



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:49 AM GMT

PDB ID : 3Q68
Title : Structure of the Vps75-Rtt109 histone chaperone-lysine acetyltransferase complex (Full-length proteins in space group P212121)
Authors : Su, D.; Thompson, J.R.; Mer, G.
Deposited on : 2010-12-30
Resolution : 2.71 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

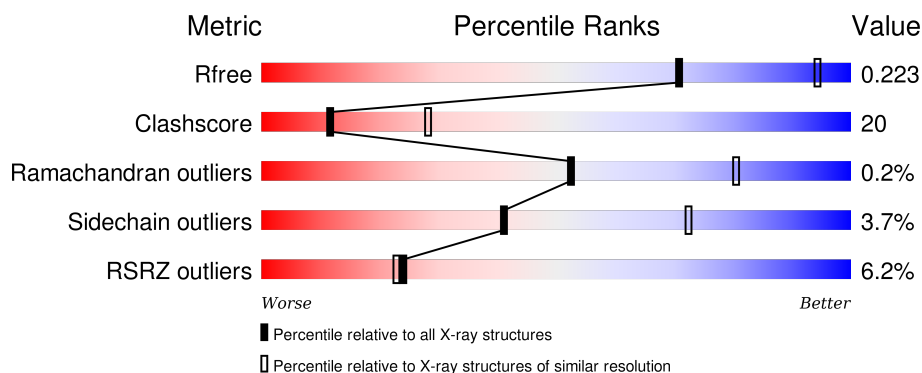
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	264	
1	B	264	
2	C	442	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7145 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 Vacuolar protein sorting-associated protein 75 (VPS75).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1921	1235	309	372	5			
1	B	221	Total	C	N	O	S	0	0	0
			1842	1185	300	352	5			

- Molecule 2 is a protein called Histone acetyltransferase RTT109.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	405	Total	C	N	O	S	0	0	0
			3292	2120	554	609	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	EXPRESSION TAG	UNP Q07794
C	-4	MET	-	EXPRESSION TAG	UNP Q07794
C	-3	ASP	-	EXPRESSION TAG	UNP Q07794
C	-2	PRO	-	EXPRESSION TAG	UNP Q07794
C	-1	ASN	-	EXPRESSION TAG	UNP Q07794
C	0	SER	-	EXPRESSION TAG	UNP Q07794

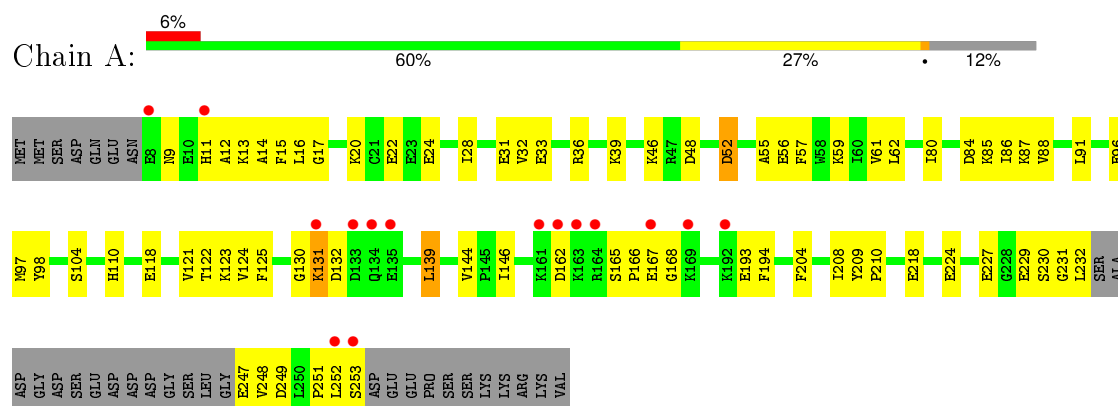
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	C	46	Total	O	0	0
			46	46		
3	B	10	Total	O	0	0
			10	10		

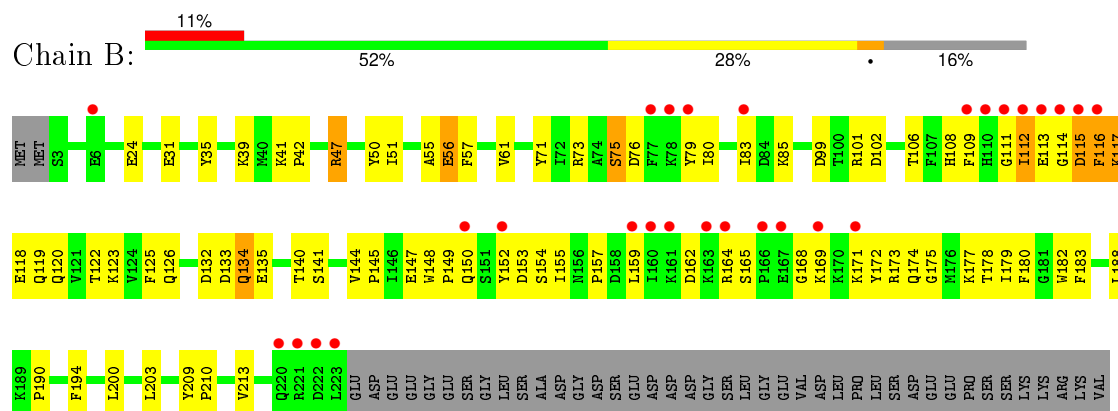
3 Residue-property plots [i](#)

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

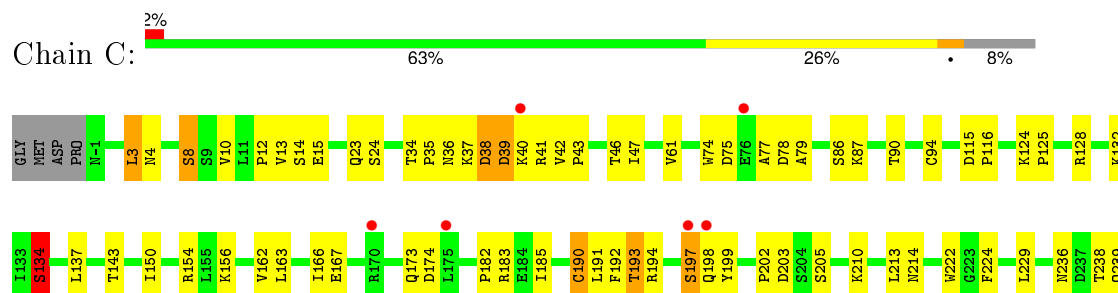
- Molecule 1: Vacuolar protein sorting-associated protein 75 (VPS75)



- Molecule 1: Vacuolar protein sorting-associated protein 75 (VPS75)



- Molecule 2: Histone acetyltransferase RTT109



K240	K241	L242	R243	I244	P245	G246	E247	D248	P249	A250	R251	V252	R253	L256	K260	Y261	P262	L263	W264	E274	N275	S276	L277	A278	V279	D287	D288	P289	K290	A291	R292	D301	R302	L303	L304	K305	V306	S307	E314	L315	Q316	Q319	E320	F321	K322	L323	S324	V325	T326	S327	S333
G334	S341	I342	F343	F344	S345	D348	V349	E368	E369	Y370	D371	N391	A392	T393	N394	L398	T399	G400	E403	HIS	ARG	GLU	ARG	ASN	GLN	PRO	VAL	PRO	ALA	SER	ASN	ILE	ASN	THR	LEU	LYS	PRO	ARG	LYS	LYS	ALA	LYS	ALA	LEU	PRO	LYS	THR				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.99 Å 98.06 Å 171.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.14 – 2.71 47.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.14-2.71) 95.7 (47.14-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.226 0.189 , 0.223	Depositor DCC
R_{free} test set	512 reflections (1.25%)	DCC
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42408 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7145	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ALY

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	1.04	0/1969	0.69	0/2652
1	B	0.87	0/1890	0.69	0/2546
2	C	1.10	2/3353 (0.1%)	0.78	2/4536 (0.0%)
All	All	1.03	2/7212 (0.0%)	0.73	2/9734 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	94	CYS	CB-SG	-5.63	1.72	1.81
2	C	190	CYS	CB-SG	-5.43	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	134	SER	N-CA-C	-6.22	94.19	111.00
2	C	325	VAL	N-CA-C	-5.86	95.19	111.00

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	1921	0	1849	69	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1842	0	1776	105	0
2	C	3292	0	3342	130	2
3	A	34	0	0	4	0
3	B	10	0	0	0	1
3	C	46	0	0	2	0
All	All	7145	0	6967	284	3

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 20.

All (284) 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)
2:C:301:ASP:OD2	1:B:177:LYS:HE3	1.47	1.13
1:B:79:TYR:HD1	1:B:116:PHE:CD2	1.68	1.11
2:C:316:GLN:HE22	2:C:323:LEU:HD13	1.16	1.10
1:A:56:GLU:OE1	1:A:59:LYS:HD3	1.49	1.09
2:C:194:ARG:NH2	2:C:321:PHE:CE1	2.23	1.06
2:C:13:VAL:HA	2:C:400:GLY:O	1.56	1.06
1:B:112:ILE:HB	1:B:116:PHE:HB3	1.36	1.05
2:C:115:ASP:OD1	2:C:116:PRO:HD2	1.55	1.04
2:C:3:LEU:HD12	2:C:3:LEU:O	1.56	1.04
1:A:253:SER:HB3	1:B:173:ARG:HG3	1.42	1.02
1:B:79:TYR:CD1	1:B:116:PHE:CD2	2.47	1.02
1:A:87:LYS:HE3	3:A:291:HOH:O	1.65	0.97
1:B:79:TYR:HD1	1:B:116:PHE:CE2	1.83	0.97
1:B:123:LYS:HE3	1:B:141:SER:OG	1.66	0.96
1:B:111:GLY:CA	1:B:118:GLU:HB3	1.97	0.94
1:A:162:ASP:HB3	1:A:165:SER:HB3	1.49	0.94
1:B:73:ARG:O	1:B:76:ASP:HB2	1.68	0.93
2:C:10:VAL:O	2:C:10:VAL:HG12	1.68	0.92
2:C:262:PRO:C	2:C:263:LEU:HD12	1.91	0.91
1:B:75:SER:HB2	1:B:152:TYR:OH	1.72	0.90
1:B:111:GLY:HA3	1:B:118:GLU:HB3	1.54	0.90
1:A:55:ALA:O	1:A:56:GLU:HB2	1.69	0.90
1:A:229:GLU:OE1	2:C:124:LYS:NZ	2.08	0.87
1:A:247:GLU:HB3	3:A:279:HOH:O	1.74	0.87
2:C:316:GLN:NE2	2:C:323:LEU:HD13	1.91	0.85
2:C:39:ASP:OD1	2:C:41:ARG:N	2.10	0.83
1:A:130:GLY:O	1:A:131:LYS:HB2	1.75	0.83
1:A:231:GLY:O	1:A:232:LEU:HB2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:GLN:OE1	2:C:203:ASP:N	2.12	0.83
2:C:263:LEU:CD1	2:C:263:LEU:N	2.42	0.82
1:B:150:GLN:O	1:B:153:ASP:HB2	1.79	0.81
1:A:24:GLU:O	1:A:28:ILE:HG13	1.82	0.80
1:B:117:LYS:HG3	1:B:118:GLU:N	1.96	0.80
1:A:11:HIS:O	1:A:15:PHE:HD2	1.65	0.79
2:C:115:ASP:OD1	2:C:116:PRO:CD	2.30	0.78
2:C:287:ASP:OD1	2:C:292:ARG:NH2	2.17	0.78
1:B:79:TYR:CD1	1:B:116:PHE:HD2	2.02	0.78
2:C:12:PRO:O	2:C:400:GLY:HA3	1.83	0.78
1:B:41:LYS:HB3	1:B:42:PRO:HD3	1.65	0.78
2:C:10:VAL:O	2:C:10:VAL:CG1	2.30	0.77
2:C:279:VAL:HG11	2:C:303:LEU:HB3	1.67	0.76
1:B:106:THR:HG1	1:B:122:THR:HG1	1.28	0.75
1:B:111:GLY:N	1:B:118:GLU:HB3	2.02	0.74
2:C:302:ARG:HH21	2:C:314:GLU:CD	1.91	0.74
2:C:143:THR:HG23	1:B:134:GLN:HG3	1.71	0.73
1:B:111:GLY:N	1:B:118:GLU:CB	2.52	0.72
1:A:130:GLY:O	1:A:131:LYS:CB	2.35	0.72
2:C:162:VAL:HG12	2:C:163:LEU:N	2.02	0.71
1:B:79:TYR:HE1	1:B:149:PRO:HB3	1.55	0.71
1:B:79:TYR:CD1	1:B:116:PHE:CE2	2.74	0.71
2:C:191:LEU:HD21	2:C:222:TRP:CG	2.26	0.71
1:B:116:PHE:HD1	1:B:117:LYS:N	1.89	0.70
2:C:190:CYS:HB3	2:C:290:ALY:HH32	1.73	0.70
1:A:162:ASP:HB3	1:A:165:SER:CB	2.21	0.70
1:B:115:ASP:C	1:B:115:ASP:OD1	2.30	0.70
2:C:306:VAL:HG12	2:C:307:SER:N	2.06	0.69
2:C:263:LEU:N	2:C:263:LEU:HD12	2.00	0.69
1:A:11:HIS:O	1:A:15:PHE:CD2	2.45	0.69
2:C:162:VAL:CG1	2:C:163:LEU:N	2.55	0.69
2:C:198:GLN:OE1	2:C:202:PRO:HA	1.92	0.69
2:C:3:LEU:HD12	2:C:3:LEU:C	2.05	0.69
2:C:12:PRO:HB2	2:C:15:GLU:HG3	1.76	0.68
2:C:262:PRO:C	2:C:263:LEU:CD1	2.61	0.68
2:C:323:LEU:CB	2:C:324:SER:HA	2.24	0.67
1:B:79:TYR:CE1	1:B:149:PRO:HB3	2.29	0.67
2:C:194:ARG:NH1	2:C:320:GLU:O	2.29	0.66
1:A:162:ASP:O	1:A:168:GLY:HA3	1.95	0.66
1:B:150:GLN:O	1:B:153:ASP:CB	2.43	0.66
1:A:121:VAL:HG21	1:A:146:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ASP:OD1	2:C:40:LYS:N	2.30	0.65
1:A:48:ASP:O	1:A:52:ASP:OD1	2.16	0.64
1:A:55:ALA:O	1:A:56:GLU:CB	2.39	0.64
1:A:33:GLU:OE2	1:A:36:ARG:NH2	2.30	0.64
2:C:306:VAL:CG1	2:C:307:SER:N	2.61	0.64
1:A:253:SER:H	1:B:173:ARG:HD3	1.63	0.64
1:B:111:GLY:CA	1:B:118:GLU:CB	2.76	0.64
2:C:238:THR:HG23	2:C:333:SER:O	1.98	0.64
1:B:171:LYS:O	1:B:174:GLN:HB2	1.98	0.64
1:B:57:PHE:O	1:B:61:VAL:HG23	1.98	0.63
2:C:197:SER:HB2	2:C:205:SER:HB3	1.79	0.63
1:A:209:TYR:HB3	1:A:210:PRO:HD3	1.80	0.63
1:B:71:TYR:CE2	1:B:203:LEU:HD22	2.34	0.63
1:A:28:ILE:O	1:A:32:VAL:HG23	1.98	0.63
2:C:274:GLU:HG3	2:C:276:SER:OG	1.99	0.63
2:C:316:GLN:HE22	2:C:323:LEU:CD1	2.03	0.63
2:C:194:ARG:O	2:C:199:TYR:OH	2.15	0.62
2:C:302:ARG:HA	2:C:305:LYS:HG3	1.81	0.62
1:B:159:LEU:HD23	1:B:159:LEU:N	2.14	0.62
1:B:51:ILE:HD13	1:B:57:PHE:CE2	2.35	0.62
2:C:13:VAL:O	2:C:14:SER:HB2	2.01	0.61
1:A:252:LEU:O	1:A:253:SER:C	2.38	0.61
2:C:262:PRO:O	2:C:263:LEU:HD12	1.99	0.61
2:C:323:LEU:HB3	2:C:324:SER:HA	1.82	0.61
1:B:134:GLN:N	1:B:134:GLN:OE1	2.33	0.61
1:B:79:TYR:HB3	1:B:116:PHE:HE2	1.66	0.61
1:B:162:ASP:OD2	1:B:165:SER:N	2.23	0.60
2:C:182:PRO:O	2:C:185:ILE:HG23	2.01	0.60
1:B:55:ALA:C	1:B:56:GLU:CG	2.70	0.60
1:A:224:GLU:O	1:A:227:GLU:HG2	2.01	0.60
2:C:239:GLN:OE1	2:C:241:LYS:NZ	2.33	0.60
1:A:218:GLU:OE2	1:A:230:SER:HB3	2.02	0.60
2:C:302:ARG:HG2	2:C:302:ARG:NH1	2.16	0.59
1:B:144:VAL:HG23	1:B:145:PRO:HD2	1.84	0.59
1:A:88:VAL:O	3:A:284:HOH:O	2.17	0.59
1:B:179:ILE:O	1:B:182:TRP:HB3	2.03	0.59
1:B:112:ILE:N	1:B:116:PHE:O	2.30	0.58
1:A:85:LYS:HG2	1:A:86:ILE:N	2.18	0.58
2:C:213:LEU:HD23	2:C:213:LEU:N	2.18	0.58
2:C:150:ILE:O	2:C:154:ARG:HG3	2.04	0.57
2:C:302:ARG:HH11	2:C:302:ARG:HG2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PRO:CD	1:A:167:GLU:H	2.17	0.57
1:A:12:ALA:O	1:A:16:LEU:HG	2.05	0.57
1:B:79:TYR:CE1	1:B:149:PRO:CB	2.89	0.56
2:C:261:TYR:CE2	2:C:263:LEU:HB2	2.40	0.56
1:B:209:TYR:HB3	1:B:210:PRO:HD3	1.88	0.56
2:C:342:LEU:HD12	2:C:343:PHE:H	1.71	0.56
1:B:79:TYR:CD2	1:B:79:TYR:N	2.73	0.56
2:C:61:VAL:O	2:C:61:VAL:HG13	2.05	0.56
1:B:99:ASP:OD1	1:B:101:ARG:HB2	2.06	0.55
2:C:47:ILE:HD12	2:C:47:ILE:N	2.21	0.55
2:C:214:ASN:C	2:C:214:ASN:OD1	2.44	0.55
2:C:166:ILE:HG23	2:C:167:GLU:N	2.22	0.55
1:B:119:GLN:HE22	1:B:147:GLU:HB3	1.71	0.55
1:A:39:LYS:NZ	1:B:31:GLU:OE2	2.36	0.55
1:B:132:ASP:OD1	1:B:133:ASP:N	2.40	0.54
1:B:80:ILE:O	1:B:83:ILE:HG13	2.07	0.54
1:A:104:SER:HB2	1:A:124:VAL:HG22	1.89	0.54
2:C:263:LEU:N	2:C:263:LEU:HD13	2.20	0.54
1:B:155:ILE:HD12	1:B:175:GLY:CA	2.38	0.54
1:A:166:PRO:HD2	1:A:167:GLU:H	1.72	0.54
1:A:96:GLU:HG2	1:A:96:GLU:O	2.07	0.54
1:A:253:SER:CB	1:B:173:ARG:HH11	2.22	0.53
2:C:39:ASP:OD1	2:C:39:ASP:C	2.46	0.53
2:C:191:LEU:HD21	2:C:222:TRP:HB3	1.91	0.53
1:B:132:ASP:HB3	1:B:135:GLU:CD	2.29	0.53
2:C:249:PRO:O	2:C:253:ARG:HB2	2.08	0.53
1:A:31:GLU:OE1	1:B:39:LYS:NZ	2.30	0.53
2:C:302:ARG:NH2	2:C:314:GLU:OE2	2.41	0.53
1:B:55:ALA:C	1:B:56:GLU:HG3	2.29	0.53
2:C:245:PRO:HD2	2:C:327:SER:O	2.09	0.53
1:A:166:PRO:CG	1:A:167:GLU:H	2.21	0.53
2:C:166:ILE:HG23	2:C:167:GLU:HG2	1.91	0.53
1:B:123:LYS:NZ	1:B:183:PHE:O	2.40	0.52
2:C:277:LEU:CD2	2:C:304:LEU:HA	2.39	0.52
1:B:169:LYS:HG3	1:B:173:ARG:NH2	2.23	0.52
1:B:178:THR:O	1:B:194:PHE:CE1	2.63	0.52
1:A:131:LYS:C	1:A:132:ASP:OD1	2.48	0.52
1:A:253:SER:HB3	1:B:173:ARG:HH11	1.75	0.51
2:C:38:ASP:OD1	2:C:38:ASP:N	2.42	0.51
1:A:46:LYS:HE3	1:B:24:GLU:OE2	2.09	0.51
1:B:123:LYS:HG2	1:B:125:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:N	1:A:210:PRO:CD	2.74	0.51
1:B:111:GLY:N	1:B:118:GLU:HB2	2.25	0.51
2:C:61:VAL:O	2:C:61:VAL:CG1	2.59	0.51
1:B:111:GLY:H	1:B:118:GLU:CB	2.24	0.51
2:C:302:ARG:HH11	2:C:302:ARG:CG	2.23	0.51
1:A:39:LYS:HZ3	1:B:31:GLU:CD	2.14	0.50
1:A:248:VAL:HG22	1:A:249:ASP:H	1.76	0.50
1:B:112:ILE:O	1:B:116:PHE:O	2.30	0.50
1:B:116:PHE:CD1	1:B:116:PHE:C	2.83	0.50
1:A:253:SER:H	1:B:173:ARG:HH11	1.60	0.50
1:B:71:TYR:HE2	1:B:203:LEU:HD22	1.74	0.50
2:C:236:ASN:OD1	2:C:236:ASN:O	2.30	0.50
1:A:252:LEU:O	1:A:253:SER:O	2.30	0.50
2:C:191:LEU:HD21	2:C:222:TRP:CB	2.40	0.50
1:B:150:GLN:HA	1:B:153:ASP:OD2	2.12	0.50
2:C:292:ARG:NH1	2:C:320:GLU:OE2	2.44	0.50
1:B:179:ILE:HG23	1:B:180:PHE:N	2.26	0.50
2:C:4:ASN:O	2:C:8:SER:OG	2.23	0.50
2:C:13:VAL:HA	2:C:400:GLY:C	2.29	0.49
1:A:166:PRO:CG	1:A:167:GLU:N	2.75	0.49
2:C:287:ASP:O	2:C:287:ASP:OD1	2.30	0.49
2:C:191:LEU:CD2	2:C:222:TRP:HB3	2.43	0.49
2:C:23:GLN:HG2	2:C:24:SER:N	2.28	0.49
1:B:83:ILE:HG12	1:B:109:PHE:CE1	2.48	0.49
1:A:166:PRO:CD	1:A:167:GLU:N	2.76	0.48
1:B:55:ALA:O	1:B:56:GLU:HG3	2.13	0.48
2:C:77:ALA:O	2:C:78:ASP:HB2	2.12	0.48
1:B:79:TYR:HD2	1:B:79:TYR:H	1.60	0.48
1:B:155:ILE:HD12	1:B:175:GLY:N	2.28	0.48
1:A:253:SER:N	1:B:173:ARG:HH11	2.12	0.48
1:B:155:ILE:HD12	1:B:175:GLY:HA2	1.96	0.48
1:B:155:ILE:O	1:B:157:PRO:HD3	2.13	0.48
1:B:178:THR:O	1:B:194:PHE:HE1	1.97	0.48
2:C:224:PHE:CD2	2:C:224:PHE:C	2.87	0.48
2:C:391:MET:O	2:C:392:ALA:C	2.50	0.47
2:C:194:ARG:HH12	2:C:320:GLU:C	2.16	0.47
1:B:150:GLN:HA	1:B:153:ASP:CG	2.34	0.47
2:C:42:VAL:HB	2:C:43:PRO:CD	2.44	0.47
2:C:393:THR:HG22	2:C:394:ASN:N	2.29	0.47
1:A:166:PRO:HG2	1:A:167:GLU:H	1.79	0.47
1:A:33:GLU:CD	1:A:36:ARG:HH21	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:LEU:HD12	2:C:343:PHE:N	2.29	0.47
2:C:46:THR:C	2:C:47:ILE:HD12	2.36	0.47
2:C:277:LEU:HD21	2:C:304:LEU:HA	1.97	0.47
1:B:41:LYS:HB3	1:B:42:PRO:CD	2.42	0.47
1:A:52:ASP:N	1:A:52:ASP:OD1	2.46	0.46
1:B:116:PHE:C	1:B:116:PHE:HD1	2.18	0.46
2:C:325:VAL:CG1	2:C:325:VAL:O	2.59	0.46
2:C:86:SER:O	2:C:87:LYS:HG3	2.15	0.46
1:A:130:GLY:C	1:A:131:LYS:HG3	2.35	0.46
2:C:238:THR:HG23	2:C:334:GLY:HA3	1.96	0.46
1:B:164:ARG:O	1:B:165:SER:C	2.52	0.46
2:C:90:THR:O	2:C:210:LYS:HE3	2.15	0.46
2:C:345:SER:H	2:C:348:ASP:HB2	1.80	0.46
2:C:398:LEU:HD12	2:C:398:LEU:C	2.36	0.46
1:B:112:ILE:O	1:B:116:PHE:N	2.48	0.46
1:B:116:PHE:CD1	1:B:117:LYS:N	2.78	0.46
2:C:229:LEU:HA	2:C:229:LEU:HD23	1.77	0.46
2:C:368:GLU:CA	2:C:368:GLU:OE1	2.63	0.45
1:A:165:SER:HG	1:A:168:GLY:HA3	1.82	0.45
2:C:247:GLU:OE2	2:C:251:ARG:NH1	2.49	0.45
1:B:79:TYR:HE1	1:B:149:PRO:CB	2.24	0.45
1:A:131:LYS:O	1:A:132:ASP:OD1	2.34	0.45
2:C:316:GLN:NE2	2:C:323:LEU:CD1	2.72	0.45
2:C:34:THR:HA	2:C:35:PRO:HD3	1.81	0.45
2:C:199:TYR:HE1	3:C:464:HOH:O	1.99	0.45
3:A:273:HOH:O	2:C:162:VAL:HG13	2.16	0.45
1:B:99:ASP:N	1:B:102:ASP:OD2	2.41	0.45
2:C:345:SER:O	2:C:348:ASP:N	2.50	0.45
2:C:368:GLU:HA	2:C:368:GLU:OE1	2.15	0.45
2:C:166:ILE:CG2	2:C:167:GLU:N	2.79	0.44
1:A:193:GLU:O	1:A:194:PHE:C	2.55	0.44
2:C:316:GLN:OE1	2:C:323:LEU:HD11	2.17	0.44
2:C:279:VAL:CG1	2:C:303:LEU:HD22	2.47	0.44
2:C:302:ARG:O	2:C:303:LEU:C	2.56	0.44
2:C:325:VAL:O	2:C:325:VAL:HG12	2.16	0.44
2:C:183:ARG:HH21	2:C:341:SER:HB3	1.82	0.44
2:C:278:ALA:HB3	3:C:461:HOH:O	2.16	0.44
1:B:169:LYS:CG	1:B:173:ARG:NH2	2.81	0.44
1:A:253:SER:CB	1:B:173:ARG:HG3	2.30	0.44
2:C:290:ALY:HH31	2:C:290:ALY:HE2	1.66	0.44
1:A:122:THR:O	1:A:144:VAL:HG11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:VAL:O	2:C:13:VAL:HG13	2.17	0.43
1:A:17:GLY:HA3	1:B:50:TYR:CZ	2.53	0.43
2:C:124:LYS:HA	2:C:125:PRO:HD3	1.86	0.43
2:C:132:LYS:HB3	2:C:174:ASP:OD2	2.18	0.43
1:B:168:GLY:O	1:B:172:TYR:HB3	2.18	0.43
1:B:188:LEU:C	1:B:190:PRO:HD3	2.38	0.43
2:C:192:PHE:CE1	2:C:289:PRO:HB2	2.54	0.43
1:A:62:LEU:HD13	1:A:80:ILE:HG23	1.99	0.43
2:C:368:GLU:OE1	2:C:369:GLU:N	2.48	0.43
2:C:320:GLU:HG3	2:C:321:PHE:HD1	1.84	0.43
1:A:229:GLU:OE1	2:C:124:LYS:CE	2.67	0.42
1:A:123:LYS:HG2	1:A:125:PHE:CE2	2.53	0.42
2:C:316:GLN:OE1	2:C:323:LEU:CD1	2.68	0.42
1:B:113:GLU:HG2	1:B:114:GLY:HA2	2.01	0.42
1:A:253:SER:HB3	1:B:173:ARG:CG	2.30	0.42
1:B:102:ASP:OD1	1:B:126:GLN:HA	2.19	0.42
2:C:301:ASP:CG	1:B:177:LYS:HE3	2.31	0.42
1:A:14:ALA:HA	1:B:50:TYR:CD1	2.54	0.42
2:C:173:GLN:OE1	2:C:173:GLN:HA	2.19	0.42
2:C:43:PRO:N	2:C:74:TRP:CZ3	2.88	0.42
1:A:110:HIS:HA	1:A:118:GLU:HG3	2.02	0.42
2:C:37:LYS:H	2:C:37:LYS:HG2	1.56	0.42
1:B:47:ARG:NH2	1:B:209:TYR:O	2.39	0.42
2:C:348:ASP:C	2:C:349:VAL:HG13	2.40	0.42
1:A:22:GLU:OE2	1:B:213:VAL:HG21	2.19	0.42
1:A:204:PHE:HA	1:A:208:ILE:HB	2.01	0.42
1:B:182:TRP:CD1	1:B:200:LEU:HD23	2.55	0.42
1:A:57:PHE:O	1:A:61:VAL:HG23	2.20	0.42
2:C:256:LEU:HD13	2:C:264:TRP:HB3	2.01	0.41
1:A:165:SER:CB	1:A:166:PRO:CD	2.98	0.41
2:C:125:PRO:HG2	2:C:128:ARG:HG2	2.02	0.41
2:C:198:GLN:CD	2:C:202:PRO:HA	2.40	0.41
1:B:144:VAL:CG2	1:B:145:PRO:HD2	2.48	0.41
1:A:139:LEU:HA	1:A:139:LEU:HD12	1.91	0.41
1:A:91:LEU:HB3	1:A:98:TYR:CD2	2.55	0.41
1:B:123:LYS:HG2	1:B:125:PHE:CZ	2.56	0.41
1:B:113:GLU:HA	1:B:114:GLY:C	2.39	0.41
1:B:85:LYS:HB3	1:B:108:HIS:HB3	2.03	0.41
1:B:35:TYR:CE2	1:B:39:LYS:HE3	2.56	0.41
2:C:391:MET:O	2:C:392:ALA:HB3	2.20	0.41
2:C:320:GLU:HG3	2:C:321:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HA	1:B:145:PRO:HD3	1.91	0.41
2:C:371:ASP:N	2:C:371:ASP:OD1	2.53	0.41
2:C:36:ASN:O	2:C:39:ASP:HB3	2.21	0.41
2:C:115:ASP:HA	2:C:116:PRO:HD3	1.88	0.40
2:C:78:ASP:HB3	2:C:79:ALA:H	1.54	0.40
2:C:193:THR:OG1	2:C:193:THR:O	2.38	0.40
1:B:148:TRP:HB3	1:B:149:PRO:HD2	2.02	0.40
1:B:150:GLN:O	1:B:153:ASP:CG	2.60	0.40
1:B:182:TRP:CE2	1:B:200:LEU:HD23	2.56	0.40
2:C:260:LYS:HA	2:C:260:LYS:HD3	1.89	0.40

All (3) 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:A:20:LYS:NZ	2:C:134:SER:OG[4_555]	1.87	0.33
1:A:97:MET:O	3:B:269:HOH:O[4_555]	2.12	0.08
1:A:9:ASN:OD1	2:C:156:LYS:O[4_555]	2.16	0.04

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	228/264 (86%)	215 (94%)	11 (5%)	2 (1%)	21	49
1	B	219/264 (83%)	212 (97%)	7 (3%)	0	100	100
2	C	402/442 (91%)	396 (98%)	6 (2%)	0	100	100
All	All	849/970 (88%)	823 (97%)	24 (3%)	2 (0%)	52	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	PRO
1	A	131	LYS

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	207/235 (88%)	203 (98%)	4 (2%)	65	88
1	B	198/235 (84%)	187 (94%)	11 (6%)	26	54
2	C	370/402 (92%)	356 (96%)	14 (4%)	40	71
All	All	775/872 (89%)	746 (96%)	29 (4%)	41	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	52	ASP
1	A	84	ASP
1	A	139	LEU
2	C	3	LEU
2	C	8	SER
2	C	38	ASP
2	C	39	ASP
2	C	75	ASP
2	C	134	SER
2	C	137	LEU
2	C	193	THR
2	C	197	SER
2	C	243	ARG
2	C	274	GLU
2	C	276	SER
2	C	302	ARG
2	C	316	GLN
1	B	47	ARG
1	B	56	GLU
1	B	75	SER

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Mol	Chain	Res	Type
1	B	112	ILE
1	B	115	ASP
1	B	116	PHE
1	B	117	LYS
1	B	120	GLN
1	B	134	GLN
1	B	140	THR
1	B	154	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ALY	C	290	2	10,11,12	0.53	0	10,12,14	1.53	2 (20%)

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	ALY	C	290	2	-	2/8/10/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	290	ALY	CD-CE-NZ	-2.47	104.97	112.19
2	C	290	ALY	CE-NZ-CH	3.24	127.66	122.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	290	ALY	CH3-CH-NZ-CE
2	C	290	ALY	OH-CH-NZ-CE

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	290	ALY	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	232/264 (87%)	0.15	15 (6%) 22 20	43, 67, 156, 252	0
1	B	221/264 (83%)	0.60	28 (12%) 5 4	51, 93, 156, 183	0
2	C	404/442 (91%)	0.11	10 (2%) 61 61	47, 72, 135, 195	0
All	All	857/970 (88%)	0.25	53 (6%) 24 23	43, 75, 149, 252	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ASP	8.9
1	B	111	GLY	6.3
1	A	134	GLN	6.3
1	B	112	ILE	6.0
1	B	164	ARG	5.5
1	B	113	GLU	5.0
1	B	160	ILE	5.0
1	A	133	ASP	4.5
1	B	116	PHE	4.5
2	C	197	SER	4.4
1	B	223	LEU	4.2
1	B	79	TYR	4.2
1	B	169	LYS	4.1
1	B	152	TYR	3.6
2	C	76	GLU	3.6
1	B	114	GLY	3.6
1	A	11	HIS	3.4
1	A	169	LYS	3.4
1	A	164	ARG	3.2
1	B	115	ASP	3.1
1	B	150	GLN	3.0
1	B	222	ASP	3.0
1	A	167	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	163	LYS	2.8
2	C	324	SER	2.8
1	B	78	LYS	2.8
1	B	166	PRO	2.8
1	B	167	GLU	2.8
1	A	163	LYS	2.7
1	B	161	LYS	2.7
1	B	171	LYS	2.6
1	B	109	PHE	2.5
1	B	77	PHE	2.5
1	B	83	ILE	2.5
1	A	252	LEU	2.4
2	C	170	ARG	2.4
1	A	161	LYS	2.4
1	B	159	LEU	2.4
2	C	319	GLN	2.4
1	B	110	HIS	2.3
1	B	220	GLN	2.3
1	A	131	LYS	2.2
2	C	323	LEU	2.2
2	C	322	LYS	2.2
1	A	253	SER	2.2
2	C	198	GLN	2.2
1	A	192	LYS	2.2
1	B	221	ARG	2.1
1	A	135	GLU	2.1
2	C	40	LYS	2.1
1	B	6	GLU	2.1
1	A	8	GLU	2.0
2	C	175	LEU	2.0

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

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	ALY	C	290	12/13	0.97	0.18	-	51,58,79,80	0

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.