



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:04 PM UTC

PDB ID : 2PUQ / pdb_00002puq
Title : Crystal structure of active site inhibited coagulation factor VIIA in complex with soluble tissue factor
Authors : Bjelke, J.R.; Rasmussen, H.B.
Deposited on : 2007-05-09
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

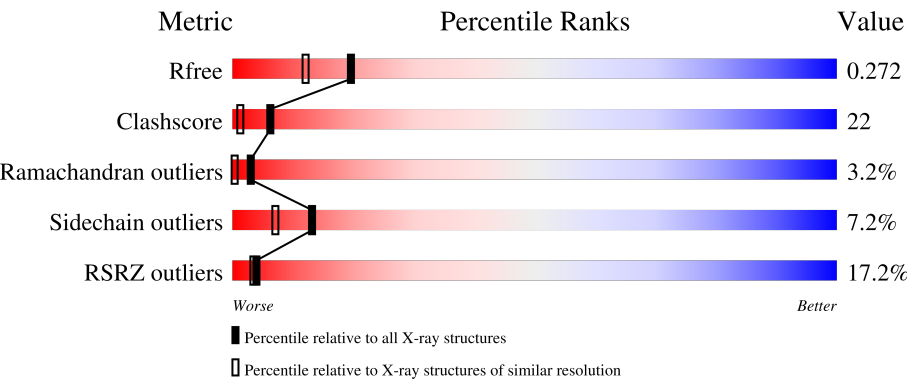
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	L	94	18% 65% 27% 9%
2	H	254	5% 62% 27% 9% •
3	T	204	31% 50% 36% 5% • 7%
4	I	5	20% 20% 40% 20%

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
5	BGC	L	143	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4306 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 Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	94	Total	C	N	O	S	0	0	0
			695	417	121	144	13			

- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	254	Total	C	N	O	S	0	0	0
			1917	1219	335	350	13			

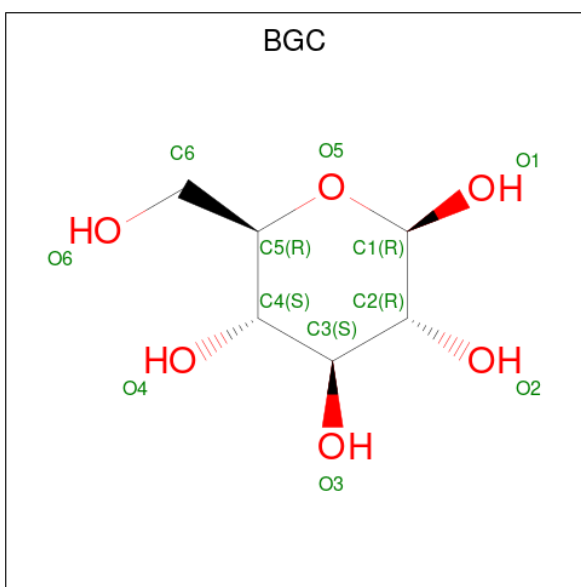
- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	190	Total	C	N	O	S	1	0	0
			1454	921	233	296	4			

- Molecule 4 is a protein called TRP-TYR-THR-ARG CHLOROMETHYLKETONE INHIBITOR.

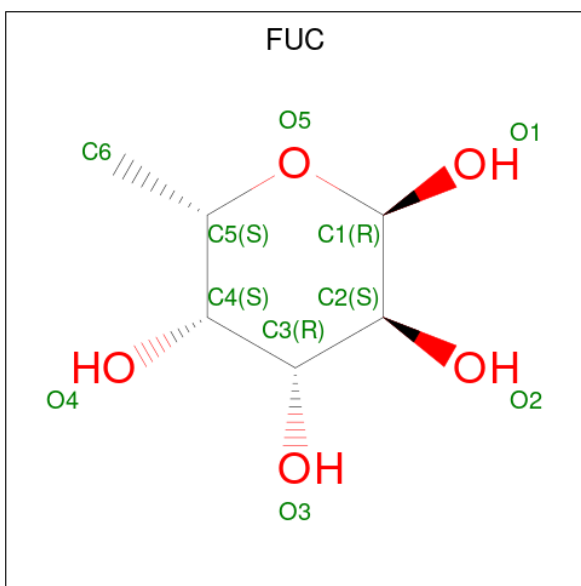
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	4	Total	C	N	O	0	0	1
			31	20	6	5			

- Molecule 5 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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

- Molecule 6 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total 1	Ca 1	0	0

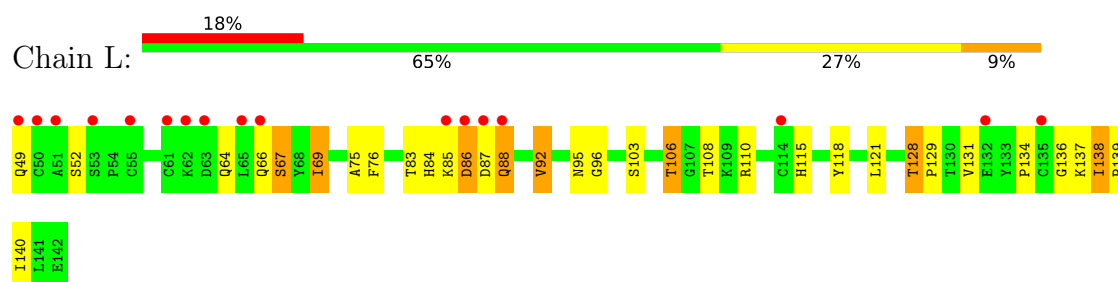
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	27	Total 27	O 27	0	0
8	H	103	Total 103	O 103	0	0
8	T	56	Total 56	O 56	0	0
8	I	1	Total 1	O 1	0	0

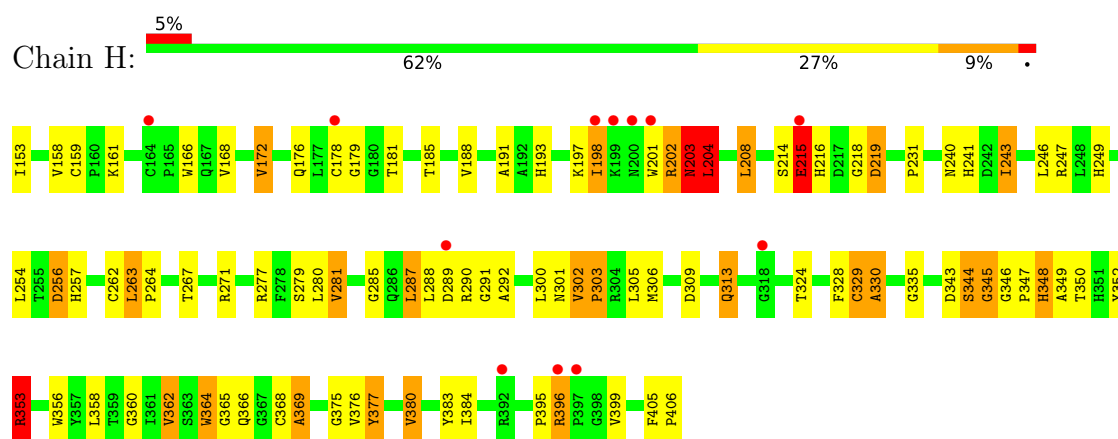
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

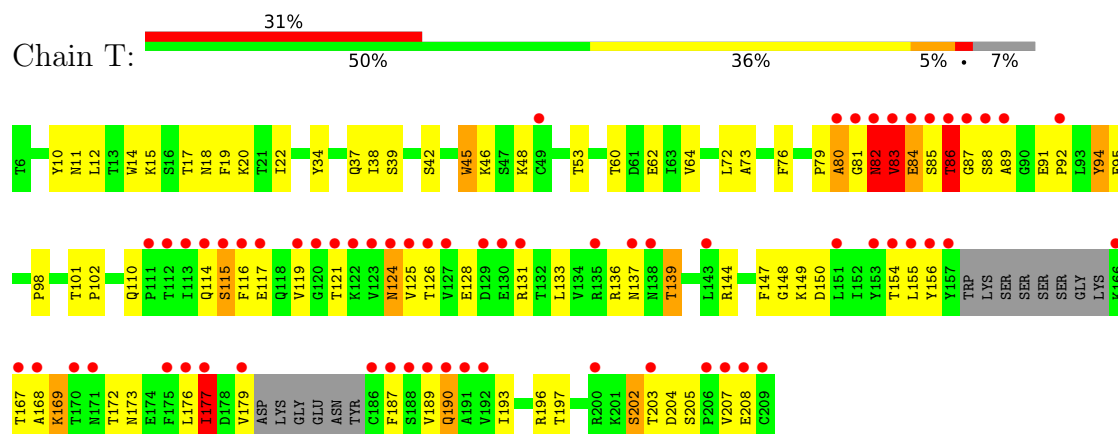
• Molecule 1: Coagulation factor VII



• Molecule 2: Coagulation factor VII

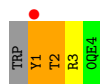


• Molecule 3: Tissue factor



- Molecule 4: TRP-TYR-THR-ARG CHLOROMETHYLKETONE INHIBITOR

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.31Å 68.83Å 78.73Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	39.15 – 2.05 39.15 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.15-2.05) 99.6 (39.15-2.05)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.273 0.229 , 0.272	Depositor DCC
R_{free} test set	2626 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.891	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.036 for h,-k,-l 0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, 0QE, FUC, AR7, CA

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	L	1.33	4/708 (0.6%)	1.28	6/956 (0.6%)
2	H	1.95	35/1966 (1.8%)	1.77	47/2683 (1.8%)
3	T	1.35	6/1484 (0.4%)	1.26	6/2027 (0.3%)
4	I	0.86	0/19	1.51	0/25
All	All	1.65	45/4177 (1.1%)	1.53	59/5691 (1.0%)

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	L	0	1
2	H	1	5
3	T	0	2
All	All	1	8

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	330	ALA	N-CA	20.98	1.71	1.46
2	H	302	VAL	CA-CB	19.39	1.79	1.54
3	T	15	LYS	CE-NZ	-12.15	1.12	1.49
2	H	303	PRO	CA-CB	-11.47	1.39	1.53
2	H	329	CYS	CA-C	11.25	1.66	1.52
2	H	330	ALA	C-O	11.13	1.37	1.23
2	H	362	VAL	CA-CB	-9.44	1.43	1.54
2	H	346	GLY	N-CA	9.03	1.57	1.44
2	H	285	GLY	C-O	8.79	1.31	1.23
2	H	362	VAL	CB-CG2	8.69	1.81	1.52
1	L	137	LYS	N-CA	7.81	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	377	TYR	CD1-CE1	7.74	1.61	1.38
3	T	83	VAL	N-CA	7.66	1.55	1.46
2	H	280	LEU	C-O	-6.82	1.15	1.24
3	T	94	TYR	CA-C	-6.67	1.44	1.52
2	H	350	THR	CB-OG1	6.61	1.54	1.43
2	H	262	CYS	N-CA	6.45	1.54	1.46
2	H	324	THR	CA-CB	-6.13	1.44	1.53
2	H	328	PHE	C-N	6.01	1.42	1.33
2	H	257	HIS	C-O	-5.96	1.16	1.24
2	H	376	VAL	CA-CB	5.89	1.61	1.54
3	T	42	SER	CA-C	5.88	1.59	1.52
2	H	305	LEU	C-O	5.76	1.31	1.24
2	H	324	THR	C-O	-5.74	1.17	1.23
2	H	301	ASN	C-N	5.74	1.39	1.33
2	H	345	GLY	CA-C	5.71	1.59	1.51
2	H	216	HIS	CA-C	-5.70	1.46	1.52
2	H	349	ALA	CA-CB	5.68	1.64	1.53
2	H	188	VAL	C-O	5.60	1.29	1.24
2	H	313	GLN	CB-CG	-5.51	1.35	1.52
2	H	300	LEU	C-O	-5.45	1.17	1.23
3	T	22	ILE	CA-C	-5.41	1.45	1.52
1	L	108	THR	CA-CB	5.36	1.63	1.53
2	H	246	LEU	C-O	5.36	1.30	1.24
2	H	208	LEU	C-O	-5.34	1.17	1.23
2	H	303	PRO	N-CA	-5.29	1.40	1.47
2	H	303	PRO	N-CD	-5.27	1.40	1.47
2	H	380	VAL	CA-CB	5.19	1.61	1.54
3	T	45	TRP	CA-CB	-5.17	1.45	1.53
2	H	288	LEU	N-CA	-5.16	1.39	1.46
1	L	106	THR	C-O	-5.14	1.17	1.24
2	H	344	SER	CA-C	-5.12	1.46	1.52
1	L	95	ASN	CG-OD1	5.06	1.33	1.23
2	H	350	THR	CA-C	5.05	1.58	1.52
2	H	287	LEU	C-N	5.04	1.39	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	345	GLY	N-CA-C	-13.90	98.15	114.69
2	H	330	ALA	N-CA-C	-13.71	87.81	108.79
2	H	289	ASP	CA-C-N	-11.74	103.87	122.65
2	H	289	ASP	C-N-CA	-11.74	103.87	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	302	VAL	CA-C-N	11.71	132.64	119.99
2	H	302	VAL	C-N-CA	11.71	132.64	119.99
2	H	303	PRO	CA-C-O	-11.28	107.94	121.48
2	H	328	PHE	CA-C-O	-9.48	111.31	121.45
2	H	329	CYS	CA-C-O	-8.30	111.74	121.11
2	H	303	PRO	CB-CA-C	-8.28	99.18	110.85
2	H	330	ALA	N-CA-CB	-8.24	98.78	111.56
2	H	290	ARG	N-CA-C	7.84	122.56	112.92
2	H	303	PRO	O-C-N	7.63	132.67	123.06
2	H	204	LEU	N-CA-C	7.59	126.97	110.80
2	H	356	TRP	CA-C-O	-7.57	112.61	121.46
3	T	80	ALA	N-CA-C	7.52	126.82	110.80
2	H	329	CYS	O-C-N	7.50	132.94	123.19
2	H	166	TRP	N-CA-C	-7.22	103.63	113.30
2	H	216	HIS	N-CA-CB	6.94	120.50	110.37
2	H	345	GLY	CA-C-N	-6.85	111.11	121.87
2	H	345	GLY	C-N-CA	-6.85	111.11	121.87
1	L	95	ASN	N-CA-C	6.76	121.11	112.86
2	H	328	PHE	N-CA-CB	-6.72	100.95	111.56
2	H	329	CYS	N-CA-C	-6.67	99.05	109.72
2	H	346	GLY	CA-C-N	6.64	128.14	119.84
2	H	346	GLY	C-N-CA	6.64	128.14	119.84
2	H	216	HIS	N-CA-C	-6.56	96.08	107.49
2	H	219	ASP	N-CA-C	6.51	121.22	113.28
2	H	263	LEU	N-CA-C	-6.43	96.96	108.47
2	H	281	VAL	CG1-CB-CG2	-6.33	96.88	110.80
2	H	290	ARG	CB-CA-C	6.33	121.25	110.56
2	H	362	VAL	CA-C-O	-6.18	113.97	121.13
1	L	138	ILE	CA-C-N	6.14	126.03	119.28
1	L	138	ILE	C-N-CA	6.14	126.03	119.28
2	H	179	GLY	N-CA-C	-6.12	102.91	112.58
2	H	376	VAL	N-CA-C	6.09	117.07	108.36
2	H	291	GLY	N-CA-C	6.08	121.31	112.55
2	H	356	TRP	N-CA-C	-6.08	100.24	109.85
2	H	369	ALA	N-CA-C	-6.04	105.87	113.23
1	L	92	VAL	N-CA-C	-5.91	106.00	112.80
2	H	353	ARG	N-CA-C	5.77	123.09	110.80
2	H	329	CYS	N-CA-CB	-5.72	101.30	111.08
2	H	302	VAL	N-CA-CB	-5.56	103.42	111.21
2	H	329	CYS	CB-CA-C	-5.56	98.38	109.33
2	H	257	HIS	N-CA-CB	5.54	119.85	110.49
3	T	95	GLU	O-C-N	5.53	129.56	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	178	CYS	CA-CB-SG	-5.44	101.89	114.40
3	T	207	VAL	N-CA-C	5.44	116.71	109.37
2	H	353	ARG	N-CA-CB	-5.39	101.39	110.49
2	H	366	GLN	CB-CA-C	-5.34	102.22	111.30
1	L	96	GLY	N-CA-C	-5.26	107.73	115.30
2	H	257	HIS	N-CA-C	-5.25	99.61	110.80
3	T	86	THR	N-CA-C	-5.24	102.77	110.52
3	T	167	THR	N-CA-C	5.14	117.83	109.24
2	H	203	ASN	CB-CA-C	-5.12	104.19	112.07
1	L	136	GLY	N-CA-C	-5.11	107.22	115.08
2	H	159	CYS	N-CA-C	-5.10	101.88	109.42
2	H	301	ASN	N-CA-C	5.06	116.55	108.41
3	T	83	VAL	N-CA-C	5.02	119.78	109.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	290	ARG	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	203	ASN	Peptide
2	H	215	GLU	Peptide
2	H	218	GLY	Peptide
2	H	256	ASP	Peptide
2	H	364	TRP	Peptide
1	L	86	ASP	Peptide
3	T	79	PRO	Peptide
3	T	82	ASN	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	L	695	0	610	26	0
2	H	1917	0	1840	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1454	0	1359	85	0
4	I	31	0	30	3	0
5	L	11	0	10	1	0
6	L	10	0	10	1	0
7	H	1	0	0	0	0
8	H	103	0	0	4	0
8	I	1	0	0	0	0
8	L	27	0	0	1	0
8	T	56	0	0	6	0
All	All	4306	0	3859	178	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 22.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:302:VAL:CA	2:H:302:VAL:CB	1.79	1.60
2:H:362:VAL:CB	2:H:362:VAL:CG2	1.81	1.55
2:H:330:ALA:N	2:H:330:ALA:CA	1.71	1.50
2:H:214:SER:O	2:H:215:GLU:HB3	1.57	1.03
3:T:84:GLU:HG3	3:T:85:SER:HB2	1.02	1.01
2:H:365:GLY:O	4:I:1:TYR:HB2	1.61	1.01
2:H:353:ARG:NH2	8:H:1075:HOH:O	1.96	0.98
2:H:158:VAL:O	8:H:1082:HOH:O	1.80	0.98
3:T:114:GLN:HG2	3:T:128:GLU:HB2	1.46	0.95
2:H:330:ALA:N	2:H:330:ALA:C	2.24	0.95
3:T:84:GLU:CG	3:T:85:SER:HB2	1.96	0.94
3:T:84:GLU:HG3	3:T:85:SER:CB	1.96	0.93
3:T:124:ASN:O	3:T:124:ASN:ND2	2.03	0.92
2:H:302:VAL:CA	2:H:302:VAL:CG2	2.53	0.86
3:T:87:GLY:H	3:T:88:SER:HB2	1.39	0.86
3:T:46:LYS:HD3	3:T:62:GLU:OE2	1.76	0.85
2:H:405:PHE:HA	2:H:406:PRO:C	2.02	0.85
2:H:302:VAL:CA	2:H:302:VAL:CG1	2.56	0.83
1:L:64:GLN:N	1:L:67:SER:O	2.12	0.82
3:T:86:THR:HG22	3:T:89:ALA:H	1.42	0.82
1:L:76:PHE:HE1	1:L:84:HIS:CD2	1.99	0.80
2:H:330:ALA:N	2:H:330:ALA:CB	2.43	0.80
2:H:362:VAL:CG2	2:H:362:VAL:CG1	2.58	0.80
1:L:49:GLN:O	5:L:143:BGC:O6	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:87:GLY:N	3:T:88:SER:HB2	1.98	0.78
2:H:329:CYS:C	2:H:330:ALA:CA	2.57	0.77
3:T:91:GLU:HB3	3:T:92:PRO:HD2	1.65	0.77
3:T:86:THR:HG23	3:T:88:SER:HB2	1.68	0.75
3:T:83:VAL:O	3:T:84:GLU:HB3	1.87	0.74
3:T:187:PHE:HB2	3:T:208:GLU:O	1.86	0.74
3:T:83:VAL:O	3:T:84:GLU:CB	2.35	0.74
2:H:214:SER:O	2:H:215:GLU:CB	2.33	0.73
2:H:362:VAL:CG2	2:H:362:VAL:CA	2.64	0.73
3:T:80:ALA:HB3	3:T:81:GLY:HA3	1.69	0.73
3:T:80:ALA:CB	3:T:81:GLY:HA3	2.19	0.73
3:T:86:THR:HG22	3:T:89:ALA:N	2.05	0.71
3:T:82:ASN:HA	3:T:83:VAL:HG22	1.73	0.71
1:L:49:GLN:NE2	1:L:67:SER:HA	2.05	0.71
3:T:81:GLY:C	3:T:82:ASN:HD22	1.99	0.70
3:T:147:PHE:O	3:T:150:ASP:HB2	1.91	0.70
3:T:202:SER:OG	3:T:203:THR:N	2.21	0.70
2:H:303:PRO:O	2:H:330:ALA:HA	1.92	0.70
3:T:86:THR:CG2	3:T:88:SER:HB2	2.23	0.69
2:H:335:GLY:HA2	2:H:369:ALA:O	1.93	0.69
3:T:48:LYS:HE3	3:T:62:GLU:CG	2.22	0.69
2:H:302:VAL:CB	2:H:302:VAL:C	2.66	0.68
2:H:191:ALA:HB2	2:H:345:GLY:HA2	1.76	0.67
1:L:92:VAL:HG12	1:L:92:VAL:O	1.95	0.66
2:H:302:VAL:CB	2:H:302:VAL:N	2.54	0.66
3:T:86:THR:N	3:T:91:GLU:O	2.28	0.66
2:H:330:ALA:N	2:H:330:ALA:O	2.29	0.65
3:T:86:THR:CG2	3:T:88:SER:CB	2.75	0.65
2:H:153:ILE:N	2:H:343:ASP:OD2	2.30	0.64
3:T:137:ASN:O	3:T:139:THR:HG23	1.98	0.64
2:H:279:SER:HB2	2:H:348:HIS:CE1	2.32	0.64
3:T:189:VAL:HG23	3:T:205:SER:HB3	1.78	0.64
2:H:309:ASP:O	2:H:313:GLN:HG3	1.98	0.64
3:T:88:SER:OG	8:T:265:HOH:O	2.09	0.63
2:H:368:CYS:O	2:H:369:ALA:HB3	1.97	0.63
2:H:396:ARG:HH11	2:H:396:ARG:HB3	1.63	0.63
3:T:34:TYR:HA	3:T:76:PHE:O	1.99	0.63
1:L:139:PRO:HD2	8:H:1043:HOH:O	1.99	0.62
3:T:18:ASN:O	3:T:19:PHE:HB2	2.01	0.61
3:T:60:THR:O	3:T:64:VAL:HG22	2.01	0.61
2:H:329:CYS:HA	2:H:375:GLY:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:THR:O	2:H:271:ARG:HB2	2.00	0.61
1:L:115:HIS:O	1:L:118:TYR:HB2	2.02	0.60
3:T:82:ASN:HD22	3:T:82:ASN:N	2.00	0.60
3:T:86:THR:HG23	3:T:88:SER:CB	2.32	0.59
1:L:76:PHE:CE1	1:L:84:HIS:CD2	2.88	0.59
3:T:20:LYS:HB2	3:T:133:LEU:CD2	2.33	0.58
2:H:176:GLN:OE1	8:H:1020:HOH:O	2.17	0.58
3:T:114:GLN:CG	3:T:128:GLU:HB2	2.28	0.58
2:H:365:GLY:O	4:I:1:TYR:CB	2.45	0.57
2:H:193:HIS:CE1	2:H:344:SER:OG	2.55	0.57
1:L:92:VAL:HG22	2:H:271:ARG:HG2	1.85	0.57
2:H:264:PRO:O	2:H:384:ILE:HD13	2.05	0.57
3:T:48:LYS:HE3	3:T:62:GLU:CD	2.31	0.56
1:L:129:PRO:HB3	1:L:134:PRO:HG3	1.88	0.56
3:T:37:GLN:O	3:T:73:ALA:HA	2.06	0.55
2:H:279:SER:CB	2:H:348:HIS:CE1	2.89	0.55
1:L:110:ARG:HD2	1:L:110:ARG:C	2.31	0.55
3:T:46:LYS:CD	3:T:62:GLU:OE2	2.51	0.55
2:H:405:PHE:CG	2:H:406:PRO:HA	2.42	0.55
3:T:168:ALA:O	3:T:169:LYS:HB2	2.06	0.55
2:H:302:VAL:H	2:H:302:VAL:HG22	1.71	0.55
3:T:39:SER:HB3	3:T:45:TRP:CE3	2.42	0.55
3:T:116:PHE:O	3:T:117:GLU:C	2.50	0.54
2:H:405:PHE:CD1	2:H:406:PRO:HA	2.41	0.54
3:T:86:THR:OG1	8:T:229:HOH:O	2.07	0.54
2:H:306:MET:CE	3:T:91:GLU:HB3	2.38	0.54
3:T:48:LYS:HE3	3:T:62:GLU:HG2	1.89	0.53
1:L:85:LYS:C	1:L:87:ASP:H	2.16	0.53
3:T:114:GLN:O	3:T:115:SER:HB3	2.08	0.53
3:T:80:ALA:CB	3:T:81:GLY:CA	2.86	0.52
2:H:364:TRP:HE3	2:H:365:GLY:H	1.57	0.52
3:T:86:THR:HG22	3:T:88:SER:CB	2.39	0.52
3:T:86:THR:CG2	3:T:88:SER:HB3	2.39	0.52
1:L:92:VAL:HG13	8:L:157:HOH:O	2.09	0.52
2:H:343:ASP:O	2:H:344:SER:C	2.52	0.52
2:H:302:VAL:CG2	2:H:302:VAL:N	2.73	0.51
3:T:155:LEU:HD23	3:T:177:ILE:HD11	1.92	0.51
2:H:181:THR:OG1	2:H:347:PRO:HG3	2.11	0.51
2:H:185:THR:HG22	2:H:254:LEU:HD21	1.91	0.51
3:T:124:ASN:ND2	3:T:124:ASN:C	2.69	0.51
1:L:92:VAL:O	1:L:92:VAL:CG1	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:121:LEU:HD21	1:L:128:THR:HB	1.93	0.50
2:H:201:TRP:O	2:H:202:ARG:C	2.54	0.50
2:H:201:TRP:O	2:H:203:ASN:N	2.44	0.50
2:H:358:LEU:HG	2:H:380:VAL:HG21	1.93	0.50
3:T:114:GLN:O	3:T:114:GLN:CD	2.54	0.50
3:T:76:PHE:CE1	3:T:92:PRO:HG2	2.46	0.50
2:H:377:TYR:CD1	2:H:377:TYR:N	2.80	0.50
1:L:85:LYS:O	1:L:87:ASP:N	2.41	0.50
3:T:86:THR:CG2	8:T:229:HOH:O	2.60	0.49
3:T:82:ASN:CA	3:T:83:VAL:HG22	2.43	0.49
3:T:114:GLN:HG2	3:T:128:GLU:CB	2.31	0.49
3:T:189:VAL:O	3:T:204:ASP:HA	2.13	0.49
1:L:85:LYS:HA	1:L:88:GLN:HE21	1.78	0.48
3:T:72:LEU:HD13	3:T:73:ALA:O	2.13	0.48
3:T:86:THR:HG21	8:T:229:HOH:O	2.12	0.48
1:L:110:ARG:HD2	1:L:110:ARG:O	2.14	0.48
3:T:144:ARG:HG3	3:T:173:ASN:HD21	1.77	0.48
1:L:69:ILE:HD11	3:T:17:THR:HB	1.96	0.47
3:T:114:GLN:O	3:T:115:SER:CB	2.61	0.47
2:H:306:MET:HE1	3:T:92:PRO:HD2	1.97	0.47
2:H:352:TYR:CE2	2:H:353:ARG:HG3	2.49	0.47
2:H:302:VAL:N	2:H:302:VAL:HG22	2.30	0.47
3:T:12:LEU:N	3:T:12:LEU:HD12	2.29	0.47
1:L:138:ILE:HA	1:L:139:PRO:HD3	1.76	0.46
2:H:197:LYS:O	2:H:198:ILE:C	2.58	0.46
2:H:161:LYS:CE	2:H:219:ASP:OD2	2.64	0.46
2:H:153:ILE:HG12	2:H:343:ASP:OD2	2.15	0.46
2:H:247:ARG:NH1	2:H:395:PRO:HG3	2.31	0.46
3:T:76:PHE:HD1	3:T:92:PRO:HB2	1.81	0.46
2:H:201:TRP:C	2:H:203:ASN:N	2.74	0.45
3:T:82:ASN:C	3:T:83:VAL:HG22	2.41	0.45
3:T:144:ARG:HG3	3:T:173:ASN:ND2	2.32	0.45
3:T:53:THR:HG22	8:T:215:HOH:O	2.17	0.45
1:L:66:GLN:O	1:L:67:SER:HB3	2.16	0.45
1:L:69:ILE:O	1:L:69:ILE:HG22	2.16	0.45
1:L:85:LYS:C	1:L:87:ASP:N	2.74	0.44
2:H:240:ASN:O	2:H:241:HIS:HB2	2.18	0.44
2:H:263:LEU:HD12	2:H:263:LEU:HA	1.62	0.44
2:H:279:SER:HB2	2:H:348:HIS:NE2	2.33	0.44
2:H:168:VAL:HG22	2:H:208:LEU:HD11	1.99	0.44
3:T:14:TRP:CD1	3:T:98:PRO:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:GLN:CD	1:L:67:SER:HA	2.44	0.43
2:H:193:HIS:CD2	4:I:2:THR:HG23	2.54	0.43
3:T:101:THR:O	3:T:102:PRO:C	2.62	0.43
3:T:189:VAL:HB	3:T:190:GLN:H	1.64	0.43
3:T:190:GLN:HE21	3:T:190:GLN:HB2	1.49	0.43
3:T:10:TYR:O	3:T:11:ASN:C	2.60	0.42
3:T:81:GLY:CA	3:T:82:ASN:HD22	2.33	0.42
6:L:144:FUC:C1	3:T:131:ARG:HH22	2.32	0.42
3:T:76:PHE:CD1	3:T:94:TYR:HB3	2.54	0.42
3:T:82:ASN:N	3:T:82:ASN:ND2	2.68	0.42
3:T:110:GLN:HB2	3:T:203:THR:HG23	2.01	0.42
2:H:302:VAL:CG1	2:H:302:VAL:N	2.81	0.42
2:H:172:VAL:HG11	2:H:198:ILE:CD1	2.50	0.42
3:T:148:GLY:C	3:T:150:ASP:H	2.28	0.42
3:T:82:ASN:CG	8:T:260:HOH:O	2.62	0.42
3:T:136:ARG:O	3:T:137:ASN:HB2	2.19	0.42
2:H:303:PRO:O	2:H:330:ALA:CA	2.66	0.42
3:T:156:TYR:CD2	3:T:156:TYR:N	2.88	0.41
2:H:302:VAL:CG2	2:H:302:VAL:H	2.32	0.41
3:T:38:ILE:HG12	3:T:39:SER:N	2.35	0.41
3:T:86:THR:HG22	3:T:88:SER:HB3	2.01	0.41
1:L:75:ALA:O	1:L:85:LYS:HB2	2.21	0.41
1:L:129:PRO:HB3	1:L:134:PRO:CG	2.50	0.41
3:T:193:ILE:HB	3:T:196:ARG:HD2	2.02	0.41
2:H:360:GLY:HA2	2:H:380:VAL:HG23	2.02	0.41
2:H:231:PRO:HD3	2:H:243:ILE:O	2.21	0.41
2:H:287:LEU:HD12	2:H:292:ALA:O	2.21	0.40
2:H:201:TRP:C	2:H:203:ASN:H	2.29	0.40
3:T:137:ASN:C	3:T:139:THR:H	2.28	0.40
2:H:241:HIS:HA	2:H:383:TYR:OH	2.22	0.40
2:H:277:ARG:O	2:H:303:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

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	L	92/94 (98%)	83 (90%)	6 (6%)	3 (3%)	3	0
2	H	252/254 (99%)	228 (90%)	18 (7%)	6 (2%)	4	1
3	T	184/204 (90%)	155 (84%)	21 (11%)	8 (4%)	2	0
4	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	529/557 (95%)	467 (88%)	45 (8%)	17 (3%)	3	0

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	198	ILE
2	H	215	GLU
2	H	256	ASP
3	T	83	VAL
3	T	84	GLU
3	T	115	SER
3	T	202	SER
1	L	86	ASP
2	H	202	ARG
2	H	353	ARG
3	T	169	LYS
1	L	67	SER
3	T	149	LYS
1	L	106	THR
2	H	204	LEU
3	T	119	VAL
3	T	177	ILE

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	L	78/82 (95%)	70 (90%)	8 (10%)	7	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	203/216 (94%)	195 (96%)	8 (4%)	28	23
3	T	161/188 (86%)	147 (91%)	14 (9%)	9	4
4	I	2/3 (67%)	0	2 (100%)	0	0
All	All	444/489 (91%)	412 (93%)	32 (7%)	13	7

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	69	ILE
1	L	83	THR
1	L	88	GLN
1	L	103	SER
1	L	128	THR
1	L	131	VAL
1	L	140	ILE
2	H	172	VAL
2	H	204	LEU
2	H	243	ILE
2	H	249	HIS
2	H	281	VAL
2	H	348	HIS
2	H	396	ARG
2	H	399	VAL
3	T	82	ASN
3	T	86	THR
3	T	121	THR
3	T	124	ASN
3	T	125	VAL
3	T	126	THR
3	T	139	THR
3	T	154	THR
3	T	172	THR
3	T	176	LEU
3	T	177	ILE
3	T	179	VAL
3	T	190	GLN
3	T	197	THR
4	I	1	TYR
4	I	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	80	ASN
1	L	84	HIS
1	L	88	GLN
1	L	115	HIS
2	H	176	GLN
2	H	250	GLN
2	H	286	GLN
2	H	308	GLN
2	H	373	HIS
3	T	82	ASN
3	T	173	ASN
3	T	190	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	AR7	I	3	4,2	10,10,11	1.86	3 (30%)	9,11,13	1.81	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AR7	I	3	4,2	-	1/9/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	AR7	C-CA	4.13	1.59	1.52
4	I	3	AR7	O-C	-3.11	1.29	1.42
4	I	3	AR7	CB-CA	2.43	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	AR7	CB-CA-C	-4.93	105.51	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	3	AR7	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
6	FUC	L	144	1	10,10,11	0.69	0	14,14,16	1.47	2 (14%)
5	BGC	L	143	1	11,11,12	0.80	0	15,15,17	1.77	4 (26%)

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	FUC	L	144	1	-	-	0/1/1/1
5	BGC	L	143	1	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	144	FUC	C2-C3-C4	-3.46	104.78	110.86
5	L	143	BGC	C1-O5-C5	3.34	116.66	112.19
5	L	143	BGC	O4-C4-C5	2.86	116.38	109.32
5	L	143	BGC	O5-C5-C6	2.77	113.05	107.66
6	L	144	FUC	O5-C5-C6	2.10	111.97	107.40
5	L	143	BGC	O5-C5-C4	-2.06	105.81	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	143	BGC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	144	FUC	1	0
5	L	143	BGC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	L	94/94 (100%)	0.85	17 (18%) 3 3	15, 38, 73, 84	0
2	H	254/254 (100%)	0.22	12 (4%) 36 36	4, 28, 62, 82	4 (1%)
3	T	190/204 (93%)	1.50	63 (33%) 1 0	12, 48, 99, 112	6 (3%)
4	I	2/5 (40%)	2.45	1 (50%) 0 0	33, 33, 33, 49	0
All	All	540/557 (96%)	0.79	93 (17%) 4 3	4, 34, 88, 112	10 (1%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	138	ASN	8.5
3	T	83	VAL	7.3
3	T	85	SER	6.6
3	T	137	ASN	6.1
1	L	61	CYS	5.5
3	T	177	ILE	5.4
3	T	80	ALA	5.3
3	T	87	GLY	5.3
3	T	179	VAL	5.2
3	T	86	THR	5.2
3	T	207	VAL	5.1
3	T	157	TYR	5.0
3	T	209	CYS	4.9
3	T	187	PHE	4.5
1	L	50	CYS	4.4
3	T	176	LEU	4.2
1	L	63	ASP	4.1
3	T	116	PHE	4.1
3	T	119	VAL	4.0
3	T	113	ILE	3.9
3	T	126	THR	3.9

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Mol	Chain	Res	Type	RSRZ
3	T	125	VAL	3.9
3	T	168	ALA	3.7
3	T	121	THR	3.7
3	T	186	CYS	3.6
1	L	65	LEU	3.6
3	T	166	LYS	3.6
2	H	201	TRP	3.5
3	T	84	GLU	3.4
3	T	189	VAL	3.4
2	H	200	ASN	3.4
1	L	49	GLN	3.4
3	T	175	PHE	3.4
3	T	81	GLY	3.3
4	I	1	TYR	3.2
3	T	88	SER	3.2
3	T	112	THR	3.2
3	T	129	ASP	3.1
3	T	131	ARG	3.1
3	T	115	SER	3.1
3	T	155	LEU	3.1
3	T	135	ARG	3.0
3	T	82	ASN	3.0
3	T	120	GLY	2.9
3	T	156	TYR	2.9
1	L	87	ASP	2.9
3	T	188	SER	2.9
3	T	123	VAL	2.8
3	T	117	GLU	2.8
2	H	396	ARG	2.8
3	T	127	VAL	2.8
2	H	318	GLY	2.7
3	T	122	LYS	2.7
2	H	397	PRO	2.7
3	T	200	ARG	2.7
1	L	66	GLN	2.6
3	T	191	ALA	2.6
3	T	143	LEU	2.6
2	H	178	CYS	2.6
2	H	215	GLU	2.6
3	T	154	THR	2.6
2	H	289	ASP	2.6
1	L	55	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	T	49	CYS	2.6
2	H	392	ARG	2.6
3	T	190	GLN	2.6
1	L	62	LYS	2.6
1	L	51	ALA	2.6
3	T	92	PRO	2.6
1	L	53	SER	2.5
3	T	192	VAL	2.4
3	T	167	THR	2.4
3	T	171	ASN	2.3
2	H	199	LYS	2.3
3	T	111	PRO	2.3
3	T	114	GLN	2.3
2	H	164	CYS	2.3
3	T	89	ALA	2.3
3	T	130	GLU	2.3
1	L	85	LYS	2.2
1	L	86	ASP	2.2
3	T	153	TYR	2.2
1	L	88	GLN	2.2
3	T	170	THR	2.2
3	T	208	GLU	2.1
3	T	206	PRO	2.1
2	H	198	ILE	2.1
1	L	135	CYS	2.1
3	T	151	LEU	2.1
1	L	114	CYS	2.1
1	L	132	GLU	2.1
3	T	203	THR	2.1
3	T	124	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AR7	I	3	11/12	0.89	0.10	22,24,30,31	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	BGC	L	143	11/12	0.76	0.17	71,72,74,76	0
6	FUC	L	144	10/11	0.87	0.11	64,66,66,66	0
7	CA	H	1001	1/1	0.98	0.08	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.