



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:12 PM UTC

PDB ID : 6YXK / pdb_00006yxk
Title : Crystal structure of ACPA 3F3 in complex with cit-vimentin 59-74
Authors : Ge, C.; Holmdahl, R.
Deposited on : 2020-05-03
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 types of validation reports are described at

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

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

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

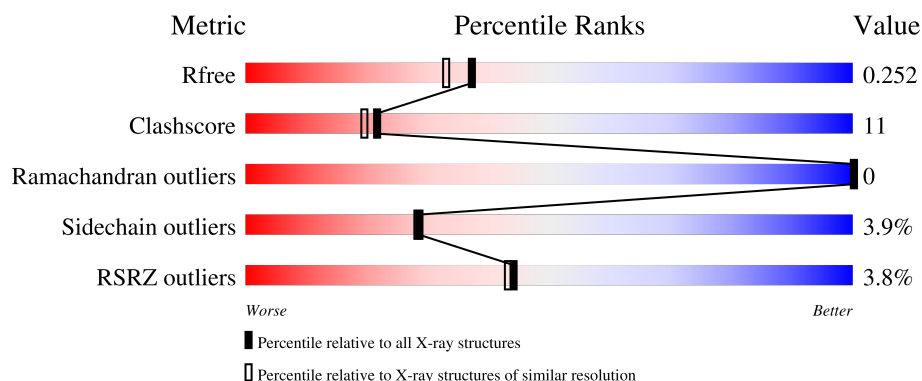
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	223	3% 77% 18% ..
2	B	218	5% 72% 23% ..
3	C	16	6% 44% 6% 6% 44%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7114 atoms, of which 3352 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 ACPA 3F3 Fab fragment - heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	220	Total	C	H	N	O	S	85	0	0
			3271	1056	1617	269	320	9			

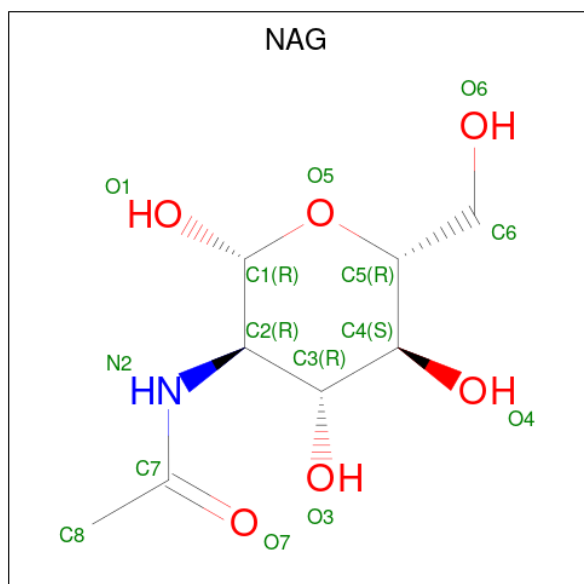
- Molecule 2 is a protein called ACPA 3F3 Fab fragment - light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	218	Total	C	H	N	O	S	109	0	0
			3321	1063	1624	285	343	6			

- Molecule 3 is a protein called Citrullinated Vimentin (59-74).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O		6	0	0
			135	38	69	13	15				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

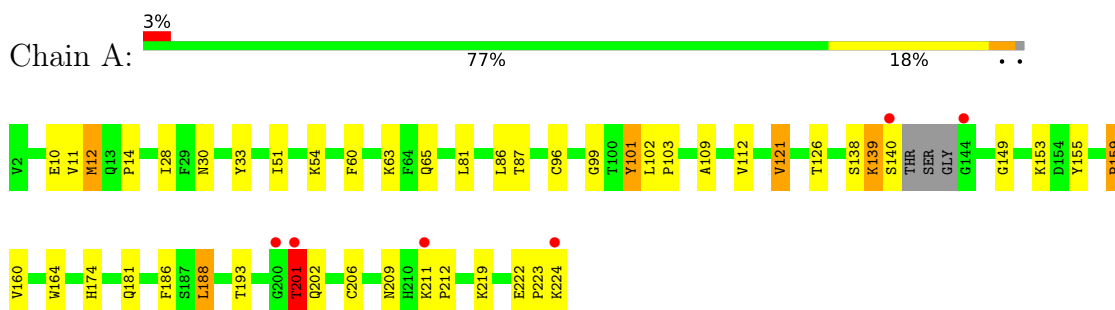
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		
5	B	157	Total	O	0	0
			157	157		
5	C	3	Total	O	0	0
			3	3		

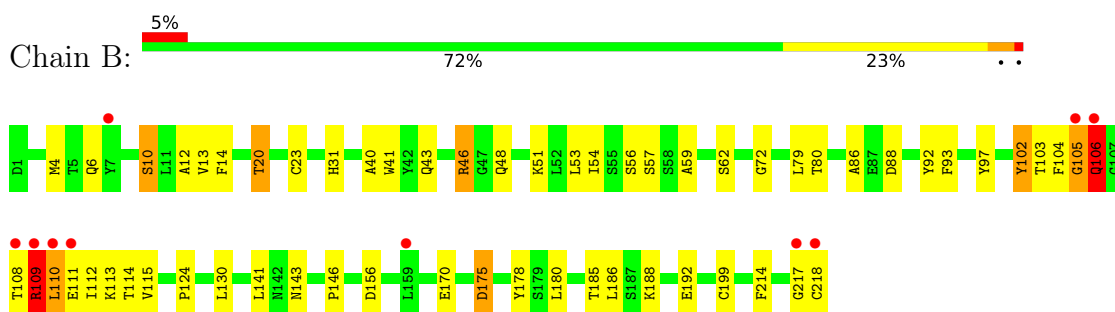
3 Residue-property plots [i](#)

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.

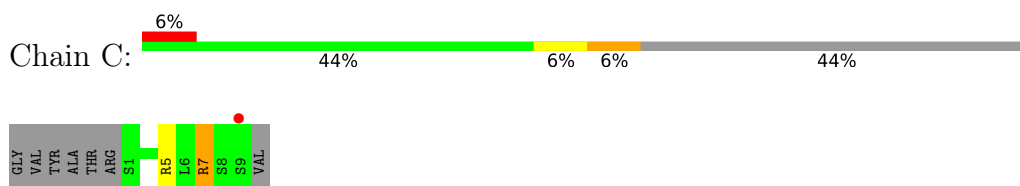
- Molecule 1: ACPA 3F3 Fab fragment - heavy chain



- Molecule 2: ACPA 3F3 Fab fragment - light chain



- Molecule 3: Citrullinated Vimentin (59-74)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.38Å 82.09Å 135.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.28 – 2.00 52.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (52.28-2.00) 99.5 (52.28-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258, REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.253 0.209 , 0.252	Depositor DCC
R_{free} test set	2026 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CIR

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	1.30	8/1698 (0.5%)	1.51	17/2319 (0.7%)
2	B	1.43	16/1735 (0.9%)	1.50	16/2353 (0.7%)
3	C	1.38	0/41	1.49	0/51
All	All	1.37	24/3474 (0.7%)	1.51	33/4723 (0.7%)

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
3	C	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	GLN	N-CA	10.34	1.59	1.46
2	B	105	GLY	C-N	9.50	1.47	1.33
2	B	106	GLN	CA-C	9.05	1.64	1.52
1	A	51	ILE	C-O	-8.22	1.15	1.24
2	B	31	HIS	CE1-NE2	7.40	1.40	1.32
1	A	96	CYS	C-O	7.33	1.32	1.23
2	B	51	LYS	C-O	7.27	1.32	1.24
2	B	41	TRP	C-O	7.14	1.33	1.24
1	A	121	VAL	C-O	6.93	1.31	1.24
2	B	92	TYR	C-O	6.75	1.32	1.24
2	B	93	PHE	C-O	6.47	1.32	1.24
2	B	103	THR	C-O	6.32	1.31	1.23
2	B	178	TYR	C-O	5.82	1.31	1.23
2	B	115	VAL	C-O	-5.71	1.18	1.24
1	A	87	THR	C-O	5.69	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	VAL	C-O	-5.64	1.18	1.24
2	B	102	TYR	C-O	5.59	1.30	1.23
2	B	59	ALA	C-O	5.51	1.30	1.24
2	B	105	GLY	N-CA	5.44	1.53	1.45
1	A	109	ALA	C-O	5.16	1.31	1.23
1	A	81	LEU	C-O	5.16	1.30	1.24
2	B	40	ALA	C-O	5.09	1.30	1.23
1	A	174	HIS	C-O	5.08	1.29	1.24
2	B	156	ASP	C-O	5.06	1.29	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	GLN	N-CA-CB	-11.63	90.83	110.49
2	B	106	GLN	O-C-N	-10.82	108.20	122.59
2	B	109	ARG	CG-CD-NE	-10.39	89.14	112.00
2	B	104	PHE	CA-C-O	-8.04	111.83	121.56
2	B	105	GLY	CA-C-O	-7.59	107.37	120.57
1	A	159	PRO	N-CA-CB	-7.25	94.63	102.60
2	B	106	GLN	N-CA-C	6.86	125.41	110.80
1	A	201	THR	CA-CB-OG1	-6.18	100.33	109.60
2	B	103	THR	N-CA-C	6.12	119.13	110.50
2	B	199	CYS	CA-CB-SG	-5.96	100.68	114.40
1	A	186	PHE	CB-CA-C	5.94	119.66	109.51
2	B	105	GLY	CA-C-N	5.89	132.80	121.54
2	B	105	GLY	C-N-CA	5.89	132.80	121.54
1	A	14	PRO	N-CA-CB	5.88	108.49	103.19
1	A	126	THR	CA-CB-OG1	-5.84	100.83	109.60
1	A	223	PRO	CA-C-O	-5.69	114.86	121.34
1	A	101	TYR	CA-C-N	5.58	127.06	120.09
1	A	101	TYR	C-N-CA	5.58	127.06	120.09
1	A	28	ILE	CA-C-N	5.43	127.86	120.54
1	A	28	ILE	C-N-CA	5.43	127.86	120.54
1	A	206	CYS	CA-C-N	5.42	129.89	122.84
1	A	206	CYS	C-N-CA	5.42	129.89	122.84
2	B	72	GLY	CA-C-O	-5.40	117.96	122.33
1	A	96	CYS	CB-CA-C	5.30	118.45	109.50
1	A	99	GLY	CA-C-N	5.27	128.19	120.71
1	A	99	GLY	C-N-CA	5.27	128.19	120.71
2	B	46	ARG	CG-CD-NE	5.26	123.58	112.00
2	B	175	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	193	THR	CA-CB-OG1	-5.21	101.79	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	146	PRO	CA-C-N	5.07	127.58	120.28
2	B	146	PRO	C-N-CA	5.07	127.58	120.28
2	B	106	GLN	CG-CD-NE2	-5.04	108.84	116.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	7	CIR	Mainchain

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	1654	1617	1610	27	0
2	B	1697	1624	1621	45	0
3	C	66	69	61	0	0
4	A	28	28	26	1	0
4	B	14	14	13	0	0
5	A	143	0	0	5	0
5	B	157	0	0	1	0
5	C	3	0	0	0	0
All	All	3762	3352	3331	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (73) 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:B:105:GLY:C	2:B:106:GLN:HG3	1.54	1.10
2:B:13:VAL:C	2:B:112:ILE:HG22	1.89	0.97
2:B:105:GLY:C	2:B:106:GLN:CG	2.37	0.93
2:B:109:ARG:CZ	2:B:109:ARG:HB3	2.00	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:C	2:B:110:LEU:HD12	2.00	0.86
1:A:10:GLU:HB3	1:A:12:MET:CE	2.06	0.85
2:B:14:PHE:CD1	2:B:112:ILE:HG23	2.12	0.84
2:B:14:PHE:N	2:B:112:ILE:HG22	1.91	0.83
1:A:10:GLU:HB3	1:A:12:MET:HE1	1.61	0.81
2:B:110:LEU:HD12	2:B:110:LEU:O	1.84	0.77
2:B:110:LEU:C	2:B:110:LEU:CD1	2.61	0.74
2:B:12:ALA:CB	2:B:110:LEU:HD11	2.19	0.72
2:B:86:ALA:HA	2:B:111:GLU:OE2	1.90	0.72
2:B:109:ARG:NH1	2:B:109:ARG:HG3	2.05	0.70
2:B:130:LEU:O	2:B:188:LYS:HD3	1.94	0.66
2:B:12:ALA:HB2	2:B:110:LEU:HD11	1.78	0.66
1:A:188:LEU:C	1:A:188:LEU:HD12	2.22	0.65
2:B:88:ASP:O	2:B:109:ARG:NH2	2.30	0.64
2:B:185:THR:O	2:B:186:LEU:HD23	1.97	0.64
2:B:20:THR:HG23	2:B:80:THR:OG1	1.97	0.64
2:B:10:SER:OG	2:B:108:THR:CG2	2.49	0.60
1:A:139:LYS:O	5:A:401:HOH:O	2.16	0.59
1:A:101:TYR:CZ	1:A:103:PRO:HG2	2.38	0.58
1:A:153:LYS:NZ	1:A:181:GLN:OE1	2.35	0.58
2:B:109:ARG:HG3	2:B:109:ARG:HH11	1.66	0.58
2:B:14:PHE:N	2:B:112:ILE:CG2	2.65	0.57
1:A:65:GLN:HG2	5:A:506:HOH:O	2.02	0.57
2:B:109:ARG:CZ	2:B:109:ARG:CB	2.61	0.56
4:A:302:NAG:O6	5:A:402:HOH:O	2.18	0.56
1:A:65:GLN:CG	5:A:506:HOH:O	2.55	0.54
2:B:10:SER:HA	2:B:108:THR:HG22	1.92	0.52
2:B:185:THR:C	2:B:186:LEU:HD23	2.34	0.52
2:B:143:ASN:ND2	2:B:175:ASP:OD2	2.43	0.51
2:B:14:PHE:CG	2:B:112:ILE:HG23	2.45	0.50
2:B:6:GLN:OE1	2:B:106:GLN:N	2.45	0.50
1:A:33:TYR:CE1	1:A:102:LEU:HD13	2.48	0.49
1:A:209:ASN:OD1	1:A:211:LYS:HE3	2.12	0.49
1:A:211:LYS:HB2	1:A:212:PRO:HD3	1.95	0.49
2:B:217:GLY:O	2:B:218:CYS:SG	2.68	0.49
2:B:12:ALA:HA	2:B:110:LEU:HD12	1.94	0.49
2:B:48:GLN:HB3	5:B:545:HOH:O	2.14	0.48
2:B:46:ARG:HD3	2:B:170:GLU:HB3	1.95	0.48
2:B:97:TYR:HA	2:B:102:TYR:CD1	2.49	0.48
1:A:12:MET:HG3	1:A:86:LEU:CD1	2.43	0.47
1:A:201:THR:HG22	1:A:202:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD12	2:B:141:LEU:N	2.28	0.47
2:B:113:LYS:HE2	2:B:114:THR:O	2.15	0.47
1:A:155:TYR:CE1	1:A:160:VAL:HG13	2.50	0.46
2:B:113:LYS:CE	2:B:114:THR:O	2.63	0.46
1:A:30:ASN:HB3	1:A:54:LYS:HE2	1.98	0.46
2:B:12:ALA:HA	2:B:110:LEU:CD1	2.46	0.46
1:A:11:VAL:C	1:A:12:MET:HE2	2.41	0.46
1:A:149:GLY:HA2	1:A:164:TRP:CH2	2.50	0.45
2:B:180:LEU:C	2:B:180:LEU:HD23	2.43	0.44
1:A:12:MET:O	1:A:121:VAL:HA	2.18	0.44
1:A:65:GLN:CD	5:A:506:HOH:O	2.61	0.43
2:B:54:ILE:HD12	2:B:79:LEU:CD1	2.49	0.43
1:A:102:LEU:N	1:A:103:PRO:CD	2.81	0.43
2:B:124:PRO:HB3	2:B:214:PHE:CZ	2.54	0.43
1:A:33:TYR:CE1	1:A:102:LEU:CD1	3.02	0.42
2:B:110:LEU:HD13	2:B:111:GLU:O	2.19	0.42
1:A:201:THR:CG2	1:A:202:GLN:N	2.83	0.42
2:B:4:MET:HE3	2:B:23:CYS:SG	2.59	0.42
2:B:56:SER:O	2:B:57:SER:HB3	2.20	0.42
2:B:12:ALA:HB1	2:B:112:ILE:HB	2.01	0.41
1:A:138:SER:C	1:A:139:LYS:HG2	2.42	0.41
1:A:188:LEU:C	1:A:188:LEU:CD1	2.90	0.41
2:B:43:GLN:HB2	2:B:53:LEU:HD11	2.02	0.41
1:A:139:LYS:O	1:A:140:SER:HB2	2.20	0.41
2:B:130:LEU:O	2:B:188:LYS:CD	2.65	0.41
2:B:56:SER:O	2:B:57:SER:CB	2.68	0.41
1:A:101:TYR:CG	1:A:103:PRO:HD2	2.57	0.40
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.92	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	A	216/223 (97%)	212 (98%)	4 (2%)	0	100	100
2	B	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	C	5/16 (31%)	5 (100%)	0	0	100	100
All	All	437/457 (96%)	424 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	185/187 (99%)	177 (96%)	8 (4%)	26	25
2	B	190/190 (100%)	183 (96%)	7 (4%)	30	30
3	C	6/11 (54%)	6 (100%)	0	100	100
All	All	381/388 (98%)	366 (96%)	15 (4%)	28	28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	63	LYS
1	A	139	LYS
1	A	159	PRO
1	A	188	LEU
1	A	201	THR
1	A	222	GLU
1	A	224	LYS
2	B	10	SER
2	B	20	THR
2	B	62	SER
2	B	106	GLN
2	B	109	ARG
2	B	110	LEU
2	B	192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CIR	C	7	3	9,10,11	1.37	1 (11%)	6,11,13	1.58	2 (33%)
3	CIR	C	5	3	9,10,11	2.19	3 (33%)	6,11,13	1.73	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIR	C	7	3	-	2/8/9/11	-
3	CIR	C	5	3	-	0/8/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	CIR	C7-N6	-5.07	1.27	1.34
3	C	5	CIR	O7-C7	-2.51	1.20	1.24
3	C	5	CIR	O-C	2.46	1.29	1.20
3	C	7	CIR	O-C	2.39	1.29	1.20

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	CIR	O7-C7-N6	-2.70	117.43	121.69
3	C	5	CIR	C5-N6-C7	2.61	126.04	122.64
3	C	7	CIR	N8-C7-N6	2.57	121.15	116.64
3	C	7	CIR	O7-C7-N8	-2.01	119.13	123.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	7	CIR	O7-C7-N6-C5
3	C	7	CIR	N8-C7-N6-C5

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	301	2	14,14,15	0.97	1 (7%)	17,19,21	2.81	9 (52%)
4	NAG	A	302	1	14,14,15	2.16	3 (21%)	17,19,21	3.24	11 (64%)
4	NAG	A	301	1	14,14,15	1.83	3 (21%)	17,19,21	3.36	8 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	301	2	-	1/6/23/26	0/1/1/1
4	NAG	A	302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	301	1	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	NAG	O5-C5	5.98	1.55	1.43
4	A	301	NAG	O5-C5	3.95	1.51	1.43
4	A	302	NAG	O5-C1	3.31	1.49	1.43
4	A	301	NAG	C3-C2	2.61	1.58	1.52
4	A	301	NAG	O4-C4	2.59	1.49	1.43
4	B	301	NAG	O4-C4	2.11	1.48	1.43
4	A	302	NAG	C1-C2	-2.08	1.49	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	NAG	O5-C1-C2	-10.29	95.37	111.29
4	A	302	NAG	O5-C1-C2	-8.05	98.84	111.29
4	B	301	NAG	C1-O5-C5	5.89	120.08	112.19
4	A	302	NAG	C1-O5-C5	5.49	119.55	112.19
4	A	301	NAG	C1-O5-C5	4.79	118.61	112.19
4	B	301	NAG	C2-N2-C7	4.71	129.21	122.90
4	A	301	NAG	C3-C4-C5	-4.69	101.73	110.23
4	B	301	NAG	C3-C4-C5	-4.51	102.05	110.23
4	B	301	NAG	O7-C7-N2	3.67	128.47	121.98
4	A	302	NAG	O7-C7-C8	3.61	128.49	122.05
4	B	301	NAG	O5-C1-C2	3.35	116.47	111.29
4	A	302	NAG	O4-C4-C5	3.25	117.32	109.32
4	A	302	NAG	C1-C2-N2	3.22	115.51	110.43
4	B	301	NAG	C8-C7-N2	-3.11	110.96	116.12
4	A	302	NAG	O3-C3-C2	-3.06	103.05	109.40
4	A	301	NAG	O4-C4-C5	3.06	116.85	109.32
4	A	302	NAG	O5-C5-C6	2.97	113.45	107.66
4	A	302	NAG	O7-C7-N2	-2.91	116.84	121.98
4	B	301	NAG	O6-C6-C5	-2.79	101.83	111.33
4	B	301	NAG	O4-C4-C3	2.52	116.32	110.38
4	A	301	NAG	C1-C2-N2	-2.50	106.50	110.43
4	A	301	NAG	C8-C7-N2	2.42	120.12	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAG	O4-C4-C5	2.37	115.17	109.32
4	A	302	NAG	O3-C3-C4	2.19	115.55	110.38
4	A	301	NAG	O7-C7-N2	-2.17	118.15	121.98
4	A	302	NAG	C4-C3-C2	-2.15	107.86	111.02
4	A	301	NAG	O4-C4-C3	2.12	115.37	110.38
4	A	302	NAG	C2-N2-C7	2.11	125.73	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	NAG	O5-C5-C6-O6
4	A	302	NAG	C4-C5-C6-O6
4	A	301	NAG	C3-C2-N2-C7
4	A	302	NAG	C3-C2-N2-C7
4	A	302	NAG	C1-C2-N2-C7
4	B	301	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	A	220/223 (98%)	0.31	6 (2%) 56 55	23, 33, 48, 70	0
2	B	218/218 (100%)	0.22	10 (4%) 37 36	23, 33, 48, 71	0
3	C	7/16 (43%)	0.99	1 (14%) 6 5	30, 33, 47, 57	0
All	All	445/457 (97%)	0.28	17 (3%) 44 43	23, 33, 48, 71	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	SER	4.9
2	B	218	CYS	3.8
2	B	109	ARG	3.7
1	A	144	GLY	3.3
2	B	106	GLN	3.2
2	B	7	TYR	3.2
2	B	105	GLY	3.2
3	C	9	SER	3.1
1	A	224	LYS	2.9
1	A	201	THR	2.8
2	B	217	GLY	2.7
1	A	200	GLY	2.6
2	B	110	LEU	2.5
2	B	111	GLU	2.4
2	B	108	THR	2.2
2	B	159	LEU	2.1
1	A	211	LYS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIR	C	5	11/12	0.93	0.09	27,33,45,53	2
3	CIR	C	7	11/12	0.94	0.08	25,31,33,35	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(Å ²)	Q<0.9
4	NAG	A	301	14/15	0.69	0.18	30,60,62,64	3
4	NAG	A	302	14/15	0.77	0.15	30,54,55,59	3
4	NAG	B	301	14/15	0.77	0.13	30,59,62,64	3

6.5 Other polymers [i](#)

There are no such residues in this entry.