



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:36 pm GMT

PDB ID : 4FHM
Title : Nup37-Nup120(aa1-961) complex from Schizosaccharomyces pombe
Authors : Bilokapic, S.; Schwartz, T.U.
Deposited on : 2012-06-06
Resolution : 4.34 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

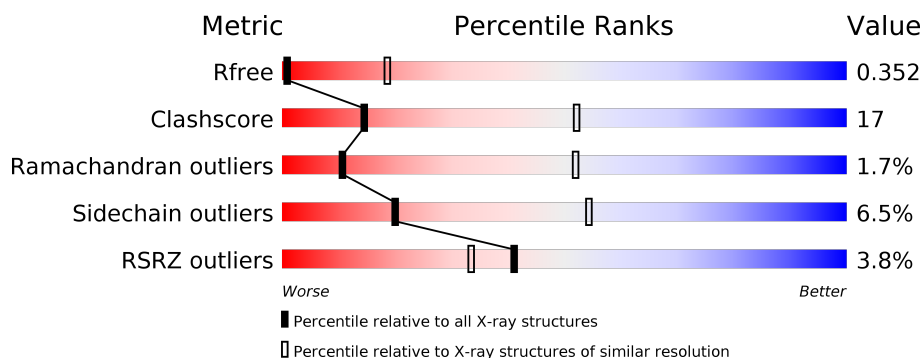
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.34 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}	100719	1023 (5.06-3.62)
Clashscore	112137	1025 (5.00-3.68)
Ramachandran outliers	110173	1015 (5.02-3.66)
Sidechain outliers	110143	1017 (5.04-3.64)
RSRZ outliers	101464	1005 (5.04-3.64)

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	394	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>• 10%</div> </div> </div>
2	B	964	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10113 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 NUCLEOPORIN NUP37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2718	1724	462	517	15	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	EXPRESSION TAG	UNP O36030
A	-1	GLY	-	EXPRESSION TAG	UNP O36030
A	0	SER	-	EXPRESSION TAG	UNP O36030

- Molecule 2 is a protein called Nucleoporin nup120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	920	7395	4779	1171	1418	27	0	0	0

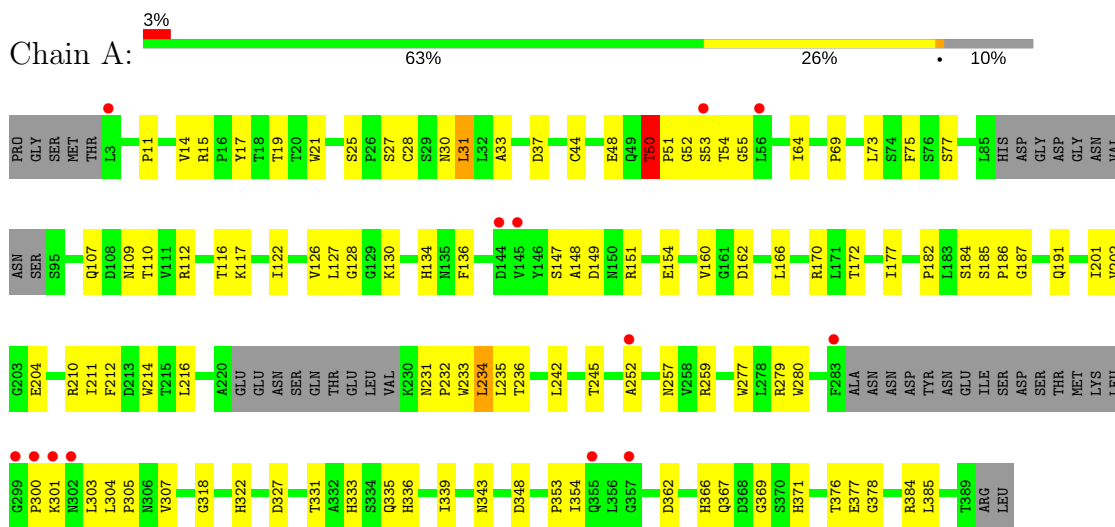
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	EXPRESSION TAG	UNP O43044
B	-1	GLY	-	EXPRESSION TAG	UNP O43044
B	0	SER	-	EXPRESSION TAG	UNP O43044

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 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: NUCLEOPORIN NUP37





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.05Å 164.05Å 310.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.50 – 4.34 64.50 – 4.34	Depositor EDS
% Data completeness (in resolution range)	99.0 (64.50-4.34) 99.1 (64.50-4.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1063)	Depositor
R, R_{free}	0.301 , 0.348 0.302 , 0.352	Depositor DCC
R_{free} test set	1451 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	202.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 284.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10113	wwPDB-VP
Average B, all atoms (Å ²)	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.26	0/2782	0.51	0/3799
2	B	0.30	0/7560	0.53	1/10259 (0.0%)
All	All	0.29	0/10342	0.52	1/14058 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	656	LEU	CA-CB-CG	5.36	127.63	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	THR	Peptide
2	B	206	GLU	Peptide
2	B	244	SER	Peptide

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	2718	0	2670	76	0
2	B	7395	0	7319	286	0
All	All	10113	0	9989	345	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 17.

All (345) 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:B:64:SER:HG	2:B:76:SER:HG	1.03	0.92
2:B:93:LYS:H	2:B:96:PRO:HG3	1.43	0.84
2:B:86:PHE:HB3	2:B:101:ASN:HD22	1.45	0.82
2:B:673:LEU:HB2	2:B:770:LEU:HD22	1.62	0.82
1:A:112:ARG:HG2	1:A:126:VAL:HG13	1.64	0.79
2:B:249:LEU:HB2	2:B:261:LEU:HB3	1.64	0.79
2:B:828:CYS:HA	2:B:831:LEU:HB2	1.65	0.77
2:B:219:LYS:HD3	2:B:220:LYS:HG3	1.68	0.76
2:B:866:SER:OG	2:B:867:LEU:N	2.17	0.76
1:A:371:HIS:NE2	1:A:384:ARG:HD2	2.01	0.76
2:B:10:PRO:HB3	2:B:433:ILE:HD11	1.67	0.75
2:B:916:LEU:HD11	2:B:948:ALA:HB3	1.67	0.74
2:B:164:PRO:HG2	2:B:195:ILE:HD13	1.70	0.74
2:B:673:LEU:HD13	2:B:770:LEU:HD13	1.69	0.73
1:A:279:ARG:HB3	1:A:307:VAL:HG12	1.70	0.73
2:B:65:ASN:HB2	2:B:75:TRP:CD1	2.23	0.73
2:B:194:LYS:HB3	2:B:205:TYR:HB2	1.69	0.73
2:B:192:LEU:HD11	2:B:251:MET:SD	2.29	0.72
1:A:117:LYS:HG2	1:A:122:ILE:HD13	1.73	0.71
1:A:371:HIS:CE1	1:A:384:ARG:HD2	2.26	0.70
2:B:337:PRO:HG3	2:B:394:HIS:HE1	1.55	0.70
2:B:310:SER:OG	2:B:311:ILE:N	2.24	0.70
2:B:743:GLU:OE2	2:B:823:LYS:NZ	2.22	0.70
2:B:81:ARG:H	2:B:109:ASN:HB3	1.58	0.69
2:B:66:LYS:HG3	2:B:119:PHE:HB2	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:H	1:A:348:ASP:HB2	1.59	0.68
2:B:90:LEU:HA	2:B:669:PRO:HG3	1.75	0.68
1:A:55:GLY:H	1:A:384:ARG:HH11	1.42	0.67
2:B:313:LYS:HB3	2:B:329:LYS:HD3	1.74	0.67
2:B:555:PRO:O	2:B:559:LEU:N	2.23	0.67
2:B:79:GLN:HB3	2:B:82:THR:HB	1.74	0.67
2:B:190:GLY:HA2	2:B:236:THR:HA	1.77	0.67
1:A:252:ALA:HB2	2:B:826:ASN:HD22	1.59	0.67
2:B:729:ARG:HH12	2:B:812:VAL:HG11	1.60	0.66
2:B:871:SER:H	2:B:883:GLN:HG2	1.60	0.66
2:B:412:ASN:ND2	2:B:594:GLU:OE2	2.29	0.66
2:B:763:LEU:HD22	2:B:771:GLN:HG2	1.76	0.66
1:A:170:ARG:HD3	1:A:214:TRP:HZ3	1.60	0.66
1:A:304:LEU:HD22	1:A:305:PRO:HD2	1.77	0.65
2:B:164:PRO:HB3	2:B:204:HIS:CD2	2.32	0.65
2:B:817:GLU:HA	2:B:844:LEU:HD11	1.79	0.65
2:B:913:ILE:HA	2:B:916:LEU:HD12	1.78	0.65
2:B:310:SER:HA	2:B:332:ILE:H	1.62	0.64
2:B:533:ILE:HD12	2:B:535:TYR:HE1	1.63	0.64
2:B:28:ALA:HB1	2:B:107:PRO:HB3	1.79	0.64
2:B:839:PRO:HB2	2:B:869:LEU:HD11	1.80	0.64
2:B:78:PHE:HZ	2:B:117:PHE:HB3	1.63	0.64
1:A:202:VAL:HB	1:A:210:ARG:HB2	1.79	0.64
2:B:247:ASN:HB3	2:B:263:LEU:HD12	1.80	0.64
2:B:130:ALA:HB3	2:B:138:TYR:HB2	1.80	0.63
2:B:349:PHE:HA	2:B:522:ILE:HD11	1.80	0.63
1:A:28:CYS:HB3	1:A:31:LEU:HD22	1.79	0.63
2:B:776:LEU:HD13	2:B:797:SER:HA	1.81	0.63
2:B:435:SER:HB2	2:B:512:LEU:HB3	1.81	0.63
1:A:149:ASP:O	1:A:151:ARG:NH1	2.32	0.62
1:A:301:LYS:HD3	2:B:479:GLN:HB3	1.81	0.62
1:A:233:TRP:HD1	2:B:413:MET:SD	2.23	0.62
2:B:535:TYR:HB2	2:B:538:LYS:O	2.00	0.62
1:A:154:GLU:HG2	1:A:172:THR:HG22	1.82	0.61
2:B:815:LEU:HD22	2:B:819:LEU:HD11	1.82	0.61
1:A:19:THR:HG22	1:A:362:ASP:HB3	1.81	0.60
2:B:67:SER:HB2	2:B:73:LEU:HG	1.82	0.60
2:B:240:MET:HG3	2:B:251:MET:HG2	1.82	0.60
2:B:817:GLU:OE2	2:B:876:PHE:N	2.24	0.60
1:A:170:ARG:HB2	1:A:177:ILE:HB	1.84	0.60
2:B:10:PRO:HG3	2:B:431:THR:HA	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:VAL:HG22	2:B:684:ILE:HD13	1.82	0.60
2:B:824:GLN:HG2	2:B:827:ALA:HB3	1.83	0.59
2:B:733:PHE:HA	2:B:834:TRP:CZ3	2.37	0.59
2:B:729:ARG:HH22	2:B:810:ASP:HB3	1.68	0.59
1:A:37:ASP:HA	1:A:69:PRO:HA	1.85	0.59
2:B:770:LEU:O	2:B:773:PHE:N	2.35	0.59
2:B:952:ASP:HB3	2:B:955:HIS:HD2	1.68	0.58
2:B:78:PHE:HD2	2:B:110:VAL:HG21	1.69	0.58
2:B:520:LEU:HD11	2:B:536:ALA:HB2	1.85	0.58
2:B:445:ASN:HB2	2:B:448:SER:HB2	1.85	0.58
2:B:65:ASN:HB2	2:B:75:TRP:HD1	1.65	0.57
2:B:690:VAL:O	2:B:693:GLU:HB2	2.05	0.57
2:B:12:ASP:HB2	2:B:433:ILE:HG23	1.87	0.57
2:B:182:GLU:HG2	2:B:196:ILE:HG13	1.86	0.57
2:B:192:LEU:O	2:B:207:GLN:N	2.30	0.57
2:B:241:ILE:HD11	2:B:292:THR:HG22	1.86	0.57
2:B:164:PRO:HD2	2:B:167:PHE:HE1	1.70	0.57
1:A:109:ASN:OD1	1:A:136:PHE:HA	2.04	0.57
2:B:293:THR:HG23	2:B:353:SER:H	1.68	0.57
2:B:835:LEU:HD21	2:B:841:ALA:HB1	1.86	0.56
1:A:136:PHE:CG	2:B:857:LYS:HG2	2.41	0.56
2:B:100:PHE:HE1	2:B:147:PHE:HA	1.69	0.56
2:B:708:TYR:HA	2:B:711:GLN:HG3	1.88	0.56
1:A:110:THR:HG22	1:A:128:GLY:HA3	1.86	0.56
1:A:170:ARG:HD3	1:A:214:TRP:CZ3	2.41	0.56
1:A:231:ASN:HD22	1:A:232:PRO:HD2	1.69	0.56
1:A:53:SER:OG	1:A:54:THR:N	2.38	0.56
1:A:166:LEU:HD22	1:A:202:VAL:HG21	1.86	0.55
2:B:13:LEU:HA	2:B:16:PHE:HD2	1.71	0.55
1:A:25:SER:HB2	1:A:77:SER:HA	1.88	0.55
2:B:615:LEU:O	2:B:699:LEU:HD13	2.07	0.55
1:A:212:PHE:HD1	1:A:233:TRP:HB3	1.71	0.54
2:B:74:ARG:HH22	2:B:144:LYS:HG2	1.72	0.54
2:B:72:THR:HG21	2:B:144:LYS:HE3	1.90	0.54
1:A:51:PRO:C	1:A:53:SER:H	2.10	0.54
2:B:668:SER:HB2	2:B:672:PHE:HD2	1.72	0.54
2:B:288:THR:OG1	2:B:348:ASP:OD1	2.18	0.54
2:B:269:VAL:HG23	2:B:322:LYS:HE2	1.90	0.54
2:B:729:ARG:NH1	2:B:812:VAL:HG11	2.23	0.53
2:B:926:LYS:HZ1	2:B:930:ASP:H	1.56	0.53
2:B:501:GLU:OE1	2:B:504:ARG:NH2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:873:THR:HG22	2:B:883:GLN:HE22	1.73	0.53
2:B:915:ALA:O	2:B:919:SER:OG	2.24	0.53
2:B:373:THR:HG21	2:B:519:ILE:HG21	1.90	0.53
2:B:693:GLU:HB3	2:B:697:PHE:CZ	2.44	0.53
2:B:311:ILE:HB	2:B:332:ILE:HG13	1.89	0.53
2:B:77:ILE:O	2:B:84:THR:OG1	2.22	0.52
2:B:463:ILE:HA	2:B:466:LEU:HG	1.90	0.52
2:B:665:SER:HB3	2:B:777:ASN:HB3	1.91	0.52
2:B:86:PHE:HB3	2:B:101:ASN:ND2	2.19	0.52
2:B:422:TRP:CZ2	2:B:499:TYR:HA	2.44	0.52
2:B:646:MET:SD	2:B:646:MET:N	2.82	0.52
2:B:18:LEU:HD13	2:B:101:ASN:HB2	1.91	0.52
2:B:629:PRO:HA	2:B:632:ILE:HD12	1.90	0.52
2:B:635:LEU:O	2:B:639:LEU:HG	2.10	0.52
2:B:173:ASP:HB2	2:B:188:PHE:CE1	2.45	0.52
2:B:913:ILE:O	2:B:916:LEU:HB2	2.10	0.52
2:B:454:LYS:HD2	2:B:457:LYS:HD2	1.92	0.52
2:B:930:ASP:HB2	2:B:933:LEU:HB3	1.91	0.52
2:B:584:HIS:HB2	2:B:693:GLU:HG2	1.92	0.52
2:B:314:LEU:HD21	2:B:325:VAL:HG13	1.92	0.51
2:B:482:PRO:HA	2:B:489:TYR:HA	1.92	0.51
2:B:816:VAL:HG12	2:B:844:LEU:HD13	1.91	0.51
2:B:741:LEU:HD23	2:B:768:THR:HG22	1.92	0.51
2:B:906:LEU:HD22	2:B:914:ASP:HB2	1.93	0.51
1:A:333:HIS:HD2	1:A:336:HIS:H	1.58	0.51
2:B:265:THR:HG22	2:B:267:GLN:HB3	1.92	0.51
2:B:518:GLU:O	2:B:536:ALA:N	2.30	0.51
2:B:838:ASP:H	2:B:841:ALA:HB3	1.75	0.51
2:B:132:THR:OG1	2:B:136:VAL:HG22	2.11	0.51
2:B:97:LEU:O	2:B:99:LYS:HG2	2.11	0.51
2:B:689:GLN:O	2:B:693:GLU:HG3	2.12	0.50
2:B:178:ILE:HD11	2:B:182:GLU:HB2	1.93	0.50
2:B:314:LEU:HD11	2:B:325:VAL:HG13	1.93	0.50
2:B:832:ILE:HG13	2:B:835:LEU:HD22	1.91	0.50
2:B:68:LYS:HG3	2:B:121:GLU:HG2	1.93	0.50
2:B:116:ALA:O	2:B:130:ALA:HA	2.11	0.50
2:B:419:SER:HB2	2:B:471:LEU:HD21	1.92	0.50
2:B:812:VAL:HG21	2:B:835:LEU:HB2	1.93	0.50
1:A:257:ASN:HB2	1:A:318:GLY:HA3	1.93	0.50
2:B:78:PHE:CZ	2:B:117:PHE:HB3	2.45	0.50
2:B:548:ILE:HD11	2:B:687:LYS:HZ2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD13	1:A:305:PRO:HG3	1.93	0.50
2:B:364:ILE:HG23	2:B:522:ILE:HD12	1.94	0.50
2:B:72:THR:OG1	2:B:73:LEU:N	2.45	0.50
2:B:237:ILE:HA	2:B:253:SER:HA	1.94	0.49
2:B:247:ASN:HB3	2:B:263:LEU:HB2	1.95	0.49
2:B:642:LEU:HD23	2:B:645:PRO:HB3	1.94	0.49
2:B:639:LEU:HD13	2:B:701:LEU:HB3	1.93	0.49
1:A:130:LYS:O	1:A:134:HIS:NE2	2.37	0.49
1:A:160:VAL:HB	1:A:187:GLY:HA3	1.92	0.49
2:B:332:ILE:HG12	2:B:388:PHE:HE2	1.77	0.49
2:B:63:THR:HB	2:B:75:TRP:HZ2	1.77	0.49
2:B:12:ASP:HB2	2:B:433:ILE:CG2	2.42	0.49
1:A:339:ILE:HB	1:A:354:ILE:HB	1.95	0.49
2:B:233:SER:O	2:B:235:ASN:N	2.43	0.49
2:B:587:MET:HG2	2:B:591:THR:HG21	1.94	0.49
2:B:926:LYS:NZ	2:B:930:ASP:H	2.10	0.49
2:B:650:ASP:OD1	2:B:651:SER:N	2.45	0.49
2:B:768:THR:C	2:B:770:LEU:H	2.15	0.49
2:B:952:ASP:HB3	2:B:955:HIS:CD2	2.46	0.49
1:A:107:GLN:HA	2:B:860:ARG:NH2	2.28	0.48
2:B:478:ILE:HD11	2:B:501:GLU:HG2	1.94	0.48
2:B:97:LEU:HB2	2:B:669:PRO:HA	1.95	0.48
2:B:768:THR:OG1	2:B:769:ALA:N	2.46	0.48
2:B:193:THR:HA	2:B:206:GLU:HA	1.95	0.48
1:A:191:GLN:OE1	1:A:259:ARG:HD2	2.13	0.48
2:B:842:VAL:HG11	2:B:865:THR:HG21	1.94	0.48
2:B:137:LEU:HB2	2:B:162:TYR:O	2.12	0.48
2:B:59:ALA:O	2:B:536:ALA:HB1	2.13	0.48
2:B:767:ASN:HB3	2:B:770:LEU:HD21	1.96	0.48
2:B:797:SER:OG	2:B:798:LEU:N	2.46	0.48
2:B:863:LYS:HZ3	2:B:961:LEU:HA	1.79	0.48
1:A:107:GLN:HE22	2:B:860:ARG:HG2	1.78	0.48
2:B:767:ASN:HB3	2:B:770:LEU:HD11	1.94	0.48
1:A:210:ARG:HH12	2:B:417:ASP:H	1.61	0.48
2:B:12:ASP:H	2:B:433:ILE:HG13	1.79	0.48
2:B:840:ILE:HG12	2:B:875:GLN:HE21	1.79	0.48
2:B:128:ILE:CG2	2:B:140:ILE:HB	2.43	0.47
2:B:632:ILE:O	2:B:636:ILE:HG12	2.14	0.47
2:B:88:VAL:HB	2:B:671:LEU:HD22	1.95	0.47
2:B:536:ALA:O	2:B:538:LYS:HD2	2.14	0.47
2:B:590:SER:O	2:B:594:GLU:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:LEU:HD22	2:B:701:LEU:HD13	1.96	0.47
2:B:332:ILE:HG12	2:B:388:PHE:CE2	2.49	0.47
2:B:192:LEU:HB2	2:B:207:GLN:CG	2.45	0.47
2:B:63:THR:OG1	2:B:521:SER:OG	2.29	0.47
2:B:235:ASN:ND2	2:B:235:ASN:O	2.45	0.47
1:A:130:LYS:HD3	2:B:609:TYR:HE1	1.80	0.47
2:B:519:ILE:HA	2:B:535:TYR:HA	1.96	0.47
2:B:636:ILE:HA	2:B:639:LEU:HD12	1.96	0.47
2:B:466:LEU:O	2:B:470:VAL:HG23	2.15	0.46
2:B:599:LEU:HA	2:B:602:LEU:HB2	1.97	0.46
2:B:174:LEU:HD21	2:B:240:MET:H	1.79	0.46
1:A:147:SER:OG	1:A:148:ALA:N	2.49	0.46
1:A:211:ILE:O	1:A:234:LEU:HB2	2.15	0.46
1:A:236:THR:HB	2:B:417:ASP:HB3	1.97	0.46
1:A:212:PHE:CD1	1:A:233:TRP:HB3	2.50	0.46
1:A:51:PRO:O	1:A:53:SER:N	2.45	0.46
2:B:178:ILE:HG21	2:B:263:LEU:HD21	1.96	0.46
2:B:644:ASN:HD22	2:B:647:ARG:HB2	1.80	0.46
2:B:849:TYR:HB3	2:B:858:ALA:HB2	1.97	0.46
1:A:233:TRP:HA	1:A:233:TRP:CE3	2.51	0.46
2:B:243:LEU:HD11	2:B:292:THR:OG1	2.15	0.46
2:B:599:LEU:HD23	2:B:602:LEU:HD12	1.96	0.46
2:B:111:MET:HA	2:B:133:HIS:HA	1.98	0.46
2:B:140:ILE:HG23	2:B:158:TRP:HD1	1.79	0.45
2:B:549:GLU:O	2:B:553:GLU:HG2	2.16	0.45
1:A:184:SER:OG	1:A:204:GLU:OE1	2.32	0.45
2:B:306:HIS:ND1	2:B:308:SER:HB3	2.31	0.45
2:B:318:ALA:HA	2:B:323:LEU:HA	1.98	0.45
2:B:764:ALA:HA	2:B:823:LYS:HZ1	1.81	0.45
2:B:815:LEU:HD23	2:B:815:LEU:HA	1.81	0.45
2:B:855:ALA:O	2:B:859:VAL:HG23	2.16	0.45
2:B:314:LEU:HG	2:B:327:ILE:HG12	1.97	0.45
2:B:579:LEU:O	2:B:583:LEU:HG	2.16	0.45
2:B:72:THR:HB	2:B:93:LYS:NZ	2.31	0.45
2:B:530:VAL:HB	2:B:541:PHE:CZ	2.51	0.45
2:B:142:LEU:HD22	2:B:146:TRP:CZ3	2.52	0.45
2:B:636:ILE:HD13	2:B:639:LEU:HD12	2.00	0.44
1:A:303:LEU:HD21	2:B:479:GLN:HA	2.00	0.44
2:B:172:PRO:HA	2:B:187:PHE:HD1	1.82	0.44
2:B:241:ILE:HG22	2:B:250:VAL:HB	1.98	0.44
2:B:71:GLN:HB3	2:B:93:LYS:HE2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:LYS:O	2:B:224:LEU:HG	2.18	0.44
2:B:453:ASN:O	2:B:457:LYS:HG3	2.17	0.44
2:B:54:CYS:SG	2:B:55:VAL:N	2.90	0.44
2:B:846:ALA:HB1	2:B:862:PHE:CZ	2.52	0.44
2:B:192:LEU:HB2	2:B:207:GLN:HG3	2.00	0.44
1:A:280:TRP:CD1	1:A:305:PRO:HA	2.52	0.44
2:B:312:TYR:HD2	2:B:327:ILE:HG21	1.83	0.44
2:B:533:ILE:HD12	2:B:535:TYR:CE1	2.48	0.44
2:B:121:GLU:HB2	2:B:125:THR:O	2.18	0.44
2:B:198:ASN:HB3	2:B:201:ASP:HB2	2.00	0.44
2:B:242:PHE:HD1	2:B:249:LEU:HD13	1.81	0.44
2:B:718:ASP:O	2:B:722:LEU:HG	2.18	0.44
1:A:162:ASP:OD1	1:A:186:PRO:HB3	2.18	0.44
2:B:311:ILE:HD11	2:B:363:LEU:HD22	2.00	0.44
2:B:498:LEU:O	2:B:502:TRP:HD1	2.00	0.44
2:B:697:PHE:O	2:B:701:LEU:HG	2.18	0.44
2:B:665:SER:CB	2:B:777:ASN:HB3	2.48	0.44
2:B:905:LYS:O	2:B:909:GLU:HG3	2.18	0.44
2:B:953:ALA:O	2:B:955:HIS:N	2.50	0.43
1:A:21:TRP:CH2	1:A:366:HIS:HD2	2.36	0.43
2:B:602:LEU:HD22	2:B:606:LEU:HB2	1.99	0.43
2:B:676:SER:O	2:B:680:VAL:HB	2.17	0.43
1:A:17:TYR:OH	2:B:961:LEU:O	2.29	0.43
2:B:436:ILE:O	2:B:440:LEU:HG	2.18	0.43
2:B:953:ALA:C	2:B:955:HIS:H	2.22	0.43
1:A:30:ASN:O	1:A:44:CYS:HA	2.19	0.43
2:B:939:HIS:O	2:B:942:LEU:HB2	2.18	0.43
2:B:885:ILE:HD12	2:B:901:HIS:ND1	2.33	0.43
1:A:322:HIS:NE2	1:A:369:GLY:O	2.36	0.43
1:A:64:ILE:HD13	1:A:116:THR:HG21	2.01	0.43
2:B:651:SER:O	2:B:655:ARG:HG3	2.19	0.43
2:B:151:ASP:OD1	2:B:152:ALA:N	2.51	0.43
2:B:241:ILE:CG2	2:B:250:VAL:HB	2.48	0.43
2:B:622:HIS:O	2:B:627:VAL:HG21	2.19	0.43
2:B:847:LEU:O	2:B:850:LEU:HB2	2.19	0.43
2:B:741:LEU:HA	2:B:768:THR:HB	2.01	0.43
2:B:859:VAL:HG12	2:B:863:LYS:HE3	1.99	0.43
1:A:335:GLN:HG3	1:A:336:HIS:CD2	2.54	0.43
2:B:652:LEU:HD23	2:B:655:ARG:NE	2.34	0.43
2:B:889:TYR:CG	2:B:933:LEU:HD13	2.53	0.43
2:B:136:VAL:HG23	2:B:138:TYR:HE1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:HG21	2:B:417:ASP:OD1	2.18	0.43
2:B:417:ASP:N	2:B:417:ASP:OD1	2.52	0.43
2:B:743:GLU:HG2	2:B:766:VAL:HG23	2.01	0.43
2:B:917:GLU:O	2:B:920:LEU:HB2	2.18	0.43
1:A:277:TRP:HZ3	1:A:307:VAL:HG13	1.84	0.42
2:B:705:GLN:O	2:B:709:GLU:HG3	2.19	0.42
2:B:454:LYS:HA	2:B:454:LYS:HD2	1.86	0.42
2:B:207:GLN:HB2	2:B:207:GLN:HE21	1.60	0.42
2:B:243:LEU:HA	2:B:243:LEU:HD23	1.88	0.42
2:B:740:LEU:HD13	2:B:827:ALA:HB1	2.00	0.42
1:A:107:GLN:NE2	2:B:860:ARG:HG2	2.35	0.42
1:A:211:ILE:HD12	1:A:235:LEU:HD23	2.02	0.42
2:B:142:LEU:HD22	2:B:146:TRP:CE3	2.54	0.42
2:B:290:ASP:N	2:B:290:ASP:OD1	2.52	0.42
2:B:543:ARG:HB3	2:B:679:ARG:HH12	1.84	0.42
2:B:652:LEU:HD23	2:B:655:ARG:HE	1.84	0.42
2:B:718:ASP:O	2:B:721:PHE:HB3	2.19	0.42
2:B:724:LEU:HD23	2:B:724:LEU:HA	1.93	0.42
2:B:845:LYS:O	2:B:849:TYR:HD2	2.01	0.42
1:A:11:PRO:HB2	1:A:14:VAL:HG23	2.02	0.42
1:A:212:PHE:CE2	1:A:214:TRP:HB3	2.55	0.42
2:B:663:ASN:OD1	2:B:796:SER:OG	2.35	0.42
2:B:584:HIS:CB	2:B:693:GLU:HG2	2.50	0.42
2:B:840:ILE:HG23	2:B:875:GLN:HE21	1.84	0.42
1:A:201:ILE:HA	1:A:210:ARG:O	2.20	0.42
2:B:812:VAL:CG2	2:B:835:LEU:HB2	2.50	0.42
2:B:350:GLN:O	2:B:363:LEU:HD12	2.20	0.42
2:B:742:LEU:HD13	2:B:826:ASN:ND2	2.35	0.42
2:B:95:GLU:O	2:B:148:GLN:NE2	2.53	0.42
2:B:759:THR:O	2:B:762:ALA:HB3	2.19	0.42
2:B:638:THR:O	2:B:642:LEU:HD13	2.20	0.41
2:B:139:TYR:O	2:B:159:CYS:HA	2.19	0.41
2:B:174:LEU:HD23	2:B:237:ILE:HD11	2.01	0.41
2:B:485:ASP:OD1	2:B:485:ASP:N	2.43	0.41
1:A:182:PRO:HB3	2:B:597:TYR:CZ	2.55	0.41
2:B:828:CYS:O	2:B:832:ILE:HB	2.20	0.41
2:B:75:TRP:HE3	2:B:86:PHE:CZ	2.39	0.41
1:A:327:ASP:O	1:A:343:ASN:HA	2.20	0.41
1:A:48:GLU:OE2	1:A:50:THR:HG23	2.20	0.41
2:B:332:ILE:HA	2:B:333:PRO:HD3	1.89	0.41
1:A:55:GLY:H	1:A:384:ARG:NH1	2.12	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:VAL:HG11	2:B:138:TYR:CE2	2.55	0.41
2:B:814:GLU:O	2:B:817:GLU:HB3	2.20	0.41
2:B:889:TYR:CD1	2:B:933:LEU:HD13	2.56	0.41
2:B:238:ILE:HG23	2:B:239:SER:H	1.85	0.41
1:A:28:CYS:O	1:A:31:LEU:HB2	2.20	0.41
2:B:492:TYR:OH	2:B:496:ARG:NH2	2.53	0.41
2:B:677:VAL:O	2:B:680:VAL:HG12	2.20	0.41
2:B:445:ASN:OD1	2:B:446:SER:N	2.53	0.41
2:B:371:LEU:HG	2:B:514:HIS:O	2.21	0.41
2:B:5:LYS:HE2	2:B:549:GLU:HG3	2.02	0.41
1:A:33:ALA:HB2	1:A:75:PHE:CZ	2.56	0.41
1:A:51:PRO:C	1:A:53:SER:N	2.74	0.41
2:B:421:ILE:HG13	2:B:421:ILE:H	1.68	0.41
1:A:15:ARG:NH1	2:B:914:ASP:OD1	2.50	0.41
2:B:300:TYR:CD2	2:B:309:PHE:HB3	2.55	0.41
2:B:450:VAL:O	2:B:454:LYS:N	2.43	0.41
2:B:454:LYS:HG3	2:B:458:PHE:CE2	2.56	0.41
2:B:838:ASP:O	2:B:842:VAL:N	2.53	0.41
2:B:71:GLN:HB3	2:B:93:LYS:HZ1	1.86	0.41
2:B:329:LYS:NZ	2:B:329:LYS:HB3	2.36	0.41
2:B:524:PHE:CE1	2:B:531:THR:HA	2.56	0.41
1:A:233:TRP:HA	1:A:233:TRP:HE3	1.86	0.41
2:B:339:ASP:O	2:B:342:ILE:HB	2.20	0.41
2:B:408:ASP:O	2:B:410:PRO:HD3	2.21	0.41
2:B:850:LEU:HA	2:B:850:LEU:HD23	1.86	0.40
2:B:174:LEU:HD21	2:B:240:MET:HB2	2.03	0.40
2:B:840:ILE:HG12	2:B:875:GLN:NE2	2.36	0.40
2:B:548:ILE:HD13	2:B:687:LYS:HD2	2.03	0.40
1:A:376:THR:O	1:A:378:GLY:N	2.55	0.40
1:A:353:PRO:HB2	1:A:385:LEU:HD22	2.03	0.40
2:B:185:VAL:HB	2:B:193:THR:HG22	2.03	0.40
1:A:303:LEU:HB3	2:B:476:SER:HA	2.03	0.40
1:A:134:HIS:HB3	2:B:605:ASP:OD1	2.22	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	346/394 (88%)	319 (92%)	22 (6%)	5 (1%)	13	54
2	B	908/964 (94%)	771 (85%)	121 (13%)	16 (2%)	10	50
All	All	1254/1358 (92%)	1090 (87%)	143 (11%)	21 (2%)	11	52

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
2	B	953	ALA
1	A	50	THR
2	B	59	ALA
2	B	410	PRO
2	B	815	LEU
2	B	856	VAL
2	B	954	ALA
2	B	287	LEU
2	B	403	GLU
2	B	495	LYS
2	B	517	ASP
2	B	626	ASN
1	A	377	GLU
2	B	115	VAL
2	B	234	PRO
1	A	52	GLY
2	B	70	SER
2	B	27	PRO
1	A	300	PRO
2	B	334	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	309/345 (90%)	299 (97%)	10 (3%)	44	72
2	B	845/886 (95%)	780 (92%)	65 (8%)	15	49
All	All	1154/1231 (94%)	1079 (94%)	75 (6%)	20	54

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	31	LEU
1	A	50	THR
1	A	73	LEU
1	A	127	LEU
1	A	185	SER
1	A	216	LEU
1	A	245	THR
1	A	331	THR
1	A	367	GLN
2	B	11	ILE
2	B	50	PHE
2	B	54	CYS
2	B	58	ASP
2	B	72	THR
2	B	88	VAL
2	B	90	LEU
2	B	159	CYS
2	B	197	LEU
2	B	207	GLN
2	B	232	ARG
2	B	235	ASN
2	B	241	ILE
2	B	289	SER
2	B	290	ASP
2	B	291	HIS
2	B	292	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	296	PHE
2	B	297	ILE
2	B	301	TYR
2	B	329	LYS
2	B	338	ASP
2	B	339	ASP
2	B	388	PHE
2	B	417	ASP
2	B	423	LEU
2	B	429	HIS
2	B	431	THR
2	B	443	PHE
2	B	450	VAL
2	B	483	ASN
2	B	512	LEU
2	B	513	ASP
2	B	515	PHE
2	B	519	ILE
2	B	524	PHE
2	B	532	TYR
2	B	533	ILE
2	B	538	LYS
2	B	539	VAL
2	B	554	GLU
2	B	579	LEU
2	B	589	PHE
2	B	642	LEU
2	B	656	LEU
2	B	672	PHE
2	B	673	LEU
2	B	680	VAL
2	B	692	ILE
2	B	703	THR
2	B	717	CYS
2	B	725	LEU
2	B	743	GLU
2	B	791	HIS
2	B	805	ASP
2	B	812	VAL
2	B	813	THR
2	B	820	PHE
2	B	831	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	835	LEU
2	B	866	SER
2	B	878	VAL
2	B	902	LEU
2	B	907	PHE
2	B	961	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	308	GLN
1	A	336	HIS
2	B	101	ASN
2	B	204	HIS
2	B	394	HIS
2	B	584	HIS
2	B	955	HIS

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 ⓘ

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, 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	354/394 (89%)	0.23	13 (3%) 42 35	177, 274, 456, 701	0
2	B	920/964 (95%)	0.20	35 (3%) 41 33	150, 305, 521, 707	0
All	All	1274/1358 (93%)	0.21	48 (3%) 41 33	150, 298, 511, 707	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	923	ASP	6.5
2	B	701	LEU	5.1
2	B	700	SER	4.7
2	B	487	THR	4.6
2	B	282	GLN	4.5
2	B	626	ASN	4.5
1	A	53	SER	4.3
1	A	299	GLY	4.1
2	B	112	LYS	4.0
2	B	97	LEU	3.7
1	A	283	PHE	3.6
1	A	301	LYS	3.5
2	B	704	SER	3.4
1	A	357	GLY	3.3
2	B	457	LYS	3.3
2	B	284	PHE	3.2
2	B	662	TYR	3.0
1	A	3	LEU	2.9
2	B	660	ASP	2.8
2	B	926	LYS	2.8
2	B	91	ASN	2.7
2	B	837	SER	2.7
1	A	302	ASN	2.7
1	A	300	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	144	LYS	2.6
2	B	481	GLU	2.6
1	A	355	GLN	2.5
2	B	304	ASN	2.5
2	B	703	THR	2.5
1	A	252	ALA	2.5
2	B	661	ILE	2.4
1	A	145	VAL	2.3
2	B	90	LEU	2.3
2	B	702	ILE	2.3
2	B	575	GLN	2.3
2	B	479	GLN	2.2
2	B	888	LYS	2.2
2	B	408	ASP	2.2
2	B	478	ILE	2.1
1	A	144	ASP	2.1
2	B	33	SER	2.1
2	B	344	TRP	2.1
2	B	148	GLN	2.1
2	B	227	PHE	2.1
1	A	56	LEU	2.1
2	B	224	LEU	2.1
2	B	705	GLN	2.0
2	B	527	SER	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.