:HIS:H	1.60	0.49
1:F:111:ARG:HD2	1:F:116:GLU:OE2	2.12	0.49
1:F:270:LEU:HD12	1:F:270:LEU:N	2.26	0.49
1:H:135:ASP:HB3	1:H:136:LEU:HD12	1.92	0.49
1:G:278:THR:HG21	1:G:282:SER:O	2.13	0.49
1:E:201:VAL:HG23	1:E:229:ARG:HH21	1.78	0.49
1:H:200:ASP:OD1	1:H:229:ARG:CZ	2.61	0.49
1:D:111:ARG:HD2	1:D:116:GLU:OE2	2.13	0.49
1:D:181:LEU:HB3	1:D:182:PRO:HD3	1.95	0.49
1:E:181:LEU:HD13	1:E:181:LEU:O	2.13	0.49
1:C:18:HIS:ND1	1:C:315:ASN:ND2	2.60	0.49
1:H:16:MET:HE3	1:H:315:ASN:HB2	1.95	0.48
1:F:2:ASN:OD1	1:F:4:ASN:HB2	2.14	0.48
1:B:278:THR:HG23	1:B:315:ASN:ND2	2.28	0.48
1:H:200:ASP:HA	1:H:229:ARG:NH1	2.28	0.48
1:A:16:MET:HB3	1:A:315:ASN:HA	1.95	0.48
1:H:207:GLU:OE1	1:H:234:LYS:HE2	2.14	0.48
1:D:15:MET:O	1:D:81:LEU:HA	2.14	0.48
1:B:15:MET:O	1:B:81:LEU:HA	2.14	0.48
1:C:344:ARG:HD2	3:C:516:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:ND2	1:D:158:TRP:H	2.09	0.48
1:H:149:ASN:ND2	1:H:158:TRP:H	2.08	0.48
1:A:2:ASN:OD1	1:A:4:ASN:HB2	2.15	0.47
1:E:15:MET:O	1:E:81:LEU:HA	2.14	0.47
1:F:2:ASN:CB	1:F:223:ASN:HD22	2.27	0.47
1:A:15:MET:O	1:A:81:LEU:HA	2.15	0.47
1:H:216:THR:O	1:H:220:LEU:HD23	2.14	0.47
1:B:219:GLU:OE2	1:B:220:LEU:HD22	2.13	0.47
1:A:87:HIS:HD1	1:A:88:HIS:H	1.60	0.47
1:C:181:LEU:HB3	1:C:182:PRO:HD3	1.96	0.47
1:C:2:ASN:OD1	1:C:4:ASN:HB2	2.14	0.47
1:D:98:VAL:O	3:D:502:HOH:O	2.20	0.47
1:E:216:THR:O	1:E:220:LEU:HD23	2.14	0.47
1:D:181:LEU:HD11	1:D:185:LYS:HE3	1.96	0.47
1:E:2:ASN:OD1	1:E:4:ASN:HB2	2.15	0.47
1:G:16:MET:HB3	1:G:315:ASN:HA	1.97	0.47
1:B:111:ARG:HD2	1:B:116:GLU:OE2	2.15	0.47
1:B:216:THR:O	1:B:220:LEU:HD23	2.14	0.47
1:D:2:ASN:OD1	1:D:4:ASN:HB2	2.14	0.47
1:H:2:ASN:CB	1:H:223:ASN:HD22	2.27	0.47
1:B:181:LEU:HB3	1:B:182:PRO:HD3	1.97	0.46
1:C:111:ARG:CD	1:C:116:GLU:OE2	2.63	0.46
1:F:111:ARG:CD	1:F:116:GLU:OE2	2.63	0.46
1:H:16:MET:HE2	1:H:313:LEU:HG	1.96	0.46
1:H:181:LEU:HB3	1:H:182:PRO:HD3	1.96	0.46
1:H:227:ASN:ND2	1:H:239:SER:HB2	2.30	0.46
1:H:2:ASN:OD1	1:H:4:ASN:HB2	2.15	0.46
1:E:111:ARG:CD	1:E:116:GLU:OE2	2.64	0.46
1:G:216:THR:O	1:G:220:LEU:HD23	2.15	0.46
1:C:216:THR:O	1:C:220:LEU:HD23	2.15	0.46
1:D:181:LEU:HD11	1:D:185:LYS:CE	2.45	0.46
1:E:181:LEU:HB3	1:E:182:PRO:HD3	1.96	0.46
1:A:111:ARG:CD	1:A:116:GLU:OE2	2.64	0.46
1:F:234:LYS:N	1:F:234:LYS:HD2	2.30	0.46
1:G:15:MET:O	1:G:81:LEU:HA	2.15	0.46
1:H:15:MET:O	1:H:81:LEU:HA	2.16	0.46
1:G:181:LEU:HB3	1:G:182:PRO:HD3	1.98	0.46
1:A:181:LEU:HB3	1:A:182:PRO:HD3	1.97	0.46
1:C:15:MET:O	1:C:81:LEU:HA	2.16	0.46
1:D:181:LEU:O	1:D:181:LEU:HD13	2.16	0.46
1:E:16:MET:HB3	1:E:315:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:C	1:A:131:TYR:CD1	2.90	0.46
1:C:227:ASN:ND2	1:C:239:SER:HB2	2.31	0.46
1:F:181:LEU:HB3	1:F:182:PRO:HD3	1.97	0.45
1:A:199:PHE:H	1:A:227:ASN:ND2	2.15	0.45
1:D:111:ARG:CD	1:D:116:GLU:OE2	2.64	0.45
1:F:148:SER:HB2	1:F:203:MET:HE1	1.97	0.45
1:G:218:ARG:NH2	1:G:236:ASP:OD1	2.48	0.45
1:C:158:TRP:CD2	1:C:203:MET:HE1	2.52	0.45
1:H:111:ARG:CD	1:H:116:GLU:OE2	2.65	0.45
1:G:148:SER:HB3	1:G:203:MET:HE1	1.99	0.45
1:F:15:MET:O	1:F:81:LEU:HA	2.17	0.45
1:F:218:ARG:NH2	1:F:236:ASP:OD1	2.46	0.45
1:C:218:ARG:NH2	1:C:236:ASP:OD1	2.48	0.44
1:G:64:PHE:CD2	1:G:113:ILE:HD12	2.52	0.44
1:H:218:ARG:NH2	1:H:236:ASP:OD1	2.48	0.44
1:E:198:TRP:CZ3	1:E:229:ARG:NH1	2.85	0.44
1:H:278:THR:HG23	1:H:280:ASN:O	2.18	0.44
1:A:118:ALA:O	1:A:122:GLN:HG2	2.17	0.44
1:D:176:PHE:HA	1:D:180:ILE:HB	2.00	0.44
1:B:111:ARG:CD	1:B:116:GLU:OE2	2.65	0.44
1:F:131:TYR:C	1:F:131:TYR:CD1	2.90	0.44
1:B:270:LEU:CD1	1:B:270:LEU:N	2.80	0.44
1:H:64:PHE:CD2	1:H:113:ILE:HD12	2.53	0.43
1:H:16:MET:CE	1:H:283:TRP:HZ3	2.30	0.43
1:D:148:SER:HB2	1:D:203:MET:HE1	1.98	0.43
1:H:16:MET:HB3	1:H:315:ASN:HA	2.00	0.43
1:D:87:HIS:HD1	1:D:88:HIS:H	1.65	0.43
1:H:131:TYR:C	1:H:131:TYR:CD1	2.92	0.43
1:B:176:PHE:HA	1:B:180:ILE:HB	2.01	0.43
1:E:131:TYR:CD1	1:E:131:TYR:C	2.92	0.43
1:A:64:PHE:CD2	1:A:113:ILE:HD12	2.54	0.43
1:B:158:TRP:CD2	1:B:203:MET:HE1	2.53	0.43
1:G:131:TYR:CD1	1:G:131:TYR:C	2.92	0.43
1:A:275:THR:CG2	1:A:305:LEU:HD13	2.49	0.43
1:F:16:MET:HB3	1:F:315:ASN:HA	2.00	0.43
1:D:1:MET:HG2	1:D:2:ASN:N	2.34	0.43
1:E:198:TRP:HZ3	1:E:229:ARG:NH1	2.17	0.43
1:E:181:LEU:HD11	1:E:185:LYS:HE3	2.01	0.42
1:G:176:PHE:HA	1:G:180:ILE:HB	2.01	0.42
1:E:176:PHE:HA	1:E:180:ILE:HB	2.02	0.42
1:G:340:ASP:HB3	1:G:344:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:SER:HB3	1:F:238:VAL:HA	2.01	0.42
1:D:131:TYR:C	1:D:131:TYR:CD1	2.92	0.42
1:D:340:ASP:HB3	1:D:344:ARG:NH1	2.34	0.42
1:A:228:SER:HB3	1:A:238:VAL:HA	2.02	0.42
1:C:131:TYR:CD1	1:C:131:TYR:C	2.92	0.42
1:C:176:PHE:HA	1:C:180:ILE:HB	2.01	0.42
1:H:270:LEU:N	1:H:270:LEU:CD1	2.83	0.42
1:C:16:MET:HB3	1:C:315:ASN:HA	2.01	0.42
1:H:176:PHE:HA	1:H:180:ILE:HB	2.02	0.42
1:A:278:THR:HG23	1:A:280:ASN:O	2.20	0.42
1:C:228:SER:HB3	1:C:238:VAL:HA	2.02	0.42
1:C:336:LYS:NZ	1:C:340:ASP:OD2	2.47	0.42
1:D:228:SER:HB3	1:D:238:VAL:HA	2.02	0.42
1:E:228:SER:HB3	1:E:238:VAL:HA	2.01	0.42
1:H:129:GLY:HA3	1:H:196:THR:OG1	2.19	0.42
1:C:129:GLY:HA3	1:C:196:THR:OG1	2.19	0.42
1:H:16:MET:HE1	1:H:283:TRP:CZ3	2.53	0.42
1:H:2:ASN:HA	1:H:223:ASN:ND2	2.34	0.42
1:C:119:GLU:HG2	1:C:123:LYS:HE2	2.02	0.41
1:E:202:PRO:HD3	1:E:229:ARG:O	2.20	0.41
1:B:227:ASN:ND2	1:B:239:SER:HB2	2.35	0.41
1:F:2:ASN:HA	1:F:223:ASN:ND2	2.35	0.41
1:F:278:THR:HG23	1:F:280:ASN:O	2.19	0.41
1:H:340:ASP:HB3	1:H:344:ARG:NH1	2.35	0.41
1:C:278:THR:HG23	1:C:280:ASN:O	2.20	0.41
1:D:16:MET:HB3	1:D:315:ASN:HA	2.01	0.41
1:D:35:SER:HB2	3:D:579:HOH:O	2.20	0.41
1:H:219:GLU:HG2	1:H:220:LEU:HD22	2.01	0.41
1:C:202:PRO:HD3	1:C:229:ARG:O	2.21	0.41
1:B:67:LYS:CE	1:G:168:ASP:OD1	2.69	0.41
1:D:278:THR:HG23	1:D:280:ASN:O	2.20	0.41
1:E:202:PRO:HG3	1:E:231:GLY:HA2	2.03	0.41
1:F:167:GLU:OE2	1:F:168:ASP:OD1	2.39	0.41
1:F:171:ASN:HA	3:F:515:HOH:O	2.20	0.41
1:H:153:THR:HG22	1:H:158:TRP:CE2	2.56	0.41
1:A:218:ARG:NH2	1:A:236:ASP:OD1	2.42	0.41
1:B:67:LYS:NZ	1:G:168:ASP:OD1	2.53	0.41
1:E:153:THR:HG22	1:E:158:TRP:CE2	2.56	0.41
1:E:168:ASP:O	1:E:169:GLN:HG2	2.21	0.41
1:A:176:PHE:HA	1:A:180:ILE:HB	2.02	0.41
1:B:103:VAL:HG21	1:B:113:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASN:ND2	1:E:171:ASN:H	2.18	0.41
1:F:176:PHE:HA	1:F:180:ILE:HB	2.02	0.41
1:H:142:ASN:ND2	1:H:171:ASN:H	2.18	0.41
1:F:270:LEU:CD1	1:F:270:LEU:N	2.83	0.41
1:H:345:LEU:HD23	1:H:345:LEU:OXT	2.21	0.41
1:B:202:PRO:HD3	1:B:229:ARG:O	2.22	0.40
1:D:218:ARG:NH2	1:D:236:ASP:OD1	2.51	0.40
1:B:2:ASN:OD1	1:B:4:ASN:HB2	2.20	0.40
1:F:18:HIS:HE2	2:F:401:FUL:H61	1.82	0.40
1:B:16:MET:HB3	1:B:315:ASN:HA	2.03	0.40
1:B:228:SER:HB3	1:B:238:VAL:HA	2.03	0.40
1:D:233:GLY:H	1:D:234:LYS:HD2	1.87	0.40
1:F:1:MET:SD	1:F:2:ASN:N	2.93	0.40

All (4) 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)
3:F:531:HOH:O	3:H:508:HOH:O[1_655]	1.79	0.41
1:F:287:TYR:CE1	1:H:287:TYR:CE1[1_655]	1.85	0.35
1:B:287:TYR:CE1	1:D:287:TYR:CE1[1_455]	1.89	0.31
1:A:123:LYS:NZ	1:E:169:GLN:O[1_556]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	325/345 (94%)	311 (96%)	12 (4%)	2 (1%)	25	19
1	B	320/345 (93%)	306 (96%)	14 (4%)	0	100	100
1	C	319/345 (92%)	305 (96%)	12 (4%)	2 (1%)	25	19
1	D	318/345 (92%)	306 (96%)	11 (4%)	1 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	323/345 (94%)	308 (95%)	14 (4%)	1 (0%)	41	37
1	F	319/345 (92%)	303 (95%)	15 (5%)	1 (0%)	41	37
1	G	313/345 (91%)	297 (95%)	15 (5%)	1 (0%)	41	37
1	H	317/345 (92%)	300 (95%)	17 (5%)	0	100	100
All	All	2554/2760 (92%)	2436 (95%)	110 (4%)	8 (0%)	41	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	232	ASN
1	C	231	GLY
1	A	35	SER
1	A	201	VAL
1	C	232	ASN
1	E	232	ASN
1	G	232	ASN
1	D	233	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	275/292 (94%)	265 (96%)	10 (4%)	35	34
1	B	272/292 (93%)	261 (96%)	11 (4%)	31	29
1	C	271/292 (93%)	264 (97%)	7 (3%)	46	48
1	D	272/292 (93%)	260 (96%)	12 (4%)	28	25
1	E	274/292 (94%)	263 (96%)	11 (4%)	31	29
1	F	271/292 (93%)	259 (96%)	12 (4%)	28	25
1	G	265/292 (91%)	251 (95%)	14 (5%)	22	18
1	H	272/292 (93%)	263 (97%)	9 (3%)	38	37
All	All	2172/2336 (93%)	2086 (96%)	86 (4%)	31	29

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	A	127	LYS
1	A	151	VAL
1	A	169	GLN
1	A	196	THR
1	A	198	TRP
1	A	200	ASP
1	A	203	MET
1	A	227	ASN
1	A	345	LEU
1	B	3	ASP
1	B	9	LYS
1	B	13	TYR
1	B	97	LYS
1	B	122	GLN
1	B	151	VAL
1	B	169	GLN
1	B	196	THR
1	B	198	TRP
1	B	278	THR
1	B	345	LEU
1	C	13	TYR
1	C	151	VAL
1	C	198	TRP
1	C	200	ASP
1	C	203	MET
1	C	287	TYR
1	C	345	LEU
1	D	9	LYS
1	D	13	TYR
1	D	97	LYS
1	D	150	ASP
1	D	151	VAL
1	D	167	GLU
1	D	196	THR
1	D	198	TRP
1	D	200	ASP
1	D	207	GLU
1	D	234	LYS
1	D	344	ARG
1	E	13	TYR
1	E	127	LYS

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Mol	Chain	Res	Type
1	E	151	VAL
1	E	167	GLU
1	E	169	GLN
1	E	196	THR
1	E	198	TRP
1	E	203	MET
1	E	227	ASN
1	E	234	LYS
1	E	278	THR
1	F	9	LYS
1	F	13	TYR
1	F	97	LYS
1	F	127	LYS
1	F	167	GLU
1	F	168	ASP
1	F	196	THR
1	F	198	TRP
1	F	200	ASP
1	F	207	GLU
1	F	234	LYS
1	F	242	ASP
1	G	13	TYR
1	G	119	GLU
1	G	127	LYS
1	G	151	VAL
1	G	152	GLU
1	G	167	GLU
1	G	169	GLN
1	G	196	THR
1	G	198	TRP
1	G	200	ASP
1	G	219	GLU
1	G	238	VAL
1	G	278	THR
1	G	287	TYR
1	H	3	ASP
1	H	9	LYS
1	H	13	TYR
1	H	167	GLU
1	H	169	GLN
1	H	198	TRP
1	H	200	ASP

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Mol	Chain	Res	Type
1	H	203	MET
1	H	345	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	211	GLN
1	A	227	ASN
1	A	232	ASN
1	C	149	ASN
1	C	306	ASN
1	C	315	ASN
1	D	149	ASN
1	D	190	ASN
1	D	306	ASN
1	D	315	ASN
1	E	142	ASN
1	E	306	ASN
1	F	110	HIS
1	F	149	ASN
1	F	223	ASN
1	F	306	ASN
1	F	315	ASN
1	G	306	ASN
1	G	315	ASN
1	H	110	HIS
1	H	142	ASN
1	H	149	ASN
1	H	169	GLN
1	H	223	ASN
1	H	306	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	FUL	E	401	-	11,11,11	1.31	1 (9%)	15,16,16	1.06	1 (6%)
2	FUL	C	401	-	11,11,11	1.34	1 (9%)	15,16,16	1.21	2 (13%)
2	FUL	B	401	-	11,11,11	1.51	1 (9%)	15,16,16	1.43	3 (20%)
2	FUL	G	401	-	11,11,11	1.35	1 (9%)	15,16,16	0.78	0
2	FUL	D	401	-	11,11,11	1.45	1 (9%)	14,16,16	2.20	4 (28%)
2	FUL	A	401	-	11,11,11	1.39	1 (9%)	15,16,16	1.47	2 (13%)
2	FUL	F	401	-	11,11,11	1.39	1 (9%)	15,16,16	1.46	2 (13%)
2	FUL	H	401	-	11,11,11	1.25	1 (9%)	15,16,16	0.87	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	FUL	E	401	-	-	-	0/1/1/1
2	FUL	C	401	-	-	-	0/1/1/1
2	FUL	B	401	-	-	-	0/1/1/1
2	FUL	G	401	-	-	-	0/1/1/1
2	FUL	A	401	-	-	-	0/1/1/1
2	FUL	F	401	-	-	-	0/1/1/1
2	FUL	H	401	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FUL	O5-C1	3.57	1.51	1.42
2	F	401	FUL	O5-C1	3.42	1.51	1.42
2	B	401	FUL	O5-C1	3.38	1.51	1.42
2	D	401	FUL	O5-C1	3.32	1.51	1.42
2	C	401	FUL	O5-C1	3.21	1.50	1.42
2	E	401	FUL	O5-C1	3.19	1.50	1.42
2	G	401	FUL	O5-C1	3.04	1.50	1.42
2	H	401	FUL	O5-C1	2.98	1.50	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FUL	O5-C5-C4	4.81	118.15	109.52
2	D	401	FUL	C3-C4-C5	4.10	116.15	109.77
2	A	401	FUL	C3-C4-C5	3.70	115.54	109.77
2	F	401	FUL	C3-C4-C5	3.68	115.51	109.77
2	B	401	FUL	O5-C5-C4	2.83	114.60	109.52
2	C	401	FUL	O5-C1-C2	2.72	115.14	110.28
2	F	401	FUL	C4-C3-C2	2.71	115.56	110.82
2	A	401	FUL	C1-C2-C3	-2.60	104.92	110.31
2	B	401	FUL	O2-C2-C1	2.58	115.15	109.16
2	B	401	FUL	C1-C2-C3	-2.51	105.10	110.31
2	D	401	FUL	C1-C2-C3	-2.48	105.17	110.31
2	D	401	FUL	O2-C2-C1	2.42	114.77	109.16
2	C	401	FUL	O4-C4-C5	2.08	114.28	109.67
2	E	401	FUL	C1-C2-C3	-2.05	106.06	110.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FUL	1	0
2	A	401	FUL	1	0
2	F	401	FUL	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	329/345 (95%)	-0.14	4 (1%) 79 78	30, 44, 64, 113	0
1	B	324/345 (93%)	-0.17	4 (1%) 79 78	29, 44, 66, 89	0
1	C	323/345 (93%)	0.13	13 (4%) 38 37	33, 53, 81, 101	0
1	D	324/345 (93%)	0.00	10 (3%) 49 48	33, 47, 76, 97	0
1	E	327/345 (94%)	0.09	8 (2%) 59 57	33, 53, 90, 116	0
1	F	323/345 (93%)	-0.03	4 (1%) 79 78	34, 49, 74, 119	0
1	G	317/345 (91%)	0.09	11 (3%) 44 43	33, 54, 84, 114	0
1	H	323/345 (93%)	0.10	13 (4%) 38 37	37, 56, 88, 108	0
All	All	2590/2760 (93%)	0.01	67 (2%) 56 54	29, 50, 82, 119	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	345	LEU	8.8
1	E	345	LEU	8.5
1	C	232	ASN	8.0
1	A	1	MET	7.8
1	E	201	VAL	6.7
1	C	231	GLY	6.5
1	D	345	LEU	6.5
1	H	345	LEU	5.6
1	G	201	VAL	5.3
1	D	232	ASN	5.3
1	F	2	ASN	5.0
1	H	245	ILE	4.8
1	C	269	PRO	4.4
1	G	245	ILE	4.0
1	F	1	MET	3.9
1	D	1	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	201	VAL	3.6
1	D	243	ALA	3.6
1	D	201	VAL	3.4
1	C	245	ILE	3.4
1	H	269	PRO	3.3
1	F	345	LEU	3.3
1	G	169	GLN	3.2
1	A	345	LEU	3.2
1	E	169	GLN	3.1
1	B	245	ILE	3.1
1	H	230	LEU	3.1
1	H	270	LEU	3.0
1	E	231	GLY	3.0
1	H	1	MET	3.0
1	G	152	GLU	3.0
1	B	198	TRP	2.9
1	B	345	LEU	2.9
1	C	201	VAL	2.8
1	A	214	TYR	2.7
1	D	267	PRO	2.7
1	C	345	LEU	2.7
1	C	220	LEU	2.6
1	H	267	PRO	2.6
1	H	234	LYS	2.6
1	D	205	LEU	2.6
1	H	214	TYR	2.6
1	E	168	ASP	2.5
1	C	270	LEU	2.5
1	C	205	LEU	2.5
1	C	226	ILE	2.5
1	A	2	ASN	2.5
1	C	151	VAL	2.4
1	E	265	PHE	2.4
1	G	232	ASN	2.4
1	H	233	GLY	2.3
1	D	174	LEU	2.3
1	D	229	ARG	2.3
1	C	168	ASP	2.2
1	G	174	LEU	2.2
1	B	148	SER	2.2
1	D	146	TYR	2.2
1	E	151	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	308	PHE	2.1
1	H	232	ASN	2.1
1	E	220	LEU	2.1
1	H	166	ASP	2.1
1	F	270	LEU	2.1
1	G	203	MET	2.1
1	C	2	ASN	2.0
1	G	242	ASP	2.0
1	G	271	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](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUL	A	401	11/11	0.84	0.13	38,45,55,63	0
2	FUL	C	401	11/11	0.86	0.16	50,61,65,72	0
2	FUL	F	401	11/11	0.86	0.15	51,58,69,75	0
2	FUL	G	401	11/11	0.87	0.14	51,57,64,68	0
2	FUL	B	401	11/11	0.88	0.14	34,48,52,61	0
2	FUL	D	401	11/11	0.91	0.11	44,52,57,59	0
2	FUL	E	401	11/11	0.92	0.19	45,52,56,60	0
2	FUL	H	401	11/11	0.93	0.12	57,60,63,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.