



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 08:54 PM EST

PDB ID : 5TOK  
Title : Crystal structure of the RSV F glycoprotein in complex with the neutralizing single-domain antibody F-VHH-L66  
Authors : Gilman, M.S.A.; Kabeche, S.C.; McLellan, J.S.  
Deposited on : 2016-10-17  
Resolution : 3.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

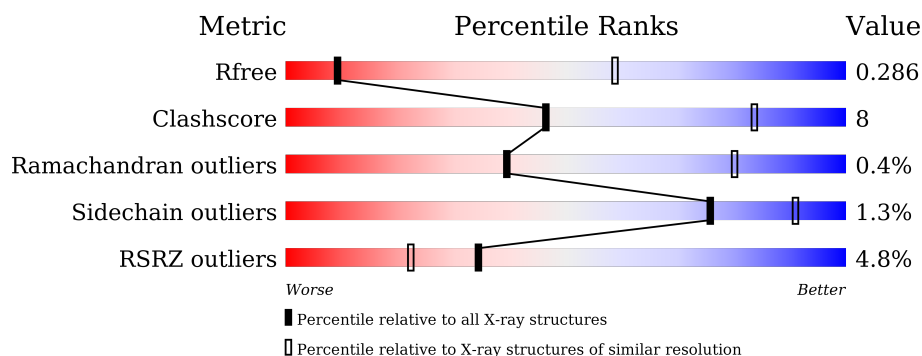
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	<div> <div>3%</div> <div>74% 13% • 13%</div> </div>
1	B	550	<div> <div>6%</div> <div>73% 13% • 13%</div> </div>
1	C	550	<div> <div>4%</div> <div>69% 17% • 13%</div> </div>
2	D	131	<div> <div>11%</div> <div>68% 26% 6%</div> </div>
2	E	131	<div> <div>70% 24% • •</div> </div>
2	F	131	<div> <div>2%</div> <div>72% 22% 6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13999 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 Fusion glycoprotein F0, Fibrin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3706	2348	610	726	22			
1	B	478	Total	C	N	O	S	0	0	0
			3706	2348	610	726	22			
1	C	478	Total	C	N	O	S	0	0	0
			3706	2348	610	726	22			

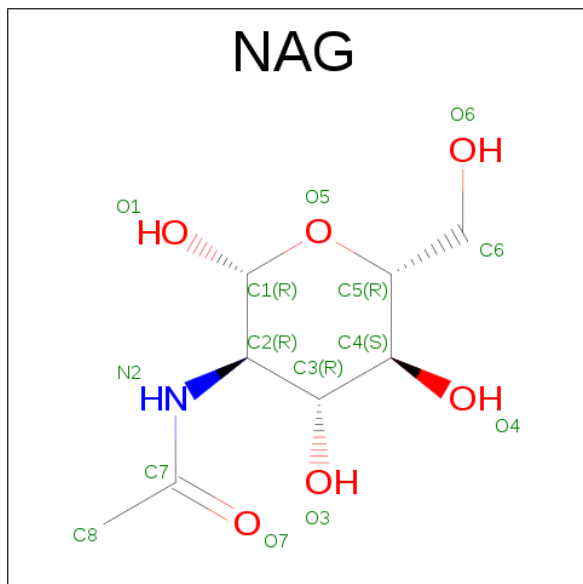
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	155	CYS	SER	engineered mutation	UNP P03420
A	190	PHE	SER	engineered mutation	UNP P03420
A	207	LEU	VAL	engineered mutation	UNP P03420
A	290	CYS	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
B	102	ALA	PRO	conflict	UNP P03420
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
C	155	CYS	SER	engineered mutation	UNP P03420
C	190	PHE	SER	engineered mutation	UNP P03420
C	207	LEU	VAL	engineered mutation	UNP P03420
C	290	CYS	SER	engineered mutation	UNP P03420
C	379	VAL	ILE	engineered mutation	UNP P03420
C	447	VAL	MET	engineered mutation	UNP P03420

- Molecule 2 is a protein called Single-domain antibody F-VHH-L66.

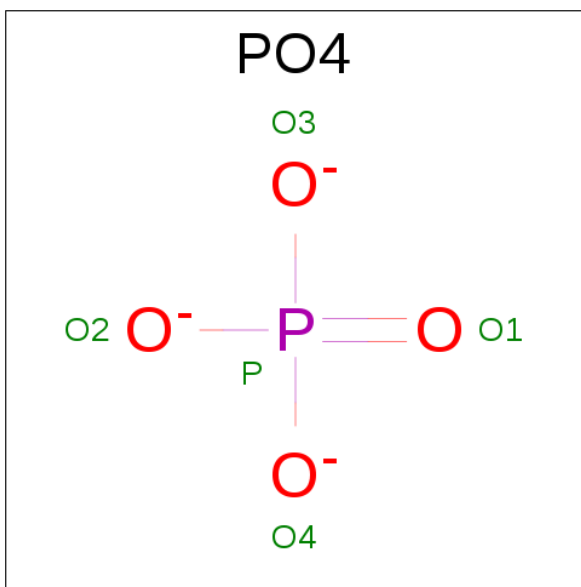
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	123	Total	C	N	O	S	0	0	0
			937	587	162	182	6			
2	E	126	Total	C	N	O	S	0	0	0
			960	600	168	186	6			
2	F	123	Total	C	N	O	S	0	0	0
			937	587	162	182	6			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



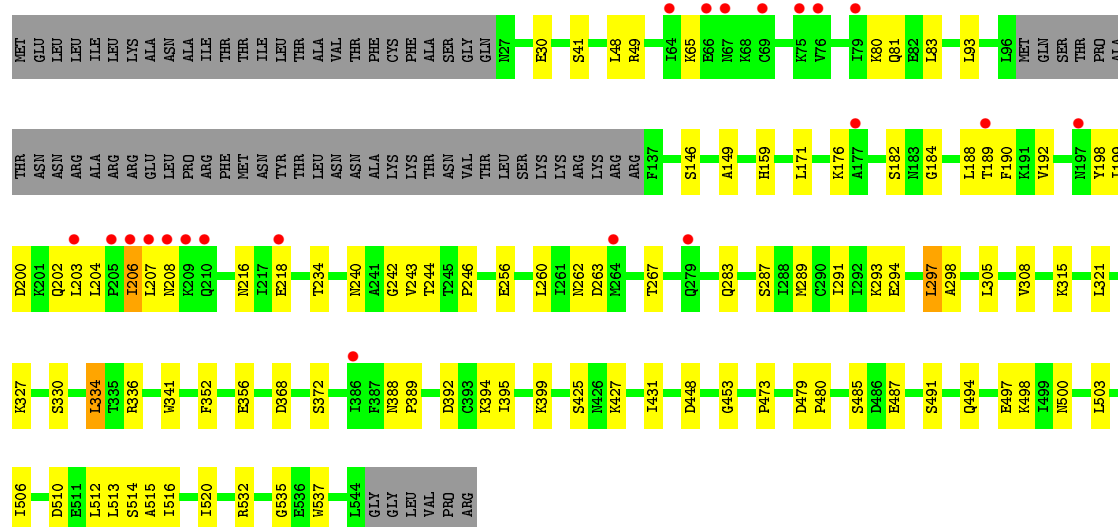
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

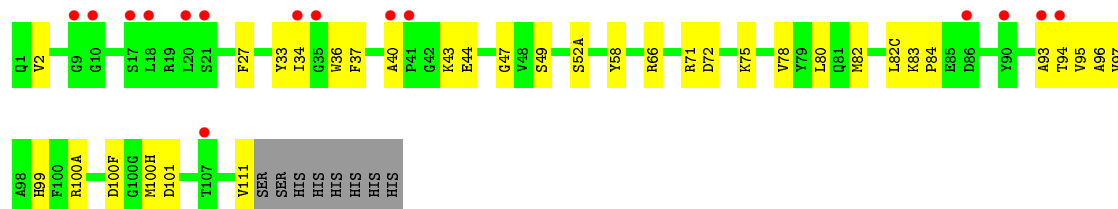


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

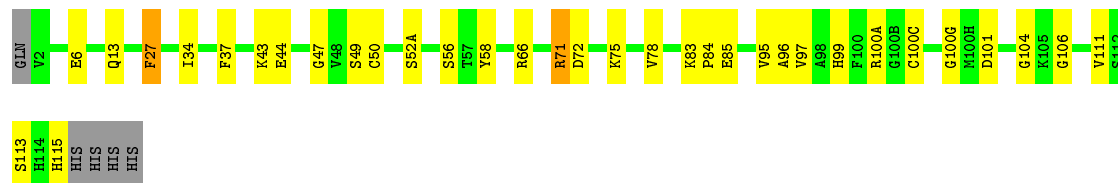




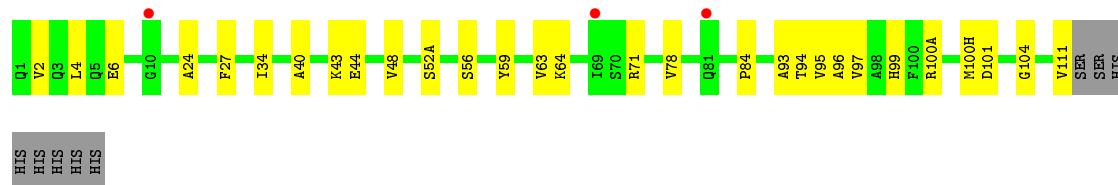
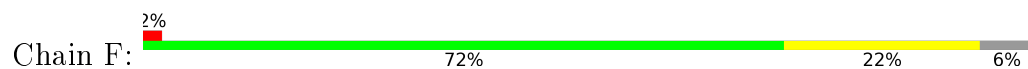
• Molecule 2: Single-domain antibody F-VHH-L66



• Molecule 2: Single-domain antibody F-VHH-L66



• Molecule 2: Single-domain antibody F-VHH-L66



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.89Å 138.89Å 221.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.38 – 3.80 50.38 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.38-3.80) 100.0 (50.38-3.80)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.247 , 0.286 0.248 , 0.286	Depositor DCC
$R_{free}$ test set	1204 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.8	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	13999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, 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	0/3763	0.60	0/5100
1	B	0.40	0/3763	0.59	1/5100 (0.0%)
1	C	0.33	0/3763	0.55	1/5100 (0.0%)
2	D	0.34	0/958	0.55	0/1296
2	E	0.47	0/983	0.68	2/1330 (0.2%)
2	F	0.32	0/958	0.53	0/1296
All	All	0.38	0/14188	0.58	4/19222 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	LEU	CA-CB-CG	5.58	128.13	115.30
2	E	50	CYS	CA-CB-SG	5.37	123.66	114.00
2	E	100(C)	CYS	N-CA-C	-5.09	97.27	111.00
1	B	334	LEU	CA-CB-CG	5.07	126.97	115.30

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	3706	0	3743	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3706	0	3741	47	0
1	C	3706	0	3743	64	0
2	D	937	0	891	28	0
2	E	960	0	904	23	0
2	F	937	0	891	21	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
4	B	5	0	0	1	0
All	All	13999	0	13952	213	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 8.

All (213) 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:B:461:LYS:NZ	4:B:602:PO4:O3	2.02	0.93
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.58	0.86
1:A:184:GLY:HA2	2:E:44:GLU:OE2	1.78	0.83
2:F:100(A):ARG:NH1	2:F:101:ASP:OD1	2.12	0.80
1:C:176:LYS:HD2	1:C:263:ASP:OD2	1.83	0.79
1:C:425:SER:HB3	1:C:431:ILE:HD13	1.63	0.79
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.16	0.74
1:C:327:LYS:HE2	1:C:330:SER:HB2	1.70	0.73
1:C:184:GLY:HA2	2:F:44:GLU:OE2	1.89	0.71
1:A:60:GLU:OE2	1:A:191:LYS:NZ	2.18	0.69
2:D:84:PRO:HA	2:D:111:VAL:HB	1.75	0.68
1:A:426:ASN:ND2	1:A:428:ASN:OD1	2.29	0.66
2:F:84:PRO:HA	2:F:111:VAL:HB	1.77	0.65
1:C:30:GLU:OE1	1:C:41:SER:OG	2.13	0.64
1:C:503:LEU:HD23	1:C:506:ILE:HD11	1.79	0.64
1:C:200:ASP:HA	1:C:204:LEU:HG	1.81	0.63
1:A:308:VAL:HG22	2:E:97:VAL:HG12	1.81	0.62
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.82	0.61
2:F:40:ALA:HB3	2:F:43:LYS:HE3	1.81	0.61
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.82	0.61
2:E:84:PRO:HA	2:E:111:VAL:HB	1.82	0.60
1:A:525:ARG:NH1	1:C:535:GLY:HA3	2.16	0.60
2:D:43:LYS:NZ	2:D:44:GLU:O	2.34	0.60
1:A:64:ILE:HD11	1:A:199:ILE:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100(A):ARG:NH1	2:E:101:ASP:OD1	2.23	0.59
1:B:200:ASP:HA	1:B:204:LEU:HG	1.83	0.59
1:A:60:GLU:HB2	1:A:191:LYS:HD2	1.84	0.59
2:F:2:VAL:HG13	2:F:27:PHE:CD1	2.38	0.59
1:B:80:LYS:NZ	1:B:207:LEU:HD22	2.17	0.59
1:A:453:GLY:O	2:F:99:HIS:NE2	2.35	0.58
1:A:426:ASN:HD22	1:A:429:ARG:HB2	1.68	0.58
1:C:487:GLU:OE2	1:C:498:LYS:HD2	2.03	0.58
2:D:33:TYR:CD1	2:D:97:VAL:HG22	2.40	0.57
2:E:43:LYS:HG3	2:E:44:GLU:N	2.20	0.57
1:B:432:ILE:HD11	1:B:447:VAL:HG22	1.87	0.56
1:A:267:THR:OG1	2:E:56:SER:OG	2.21	0.56
2:E:34:ILE:HG21	2:E:78:VAL:HG21	1.87	0.56
1:A:432:ILE:HD11	1:A:447:VAL:HG22	1.88	0.55
1:A:427:LYS:HG2	1:A:448:ASP:OD2	2.06	0.55
1:C:199:ILE:HG23	1:C:203:LEU:HB2	1.87	0.55
1:B:520:ILE:HB	1:B:532:ARG:HH12	1.72	0.55
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.88	0.55
2:E:115:HIS:ND1	2:E:115:HIS:O	2.38	0.55
1:A:399:LYS:HD2	1:C:494:GLN:HG3	1.89	0.54
2:D:100(A):ARG:NH1	2:D:101:ASP:OD1	2.19	0.54
1:C:513:LEU:HG	1:C:516:ILE:HD11	1.90	0.54
1:A:80:LYS:NZ	1:A:207:LEU:HD22	2.22	0.54
2:E:6:GLU:OE2	2:E:104:GLY:HA3	2.08	0.54
2:F:34:ILE:HG13	2:F:78:VAL:HG21	1.90	0.54
1:B:167:ILE:HG23	1:B:189:THR:HG21	1.89	0.53
1:A:137:PHE:N	1:A:354:GLN:OE1	2.41	0.53
2:F:6:GLU:OE2	2:F:104:GLY:HA3	2.09	0.53
1:B:310:ASP:OD1	1:B:364:ARG:NH1	2.36	0.52
1:B:184:GLY:HA2	2:D:44:GLU:OE2	2.09	0.52
1:B:80:LYS:HZ3	1:B:207:LEU:HD22	1.71	0.52
1:C:80:LYS:NZ	1:C:207:LEU:HD22	2.25	0.52
1:C:204:LEU:O	1:C:208:ASN:HB2	2.09	0.52
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.45	0.52
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.45	0.51
1:B:167:ILE:HD13	1:B:179:VAL:HG21	1.91	0.51
1:C:453:GLY:O	2:D:99:HIS:NE2	2.39	0.51
1:C:48:LEU:HB2	1:C:308:VAL:HB	1.92	0.51
1:A:80:LYS:HZ3	1:A:207:LEU:HD22	1.75	0.50
2:D:2:VAL:HG13	2:D:27:PHE:CD1	2.46	0.50
2:D:95:VAL:HG12	2:D:96:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:HG22	1:A:402:VAL:HG23	1.91	0.50
1:B:236:GLU:OE2	1:B:248:SER:OG	2.18	0.50
1:B:146:SER:HB3	1:B:149:ALA:HB2	1.94	0.50
1:C:308:VAL:HG22	2:F:97:VAL:HG12	1.94	0.50
1:C:49:ARG:HE	1:C:368:ASP:CG	2.15	0.50
1:A:146:SER:HB3	1:A:149:ALA:HB2	1.92	0.50
1:C:427:LYS:N	1:C:448:ASP:OD2	2.38	0.50
2:D:40:ALA:HB3	2:D:43:LYS:HE3	1.94	0.50
1:A:356:GLU:CD	1:A:356:GLU:H	2.15	0.50
2:D:95:VAL:HG23	2:D:100(H):MET:SD	2.51	0.50
1:B:308:VAL:HG22	2:D:97:VAL:HG12	1.94	0.49
1:B:449:THR:HB	1:B:456:LEU:HD11	1.93	0.49
1:C:198:TYR:O	1:C:202:GLN:HB2	2.11	0.49
1:A:426:ASN:ND2	1:A:429:ARG:HE	2.10	0.49
2:E:72:ASP:OD2	2:E:75:LYS:HD3	2.12	0.49
1:A:399:LYS:NZ	1:C:497:GLU:OE1	2.45	0.48
1:B:451:SER:HB3	2:E:99:HIS:NE2	2.28	0.48
1:B:293:LYS:HG2	1:B:294:GLU:HG3	1.96	0.48
1:C:427:LYS:HG2	1:C:448:ASP:OD2	2.13	0.48
1:C:513:LEU:O	1:C:516:ILE:HG13	2.13	0.48
1:C:267:THR:HG1	2:F:56:SER:HG	1.55	0.48
2:F:34:ILE:HG23	2:F:94:THR:HG22	1.95	0.48
1:B:487:GLU:HB3	1:B:490:ALA:HB2	1.94	0.48
1:C:146:SER:HB3	1:C:149:ALA:HB2	1.95	0.48
1:B:48:LEU:HB2	1:B:308:VAL:HB	1.96	0.48
1:C:510:ASP:O	1:C:514:SER:N	2.47	0.48
2:D:34:ILE:HG23	2:D:94:THR:HG22	1.94	0.48
1:A:398:SER:HA	1:A:485:SER:O	2.14	0.47
1:C:336:ARG:HA	1:C:395:ILE:HG22	1.95	0.47
2:D:34:ILE:HG21	2:D:78:VAL:HG21	1.95	0.47
2:E:85:GLU:OE1	2:E:85:GLU:N	2.33	0.47
1:B:176:LYS:HB3	1:B:190:PHE:HE1	1.80	0.47
2:D:93:ALA:HB3	2:D:100(H):MET:HE3	1.96	0.47
1:B:198:TYR:O	1:B:202:GLN:HB2	2.15	0.47
2:D:82:MET:HB3	2:D:82(C):LEU:HD21	1.97	0.47
2:F:93:ALA:HB3	2:F:100(H):MET:HE3	1.96	0.47
1:B:171:LEU:HD11	1:B:189:THR:HG22	1.97	0.47
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.96	0.47
2:E:52(A):SER:O	2:E:71:ARG:NE	2.24	0.47
1:C:188:LEU:HD13	1:C:260:LEU:HD12	1.96	0.47
1:B:204:LEU:HD22	1:B:208:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LYS:HG3	1:C:330:SER:HB3	1.96	0.47
1:B:356:GLU:CD	1:B:356:GLU:H	2.19	0.46
1:A:399:LYS:NZ	1:C:497:GLU:CD	2.68	0.46
1:C:293:LYS:HG2	1:C:294:GLU:HG3	1.96	0.46
1:A:297:LEU:HD12	1:A:298:ALA:N	2.30	0.46
1:C:204:LEU:HD22	1:C:208:ASN:ND2	2.30	0.46
2:D:36:TRP:CD1	2:D:80:LEU:HB2	2.51	0.46
1:A:79:ILE:HD11	1:A:220:VAL:HG22	1.96	0.46
1:A:28:ILE:HD13	1:A:44:TYR:CZ	2.50	0.46
1:A:188:LEU:HD23	1:A:260:LEU:HD12	1.97	0.46
1:A:49:ARG:HE	1:A:368:ASP:CG	2.19	0.46
1:B:216:ASN:OD1	1:B:216:ASN:N	2.49	0.45
2:D:34:ILE:HG13	2:D:78:VAL:HG21	1.98	0.45
1:C:242:GLY:O	1:C:289:MET:N	2.43	0.45
2:E:37:PHE:CD2	2:E:47:GLY:HA2	2.52	0.45
1:C:171:LEU:HD11	1:C:189:THR:HG22	1.98	0.45
1:A:336:ARG:HA	1:A:395:ILE:HG22	1.97	0.45
1:C:356:GLU:CD	1:C:356:GLU:H	2.20	0.45
2:D:33:TYR:HE1	2:D:97:VAL:HG13	1.82	0.45
2:D:52(A):SER:HA	2:D:71:ARG:HD3	1.99	0.45
1:B:291:ILE:HD11	1:B:293:LYS:HE2	1.97	0.45
1:B:334:LEU:HB3	1:B:475:ILE:HD13	1.99	0.45
2:E:95:VAL:HG12	2:E:96:ALA:O	2.16	0.45
1:A:80:LYS:HZ3	1:A:207:LEU:CD2	2.30	0.44
1:B:240:ASN:HB3	1:B:243:VAL:O	2.15	0.44
1:A:514:SER:O	1:A:516:ILE:N	2.51	0.44
1:A:206:ILE:CD1	1:A:207:LEU:HG	2.48	0.44
1:C:388:ASN:HA	1:C:389:PRO:HD3	1.79	0.44
2:E:66:ARG:CZ	2:E:83:LYS:HE2	2.47	0.44
1:C:352:PHE:CE2	1:C:372:SER:HB3	2.53	0.44
1:C:497:GLU:O	1:C:500:ASN:HB2	2.18	0.44
2:F:4:LEU:HD23	2:F:24:ALA:HA	1.99	0.44
2:F:59:TYR:HB2	2:F:64:LYS:HG3	1.99	0.44
2:D:66:ARG:CZ	2:D:83:LYS:HE2	2.48	0.44
2:D:49:SER:HA	2:D:58:TYR:O	2.18	0.44
2:E:27:PHE:CD1	2:E:27:PHE:N	2.86	0.44
1:B:285:SER:OG	1:B:303:LEU:HD23	2.17	0.44
2:D:72:ASP:OD2	2:D:75:LYS:HD3	2.18	0.44
2:E:43:LYS:HG3	2:E:44:GLU:H	1.82	0.44
1:A:514:SER:C	1:A:516:ILE:H	2.20	0.43
1:C:267:THR:OG1	2:F:56:SER:OG	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:VAL:HG13	2:F:63:VAL:HG21	1.99	0.43
2:D:71:ARG:HG3	2:D:71:ARG:O	2.18	0.43
2:F:95:VAL:HG23	2:F:100(H):MET:SD	2.58	0.43
1:A:465:LYS:HE3	1:A:465:LYS:HB2	1.80	0.43
1:A:171:LEU:HD13	1:A:191:LYS:HB2	2.01	0.43
1:C:240:ASN:HB3	1:C:243:VAL:O	2.18	0.43
2:F:52(A):SER:O	2:F:71:ARG:NE	2.51	0.43
1:B:252:LEU:O	1:B:282:ARG:NH2	2.48	0.43
1:C:512:LEU:HD23	1:C:512:LEU:HA	1.76	0.43
2:E:100(A):ARG:HE	2:E:100(G):GLY:HA2	1.82	0.43
1:A:150:SER:OG	1:A:302:GLN:OE1	2.34	0.43
1:C:297:LEU:HD12	1:C:298:ALA:N	2.34	0.43
1:C:394:LYS:HB3	1:C:394:LYS:HE3	1.75	0.43
1:A:508:LYS:HE2	1:A:512:LEU:HD11	2.00	0.43
1:C:532:ARG:NH1	1:C:537:TRP:CD1	2.87	0.43
1:A:506:ILE:HA	1:A:509:SER:HG	1.84	0.42
1:B:49:ARG:O	1:B:369:THR:HG23	2.19	0.42
1:C:399:LYS:HE2	1:C:485:SER:OG	2.17	0.42
1:C:216:ASN:HB2	1:C:218:GLU:OE1	2.19	0.42
1:B:204:LEU:O	1:B:208:ASN:HB2	2.20	0.42
1:B:427:LYS:HG3	1:B:428:ASN:N	2.35	0.42
1:A:216:ASN:OD1	1:A:216:ASN:N	2.53	0.42
2:D:33:TYR:HD1	2:D:97:VAL:HG22	1.84	0.42
1:B:334:LEU:HD21	1:B:474:ILE:HD11	2.02	0.42
1:C:392:ASP:OD2	1:C:491:SER:OG	2.24	0.42
2:D:2:VAL:HG13	2:D:27:PHE:CE1	2.55	0.42
1:B:297:LEU:HD12	1:B:298:ALA:N	2.35	0.42
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.69	0.42
2:E:13:GLN:N	2:E:13:GLN:OE1	2.51	0.42
1:A:93:LEU:HG	1:A:234:THR:HG23	2.01	0.42
1:C:80:LYS:HZ3	1:C:207:LEU:CD2	2.33	0.42
2:E:95:VAL:HG21	2:E:100(G):GLY:O	2.20	0.42
1:A:176:LYS:HE2	1:A:176:LYS:HB3	1.83	0.42
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.70	0.42
1:B:50:THR:HG21	1:B:308:VAL:HG23	2.01	0.42
1:C:427:LYS:O	2:D:100(F):ASP:HA	2.20	0.42
1:B:523:ALA:HB2	1:B:537:TRP:CE2	2.55	0.41
1:C:315:LYS:HD2	1:C:341:TRP:CZ2	2.55	0.41
2:D:37:PHE:CD2	2:D:47:GLY:HA2	2.55	0.41
1:C:479:ASP:HA	1:C:480:PRO:HD3	1.86	0.41
1:A:202:GLN:O	1:A:205:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PHE:O	1:B:544:LEU:HD23	2.20	0.41
1:C:80:LYS:HZ3	1:C:207:LEU:HD22	1.86	0.41
2:F:71:ARG:HG3	2:F:71:ARG:O	2.20	0.41
1:B:65:LYS:HB2	1:B:66:GLU:H	1.67	0.41
1:C:244:THR:OG1	1:C:287:SER:HB3	2.20	0.41
1:A:520:ILE:HG23	1:A:532:ARG:NH1	2.35	0.41
1:C:206:ILE:CD1	1:C:207:LEU:HG	2.50	0.41
1:C:192:VAL:HB	1:C:256:GLU:OE2	2.20	0.41
1:C:159:HIS:CD2	1:C:291:ILE:HD12	2.56	0.41
1:B:206:ILE:CD1	1:B:207:LEU:HG	2.51	0.41
2:D:52(A):SER:O	2:D:71:ARG:NE	2.54	0.41
1:C:216:ASN:N	1:C:216:ASN:OD1	2.53	0.41
1:C:93:LEU:HG	1:C:234:THR:HG23	2.03	0.41
2:E:6:GLU:CD	2:E:106:GLY:H	2.24	0.41
1:C:513:LEU:C	1:C:515:ALA:H	2.24	0.41
2:E:49:SER:HA	2:E:58:TYR:O	2.21	0.41
2:F:95:VAL:HG12	2:F:96:ALA:O	2.21	0.41
1:A:399:LYS:HE3	1:A:485:SER:OG	2.21	0.40
1:B:47:ALA:HB2	1:B:364:ARG:HD2	2.02	0.40
1:B:379:VAL:HG23	1:B:391:TYR:CE2	2.56	0.40
1:B:83:LEU:O	1:B:86:TYR:HB3	2.20	0.40
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.88	0.40
1:B:64:ILE:HD11	1:B:199:ILE:HG21	2.02	0.40
2:F:43:LYS:HE3	2:F:43:LYS:HB3	1.91	0.40
1:B:520:ILE:HD11	1:C:520:ILE:HD12	2.03	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	474/550 (86%)	457 (96%)	14 (3%)	3 (1%)	30 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/550 (86%)	461 (97%)	11 (2%)	2 (0%)	39	80
1	C	474/550 (86%)	455 (96%)	17 (4%)	2 (0%)	39	80
2	D	121/131 (92%)	117 (97%)	4 (3%)	0	100	100
2	E	124/131 (95%)	120 (97%)	4 (3%)	0	100	100
2	F	121/131 (92%)	118 (98%)	3 (2%)	0	100	100
All	All	1788/2043 (88%)	1728 (97%)	53 (3%)	7 (0%)	39	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	182	SER
1	B	65	LYS
1	B	182	SER
1	C	182	SER
1	C	65	LYS
1	A	515	ALA

### 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	432/494 (87%)	425 (98%)	7 (2%)	70	89
1	B	432/494 (87%)	428 (99%)	4 (1%)	84	93
1	C	432/494 (87%)	426 (99%)	6 (1%)	74	90
2	D	98/106 (92%)	98 (100%)	0	100	100
2	E	101/106 (95%)	98 (97%)	3 (3%)	48	80
2	F	98/106 (92%)	98 (100%)	0	100	100
All	All	1593/1800 (88%)	1573 (99%)	20 (1%)	76	91

All (20) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	81	GLN
1	A	190	PHE
1	A	206	ILE
1	A	297	LEU
1	A	334	LEU
1	A	472	GLU
1	A	516	ILE
1	B	183	ASN
1	B	206	ILE
1	B	297	LEU
1	B	334	LEU
1	C	81	GLN
1	C	190	PHE
1	C	206	ILE
1	C	262	ASN
1	C	297	LEU
1	C	334	LEU
2	E	27	PHE
2	E	71	ARG
2	E	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	426	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	800	1	14,14,15	0.21	0	15,19,21	0.61	0
3	NAG	B	601	1	14,14,15	0.44	0	15,19,21	0.31	0
4	PO4	B	602	1	4,4,4	0.75	0	6,6,6	0.27	0
3	NAG	C	800	1	14,14,15	0.69	1 (7%)	15,19,21	0.46	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	A	800	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	PO4	B	602	1	-	0/0/0/0	0/0/0/0
3	NAG	C	800	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	NAG	O5-C1	-2.47	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	PO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	478/550 (86%)	-0.06	16 (3%) 50 34	57, 96, 209, 273	0
1	B	478/550 (86%)	0.17	32 (6%) 21 12	59, 100, 260, 313	0
1	C	478/550 (86%)	0.14	21 (4%) 38 25	75, 126, 229, 295	0
2	D	123/131 (93%)	0.74	15 (12%) 5 5	105, 143, 187, 210	0
2	E	126/131 (96%)	-0.26	0 100 100	53, 73, 95, 135	0
2	F	123/131 (93%)	0.45	3 (2%) 62 46	129, 153, 181, 207	0
All	All	1806/2043 (88%)	0.13	87 (4%) 34 22	53, 114, 223, 313	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	ILE	6.2
1	B	298	ALA	5.5
1	C	207	LEU	5.3
1	B	72	THR	5.0
1	B	215	SER	4.7
1	C	79	ILE	4.7
1	B	76	VAL	4.5
1	B	297	LEU	4.5
1	A	207	LEU	4.5
1	A	208	ASN	4.4
1	B	219	THR	4.3
1	B	208	ASN	4.3
1	B	216	ASN	4.2
2	F	10	GLY	4.2
1	A	215	SER	4.1
1	B	68	LYS	4.0
1	B	73	ASP	3.9
1	C	218	GLU	3.8
1	B	211	SER	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	72	THR	3.8
1	B	210	GLN	3.7
1	B	207	LEU	3.7
1	B	204	LEU	3.6
1	C	189	THR	3.5
2	D	40	ALA	3.5
1	C	203	LEU	3.4
1	B	227	ASN	3.4
2	D	34	ILE	3.4
1	B	167	ILE	3.4
1	A	64	ILE	3.4
1	B	203	LEU	3.3
2	F	69	ILE	3.3
2	D	86	ASP	3.2
1	C	75	LYS	3.1
1	B	66	GLU	3.0
1	A	204	LEU	3.0
1	A	67	ASN	3.0
2	D	94	THR	3.0
1	B	65	LYS	3.0
1	B	61	LEU	2.9
1	C	208	ASN	2.9
1	A	203	LEU	2.8
2	D	90	TYR	2.8
2	D	107	THR	2.8
2	D	17	SER	2.7
1	A	206	ILE	2.7
1	B	80	LYS	2.7
1	A	210	GLN	2.7
1	A	66	GLU	2.6
1	C	279	GLN	2.6
1	C	64	ILE	2.5
1	C	205	PRO	2.5
1	B	67	ASN	2.5
1	B	220	VAL	2.5
2	D	41	PRO	2.5
1	B	223	PHE	2.4
2	D	35	GLY	2.4
1	B	291	ILE	2.3
1	A	61	LEU	2.3
1	B	91	THR	2.3
2	D	20	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	177	ALA	2.3
1	A	209	LYS	2.2
1	B	289	MET	2.2
1	C	197	ASN	2.2
1	B	296	VAL	2.2
1	B	63	ASN	2.2
1	C	67	ASN	2.2
2	D	93	ALA	2.2
1	C	210	GLN	2.2
2	D	18	LEU	2.1
1	A	62	SER	2.1
1	B	174	THR	2.1
1	C	76	VAL	2.1
1	B	206	ILE	2.1
1	C	209	LYS	2.1
1	C	386	ILE	2.1
2	D	21	SER	2.1
1	B	59	ILE	2.1
1	C	66	GLU	2.1
1	C	69	CYS	2.1
1	C	264	MET	2.0
2	F	81	GLN	2.0
2	D	10	GLY	2.0
1	A	467	LEU	2.0
2	D	9	GLY	2.0
1	A	65	LYS	2.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	B	602	5/5	0.76	0.27	0.99	148,148,148,150	0
3	NAG	A	800	14/15	0.90	0.21	-0.14	104,109,111,112	0
3	NAG	C	800	14/15	0.80	0.31	-	126,133,136,137	0
3	NAG	B	601	14/15	0.87	0.24	-	105,112,114,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.