Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:58 am BST

PDB ID	:	6HJY
Title	:	X-ray structure of a pentameric ligand gated ion channel from Erwinia chrysanthemi (ELIC) Delta8 truncation mutant in complex with nanobody 72
Authors	:	Spurny, R.; Govaerts, C.; Evans, G.L.; Pardon, E.; Steyaert, J.; Ulens, C.
Deposited on	:	2018-09-04
Resolution	:	2.78 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 following versions of software and data (see references ①) were used in the production of this report:

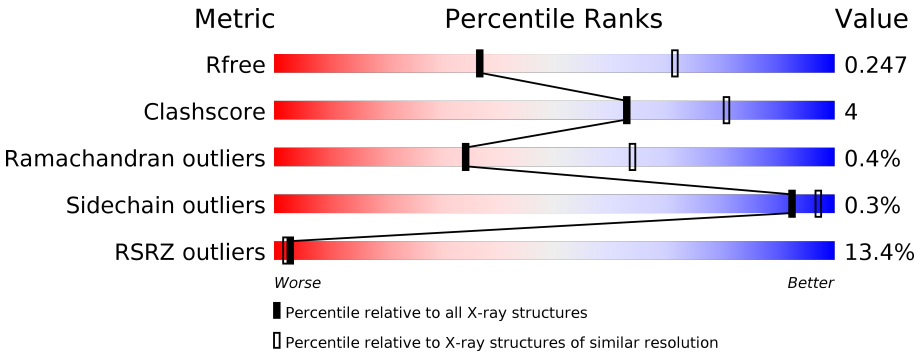
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.78 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 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 <=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	277	10% 91% 9%
2	B	280	10% 88% 12%
2	C	280	17% 88% 11%
3	D	276	14% 89% 10%
4	E	278	11% 90% 10%
5	F	124	7% 93% 7%

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Mol	Chain	Length	Quality of chain
5	J	124	22% 90% 10%
6	G	123	16% 93% 7%
6	H	123	23% 92% 8%
6	I	123	11% 93% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16066 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2274	1481	377	411	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 2 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2289	1490	379	415	5			
2	C	279	Total	C	N	O	S	0	0	0
			2289	1490	379	415	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	PRO	-	expression tag	UNP P0C7B7
B	7	VAL	-	expression tag	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	238	CYS	LEU	conflict	UNP P0C7B7
C	6	PRO	-	expression tag	UNP P0C7B7
C	7	VAL	-	expression tag	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 3 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	276	Total	C	N	O	S	0	0	0
			2269	1478	376	410	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	164	GLY	-	insertion	UNP P0C7B7
D	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 4 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	278	Total	C	N	O	S	0	0	0
			2282	1485	378	414	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	164	GLY	-	insertion	UNP P0C7B7
E	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 5 is a protein called nanobody 72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	124	Total	C	N	O	S	0	0	0
			938	584	170	179	5			
5	J	124	Total	C	N	O	S	0	0	0
			938	584	170	179	5			

- Molecule 6 is a protein called nanobody 72.

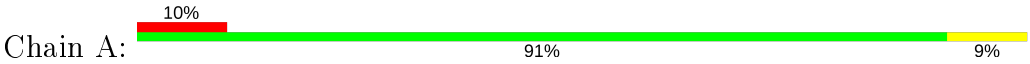
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	123	Total	C	N	O	S	0	0	0
			929	579	168	177	5			
6	H	123	Total	C	N	O	S	0	0	0
			929	579	168	177	5			
6	I	123	Total	C	N	O	S	0	0	0
			929	579	168	177	5			

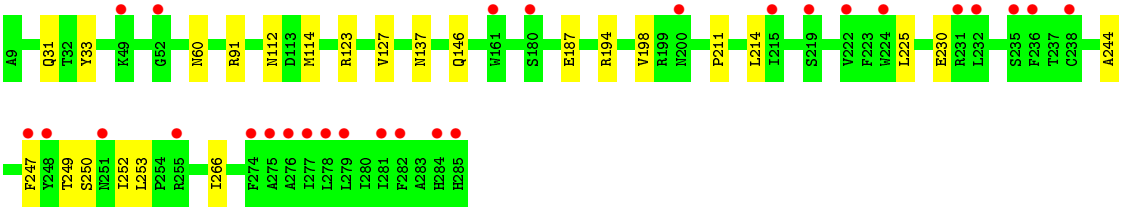
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Cys-loop ligand-gated ion channel

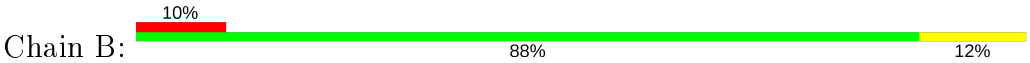
Chain A:

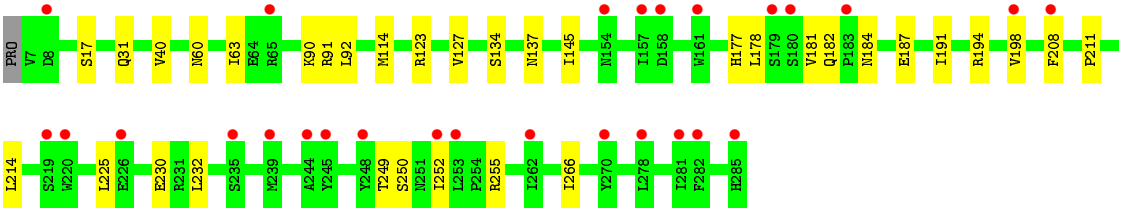




- Molecule 2: Cys-loop ligand-gated ion channel

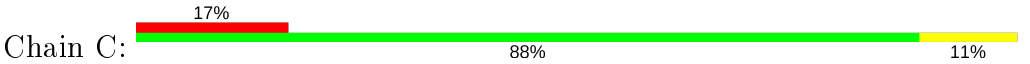
Chain B:

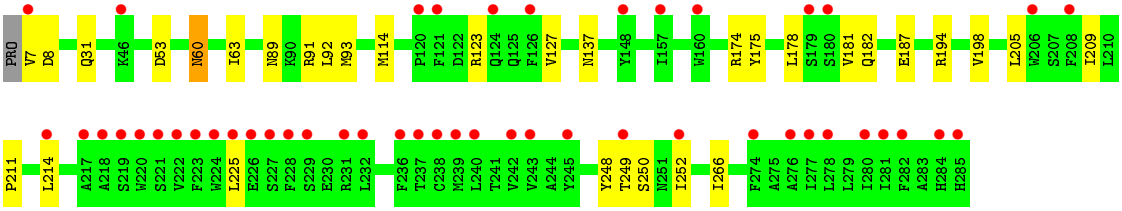




- Molecule 2: Cys-loop ligand-gated ion channel

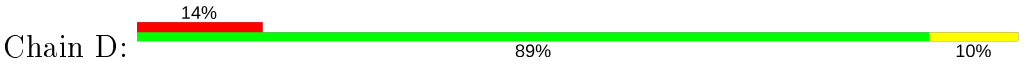
Chain C:

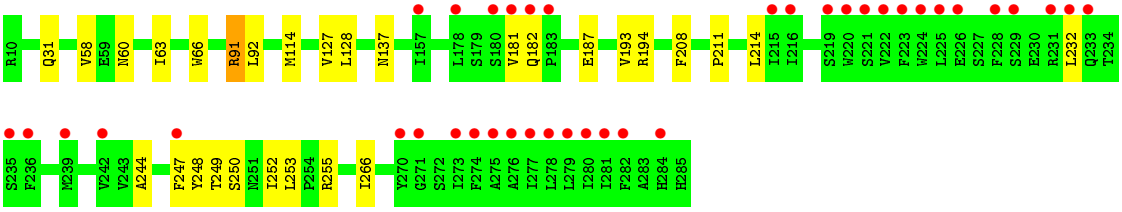




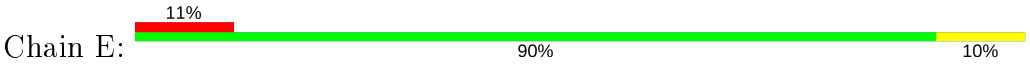
- Molecule 3: Cys-loop ligand-gated ion channel

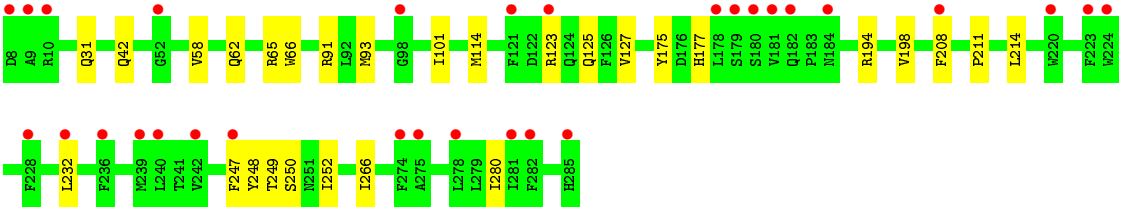
Chain D:



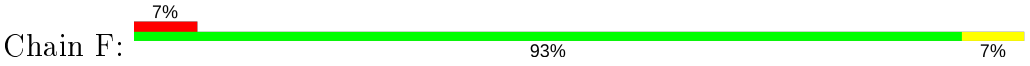


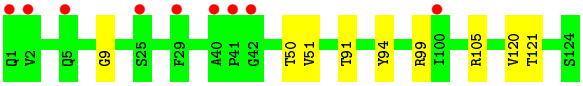
• Molecule 4: Cys-loop ligand-gated ion channel



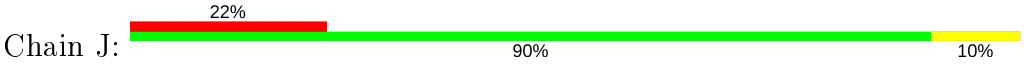


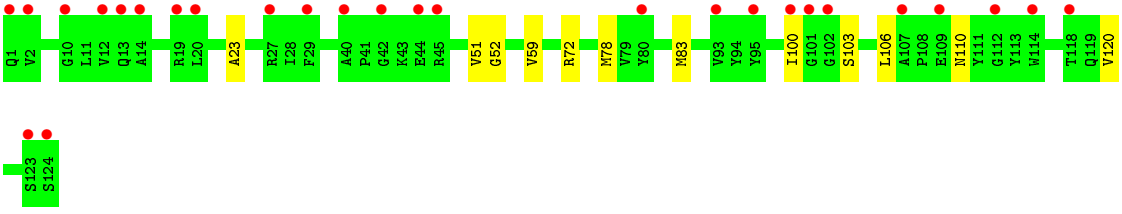
• Molecule 5: nanobody 72



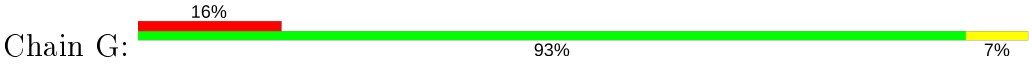


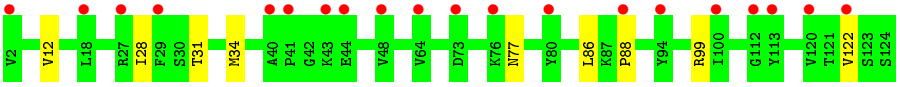
• Molecule 5: nanobody 72



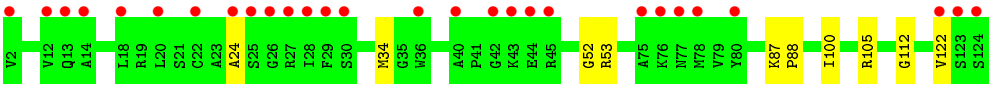


• Molecule 6: nanobody 72



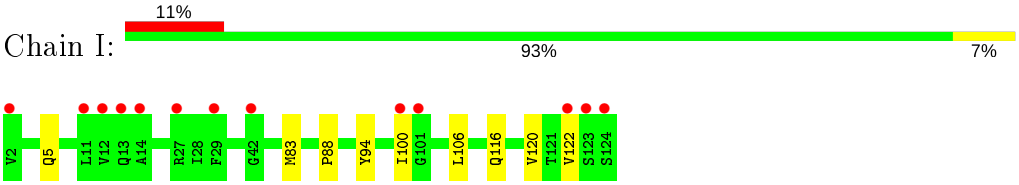


• Molecule 6: nanobody 72



• Molecule 6: nanobody 72

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.67Å 155.09Å 101.62Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	49.49 – 2.78 48.49 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.49-2.78) 99.3 (48.49-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.233 0.237 , 0.247	Depositor DCC
R_{free} test set	3602 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16066	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0/2339	0.65	0/3190
2	B	0.45	0/2354	0.65	0/3211
2	C	0.43	0/2354	0.65	0/3211
3	D	0.43	0/2334	0.66	0/3183
4	E	0.42	0/2347	0.64	0/3201
5	F	0.37	0/955	0.65	0/1287
5	J	0.44	0/955	0.67	0/1287
6	G	0.36	0/946	0.63	0/1275
6	H	0.40	0/946	0.65	0/1275
6	I	0.39	0/946	0.65	0/1275
All	All	0.42	0/16476	0.65	0/22395

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

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	2274	0	2229	18	0
2	B	2289	0	2242	23	0
2	C	2289	0	2242	21	0
3	D	2269	0	2224	25	0
4	E	2282	0	2233	25	0
5	F	938	0	914	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	938	0	914	16	0
6	G	929	0	903	4	0
6	H	929	0	903	11	0
6	I	929	0	903	5	0
All	All	16066	0	15707	138	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 4.

All (138) 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)
5:J:51:VAL:CG2	5:J:72:ARG:HH22	1.69	1.05
5:J:51:VAL:HB	5:J:72:ARG:NH2	1.86	0.90
5:J:72:ARG:O	5:J:78:MET:O	1.92	0.87
6:H:88:PRO:HA	6:H:122:VAL:HG13	1.56	0.84
5:J:51:VAL:CG2	5:J:72:ARG:NH2	2.43	0.82
4:E:91:ARG:NH1	4:E:93:MET:HB2	1.96	0.80
5:J:51:VAL:HG21	5:J:72:ARG:HH22	1.45	0.80
5:J:51:VAL:CB	5:J:72:ARG:NH2	2.50	0.73
4:E:232:LEU:HD12	4:E:280:ILE:HG21	1.73	0.69
6:I:5:GLN:HG3	6:I:116:GLN:HE22	1.59	0.68
6:H:52:GLY:C	6:H:105:ARG:HH12	1.96	0.68
4:E:42:GLN:HG3	4:E:101:ILE:HG12	1.75	0.67
2:C:252:ILE:HD11	3:D:250:SER:HB2	1.78	0.66
4:E:91:ARG:HH12	4:E:93:MET:HB2	1.58	0.66
2:C:225:LEU:HD21	3:D:232:LEU:HD22	1.79	0.65
1:A:250:SER:HB2	4:E:252:ILE:HD11	1.79	0.65
5:J:51:VAL:HB	5:J:72:ARG:HH21	1.62	0.65
6:H:24:ALA:HB2	6:H:34:MET:CE	2.26	0.65
1:A:137:ASN:HD21	1:A:187:GLU:HB3	1.65	0.61
3:D:128:LEU:HB2	3:D:193:VAL:HG22	1.81	0.61
1:A:112:ASN:ND2	1:A:127:VAL:HG22	2.14	0.61
1:A:137:ASN:ND2	1:A:187:GLU:HB3	2.16	0.61
5:J:51:VAL:HG22	5:J:52:GLY:O	2.02	0.59
3:D:249:THR:HG23	3:D:253:LEU:HD13	1.85	0.59
3:D:208:PHE:HE2	3:D:249:THR:HA	1.69	0.58
6:H:24:ALA:HB2	6:H:34:MET:HE2	1.84	0.58
2:C:60:ASN:O	2:C:63:ILE:HB	2.04	0.57
1:A:244:ALA:HA	1:A:247:PHE:CE2	2.38	0.57
1:A:249:THR:HG23	1:A:253:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:51:VAL:HG23	5:J:72:ARG:HH22	1.62	0.56
6:H:53:ARG:N	6:H:105:ARG:HH12	2.03	0.56
2:C:248:TYR:HE1	3:D:250:SER:HB3	1.70	0.56
4:E:232:LEU:CD1	4:E:280:ILE:HG21	2.34	0.56
4:E:123:ARG:HG2	4:E:198:VAL:HG22	1.88	0.56
1:A:225:LEU:HD22	1:A:230:GLU:HB3	1.88	0.56
3:D:181:VAL:O	3:D:182:GLN:HG3	2.06	0.56
2:C:60:ASN:HD21	2:C:89:ASN:HA	1.71	0.56
3:D:244:ALA:HA	3:D:247:PHE:CE2	2.41	0.55
1:A:252:ILE:HD11	2:B:250:SER:HB2	1.87	0.55
6:H:100:ILE:HD11	6:H:112:GLY:HA3	1.87	0.55
2:C:249:THR:HG21	2:C:266:ILE:HD11	1.89	0.55
2:C:123:ARG:HG2	2:C:198:VAL:HG22	1.89	0.54
2:C:137:ASN:HD21	2:C:187:GLU:HB3	1.73	0.54
2:B:137:ASN:HD21	2:B:187:GLU:HB3	1.71	0.53
2:B:177:HIS:O	2:B:178:LEU:HG	2.08	0.53
2:B:123:ARG:HG2	2:B:198:VAL:HG22	1.90	0.53
2:C:91:ARG:HH11	2:C:93:MET:HB2	1.74	0.53
2:B:181:VAL:O	2:B:182:GLN:HG3	2.07	0.53
3:D:255:ARG:HA	3:D:255:ARG:NE	2.23	0.53
2:B:252:ILE:HD11	2:C:250:SER:HB2	1.91	0.53
2:B:137:ASN:ND2	2:B:187:GLU:HB3	2.23	0.53
1:A:127:VAL:HG12	1:A:194:ARG:HG3	1.91	0.53
1:A:247:PHE:HB3	4:E:248:TYR:HB2	1.92	0.52
2:C:181:VAL:HG12	2:C:182:GLN:HG3	1.92	0.52
2:C:91:ARG:NH1	2:C:93:MET:HB2	2.24	0.52
1:A:33:TYR:HE1	1:A:112:ASN:HB2	1.76	0.51
2:B:127:VAL:HG12	2:B:194:ARG:HG3	1.92	0.51
2:C:137:ASN:ND2	2:C:187:GLU:HB3	2.26	0.50
1:A:123:ARG:HG2	1:A:198:VAL:HG22	1.93	0.50
5:J:83:MET:HE1	5:J:120:VAL:HG21	1.94	0.50
2:C:91:ARG:HG2	2:C:92:LEU:N	2.26	0.49
5:J:51:VAL:HG22	5:J:52:GLY:N	2.27	0.49
2:B:225:LEU:HD22	2:B:230:GLU:HB3	1.95	0.49
3:D:127:VAL:HG12	3:D:194:ARG:HG3	1.95	0.49
2:B:145:ILE:HD13	2:B:191:ILE:HD13	1.94	0.49
2:C:7:VAL:HG12	2:C:8:ASP:N	2.27	0.49
5:J:51:VAL:HG23	5:J:72:ARG:NH2	2.25	0.49
6:H:24:ALA:HB2	6:H:34:MET:HE1	1.94	0.48
6:H:100:ILE:CD1	6:H:112:GLY:HA3	2.42	0.48
3:D:248:TYR:HA	4:E:247:PHE:HD1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:249:THR:HG21	3:D:266:ILE:HD11	1.95	0.48
1:A:31:GLN:HA	1:A:114:MET:HE2	1.95	0.48
6:H:87:LYS:O	6:H:122:VAL:HG11	2.14	0.48
5:F:50:THR:HG21	5:F:105:ARG:HB2	1.94	0.48
4:E:31:GLN:HA	4:E:114:MET:HE2	1.96	0.47
2:B:255:ARG:CZ	2:B:255:ARG:HA	2.44	0.47
6:G:28:ILE:CG2	6:G:77:ASN:HD21	2.28	0.47
3:D:248:TYR:HD1	4:E:247:PHE:HA	1.79	0.47
6:H:53:ARG:N	6:H:105:ARG:NH1	2.63	0.47
4:E:211:PRO:HA	4:E:214:LEU:HD12	1.98	0.46
3:D:31:GLN:HA	3:D:114:MET:HE2	1.98	0.46
4:E:127:VAL:HG12	4:E:194:ARG:HG3	1.98	0.46
5:F:91:THR:HG23	5:F:121:THR:HA	1.98	0.45
6:I:94:TYR:CE1	6:I:120:VAL:HG22	2.52	0.45
3:D:137:ASN:HD21	3:D:187:GLU:HB3	1.81	0.45
4:E:208:PHE:CD2	4:E:249:THR:HG22	2.52	0.45
2:B:178:LEU:HA	2:B:181:VAL:HG23	1.98	0.45
2:B:31:GLN:HA	2:B:114:MET:HE2	1.98	0.45
4:E:125:GLN:HB2	5:J:103:SER:OG	2.16	0.45
3:D:63:ILE:HD11	3:D:91:ARG:HA	1.98	0.44
4:E:232:LEU:CD1	4:E:280:ILE:CG2	2.94	0.44
2:B:208:PHE:HE1	2:B:249:THR:HA	1.83	0.44
4:E:62:GLN:OE1	4:E:65:ARG:HD3	2.17	0.44
4:E:232:LEU:HD11	4:E:280:ILE:HG22	2.00	0.44
1:A:91:ARG:HD2	2:B:134:SER:HB3	2.00	0.44
2:C:127:VAL:HG12	2:C:194:ARG:HG3	2.00	0.43
5:F:94:TYR:CE1	5:F:120:VAL:HG22	2.52	0.43
3:D:211:PRO:HA	3:D:214:LEU:HD12	2.00	0.43
3:D:249:THR:HG21	3:D:266:ILE:CD1	2.49	0.43
2:C:205:LEU:HA	2:C:209:ILE:HD12	1.99	0.43
3:D:63:ILE:HG23	3:D:92:LEU:HD11	2.00	0.43
4:E:232:LEU:HD11	4:E:280:ILE:CG2	2.49	0.43
5:J:59:VAL:HG11	5:J:106:LEU:HD21	2.01	0.43
1:A:211:PRO:HA	1:A:214:LEU:HD12	2.01	0.43
2:C:175:TYR:HB2	2:C:178:LEU:HD12	2.00	0.43
4:E:58:VAL:HG11	4:E:66:TRP:CD1	2.54	0.43
4:E:208:PHE:HD2	4:E:249:THR:HG22	1.84	0.42
6:I:5:GLN:HG3	6:I:116:GLN:NE2	2.30	0.42
6:I:83:MET:HE1	6:I:120:VAL:HG11	2.01	0.42
1:A:249:THR:HG21	1:A:266:ILE:HD11	2.00	0.42
6:I:88:PRO:HA	6:I:122:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:175:TYR:HB3	4:E:177:HIS:CE1	2.54	0.42
6:G:88:PRO:HA	6:G:122:VAL:HB	2.02	0.42
6:H:52:GLY:C	6:H:105:ARG:NH1	2.67	0.42
2:B:17:SER:HB2	2:B:40:VAL:HB	2.02	0.42
4:E:249:THR:HG21	4:E:266:ILE:HD11	2.01	0.42
2:B:249:THR:HG21	2:B:266:ILE:HD11	2.01	0.42
1:A:33:TYR:CE1	1:A:112:ASN:HB2	2.54	0.42
1:A:225:LEU:HD21	2:B:232:LEU:HD23	2.01	0.42
2:C:211:PRO:HA	2:C:214:LEU:HD12	2.01	0.42
3:D:248:TYR:HB2	4:E:247:PHE:HB2	2.02	0.42
3:D:31:GLN:HG2	3:D:114:MET:HB2	2.02	0.42
3:D:252:ILE:HD11	4:E:250:SER:HB3	2.02	0.42
3:D:137:ASN:ND2	3:D:187:GLU:HB3	2.35	0.41
2:B:145:ILE:HD13	2:B:191:ILE:HG21	2.02	0.41
6:G:31:THR:HG22	6:G:34:MET:HE3	2.02	0.41
2:B:211:PRO:HA	2:B:214:LEU:HD12	2.02	0.41
2:B:63:ILE:HD12	2:B:90:LYS:HG3	2.03	0.41
3:D:58:VAL:HG11	3:D:66:TRP:CD1	2.55	0.41
5:J:23:ALA:HA	5:J:78:MET:HG2	2.02	0.41
5:F:9:GLY:HA2	5:F:120:VAL:HG12	2.03	0.41
5:J:100:ILE:HG22	5:J:110:ASN:O	2.21	0.41
2:C:174:ARG:HG3	2:C:187:GLU:HG3	2.04	0.40
3:D:244:ALA:HA	3:D:247:PHE:CZ	2.56	0.40
2:B:91:ARG:HG2	2:B:92:LEU:N	2.36	0.40
2:B:208:PHE:CD1	2:B:249:THR:HG22	2.55	0.40
2:C:31:GLN:HG2	2:C:114:MET:HB2	2.03	0.40
6:G:12:VAL:HG11	6:G:86:LEU:HD13	2.02	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	275/277 (99%)	268 (98%)	6 (2%)	1 (0%)	34 64
2	B	277/280 (99%)	271 (98%)	4 (1%)	2 (1%)	22 50
2	C	277/280 (99%)	267 (96%)	9 (3%)	1 (0%)	34 64
3	D	274/276 (99%)	269 (98%)	4 (2%)	1 (0%)	34 64
4	E	276/278 (99%)	270 (98%)	6 (2%)	0	100 100
5	F	122/124 (98%)	118 (97%)	3 (2%)	1 (1%)	19 47
5	J	122/124 (98%)	114 (93%)	8 (7%)	0	100 100
6	G	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	19 47
6	H	121/123 (98%)	116 (96%)	5 (4%)	0	100 100
6	I	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	19 47
All	All	1986/2008 (99%)	1927 (97%)	51 (3%)	8 (0%)	34 64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
6	I	100	ILE
2	B	60	ASN
3	D	60	ASN
6	G	99	ARG
2	B	184	ASN
2	C	60	ASN
5	F	99	ARG

5.3.2 Protein sidechains (i)

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	250/250 (100%)	249 (100%)	1 (0%)	91 96
2	B	252/253 (100%)	252 (100%)	0	100 100
2	C	252/253 (100%)	251 (100%)	1 (0%)	91 96
3	D	250/250 (100%)	249 (100%)	1 (0%)	91 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	251/251 (100%)	251 (100%)	0	100 100
5	F	96/96 (100%)	95 (99%)	1 (1%)	76 91
5	J	96/96 (100%)	96 (100%)	0	100 100
6	G	95/95 (100%)	95 (100%)	0	100 100
6	H	95/95 (100%)	95 (100%)	0	100 100
6	I	95/95 (100%)	94 (99%)	1 (1%)	73 90
All	All	1732/1734 (100%)	1727 (100%)	5 (0%)	92 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
2	C	53	ASP
3	D	91	ARG
5	F	51	VAL
6	I	106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
2	B	137	ASN
2	C	60	ASN
2	C	137	ASN
3	D	137	ASN
4	E	112	ASN
6	G	77	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	277/277 (100%)	0.69	28 (10%) 7 4	58, 80, 172, 216	0
2	B	279/280 (99%)	0.53	27 (9%) 7 5	56, 87, 191, 213	0
2	C	279/280 (99%)	0.99	48 (17%) 1 1	53, 88, 205, 230	0
3	D	276/276 (100%)	0.90	39 (14%) 2 2	53, 79, 200, 219	0
4	E	278/278 (100%)	0.63	30 (10%) 5 4	57, 88, 170, 220	0
5	F	124/124 (100%)	0.46	9 (7%) 15 10	60, 80, 118, 150	0
5	J	124/124 (100%)	1.24	27 (21%) 0 0	81, 119, 157, 186	0
6	G	123/123 (100%)	1.06	20 (16%) 1 1	72, 111, 144, 170	0
6	H	123/123 (100%)	1.23	28 (22%) 0 0	79, 117, 160, 183	0
6	I	123/123 (100%)	0.62	13 (10%) 6 4	58, 79, 120, 150	0
All	All	2006/2008 (99%)	0.80	269 (13%) 3 2	53, 91, 177, 230	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	285	HIS	14.5
2	C	225	LEU	11.8
1	A	282	PHE	11.2
6	H	29	PHE	10.7
3	D	228	PHE	9.9
3	D	231	ARG	9.6
5	J	29	PHE	9.6
2	C	223	PHE	9.3
6	H	27	ARG	9.2
2	C	226	GLU	9.1
3	D	277	ILE	9.1
4	E	278	LEU	9.0
3	D	220	TRP	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	281	ILE	8.8
6	I	27	ARG	8.6
3	D	223	PHE	8.4
1	A	285	HIS	8.3
3	D	222	VAL	8.0
3	D	275	ALA	8.0
3	D	235	SER	8.0
6	H	26	GLY	7.9
6	H	76	LYS	7.8
3	D	229	SER	7.8
3	D	225	LEU	7.7
2	C	228	PHE	7.6
5	F	1	GLN	7.5
2	B	282	PHE	7.5
2	C	222	VAL	7.5
2	C	218	ALA	7.3
3	D	282	PHE	7.2
2	C	221	SER	7.2
3	D	232	LEU	7.2
6	I	29	PHE	7.0
2	C	281	ILE	6.8
6	G	29	PHE	6.7
5	J	42	GLY	6.6
3	D	273	ILE	6.4
3	D	281	ILE	6.4
6	G	2	VAL	6.4
5	J	27	ARG	6.3
3	D	278	LEU	6.1
4	E	224	TRP	6.1
3	D	224	TRP	6.1
6	H	24	ALA	6.0
6	H	2	VAL	5.9
4	E	8	ASP	5.9
2	C	227	SER	5.8
4	E	228	PHE	5.8
3	D	271	GLY	5.8
2	C	232	LEU	5.7
2	C	284	HIS	5.6
3	D	216	ILE	5.6
4	E	181	VAL	5.6
6	I	124	SER	5.5
6	H	28	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
6	I	13	GLN	5.4
3	D	219	SER	5.4
4	E	274	PHE	5.4
4	E	285	HIS	5.2
2	B	220	TRP	5.1
2	C	236	PHE	4.9
4	E	236	PHE	4.9
4	E	281	ILE	4.8
4	E	232	LEU	4.8
2	C	224	TRP	4.7
3	D	270	TYR	4.7
4	E	223	PHE	4.7
5	J	100	ILE	4.7
6	H	124	SER	4.7
5	J	2	VAL	4.6
1	A	278	LEU	4.6
6	H	77	ASN	4.5
2	C	282	PHE	4.5
6	H	25	SER	4.5
5	F	41	PRO	4.4
6	H	13	GLN	4.4
5	J	102	GLY	4.4
3	D	274	PHE	4.3
5	J	1	GLN	4.3
3	D	233	GLN	4.3
1	A	247	PHE	4.3
1	A	277	ILE	4.3
2	C	121	PHE	4.2
2	C	217	ALA	4.2
6	G	27	ARG	4.2
1	A	276	ALA	4.1
2	C	214	LEU	4.1
6	I	123	SER	4.1
6	H	40	ALA	4.1
6	H	14	ALA	4.0
1	A	232	LEU	4.0
3	D	279	LEU	4.0
5	F	40	ALA	4.0
6	I	2	VAL	4.0
6	I	100	ILE	4.0
6	G	40	ALA	4.0
4	E	180	SER	3.9

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Mol	Chain	Res	Type	RSRZ
5	J	123	SER	3.9
2	B	270	TYR	3.9
6	H	123	SER	3.9
6	G	113	TYR	3.9
4	E	282	PHE	3.9
6	G	120	VAL	3.9
1	A	231	ARG	3.9
3	D	215	ILE	3.8
1	A	52	GLY	3.8
2	C	7	VAL	3.8
6	G	100	ILE	3.7
6	H	42	GLY	3.6
5	J	45	ARG	3.6
6	H	78	MET	3.6
2	C	278	LEU	3.6
2	C	276	ALA	3.5
2	C	242	VAL	3.5
6	I	11	LEU	3.5
1	A	248	TYR	3.5
1	A	238	CYS	3.5
5	J	112	GLY	3.4
2	C	219	SER	3.4
6	H	30	SER	3.4
5	F	5	GLN	3.4
4	E	9	ALA	3.4
4	E	179	SER	3.4
2	C	157	ILE	3.3
3	D	221	SER	3.3
6	H	44	GLU	3.3
6	G	41	PRO	3.3
5	F	2	VAL	3.2
2	B	219	SER	3.2
3	D	180	SER	3.2
1	A	215	ILE	3.1
6	H	75	ALA	3.1
6	G	88	PRO	3.1
6	I	14	ALA	3.1
2	B	226	GLU	3.1
3	D	276	ALA	3.0
2	C	239	MET	3.0
6	I	122	VAL	3.0
3	D	284	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	279	LEU	3.0
5	J	80	TYR	3.0
1	A	275	ALA	3.0
2	C	229	SER	2.9
3	D	236	PHE	2.9
2	B	161	TRP	2.9
6	G	43	LYS	2.9
2	C	245	TYR	2.9
4	E	182	GLN	2.8
6	H	80	TYR	2.8
2	C	206	TRP	2.8
5	J	124	SER	2.8
2	C	208	PHE	2.8
2	B	285	HIS	2.8
6	G	94	TYR	2.8
2	B	154	ASN	2.8
6	G	64	VAL	2.7
1	A	161	TRP	2.7
6	G	122	VAL	2.7
5	J	10	GLY	2.7
5	J	44	GLU	2.7
3	D	226	GLU	2.7
2	C	243	VAL	2.7
2	B	157	ILE	2.7
2	C	220	TRP	2.7
5	J	118	THR	2.7
2	C	46	LYS	2.7
2	B	180	SER	2.6
5	F	29	PHE	2.6
2	C	180	SER	2.6
1	A	284	HIS	2.6
5	F	25	SER	2.6
2	C	277	ILE	2.6
4	E	10	ARG	2.6
5	J	95	TYR	2.6
2	B	252	ILE	2.6
2	B	245	TYR	2.5
2	B	253	LEU	2.5
6	H	12	VAL	2.5
2	C	238	CYS	2.5
1	A	255	ARG	2.5
1	A	180	SER	2.5

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Mol	Chain	Res	Type	RSRZ
6	H	43	LYS	2.5
3	D	157	ILE	2.5
4	E	123	ARG	2.5
2	B	235	SER	2.4
2	C	148	TYR	2.4
5	J	109	GLU	2.4
5	J	14	ALA	2.4
1	A	200	ASN	2.4
2	B	248	TYR	2.4
1	A	251	ASN	2.4
4	E	208	PHE	2.4
6	G	18	LEU	2.4
6	G	80	TYR	2.4
3	D	183	PRO	2.4
2	C	179	SER	2.3
6	I	101	GLY	2.3
5	J	93	VAL	2.3
2	C	231	ARG	2.3
5	J	19	ARG	2.3
1	A	274	PHE	2.3
2	B	8	ASP	2.3
6	H	18	LEU	2.3
3	D	280	ILE	2.3
5	J	12	VAL	2.3
6	G	48	VAL	2.3
1	A	224	TRP	2.3
4	E	220	TRP	2.3
4	E	239	MET	2.3
6	H	20	LEU	2.3
5	J	107	ALA	2.3
3	D	181	VAL	2.3
5	J	20	LEU	2.3
6	H	36	TRP	2.3
2	C	237	THR	2.3
4	E	242	VAL	2.3
6	H	45	ARG	2.2
3	D	247	PHE	2.2
1	A	222	VAL	2.2
6	G	76	LYS	2.2
5	J	101	GLY	2.2
6	G	44	GLU	2.2
2	B	278	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	240	LEU	2.2
2	C	160	TRP	2.2
4	E	275	ALA	2.2
4	E	52	GLY	2.2
6	G	73	ASP	2.2
6	I	12	VAL	2.2
3	D	182	GLN	2.2
2	B	244	ALA	2.2
6	I	42	GLY	2.2
1	A	235	SER	2.2
2	B	198	VAL	2.2
2	B	281	ILE	2.2
3	D	239	MET	2.2
2	C	280	ILE	2.1
3	D	178	LEU	2.1
4	E	98	GLY	2.1
5	F	42	GLY	2.1
1	A	236	PHE	2.1
2	C	274	PHE	2.1
1	A	219	SER	2.1
6	G	112	GLY	2.1
5	J	114	TRP	2.1
2	B	262	ILE	2.1
5	J	13	GLN	2.1
4	E	184	ASN	2.1
4	E	240	LEU	2.1
6	H	22	CYS	2.1
2	C	249	THR	2.1
3	D	242	VAL	2.1
6	H	122	VAL	2.1
2	C	120	PRO	2.1
2	C	124	GLN	2.1
2	B	208	PHE	2.1
2	C	252	ILE	2.1
2	B	158	ASP	2.1
4	E	121	PHE	2.1
1	A	49	LYS	2.0
4	E	178	LEU	2.0
5	F	100	ILE	2.0
5	J	40	ALA	2.0
4	E	247	PHE	2.0
2	B	179	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	239	MET	2.0
2	C	126	PHE	2.0
2	B	65	ARG	2.0
2	B	183	PRO	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.