



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:00 AM UTC

PDB ID : 7K93 / pdb_00007k93
Title : DENV2 NS1 in complex with neutralizing 2B7 single chain Fab variable region (scFv)
Authors : Akey, D.L.; Smith, J.L.
Deposited on : 2020-09-28
Resolution : 2.89 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:

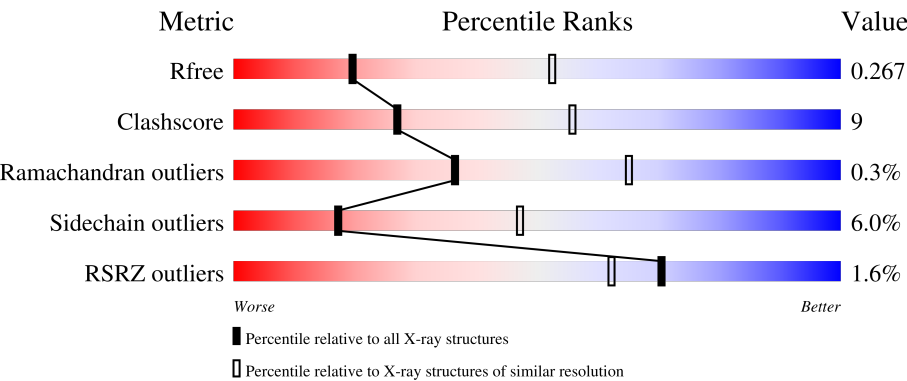
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	376	2% 58% 27% • 13%
1	B	376	2% 66% 20% • 13%
1	C	376	2% 61% 27% • 11%
1	D	376	% 62% 23% • 14%
2	E	251	2% 75% 16% • 7%

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Mol	Chain	Length	Quality of chain
2	G	251	75% 16% • 8%
2	I	251	% 75% 17% • 8%
2	K	251	74% 16% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17581 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2597	1632	450	495	20			
1	B	328	Total	C	N	O	S	0	0	0
			2600	1635	450	495	20			
1	C	335	Total	C	N	O	S	0	0	0
			2642	1663	457	502	20			
1	D	325	Total	C	N	O	S	0	0	0
			2578	1622	446	490	20			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	ALA	-	expression tag	UNP D0EPS0
A	-22	HIS	-	expression tag	UNP D0EPS0
A	-21	HIS	-	expression tag	UNP D0EPS0
A	-20	HIS	-	expression tag	UNP D0EPS0
A	-19	HIS	-	expression tag	UNP D0EPS0
A	-18	HIS	-	expression tag	UNP D0EPS0
A	-17	HIS	-	expression tag	UNP D0EPS0
A	-16	SER	-	expression tag	UNP D0EPS0
A	-15	SER	-	expression tag	UNP D0EPS0
A	-14	GLY	-	expression tag	UNP D0EPS0
A	-13	VAL	-	expression tag	UNP D0EPS0
A	-12	ASP	-	expression tag	UNP D0EPS0
A	-11	LEU	-	expression tag	UNP D0EPS0
A	-10	GLY	-	expression tag	UNP D0EPS0
A	-9	THR	-	expression tag	UNP D0EPS0
A	-8	GLU	-	expression tag	UNP D0EPS0
A	-7	ASN	-	expression tag	UNP D0EPS0
A	-6	LEU	-	expression tag	UNP D0EPS0
A	-5	TYR	-	expression tag	UNP D0EPS0
A	-4	PHE	-	expression tag	UNP D0EPS0
A	-3	GLN	-	expression tag	UNP D0EPS0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D0EPS0
A	-1	ASN	-	expression tag	UNP D0EPS0
B	-23	ALA	-	expression tag	UNP D0EPS0
B	-22	HIS	-	expression tag	UNP D0EPS0
B	-21	HIS	-	expression tag	UNP D0EPS0
B	-20	HIS	-	expression tag	UNP D0EPS0
B	-19	HIS	-	expression tag	UNP D0EPS0
B	-18	HIS	-	expression tag	UNP D0EPS0
B	-17	HIS	-	expression tag	UNP D0EPS0
B	-16	SER	-	expression tag	UNP D0EPS0
B	-15	SER	-	expression tag	UNP D0EPS0
B	-14	GLY	-	expression tag	UNP D0EPS0
B	-13	VAL	-	expression tag	UNP D0EPS0
B	-12	ASP	-	expression tag	UNP D0EPS0
B	-11	LEU	-	expression tag	UNP D0EPS0
B	-10	GLY	-	expression tag	UNP D0EPS0
B	-9	THR	-	expression tag	UNP D0EPS0
B	-8	GLU	-	expression tag	UNP D0EPS0
B	-7	ASN	-	expression tag	UNP D0EPS0
B	-6	LEU	-	expression tag	UNP D0EPS0
B	-5	TYR	-	expression tag	UNP D0EPS0
B	-4	PHE	-	expression tag	UNP D0EPS0
B	-3	GLN	-	expression tag	UNP D0EPS0
B	-2	SER	-	expression tag	UNP D0EPS0
B	-1	ASN	-	expression tag	UNP D0EPS0
C	-23	ALA	-	expression tag	UNP D0EPS0
C	-22	HIS	-	expression tag	UNP D0EPS0
C	-21	HIS	-	expression tag	UNP D0EPS0
C	-20	HIS	-	expression tag	UNP D0EPS0
C	-19	HIS	-	expression tag	UNP D0EPS0
C	-18	HIS	-	expression tag	UNP D0EPS0
C	-17	HIS	-	expression tag	UNP D0EPS0
C	-16	SER	-	expression tag	UNP D0EPS0
C	-15	SER	-	expression tag	UNP D0EPS0
C	-14	GLY	-	expression tag	UNP D0EPS0
C	-13	VAL	-	expression tag	UNP D0EPS0
C	-12	ASP	-	expression tag	UNP D0EPS0
C	-11	LEU	-	expression tag	UNP D0EPS0
C	-10	GLY	-	expression tag	UNP D0EPS0
C	-9	THR	-	expression tag	UNP D0EPS0
C	-8	GLU	-	expression tag	UNP D0EPS0
C	-7	ASN	-	expression tag	UNP D0EPS0

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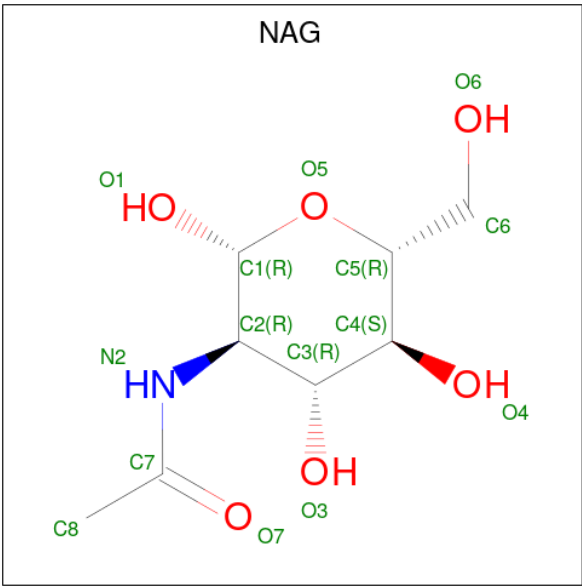
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	expression tag	UNP D0EPS0
C	-5	TYR	-	expression tag	UNP D0EPS0
C	-4	PHE	-	expression tag	UNP D0EPS0
C	-3	GLN	-	expression tag	UNP D0EPS0
C	-2	SER	-	expression tag	UNP D0EPS0
C	-1	ASN	-	expression tag	UNP D0EPS0
D	-23	ALA	-	expression tag	UNP D0EPS0
D	-22	HIS	-	expression tag	UNP D0EPS0
D	-21	HIS	-	expression tag	UNP D0EPS0
D	-20	HIS	-	expression tag	UNP D0EPS0
D	-19	HIS	-	expression tag	UNP D0EPS0
D	-18	HIS	-	expression tag	UNP D0EPS0
D	-17	HIS	-	expression tag	UNP D0EPS0
D	-16	SER	-	expression tag	UNP D0EPS0
D	-15	SER	-	expression tag	UNP D0EPS0
D	-14	GLY	-	expression tag	UNP D0EPS0
D	-13	VAL	-	expression tag	UNP D0EPS0
D	-12	ASP	-	expression tag	UNP D0EPS0
D	-11	LEU	-	expression tag	UNP D0EPS0
D	-10	GLY	-	expression tag	UNP D0EPS0
D	-9	THR	-	expression tag	UNP D0EPS0
D	-8	GLU	-	expression tag	UNP D0EPS0
D	-7	ASN	-	expression tag	UNP D0EPS0
D	-6	LEU	-	expression tag	UNP D0EPS0
D	-5	TYR	-	expression tag	UNP D0EPS0
D	-4	PHE	-	expression tag	UNP D0EPS0
D	-3	GLN	-	expression tag	UNP D0EPS0
D	-2	SER	-	expression tag	UNP D0EPS0
D	-1	ASN	-	expression tag	UNP D0EPS0

- Molecule 2 is a protein called 2B7 single chain fab variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	233	Total	C	N	O	S	0	0	0
			1780	1118	294	355	13			
2	G	232	Total	C	N	O	S	0	0	0
			1776	1116	293	354	13			
2	I	232	Total	C	N	O	S	0	0	0
			1776	1116	293	354	13			
2	K	232	Total	C	N	O	S	0	0	0
			1776	1116	293	354	13			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

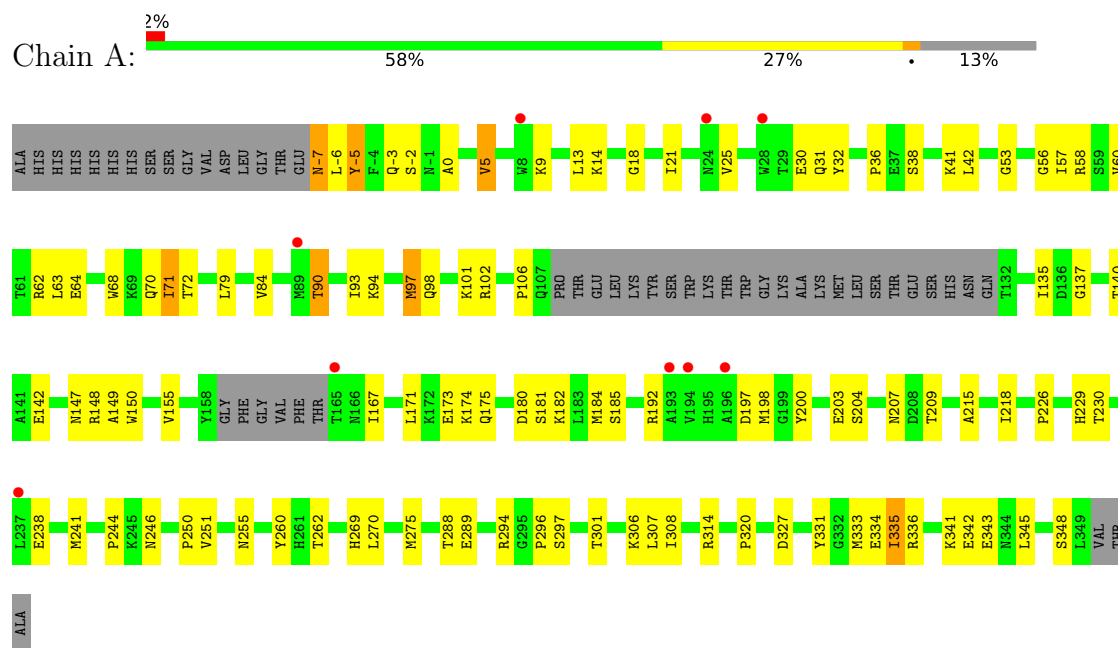


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

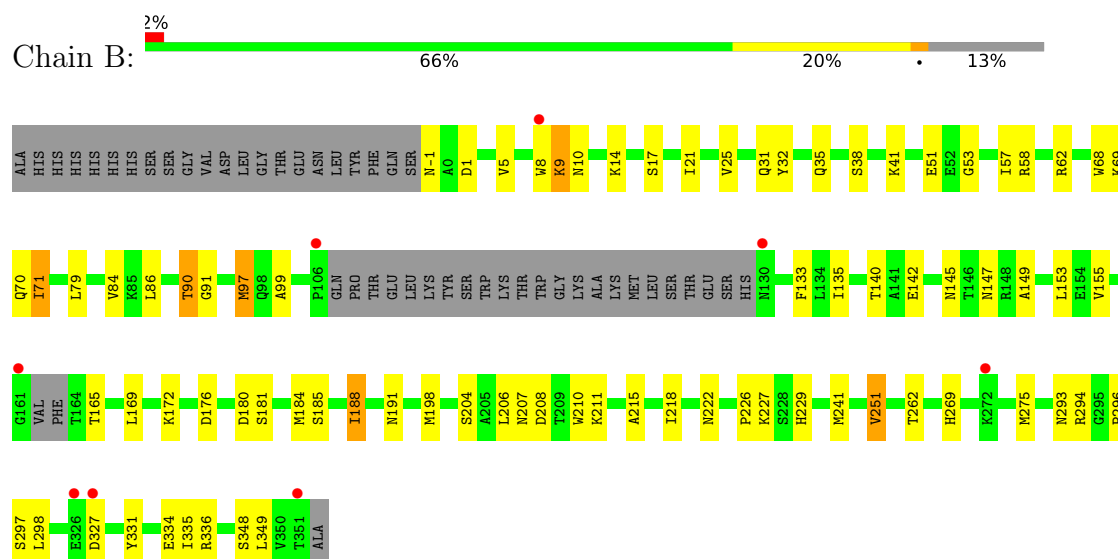
3 Residue-property plots [i](#)

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.

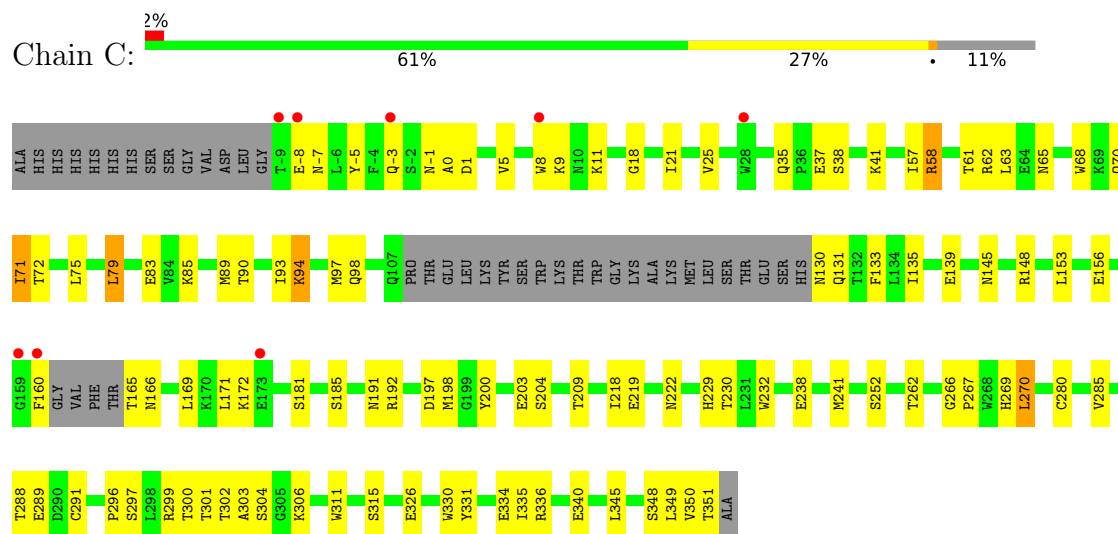
• Molecule 1: Non-structural protein 1



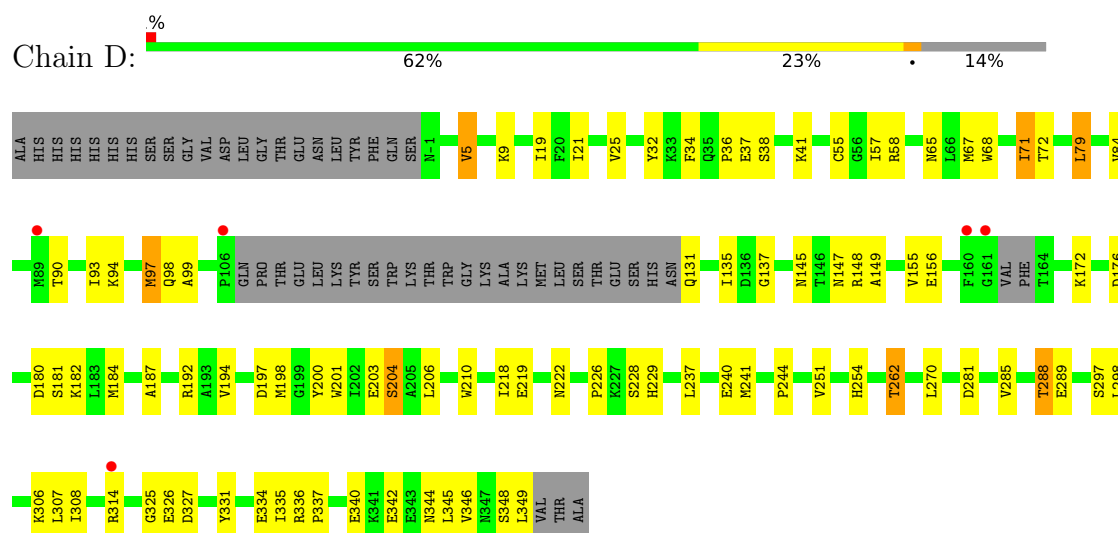
• Molecule 1: Non-structural protein 1



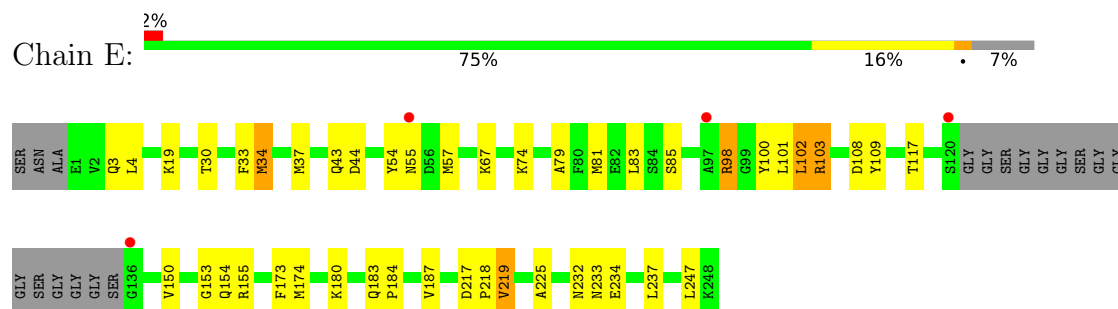
- Molecule 1: Non-structural protein 1



- Molecule 1: Non-structural protein 1

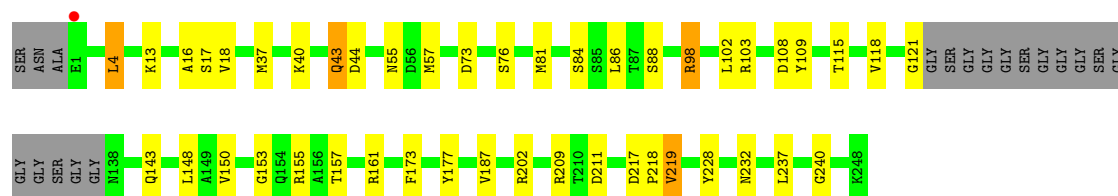


- Molecule 2: 2B7 single chain fab variable region

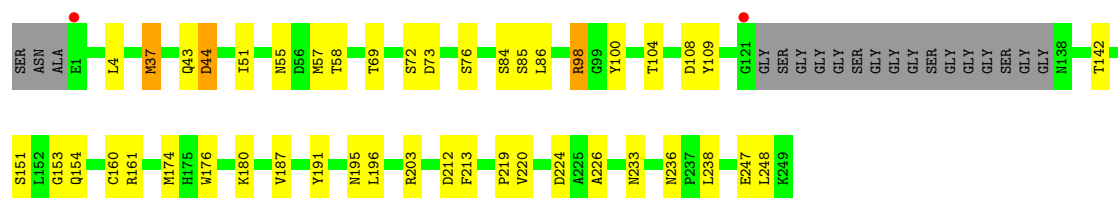


- Molecule 2: 2B7 single chain fab variable region

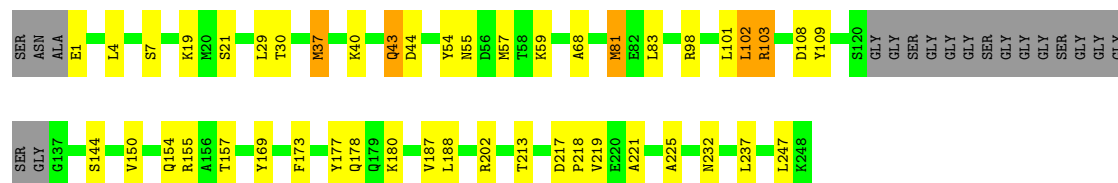
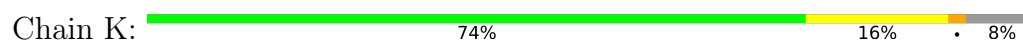




- Molecule 2: 2B7 single chain fab variable region



- Molecule 2: 2B7 single chain fab variable region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.63Å 165.59Å 258.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.89 47.38 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.38-2.89) 89.4 (47.38-2.89)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.223 , 0.269 0.229 , 0.267	Depositor DCC
R_{free} test set	2412 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17581	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

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	0.41	0/2657	0.65	0/3599
1	B	0.44	0/2660	0.65	0/3603
1	C	0.53	0/2703	0.74	0/3663
1	D	0.48	0/2638	0.66	0/3572
2	E	0.40	0/1820	0.69	0/2467
2	G	0.40	0/1816	0.68	0/2462
2	I	0.43	0/1816	0.69	0/2462
2	K	0.41	0/1816	0.66	0/2462
All	All	0.45	0/17926	0.68	0/24290

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2518	75	0
1	B	2600	0	2530	52	0
1	C	2642	0	2547	62	0
1	D	2578	0	2508	58	0
2	E	1780	0	1709	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1776	0	1706	28	0
2	I	1776	0	1706	26	0
2	K	1776	0	1706	27	0
3	A	14	0	13	1	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
All	All	17581	0	16982	318	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 9.

All (318) 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:289:GLU:HA	1:D:314:ARG:HG3	1.41	0.99
1:B:184:MET:HE2	1:B:226:PRO:HD2	1.64	0.80
1:C:94:LYS:NZ	1:C:139:GLU:OE2	2.19	0.76
1:C:35:GLN:OE1	1:C:166:ASN:ND2	2.20	0.74
2:I:98:ARG:NH1	2:I:108:ASP:OD2	2.20	0.74
2:I:55:ASN:HB3	2:I:57:MET:HG3	1.67	0.74
1:C:25:VAL:HG13	1:C:218:ILE:HG12	1.70	0.73
1:B:296:PRO:O	1:B:336:ARG:NH1	2.21	0.71
1:A:182:LYS:HG2	1:B:191:ASN:HD21	1.56	0.70
2:G:55:ASN:HB3	2:G:57:MET:HG3	1.74	0.70
1:A:58:ARG:NH1	1:A:137:GLY:O	2.25	0.69
1:A:53:GLY:O	1:A:147:ASN:ND2	2.24	0.69
1:D:331:TYR:HB3	1:D:335:ILE:HB	1.74	0.67
1:D:172:LYS:NZ	1:D:176:ASP:OD1	2.27	0.67
1:D:270:LEU:HD13	1:D:325:GLY:HA3	1.76	0.67
1:D:21:ILE:HG13	1:D:187:ALA:HB2	1.77	0.67
1:A:31:GLN:HE21	1:B:14:LYS:NZ	1.92	0.66
2:I:180:LYS:HD3	2:I:226:ALA:HB2	1.79	0.65
2:G:98:ARG:NH1	2:G:108:ASP:OD2	2.30	0.64
1:B:227:LYS:HE2	1:B:251:VAL:HG11	1.79	0.64
1:A:25:VAL:HG13	1:A:218:ILE:HG12	1.80	0.64
2:E:55:ASN:HB3	2:E:57:MET:HG3	1.78	0.64
2:G:108:ASP:HB3	2:G:109:TYR:CD2	2.33	0.63
1:A:244:PRO:HG3	1:A:262:THR:HG22	1.80	0.63
1:D:58:ARG:HD2	1:D:145:ASN:OD1	1.98	0.63
1:D:184:MET:HE2	1:D:226:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LYS:NZ	1:B:91:GLY:O	2.32	0.62
1:C:38:SER:HB3	1:C:41:LYS:HB2	1.80	0.62
1:C:58:ARG:HD2	1:C:145:ASN:OD1	2.01	0.61
1:C:296:PRO:O	1:C:336:ARG:NH1	2.27	0.61
1:A:21:ILE:HD12	1:A:185:SER:HB2	1.83	0.61
1:A:38:SER:HB3	1:A:41:LYS:HB2	1.82	0.60
1:D:99:ALA:H	1:D:222:ASN:HD22	1.49	0.60
1:D:308:ILE:HG13	1:D:345:LEU:HD21	1.84	0.60
1:C:267:PRO:HB2	1:C:270:LEU:HD22	1.83	0.59
1:A:36:PRO:HG3	1:A:71:ILE:HD11	1.84	0.59
1:D:336:ARG:HD3	1:D:342:GLU:OE2	2.03	0.59
1:A:308:ILE:HG13	1:A:345:LEU:HD21	1.84	0.59
1:A:296:PRO:O	1:A:336:ARG:NH1	2.27	0.58
1:A:30:GLU:OE2	1:A:62:ARG:NH1	2.36	0.58
2:G:73:ASP:OD2	2:G:76:SER:HB3	2.02	0.58
2:E:155:ARG:HB2	2:E:217:ASP:OD2	2.04	0.58
2:K:232:ASN:HA	2:K:237:LEU:HD22	1.86	0.58
2:E:54:TYR:HA	2:E:74:LYS:HG2	1.85	0.57
1:A:184:MET:HE2	1:A:226:PRO:HD2	1.85	0.57
2:K:103:ARG:HB3	2:K:173:PHE:CE2	2.41	0.56
1:C:288:THR:HG23	1:C:291:CYS:HB2	1.88	0.56
1:A:-7:ASN:OD1	1:A:-7:ASN:N	2.36	0.56
1:D:36:PRO:HG3	1:D:71:ILE:HD11	1.87	0.56
1:C:89:MET:HE3	2:G:121:GLY:HA3	1.87	0.55
1:D:288:THR:O	1:D:314:ARG:HA	2.06	0.55
1:A:68:TRP:O	1:A:72:THR:OG1	2.22	0.55
1:A:341:LYS:HB3	1:A:343:GLU:OE1	2.07	0.55
1:C:153:LEU:HD13	1:C:169:LEU:HD23	1.88	0.55
1:B:32:TYR:CD2	1:B:198:MET:HE1	2.42	0.55
1:A:5:VAL:CG1	1:B:1:ASP:HB3	2.37	0.55
1:A:269:HIS:HE1	1:A:348:SER:HB3	1.70	0.55
2:G:143:GLN:HG3	2:G:240:GLY:HA3	1.88	0.55
1:D:244:PRO:HG3	1:D:262:THR:HG22	1.89	0.55
2:G:103:ARG:HB3	2:G:173:PHE:CE2	2.42	0.55
1:A:14:LYS:NZ	1:B:31:GLN:HE21	2.04	0.54
1:A:331:TYR:HB3	1:A:335:ILE:HB	1.89	0.54
1:C:197:ASP:HB3	1:C:200:TYR:H	1.72	0.54
1:A:5:VAL:HG11	1:B:1:ASP:HB3	1.90	0.54
2:G:177:TYR:HE2	2:G:187:VAL:HG22	1.71	0.54
1:A:182:LYS:HG2	1:B:191:ASN:ND2	2.23	0.54
1:A:174:LYS:HD2	1:A:175:GLN:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HE21	1:B:14:LYS:HZ3	1.56	0.53
1:D:57:ILE:HG22	1:D:149:ALA:HB3	1.90	0.53
1:A:197:ASP:HB3	1:A:200:TYR:H	1.74	0.53
1:D:340:GLU:OE1	1:D:344:ASN:ND2	2.41	0.53
1:A:269:HIS:CE1	1:A:348:SER:HB3	2.43	0.53
2:I:44:ASP:OD1	2:I:44:ASP:N	2.35	0.53
1:A:215:ALA:HB3	1:A:275:MET:HE2	1.90	0.53
1:C:62:ARG:HA	1:C:97:MET:HE1	1.90	0.53
1:C:241:MET:O	1:C:262:THR:HG23	2.08	0.53
2:K:108:ASP:HB3	2:K:109:TYR:CD2	2.43	0.53
1:A:207:ASN:HD22	3:A:401:NAG:H83	1.74	0.52
1:D:197:ASP:HB3	1:D:200:TYR:H	1.74	0.52
1:C:266:GLY:HA2	1:C:297:SER:OG	2.10	0.52
1:A:-2:SER:O	1:B:9:LYS:NZ	2.34	0.52
1:A:93:ILE:HG21	1:A:97:MET:HE2	1.91	0.52
1:C:57:ILE:HG23	1:C:133:PHE:CE2	2.43	0.52
1:C:97:MET:HE3	1:C:219:GLU:HB2	1.92	0.52
2:I:108:ASP:HB3	2:I:109:TYR:CD2	2.44	0.52
2:E:98:ARG:NH1	2:E:100:TYR:OH	2.43	0.52
2:K:1:GLU:HA	2:K:109:TYR:CZ	2.45	0.52
1:B:62:ARG:HA	1:B:97:MET:HE1	1.92	0.52
1:A:307:LEU:HD22	2:E:30:THR:HG21	1.92	0.52
1:C:181:SER:HB2	1:C:229:HIS:CE1	2.45	0.52
1:D:38:SER:HB3	1:D:41:LYS:HB2	1.91	0.52
1:D:94:LYS:HE3	1:D:98:GLN:H	1.74	0.52
2:K:55:ASN:HB3	2:K:57:MET:HG3	1.91	0.51
1:C:238:GLU:HA	1:C:241:MET:HG3	1.92	0.51
1:B:68:TRP:HA	1:B:71:ILE:HG22	1.92	0.51
1:A:336:ARG:HD3	1:A:342:GLU:OE1	2.11	0.51
1:C:269:HIS:HE1	1:C:348:SER:HB3	1.75	0.51
1:B:90:THR:HB	1:B:135:ILE:HB	1.92	0.51
2:K:19:LYS:HA	2:K:81:MET:O	2.11	0.51
1:C:37:GLU:OE2	1:C:156:GLU:HG2	2.10	0.51
1:B:86:LEU:HD11	1:B:133:PHE:HB2	1.91	0.50
1:B:21:ILE:HD12	1:B:185:SER:HB2	1.93	0.50
1:D:297:SER:OG	1:D:331:TYR:O	2.29	0.50
1:B:327:ASP:HB3	2:G:102:LEU:HB3	1.94	0.50
1:C:62:ARG:CA	1:C:97:MET:HE1	2.42	0.50
2:G:150:VAL:HG13	2:G:219:VAL:HG21	1.93	0.50
1:D:68:TRP:HA	1:D:71:ILE:HG22	1.94	0.50
1:A:173:GLU:HG3	1:A:174:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:CYS:SG	1:D:147:ASN:HB3	2.52	0.49
2:E:180:LYS:HD3	2:E:225:ALA:HB2	1.94	0.49
1:A:68:TRP:HA	1:A:71:ILE:HG22	1.93	0.49
1:A:5:VAL:O	1:A:13:LEU:HD12	2.12	0.49
2:I:191:TYR:O	2:I:195:ASN:HB2	2.13	0.49
1:A:57:ILE:HG22	1:A:149:ALA:HB3	1.93	0.49
2:K:180:LYS:HD3	2:K:225:ALA:HB2	1.93	0.49
1:C:94:LYS:HE3	1:C:98:GLN:H	1.78	0.49
1:C:65:ASN:HB3	1:C:93:ILE:HD11	1.95	0.49
1:D:97:MET:HE3	1:D:219:GLU:HB2	1.94	0.49
1:C:-7:ASN:C	1:C:-5:TYR:H	2.21	0.49
1:D:348:SER:O	1:D:349:LEU:HG	2.13	0.48
2:G:18:VAL:HG12	2:G:86:LEU:HD11	1.95	0.48
1:C:62:ARG:HD3	1:C:218:ILE:HG22	1.95	0.48
1:B:215:ALA:HB3	1:B:275:MET:HE2	1.94	0.48
1:C:302:THR:HG22	1:C:304:SER:H	1.79	0.48
2:E:232:ASN:HA	2:E:237:LEU:HD22	1.96	0.48
1:D:34:PHE:HB2	1:D:67:MET:HB2	1.95	0.48
1:D:25:VAL:HG13	1:D:218:ILE:HG13	1.95	0.48
2:E:150:VAL:HG22	2:E:154:GLN:HB2	1.96	0.48
1:C:57:ILE:HD11	1:C:68:TRP:CE2	2.48	0.47
1:A:140:THR:OG1	1:A:142:GLU:HG2	2.14	0.47
1:C:68:TRP:HA	1:C:71:ILE:HG22	1.96	0.47
1:C:192:ARG:HD2	1:C:203:GLU:OE2	2.15	0.47
1:D:37:GLU:OE2	1:D:156:GLU:HG2	2.14	0.47
1:D:194:VAL:HG11	1:D:201:TRP:CH2	2.49	0.47
2:K:155:ARG:HB2	2:K:217:ASP:OD2	2.13	0.47
1:A:9:LYS:HE2	1:B:-1:ASN:HA	1.96	0.47
1:A:14:LYS:HA	1:A:14:LYS:HD2	1.71	0.47
1:A:14:LYS:HZ1	1:B:31:GLN:HE21	1.62	0.47
2:I:51:ILE:HD11	2:I:72:SER:HB3	1.96	0.47
1:A:238:GLU:HA	1:A:241:MET:HG3	1.97	0.47
2:E:34:MET:HE2	2:E:79:ALA:HB2	1.96	0.47
2:E:154:GLN:O	2:E:219:VAL:HG12	2.13	0.47
2:G:161:ARG:HD2	2:G:211:ASP:HA	1.95	0.47
2:I:37:MET:HE2	2:I:37:MET:HB3	1.57	0.47
1:D:241:MET:O	1:D:262:THR:HA	2.14	0.47
2:E:183:GLN:HG2	2:E:184:PRO:HD2	1.97	0.47
1:A:36:PRO:HG3	1:A:71:ILE:CD1	2.45	0.47
1:A:42:LEU:HD12	1:A:171:LEU:HD11	1.95	0.47
1:A:94:LYS:HE3	1:A:98:GLN:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:HIS:CD2	1:B:188:ILE:HD12	2.50	0.46
1:B:57:ILE:HG12	1:B:135:ILE:HG12	1.96	0.46
1:B:14:LYS:HA	1:B:14:LYS:HD2	1.64	0.46
1:B:331:TYR:HB3	1:B:335:ILE:HB	1.97	0.46
1:B:8:TRP:H	1:B:8:TRP:CD1	2.33	0.46
2:I:233:ASN:HA	2:I:238:LEU:HD22	1.98	0.46
1:A:56:GLY:O	1:A:148:ARG:HA	2.16	0.46
1:B:57:ILE:HG22	1:B:149:ALA:HB3	1.96	0.46
1:C:68:TRP:O	1:C:72:THR:OG1	2.23	0.46
1:C:70:GLN:HA	2:G:16:ALA:HB1	1.98	0.46
1:D:184:MET:HB3	1:D:184:MET:HE3	1.65	0.46
1:D:204:SER:OG	1:D:254:HIS:HB3	2.15	0.46
1:C:299:ARG:HA	1:C:330:TRP:HA	1.96	0.46
1:C:70:GLN:HG3	2:G:17:SER:H	1.80	0.46
1:D:68:TRP:O	1:D:72:THR:OG1	2.27	0.45
1:D:281:ASP:OD1	2:K:29:LEU:HD21	2.16	0.45
1:A:31:GLN:HE21	1:B:14:LYS:HZ1	1.62	0.45
1:C:-1:ASN:HA	1:D:9:LYS:HE2	1.99	0.45
1:C:21:ILE:HD12	1:C:185:SER:HB2	1.98	0.45
1:D:346:VAL:HG13	2:K:169:TYR:CG	2.52	0.45
2:I:174:MET:HG2	2:I:213:PHE:CD2	2.50	0.45
1:B:181:SER:HA	1:B:184:MET:HG2	1.99	0.45
1:D:192:ARG:HD2	1:D:203:GLU:OE2	2.15	0.45
2:E:103:ARG:HB3	2:E:173:PHE:CE2	2.52	0.45
1:B:153:LEU:HD13	1:B:169:LEU:HD23	1.99	0.45
1:A:0:ALA:HB1	1:A:18:GLY:O	2.17	0.45
1:B:53:GLY:O	1:B:147:ASN:ND2	2.49	0.45
1:C:241:MET:O	1:C:262:THR:HA	2.16	0.45
2:G:143:GLN:OE1	2:G:228:TYR:HA	2.17	0.45
1:C:63:LEU:HD11	1:C:198:MET:HE2	1.99	0.45
1:D:57:ILE:HG12	1:D:135:ILE:HG12	1.99	0.45
2:K:29:LEU:HA	2:K:54:TYR:HD2	1.82	0.45
1:C:70:GLN:HG3	2:G:16:ALA:HB1	1.99	0.45
1:A:182:LYS:HE3	1:B:191:ASN:ND2	2.32	0.45
1:B:38:SER:HB3	1:B:41:LYS:HB2	1.98	0.45
2:K:177:TYR:CE2	2:K:187:VAL:HG22	2.52	0.45
1:A:106:PRO:HA	1:A:171:LEU:HD22	1.99	0.45
2:I:153:GLY:HA2	2:I:219:PRO:HB2	1.98	0.45
1:C:85:LYS:H	1:C:85:LYS:HG2	1.40	0.44
2:G:88:SER:HA	2:G:118:VAL:HB	1.99	0.44
1:B:241:MET:O	1:B:262:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD11	1:A:198:MET:HE2	1.99	0.44
2:K:37:MET:HE3	2:K:37:MET:HB3	1.59	0.44
1:D:327:ASP:HA	2:K:102:LEU:H	1.82	0.44
2:K:103:ARG:HB3	2:K:173:PHE:CZ	2.53	0.44
1:A:230:THR:HG21	1:A:251:VAL:O	2.17	0.44
1:C:326:GLU:OE2	2:I:236:ASN:ND2	2.50	0.44
1:D:326:GLU:OE2	2:K:59:LYS:HD3	2.18	0.44
2:E:19:LYS:HA	2:E:81:MET:O	2.18	0.44
2:I:84:SER:HB3	2:I:85:SER:H	1.54	0.44
2:I:151:SER:HB2	2:I:154:GLN:HG3	2.00	0.44
1:C:0:ALA:HB1	1:C:18:GLY:O	2.17	0.44
2:E:67:LYS:NZ	2:E:85:SER:O	2.48	0.44
2:K:83:LEU:HD23	2:K:83:LEU:HA	1.79	0.44
1:A:241:MET:O	1:A:262:THR:HA	2.18	0.44
1:A:288:THR:O	1:A:314:ARG:HA	2.18	0.44
1:D:298:LEU:HD12	1:D:337:PRO:HD3	2.00	0.44
2:G:57:MET:HB3	2:G:57:MET:HE2	1.85	0.44
2:K:101:LEU:HD23	2:K:101:LEU:HA	1.80	0.44
1:C:230:THR:HG22	1:C:252:SER:HB2	2.00	0.43
1:C:57:ILE:HG12	1:C:135:ILE:HG12	2.01	0.43
1:D:307:LEU:HD22	2:K:30:THR:HG21	1.99	0.43
2:I:98:ARG:O	2:I:98:ARG:HG3	2.15	0.43
2:K:202:ARG:HD3	2:K:218:PRO:O	2.18	0.43
1:B:206:LEU:HD13	1:B:210:TRP:CD1	2.53	0.43
2:G:153:GLY:HA2	2:G:218:PRO:HB2	1.99	0.43
2:I:55:ASN:HB3	2:I:57:MET:H	1.83	0.43
1:B:90:THR:CB	1:B:135:ILE:HB	2.49	0.43
1:B:207:ASN:O	1:B:208:ASP:HB2	2.19	0.43
1:C:1:ASP:HB3	1:D:5:VAL:HG11	2.01	0.43
2:I:180:LYS:CD	2:I:226:ALA:HB2	2.46	0.43
2:K:178:GLN:HB2	2:K:188:LEU:HD11	2.01	0.43
1:A:184:MET:H	1:A:184:MET:HG2	1.62	0.43
1:A:260:TYR:OH	1:A:320:PRO:HA	2.18	0.43
1:B:172:LYS:NZ	1:B:176:ASP:OD1	2.41	0.43
2:E:101:LEU:HA	2:E:101:LEU:HD23	1.77	0.43
1:C:8:TRP:O	1:C:11:LYS:HG3	2.19	0.43
1:B:58:ARG:HD2	1:B:145:ASN:OD1	2.18	0.43
2:G:86:LEU:HD23	2:G:86:LEU:HA	1.83	0.43
1:C:75:LEU:O	1:C:79:LEU:HD22	2.19	0.43
1:C:340:GLU:HG2	1:C:345:LEU:HD11	2.00	0.43
1:A:64:GLU:HG2	1:A:68:TRP:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:HB3	1:D:5:VAL:CG1	2.49	0.42
2:I:100:TYR:HB2	2:I:104:THR:HB	2.01	0.42
1:B:155:VAL:HG23	1:B:180:ASP:OD2	2.20	0.42
2:G:177:TYR:CE2	2:G:187:VAL:HG22	2.52	0.42
1:A:301:THR:HA	1:A:306:LYS:O	2.19	0.42
1:A:327:ASP:HB3	2:E:102:LEU:HB3	2.01	0.42
1:D:79:LEU:HD12	1:D:79:LEU:HA	1.76	0.42
2:G:155:ARG:NE	2:G:217:ASP:OD2	2.45	0.42
1:A:90:THR:HG22	1:A:135:ILE:HB	2.00	0.42
2:E:83:LEU:HD23	2:E:83:LEU:HA	1.88	0.42
2:E:217:ASP:HA	2:E:218:PRO:HA	1.79	0.42
2:E:233:ASN:O	2:E:234:GLU:HG3	2.19	0.42
2:G:232:ASN:HA	2:G:237:LEU:HD22	2.01	0.42
1:C:191:ASN:ND2	1:D:182:LYS:HG2	2.33	0.42
2:E:153:GLY:HA2	2:E:218:PRO:HB2	2.02	0.42
1:C:131:GLN:H	1:C:131:GLN:HG2	1.67	0.42
1:B:269:HIS:HE1	1:B:348:SER:HB3	1.84	0.42
1:C:160:PHE:O	1:C:165:THR:HG22	2.20	0.42
1:D:32:TYR:CD2	1:D:198:MET:HE1	2.54	0.42
1:D:206:LEU:HB2	1:D:210:TRP:CE2	2.54	0.42
2:E:174:MET:HE2	2:E:174:MET:HB2	1.81	0.42
2:I:160:CYS:HB2	2:I:176:TRP:CH2	2.55	0.42
1:A:62:ARG:HD3	1:A:218:ILE:HG22	2.01	0.42
1:A:184:MET:HB2	1:A:229:HIS:CD2	2.55	0.42
1:B:207:ASN:HB3	1:B:211:LYS:HZ1	1.84	0.42
1:A:32:TYR:CD1	1:A:167:ILE:HD11	2.54	0.41
1:B:140:THR:OG1	1:B:142:GLU:HG2	2.20	0.41
1:D:58:ARG:HG2	1:D:148:ARG:HD2	2.00	0.41
1:D:181:SER:HB2	1:D:229:HIS:CE1	2.55	0.41
2:I:51:ILE:HG13	2:I:58:THR:HG22	2.02	0.41
2:K:217:ASP:HA	2:K:218:PRO:HA	1.85	0.41
1:A:60:VAL:HG22	1:A:150:TRP:CD1	2.54	0.41
1:A:101:LYS:HA	1:A:101:LYS:HD3	1.84	0.41
1:C:57:ILE:HG21	1:C:57:ILE:HD13	1.62	0.41
2:G:4:LEU:HD12	2:G:4:LEU:HA	1.91	0.41
1:A:9:LYS:CG	1:B:-1:ASN:HA	2.50	0.41
1:C:58:ARG:HG2	1:C:148:ARG:HD2	2.01	0.41
1:D:65:ASN:HB3	1:D:93:ILE:HD11	2.01	0.41
2:E:30:THR:O	2:E:33:PHE:HE1	2.02	0.41
2:G:202:ARG:HD3	2:G:218:PRO:O	2.20	0.41
1:B:293:ASN:O	1:B:336:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:HIS:CE1	1:C:348:SER:HB3	2.55	0.41
1:D:237:LEU:HD13	1:D:240:GLU:HG3	2.01	0.41
2:E:108:ASP:HB3	2:E:109:TYR:CD2	2.55	0.41
2:E:150:VAL:O	2:E:247:LEU:HD23	2.21	0.41
2:G:209:ARG:CZ	2:G:209:ARG:HB3	2.51	0.41
2:K:150:VAL:HG22	2:K:154:GLN:HB2	2.02	0.41
1:A:9:LYS:HG2	1:B:-1:ASN:HA	2.02	0.41
1:A:241:MET:HE3	1:A:250:PRO:O	2.21	0.41
1:B:99:ALA:H	1:B:222:ASN:HD22	1.69	0.41
2:I:161:ARG:HD2	2:I:212:ASP:OD1	2.20	0.41
2:I:203:ARG:NH1	2:I:224:ASP:OD1	2.53	0.41
1:D:57:ILE:HD11	1:D:68:TRP:CE2	2.56	0.41
1:D:155:VAL:HG23	1:D:180:ASP:OD2	2.21	0.41
2:I:86:LEU:HD23	2:I:86:LEU:HA	1.91	0.41
2:I:247:GLU:HG2	2:I:248:LEU:N	2.36	0.41
1:C:280:CYS:HB3	1:C:300:THR:HG21	2.03	0.41
2:K:7:SER:HB3	2:K:21:SER:OG	2.21	0.41
1:A:-6:LEU:C	1:A:-5:TYR:HD2	2.28	0.41
1:B:25:VAL:HG13	1:B:218:ILE:HG13	2.02	0.41
1:C:232:TRP:CG	1:D:228:SER:HA	2.56	0.41
2:K:68:ALA:HA	2:K:83:LEU:HD23	2.03	0.41
1:A:102:ARG:O	1:A:149:ALA:HA	2.21	0.41
1:B:327:ASP:HA	2:G:102:LEU:H	1.85	0.41
1:C:71:ILE:HD13	1:C:71:ILE:HG21	1.74	0.41
1:C:331:TYR:HB3	1:C:335:ILE:HB	2.03	0.41
1:C:349:LEU:HD23	1:C:349:LEU:HA	1.76	0.41
1:D:36:PRO:HG3	1:D:71:ILE:CD1	2.51	0.41
1:D:58:ARG:NH1	1:D:137:GLY:O	2.54	0.41
2:K:40:LYS:HB2	2:K:43:GLN:CB	2.50	0.41
2:G:40:LYS:HB2	2:G:43:GLN:CB	2.51	0.41
2:K:221:ALA:HA	2:K:247:LEU:HD11	2.03	0.41
1:A:192:ARG:HD2	1:A:203:GLU:OE2	2.22	0.40
1:D:285:VAL:HG11	1:D:335:ILE:HD12	2.03	0.40
1:A:333:MET:HE2	1:A:333:MET:HB3	1.78	0.40
1:B:184:MET:HB2	1:B:229:HIS:CD2	2.55	0.40
1:C:302:THR:HG22	1:C:303:ALA:N	2.35	0.40
2:I:55:ASN:CB	2:I:57:MET:HG3	2.45	0.40
1:C:285:VAL:HG22	1:C:311:TRP:HB2	2.04	0.40
1:C:301:THR:HA	1:C:306:LYS:O	2.22	0.40
1:A:155:VAL:HG23	1:A:180:ASP:OD2	2.22	0.40
1:A:241:MET:HA	1:A:255:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.72	0.40
1:B:181:SER:HA	1:B:184:MET:CG	2.52	0.40
1:D:184:MET:HB2	1:D:229:HIS:CD2	2.56	0.40
2:I:73:ASP:OD2	2:I:76:SER:HB3	2.20	0.40
1:D:345:LEU:HD23	1:D:345:LEU:HA	1.93	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	321/376 (85%)	306 (95%)	15 (5%)	0	100	100
1	B	322/376 (86%)	308 (96%)	14 (4%)	0	100	100
1	C	329/376 (88%)	308 (94%)	17 (5%)	4 (1%)	10	34
1	D	319/376 (85%)	305 (96%)	14 (4%)	0	100	100
2	E	229/251 (91%)	217 (95%)	11 (5%)	1 (0%)	30	59
2	G	228/251 (91%)	216 (95%)	11 (5%)	1 (0%)	30	59
2	I	228/251 (91%)	215 (94%)	13 (6%)	0	100	100
2	K	228/251 (91%)	214 (94%)	13 (6%)	1 (0%)	30	59
All	All	2204/2508 (88%)	2089 (95%)	108 (5%)	7 (0%)	36	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-3	GLN
1	C	-8	GLU
2	G	84	SER
1	C	94	LYS
2	E	102	LEU

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Mol	Chain	Res	Type
2	K	102	LEU
1	C	350	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/331 (87%)	268 (93%)	20 (7%)	14	41
1	B	289/331 (87%)	268 (93%)	21 (7%)	13	38
1	C	289/331 (87%)	270 (93%)	19 (7%)	15	43
1	D	286/331 (86%)	272 (95%)	14 (5%)	22	54
2	E	196/203 (97%)	185 (94%)	11 (6%)	19	50
2	G	196/203 (97%)	185 (94%)	11 (6%)	19	50
2	I	196/203 (97%)	186 (95%)	10 (5%)	21	53
2	K	196/203 (97%)	185 (94%)	11 (6%)	19	50
All	All	1936/2136 (91%)	1819 (94%)	117 (6%)	17	47

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	ASN
1	A	-5	TYR
1	A	-3	GLN
1	A	5	VAL
1	A	70	GLN
1	A	71	ILE
1	A	79	LEU
1	A	84	VAL
1	A	90	THR
1	A	97	MET
1	A	181	SER
1	A	204	SER
1	A	209	THR

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Mol	Chain	Res	Type
1	A	246	ASN
1	A	270	LEU
1	A	289	GLU
1	A	294	ARG
1	A	297	SER
1	A	334	GLU
1	A	335	ILE
1	B	5	VAL
1	B	9	LYS
1	B	10	ASN
1	B	17	SER
1	B	35	GLN
1	B	51	GLU
1	B	70	GLN
1	B	71	ILE
1	B	79	LEU
1	B	84	VAL
1	B	90	THR
1	B	97	MET
1	B	165	THR
1	B	188	ILE
1	B	204	SER
1	B	251	VAL
1	B	294	ARG
1	B	297	SER
1	B	298	LEU
1	B	334	GLU
1	B	349	LEU
1	C	5	VAL
1	C	9	LYS
1	C	58	ARG
1	C	61	THR
1	C	71	ILE
1	C	79	LEU
1	C	83	GLU
1	C	90	THR
1	C	130	ASN
1	C	171	LEU
1	C	172	LYS
1	C	204	SER
1	C	209	THR
1	C	222	ASN

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Mol	Chain	Res	Type
1	C	270	LEU
1	C	289	GLU
1	C	315	SER
1	C	334	GLU
1	C	351	THR
1	D	5	VAL
1	D	19	ILE
1	D	71	ILE
1	D	79	LEU
1	D	84	VAL
1	D	90	THR
1	D	97	MET
1	D	131	GLN
1	D	204	SER
1	D	251	VAL
1	D	262	THR
1	D	288	THR
1	D	306	LYS
1	D	334	GLU
2	E	3	GLN
2	E	4	LEU
2	E	34	MET
2	E	37	MET
2	E	43	GLN
2	E	44	ASP
2	E	98	ARG
2	E	103	ARG
2	E	117	THR
2	E	187	VAL
2	E	219	VAL
2	G	4	LEU
2	G	13	LYS
2	G	37	MET
2	G	43	GLN
2	G	44	ASP
2	G	81	MET
2	G	98	ARG
2	G	115	THR
2	G	148	LEU
2	G	157	THR
2	G	219	VAL
2	I	4	LEU

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Mol	Chain	Res	Type
2	I	37	MET
2	I	43	GLN
2	I	44	ASP
2	I	69	THR
2	I	98	ARG
2	I	142	THR
2	I	187	VAL
2	I	196	LEU
2	I	220	VAL
2	K	4	LEU
2	K	37	MET
2	K	43	GLN
2	K	44	ASP
2	K	81	MET
2	K	98	ARG
2	K	103	ARG
2	K	144	SER
2	K	157	THR
2	K	213	THR
2	K	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	31	GLN
1	A	191	ASN
1	A	222	ASN
1	A	224	HIS
1	A	261	HIS
1	B	-1	ASN
1	B	31	GLN
1	B	35	GLN
1	B	50	HIS
1	B	70	GLN
1	B	98	GLN
1	B	191	ASN
1	B	222	ASN
1	B	224	HIS
1	B	269	HIS
1	B	344	ASN
1	C	24	ASN

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Mol	Chain	Res	Type
1	C	31	GLN
1	C	47	GLN
1	C	130	ASN
1	C	131	GLN
1	C	191	ASN
1	C	222	ASN
1	C	269	HIS
1	D	-1	ASN
1	D	24	ASN
1	D	47	GLN
1	D	77	HIS
1	D	222	ASN
1	D	229	HIS
1	D	269	HIS
2	E	154	GLN
2	G	194	ASN
2	I	154	GLN
2	I	195	ASN
2	K	154	GLN
2	K	194	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
3	NAG	C	401	1	14,14,15	0.87	1 (7%)	17,19,21	0.67	1 (5%)
3	NAG	B	401	1	14,14,15	0.82	1 (7%)	17,19,21	0.42	0
3	NAG	A	401	1	14,14,15	0.36	0	17,19,21	0.62	1 (5%)
3	NAG	D	401	1	14,14,15	0.99	2 (14%)	17,19,21	0.71	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
3	NAG	C	401	1	-	3/6/23/26	0/1/1/1
3	NAG	B	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	4/6/23/26	0/1/1/1
3	NAG	D	401	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAG	C1-C2	2.79	1.56	1.52
3	B	401	NAG	O5-C1	2.64	1.48	1.43
3	C	401	NAG	O5-C1	2.64	1.48	1.43
3	D	401	NAG	O5-C1	2.31	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAG	C1-O5-C5	2.30	115.27	112.19
3	A	401	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	401	NAG	C4-C5-C6-O6
3	A	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	C	401	NAG	C8-C7-N2-C2
3	C	401	NAG	O7-C7-N2-C2
3	B	401	NAG	C4-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	D	401	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	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 ⓘ

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	327/376 (86%)	0.31	9 (2%)	55	46	64, 90, 155, 172	0
1	B	328/376 (87%)	0.18	8 (2%)	59	50	67, 82, 114, 125	0
1	C	335/376 (89%)	0.07	8 (2%)	59	50	55, 66, 94, 115	0
1	D	325/376 (86%)	0.10	5 (1%)	72	64	57, 81, 107, 122	0
2	E	233/251 (92%)	0.11	4 (1%)	69	61	68, 85, 110, 120	0
2	G	232/251 (92%)	-0.03	1 (0%)	88	85	64, 78, 90, 99	0
2	I	232/251 (92%)	0.16	2 (0%)	81	75	66, 81, 131, 152	0
2	K	232/251 (92%)	0.04	0	100	100	67, 83, 105, 119	0
All	All	2244/2508 (89%)	0.13	37 (1%)	70	62	55, 80, 123, 172	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	121	GLY	4.3
1	C	-9	THR	4.3
1	A	28	TRP	3.8
2	E	136	GLY	3.4
1	C	28	TRP	2.9
1	D	106	PRO	2.8
1	C	-8	GLU	2.7
1	C	-3	GLN	2.7
1	A	237	LEU	2.7
1	D	160	PHE	2.6
1	C	160	PHE	2.6
1	B	106	PRO	2.6
1	B	326	GLU	2.6
1	C	173	GLU	2.6
1	B	161	GLY	2.5
1	D	89	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	351	THR	2.5
2	G	1	GLU	2.5
1	A	196	ALA	2.5
2	E	55	ASN	2.5
1	A	89	MET	2.4
1	A	165	THR	2.4
1	B	130	ASN	2.4
1	C	159	GLY	2.3
1	D	314	ARG	2.3
1	A	24	ASN	2.3
1	B	327	ASP	2.3
1	C	8	TRP	2.2
2	E	120	SER	2.2
2	I	1	GLU	2.2
2	E	97	ALA	2.2
1	A	194	VAL	2.1
1	B	272	LYS	2.1
1	B	8	TRP	2.1
1	A	193	ALA	2.1
1	D	161	GLY	2.1
1	A	8	TRP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	NAG	A	401	14/15	0.68	0.10	91,91,91,91	0
3	NAG	C	401	14/15	0.68	0.11	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	401	14/15	0.75	0.09	87,87,87,87	0
3	NAG	B	401	14/15	0.84	0.08	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.