



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 AM GMT

PDB ID : 2J3U
Title : L-FICOLIN COMPLEXED TO GALACTOSE
Authors : Garlatti, V.; Gaboriaud, C.
Deposited on : 2006-08-23
Resolution : 2.15 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

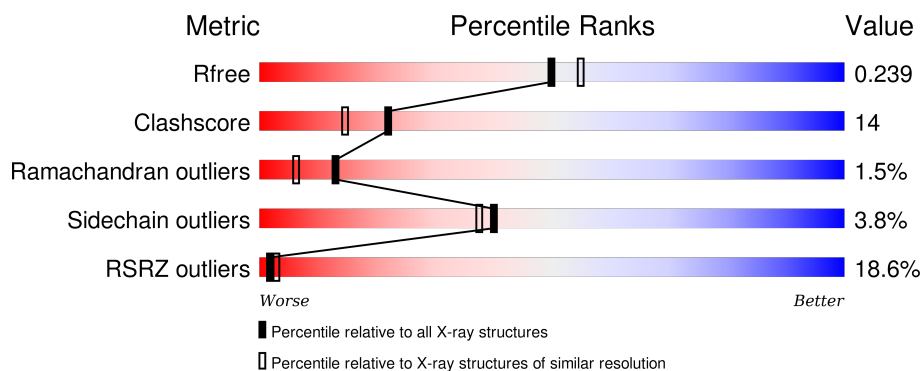
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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>41%</div> <div>65%</div> <div>27%</div> <div>6%</div> </div>
1	B	218	<div> <div>6%</div> <div>81%</div> <div>18%</div> </div>
1	C	218	<div> <div>12%</div> <div>84%</div> <div>13%</div> </div>
1	D	218	<div> <div>33%</div> <div>69%</div> <div>25%</div> </div>
1	E	218	<div> <div>7%</div> <div>82%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	218	

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
3	ACT	B	1290	-	-	X	-
3	ACT	E	1290	-	-	X	-
4	EPE	C	1289	-	-	-	X
4	EPE	F	1289	-	-	-	X
5	GLA	B	1291	-	-	-	X
5	GLA	C	1290	-	-	-	X
5	GLA	E	1289	-	-	-	X
5	GLA	F	1290	-	-	-	X
6	NAG	B	1293	-	-	-	X
6	NAG	E	1292	-	-	-	X
8	P4C	B	1296	-	-	-	X
8	P4C	C	1294	-	-	-	X
8	P4C	E	1295	-	-	-	X
8	P4C	E	1296	-	-	-	X
8	P4C	F	1294	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11129 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	217	Total	C	N	O	S	1	3	0
			1767	1112	312	334	9			
1	B	218	Total	C	N	O	S	3	1	0
			1752	1101	310	332	9			
1	C	214	Total	C	N	O	S	5	1	0
			1721	1082	302	329	8			
1	D	216	Total	C	N	O	S	2	1	0
			1738	1092	306	331	9			
1	E	218	Total	C	N	O	S	0	1	0
			1752	1100	309	334	9			
1	F	217	Total	C	N	O	S	0	0	0
			1736	1092	305	330	9			

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

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

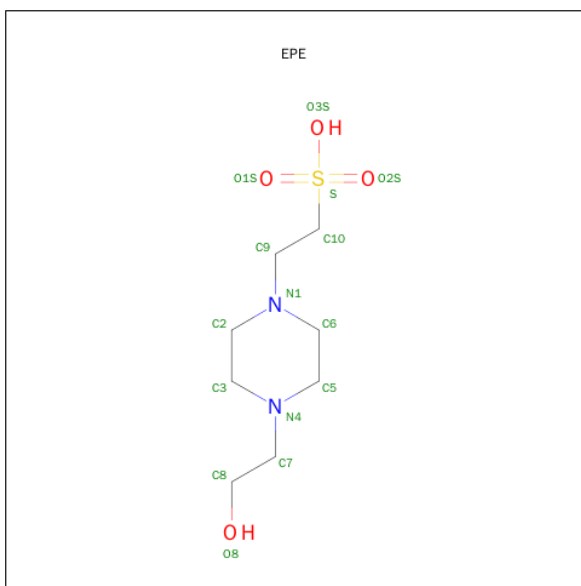
- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

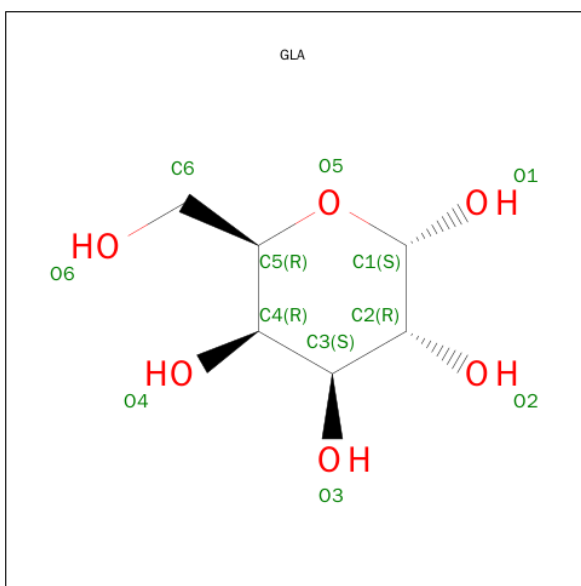
- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
4	F	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

- Molecule 5 is SUGAR (ALPHA D-GALACTOSE) (three-letter code: GLA) (formula: $C_6H_{12}O_6$).

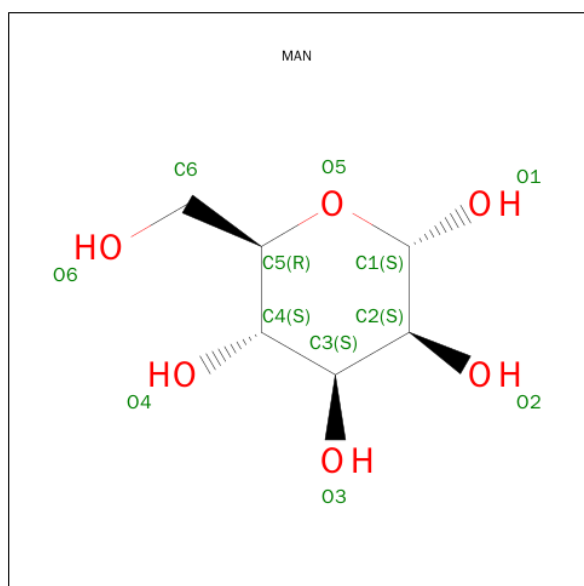


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			12	6	6		
5	C	1	Total	C	O	0	0
			12	6	6		
5	E	1	Total	C	O	0	0
			12	6	6		
5	F	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

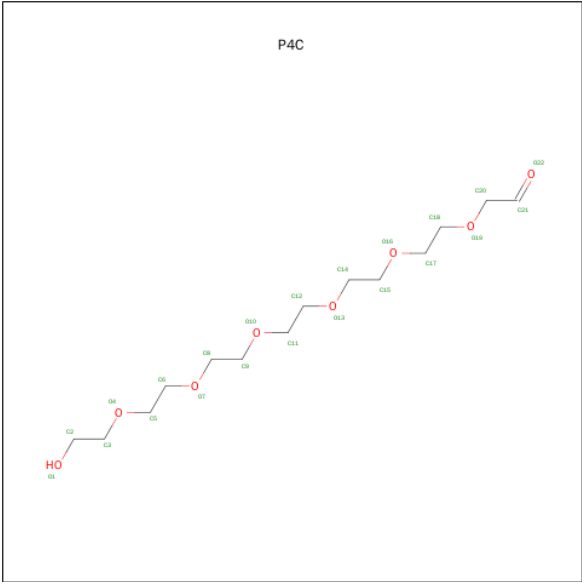
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



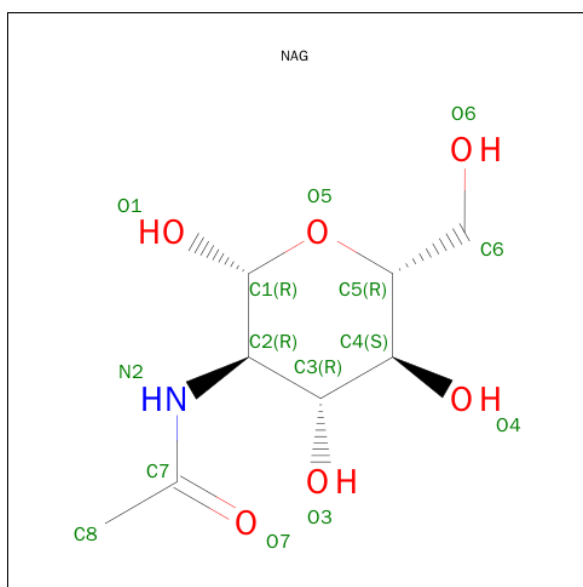
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (three-letter code: P4C) (formula: $C_{14}H_{28}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			22	14	8		
8	C	1	Total	C	O	0	0
			22	14	8		
8	E	1	Total	C	O	0	0
			22	14	8		
8	E	1	Total	C	O	0	0
			22	14	8		
8	F	1	Total	C	O	0	0
			22	14	8		

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			15	8	1	6		
9	F	1	Total	C	N	O	0	0
			15	8	1	6		

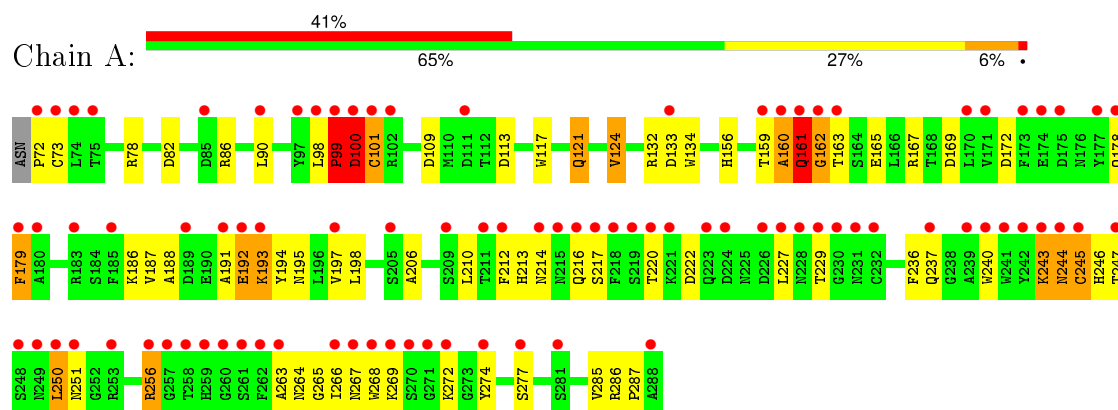
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	29	Total	O	0	0
			29	29		
10	B	89	Total	O	0	0
			89	89		
10	C	59	Total	O	0	0
			59	59		
10	D	32	Total	O	0	0
			32	32		
10	E	64	Total	O	0	0
			64	64		
10	F	62	Total	O	0	0
			62	62		

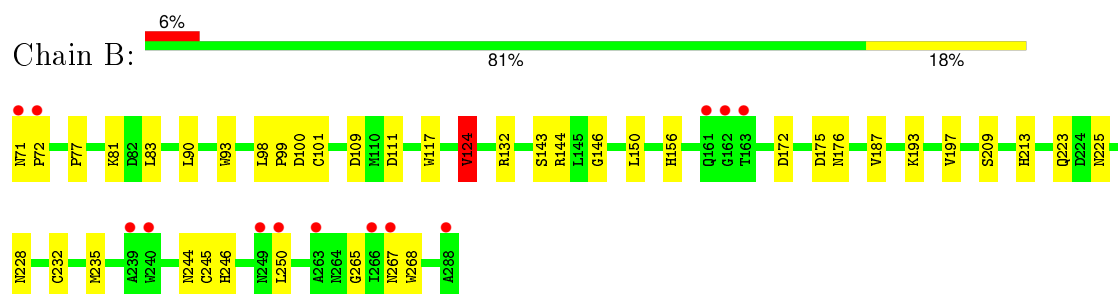
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

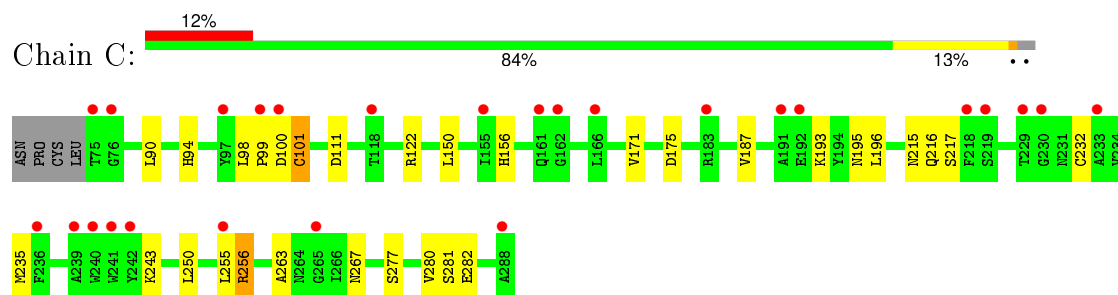
• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2

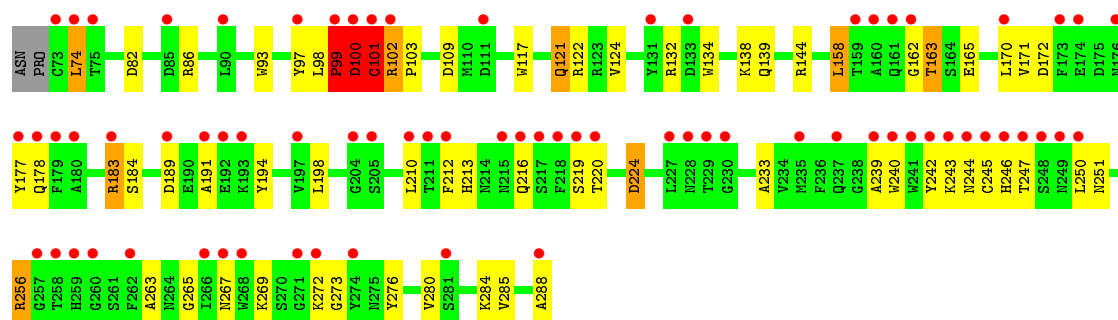


• Molecule 1: FICOLIN-2

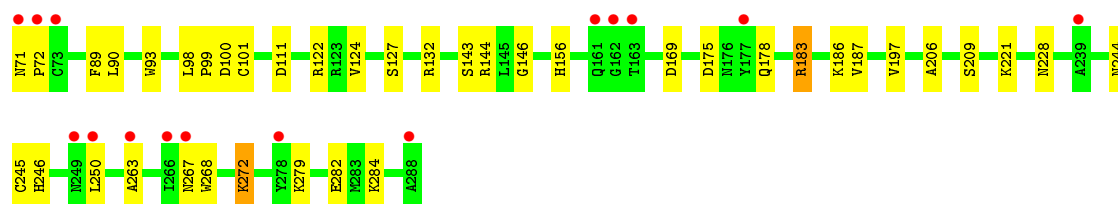
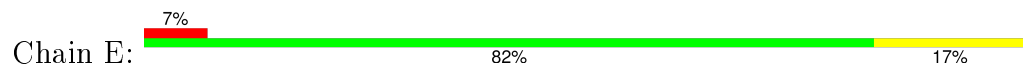


• Molecule 1: FICOLIN-2

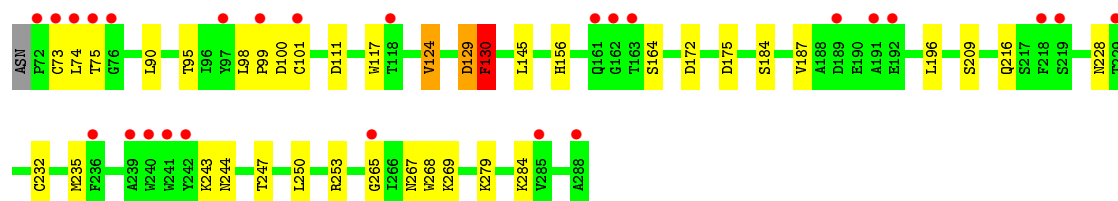
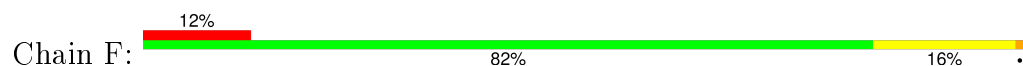




• Molecule 1: FICOLIN-2



• Molecule 1: FICOLIN-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	96.08 Å 96.08 Å 140.98 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.15) 99.1 (19.95-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.15 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.237 0.191 , 0.239	Depositor DCC
R_{free} test set	3923 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
Estimated twinning fraction	0.029 for -h,-k,l 0.470 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78446 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11129	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, GLA, CA, P4C, ACT, EPE, MAN

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	0.95	7/1816 (0.4%)	0.94	10/2455 (0.4%)
1	B	0.44	1/1803 (0.1%)	0.59	1/2439 (0.0%)
1	C	0.40	0/1771	0.59	0/2395
1	D	1.46	2/1785 (0.1%)	0.61	3/2414 (0.1%)
1	E	0.42	0/1800	0.58	0/2436
1	F	0.42	0/1784	0.62	1/2413 (0.0%)
All	All	0.79	10/10759 (0.1%)	0.67	15/14552 (0.1%)

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	A	2	5
1	D	2	4
1	F	0	1
All	All	4	10

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	74	LEU	C-O	57.69	2.33	1.23
1	A	256	ARG	C-O	19.96	1.61	1.23
1	A	100	ASP	CA-CB	-19.80	1.10	1.53
1	D	256	ARG	C-O	16.04	1.53	1.23
1	A	99	PRO	N-CA	-13.59	1.24	1.47
1	A	162	GLY	N-CA	13.58	1.66	1.46
1	A	99	PRO	CA-CB	-10.76	1.32	1.53
1	A	161	GLN	C-N	6.03	1.43	1.33
1	A	100	ASP	CA-C	5.86	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	LYS	CG-CD	5.36	1.70	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	PRO	N-CA-CB	22.13	129.86	103.30
1	A	100	ASP	N-CA-CB	14.57	136.84	110.60
1	D	256	ARG	CA-C-O	-12.66	93.51	120.10
1	A	100	ASP	CB-CA-C	12.09	134.58	110.40
1	A	99	PRO	CA-N-CD	-11.60	95.26	111.50
1	A	256	ARG	CA-C-O	-11.11	96.77	120.10
1	A	256	ARG	O-C-N	-10.52	105.31	123.20
1	D	74	LEU	CA-C-O	-9.72	99.68	120.10
1	A	100	ASP	N-CA-C	-8.37	88.40	111.00
1	A	99	PRO	CA-CB-CG	-8.00	88.80	104.00
1	A	161	GLN	CA-C-O	-6.55	106.35	120.10
1	F	130	PHE	N-CA-C	-5.93	94.98	111.00
1	A	161	GLN	O-C-N	-5.61	113.66	123.20
1	B	81	LYS	CB-CG-CD	-5.39	97.58	111.60
1	D	100	ASP	CB-CG-OD2	5.17	122.96	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	99	PRO	CA
1	A	100	ASP	CA
1	D	100	ASP	CA
1	D	101	CYS	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Peptide
1	A	161	GLN	Mainchain,Peptide
1	A	162	GLY	Peptide
1	A	256	ARG	Mainchain
1	D	100	ASP	Peptide
1	D	256	ARG	Mainchain
1	D	74	LEU	Mainchain
1	D	99	PRO	Peptide
1	F	129	ASP	Peptide

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	1767	0	1636	77	0
1	B	1752	0	1624	38	0
1	C	1721	0	1591	23	0
1	D	1738	0	1608	65	0
1	E	1752	0	1616	43	0
1	F	1736	0	1609	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	8	0	6	10	0
3	C	4	0	3	0	0
3	E	4	0	3	14	0
3	F	4	0	3	0	0
4	B	12	0	12	1	0
4	C	12	0	12	0	0
4	F	12	0	12	1	0
5	B	12	0	12	0	0
5	C	12	0	12	1	0
5	E	12	0	12	5	0
5	F	12	0	12	1	0
6	B	28	0	25	0	0
6	E	28	0	25	2	0
7	B	11	0	10	0	0
7	E	11	0	10	2	0
8	B	22	0	27	3	0
8	C	22	0	27	1	0
8	E	44	0	54	3	0
8	F	22	0	27	4	0
9	C	15	0	15	1	0
9	F	15	0	15	0	0
10	A	29	0	0	10	0
10	B	89	0	0	3	0
10	C	59	0	0	3	0
10	D	32	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	64	0	0	0	0
10	F	62	0	0	2	0
All	All	11129	0	10018	287	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 14.

All (287) 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:101:CYS:CB	1:D:102:ARG:HA	1.24	1.44
1:D:101:CYS:HB3	1:D:102:ARG:CA	1.52	1.36
1:D:101:CYS:CB	1:D:102:ARG:CA	2.15	1.16
1:D:101:CYS:HB2	1:D:102:ARG:HA	1.21	1.13
1:C:255:LEU:O	1:C:277:SER:HB3	1.49	1.13
1:F:73:CYS:CB	1:F:74:LEU:HB2	1.82	1.10
1:F:74:LEU:N	1:F:75:THR:HA	1.58	1.10
1:D:269:LYS:HB3	10:D:2030:HOH:O	1.51	1.09
1:C:243:LYS:HE2	10:C:2036:HOH:O	1.52	1.08
1:F:73:CYS:HB2	1:F:74:LEU:HB2	1.06	1.05
1:A:98:LEU:O	1:A:101:CYS:HA	1.57	1.04
1:D:102:ARG:HB3	1:D:103:PRO:HD2	1.38	1.02
1:A:269:LYS:HE3	10:A:2020:HOH:O	1.61	1.00
1:A:265:GLY:HA3	10:A:2026:HOH:O	1.62	1.00
1:F:216:GLN:HG2	1:F:243:LYS:HE3	1.45	0.97
1:A:243:LYS:C	1:A:245:CYS:H	1.63	0.96
1:D:97:TYR:HD1	1:D:101:CYS:HG	1.15	0.92
1:D:101:CYS:HB3	1:D:102:ARG:HA	0.92	0.91
1:A:169:ASP:OD1	1:A:179:PHE:CD2	2.25	0.89
1:D:101:CYS:HB3	1:D:102:ARG:C	1.93	0.88
1:A:198:LEU:H	1:A:214:ASN:HD21	1.19	0.88
1:B:245:CYS:H	3:B:1290:ACT:CH3	1.87	0.87
1:D:99:PRO:HA	1:D:100:ASP:OD1	1.75	0.87
1:A:198:LEU:H	1:A:214:ASN:ND2	1.73	0.86
1:B:223:GLN:HE21	1:B:225:ASN:HD21	1.21	0.86
1:F:73:CYS:HB2	1:F:74:LEU:CB	2.01	0.84
1:A:191:ALA:O	1:A:192:GLU:HB2	1.75	0.84
1:A:179:PHE:HA	10:A:2016:HOH:O	1.77	0.84
1:C:215:ASN:ND2	9:C:1293:NAG:O5	2.10	0.83
1:C:100:ASP:O	1:C:101:CYS:HB2	1.76	0.82
1:D:138:LYS:HB2	10:D:2022:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:O	1:A:245:CYS:HB2	1.80	0.81
1:A:192:GLU:O	1:A:193:LYS:HG2	1.81	0.80
1:F:232:CYS:HA	1:F:235:MET:HE2	1.64	0.79
1:E:71:ASN:N	1:E:72:PRO:HD2	1.96	0.79
1:A:265:GLY:CA	10:A:2026:HOH:O	2.22	0.77
1:E:246:HIS:H	3:E:1290:ACT:CH3	1.97	0.77
1:E:71:ASN:N	1:E:72:PRO:CD	2.49	0.76
1:B:245:CYS:H	3:B:1290:ACT:H3	1.50	0.76
1:A:169:ASP:HA	1:A:179:PHE:HB3	1.66	0.76
1:A:188:ALA:CB	10:A:2017:HOH:O	2.33	0.76
1:C:156:HIS:HE1	10:C:2029:HOH:O	1.69	0.75
1:B:71:ASN:N	1:B:72:PRO:CD	2.49	0.74
1:A:277:SER:HB2	10:A:2026:HOH:O	1.86	0.74
1:D:244:ASN:N	1:D:245:CYS:HA	2.02	0.74
1:A:160:ALA:O	1:A:186:LYS:HD3	1.88	0.73
1:A:243:LYS:C	1:A:245:CYS:N	2.36	0.73
1:F:100:ASP:O	1:F:101:CYS:HB2	1.88	0.71
1:A:169:ASP:OD1	1:A:179:PHE:HD2	1.72	0.70
1:B:246:HIS:H	3:B:1290:ACT:CH3	2.05	0.69
1:D:224:ASP:HB3	10:D:2028:HOH:O	1.90	0.69
1:E:127:SER:HA	8:F:1294:P4C:H121	1.74	0.69
1:D:102:ARG:CB	1:D:103:PRO:HD2	2.20	0.69
1:C:232:CYS:HA	1:C:235:MET:HE2	1.76	0.68
1:A:266:ILE:N	10:A:2026:HOH:O	2.26	0.68
1:E:246:HIS:H	3:E:1290:ACT:H1	1.58	0.68
1:A:179:PHE:HD1	1:A:179:PHE:N	1.93	0.67
1:F:216:GLN:CG	1:F:243:LYS:HG2	2.24	0.67
1:A:237:GLN:NE2	1:A:264:ASN:HD22	1.93	0.67
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.77	0.66
1:B:197:VAL:HG22	10:B:2040:HOH:O	1.97	0.65
1:D:233:ALA:HB2	10:D:2026:HOH:O	1.96	0.65
1:E:127:SER:HA	8:F:1294:P4C:C12	2.27	0.65
1:E:156:HIS:HD2	1:E:187:VAL:O	1.79	0.65
1:A:172:ASP:HB3	1:A:272:LYS:HE2	1.77	0.65
1:E:221:LYS:HZ1	5:E:1289:GLA:H62	1.62	0.64
1:F:73:CYS:C	1:F:75:THR:HA	2.18	0.64
1:E:122:ARG:HG3	1:E:282:GLU:HG2	1.80	0.64
1:B:156:HIS:HD2	1:B:187:VAL:O	1.80	0.64
1:D:102:ARG:HB3	1:D:103:PRO:CD	2.22	0.64
1:A:210:LEU:HG	1:A:268:TRP:CH2	2.33	0.64
1:B:124:VAL:HG22	8:B:1296:P4C:H172	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:HB3	1:A:243:LYS:HD3	1.79	0.63
1:E:228:ASN:ND2	1:E:244[A]:ASN:OD1	2.26	0.63
1:D:243:LYS:HG2	1:D:244:ASN:N	2.14	0.63
1:D:212:PHE:HD1	10:D:2025:HOH:O	1.82	0.62
1:B:246:HIS:H	3:B:1290:ACT:H1	1.63	0.62
1:C:122:ARG:HD2	1:C:282:GLU:OE2	1.99	0.62
1:C:255:LEU:O	1:C:277:SER:CB	2.37	0.61
1:A:179:PHE:CD1	1:A:179:PHE:N	2.67	0.61
1:B:245:CYS:HB2	3:B:1290:ACT:CH3	2.31	0.61
1:F:216:GLN:HG2	1:F:243:LYS:CE	2.25	0.61
1:D:134:TRP:HA	1:D:220:THR:HG21	1.82	0.61
1:E:246:HIS:H	3:E:1290:ACT:H3	1.65	0.61
1:A:188:ALA:HB3	10:A:2017:HOH:O	1.94	0.60
1:A:167:ARG:NH2	1:A:179:PHE:CD2	2.69	0.60
1:E:183:ARG:O	1:E:183:ARG:HD3	2.01	0.60
1:D:183:ARG:HG3	1:D:183:ARG:HH11	1.67	0.59
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.83	0.59
1:F:156:HIS:HE1	10:F:2036:HOH:O	1.84	0.59
1:D:246:HIS:ND1	10:D:2029:HOH:O	2.32	0.59
1:D:82:ASP:O	1:D:86:ARG:HB2	2.02	0.59
1:B:143:SER:HB2	5:C:1290:GLA:O5	2.03	0.59
1:F:253:ARG:NH2	10:F:2056:HOH:O	2.35	0.59
1:D:194:TYR:CE2	10:D:2022:HOH:O	2.52	0.58
1:B:245:CYS:HB2	3:B:1290:ACT:H1	1.84	0.58
1:D:219:SER:HB2	10:D:2026:HOH:O	2.03	0.58
1:A:188:ALA:HB1	1:A:192:GLU:OE1	2.04	0.58
1:A:191:ALA:O	1:A:192:GLU:CB	2.47	0.58
1:A:132:ARG:NH2	1:B:111:ASP:OD1	2.37	0.57
1:F:74:LEU:N	1:F:75:THR:CA	2.48	0.57
1:F:100:ASP:O	1:F:101:CYS:CB	2.53	0.56
1:F:156:HIS:HD2	1:F:187:VAL:O	1.88	0.56
1:A:101:CYS:O	1:A:101:CYS:SG	2.63	0.56
1:D:194:TYR:HE2	10:D:2022:HOH:O	1.86	0.56
1:E:245:CYS:HB2	3:E:1290:ACT:H1	1.86	0.56
1:E:221:LYS:HZ3	5:E:1289:GLA:H5	1.71	0.56
1:D:272:LYS:HD3	1:D:276:TYR:CD2	2.40	0.56
1:B:223:GLN:NE2	1:B:225:ASN:HD21	1.97	0.56
1:B:245:CYS:H	3:B:1290:ACT:H2	1.67	0.56
1:D:172:ASP:CB	1:D:272:LYS:HE3	2.37	0.55
1:D:121[A]:GLN:OE1	1:D:251:ASN:OD1	2.24	0.55
1:D:97:TYR:HD1	1:D:101:CYS:SG	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:SER:HB2	5:F:1290:GLA:O5	2.05	0.55
1:B:71:ASN:N	1:B:72:PRO:HD3	2.20	0.55
1:B:209:SER:HB2	1:B:268:TRP:CE2	2.42	0.54
1:E:245:CYS:N	3:E:1290:ACT:H2	2.16	0.54
1:F:74:LEU:H	1:F:75:THR:HA	1.61	0.54
1:A:243:LYS:O	1:A:245:CYS:N	2.40	0.54
1:C:156:HIS:HD2	1:C:187:VAL:O	1.89	0.54
1:F:279:LYS:HE3	8:F:1294:P4C:H52	1.90	0.54
1:D:98:LEU:O	1:D:100:ASP:N	2.36	0.53
1:A:167:ARG:NH2	1:A:179:PHE:CE2	2.57	0.53
1:A:210:LEU:HG	1:A:268:TRP:HH2	1.71	0.53
1:E:272:LYS:HE3	8:E:1296:P4C:H92	1.91	0.53
1:A:73:CYS:O	1:A:78:ARG:HD3	2.08	0.53
1:B:245:CYS:N	3:B:1290:ACT:CH3	2.67	0.53
1:D:170:LEU:O	1:D:177:TYR:O	2.25	0.53
1:D:219:SER:CB	10:D:2026:HOH:O	2.57	0.52
1:E:132:ARG:HB3	5:E:1289:GLA:HO1	1.74	0.52
1:B:246:HIS:H	3:B:1290:ACT:H3	1.75	0.52
1:B:144:ARG:NH2	1:C:94:HIS:NE2	2.57	0.52
1:C:193:LYS:CB	1:C:217:SER:HB3	2.39	0.52
1:A:247:THR:O	1:A:269:LYS:HG2	2.10	0.52
1:D:172:ASP:HB3	1:D:272:LYS:HE3	1.92	0.52
1:D:121[A]:GLN:HG3	1:D:122:ARG:N	2.17	0.52
1:A:172:ASP:CB	1:A:272:LYS:HE2	2.39	0.52
1:F:209:SER:HB3	1:F:247:THR:HG22	1.92	0.52
1:E:132:ARG:HD2	5:E:1289:GLA:H3	1.91	0.51
1:E:132:ARG:NH2	1:F:111:ASP:OD2	2.41	0.51
1:A:72:PRO:HA	1:A:99:PRO:HB3	1.91	0.51
1:E:186:LYS:HB3	1:E:197:VAL:HB	1.92	0.50
1:E:169:ASP:OD2	1:E:284:LYS:NZ	2.42	0.50
1:B:244:ASN:HB3	10:B:2063:HOH:O	2.10	0.50
1:E:209:SER:HB2	1:E:268:TRP:CE2	2.46	0.50
1:E:244[A]:ASN:N	1:E:245:CYS:HA	2.27	0.50
1:A:216:GLN:HG2	1:A:243:LYS:NZ	2.27	0.50
1:D:246:HIS:HE1	1:D:263:ALA:O	1.95	0.49
1:E:245:CYS:N	3:E:1290:ACT:CH3	2.62	0.49
1:E:244[B]:ASN:N	1:E:245:CYS:HA	2.28	0.49
1:A:117:TRP:CZ3	1:A:286:ARG:HG2	2.48	0.49
1:B:132:ARG:HH22	1:C:111:ASP:CG	2.15	0.49
1:A:160:ALA:O	1:A:161:GLN:HG2	2.12	0.49
1:C:98:LEU:HB3	1:C:99:PRO:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:GLY:H	1:F:267:ASN:HD21	1.60	0.49
1:F:117:TRP:HB3	1:F:284:LYS:HB2	1.95	0.48
1:E:245:CYS:HB2	3:E:1290:ACT:CH3	2.42	0.48
1:A:82:ASP:O	1:A:86:ARG:HG3	2.13	0.48
1:D:265:GLY:H	1:D:267:ASN:HD21	1.62	0.48
1:F:175:ASP:OD2	8:F:1294:P4C:H151	2.13	0.48
1:C:193:LYS:HB2	1:C:217:SER:HB3	1.94	0.48
1:E:178:GLN:HB3	1:E:206:ALA:HB2	1.95	0.48
1:F:98:LEU:HB3	1:F:99:PRO:CD	2.43	0.48
1:A:188:ALA:O	1:A:194:TYR:HA	2.13	0.47
1:C:263:ALA:HA	1:C:267:ASN:ND2	2.28	0.47
1:F:209:SER:HB2	1:F:268:TRP:CE2	2.49	0.47
1:E:100:ASP:O	1:E:101:CYS:HB2	2.14	0.47
1:A:212[B]:PHE:N	1:A:212[B]:PHE:CD2	2.82	0.47
1:A:198:LEU:N	1:A:214:ASN:ND2	2.53	0.47
1:A:227:LEU:HG	1:A:243:LYS:HG3	1.96	0.47
1:A:187:VAL:HA	1:A:195:ASN:O	2.15	0.47
1:A:113:ASP:OD2	1:A:167:ARG:NH1	2.47	0.47
1:D:244:ASN:N	1:D:245:CYS:CA	2.76	0.47
1:A:121[A]:GLN:OE1	1:A:251:ASN:OD1	2.33	0.47
1:B:100:ASP:O	1:B:101:CYS:HB2	2.15	0.47
1:D:99:PRO:CA	1:D:100:ASP:OD1	2.56	0.47
1:E:175:ASP:OD1	8:E:1295:P4C:H112	2.14	0.47
1:A:240:TRP:CH2	1:A:250:LEU:HB2	2.50	0.46
1:A:263:ALA:HB2	1:A:274:TYR:HB3	1.96	0.46
1:D:98:LEU:HB3	1:D:99:PRO:HD2	1.96	0.46
1:A:156:HIS:HD2	1:A:187:VAL:O	1.98	0.46
1:D:243:LYS:CG	1:D:244:ASN:N	2.77	0.46
6:E:1293:NAG:O4	7:E:1294:MAN:H2	2.15	0.46
1:A:192:GLU:C	1:A:193:LYS:HG2	2.35	0.46
1:A:195:ASN:HB3	10:A:2017:HOH:O	2.15	0.46
1:A:178:GLN:HB3	1:A:206:ALA:HB2	1.97	0.46
1:A:165:GLU:O	1:A:285:VAL:HA	2.15	0.46
1:D:242:TYR:HD2	10:D:2026:HOH:O	1.98	0.46
1:A:263:ALA:HA	1:A:267:ASN:ND2	2.31	0.46
1:B:144:ARG:NH1	10:B:2028:HOH:O	2.48	0.46
1:D:101:CYS:HB2	1:D:102:ARG:CA	2.14	0.46
1:D:102:ARG:CB	1:D:103:PRO:CD	2.88	0.46
1:A:212[B]:PHE:N	1:A:212[B]:PHE:HD2	2.14	0.46
1:F:216:GLN:HG3	1:F:243:LYS:HG2	1.96	0.45
1:A:214:ASN:O	1:A:216:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:C	1:D:224:ASP:OD1	2.54	0.45
1:A:216:GLN:HG2	1:A:243:LYS:HZ2	1.82	0.45
1:A:244:ASN:O	1:A:245:CYS:CB	2.60	0.45
1:C:171:VAL:HB	1:C:280:VAL:HB	1.98	0.45
1:A:134:TRP:HA	1:A:220:THR:HG21	1.99	0.45
1:E:221:LYS:NZ	5:E:1289:GLA:H62	2.30	0.45
1:F:164:SER:O	1:F:184:SER:HA	2.17	0.45
1:A:213:HIS:CE1	1:A:246:HIS:HA	2.52	0.44
1:D:139:GLN:HG2	1:E:89:PHE:CE2	2.52	0.44
1:B:265:GLY:H	1:B:267:ASN:HD21	1.65	0.44
1:D:100:ASP:N	1:D:100:ASP:OD1	2.50	0.44
1:A:188:ALA:N	10:A:2017:HOH:O	2.21	0.44
1:B:109:ASP:HB3	1:B:117:TRP:HB2	1.99	0.44
1:A:193:LYS:HG3	1:A:217:SER:CB	2.47	0.44
1:B:71:ASN:N	1:B:72:PRO:HD2	2.30	0.44
8:B:1296:P4C:H52	8:B:1296:P4C:H21A	1.37	0.44
1:D:247:THR:HB	10:D:2030:HOH:O	2.17	0.44
1:D:98:LEU:CD2	1:D:158:LEU:HD13	2.47	0.44
6:E:1293:NAG:O4	7:E:1294:MAN:C2	2.65	0.44
1:D:240:TRP:CH2	1:D:250:LEU:HB2	2.52	0.44
1:F:216:GLN:HE21	1:F:243:LYS:HE2	1.83	0.44
1:C:175:ASP:HB3	8:C:1294:P4C:H171	1.99	0.44
1:F:129:ASP:OD1	1:F:130:PHE:N	2.51	0.44
1:D:189:ASP:OD1	1:D:191:ALA:HB3	2.18	0.44
1:F:73:CYS:CB	1:F:101:CYS:HG	2.30	0.43
1:F:216:GLN:CG	1:F:243:LYS:CG	2.96	0.43
1:D:171:VAL:HB	1:D:280:VAL:HB	1.99	0.43
1:F:216:GLN:HG2	1:F:243:LYS:HG2	2.01	0.43
1:B:93:TRP:CZ2	1:B:144:ARG:HA	2.53	0.43
1:E:132:ARG:HH22	1:F:111:ASP:CG	2.21	0.43
1:D:165:GLU:O	1:D:285:VAL:HA	2.18	0.43
1:D:162:GLY:O	1:D:163:THR:HG22	2.19	0.43
1:D:269:LYS:HA	1:D:273:GLY:HA2	2.01	0.43
1:A:247:THR:HB	1:A:269:LYS:HE2	1.99	0.43
4:B:1289:EPE:H62	4:B:1289:EPE:H102	1.56	0.43
1:A:98:LEU:O	1:A:101:CYS:CA	2.48	0.42
1:D:213:HIS:CE1	1:D:246:HIS:HA	2.54	0.42
4:F:1289:EPE:H21	4:F:1289:EPE:H101	1.68	0.42
1:B:132:ARG:NH2	1:C:111:ASP:OD2	2.48	0.42
1:D:132:ARG:NH2	1:E:111:ASP:OD1	2.52	0.42
1:A:227:LEU:CD1	1:A:243:LYS:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:HIS:N	3:E:1290:ACT:H1	2.29	0.42
1:B:77:PRO:HG3	1:B:83:LEU:HD21	2.00	0.42
1:C:187:VAL:HA	1:C:195:ASN:O	2.20	0.42
1:B:175:ASP:OD1	8:B:1296:P4C:H112	2.20	0.42
1:D:243:LYS:N	1:D:245:CYS:O	2.26	0.42
1:A:73:CYS:HB3	1:A:78:ARG:HG2	2.01	0.42
1:C:216:GLN:HB2	1:C:243:LYS:HE3	2.02	0.42
1:A:243:LYS:HD2	1:A:243:LYS:HA	1.82	0.42
1:A:159:THR:O	1:A:160:ALA:C	2.58	0.42
1:E:122:ARG:HD2	1:E:282:GLU:OE2	2.20	0.42
1:D:117:TRP:HB3	1:D:284:LYS:HB2	2.02	0.42
1:E:263:ALA:HA	1:E:267:ASN:ND2	2.34	0.42
1:A:167:ARG:HE	1:A:179:PHE:HD2	1.68	0.41
1:A:133:ASP:HB2	1:A:222:ASP:OD2	2.19	0.41
1:D:93:TRP:CZ2	1:D:144:ARG:HA	2.55	0.41
1:B:193:LYS:HD3	1:B:225:ASN:CG	2.41	0.41
1:F:145:LEU:HD12	1:F:145:LEU:N	2.34	0.41
1:E:156:HIS:CD2	1:E:187:VAL:O	2.67	0.41
1:E:93:TRP:CZ2	1:E:144:ARG:HA	2.56	0.41
1:B:232:CYS:HA	1:B:235:MET:HE3	2.03	0.41
1:C:256:ARG:H	1:C:256:ARG:HG3	1.52	0.41
1:B:172:ASP:OD2	1:B:176:ASN:HB2	2.21	0.41
1:F:172:ASP:C	1:F:172:ASP:OD1	2.58	0.41
1:A:236:PHE:HE2	1:A:245:CYS:SG	2.43	0.41
1:B:245:CYS:HB2	3:B:1290:ACT:H2	2.03	0.41
1:C:122:ARG:NH2	10:C:2015:HOH:O	2.38	0.41
1:A:109:ASP:HB3	1:A:117:TRP:HB2	2.01	0.41
1:D:243:LYS:C	1:D:245:CYS:HA	2.40	0.41
1:D:239:ALA:O	1:D:251:ASN:HB2	2.19	0.41
1:A:286:ARG:O	1:A:287:PRO:C	2.58	0.41
1:B:98:LEU:HB3	1:B:99:PRO:HD2	2.03	0.41
1:E:246:HIS:C	1:E:246:HIS:CD2	2.93	0.41
1:B:213:HIS:CE1	1:B:246:HIS:HA	2.56	0.41
1:E:279:LYS:HZ2	8:E:1295:P4C:H52	1.86	0.41
1:F:228:ASN:ND2	1:F:244:ASN:OD1	2.53	0.41
1:D:198:LEU:HD22	1:D:210:LEU:HG	2.03	0.41
1:D:165:GLU:HG3	1:D:288:ALA:CB	2.51	0.40
1:E:272:LYS:HE2	1:E:272:LYS:HB3	1.83	0.40
1:D:216:GLN:HE22	1:D:243:LYS:HG3	1.86	0.40
1:F:247:THR:HG23	1:F:269:LYS:HB3	2.02	0.40
1:B:228:ASN:ND2	1:B:244:ASN:OD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:CYS:H	1:F:74:LEU:C	2.25	0.40
1:D:109:ASP:HB3	1:D:117:TRP:HB2	2.03	0.40
1:A:156:HIS:CD2	1:A:187:VAL:O	2.74	0.40
1:E:98:LEU:HB3	1:E:99:PRO:HD2	2.03	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	218/218 (100%)	188 (86%)	22 (10%)	8 (4%)	4	1
1	B	217/218 (100%)	207 (95%)	8 (4%)	2 (1%)	21	13
1	C	213/218 (98%)	201 (94%)	11 (5%)	1 (0%)	34	26
1	D	215/218 (99%)	192 (89%)	18 (8%)	5 (2%)	8	2
1	E	217/218 (100%)	204 (94%)	11 (5%)	2 (1%)	21	13
1	F	215/218 (99%)	202 (94%)	12 (6%)	1 (0%)	34	26
All	All	1295/1308 (99%)	1194 (92%)	82 (6%)	19 (2%)	13	6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	GLU
1	A	244	ASN
1	A	245	CYS
1	D	100	ASP
1	D	178	GLN
1	C	256	ARG
1	A	99	PRO
1	A	160	ALA

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Mol	Chain	Res	Type
1	A	100	ASP
1	D	99	PRO
1	D	101	CYS
1	A	163	THR
1	A	124	VAL
1	B	124	VAL
1	E	124	VAL
1	B	146	GLY
1	F	124	VAL
1	D	124	VAL
1	E	146	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	185/183 (101%)	172 (93%)	13 (7%)	19	12
1	B	184/183 (100%)	180 (98%)	4 (2%)	60	63
1	C	180/183 (98%)	174 (97%)	6 (3%)	45	44
1	D	182/183 (100%)	172 (94%)	10 (6%)	27	21
1	E	184/183 (100%)	180 (98%)	4 (2%)	60	63
1	F	182/183 (100%)	176 (97%)	6 (3%)	45	44
All	All	1097/1098 (100%)	1054 (96%)	43 (4%)	40	36

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	99	PRO
1	A	101	CYS
1	A	121[A]	GLN
1	A	121[B]	GLN
1	A	124	VAL
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	179	PHE
1	A	193	LYS
1	A	197	VAL
1	A	229	THR
1	A	243	LYS
1	A	250	LEU
1	B	90	LEU
1	B	124	VAL
1	B	150	LEU
1	B	250	LEU
1	C	90	LEU
1	C	101	CYS
1	C	150	LEU
1	C	196	LEU
1	C	250	LEU
1	C	281	SER
1	D	100	ASP
1	D	101	CYS
1	D	102	ARG
1	D	121[A]	GLN
1	D	121[B]	GLN
1	D	158	LEU
1	D	163	THR
1	D	183	ARG
1	D	184	SER
1	D	224	ASP
1	E	90	LEU
1	E	183	ARG
1	E	250	LEU
1	E	272	LYS
1	F	90	LEU
1	F	95	THR
1	F	124	VAL
1	F	130	PHE
1	F	196	LEU
1	F	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	195	ASN
1	A	214	ASN
1	A	228	ASN
1	A	237	GLN
1	A	246	HIS
1	A	267	ASN
1	B	71	ASN
1	B	156	HIS
1	B	225	ASN
1	B	246	HIS
1	B	267	ASN
1	C	156	HIS
1	C	195	ASN
1	C	223	GLN
1	C	267	ASN
1	D	156	HIS
1	D	195	ASN
1	D	216	GLN
1	D	246	HIS
1	D	267	ASN
1	E	156	HIS
1	E	161	GLN
1	E	246	HIS
1	E	267	ASN
1	E	275	ASN
1	F	156	HIS
1	F	195	ASN
1	F	216	GLN
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 ⓘ

4 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	$\# Z > 2$
6	NAG	B	1293	1,6	14,14,15	0.57	0	15,19,21	0.97	1 (6%)
6	NAG	B	1294	6	14,14,15	0.37	0	15,19,21	0.95	0
6	NAG	E	1292	1,6	14,14,15	0.66	0	15,19,21	1.13	1 (6%)
6	NAG	E	1293	6	14,14,15	0.51	0	15,19,21	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
6	NAG	B	1293	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1294	6	-	0/6/23/26	0/1/1/1
6	NAG	E	1292	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1293	6	-	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(°)
6	E	1292	NAG	C3-C4-C5	-2.95	105.05	110.20
6	B	1293	NAG	C3-C4-C5	-2.74	105.42	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1293	NAG	2	0

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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$
4	EPE	B	1289	-	11,12,15	0.46	0	12,16,20	1.90	2 (16%)
3	ACT	B	1290	-	1,3,3	0.30	0	0,3,3	0.00	-
5	GLA	B	1291	-	12,12,12	0.64	0	17,17,17	0.83	0
7	MAN	B	1295	-	11,11,12	0.55	0	14,15,17	0.71	0
8	P4C	B	1296	-	21,21,21	1.25	2 (9%)	19,20,20	0.43	0
3	ACT	B	407	-	1,3,3	1.48	0	0,3,3	0.00	-
4	EPE	C	1289	-	11,12,15	0.45	0	12,16,20	1.38	3 (25%)
5	GLA	C	1290	-	12,12,12	0.51	0	17,17,17	0.52	0
3	ACT	C	1291	-	1,3,3	1.27	0	0,3,3	0.00	-
9	NAG	C	1293	-	15,15,15	0.45	0	17,21,21	0.65	0
8	P4C	C	1294	-	21,21,21	1.27	2 (9%)	19,20,20	0.40	0
5	GLA	E	1289	-	12,12,12	0.77	0	17,17,17	1.48	2 (11%)
3	ACT	E	1290	-	1,3,3	0.08	0	0,3,3	0.00	-
7	MAN	E	1294	-	11,11,12	0.58	0	14,15,17	1.31	3 (21%)
8	P4C	E	1295	-	21,21,21	1.25	2 (9%)	19,20,20	0.49	0
8	P4C	E	1296	-	21,21,21	1.28	2 (9%)	19,20,20	0.41	0
4	EPE	F	1289	-	11,12,15	0.36	0	12,16,20	1.58	3 (25%)
5	GLA	F	1290	-	12,12,12	0.49	0	17,17,17	0.69	0
3	ACT	F	1291	-	1,3,3	1.23	0	0,3,3	0.00	-
9	NAG	F	1293	-	15,15,15	0.50	0	17,21,21	0.85	0
8	P4C	F	1294	-	21,21,21	1.27	2 (9%)	19,20,20	0.40	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
4	EPE	B	1289	-	-	0/6/14/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	1290	-	-	0/0/0/0	0/0/0/0
5	GLA	B	1291	-	-	0/2/22/22	0/1/1/1
7	MAN	B	1295	-	-	0/2/19/22	0/1/1/1
8	P4C	B	1296	-	-	0/18/19/19	0/0/0/0
3	ACT	B	407	-	-	0/0/0/0	0/0/0/0
4	EPE	C	1289	-	-	0/6/14/19	0/1/1/1
5	GLA	C	1290	-	-	0/2/22/22	0/1/1/1
3	ACT	C	1291	-	-	0/0/0/0	0/0/0/0
9	NAG	C	1293	-	-	0/6/26/26	0/1/1/1
8	P4C	C	1294	-	-	0/18/19/19	0/0/0/0
5	GLA	E	1289	-	-	0/2/22/22	0/1/1/1
3	ACT	E	1290	-	-	0/0/0/0	0/0/0/0
7	MAN	E	1294	-	-	0/2/19/22	0/1/1/1
8	P4C	E	1295	-	-	0/18/19/19	0/0/0/0
8	P4C	E	1296	-	-	0/18/19/19	0/0/0/0
4	EPE	F	1289	-	-	0/6/14/19	0/1/1/1
5	GLA	F	1290	-	-	0/2/22/22	0/1/1/1
3	ACT	F	1291	-	-	0/0/0/0	0/0/0/0
9	NAG	F	1293	-	-	0/6/26/26	0/1/1/1
8	P4C	F	1294	-	-	0/18/19/19	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1294	P4C	O1-C2	-3.62	1.22	1.42
8	E	1296	P4C	O1-C2	-3.59	1.22	1.42
8	C	1294	P4C	O1-C2	-3.52	1.23	1.42
8	E	1295	P4C	O1-C2	-3.50	1.23	1.42
8	B	1296	P4C	O1-C2	-3.48	1.23	1.42
8	F	1294	P4C	O22-C21	3.77	1.44	1.19
8	C	1294	P4C	O22-C21	3.77	1.44	1.19
8	E	1296	P4C	O22-C21	3.77	1.44	1.19
8	E	1295	P4C	O22-C21	3.78	1.44	1.19
8	B	1296	P4C	O22-C21	3.80	1.44	1.19

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1289	EPE	O1S-S-C10	2.14	108.73	106.91
7	E	1294	MAN	C2-C3-C4	2.23	114.82	111.04
7	E	1294	MAN	C1-C2-C3	2.56	112.57	109.54
4	C	1289	EPE	C5-N4-C3	2.58	118.89	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	1294	MAN	C3-C4-C5	2.62	114.77	110.20
4	C	1289	EPE	O2S-S-C10	2.71	109.21	106.91
4	F	1289	EPE	O2S-S-C10	2.81	109.30	106.91
4	F	1289	EPE	C5-N4-C3	2.92	120.02	110.33
4	F	1289	EPE	O1S-S-C10	3.04	109.50	106.91
5	E	1289	GLA	C4-C3-C2	3.22	116.80	110.79
4	B	1289	EPE	C5-N4-C3	3.25	121.12	110.33
5	E	1289	GLA	C3-C4-C5	3.81	116.83	110.20
4	B	1289	EPE	O2S-S-C10	5.01	111.18	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1289	EPE	1	0
3	B	1290	ACT	10	0
8	B	1296	P4C	3	0
5	C	1290	GLA	1	0
9	C	1293	NAG	1	0
8	C	1294	P4C	1	0
5	E	1289	GLA	5	0
3	E	1290	ACT	14	0
7	E	1294	MAN	2	0
8	E	1295	P4C	2	0
8	E	1296	P4C	1	0
4	F	1289	EPE	1	0
5	F	1290	GLA	1	0
8	F	1294	P4C	4	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	217/218 (99%)	1.90	89 (41%) 0 1	28, 38, 45, 52	0
1	B	218/218 (100%)	0.37	13 (5%) 25 34	34, 38, 44, 53	2 (0%)
1	C	214/218 (98%)	0.55	26 (12%) 6 9	32, 38, 45, 51	1 (0%)
1	D	216/218 (99%)	1.77	73 (33%) 0 1	28, 38, 45, 58	1 (0%)
1	E	218/218 (100%)	0.35	15 (6%) 20 27	32, 38, 45, 53	0
1	F	217/218 (99%)	0.63	26 (11%) 6 9	32, 38, 46, 63	0
All	All	1300/1308 (99%)	0.93	242 (18%) 2 3	28, 38, 45, 63	4 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	LEU	10.7
1	A	229	THR	10.0
1	D	229	THR	9.2
1	F	75	THR	8.7
1	A	244	ASN	8.3
1	A	179	PHE	8.1
1	D	101	CYS	7.9
1	F	74	LEU	7.5
1	D	102	ARG	7.5
1	A	216	GLN	7.4
1	F	73	CYS	7.3
1	A	271	GLY	7.0
1	A	227	LEU	7.0
1	D	212	PHE	7.0
1	D	260	GLY	7.0
1	A	218	PHE	6.7
1	C	99	PRO	6.6
1	A	100	ASP	6.6
1	D	218	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	100	ASP	6.3
1	D	73	CYS	6.2
1	F	161	GLN	6.2
1	C	162	GLY	6.2
1	F	162	GLY	6.0
1	A	260	GLY	6.0
1	D	227	LEU	5.9
1	A	73	CYS	5.9
1	A	240	TRP	5.8
1	A	241	TRP	5.8
1	A	74	LEU	5.7
1	D	191	ALA	5.7
1	D	177	TYR	5.6
1	A	250	LEU	5.5
1	D	241	TRP	5.4
1	D	240	TRP	5.3
1	A	268	TRP	5.2
1	A	258	THR	5.1
1	A	245	CYS	5.1
1	C	161	GLN	5.1
1	A	163	THR	5.1
1	D	228	ASN	5.0
1	D	230	GLY	5.0
1	A	191	ALA	5.0
1	A	192	GLU	4.9
1	D	160	ALA	4.9
1	D	250	LEU	4.8
1	A	101	CYS	4.8
1	D	271	GLY	4.8
1	D	258	THR	4.8
1	E	250	LEU	4.8
1	A	212[A]	PHE	4.8
1	D	243	LYS	4.8
1	A	288	ALA	4.7
1	A	72	PRO	4.7
1	D	162	GLY	4.7
1	D	288	ALA	4.6
1	B	250	LEU	4.6
1	A	177	TYR	4.5
1	A	160	ALA	4.5
1	A	193	LYS	4.5
1	F	99	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	216	GLN	4.4
1	F	72	PRO	4.4
1	E	266	ILE	4.3
1	C	242	TYR	4.2
1	A	243	LYS	4.2
1	C	76	GLY	4.2
1	D	245	CYS	4.1
1	A	197	VAL	4.0
1	D	111	ASP	4.0
1	D	193	LYS	4.0
1	B	266	ILE	4.0
1	A	228	ASN	3.9
1	C	229	THR	3.9
1	E	72	PRO	3.9
1	D	244	ASN	3.9
1	A	248	SER	3.8
1	A	249	ASN	3.8
1	C	75	THR	3.8
1	B	71	ASN	3.7
1	A	99	PRO	3.7
1	D	178	GLN	3.7
1	D	173	PHE	3.6
1	D	268	TRP	3.6
1	F	242	TYR	3.6
1	A	262	PHE	3.6
1	F	229	THR	3.6
1	B	288	ALA	3.6
1	A	230	GLY	3.5
1	D	211	THR	3.5
1	D	249	ASN	3.5
1	A	259	HIS	3.5
1	D	239	ALA	3.5
1	E	71	ASN	3.5
1	A	239	ALA	3.5
1	A	266	ILE	3.5
1	A	102	ARG	3.4
1	D	219	SER	3.4
1	D	179	PHE	3.4
1	D	266	ILE	3.4
1	D	176	ASN	3.3
1	F	236	PHE	3.3
1	D	259	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	111	ASP	3.3
1	F	288	ALA	3.3
1	D	161	GLN	3.3
1	B	72	PRO	3.3
1	A	215	ASN	3.2
1	A	211	THR	3.2
1	D	174	GLU	3.2
1	E	161	GLN	3.2
1	A	180	ALA	3.2
1	F	239	ALA	3.2
1	D	192	GLU	3.2
1	D	90	LEU	3.2
1	E	163	THR	3.1
1	A	161	GLN	3.1
1	D	215	ASN	3.1
1	A	75	THR	3.1
1	A	174	GLU	3.0
1	D	248	SER	3.0
1	A	261	SER	3.0
1	B	162	GLY	3.0
1	D	242	TYR	3.0
1	D	262	PHE	3.0
1	A	221	LYS	3.0
1	A	205	SER	3.0
1	E	263	ALA	3.0
1	A	257	GLY	2.9
1	A	242	TYR	2.9
1	A	267	ASN	2.9
1	A	263	ALA	2.9
1	A	269	LYS	2.9
1	A	97	TYR	2.9
1	F	76	GLY	2.9
1	A	272	LYS	2.9
1	A	90	LEU	2.9
1	D	75	THR	2.9
1	D	85	ASP	2.8
1	F	285	VAL	2.8
1	B	163	THR	2.8
1	C	236	PHE	2.8
1	C	97	TYR	2.8
1	F	218	PHE	2.8
1	C	230	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	210	LEU	2.8
1	D	204	GLY	2.7
1	C	239	ALA	2.7
1	A	217	SER	2.7
1	C	288	ALA	2.7
1	D	99	PRO	2.7
1	A	170	LEU	2.7
1	C	255	LEU	2.7
1	F	240	TRP	2.7
1	C	100	ASP	2.7
1	D	217	SER	2.7
1	A	224	ASP	2.6
1	A	223	GLN	2.6
1	C	219	SER	2.6
1	F	265	GLY	2.6
1	D	220	THR	2.6
1	A	133	ASP	2.6
1	E	162	GLY	2.6
1	B	239	ALA	2.6
1	E	239	ALA	2.6
1	E	267	ASN	2.6
1	C	191	ALA	2.5
1	D	197	VAL	2.5
1	D	97	TYR	2.5
1	F	219	SER	2.5
1	B	249	ASN	2.5
1	A	162	GLY	2.5
1	E	288	ALA	2.5
1	A	237	GLN	2.5
1	A	256	ARG	2.4
1	A	173	PHE	2.4
1	E	177	TYR	2.4
1	A	220	THR	2.4
1	C	118	THR	2.4
1	A	281	SER	2.4
1	D	274	TYR	2.4
1	A	226	ASP	2.4
1	F	191	ALA	2.4
1	A	214	ASN	2.4
1	A	183[A]	ARG	2.4
1	A	270	SER	2.4
1	D	180	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	155	ILE	2.3
1	A	277	SER	2.3
1	A	98	LEU	2.3
1	D	237	GLN	2.3
1	F	118	THR	2.3
1	F	101	CYS	2.3
1	D	281	SER	2.3
1	B	263	ALA	2.3
1	F	97	TYR	2.3
1	A	85	ASP	2.3
1	A	189	ASP	2.3
1	A	231	ASN	2.3
1	D	189	ASP	2.3
1	C	265	GLY	2.3
1	E	73	CYS	2.3
1	C	218	PHE	2.2
1	A	171	VAL	2.2
1	A	247	THR	2.2
1	D	159	THR	2.2
1	D	183	ARG	2.2
1	A	251	ASN	2.2
1	B	267	ASN	2.2
1	E	249	ASN	2.2
1	C	183	ARG	2.2
1	A	159	THR	2.2
1	A	232	CYS	2.2
1	F	241	TRP	2.2
1	F	163	THR	2.2
1	A	178	GLN	2.1
1	B	161	GLN	2.1
1	D	246	HIS	2.1
1	D	205	SER	2.1
1	D	257	GLY	2.1
1	D	267	ASN	2.1
1	D	131	TYR	2.1
1	E	278	TYR	2.1
1	C	192[A]	GLU	2.1
1	D	133	ASP	2.1
1	A	209	SER	2.1
1	A	185	PHE	2.1
1	A	274	TYR	2.1
1	C	233	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	235	MET	2.1
1	D	247	THR	2.1
1	F	192	GLU	2.1
1	C	166	LEU	2.1
1	A	253	ARG	2.1
1	A	175	ASP	2.1
1	F	189	ASP	2.1
1	C	240	TRP	2.0
1	A	219	SER	2.0
1	D	272	LYS	2.0
1	B	240	TRP	2.0
1	C	241	TRP	2.0
1	D	170	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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
6	NAG	B	1293	14/15	0.86	0.26	9.27	41,43,44,45	0
6	NAG	E	1292	14/15	0.94	0.20	4.30	35,36,39,41	0
6	NAG	B	1294	14/15	0.91	0.33	-	44,45,47,47	0
6	NAG	E	1293	14/15	0.92	0.29	-	38,40,42,42	0

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. 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
5	GLA	E	1289	12/12	0.67	0.45	14.81	53,57,59,59	0
4	EPE	C	1289	12/15	0.89	0.39	10.35	51,53,53,54	0
8	P4C	E	1296	22/22	0.78	0.40	9.09	50,54,56,57	0
4	EPE	F	1289	12/15	0.91	0.38	7.10	47,49,51,52	0
8	P4C	C	1294	22/22	0.58	0.39	6.52	62,66,69,70	0
5	GLA	C	1290	12/12	0.83	0.29	5.91	52,54,55,55	0
5	GLA	F	1290	12/12	0.83	0.22	3.68	51,53,54,55	0
5	GLA	B	1291	12/12	0.78	0.27	3.13	45,47,47,48	0
8	P4C	F	1294	22/22	0.72	0.39	3.10	59,59,62,62	0
8	P4C	E	1295	22/22	0.71	0.29	2.99	50,53,62,62	0
8	P4C	B	1296	22/22	0.78	0.29	2.69	47,51,56,57	0
3	ACT	C	1291	4/4	0.95	0.22	1.13	36,36,36,37	0
3	ACT	F	1291	4/4	0.94	0.20	0.51	36,36,37,38	0
3	ACT	B	1290	4/4	0.96	0.16	0.38	36,37,37,38	0
2	CA	B	1292	1/1	0.99	0.12	0.22	26,26,26,26	0
2	CA	F	1292	1/1	0.99	0.16	-0.11	40,40,40,40	0
2	CA	D	1289	1/1	0.96	0.27	-0.70	62,62,62,62	0
2	CA	A	1289	1/1	0.52	0.29	-0.83	83,83,83,83	0
2	CA	C	1292	1/1	0.98	0.11	-0.84	42,42,42,42	0
3	ACT	E	1290	4/4	0.97	0.11	-0.90	37,38,38,39	0
2	CA	E	1291	1/1	1.00	0.10	-1.18	23,23,23,23	0
9	NAG	F	1293	15/15	0.27	0.44	-	67,69,70,70	0
9	NAG	C	1293	15/15	0.63	0.40	-	64,65,66,66	0
4	EPE	B	1289	12/15	0.85	0.47	-	59,64,65,65	0
3	ACT	B	407	4/4	0.81	0.40	-	67,67,67,67	0
7	MAN	B	1295	11/12	0.31	0.48	-	82,83,83,83	0
7	MAN	E	1294	11/12	0.63	0.40	-	59,59,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.