



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2017 – 01:33 PM EST

PDB ID : 5TLJ
Title : COMPLEX BETWEEN HUMAN CD27 AND FAB FRAGMENTS OF ANTIBODIES M2177 AND M2191
Authors : Teplyakov, A.; Obmolova, G.; Malia, T.; Gilliland, G.L.
Deposited on : 2016-10-11
Resolution : 3.50 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

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

with specific help available everywhere you see the ⓘ symbol.

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

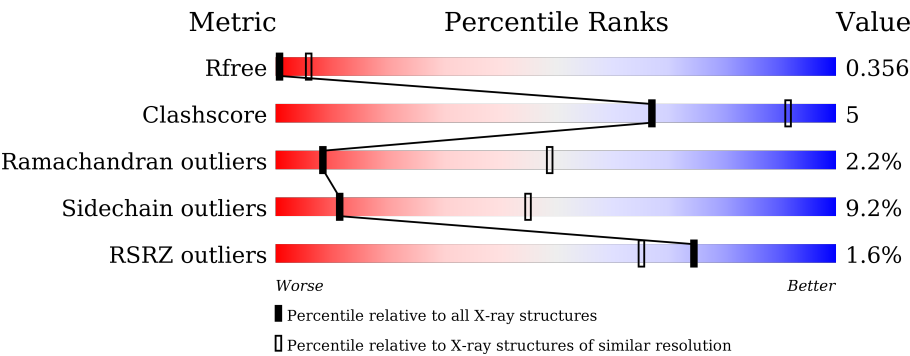
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 ≥ 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	218	<div><div></div><div>74%21%..</div></div>
1	E	218	<div><div></div><div>72%24%..</div></div>
2	B	229	<div><div>3%</div><div>78%16%..</div></div>
2	F	229	<div><div>3%</div><div>79%15%..</div></div>
3	C	218	<div><div></div><div>83%14%..</div></div>
3	G	218	<div><div>%</div><div>76%22%..</div></div>

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Mol	Chain	Length	Quality of chain
4	D	226	 % 81% 13% • •
4	H	226	 3% 75% 19% • •
5	X	109	 2% 54% 13% • 32%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13732 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 M2177 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1647	1029	274	339	5			
1	E	215	Total	C	N	O	S	0	0	0
			1647	1029	274	339	5			

- Molecule 2 is a protein called M2177 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1632	1034	267	325	6			
2	F	220	Total	C	N	O	S	0	0	0
			1632	1034	267	325	6			

- Molecule 3 is a protein called M2191 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1656	1040	281	330	5			
3	G	215	Total	C	N	O	S	0	0	0
			1656	1040	281	330	5			

- Molecule 4 is a protein called M2191 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	217	Total	C	N	O	S	0	0	0
			1632	1027	276	322	7			
4	H	217	Total	C	N	O	S	0	0	0
			1632	1027	276	322	7			

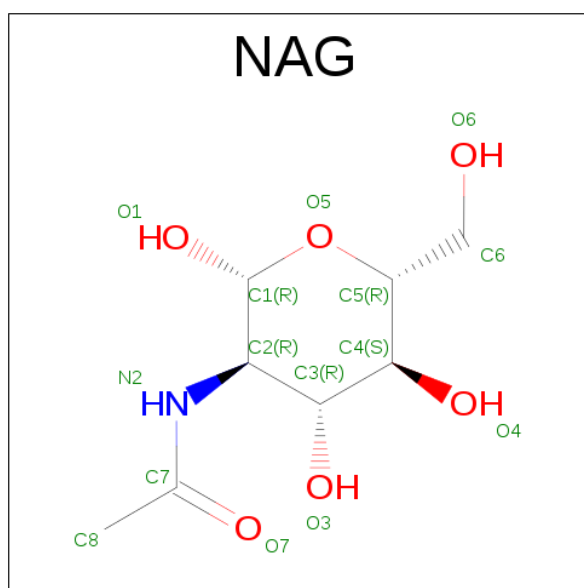
- Molecule 5 is a protein called CD27 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	74	Total	C	N	O	S	0	0	0
			570	343	109	105	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	102	GLY	-	expression tag	UNP P26842
X	103	GLY	-	expression tag	UNP P26842
X	104	HIS	-	expression tag	UNP P26842
X	105	HIS	-	expression tag	UNP P26842
X	106	HIS	-	expression tag	UNP P26842
X	107	HIS	-	expression tag	UNP P26842
X	108	HIS	-	expression tag	UNP P26842
X	109	HIS	-	expression tag	UNP P26842

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

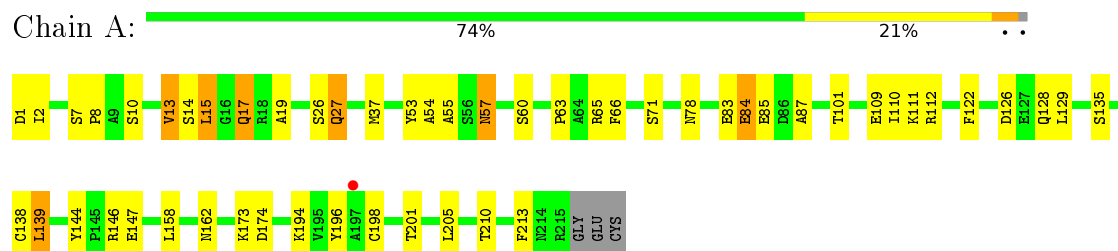


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	X	1	Total	C	N	O	0	0
			14	8	1	5		
6	X	1	Total	C	N	O	0	0
			14	8	1	5		

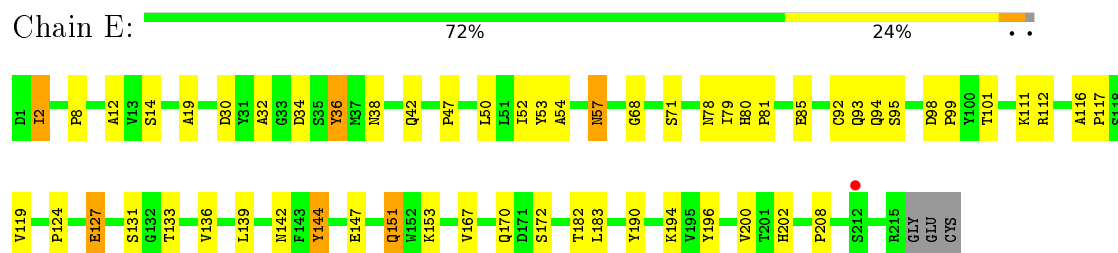
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

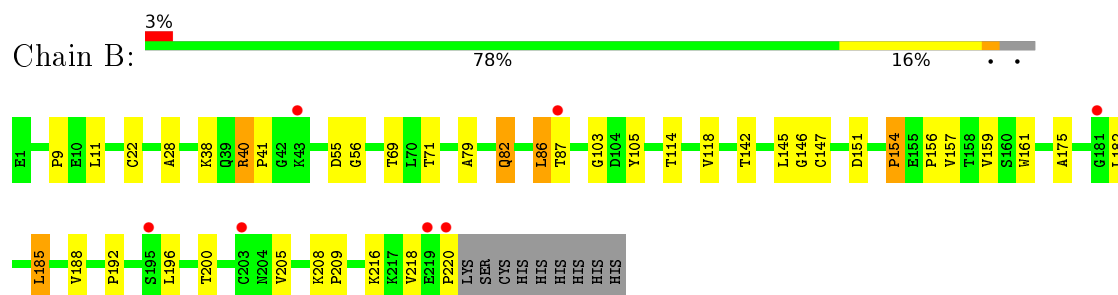
• Molecule 1: M2177 LIGHT CHAIN



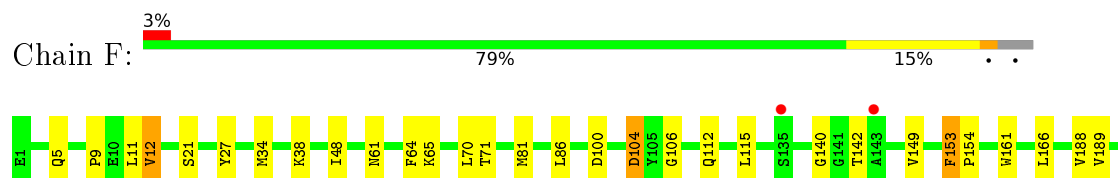
• Molecule 1: M2177 LIGHT CHAIN

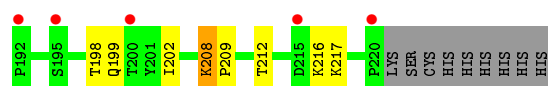


• Molecule 2: M2177 HEAVY CHAIN



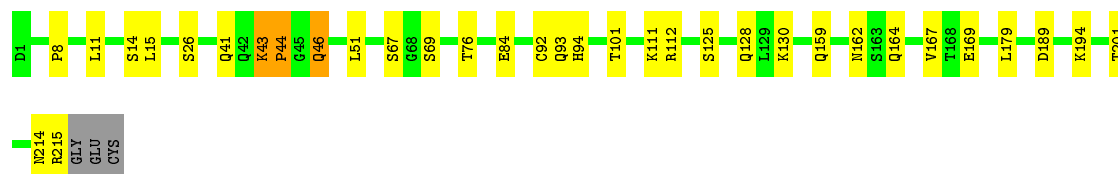
• Molecule 2: M2177 HEAVY CHAIN





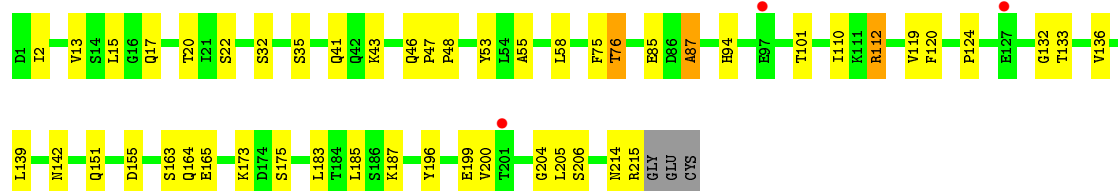
• Molecule 3: M2191 LIGHT CHAIN

Chain C: 83% 14% ..



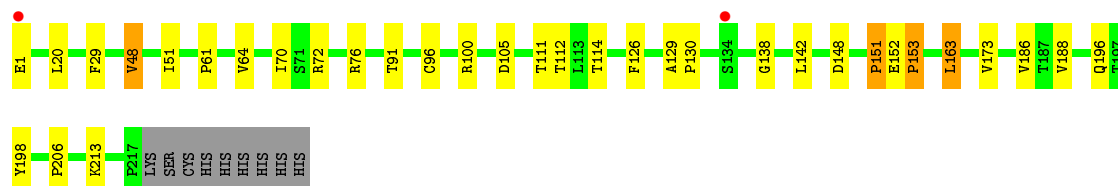
• Molecule 3: M2191 LIGHT CHAIN

Chain G: 76% 22% ..



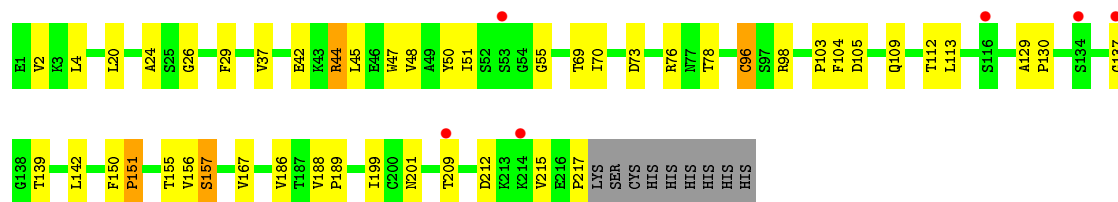
• Molecule 4: M2191 HEAVY CHAIN

Chain D: 81% 13% ..



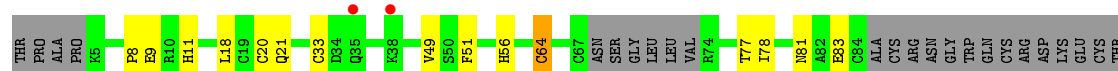
• Molecule 4: M2191 HEAVY CHAIN

Chain H: 75% 19% ..



• Molecule 5: CD27 antigen

Chain X: 54% 13% 32%



GLU
CYS
ASP
GLY
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	141.08 Å 52.96 Å 143.41 Å 90.00° 112.19° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 29.25 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.50) 98.2 (29.25-3.49)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.47 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.283 , 0.356 0.283 , 0.356	Depositor DCC
R_{free} test set	1254 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.068 for l,-k,h	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.95 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1899e-04.*

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: PCA, 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	0.42	0/1683	0.62	0/2288
1	E	0.41	0/1683	0.66	0/2288
2	B	0.46	0/1668	0.64	1/2275 (0.0%)
2	F	0.44	0/1668	0.64	0/2275
3	C	0.41	0/1695	0.65	1/2303 (0.0%)
3	G	0.44	0/1695	0.63	0/2303
4	D	0.43	0/1673	0.65	0/2276
4	H	0.45	0/1673	0.65	0/2276
5	X	0.41	0/585	0.64	0/790
All	All	0.43	0/14023	0.64	2/19074 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	15	LEU	CA-CB-CG	5.23	127.32	115.30
2	B	185	LEU	CA-CB-CG	5.11	127.06	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	1647	0	1583	17	0
1	E	1647	0	1583	22	0
2	B	1632	0	1574	16	0
2	F	1632	0	1574	13	0
3	C	1656	0	1611	11	0
3	G	1656	0	1611	20	0
4	D	1632	0	1597	13	0
4	H	1632	0	1597	20	0
5	X	570	0	509	4	0
6	X	28	0	25	0	0
All	All	13732	0	13264	129	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 5.

All (129) 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)
4:D:91:THR:HG23	4:D:114:THR:HA	1.73	0.69
2:F:9:PRO:HD2	2:F:208:LYS:HD3	1.74	0.69
1:E:14:SER:HA	1:E:111:LYS:HB2	1.76	0.68
3:C:194:LYS:HE3	3:C:214:ASN:HB3	1.77	0.67
1:A:196:TYR:HB2	1:A:213:PHE:CE1	2.31	0.66
3:G:43:LYS:HB2	3:G:46:GLN:HB2	1.78	0.66
4:D:151:PRO:HD2	4:D:206:PRO:HG2	1.79	0.64
4:D:130:PRO:HG3	4:D:142:LEU:HB3	1.79	0.64
3:G:87:ALA:HB2	3:G:110:ILE:HG12	1.81	0.62
4:H:157:SER:H	4:H:201:ASN:HB2	1.66	0.61
3:G:41:GLN:O	3:G:48:PRO:HA	2.00	0.61
1:A:13:VAL:HG21	1:A:19:ALA:HB2	1.83	0.60
1:E:36:TYR:HA	1:E:54:ALA:HA	1.81	0.60
1:E:2:ILE:HG21	1:E:94:GLN:HG2	1.81	0.60
2:B:196:LEU:HB3	2:B:220:PRO:HG3	1.84	0.59
1:A:196:TYR:HB2	1:A:213:PHE:HE1	1.67	0.58
3:C:43:LYS:HD2	3:C:44:PRO:HD2	1.85	0.58
2:F:166:LEU:HD21	2:F:189:VAL:HG21	1.85	0.57
3:G:120:PHE:HB2	3:G:139:LEU:HB3	1.87	0.57
3:C:69:SER:HB2	3:C:76:THR:HB	1.87	0.56
3:G:22:SER:HA	3:G:76:THR:HA	1.88	0.56
2:F:61:ASN:HB3	2:F:64:PHE:HD2	1.72	0.55
5:X:20:CYS:SG	5:X:33:CYS:N	2.80	0.54
3:G:196:TYR:HE1	3:G:215:ARG:HD3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:24:ALA:HB3	4:H:29:PHE:HE1	1.73	0.53
1:E:38:ASN:HB2	1:E:93:GLN:HB3	1.90	0.53
1:A:14:SER:HB2	1:A:17:GLN:HG3	1.90	0.53
3:C:164:GLN:HB3	4:D:173:VAL:HG11	1.90	0.53
1:A:128:GLN:HE22	1:A:135:SER:HB2	1.73	0.53
1:E:136:VAL:HB	1:E:183:LEU:HB3	1.91	0.53
3:G:112:ARG:HE	3:G:175:SER:HB2	1.72	0.53
3:G:151:GLN:HB2	3:G:199:GLU:HB3	1.90	0.52
1:A:53:TYR:HB2	2:B:105:TYR:HB3	1.91	0.51
4:H:129:ALA:HA	4:H:215:VAL:HG12	1.91	0.51
4:H:167:VAL:HG22	4:H:186:VAL:HG23	1.92	0.51
2:B:142:THR:HA	2:B:192:PRO:HA	1.92	0.51
1:E:190:TYR:HA	1:E:196:TYR:OH	2.11	0.51
5:X:49:VAL:O	5:X:64:CYS:HB2	2.09	0.51
3:C:43:LYS:HB2	3:C:46:GLN:HB2	1.93	0.51
2:B:146:GLY:HA3	2:B:188:VAL:HG12	1.92	0.50
3:C:41:GLN:HB2	3:C:51:LEU:HD11	1.93	0.50
4:H:2:VAL:HA	4:H:26:GLY:HA3	1.93	0.50
1:A:111:LYS:HA	1:A:144:TYR:OH	2.11	0.50
4:H:24:ALA:HB3	4:H:29:PHE:CE1	2.46	0.50
3:G:94:HIS:CE1	3:G:101:THR:H	2.30	0.50
3:G:132:GLY:HA2	3:G:187:LYS:HB2	1.92	0.50
1:A:66:PHE:HA	1:A:78:ASN:O	2.12	0.49
1:E:151:GLN:HE22	1:E:153:LYS:HE3	1.77	0.49
2:B:159:VAL:HG22	2:B:205:VAL:HA	1.93	0.49
2:F:70:LEU:HD23	2:F:81:MET:HG3	1.95	0.49
4:H:4:LEU:HD23	4:H:24:ALA:HB2	1.93	0.49
4:D:48:VAL:HG12	4:D:64:VAL:HG21	1.94	0.48
2:B:86:LEU:HB3	2:B:118:VAL:HG21	1.95	0.48
2:B:11:LEU:HD13	2:B:154:PRO:HG3	1.96	0.48
4:D:51:ILE:HD12	4:D:70:ILE:HG23	1.95	0.48
4:D:61:PRO:HG2	4:D:64:VAL:HG22	1.95	0.48
1:E:124:PRO:HD3	1:E:136:VAL:HG22	1.96	0.47
3:C:159:GLN:HB3	3:C:162:ASN:HD21	1.78	0.47
4:H:4:LEU:HD22	4:H:96:CYS:HB3	1.96	0.47
3:G:124:PRO:HG3	3:G:136:VAL:HG22	1.97	0.47
2:B:22:CYS:HB3	2:B:79:ALA:HB3	1.96	0.47
1:E:119:VAL:HG21	1:E:200:VAL:HG21	1.96	0.47
1:E:50:LEU:HD21	1:E:53:TYR:HB3	1.95	0.47
4:H:47:TRP:HZ2	4:H:50:TYR:HB2	1.80	0.47
3:G:2:ILE:HD12	3:G:94:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HG12	1:A:27:GLN:HB2	1.97	0.46
3:G:196:TYR:CE1	3:G:215:ARG:HD3	2.51	0.46
3:G:119:VAL:HG21	3:G:200:VAL:HG21	1.97	0.46
4:H:130:PRO:HG2	4:H:217:PRO:HB3	1.96	0.46
2:B:151:ASP:HB3	2:B:182:LEU:HD13	1.98	0.45
2:B:69:THR:HB	2:B:82:GLN:HB3	1.99	0.45
1:E:111:LYS:HA	1:E:144:TYR:OH	2.17	0.45
4:D:152:GLU:HA	4:D:153:PRO:HA	1.73	0.45
2:F:12:VAL:HG21	2:F:86:LEU:HD13	1.99	0.45
5:X:11:HIS:NE2	5:X:21:GLN:HG2	2.31	0.45
1:E:54:ALA:HB3	1:E:57:ASN:ND2	2.32	0.45
4:H:42:GLU:HB2	4:H:44:ARG:HG2	1.99	0.44
1:E:127:GLU:HG2	1:E:127:GLU:H	1.58	0.44
2:F:38:LYS:HB2	2:F:48:ILE:HD11	1.99	0.44
4:D:163:LEU:HD21	4:D:186:VAL:HG21	1.99	0.44
4:H:73:ASP:HB3	4:H:78:THR:HB	1.99	0.44
4:D:196:GLN:HG2	4:D:198:TYR:CZ	2.52	0.44
1:E:139:LEU:HD13	2:F:188:VAL:HG21	1.99	0.44
1:A:13:VAL:HG12	1:A:17:GLN:HB2	2.00	0.43
3:G:163:SER:HB3	3:G:183:LEU:HD12	2.00	0.43
1:E:12:ALA:HB1	1:E:111:LYS:HD2	2.01	0.43
5:X:51:PHE:CE1	5:X:81:ASN:HB3	2.54	0.43
1:E:19:ALA:HB3	1:E:79:ILE:HB	2.00	0.43
4:H:37:VAL:HG13	4:H:47:TRP:HA	2.01	0.43
2:F:153:PHE:HA	2:F:154:PRO:HA	1.77	0.43
4:H:150:PHE:HA	4:H:151:PRO:HA	1.69	0.43
2:F:11:LEU:HB2	2:F:154:PRO:HG3	2.00	0.43
1:E:52:ILE:HG21	1:E:68:GLY:HA3	2.00	0.42
2:B:9:PRO:HA	2:B:114:THR:HG23	2.02	0.42
3:C:8:PRO:HG3	3:C:11:LEU:HD13	2.01	0.42
4:H:188:VAL:HA	4:H:189:PRO:HD2	1.83	0.42
4:H:156:VAL:HA	4:H:201:ASN:O	2.19	0.42
2:B:38:LYS:HD3	2:B:40:ARG:HD2	2.01	0.42
3:G:35:SER:HB3	3:G:75:PHE:HZ	1.84	0.42
1:A:54:ALA:HB3	1:A:57:ASN:ND2	2.35	0.42
2:F:161:TRP:HB3	2:F:166:LEU:HD23	2.01	0.42
1:A:84:GLU:HA	1:A:110:ILE:HG13	2.01	0.42
2:F:34:MET:HE2	2:F:34:MET:HB2	1.88	0.41
1:A:7:SER:HA	1:A:8:PRO:HA	1.83	0.41
1:E:117:PRO:HD3	1:E:202:HIS:CD2	2.55	0.41
1:E:47:PRO:HG3	2:F:112:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:ASP:C	2:F:106:GLY:H	2.24	0.41
3:C:194:LYS:HA	3:C:215:ARG:HD3	2.01	0.41
4:H:139:THR:HA	4:H:189:PRO:HA	2.02	0.41
2:B:146:GLY:HA2	2:B:161:TRP:HZ2	1.85	0.41
1:A:37:MET:HB3	1:A:55:ALA:HB2	2.02	0.41
1:E:116:ALA:HA	1:E:202:HIS:HD2	1.86	0.41
3:G:164:GLN:HB3	3:G:165:GLU:H	1.76	0.41
1:A:122:PHE:HE1	1:A:139:LEU:HD23	1.86	0.41
2:B:208:LYS:N	2:B:209:PRO:CD	2.84	0.41
1:E:98:ASP:HA	1:E:99:PRO:HA	1.83	0.41
1:A:63:PRO:HB2	1:A:65:ARG:HG3	2.01	0.41
2:B:175:ALA:HA	2:B:185:LEU:HB3	2.03	0.41
3:C:14:SER:HA	3:C:111:LYS:HB2	2.03	0.41
1:E:80:HIS:HA	1:E:81:PRO:HA	1.78	0.41
2:B:40:ARG:HA	2:B:41:PRO:HD2	1.85	0.40
4:D:29:PHE:O	4:D:72:ARG:NH2	2.54	0.40
4:H:51:ILE:HD12	4:H:70:ILE:HG23	2.03	0.40
3:G:53:TYR:HB2	4:H:103:PRO:HG3	2.04	0.40
3:G:47:PRO:HG2	4:H:109:GLN:HA	2.04	0.40
3:G:35:SER:HB3	3:G:75:PHE:CZ	2.56	0.40
4:D:129:ALA:HA	4:D:130:PRO:HD3	1.96	0.40
1:A:126:ASP:HA	1:A:129:LEU:HD12	2.02	0.40
3:C:128:GLN:HG3	4:D:126:PHE:CE2	2.57	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	213/218 (98%)	189 (89%)	19 (9%)	5 (2%)	8	48
1	E	213/218 (98%)	189 (89%)	17 (8%)	7 (3%)	5	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	218/229 (95%)	186 (85%)	26 (12%)	6 (3%)	6	43
2	F	218/229 (95%)	187 (86%)	27 (12%)	4 (2%)	11	53
3	C	213/218 (98%)	194 (91%)	17 (8%)	2 (1%)	21	68
3	G	213/218 (98%)	186 (87%)	20 (9%)	7 (3%)	5	39
4	D	215/226 (95%)	195 (91%)	16 (7%)	4 (2%)	10	51
4	H	215/226 (95%)	188 (87%)	24 (11%)	3 (1%)	14	58
5	X	70/109 (64%)	61 (87%)	8 (11%)	1 (1%)	14	58
All	All	1788/1891 (95%)	1575 (88%)	174 (10%)	39 (2%)	8	49

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
2	B	28	ALA
2	B	86	LEU
1	E	8	PRO
3	G	142	ASN
4	H	151	PRO
1	A	147	GLU
1	E	32	ALA
3	G	32	SER
1	E	36	TYR
2	F	65	LYS
2	F	198	THR
3	G	55	ALA
3	G	204	GLY
4	H	137	GLY
1	A	87	ALA
1	A	162	ASN
2	B	103	GLY
3	C	26	SER
4	D	148	ASP
4	D	151	PRO
4	D	153	PRO
1	E	142	ASN
1	E	172	SER
3	G	15	LEU
1	A	17	GLN
1	E	170	GLN
2	F	209	PRO

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Mol	Chain	Res	Type
1	E	208	PRO
3	G	87	ALA
3	G	206	SER
4	D	138	GLY
2	B	154	PRO
2	F	140	GLY
4	H	55	GLY
2	B	56	GLY
3	C	44	PRO
5	X	8	PRO
2	B	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/187 (99%)	159 (86%)	26 (14%)	4	24
1	E	185/187 (99%)	164 (89%)	21 (11%)	7	33
2	B	179/190 (94%)	168 (94%)	11 (6%)	23	64
2	F	179/190 (94%)	162 (90%)	17 (10%)	11	43
3	C	187/189 (99%)	171 (91%)	16 (9%)	13	49
3	G	187/189 (99%)	174 (93%)	13 (7%)	19	59
4	D	185/194 (95%)	173 (94%)	12 (6%)	21	62
4	H	185/194 (95%)	167 (90%)	18 (10%)	10	42
5	X	65/95 (68%)	58 (89%)	7 (11%)	8	37
All	All	1537/1615 (95%)	1396 (91%)	141 (9%)	11	45

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	10	SER
1	A	13	VAL

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Mol	Chain	Res	Type
1	A	15	LEU
1	A	26	SER
1	A	27	GLN
1	A	57	ASN
1	A	60	SER
1	A	71	SER
1	A	83	GLU
1	A	84	GLU
1	A	85	GLU
1	A	101	THR
1	A	109	GLU
1	A	112	ARG
1	A	138	CYS
1	A	139	LEU
1	A	146	ARG
1	A	158	LEU
1	A	173	LYS
1	A	174	ASP
1	A	194	LYS
1	A	198	CYS
1	A	201	THR
1	A	205	LEU
1	A	210	THR
2	B	40	ARG
2	B	55	ASP
2	B	71	THR
2	B	82	GLN
2	B	87	THR
2	B	145	LEU
2	B	147	CYS
2	B	157	VAL
2	B	200	THR
2	B	216	LYS
2	B	218	VAL
3	C	43	LYS
3	C	46	GLN
3	C	67	SER
3	C	84	GLU
3	C	92	CYS
3	C	93	GLN
3	C	94	HIS
3	C	101	THR

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Mol	Chain	Res	Type
3	C	112	ARG
3	C	125	SER
3	C	130	LYS
3	C	167	VAL
3	C	169	GLU
3	C	179	LEU
3	C	189	ASP
3	C	201	THR
4	D	1	GLU
4	D	20	LEU
4	D	48	VAL
4	D	76	ARG
4	D	96	CYS
4	D	100	ARG
4	D	105	ASP
4	D	111	THR
4	D	112	THR
4	D	163	LEU
4	D	188	VAL
4	D	213	LYS
1	E	2	ILE
1	E	30	ASP
1	E	34	ASP
1	E	42	GLN
1	E	57	ASN
1	E	71	SER
1	E	78	ASN
1	E	85	GLU
1	E	92	CYS
1	E	95	SER
1	E	101	THR
1	E	112	ARG
1	E	127	GLU
1	E	131	SER
1	E	133	THR
1	E	144	TYR
1	E	147	GLU
1	E	151	GLN
1	E	167	VAL
1	E	182	THR
1	E	194	LYS
2	F	5	GLN

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Mol	Chain	Res	Type
2	F	12	VAL
2	F	21	SER
2	F	27	TYR
2	F	71	THR
2	F	100	ASP
2	F	104	ASP
2	F	115	LEU
2	F	142	THR
2	F	149	VAL
2	F	153	PHE
2	F	199	GLN
2	F	202	ILE
2	F	208	LYS
2	F	212	THR
2	F	216	LYS
2	F	217	LYS
3	G	13	VAL
3	G	17	GLN
3	G	20	THR
3	G	58	LEU
3	G	76	THR
3	G	85	GLU
3	G	112	ARG
3	G	133	THR
3	G	155	ASP
3	G	173	LYS
3	G	185	LEU
3	G	205	LEU
3	G	214	ASN
4	H	20	LEU
4	H	44	ARG
4	H	45	LEU
4	H	48	VAL
4	H	69	THR
4	H	76	ARG
4	H	96	CYS
4	H	98	ARG
4	H	104	PHE
4	H	105	ASP
4	H	112	THR
4	H	113	LEU
4	H	142	LEU

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Mol	Chain	Res	Type
4	H	155	THR
4	H	157	SER
4	H	199	ILE
4	H	209	THR
4	H	212	ASP
5	X	9	GLU
5	X	18	LEU
5	X	56	HIS
5	X	64	CYS
5	X	77	THR
5	X	78	ILE
5	X	83	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	42	GLN
1	A	78	ASN
1	A	96	ASN
1	A	128	GLN
2	B	39	GLN
3	C	93	GLN
3	C	128	GLN
3	C	170	GLN
3	C	202	HIS
4	D	57	ASN
4	D	77	ASN
4	D	109	GLN
1	E	151	GLN
1	E	202	HIS
3	G	42	GLN
3	G	78	ASN
3	G	93	GLN
3	G	94	HIS
3	G	142	ASN
3	G	170	GLN
4	H	77	ASN
5	X	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PCA	B	1	2	7,8,9	0.57	0	9,10,12	1.11	1 (11%)
2	PCA	F	1	2	7,8,9	0.53	0	9,10,12	1.16	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	PCA	O-C-CA	-2.33	119.31	125.69
2	F	1	PCA	O-C-CA	-2.07	120.04	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
6	NAG	X	301	5,6	14,14,15	0.71	0	15,19,21	2.29	6 (40%)
6	NAG	X	302	6	14,14,15	0.56	0	15,19,21	1.05	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	301	5,6	-	0/6/23/26	0/1/1/1
6	NAG	X	302	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	302	NAG	C4-C3-C2	2.02	114.47	111.34
6	X	301	NAG	C8-C7-N2	2.09	120.09	116.10
6	X	301	NAG	O5-C5-C6	2.21	112.07	107.34
6	X	302	NAG	C1-O5-C5	2.56	115.90	112.14
6	X	301	NAG	O5-C5-C4	2.72	114.64	110.13
6	X	301	NAG	C3-C4-C5	3.48	116.42	110.23
6	X	301	NAG	C4-C3-C2	4.26	117.95	111.34
6	X	301	NAG	C1-O5-C5	4.85	119.27	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	215/218 (98%)	-0.19	1 (0%) 91 88	26, 53, 89, 99	0
1	E	215/218 (98%)	-0.06	1 (0%) 91 88	34, 69, 96, 99	0
2	B	219/229 (95%)	0.26	7 (3%) 51 42	39, 72, 99, 99	0
2	F	219/229 (95%)	0.01	7 (3%) 51 42	27, 64, 99, 99	0
3	C	215/218 (98%)	-0.43	0 100 100	16, 40, 66, 83	0
3	G	215/218 (98%)	0.19	3 (1%) 78 68	45, 75, 98, 99	0
4	D	217/226 (96%)	-0.40	2 (0%) 85 78	14, 39, 65, 96	0
4	H	217/226 (96%)	0.23	6 (2%) 56 46	50, 75, 97, 99	0
5	X	74/109 (67%)	0.08	2 (2%) 58 47	24, 46, 63, 66	0
All	All	1806/1891 (95%)	-0.04	29 (1%) 74 65	14, 62, 96, 99	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	214	LYS	4.3
2	F	220	PRO	3.7
2	F	215	ASP	3.1
4	H	116	SER	3.1
2	F	143	ALA	3.0
2	B	220	PRO	3.0
3	G	201	THR	3.0
2	B	87	THR	2.7
4	D	134	SER	2.7
2	F	195	SER	2.6
2	B	181	GLY	2.6
4	H	137	GLY	2.5
4	H	53	SER	2.5
5	X	35	GLN	2.4
1	A	197	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	97	GLU	2.2
2	F	135	SER	2.2
2	F	192	PRO	2.2
3	G	127	GLU	2.2
4	D	1	GLU	2.2
2	F	200	THR	2.2
1	E	212	SER	2.1
2	B	43	LYS	2.1
2	B	195	SER	2.1
2	B	219	GLU	2.1
2	B	203	CYS	2.1
4	H	134	SER	2.0
5	X	38	LYS	2.0
4	H	209	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	PCA	B	1	8/9	0.91	0.29	-	59,60,62,64	0
2	PCA	F	1	8/9	0.81	0.25	-	66,68,77,79	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	X	302	14/15	0.80	0.30	-	75,93,99,99	0
6	NAG	X	301	14/15	0.79	0.30	-	54,63,72,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.