



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:04 PM GMT

PDB ID : 1DZL
Title : L1 PROTEIN OF HUMAN PAPILLOMAVIRUS 16
Authors : Chen, X.J.; Garcea, B.; Goldberge, I.; Harrison, S.C.
Deposited on : 2000-03-01
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

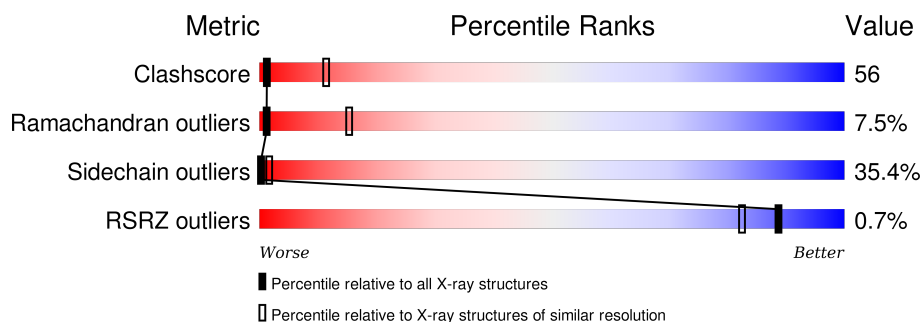
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3578 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 LATE MAJOR CAPSID PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3578	2281	600	676	21			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLN	ASN	CONFLICT	UNP Q9WPH4
A	181	GLN	ASN	CONFLICT	UNP Q9WPH4
A	258	ARG	GLY	CONFLICT	UNP Q9WPH4
A	266	THR	ALA	CONFLICT	UNP Q9WPH4
A	472	LEU	ALA	ENGINEERED	UNP Q9WPH4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	387.00Å 387.00Å 387.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50 29.86 – 3.51	Depositor EDS
% Data completeness (in resolution range)	89.0 (15.00-3.50) 75.0 (29.86-3.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.56Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.280 , 0.290 0.371 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	91.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 33.0	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 202236 reflections	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	3578	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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](#)

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	0.43	0/3674	0.60	0/5002

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 [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	3578	0	3478	392	0
All	All	3578	0	3478	392	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 56.

All (392) 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:54:LYS:HB3	1:A:57:ASN:HB3	1.45	0.96
1:A:378:LEU:HD12	1:A:379:CYS:H	1.31	0.95
1:A:156:LEU:HG	1:A:334:VAL:HB	1.50	0.93
1:A:39:THR:HG23	1:A:372:LEU:H	1.32	0.92
1:A:71:ARG:HH11	1:A:71:ARG:HA	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG23	1:A:304:ALA:HB2	1.53	0.89
1:A:121:PRO:HD3	1:A:222:LEU:HD21	1.57	0.84
1:A:329:LEU:HD23	1:A:330:PHE:H	1.44	0.82
1:A:29:ALA:HB3	1:A:380:LYS:HG3	1.59	0.82
1:A:258:ARG:HB3	1:A:294:THR:HB	1.63	0.81
1:A:165:ILE:H	1:A:237:MET:HE1	1.44	0.81
1:A:151:TYR:CD1	1:A:203:THR:HB	2.16	0.81
1:A:432:THR:C	1:A:434:PRO:HD3	2.04	0.78
1:A:119:GLY:O	1:A:222:LEU:HD22	1.83	0.78
1:A:156:LEU:HD12	1:A:156:LEU:C	2.05	0.78
1:A:344:LEU:H	1:A:344:LEU:HD23	1.48	0.77
1:A:130:GLU:HB2	1:A:260:LEU:HD13	1.66	0.77
1:A:75:ILE:H	1:A:75:ILE:HD12	1.50	0.77
1:A:30:ARG:HB3	1:A:377:GLN:NE2	1.99	0.76
1:A:24:THR:HG23	1:A:320:ASN:HA	1.67	0.76
1:A:75:ILE:HD13	1:A:329:LEU:HB3	1.68	0.76
1:A:378:LEU:HD12	1:A:379:CYS:N	2.00	0.76
1:A:75:ILE:HD11	1:A:331:VAL:HG23	1.68	0.75
1:A:96:GLN:NE2	1:A:382:THR:HG23	2.01	0.75
1:A:39:THR:CG2	1:A:372:LEU:H	2.00	0.74
1:A:111:GLN:NE2	1:A:111:GLN:HA	2.03	0.74
1:A:121:PRO:HA	1:A:146:CYS:SG	2.27	0.73
1:A:273:ASP:HA	1:A:276:TYR:CE1	2.23	0.73
1:A:53:LYS:HD3	1:A:58:ASN:HA	1.69	0.73
1:A:168:HIS:O	1:A:191:ILE:HD12	1.89	0.73
1:A:65:VAL:HA	1:A:69:GLN:HE22	1.54	0.72
1:A:222:LEU:H	1:A:222:LEU:HD22	1.54	0.72
1:A:384:THR:HG23	1:A:387:VAL:HG21	1.71	0.72
1:A:387:VAL:O	1:A:391:ILE:HD12	1.90	0.72
1:A:302:SER:O	1:A:305:GLN:HB2	1.89	0.72
1:A:374:PHE:HB2	1:A:376:PHE:CE1	2.25	0.72
1:A:260:LEU:N	1:A:260:LEU:HD12	2.03	0.72
1:A:106:GLU:HG2	1:A:310:PRO:HA	1.74	0.70
1:A:374:PHE:CD1	1:A:374:PHE:N	2.60	0.70
1:A:149:MET:HE2	1:A:295:PRO:HD2	1.73	0.70
1:A:280:SER:H	1:A:284:ALA:N	1.90	0.69
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.73	0.69
1:A:31:THR:HG23	1:A:378:LEU:O	1.91	0.69
1:A:66:SER:H	1:A:69:GLN:NE2	1.91	0.69
1:A:220:VAL:HB	1:A:224:ILE:HD11	1.74	0.69
1:A:65:VAL:HA	1:A:69:GLN:NE2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:OD1	1:A:236:LYS:HB2	1.94	0.67
1:A:152:LYS:HB2	1:A:255:MET:HB2	1.75	0.67
1:A:165:ILE:N	1:A:237:MET:HE1	2.08	0.67
1:A:214:GLN:OE1	1:A:219:GLU:HB2	1.94	0.67
1:A:305:GLN:HA	1:A:305:GLN:NE2	2.08	0.67
1:A:52:ILE:HB	1:A:62:VAL:HB	1.77	0.66
1:A:368:GLU:HG3	1:A:370:TYR:HE1	1.59	0.66
1:A:270:ASN:HD22	1:A:271:VAL:H	1.44	0.66
1:A:159:ILE:HA	1:A:330:PHE:O	1.96	0.65
1:A:92:ASN:O	1:A:96:GLN:HG2	1.96	0.65
1:A:439:ASP:OD1	1:A:441:LEU:HD12	1.95	0.65
1:A:432:THR:O	1:A:434:PRO:HD3	1.96	0.65
1:A:431:HIS:C	1:A:433:PRO:HD3	2.17	0.65
1:A:164:PRO:C	1:A:195:ILE:HD12	2.18	0.64
1:A:121:PRO:C	1:A:122:LEU:HD23	2.17	0.64
1:A:49:TYR:O	1:A:64:LYS:HE2	1.96	0.64
1:A:120:HIS:CE1	1:A:122:LEU:H	2.15	0.64
1:A:470:LEU:HD23	1:A:471:GLN:N	2.13	0.64
1:A:72:VAL:HG23	1:A:197:ASP:HA	1.80	0.64
1:A:155:GLN:HG2	1:A:307:PHE:CE2	2.33	0.64
1:A:152:LYS:HB2	1:A:255:MET:CB	2.28	0.63
1:A:413:THR:HG22	1:A:415:GLU:H	1.63	0.63
1:A:154:THR:O	1:A:336:THR:HG23	1.98	0.63
1:A:54:LYS:HB3	1:A:57:ASN:CB	2.26	0.63
1:A:150:ASP:O	1:A:296:SER:HA	1.97	0.63
1:A:47:HIS:HB3	1:A:50:PHE:O	1.98	0.63
1:A:301:THR:HG23	1:A:304:ALA:CB	2.28	0.62
1:A:123:LEU:HD11	1:A:220:VAL:N	2.14	0.62
1:A:124:ASN:HB3	1:A:263:ARG:HH11	1.64	0.62
1:A:24:THR:CG2	1:A:320:ASN:HA	2.29	0.62
1:A:417:THR:O	1:A:420:PHE:HB3	1.99	0.62
1:A:157:CYS:HA	1:A:332:THR:O	1.99	0.62
1:A:170:GLY:N	1:A:191:ILE:HD11	2.14	0.62
1:A:221:PRO:O	1:A:224:ILE:HG12	2.00	0.62
1:A:165:ILE:N	1:A:165:ILE:HD12	2.15	0.62
1:A:72:VAL:HG13	1:A:332:THR:HG23	1.82	0.62
1:A:75:ILE:CD1	1:A:331:VAL:HG23	2.30	0.62
1:A:79:ASP:HB3	1:A:82:LYS:HB2	1.82	0.61
1:A:237:MET:O	1:A:240:GLU:HB2	2.00	0.61
1:A:121:PRO:O	1:A:122:LEU:HD23	2.01	0.61
1:A:221:PRO:HD2	1:A:224:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:HIS:HE1	1:A:49:TYR:HB2	1.65	0.61
1:A:246:LEU:O	1:A:246:LEU:HG	2.00	0.61
1:A:154:THR:H	1:A:336:THR:CG2	2.13	0.61
1:A:259:HIS:HB2	1:A:294:THR:OG1	2.01	0.61
1:A:85:PHE:HB3	1:A:86:PRO:HD2	1.82	0.61
1:A:180:VAL:HG12	1:A:184:ASP:HB2	1.83	0.60
1:A:333:VAL:HG12	1:A:334:VAL:N	2.16	0.60
1:A:424:GLN:HE21	1:A:425:ALA:N	1.98	0.60
1:A:235:ILE:O	1:A:238:VAL:HG23	2.02	0.60
1:A:39:THR:HG23	1:A:372:LEU:N	2.11	0.60
1:A:86:PRO:HG2	1:A:87:ASP:H	1.67	0.60
1:A:272:PRO:O	1:A:275:LEU:HG	2.01	0.60
1:A:158:LEU:C	1:A:159:ILE:HD13	2.21	0.59
1:A:154:THR:HG23	1:A:253:GLU:HB3	1.83	0.59
1:A:395:ASN:HD22	1:A:395:ASN:C	2.06	0.59
1:A:384:THR:OG1	1:A:387:VAL:HG23	2.02	0.59
1:A:235:ILE:N	1:A:235:ILE:HD12	2.18	0.59
1:A:329:LEU:HD23	1:A:330:PHE:N	2.16	0.59
1:A:417:THR:O	1:A:421:VAL:HG23	2.03	0.58
1:A:149:MET:CE	1:A:295:PRO:HD2	2.33	0.58
1:A:164:PRO:HG3	1:A:332:THR:HG21	1.86	0.58
1:A:103:VAL:HG23	1:A:375:ILE:HG22	1.85	0.58
1:A:196:GLN:HG2	1:A:445:THR:O	2.04	0.58
1:A:395:ASN:ND2	1:A:395:ASN:C	2.56	0.58
1:A:356:LYS:HB2	1:A:359:ASN:HB2	1.86	0.58
1:A:147:ILE:HG22	1:A:148:SER:H	1.67	0.58
1:A:47:HIS:CE1	1:A:49:TYR:HB2	2.39	0.58
1:A:21:VAL:HG12	1:A:22:VAL:N	2.19	0.57
1:A:123:LEU:HB3	1:A:147:ILE:HD13	1.87	0.57
1:A:210:PHE:HE2	1:A:229:CYS:HB2	1.68	0.57
1:A:165:ILE:H	1:A:237:MET:CE	2.14	0.57
1:A:209:ASP:HA	1:A:228:ILE:HG13	1.86	0.57
1:A:329:LEU:CD2	1:A:330:PHE:H	2.16	0.57
1:A:24:THR:HG21	1:A:323:ILE:CG1	2.35	0.57
1:A:209:ASP:HA	1:A:228:ILE:CG1	2.35	0.57
1:A:147:ILE:HD12	1:A:147:ILE:N	2.20	0.56
1:A:344:LEU:N	1:A:344:LEU:HD23	2.19	0.56
1:A:156:LEU:CG	1:A:334:VAL:HB	2.31	0.56
1:A:120:HIS:HA	1:A:222:LEU:HD21	1.86	0.56
1:A:222:LEU:HA	1:A:225:CYS:HB2	1.86	0.56
1:A:299:MET:HG2	1:A:300:VAL:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:CD1	1:A:232:PRO:HD2	2.41	0.56
1:A:54:LYS:HZ2	1:A:54:LYS:HA	1.70	0.56
1:A:154:THR:H	1:A:336:THR:HG21	1.71	0.56
1:A:102:CYS:SG	1:A:313:LEU:HD11	2.47	0.55
1:A:222:LEU:O	1:A:224:ILE:N	2.39	0.55
1:A:96:GLN:HE22	1:A:382:THR:HG23	1.70	0.55
1:A:323:ILE:N	1:A:323:ILE:HD13	2.21	0.55
1:A:197:ASP:HB3	1:A:446:PHE:HA	1.87	0.55
1:A:120:HIS:HB3	1:A:123:LEU:HD13	1.88	0.55
1:A:49:TYR:HA	1:A:223:ASP:HB3	1.89	0.55
1:A:71:ARG:HH12	1:A:198:GLY:H	1.55	0.54
1:A:211:THR:HG23	1:A:226:THR:HA	1.89	0.54
1:A:71:ARG:HA	1:A:71:ARG:NH1	2.15	0.54
1:A:24:THR:HG21	1:A:323:ILE:HG12	1.89	0.54
1:A:280:SER:O	1:A:283:THR:HG23	2.07	0.54
1:A:100:TRP:HA	1:A:100:TRP:CE3	2.41	0.54
1:A:341:ASN:HD22	1:A:366:HIS:HB2	1.72	0.54
1:A:172:GLY:O	1:A:187:PRO:HG2	2.08	0.54
1:A:71:ARG:HH12	1:A:198:GLY:N	2.05	0.54
1:A:125:LYS:NZ	1:A:127:ASP:HA	2.23	0.54
1:A:42:LEU:HD23	1:A:42:LEU:N	2.23	0.53
1:A:105:VAL:HG13	1:A:374:PHE:CD2	2.44	0.53
1:A:128:ASP:OD1	1:A:130:GLU:HB3	2.08	0.53
1:A:168:HIS:CE1	1:A:191:ILE:HB	2.43	0.53
1:A:54:LYS:HZ1	1:A:55:PRO:HD2	1.72	0.53
1:A:69:GLN:HB3	1:A:198:GLY:HA2	1.89	0.53
1:A:60:ILE:HD13	1:A:60:ILE:N	2.24	0.53
1:A:396:SER:O	1:A:399:LEU:HD12	2.09	0.53
1:A:168:HIS:O	1:A:190:LEU:HD12	2.09	0.53
1:A:413:THR:O	1:A:417:THR:HG23	2.09	0.52
1:A:372:LEU:O	1:A:373:GLN:HG3	2.10	0.52
1:A:391:ILE:O	1:A:394:MET:HB3	2.09	0.52
1:A:151:TYR:CG	1:A:203:THR:HB	2.44	0.52
1:A:156:LEU:CD1	1:A:156:LEU:C	2.74	0.52
1:A:241:PRO:HG2	1:A:242:TYR:H	1.74	0.52
1:A:49:TYR:O	1:A:223:ASP:HA	2.10	0.52
1:A:80:PRO:HB2	1:A:98:LEU:HB2	1.91	0.51
1:A:164:PRO:HB2	1:A:195:ILE:HD13	1.92	0.51
1:A:126:LEU:HD22	1:A:264:ALA:HA	1.92	0.51
1:A:247:PHE:CE2	1:A:322:GLY:HA2	2.46	0.51
1:A:156:LEU:HD12	1:A:157:CYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LYS:HZ2	1:A:127:ASP:HA	1.75	0.51
1:A:307:PHE:O	1:A:308:ASN:HB2	2.10	0.51
1:A:423:SER:O	1:A:426:ILE:HG13	2.10	0.51
1:A:36:HIS:C	1:A:36:HIS:ND1	2.64	0.51
1:A:290:ASN:N	1:A:290:ASN:HD22	2.08	0.51
1:A:50:PHE:HB2	1:A:51:PRO:HD2	1.93	0.51
1:A:237:MET:HB3	1:A:246:LEU:HD23	1.93	0.51
1:A:280:SER:N	1:A:284:ALA:HA	2.25	0.51
1:A:250:LEU:HD12	1:A:250:LEU:N	2.26	0.51
1:A:210:PHE:CE2	1:A:229:CYS:HB2	2.46	0.51
1:A:54:LYS:NZ	1:A:55:PRO:HD2	2.26	0.50
1:A:120:HIS:ND1	1:A:121:PRO:HD2	2.25	0.50
1:A:88:THR:HA	1:A:90:PHE:CE1	2.46	0.50
1:A:106:GLU:HG2	1:A:310:PRO:CA	2.40	0.50
1:A:74:ARG:HH21	1:A:441:LEU:HD13	1.76	0.50
1:A:27:TYR:N	1:A:27:TYR:CD1	2.79	0.50
1:A:120:HIS:HA	1:A:222:LEU:CD2	2.42	0.50
1:A:255:MET:HG2	1:A:256:PHE:N	2.27	0.50
1:A:335:ASP:C	1:A:335:ASP:OD1	2.49	0.50
1:A:468:PHE:O	1:A:471:GLN:HB3	2.12	0.49
1:A:121:PRO:CD	1:A:222:LEU:HD21	2.35	0.49
1:A:348:ILE:HG22	1:A:359:ASN:OD1	2.12	0.49
1:A:439:ASP:OD2	1:A:442:LYS:HA	2.13	0.49
1:A:368:GLU:HG3	1:A:370:TYR:CE1	2.46	0.49
1:A:43:LEU:CD1	1:A:369:GLU:HA	2.42	0.49
1:A:123:LEU:HD11	1:A:220:VAL:CA	2.43	0.49
1:A:151:TYR:OH	1:A:221:PRO:HB2	2.13	0.49
1:A:262:ASN:HD22	1:A:263:ARG:H	1.59	0.49
1:A:166:GLY:N	1:A:195:ILE:HD11	2.28	0.48
1:A:181:GLN:O	1:A:184:ASP:HB2	2.13	0.48
1:A:240:GLU:HB3	1:A:243:GLY:HA2	1.94	0.48
1:A:197:ASP:CB	1:A:446:PHE:HA	2.43	0.48
1:A:416:ASP:O	1:A:417:THR:C	2.51	0.48
1:A:79:ASP:OD1	1:A:81:ASN:N	2.46	0.48
1:A:81:ASN:OD1	1:A:97:ARG:HD3	2.14	0.48
1:A:387:VAL:O	1:A:388:MET:C	2.52	0.48
1:A:160:GLY:HA2	1:A:247:PHE:CZ	2.48	0.48
1:A:216:ASN:OD1	1:A:219:GLU:HG2	2.13	0.48
1:A:323:ILE:O	1:A:325:TRP:N	2.46	0.48
1:A:233:ASP:O	1:A:234:TYR:C	2.52	0.48
1:A:234:TYR:O	1:A:235:ILE:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HB2	1:A:195:ILE:CD1	2.43	0.48
1:A:262:ASN:HD22	1:A:263:ARG:N	2.11	0.48
1:A:36:HIS:CG	1:A:37:ALA:N	2.82	0.48
1:A:169:TRP:HB2	1:A:208:MET:HB3	1.94	0.48
1:A:123:LEU:HD11	1:A:219:GLU:C	2.34	0.47
1:A:387:VAL:HG12	1:A:391:ILE:CD1	2.44	0.47
1:A:74:ARG:HH22	1:A:439:ASP:CG	2.18	0.47
1:A:465:GLY:O	1:A:466:ARG:C	2.51	0.47
1:A:24:THR:HA	1:A:27:TYR:CZ	2.49	0.47
1:A:255:MET:CG	1:A:256:PHE:N	2.76	0.47
1:A:388:MET:O	1:A:389:THR:C	2.53	0.47
1:A:396:SER:O	1:A:397:THR:C	2.52	0.47
1:A:235:ILE:HD12	1:A:235:ILE:H	1.79	0.47
1:A:413:THR:HG22	1:A:415:GLU:N	2.30	0.47
1:A:33:ILE:N	1:A:33:ILE:HD13	2.29	0.47
1:A:165:ILE:N	1:A:195:ILE:HD12	2.29	0.47
1:A:375:ILE:HD12	1:A:464:LEU:HD13	1.97	0.47
1:A:387:VAL:HG12	1:A:391:ILE:HD11	1.97	0.47
1:A:52:ILE:O	1:A:52:ILE:HG22	2.13	0.47
1:A:181:GLN:O	1:A:182:PRO:C	2.51	0.47
1:A:156:LEU:HD12	1:A:156:LEU:O	2.15	0.47
1:A:43:LEU:HD12	1:A:368:GLU:O	2.14	0.47
1:A:437:LYS:CD	1:A:437:LYS:H	2.26	0.47
1:A:419:ARG:CB	1:A:419:ARG:HH11	2.28	0.47
1:A:68:LEU:O	1:A:201:VAL:HG23	2.14	0.47
1:A:373:GLN:HB3	1:A:464:LEU:HD12	1.95	0.47
1:A:191:ILE:HD12	1:A:191:ILE:N	2.30	0.47
1:A:28:VAL:HA	1:A:381:ILE:HG12	1.97	0.46
1:A:424:GLN:O	1:A:427:ALA:HB3	2.14	0.46
1:A:375:ILE:CD1	1:A:464:LEU:HD13	2.46	0.46
1:A:119:GLY:O	1:A:221:PRO:HA	2.14	0.46
1:A:124:ASN:OD1	1:A:264:ALA:HB3	2.16	0.46
1:A:312:TRP:CH2	1:A:468:PHE:HB2	2.51	0.46
1:A:79:ASP:HA	1:A:327:ASN:ND2	2.30	0.46
1:A:144:ARG:C	1:A:145:GLU:HG2	2.35	0.46
1:A:70:TYR:CD2	1:A:201:VAL:HG22	2.50	0.46
1:A:109:ARG:HA	1:A:109:ARG:HD2	1.54	0.46
1:A:123:LEU:O	1:A:125:LYS:N	2.43	0.46
1:A:397:THR:OG1	1:A:398:ILE:N	2.49	0.46
1:A:307:PHE:O	1:A:309:LYS:HG3	2.14	0.46
1:A:75:ILE:HD12	1:A:329:LEU:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:C	1:A:195:ILE:HD11	2.36	0.46
1:A:104:GLY:O	1:A:374:PHE:HA	2.16	0.46
1:A:385:ALA:O	1:A:386:ASP:C	2.54	0.46
1:A:155:GLN:OE1	1:A:306:ILE:HB	2.15	0.46
1:A:98:LEU:HA	1:A:379:CYS:O	2.16	0.45
1:A:111:GLN:NE2	1:A:111:GLN:CA	2.78	0.45
1:A:101:ALA:HA	1:A:322:GLY:O	2.16	0.45
1:A:329:LEU:CD2	1:A:330:PHE:N	2.77	0.45
1:A:24:THR:O	1:A:28:VAL:HG23	2.16	0.45
1:A:336:THR:O	1:A:338:ARG:N	2.50	0.45
1:A:371:ASP:C	1:A:372:LEU:HD23	2.37	0.45
1:A:431:HIS:O	1:A:433:PRO:HD3	2.15	0.45
1:A:58:ASN:O	1:A:60:ILE:HD13	2.17	0.45
1:A:375:ILE:HD13	1:A:464:LEU:HD22	1.99	0.45
1:A:273:ASP:C	1:A:275:LEU:H	2.19	0.45
1:A:80:PRO:HB2	1:A:98:LEU:CB	2.46	0.45
1:A:120:HIS:ND1	1:A:121:PRO:N	2.64	0.45
1:A:57:ASN:CG	1:A:58:ASN:H	2.20	0.45
1:A:49:TYR:OH	1:A:118:SER:HA	2.17	0.45
1:A:30:ARG:HB3	1:A:377:GLN:HE21	1.79	0.45
1:A:431:HIS:N	1:A:431:HIS:ND1	2.64	0.45
1:A:75:ILE:CD1	1:A:329:LEU:HB3	2.43	0.45
1:A:397:THR:O	1:A:398:ILE:C	2.55	0.45
1:A:155:GLN:OE1	1:A:306:ILE:N	2.50	0.45
1:A:381:ILE:O	1:A:383:LEU:HG	2.18	0.44
1:A:283:THR:O	1:A:284:ALA:C	2.55	0.44
1:A:150:ASP:N	1:A:150:ASP:OD1	2.50	0.44
1:A:75:ILE:HB	1:A:329:LEU:HB3	1.99	0.44
1:A:383:LEU:HB3	1:A:388:MET:CE	2.47	0.44
1:A:235:ILE:CD1	1:A:235:ILE:N	2.79	0.44
1:A:88:THR:HA	1:A:90:PHE:HE1	1.82	0.44
1:A:468:PHE:O	1:A:469:LEU:C	2.56	0.44
1:A:109:ARG:HB3	1:A:338:ARG:CZ	2.48	0.44
1:A:98:LEU:HB3	1:A:378:LEU:HD11	1.99	0.44
1:A:42:LEU:O	1:A:43:LEU:HD13	2.17	0.44
1:A:387:VAL:C	1:A:391:ILE:HD12	2.37	0.44
1:A:351:SER:HB2	1:A:352:GLU:H	1.45	0.44
1:A:415:GLU:O	1:A:418:TYR:HB3	2.17	0.44
1:A:108:GLY:N	1:A:371:ASP:O	2.46	0.44
1:A:335:ASP:OD1	1:A:337:THR:HG23	2.18	0.44
1:A:24:THR:HG21	1:A:323:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HD12	1:A:277:ILE:N	2.32	0.44
1:A:191:ILE:HD12	1:A:191:ILE:H	1.81	0.44
1:A:305:GLN:CA	1:A:305:GLN:NE2	2.78	0.44
1:A:471:GLN:OE1	1:A:472:LEU:N	2.51	0.44
1:A:120:HIS:HB2	1:A:221:PRO:HA	2.00	0.43
1:A:120:HIS:ND1	1:A:120:HIS:C	2.71	0.43
1:A:381:ILE:HG22	1:A:383:LEU:HD23	2.00	0.43
1:A:91:TYR:HD2	1:A:96:GLN:HG3	1.84	0.43
1:A:96:GLN:HB3	1:A:382:THR:HA	2.00	0.43
1:A:124:ASN:HB3	1:A:263:ARG:NH1	2.30	0.43
1:A:155:GLN:HG2	1:A:307:PHE:HE2	1.83	0.43
1:A:451:LEU:O	1:A:453:GLU:N	2.51	0.43
1:A:120:HIS:CD2	1:A:218:SER:HA	2.53	0.43
1:A:178:VAL:O	1:A:180:VAL:N	2.50	0.43
1:A:276:TYR:C	1:A:277:ILE:HD12	2.39	0.43
1:A:307:PHE:HA	1:A:311:TYR:OH	2.19	0.43
1:A:351:SER:O	1:A:352:GLU:O	2.36	0.43
1:A:103:VAL:O	1:A:313:LEU:HG	2.18	0.43
1:A:89:SER:O	1:A:91:TYR:N	2.52	0.43
1:A:222:LEU:C	1:A:224:ILE:N	2.72	0.43
1:A:259:HIS:C	1:A:260:LEU:HD12	2.39	0.43
1:A:111:GLN:HE21	1:A:111:GLN:HA	1.80	0.43
1:A:235:ILE:CD1	1:A:235:ILE:H	2.30	0.43
1:A:135:TYR:CE2	1:A:287:ALA:HB2	2.53	0.43
1:A:43:LEU:HD12	1:A:369:GLU:HA	2.01	0.42
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.53	0.42
1:A:175:CYS:HB3	1:A:177:GLN:NE2	2.34	0.42
1:A:159:ILE:CG2	1:A:331:VAL:HG22	2.49	0.42
1:A:70:TYR:CE2	1:A:201:VAL:HA	2.53	0.42
1:A:233:ASP:O	1:A:233:ASP:OD1	2.36	0.42
1:A:306:ILE:HD12	1:A:306:ILE:HA	1.81	0.42
1:A:124:ASN:N	1:A:218:SER:O	2.44	0.42
1:A:26:GLU:HA	1:A:26:GLU:OE1	2.19	0.42
1:A:70:TYR:O	1:A:71:ARG:NH1	2.52	0.42
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.82	0.42
1:A:99:VAL:HG21	1:A:381:ILE:HD12	2.02	0.42
1:A:386:ASP:OD1	1:A:386:ASP:N	2.53	0.42
1:A:417:THR:OG1	1:A:418:TYR:N	2.52	0.42
1:A:86:PRO:CG	1:A:87:ASP:H	2.33	0.42
1:A:157:CYS:SG	1:A:158:LEU:N	2.92	0.42
1:A:280:SER:N	1:A:284:ALA:CA	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASP:OD1	1:A:212:THR:HG23	2.19	0.42
1:A:399:LEU:O	1:A:400:GLU:C	2.58	0.42
1:A:117:ILE:HG13	1:A:149:MET:O	2.20	0.42
1:A:413:THR:O	1:A:414:LEU:C	2.58	0.42
1:A:458:ASP:N	1:A:458:ASP:OD1	2.49	0.42
1:A:120:HIS:ND1	1:A:121:PRO:CD	2.83	0.42
1:A:147:ILE:HG22	1:A:148:SER:N	2.34	0.42
1:A:115:VAL:HA	1:A:339:SER:OG	2.19	0.42
1:A:71:ARG:NH1	1:A:197:ASP:OD1	2.52	0.42
1:A:170:GLY:HA2	1:A:213:LEU:HD21	2.01	0.42
1:A:466:ARG:O	1:A:467:LYS:C	2.58	0.42
1:A:333:VAL:HG12	1:A:334:VAL:H	1.84	0.42
1:A:66:SER:N	1:A:69:GLN:NE2	2.64	0.42
1:A:110:GLY:HA3	1:A:369:GLU:CD	2.40	0.42
1:A:119:GLY:HA3	1:A:148:SER:HA	2.01	0.42
1:A:60:ILE:N	1:A:60:ILE:CD1	2.83	0.41
1:A:384:THR:O	1:A:387:VAL:HB	2.20	0.41
1:A:351:SER:O	1:A:352:GLU:C	2.58	0.41
1:A:446:PHE:CD1	1:A:446:PHE:N	2.87	0.41
1:A:180:VAL:HG12	1:A:184:ASP:CB	2.49	0.41
1:A:348:ILE:CG2	1:A:359:ASN:OD1	2.68	0.41
1:A:459:LEU:H	1:A:459:LEU:HG	1.49	0.41
1:A:43:LEU:HA	1:A:43:LEU:HD12	1.72	0.41
1:A:233:ASP:CG	1:A:236:LYS:HB2	2.41	0.41
1:A:162:LYS:C	1:A:330:PHE:CD2	2.94	0.41
1:A:270:ASN:HD22	1:A:271:VAL:N	2.13	0.41
1:A:439:ASP:C	1:A:439:ASP:OD1	2.58	0.41
1:A:420:PHE:O	1:A:421:VAL:C	2.58	0.41
1:A:108:GLY:O	1:A:370:TYR:HA	2.20	0.41
1:A:193:THR:HG21	1:A:230:LYS:HD3	2.03	0.41
1:A:71:ARG:HD3	1:A:71:ARG:HA	1.85	0.41
1:A:242:TYR:CZ	1:A:394:MET:HA	2.56	0.41
1:A:333:VAL:CG1	1:A:334:VAL:N	2.82	0.41
1:A:196:GLN:OE1	1:A:444:TYR:HA	2.21	0.41
1:A:292:PHE:HA	1:A:293:PRO:HD3	1.88	0.41
1:A:119:GLY:HA3	1:A:147:ILE:O	2.21	0.41
1:A:222:LEU:C	1:A:224:ILE:H	2.24	0.41
1:A:386:ASP:O	1:A:387:VAL:C	2.58	0.41
1:A:388:MET:HG3	1:A:399:LEU:CD2	2.51	0.41
1:A:280:SER:N	1:A:283:THR:OG1	2.54	0.41
1:A:419:ARG:HB2	1:A:419:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.85	0.41
1:A:168:HIS:CE1	1:A:191:ILE:HD13	2.56	0.41
1:A:75:ILE:HD11	1:A:331:VAL:H	1.86	0.40
1:A:467:LYS:O	1:A:468:PHE:C	2.60	0.40
1:A:42:LEU:HD13	1:A:447:TRP:CZ2	2.57	0.40
1:A:236:LYS:HA	1:A:239:SER:OG	2.22	0.40
1:A:307:PHE:CE2	1:A:335:ASP:HB2	2.56	0.40
1:A:41:ARG:HD3	1:A:43:LEU:HD22	2.03	0.40
1:A:300:VAL:HG11	1:A:337:THR:HA	2.03	0.40
1:A:418:TYR:O	1:A:419:ARG:C	2.60	0.40
1:A:56:ASN:H	1:A:56:ASN:ND2	2.19	0.40
1:A:47:HIS:O	1:A:64:LYS:HA	2.21	0.40
1:A:77:LEU:HB2	1:A:327:ASN:HB3	2.03	0.40
1:A:424:GLN:HE21	1:A:424:GLN:C	2.24	0.40
1:A:209:ASP:CG	1:A:212:THR:HG23	2.42	0.40
1:A:406:LEU:HD12	1:A:406:LEU:N	2.36	0.40
1:A:260:LEU:N	1:A:260:LEU:CD1	2.75	0.40
1:A:23:SER:HA	1:A:319:HIS:O	2.21	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	453/505 (90%)	346 (76%)	73 (16%)	34 (8%)	1 15

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PHE
1	A	180	VAL
1	A	235	ILE

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Mol	Chain	Res	Type
1	A	337	THR
1	A	352	GLU
1	A	385	ALA
1	A	387	VAL
1	A	57	ASN
1	A	179	ALA
1	A	223	ASP
1	A	305	GLN
1	A	397	THR
1	A	398	ILE
1	A	452	LYS
1	A	469	LEU
1	A	86	PRO
1	A	117	ILE
1	A	124	ASN
1	A	137	ALA
1	A	218	SER
1	A	324	CYS
1	A	396	SER
1	A	241	PRO
1	A	280	SER
1	A	433	PRO
1	A	467	LYS
1	A	41	ARG
1	A	178	VAL
1	A	416	ASP
1	A	421	VAL
1	A	426	ILE
1	A	182	PRO
1	A	463	PRO
1	A	174	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	396/442 (90%)	256 (65%)	140 (35%)	0 2

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	23	SER
1	A	27	TYR
1	A	32	ASN
1	A	36	HIS
1	A	39	THR
1	A	40	SER
1	A	42	LEU
1	A	43	LEU
1	A	53	LYS
1	A	54	LYS
1	A	59	LYS
1	A	60	ILE
1	A	66	SER
1	A	71	ARG
1	A	74	ARG
1	A	95	THR
1	A	96	GLN
1	A	103	VAL
1	A	106	GLU
1	A	109	ARG
1	A	113	LEU
1	A	120	HIS
1	A	122	LEU
1	A	125	LYS
1	A	126	LEU
1	A	127	ASP
1	A	129	THR
1	A	133	SER
1	A	138	ASN
1	A	141	VAL
1	A	142	ASP
1	A	144	ARG
1	A	145	GLU
1	A	147	ILE

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Mol	Chain	Res	Type
1	A	148	SER
1	A	149	MET
1	A	155	GLN
1	A	156	LEU
1	A	157	CYS
1	A	158	LEU
1	A	159	ILE
1	A	173	SER
1	A	176	THR
1	A	180	VAL
1	A	191	ILE
1	A	193	THR
1	A	196	GLN
1	A	200	MET
1	A	208	MET
1	A	211	THR
1	A	213	LEU
1	A	217	LYS
1	A	218	SER
1	A	222	LEU
1	A	224	ILE
1	A	225	CYS
1	A	226	THR
1	A	227	SER
1	A	229	CYS
1	A	235	ILE
1	A	236	LYS
1	A	238	VAL
1	A	239	SER
1	A	245	SER
1	A	246	LEU
1	A	247	PHE
1	A	250	LEU
1	A	251	ARG
1	A	252	ARG
1	A	254	GLN
1	A	255	MET
1	A	257	VAL
1	A	258	ARG
1	A	260	LEU
1	A	262	ASN
1	A	270	ASN

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Mol	Chain	Res	Type
1	A	273	ASP
1	A	280	SER
1	A	282	SER
1	A	283	THR
1	A	291	TYR
1	A	299	MET
1	A	301	THR
1	A	305	GLN
1	A	306	ILE
1	A	313	LEU
1	A	315	ARG
1	A	317	GLN
1	A	329	LEU
1	A	332	THR
1	A	336	THR
1	A	339	SER
1	A	340	THR
1	A	341	ASN
1	A	342	MET
1	A	343	SER
1	A	345	CYS
1	A	349	SER
1	A	350	THR
1	A	351	SER
1	A	353	THR
1	A	354	THR
1	A	358	THR
1	A	368	GLU
1	A	374	PHE
1	A	375	ILE
1	A	380	LYS
1	A	382	THR
1	A	384	THR
1	A	386	ASP
1	A	388	MET
1	A	389	THR
1	A	393	SER
1	A	395	ASN
1	A	399	LEU
1	A	406	LEU
1	A	407	GLN
1	A	414	LEU

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Mol	Chain	Res	Type
1	A	415	GLU
1	A	416	ASP
1	A	419	ARG
1	A	422	THR
1	A	423	SER
1	A	424	GLN
1	A	428	CYS
1	A	431	HIS
1	A	437	LYS
1	A	441	LEU
1	A	443	LYS
1	A	446	PHE
1	A	449	VAL
1	A	454	LYS
1	A	458	ASP
1	A	459	LEU
1	A	464	LEU
1	A	467	LYS
1	A	470	LEU
1	A	472	LEU
1	A	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	69	GLN
1	A	111	GLN
1	A	254	GLN
1	A	262	ASN
1	A	270	ASN
1	A	290	ASN
1	A	319	HIS
1	A	328	GLN
1	A	341	ASN
1	A	377	GLN
1	A	395	ASN
1	A	424	GLN
1	A	461	GLN

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	455/505 (90%)	-0.33	3 (0%) 89 82	23, 54, 98, 100	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	LYS	2.5
1	A	432	THR	2.3
1	A	137	ALA	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.