



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:56 AM UTC

PDB ID : 6XXN / pdb_00006xxn
Title : Crystal structure of NB7, a nanobody targeting prostate specific membrane antigen
Authors : Shahar, A.; Rosenfeld, L.; Papo, N.
Deposited on : 2020-01-28
Resolution : 2.65 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

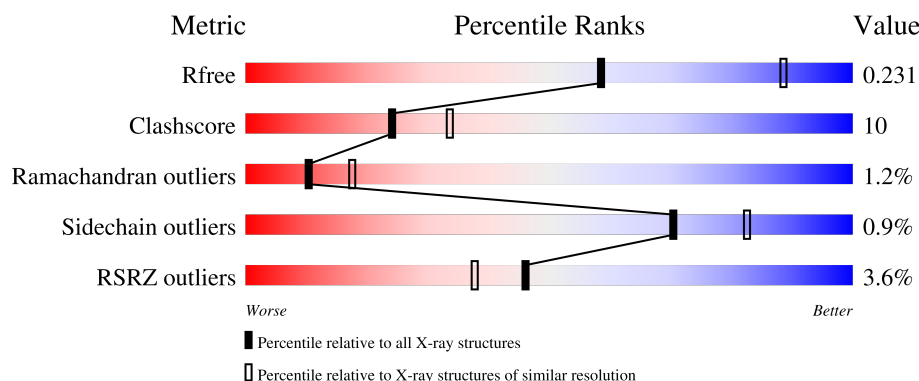
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	146	3% 67% 16% .. 14%
1	B	146	3% 69% 15% • 14%
1	C	146	3% 68% 16% • 14%
1	D	146	3% 65% 17% • 15%
1	E	146	0% 65% 19% • 15%

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Mol	Chain	Length	Quality of chain
1	F	146	
2	G	146	
3	H	146	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7731 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 NB_7_a,b,c,f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			955	592	164	192	7			
1	B	125	Total	C	N	O	S	0	0	0
			955	592	164	192	7			
1	C	125	Total	C	N	O	S	0	0	0
			955	592	164	192	7			
1	D	124	Total	C	N	O	S	0	0	0
			949	589	163	190	7			
1	E	124	Total	C	N	O	S	0	0	0
			949	589	163	190	7			
1	F	125	Total	C	N	O	S	0	0	0
			955	592	164	192	7			

- Molecule 2 is a protein called NB_7_g.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	124	Total	C	N	O	S	0	0	0
			947	588	162	190	7			

- Molecule 3 is a protein called NB_7_h.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	124	Total	C	N	O	S	0	0	0
			950	588	164	191	7			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

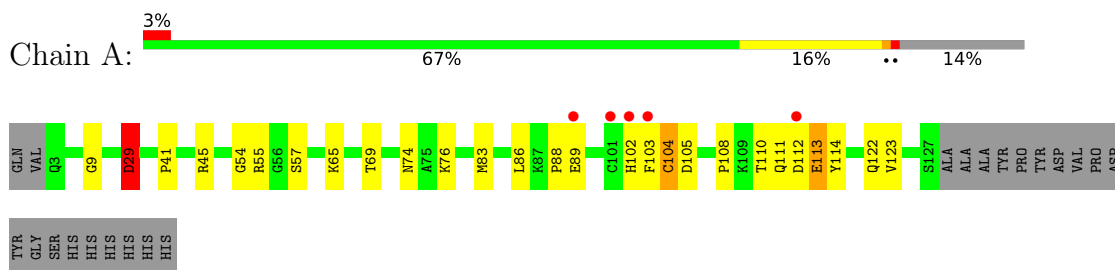
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total O 2 2	0	0
5	E	3	Total O 3 3	0	0
5	F	1	Total O 1 1	0	0
5	G	3	Total O 3 3	0	0
5	H	2	Total O 2 2	0	0

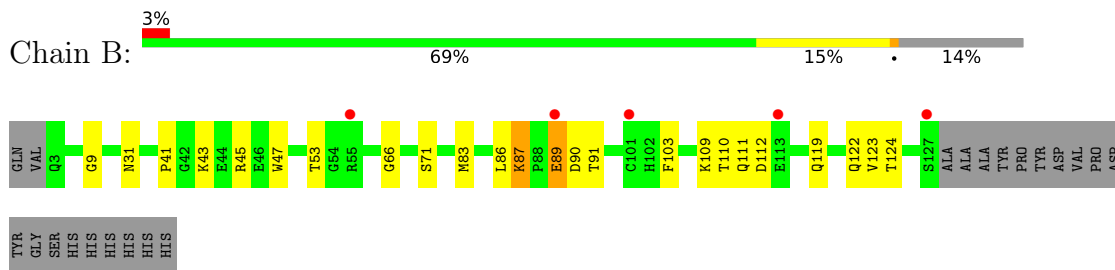
3 Residue-property plots [i](#)

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.

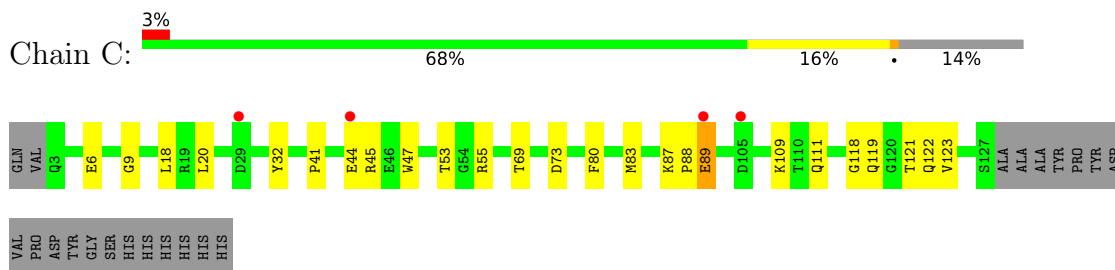
- Molecule 1: NB_7_a,b,c,f



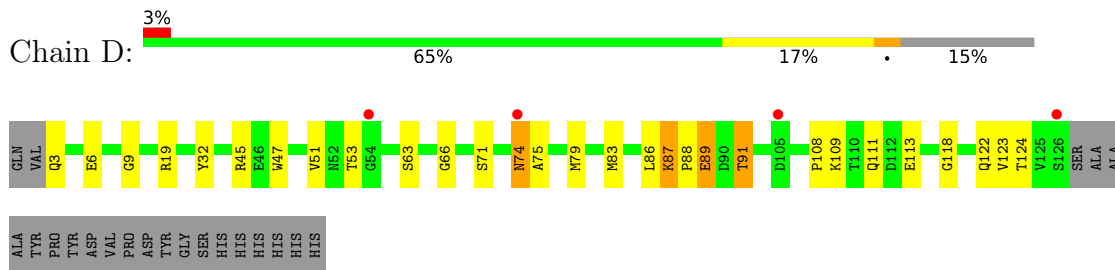
- Molecule 1: NB_7_a,b,c,f



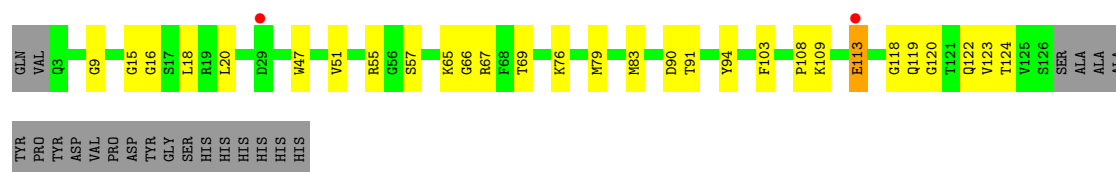
- Molecule 1: NB_7_a,b,c,f



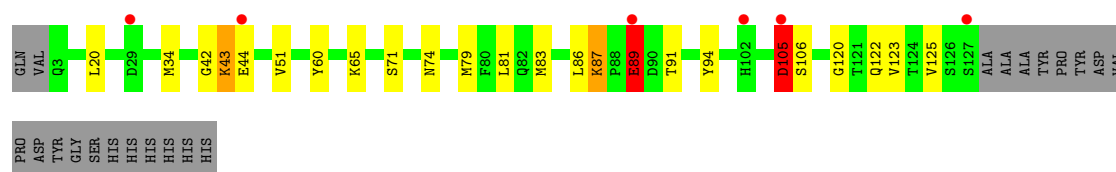
- Molecule 1: NB_7_a,b,c,f



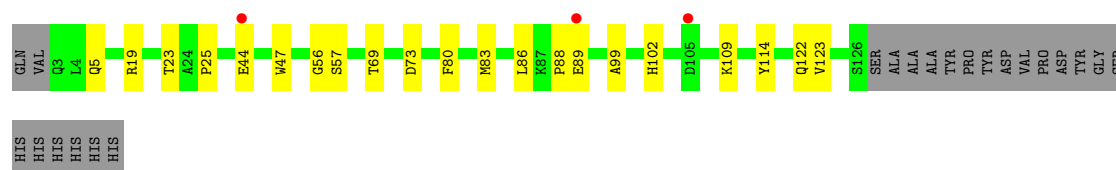
- Molecule 1: NB_7_a,b,c,f



- Molecule 1: NB_7_a,b,c,f



- Molecule 2: NB_7_g



- Molecule 3: NB_7_h



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.56Å 171.72Å 83.48Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	47.20 – 2.65 47.20 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.20-2.65) 99.0 (47.20-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.182 , 0.231 0.188 , 0.231	Depositor DCC
R_{free} test set	2120 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7731	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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: SO4

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	0.49	0/976	1.06	11/1322 (0.8%)
1	B	0.52	0/976	0.91	4/1322 (0.3%)
1	C	0.48	0/976	0.92	5/1322 (0.4%)
1	D	0.58	0/970	0.91	4/1314 (0.3%)
1	E	0.47	0/970	0.88	6/1314 (0.5%)
1	F	0.59	1/976 (0.1%)	1.01	7/1322 (0.5%)
2	G	0.50	1/968 (0.1%)	0.93	5/1312 (0.4%)
3	H	0.72	2/971 (0.2%)	0.98	3/1315 (0.2%)
All	All	0.55	4/7783 (0.1%)	0.95	45/10543 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	2
2	G	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	89	GLU	CB-CG	6.65	1.72	1.52
1	F	87	LYS	CA-C	5.98	1.58	1.52
3	H	95	TYR	C-O	-5.93	1.16	1.24
3	H	6	GLU	C-O	-5.04	1.17	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	89	GLU	CA-CB-CG	11.43	136.96	114.10
1	F	105	ASP	CB-CA-C	-11.08	93.48	110.88
2	G	88	PRO	CA-C-N	-10.13	105.83	122.65
2	G	88	PRO	C-N-CA	-10.13	105.83	122.65
1	A	88	PRO	CA-C-N	-8.87	107.31	122.56
1	A	88	PRO	C-N-CA	-8.87	107.31	122.56
2	G	89	GLU	CB-CG-CD	8.13	126.43	112.60
1	F	89	GLU	CB-CA-C	-8.05	94.40	110.42
1	F	89	GLU	CA-CB-CG	7.98	130.05	114.10
1	B	87	LYS	N-CA-CB	-7.97	97.62	111.17
1	D	91	THR	CA-CB-OG1	-7.75	97.98	109.60
3	H	43	LYS	CA-C-N	7.71	132.16	120.82
3	H	43	LYS	C-N-CA	7.71	132.16	120.82
1	C	119	GLN	CA-CB-CG	-7.29	99.52	114.10
1	D	74	ASN	CB-CA-C	-7.22	99.45	110.92
1	D	88	PRO	CA-N-CD	-7.15	101.99	112.00
1	C	89	GLU	CA-CB-CG	-6.95	100.21	114.10
1	A	89	GLU	CA-CB-CG	6.72	127.55	114.10
1	A	76	LYS	CD-CE-NZ	-6.38	91.50	111.90
1	B	87	LYS	CG-CD-CE	-6.20	97.05	111.30
1	C	44	GLU	CA-CB-CG	6.15	126.39	114.10
1	A	113	GLU	CA-CB-CG	-6.14	101.81	114.10
1	E	113	GLU	CA-CB-CG	6.12	126.34	114.10
1	F	43	LYS	CA-CB-CG	-6.05	102.00	114.10
1	A	104	CYS	CA-C-N	5.95	132.46	121.52
1	A	104	CYS	C-N-CA	5.95	132.46	121.52
3	H	101	CYS	N-CA-CB	-5.94	100.25	111.00
1	A	89	GLU	CB-CG-CD	5.93	122.68	112.60
1	A	65	LYS	CD-CE-NZ	5.87	130.70	111.90
1	F	43	LYS	CB-CG-CD	5.81	124.66	111.30
1	A	76	LYS	CA-CB-CG	-5.60	102.91	114.10
1	E	118	GLY	CA-C-N	-5.54	113.96	122.60
1	E	118	GLY	C-N-CA	-5.54	113.96	122.60
1	F	74	ASN	CB-CA-C	5.54	121.30	110.67
1	A	29	ASP	CB-CA-C	-5.46	99.56	110.42
1	E	119	GLN	CA-CB-CG	-5.38	103.33	114.10
1	E	76	LYS	CA-CB-CG	5.36	124.82	114.10
1	E	65	LYS	CA-CB-CG	-5.35	103.40	114.10
1	D	87	LYS	O-C-N	5.16	125.74	121.35
1	B	87	LYS	O-C-N	-5.09	118.29	121.85
2	G	44	GLU	CA-CB-CG	-5.09	103.92	114.10
1	C	88	PRO	CA-C-N	5.02	127.71	120.38
1	C	88	PRO	C-N-CA	5.02	127.71	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	GLN	CB-CA-C	-5.02	100.14	110.38
1	F	44	GLU	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ASP	Peptide
1	F	105	ASP	Peptide
1	F	89	GLU	Sidechain
2	G	56	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	955	0	893	24	0
1	B	955	0	894	18	1
1	C	955	0	894	17	0
1	D	949	0	889	20	0
1	E	949	0	889	22	0
1	F	955	0	894	16	0
2	G	947	0	888	14	0
3	H	950	0	886	33	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
4	C	15	0	0	0	0
4	D	5	0	0	0	1
4	E	20	0	0	0	0
4	F	15	0	0	0	0
4	G	15	0	0	1	0
4	H	15	0	0	1	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
5	G	3	0	0	0	0
5	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7731	0	7127	148	1

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 10.

All (148) 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:A:113:GLU:OE1	1:A:113:GLU:N	1.56	1.36
1:A:110:THR:OG1	1:A:113:GLU:OE2	1.54	1.24
1:B:87:LYS:HE3	1:B:89:GLU:OE2	1.33	1.24
1:D:89:GLU:N	1:D:89:GLU:OE2	1.87	1.06
1:A:113:GLU:H	1:A:113:GLU:CD	1.62	1.02
1:F:91:THR:HG22	1:F:125:VAL:H	1.29	0.92
1:D:74:ASN:OD1	1:D:75:ALA:N	2.03	0.92
3:H:6:GLU:OE1	3:H:119:GLN:N	2.02	0.91
1:B:87:LYS:HB3	1:B:89:GLU:CD	2.02	0.84
1:F:91:THR:CG2	1:F:125:VAL:H	1.92	0.81
2:G:19:ARG:NH2	2:G:80:PHE:CE2	2.47	0.81
1:F:87:LYS:HB2	1:F:89:GLU:OE1	1.82	0.80
1:B:87:LYS:CE	1:B:89:GLU:OE2	2.26	0.78
3:H:6:GLU:CD	3:H:119:GLN:H	1.91	0.76
1:B:45:ARG:HB3	1:B:111:GLN:NE2	2.01	0.76
3:H:32:TYR:HA	3:H:101:CYS:HB2	1.67	0.76
1:A:108:PRO:HB2	1:A:113:GLU:HG3	1.69	0.73
3:H:20:LEU:HD21	3:H:122:GLN:HE22	1.53	0.73
3:H:118:GLY:O	3:H:119:GLN:HB3	1.90	0.72
1:D:51:VAL:HG11	1:D:79:MET:HE2	1.71	0.72
1:A:45:ARG:HB3	1:A:111:GLN:HE21	1.56	0.70
2:G:102:HIS:N	4:G:201:SO4:O3	2.26	0.69
1:A:112:ASP:N	1:A:113:GLU:OE1	2.25	0.68
1:F:91:THR:HG22	1:F:125:VAL:N	2.06	0.68
1:B:87:LYS:HB3	1:B:89:GLU:OE2	1.93	0.67
1:E:108:PRO:CB	1:E:113:GLU:HG3	2.23	0.67
3:H:51:VAL:HG11	3:H:79:MET:HE3	1.77	0.67
1:A:103:PHE:HB3	1:A:105:ASP:HB3	1.77	0.67
1:F:51:VAL:HG11	1:F:79:MET:HE2	1.77	0.66
1:A:45:ARG:HB3	1:A:111:GLN:NE2	2.09	0.66
1:A:103:PHE:CB	1:A:105:ASP:HB3	2.25	0.66
1:E:91:THR:HG23	1:E:124:THR:HA	1.79	0.65
1:B:83:MET:HE3	1:B:86:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:HD2	1:C:111:GLN:OE1	1.96	0.64
1:F:105:ASP:HB2	1:F:106:SER:HB3	1.79	0.64
1:D:83:MET:HE3	1:D:86:LEU:HD21	1.79	0.64
2:G:5:GLN:HE22	2:G:25:PRO:HG3	1.63	0.64
3:H:13:GLN:HA	3:H:125:VAL:HG22	1.81	0.63
1:C:20:LEU:HG	1:C:83:MET:HE2	1.82	0.61
1:A:83:MET:HE3	1:A:86:LEU:HD21	1.83	0.61
1:A:112:ASP:C	1:A:113:GLU:OE1	2.41	0.61
1:C:87:LYS:HB2	1:C:89:GLU:CD	2.25	0.61
1:A:102:HIS:HB3	4:A:202:SO4:O1	2.01	0.60
1:A:110:THR:CB	1:A:113:GLU:OE2	2.50	0.60
1:D:89:GLU:H	1:D:89:GLU:CD	2.05	0.60
1:E:15:GLY:O	3:H:74:ASN:OD1	2.20	0.60
1:E:69:THR:HG23	3:H:71:SER:HB2	1.85	0.59
1:A:108:PRO:CB	1:A:113:GLU:HG3	2.34	0.58
1:E:67:ARG:NH2	1:E:90:ASP:OD2	2.37	0.58
1:F:60:TYR:HB2	1:F:65:LYS:HG3	1.86	0.58
1:B:89:GLU:HG2	1:B:90:ASP:N	2.19	0.57
1:A:113:GLU:N	1:A:113:GLU:CD	2.37	0.57
1:E:20:LEU:HG	1:E:83:MET:HE2	1.85	0.56
1:F:42:GLY:C	1:F:43:LYS:HG2	2.30	0.56
1:A:55:ARG:NH2	1:A:105:ASP:O	2.39	0.56
1:B:45:ARG:HB3	1:B:111:GLN:HE22	1.71	0.55
1:B:103:PHE:N	4:B:202:SO4:O1	2.38	0.55
3:H:20:LEU:HD21	3:H:122:GLN:NE2	2.21	0.55
1:B:110:THR:HG22	1:B:112:ASP:H	1.72	0.55
1:E:16:GLY:HA2	3:H:74:ASN:OD1	2.07	0.54
2:G:83:MET:HB3	2:G:86:LEU:HD21	1.90	0.54
1:D:47:TRP:CZ3	1:D:109:LYS:HD3	2.42	0.54
3:H:31:ASN:HD22	3:H:53:THR:HG22	1.73	0.54
2:G:47:TRP:CZ3	2:G:109:LYS:HD3	2.42	0.54
3:H:68:PHE:CE2	3:H:83:MET:HE2	2.43	0.53
3:H:119:GLN:HG2	3:H:119:GLN:O	2.06	0.53
1:C:73:ASP:HB2	1:C:80:PHE:HE1	1.72	0.53
1:B:87:LYS:CB	1:B:89:GLU:OE2	2.56	0.53
1:D:108:PRO:HB3	1:D:113:GLU:HG3	1.90	0.53
1:C:69:THR:HG23	1:F:71:SER:HB2	1.90	0.53
1:D:19:ARG:NH2	2:G:69:THR:OG1	2.42	0.52
1:D:66:GLY:O	2:G:57:SER:HA	2.10	0.52
1:D:71:SER:HB2	2:G:69:THR:HG23	1.91	0.52
1:E:57:SER:HA	3:H:66:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:HD2	1:E:55:ARG:HG2	1.92	0.52
1:E:9:GLY:HA2	1:E:18:LEU:HD13	1.92	0.51
1:A:103:PHE:HB2	1:A:105:ASP:HB3	1.92	0.51
1:A:69:THR:HG23	1:B:71:SER:HB2	1.93	0.50
1:D:108:PRO:CB	1:D:113:GLU:HG3	2.42	0.50
1:A:74:ASN:HB2	1:C:73:ASP:OD2	2.12	0.50
1:E:108:PRO:CG	1:E:113:GLU:HG3	2.42	0.50
1:A:54:GLY:HA3	1:A:104:CYS:HB3	1.94	0.50
1:B:91:THR:HG23	1:B:124:THR:HA	1.94	0.50
1:E:69:THR:CG2	3:H:71:SER:HB2	2.41	0.49
3:H:18:LEU:HD13	3:H:122:GLN:NE2	2.27	0.49
2:G:5:GLN:HB2	2:G:23:THR:HB	1.94	0.49
1:B:31:ASN:HD22	1:B:53:THR:HG22	1.77	0.49
3:H:89:GLU:H	3:H:89:GLU:CD	2.19	0.49
2:G:19:ARG:NH2	2:G:80:PHE:HE2	2.03	0.49
3:H:94:TYR:CD1	3:H:122:GLN:HG2	2.47	0.49
1:D:45:ARG:NH1	1:D:111:GLN:OE1	2.43	0.48
1:E:66:GLY:O	3:H:72:GLN:HG3	2.13	0.48
3:H:51:VAL:CG1	3:H:79:MET:HE3	2.42	0.48
2:G:122:GLN:HG3	2:G:123:VAL:N	2.27	0.48
1:D:3:GLN:O	1:D:3:GLN:HG3	2.14	0.48
1:F:83:MET:HE2	1:F:86:LEU:HD21	1.96	0.47
3:H:32:TYR:HA	3:H:101:CYS:CB	2.41	0.47
1:C:6:GLU:OE1	1:C:118:GLY:HA3	2.14	0.47
1:C:32:TYR:H	1:C:53:THR:HB	1.80	0.47
1:E:108:PRO:HB3	1:E:113:GLU:CG	2.45	0.47
3:H:31:ASN:ND2	3:H:53:THR:HG22	2.30	0.47
1:A:57:SER:HA	1:B:66:GLY:O	2.14	0.46
1:D:122:GLN:HG3	1:D:123:VAL:N	2.30	0.46
3:H:30:SER:HA	4:H:203:SO4:O1	2.14	0.46
1:C:47:TRP:CH2	1:C:109:LYS:HD3	2.51	0.46
1:C:87:LYS:HD2	1:C:89:GLU:OE2	2.15	0.46
1:F:94:TYR:O	1:F:120:GLY:HA2	2.16	0.46
2:G:73:ASP:HB2	2:G:80:PHE:HE1	1.81	0.46
1:C:9:GLY:HA3	1:C:121:THR:CG2	2.46	0.46
1:C:73:ASP:HB2	1:C:80:PHE:CE1	2.51	0.45
1:D:6:GLU:OE2	1:D:118:GLY:HA3	2.17	0.45
1:E:51:VAL:HG11	1:E:79:MET:HE2	1.98	0.45
1:E:103:PHE:HD2	1:F:87:LYS:HE2	1.80	0.45
1:C:47:TRP:CZ3	1:C:109:LYS:HD3	2.52	0.45
1:A:108:PRO:O	1:A:114:TYR:OH	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:HIS:ND1	1:A:103:PHE:HD1	2.15	0.44
1:E:94:TYR:O	1:E:120:GLY:HA2	2.17	0.44
1:D:91:THR:HG23	1:D:124:THR:HA	1.99	0.44
1:E:108:PRO:CB	1:E:113:GLU:CG	2.94	0.44
3:H:6:GLU:OE1	3:H:118:GLY:HA3	2.16	0.44
1:F:34:MET:SD	1:F:79:MET:HB2	2.58	0.43
1:B:112:ASP:N	1:B:112:ASP:OD1	2.51	0.43
2:G:5:GLN:HE22	2:G:25:PRO:CG	2.28	0.43
3:H:13:GLN:NE2	3:H:125:VAL:HG21	2.33	0.43
3:H:18:LEU:CD1	3:H:122:GLN:NE2	2.82	0.43
2:G:99:ALA:HB2	2:G:114:TYR:HA	2.01	0.42
3:H:67:ARG:C	3:H:68:PHE:HD1	2.27	0.42
1:C:122:GLN:HG3	1:C:123:VAL:N	2.33	0.42
1:D:74:ASN:CG	1:D:75:ALA:H	2.09	0.42
3:H:73:ASP:HB2	3:H:80:PHE:CE2	2.55	0.42
3:H:11:SER:HA	3:H:123:VAL:O	2.20	0.41
1:B:122:GLN:HG3	1:B:123:VAL:N	2.34	0.41
1:F:122:GLN:HG3	1:F:123:VAL:N	2.35	0.41
1:E:103:PHE:CD2	1:F:87:LYS:HE2	2.55	0.41
1:C:18:LEU:HB2	1:C:83:MET:HE3	2.01	0.41
1:E:47:TRP:CZ3	1:E:109:LYS:HD3	2.55	0.41
1:B:47:TRP:CZ3	1:B:109:LYS:HD3	2.56	0.41
1:C:9:GLY:HA3	1:C:121:THR:HG23	2.01	0.41
1:D:47:TRP:CH2	1:D:109:LYS:HD3	2.56	0.41
1:A:122:GLN:HG3	1:A:123:VAL:N	2.34	0.41
3:H:89:GLU:OE1	3:H:89:GLU:N	2.35	0.41
3:H:94:TYR:CE1	3:H:122:GLN:HG2	2.56	0.40
1:F:20:LEU:HB2	1:F:81:LEU:HB3	2.03	0.40
1:E:108:PRO:HG2	1:E:113:GLU:HG3	2.03	0.40
1:E:122:GLN:HG3	1:E:123:VAL:N	2.32	0.40
3:H:83:MET:HE2	3:H:83:MET:HB3	1.92	0.40
1:D:32:TYR:H	1:D:53:THR:HB	1.86	0.40
1:D:79:MET:HE3	1:D:79:MET:HB3	2.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:NZ	4:D:201:SO4:O2[2_757]	1.30	0.90

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	123/146 (84%)	117 (95%)	3 (2%)	3 (2%)	4	7
1	B	123/146 (84%)	118 (96%)	2 (2%)	3 (2%)	4	7
1	C	123/146 (84%)	118 (96%)	4 (3%)	1 (1%)	16	27
1	D	122/146 (84%)	119 (98%)	2 (2%)	1 (1%)	16	27
1	E	122/146 (84%)	117 (96%)	5 (4%)	0	100	100
1	F	123/146 (84%)	117 (95%)	6 (5%)	0	100	100
2	G	122/146 (84%)	120 (98%)	2 (2%)	0	100	100
3	H	122/146 (84%)	113 (93%)	5 (4%)	4 (3%)	3	4
All	All	980/1168 (84%)	939 (96%)	29 (3%)	12 (1%)	10	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	119	GLN
1	A	29	ASP
1	B	9	GLY
1	D	9	GLY
3	H	9	GLY
1	A	9	GLY
1	B	89	GLU
1	A	41	PRO
1	B	41	PRO
1	C	41	PRO
3	H	41	PRO
3	H	125	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	102/119 (86%)	102 (100%)	0	100	100
1	B	102/119 (86%)	102 (100%)	0	100	100
1	C	102/119 (86%)	102 (100%)	0	100	100
1	D	101/119 (85%)	98 (97%)	3 (3%)	36	57
1	E	101/119 (85%)	101 (100%)	0	100	100
1	F	102/119 (86%)	102 (100%)	0	100	100
2	G	101/119 (85%)	101 (100%)	0	100	100
3	H	101/119 (85%)	97 (96%)	4 (4%)	28	47
All	All	812/952 (85%)	805 (99%)	7 (1%)	70	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	63	SER
1	D	87	LYS
1	D	89	GLU
3	H	28	THR
3	H	29	ASP
3	H	30	SER
3	H	93	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	111	GLN
1	B	31	ASN
1	C	74	ASN
1	D	3	GLN
1	D	31	ASN
1	D	82	GLN
1	D	84	ASN
1	E	13	GLN
1	E	74	ASN
1	F	84	ASN

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Mol	Chain	Res	Type
2	G	5	GLN
2	G	39	GLN
2	G	74	ASN
3	H	31	ASN
3	H	74	ASN
3	H	122	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](#)

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](#)

21 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	SO4	B	202	-	4,4,4	0.32	0	6,6,6	0.29	0
4	SO4	A	201	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	G	201	-	4,4,4	0.34	0	6,6,6	0.43	0
4	SO4	C	202	-	4,4,4	0.24	0	6,6,6	0.23	0
4	SO4	A	202	-	4,4,4	0.20	0	6,6,6	0.30	0
4	SO4	F	201	-	4,4,4	0.32	0	6,6,6	0.17	0
4	SO4	E	204	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	F	203	-	4,4,4	0.30	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	201	-	4,4,4	0.31	0	6,6,6	0.14	0
4	SO4	C	201	-	4,4,4	0.25	0	6,6,6	0.32	0
4	SO4	C	203	-	4,4,4	0.23	0	6,6,6	0.31	0
4	SO4	H	201	-	4,4,4	0.27	0	6,6,6	0.35	0
4	SO4	D	201	-	4,4,4	0.30	0	6,6,6	0.23	0
4	SO4	G	202	-	4,4,4	0.24	0	6,6,6	0.13	0
4	SO4	F	202	-	4,4,4	0.32	0	6,6,6	0.18	0
4	SO4	E	202	-	4,4,4	0.26	0	6,6,6	0.23	0
4	SO4	G	203	-	4,4,4	0.30	0	6,6,6	0.25	0
4	SO4	H	202	-	4,4,4	0.30	0	6,6,6	0.15	0
4	SO4	H	203	-	4,4,4	0.21	0	6,6,6	0.44	0
4	SO4	E	201	-	4,4,4	0.22	0	6,6,6	0.47	0
4	SO4	E	203	-	4,4,4	0.24	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	SO4	1	0
4	G	201	SO4	1	0
4	A	202	SO4	1	0
4	D	201	SO4	0	1
4	H	203	SO4	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	125/146 (85%)	0.22	5 (4%)	42	34	36, 51, 85, 109	0
1	B	125/146 (85%)	0.27	5 (4%)	42	34	36, 52, 78, 100	0
1	C	125/146 (85%)	0.12	4 (3%)	50	42	35, 49, 76, 108	0
1	D	124/146 (84%)	0.20	4 (3%)	50	42	38, 53, 82, 99	0
1	E	124/146 (84%)	0.16	2 (1%)	70	66	34, 49, 75, 91	0
1	F	125/146 (85%)	0.27	6 (4%)	35	28	36, 48, 87, 107	0
2	G	124/146 (84%)	0.14	3 (2%)	59	53	34, 51, 77, 106	0
3	H	124/146 (84%)	0.26	7 (5%)	30	24	32, 48, 81, 113	0
All	All	996/1168 (85%)	0.21	36 (3%)	46	38	32, 50, 81, 113	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	113	GLU	4.1
1	D	105	ASP	3.8
1	B	89	GLU	3.6
1	C	89	GLU	3.3
1	B	113	GLU	3.2
3	H	74	ASN	3.1
1	F	105	ASP	3.1
3	H	118	GLY	3.1
1	A	103	PHE	3.0
1	A	89	GLU	2.9
2	G	89	GLU	2.9
1	F	127	SER	2.9
1	F	89	GLU	2.8
1	A	102	HIS	2.7
1	A	101	CYS	2.7
3	H	122	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	29	ASP	2.6
1	B	127	SER	2.5
1	F	102	HIS	2.5
3	H	44	GLU	2.4
3	H	56	GLY	2.4
3	H	28	THR	2.4
1	F	29	ASP	2.4
1	A	112	ASP	2.3
1	C	105	ASP	2.3
1	D	126	SER	2.3
3	H	125	VAL	2.3
2	G	105	ASP	2.2
1	C	44	GLU	2.2
2	G	44	GLU	2.2
1	B	55	ARG	2.2
1	D	54	GLY	2.2
1	D	74	ASN	2.1
1	E	29	ASP	2.1
1	F	44	GLU	2.1
1	B	101	CYS	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(Å ²)	Q<0.9
4	SO4	H	203	5/5	0.39	0.18	105,108,110,113	0
4	SO4	E	204	5/5	0.69	0.17	94,96,97,99	0
4	SO4	F	202	5/5	0.70	0.12	100,103,105,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	H	202	5/5	0.79	0.18	101,101,104,105	0
4	SO4	F	203	5/5	0.83	0.15	83,85,87,89	0
4	SO4	H	201	5/5	0.83	0.18	78,80,87,93	0
4	SO4	A	202	5/5	0.83	0.13	96,99,103,106	0
4	SO4	B	202	5/5	0.83	0.14	79,82,85,87	0
4	SO4	C	203	5/5	0.87	0.15	91,92,94,96	0
4	SO4	G	202	5/5	0.87	0.13	87,91,92,93	0
4	SO4	E	203	5/5	0.87	0.12	92,92,95,95	0
4	SO4	B	201	5/5	0.87	0.20	83,84,86,92	0
4	SO4	A	201	5/5	0.87	0.17	84,87,87,93	0
4	SO4	G	203	5/5	0.89	0.17	86,91,92,93	0
4	SO4	F	201	5/5	0.89	0.16	83,83,88,89	0
4	SO4	G	201	5/5	0.94	0.09	73,76,82,83	0
4	SO4	C	201	5/5	0.94	0.10	65,67,74,75	0
4	SO4	E	201	5/5	0.95	0.10	56,60,67,68	0
4	SO4	E	202	5/5	0.96	0.13	62,63,68,69	0
4	SO4	C	202	5/5	0.96	0.08	58,73,79,82	0
4	SO4	D	201	5/5	0.97	0.07	73,79,82,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.