



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:58 AM EDT

PDB ID : 2R7Q  
Title : Crystal Structure of VP1 apoenzyme of Rotavirus SA11 (C-terminal hexahistidine-tagged)  
Authors : Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.  
Deposited on : 2007-09-09  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

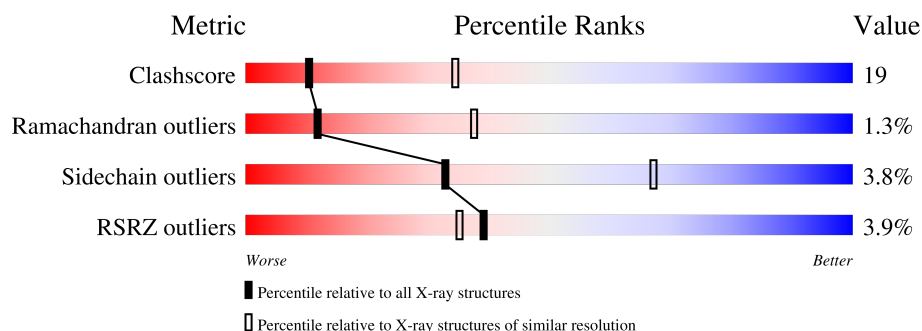
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	1095	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8686 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.

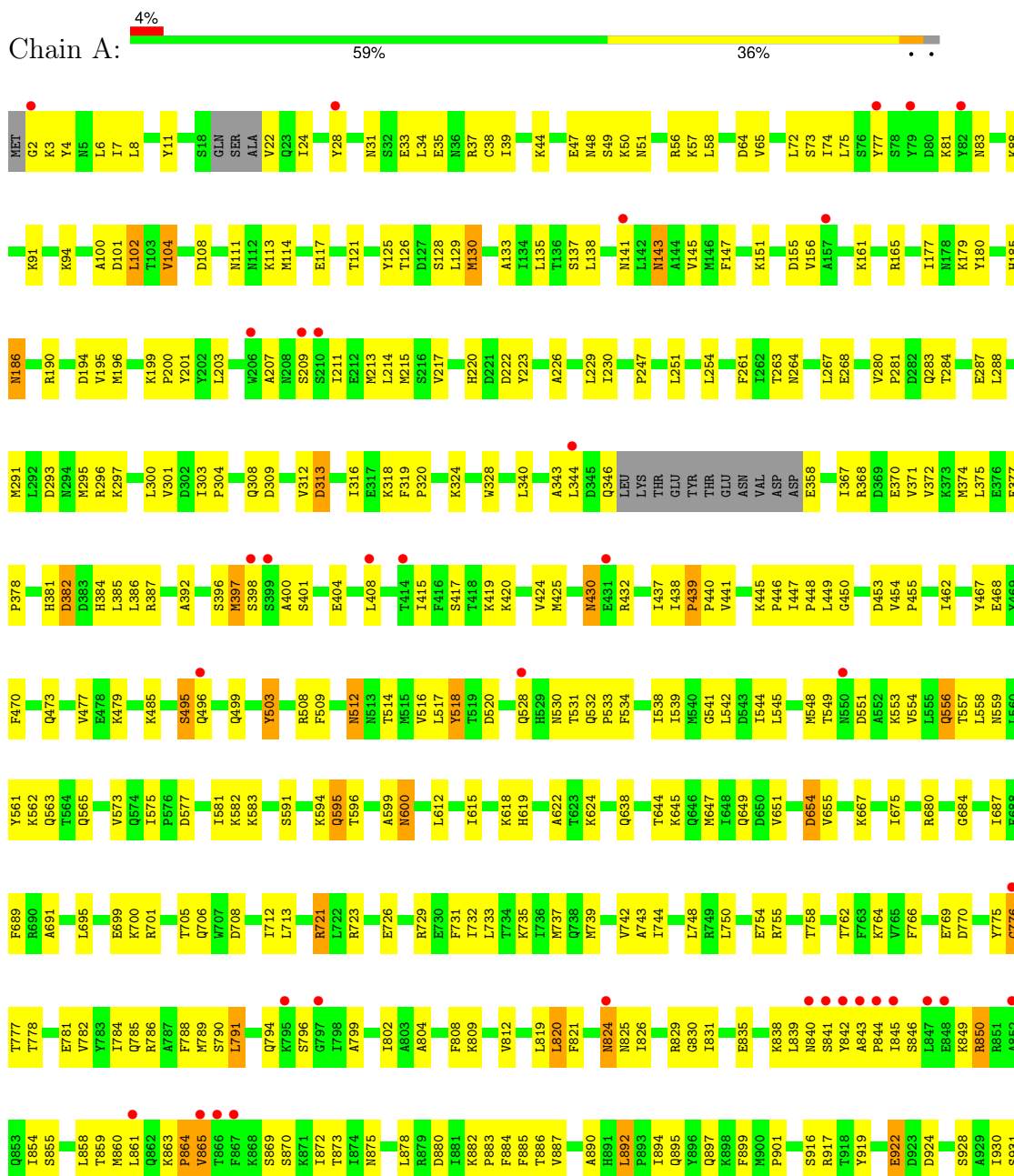
- Molecule 1 is a protein called RNA-dependent RNA polymerase.

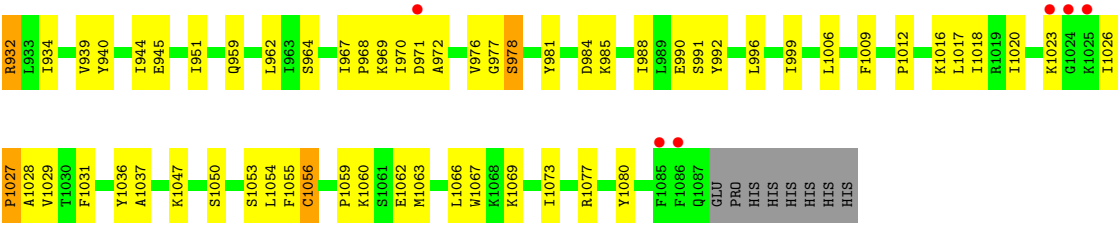
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1072	Total	C	N	O	S	0	0	0
			8686	5571	1446	1631	38			

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: RNA-dependent RNA polymerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.38Å 112.47Å 143.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.81 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.90) 96.2 (29.81-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.290 0.230 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/8857	0.58	1/11973 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	ASN	N-CA-C	7.10	130.18	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	8686	0	8776	325	0
All	All	8686	0	8776	325	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 19.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HB2	1:A:83:ASN:HD22	1.21	0.98
1:A:556:GLN:HA	1:A:556:GLN:HE21	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD23	1:A:479:LYS:HE2	1.57	0.86
1:A:470:PHE:HE1	1:A:594:LYS:HD3	1.40	0.85
1:A:254:LEU:HD23	1:A:280:VAL:HG21	1.59	0.84
1:A:186:ASN:HD21	1:A:190:ARG:H	1.24	0.84
1:A:705:THR:HB	1:A:850:ARG:NH1	1.94	0.82
1:A:789:MET:HE1	1:A:873:THR:HG21	1.63	0.80
1:A:102:LEU:HD22	1:A:102:LEU:H	1.47	0.78
1:A:438:ILE:HD12	1:A:563:GLN:HB3	1.65	0.78
1:A:398:SER:HB2	1:A:838:LYS:HE2	1.68	0.76
1:A:959:GLN:HG2	1:A:976:VAL:HG21	1.68	0.76
1:A:186:ASN:ND2	1:A:190:ARG:H	1.82	0.76
1:A:296:ARG:HH22	1:A:308:GLN:NE2	1.84	0.76
1:A:470:PHE:CE1	1:A:594:LYS:HD3	2.21	0.75
1:A:81:LYS:HB2	1:A:83:ASN:ND2	2.01	0.75
1:A:180:TYR:HB3	1:A:199:LYS:HG2	1.69	0.74
1:A:1059:PRO:HB2	1:A:1062:GLU:HB2	1.70	0.73
1:A:3:LYS:O	1:A:7:ILE:HG12	1.88	0.72
1:A:840:ASN:O	1:A:846:SER:HB3	1.90	0.72
1:A:177:ILE:HD13	1:A:203:LEU:HD11	1.71	0.71
1:A:503:TYR:HB2	1:A:687:ILE:HD13	1.72	0.71
1:A:88:LYS:HA	1:A:91:LYS:HE2	1.72	0.71
1:A:972:ALA:O	1:A:976:VAL:HG23	1.92	0.70
1:A:283:GLN:OE1	1:A:649:GLN:HG3	1.92	0.70
1:A:764:LYS:HD3	1:A:1080:TYR:CG	2.27	0.70
1:A:622:ALA:HB3	1:A:638:GLN:HB3	1.74	0.69
1:A:453:ASP:HB2	1:A:699:GLU:HG3	1.73	0.69
1:A:762:THR:HA	1:A:1077:ARG:O	1.93	0.69
1:A:44:LYS:HB3	1:A:58:LEU:HD21	1.74	0.69
1:A:473:GLN:HG2	1:A:561:TYR:CE1	2.27	0.68
1:A:556:GLN:HA	1:A:556:GLN:NE2	2.08	0.68
1:A:145:VAL:HG21	1:A:211:ILE:HG23	1.76	0.67
1:A:528:GLN:O	1:A:531:THR:HG22	1.94	0.67
1:A:1023:LYS:HB3	1:A:1060:LYS:HE2	1.75	0.67
1:A:316:ILE:HD13	1:A:684:GLY:HA3	1.75	0.67
1:A:781:GLU:O	1:A:784:ILE:HG22	1.95	0.67
1:A:796:SER:HB2	1:A:849:LYS:HE3	1.77	0.67
1:A:887:VAL:HG22	1:A:1054:LEU:HD11	1.75	0.67
1:A:744:ILE:HD13	1:A:748:LEU:HG	1.77	0.66
1:A:968:PRO:HG2	1:A:971:ASP:HB2	1.78	0.66
1:A:843:ALA:HB3	1:A:844:PRO:HD3	1.78	0.66
1:A:744:ILE:HD11	1:A:750:LEU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:O	1:A:557:THR:HG21	1.97	0.65
1:A:367:ILE:O	1:A:371:VAL:HG23	1.97	0.64
1:A:1059:PRO:O	1:A:1063:MET:HG3	1.97	0.64
1:A:392:ALA:HB2	1:A:939:VAL:HG21	1.79	0.64
1:A:591:SER:HB2	1:A:596:THR:HG21	1.80	0.63
1:A:449:LEU:HD13	1:A:573:VAL:HG13	1.78	0.63
1:A:309:ASP:O	1:A:312:VAL:HG22	1.99	0.63
1:A:381:HIS:O	1:A:382:ASP:HB2	1.97	0.63
1:A:430:ASN:O	1:A:432:ARG:HG3	1.99	0.63
1:A:735:LYS:O	1:A:739:MET:HG3	1.98	0.63
1:A:864:PRO:O	1:A:865:VAL:HG12	1.98	0.63
1:A:370:GLU:O	1:A:374:MET:HG3	1.98	0.62
1:A:573:VAL:HG12	1:A:575:ILE:HG13	1.80	0.62
1:A:777:THR:HG21	1:A:882:LYS:HE3	1.80	0.62
1:A:296:ARG:HH22	1:A:308:GLN:HE21	1.45	0.62
1:A:324:LYS:O	1:A:328:TRP:HD1	1.82	0.61
1:A:951:ILE:HG12	1:A:985:LYS:HA	1.81	0.61
1:A:186:ASN:C	1:A:186:ASN:HD22	2.03	0.61
1:A:514:THR:HG22	1:A:638:GLN:HG3	1.82	0.61
1:A:820:LEU:HD22	1:A:824:ASN:ND2	2.15	0.61
1:A:855:SER:HA	1:A:858:LEU:HD12	1.83	0.61
1:A:530:ASN:O	1:A:533:PRO:HD2	2.01	0.61
1:A:945:GLU:HG2	1:A:992:TYR:HE1	1.66	0.61
1:A:612:LEU:HD23	1:A:615:ILE:HD11	1.83	0.60
1:A:840:ASN:HD21	1:A:849:LYS:NZ	1.99	0.60
1:A:31:ASN:OD1	1:A:33:GLU:HG2	2.02	0.60
1:A:165:ARG:HD3	1:A:223:TYR:HB2	1.84	0.60
1:A:829:ARG:HG3	1:A:830:GLY:N	2.16	0.60
1:A:721:ARG:HD2	1:A:726:GLU:HG3	1.84	0.60
1:A:769:GLU:HG2	1:A:1047:LYS:HE2	1.84	0.60
1:A:4:TYR:HD1	1:A:733:LEU:HD22	1.66	0.60
1:A:538:ILE:O	1:A:542:LEU:HG	2.01	0.60
1:A:293:ASP:O	1:A:297:LYS:HG2	2.02	0.59
1:A:372:VAL:HA	1:A:545:LEU:HD21	1.83	0.59
1:A:820:LEU:HD13	1:A:824:ASN:HB2	1.83	0.59
1:A:8:LEU:HD23	1:A:74:ILE:HD12	1.85	0.59
1:A:447:ILE:HG22	1:A:448:PRO:O	2.03	0.58
1:A:264:ASN:HD21	1:A:268:GLU:HG3	1.68	0.58
1:A:1029:VAL:HG13	1:A:1066:LEU:HD23	1.86	0.58
1:A:28:TYR:CZ	1:A:784:ILE:HD13	2.38	0.58
1:A:553:LYS:O	1:A:557:THR:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ILE:O	1:A:894:ILE:HG13	2.03	0.58
1:A:778:THR:O	1:A:782:VAL:HG23	2.03	0.58
1:A:959:GLN:CG	1:A:976:VAL:HG21	2.34	0.57
1:A:882:LYS:HB3	1:A:883:PRO:HD3	1.86	0.57
1:A:755:ARG:HD2	1:A:781:GLU:HG2	1.86	0.57
1:A:161:LYS:O	1:A:165:ARG:HG3	2.05	0.57
1:A:295:MET:HE2	1:A:300:LEU:HD22	1.87	0.57
1:A:312:VAL:HG23	1:A:313:ASP:N	2.20	0.57
1:A:930:ILE:O	1:A:934:ILE:HG13	2.03	0.57
1:A:962:LEU:O	1:A:967:ILE:HB	2.05	0.57
1:A:446:PRO:HG2	1:A:583:LYS:HD3	1.87	0.56
1:A:24:ILE:HB	1:A:75:LEU:HB3	1.87	0.56
1:A:303:ILE:HB	1:A:304:PRO:HD3	1.86	0.56
1:A:916:SER:HB2	1:A:1006:LEU:O	2.05	0.56
1:A:1018:ILE:HD12	1:A:1037:ALA:HB1	1.86	0.56
1:A:705:THR:HB	1:A:850:ARG:HH11	1.69	0.56
1:A:924:ASP:C	1:A:944:ILE:HD13	2.25	0.56
1:A:544:ILE:O	1:A:548:MET:HG3	2.06	0.55
1:A:969:LYS:NZ	1:A:969:LYS:HB2	2.21	0.55
1:A:400:ALA:HB2	1:A:470:PHE:CE2	2.42	0.55
1:A:135:LEU:HB3	1:A:706:GLN:HG2	1.90	0.54
1:A:340:LEU:O	1:A:344:LEU:HB2	2.08	0.54
1:A:419:LYS:HE3	1:A:841:SER:OG	2.07	0.54
1:A:824:ASN:O	1:A:826:ILE:N	2.41	0.54
1:A:343:ALA:O	1:A:346:GLN:HG3	2.08	0.54
1:A:368:ARG:HG3	1:A:541:GLY:N	2.23	0.54
1:A:398:SER:HB2	1:A:838:LYS:CE	2.37	0.54
1:A:319:PHE:N	1:A:320:PRO:CD	2.71	0.53
1:A:554:VAL:O	1:A:558:LEU:HB2	2.08	0.53
1:A:596:THR:O	1:A:600:ASN:HB2	2.07	0.53
1:A:75:LEU:HG	1:A:748:LEU:HD11	1.89	0.53
1:A:396:SER:O	1:A:398:SER:N	2.41	0.53
1:A:556:GLN:HE21	1:A:556:GLN:CA	2.04	0.53
1:A:840:ASN:HD21	1:A:849:LYS:HZ1	1.55	0.53
1:A:6:LEU:N	1:A:6:LEU:HD22	2.24	0.53
1:A:539:ILE:HG23	1:A:562:LYS:HG3	1.91	0.53
1:A:392:ALA:HB2	1:A:939:VAL:CG2	2.39	0.53
1:A:419:LYS:HE3	1:A:841:SER:CB	2.39	0.53
1:A:102:LEU:HD22	1:A:102:LEU:N	2.22	0.52
1:A:618:LYS:HD3	1:A:654:ASP:OD2	2.09	0.52
1:A:1018:ILE:HD12	1:A:1037:ALA:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASN:ND2	1:A:186:ASN:C	2.64	0.52
1:A:551:ASP:HB3	1:A:554:VAL:HB	1.91	0.51
1:A:981:TYR:O	1:A:985:LYS:HG3	2.09	0.51
1:A:44:LYS:CB	1:A:58:LEU:HD21	2.39	0.51
1:A:207:ALA:O	1:A:211:ILE:HG13	2.11	0.51
1:A:860:MET:HE1	1:A:864:PRO:HB3	1.93	0.51
1:A:791:LEU:HD23	1:A:791:LEU:H	1.75	0.51
1:A:886:THR:OG1	1:A:1055:PHE:HB3	2.11	0.51
1:A:651:VAL:O	1:A:655:VAL:HG23	2.10	0.51
1:A:804:ALA:O	1:A:809:LYS:HE3	2.11	0.51
1:A:820:LEU:HD13	1:A:824:ASN:CB	2.40	0.51
1:A:854:ILE:O	1:A:858:LEU:HG	2.11	0.51
1:A:217:VAL:HG13	1:A:222:ASP:HB2	1.91	0.51
1:A:56:ARG:HH12	1:A:57:LYS:HD3	1.76	0.50
1:A:209:SER:O	1:A:213:MET:HG3	2.10	0.50
1:A:425:MET:HE1	1:A:802:ILE:HD11	1.92	0.50
1:A:485:LYS:HZ2	1:A:495:SER:HA	1.76	0.50
1:A:644:THR:OG1	1:A:647:MET:HG3	2.11	0.50
1:A:2:GLY:HA2	1:A:754:GLU:OE1	2.12	0.50
1:A:928:SER:O	1:A:932:ARG:HD2	2.11	0.50
1:A:518:TYR:N	1:A:518:TYR:CD2	2.79	0.50
1:A:532:GLN:HB2	1:A:533:PRO:HD3	1.93	0.50
1:A:899:PHE:O	1:A:901:PRO:HD3	2.11	0.50
1:A:880:ASP:OD2	1:A:1069:LYS:HE2	2.11	0.50
1:A:885:PHE:CE1	1:A:1056:CYS:HB2	2.47	0.50
1:A:420:LYS:O	1:A:424:VAL:HG23	2.11	0.49
1:A:138:LEU:HA	1:A:141:ASN:HD22	1.77	0.49
1:A:217:VAL:HG13	1:A:222:ASP:CB	2.42	0.49
1:A:473:GLN:HG2	1:A:561:TYR:CD1	2.48	0.49
1:A:473:GLN:HE21	1:A:594:LYS:HB3	1.76	0.49
1:A:680:ARG:HB3	1:A:689:PHE:CE1	2.47	0.49
1:A:970:ILE:HG23	1:A:971:ASP:OD1	2.13	0.49
1:A:999:ILE:HD11	1:A:1009:PHE:CZ	2.48	0.49
1:A:882:LYS:HE2	1:A:1036:TYR:OH	2.13	0.49
1:A:324:LYS:O	1:A:328:TRP:CD1	2.64	0.49
1:A:384:HIS:HE1	1:A:939:VAL:HB	1.78	0.49
1:A:820:LEU:HD22	1:A:824:ASN:HD22	1.78	0.49
1:A:758:THR:HG22	1:A:766:PHE:O	2.12	0.49
1:A:145:VAL:CG2	1:A:211:ILE:HG23	2.42	0.49
1:A:213:MET:HB3	1:A:328:TRP:HZ3	1.78	0.49
1:A:397:MET:CE	1:A:467:TYR:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:SG	1:A:65:VAL:HG13	2.53	0.49
1:A:775:TYR:O	1:A:777:THR:HG23	2.13	0.49
1:A:6:LEU:HD22	1:A:6:LEU:H	1.78	0.48
1:A:101:ASP:O	1:A:104:VAL:HG23	2.13	0.48
1:A:226:ALA:O	1:A:230:ILE:HG13	2.13	0.48
1:A:301:VAL:C	1:A:304:PRO:HD2	2.33	0.48
1:A:8:LEU:CD2	1:A:74:ILE:HD12	2.43	0.48
1:A:976:VAL:O	1:A:976:VAL:HG12	2.13	0.48
1:A:977:GLY:O	1:A:978:SER:O	2.30	0.48
1:A:137:SER:HB2	1:A:185:HIS:CD2	2.48	0.48
1:A:820:LEU:HD22	1:A:824:ASN:CB	2.44	0.48
1:A:439:PRO:HG2	1:A:468:GLU:OE1	2.13	0.48
1:A:126:THR:HG23	1:A:126:THR:O	2.14	0.48
1:A:885:PHE:CZ	1:A:1056:CYS:HB2	2.49	0.48
1:A:397:MET:HE2	1:A:470:PHE:HD2	1.77	0.48
1:A:509:PHE:CD2	1:A:624:LYS:HB3	2.48	0.48
1:A:8:LEU:HA	1:A:737:MET:SD	2.54	0.47
1:A:776:GLY:HA3	1:A:785:GLN:NE2	2.29	0.47
1:A:880:ASP:O	1:A:883:PRO:HD2	2.13	0.47
1:A:892:LEU:HD22	1:A:1017:LEU:HD11	1.96	0.47
1:A:133:ALA:CB	1:A:701:ARG:HG3	2.45	0.47
1:A:559:ASN:O	1:A:562:LYS:HB3	2.14	0.47
1:A:35:GLU:O	1:A:39:ILE:HG13	2.15	0.47
1:A:114:MET:HB2	1:A:117:GLU:HG2	1.95	0.47
1:A:992:TYR:CE2	1:A:996:LEU:HD11	2.50	0.47
1:A:377:GLU:HB2	1:A:378:PRO:HD3	1.97	0.47
1:A:449:LEU:HD22	1:A:573:VAL:CG1	2.45	0.47
1:A:1012:PRO:O	1:A:1016:LYS:HG3	2.15	0.47
1:A:699:GLU:OE1	1:A:700:LYS:HE3	2.15	0.47
1:A:790:SER:OG	1:A:791:LEU:HD23	2.15	0.47
1:A:808:PHE:O	1:A:812:VAL:HG23	2.14	0.47
1:A:860:MET:HA	1:A:860:MET:HE3	1.97	0.47
1:A:419:LYS:HE3	1:A:841:SER:HB2	1.97	0.47
1:A:539:ILE:CG2	1:A:562:LYS:HE3	2.45	0.47
1:A:708:ASP:O	1:A:712:ILE:HG13	2.14	0.47
1:A:161:LYS:HB3	1:A:165:ARG:NH1	2.30	0.47
1:A:368:ARG:O	1:A:372:VAL:HG23	2.15	0.46
1:A:534:PHE:HZ	1:A:599:ALA:HB1	1.81	0.46
1:A:165:ARG:HE	1:A:220:HIS:HA	1.79	0.46
1:A:108:ASP:HB2	1:A:113:LYS:NZ	2.31	0.46
1:A:114:MET:HE1	1:A:200:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:O	1:A:251:LEU:HG	2.16	0.46
1:A:794:GLN:O	1:A:849:LYS:HE2	2.14	0.46
1:A:878:LEU:HD22	1:A:1036:TYR:CD1	2.51	0.46
1:A:1028:ALA:HB3	1:A:1067:TRP:HD1	1.80	0.46
1:A:581:ILE:O	1:A:581:ILE:HG22	2.14	0.46
1:A:802:ILE:HG21	1:A:839:LEU:HD13	1.97	0.46
1:A:835:GLU:O	1:A:839:LEU:HG	2.15	0.46
1:A:34:LEU:O	1:A:37:ARG:HB2	2.15	0.46
1:A:283:GLN:CD	1:A:649:GLN:HG3	2.35	0.46
1:A:56:ARG:NH1	1:A:57:LYS:HD3	2.30	0.46
1:A:100:ALA:O	1:A:102:LEU:HD22	2.16	0.46
1:A:691:ALA:HB2	1:A:723:ARG:HB2	1.98	0.46
1:A:75:LEU:HD12	1:A:750:LEU:HD13	1.97	0.46
1:A:917:ARG:HD2	1:A:919:TYR:CE1	2.51	0.46
1:A:133:ALA:HB1	1:A:701:ARG:HG3	1.97	0.45
1:A:261:PHE:CD2	1:A:899:PHE:HB3	2.51	0.45
1:A:984:ASP:O	1:A:988:ILE:HG12	2.15	0.45
1:A:375:LEU:C	1:A:378:PRO:HD2	2.37	0.45
1:A:437:ILE:O	1:A:439:PRO:HD3	2.15	0.45
1:A:102:LEU:H	1:A:102:LEU:CD2	2.25	0.45
1:A:143:ASN:HD22	1:A:143:ASN:HA	1.56	0.45
1:A:147:PHE:O	1:A:151:LYS:HG2	2.17	0.45
1:A:622:ALA:N	1:A:638:GLN:O	2.50	0.45
1:A:415:ILE:HB	1:A:842:TYR:OH	2.15	0.45
1:A:542:LEU:HA	1:A:545:LEU:HD12	1.99	0.45
1:A:819:LEU:HD11	1:A:940:TYR:HB2	1.99	0.45
1:A:37:ARG:HH21	1:A:64:ASP:CG	2.20	0.44
1:A:439:PRO:HA	1:A:440:PRO:HD3	1.79	0.44
1:A:824:ASN:ND2	1:A:964:SER:O	2.50	0.44
1:A:1026:ILE:HA	1:A:1027:PRO:HD2	1.78	0.44
1:A:397:MET:O	1:A:400:ALA:HB3	2.17	0.44
1:A:897:GLN:OE1	1:A:897:GLN:N	2.43	0.44
1:A:49:SER:C	1:A:51:ASN:H	2.21	0.44
1:A:75:LEU:CD1	1:A:750:LEU:HD13	2.47	0.44
1:A:786:ARG:HD3	1:A:869:SER:HB2	2.00	0.44
1:A:924:ASP:HA	1:A:944:ILE:HB	2.00	0.44
1:A:1020:ILE:HG12	1:A:1056:CYS:HB3	1.99	0.44
1:A:473:GLN:O	1:A:477:VAL:HG23	2.17	0.44
1:A:111:ASN:O	1:A:113:LYS:N	2.48	0.44
1:A:495:SER:OG	1:A:496:GLN:N	2.51	0.44
1:A:922:GLU:HG3	1:A:991:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:HA	1:A:50:LYS:HG2	1.99	0.44
1:A:440:PRO:O	1:A:445:LYS:HB3	2.17	0.44
1:A:479:LYS:HD3	1:A:479:LYS:HA	1.86	0.44
1:A:831:ILE:O	1:A:835:GLU:HG2	2.18	0.44
1:A:264:ASN:ND2	1:A:268:GLU:HG3	2.32	0.43
1:A:129:LEU:HB2	1:A:201:TYR:CE2	2.53	0.43
1:A:1026:ILE:O	1:A:1026:ILE:HG13	2.17	0.43
1:A:129:LEU:HB2	1:A:201:TYR:HE2	1.83	0.43
1:A:534:PHE:CZ	1:A:599:ALA:HB1	2.53	0.43
1:A:872:ILE:HG22	1:A:1073:ILE:HA	2.00	0.43
1:A:50:LYS:O	1:A:50:LYS:HG3	2.19	0.43
1:A:473:GLN:OE1	1:A:595:GLN:HG2	2.18	0.43
1:A:990:GLU:HG3	1:A:1031:PHE:CE1	2.54	0.43
1:A:404:GLU:H	1:A:404:GLU:HG2	1.62	0.43
1:A:967:ILE:HD12	1:A:967:ILE:N	2.34	0.43
1:A:215:MET:HE3	1:A:731:PHE:HB2	2.01	0.43
1:A:385:LEU:HD13	1:A:939:VAL:HG23	2.00	0.43
1:A:577:ASP:OD1	1:A:582:LYS:HE2	2.18	0.43
1:A:784:ILE:HG13	1:A:788:PHE:CE2	2.54	0.43
1:A:263:THR:HG23	1:A:267:LEU:HA	1.99	0.43
1:A:387:ARG:NH1	1:A:387:ARG:HB3	2.34	0.43
1:A:520:ASP:HB3	1:A:667:LYS:HB3	2.01	0.43
1:A:791:LEU:HD21	1:A:860:MET:SD	2.59	0.43
1:A:821:PHE:N	1:A:821:PHE:HD2	2.17	0.43
1:A:512:ASN:N	1:A:512:ASN:HD22	2.17	0.42
1:A:22:VAL:CG2	1:A:77:TYR:HB3	2.49	0.42
1:A:101:ASP:OD1	1:A:101:ASP:C	2.56	0.42
1:A:804:ALA:HA	1:A:809:LYS:HE3	2.00	0.42
1:A:826:ILE:O	1:A:829:ARG:HG2	2.19	0.42
1:A:538:ILE:HD12	1:A:565:GLN:NE2	2.35	0.42
1:A:514:THR:HG22	1:A:638:GLN:HA	2.00	0.42
1:A:516:VAL:HG21	1:A:675:ILE:CG2	2.49	0.42
1:A:863:LYS:HA	1:A:864:PRO:HD3	1.70	0.42
1:A:288:LEU:HD12	1:A:288:LEU:O	2.19	0.42
1:A:454:VAL:HG22	1:A:455:PRO:N	2.35	0.42
1:A:821:PHE:N	1:A:821:PHE:CD2	2.86	0.42
1:A:499:GLN:OE1	1:A:680:ARG:NH1	2.44	0.42
1:A:165:ARG:HD3	1:A:223:TYR:CB	2.48	0.42
1:A:742:VAL:HG12	1:A:743:ALA:N	2.34	0.42
1:A:214:LEU:HA	1:A:217:VAL:HG23	2.01	0.42
1:A:73:SER:OG	1:A:750:LEU:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG23	1:A:196:MET:N	2.35	0.41
1:A:477:VAL:HG21	1:A:594:LYS:HG3	2.02	0.41
1:A:713:LEU:CD2	1:A:732:ILE:HG23	2.50	0.41
1:A:890:ALA:HB2	1:A:1053:SER:HB2	2.02	0.41
1:A:408:LEU:HD12	1:A:417:SER:HB3	2.02	0.41
1:A:799:ALA:HB2	1:A:845:ILE:HG23	2.02	0.41
1:A:1026:ILE:HD11	1:A:1067:TRP:CD1	2.55	0.41
1:A:549:THR:HG21	1:A:554:VAL:HG11	2.02	0.41
1:A:892:LEU:HD13	1:A:1017:LEU:HD21	2.03	0.41
1:A:151:LYS:HA	1:A:151:LYS:HD3	1.88	0.41
1:A:161:LYS:CB	1:A:165:ARG:HH12	2.33	0.41
1:A:179:LYS:HD3	1:A:180:TYR:CE2	2.56	0.41
1:A:542:LEU:HD11	1:A:561:TYR:HD2	1.86	0.41
1:A:441:VAL:HB	1:A:447:ILE:HD11	2.02	0.41
1:A:450:GLY:O	1:A:462:ILE:N	2.48	0.41
1:A:721:ARG:HH11	1:A:721:ARG:CG	2.34	0.41
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.92	0.41
1:A:517:LEU:HD23	1:A:517:LEU:C	2.41	0.41
1:A:729:ARG:HE	1:A:770:ASP:CG	2.23	0.41
1:A:864:PRO:HB2	1:A:865:VAL:H	1.53	0.41
1:A:899:PHE:C	1:A:901:PRO:HD3	2.41	0.41
1:A:951:ILE:HG13	1:A:985:LYS:HG2	2.03	0.41
1:A:11:TYR:HA	1:A:147:PHE:CE1	2.56	0.41
1:A:108:ASP:HB2	1:A:113:LYS:HZ1	1.85	0.40
1:A:541:GLY:O	1:A:545:LEU:HG	2.21	0.40
1:A:72:LEU:HD23	1:A:861:LEU:O	2.21	0.40
1:A:130:MET:SD	1:A:130:MET:C	2.99	0.40
1:A:385:LEU:CD1	1:A:939:VAL:HG23	2.51	0.40
1:A:125:TYR:CG	1:A:126:THR:N	2.88	0.40
1:A:287:GLU:O	1:A:291:MET:HG3	2.22	0.40
1:A:430:ASN:OD1	1:A:430:ASN:N	2.55	0.40
1:A:775:TYR:HD1	1:A:875:ASN:OD1	2.04	0.40
1:A:884:PHE:CD1	1:A:1059:PRO:HD3	2.56	0.40
1:A:281:PRO:HG2	1:A:284:THR:OG1	2.21	0.40
1:A:318:LYS:HB2	1:A:318:LYS:NZ	2.37	0.40
1:A:185:HIS:CD2	1:A:185:HIS:H	2.38	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	1066/1095 (97%)	988 (93%)	64 (6%)	14 (1%)	12	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	MET
1	A	825	ASN
1	A	864	PRO
1	A	978	SER
1	A	382	ASP
1	A	495	SER
1	A	776	GLY
1	A	128	SER
1	A	430	ASN
1	A	870	SER
1	A	94	LYS
1	A	865	VAL
1	A	439	PRO
1	A	1027	PRO

### 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	973/996 (98%)	936 (96%)	37 (4%)	33	67

All (37) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	48	ASN
1	A	102	LEU
1	A	104	VAL
1	A	121	THR
1	A	130	MET
1	A	143	ASN
1	A	155	ASP
1	A	156	VAL
1	A	186	ASN
1	A	194	ASP
1	A	229	LEU
1	A	313	ASP
1	A	358	GLU
1	A	401	SER
1	A	503	TYR
1	A	508	ARG
1	A	512	ASN
1	A	518	TYR
1	A	556	GLN
1	A	595	GLN
1	A	600	ASN
1	A	619	HIS
1	A	645	LYS
1	A	654	ASP
1	A	695	LEU
1	A	721	ARG
1	A	791	LEU
1	A	820	LEU
1	A	850	ARG
1	A	859	THR
1	A	892	LEU
1	A	895	GLN
1	A	922	GLU
1	A	931	SER
1	A	932	ARG
1	A	1050	SER
1	A	1056	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	42	HIS

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Mol	Chain	Res	Type
1	A	48	ASN
1	A	83	ASN
1	A	143	ASN
1	A	185	HIS
1	A	186	ASN
1	A	290	GLN
1	A	294	ASN
1	A	308	GLN
1	A	384	HIS
1	A	423	HIS
1	A	473	GLN
1	A	512	ASN
1	A	528	GLN
1	A	556	GLN
1	A	563	GLN
1	A	565	GLN
1	A	574	GLN
1	A	653	ASN
1	A	698	ASN
1	A	760	ASN
1	A	794	GLN
1	A	810	ASN
1	A	824	ASN
1	A	840	ASN
1	A	853	GLN
1	A	862	GLN
1	A	895	GLN
1	A	912	GLN
1	A	1057	ASN
1	A	1087	GLN

### 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 [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1072/1095 (97%)	0.02	42 (3%) 39 35	16, 53, 97, 147	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	866	THR	7.5
1	A	1023	LYS	4.5
1	A	79	TYR	4.4
1	A	847	LEU	4.2
1	A	399	SER	4.1
1	A	844	PRO	4.1
1	A	408	LEU	4.0
1	A	1025	LYS	3.7
1	A	867	PHE	3.5
1	A	841	SER	3.5
1	A	845	ILE	3.2
1	A	398	SER	3.1
1	A	852	ALA	3.0
1	A	824	ASN	3.0
1	A	209	SER	2.9
1	A	842	TYR	2.9
1	A	528	GLN	2.8
1	A	1024	GLY	2.7
1	A	77	TYR	2.7
1	A	210	SER	2.6
1	A	28	TYR	2.6
1	A	414	THR	2.6
1	A	840	ASN	2.5
1	A	795	LYS	2.5
1	A	157	ALA	2.5
1	A	848	GLU	2.4
1	A	797	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	865	VAL	2.4
1	A	1086	PHE	2.4
1	A	431	GLU	2.3
1	A	861	LEU	2.3
1	A	82	TYR	2.3
1	A	843	ALA	2.2
1	A	550	ASN	2.2
1	A	971	ASP	2.1
1	A	206	TRP	2.1
1	A	496	GLN	2.0
1	A	1085	PHE	2.0
1	A	2	GLY	2.0
1	A	141	ASN	2.0
1	A	776	GLY	2.0
1	A	344	LEU	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 monosaccharides 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.