



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 PM GMT

PDB ID : 4GPO
Title : Oligomeic Turkey Beta1-Adrenergic G Protein-Coupled Receptor
Authors : Huang, J.J.; Chen, S.; Zhang, J.J.; Huang, X.Y.
Deposited on : 2012-08-21
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

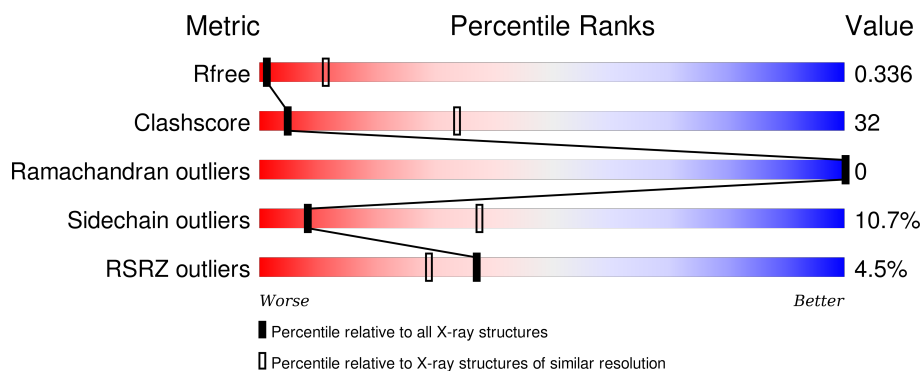
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

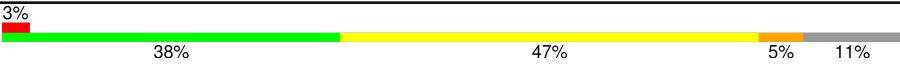
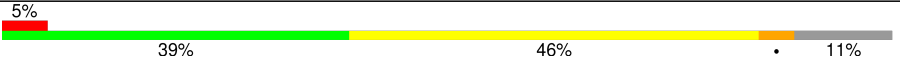
The reported resolution of this entry is 3.50 Å.

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))
R_{free}	91344	1051 (3.60-3.40)
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	313	 3% 38% 47% 5% 11%
1	B	313	 5% 39% 46% • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4442 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 Beta-1 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2217	1466	362	369	20			
1	B	280	Total	C	N	O	S	0	0	0
			2225	1472	363	370	20			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	VAL	CONFLICT	UNP P07700
A	32	GLY	SER	CONFLICT	UNP P07700
A	68	SER	ARG	CONFLICT	UNP P07700
A	90	VAL	MET	CONFLICT	UNP P07700
A	116	LEU	CYS	CONFLICT	UNP P07700
A	227	ALA	TYR	CONFLICT	UNP P07700
A	?	-	ARG	DELETION	UNP P07700
A	?	-	CYS	DELETION	UNP P07700
A	?	-	GLU	DELETION	UNP P07700
A	?	-	GLY	DELETION	UNP P07700
A	?	-	ARG	DELETION	UNP P07700
A	?	-	PHE	DELETION	UNP P07700
A	?	-	TYR	DELETION	UNP P07700
A	?	-	GLY	DELETION	UNP P07700
A	?	-	SER	DELETION	UNP P07700
A	?	-	GLN	DELETION	UNP P07700
A	?	-	GLU	DELETION	UNP P07700
A	?	-	GLN	DELETION	UNP P07700
A	?	-	PRO	DELETION	UNP P07700
A	?	-	GLN	DELETION	UNP P07700
A	?	-	PRO	DELETION	UNP P07700
A	?	-	PRO	DELETION	UNP P07700
A	?	-	PRO	DELETION	UNP P07700
A	?	-	LEU	DELETION	UNP P07700
A	?	-	PRO	DELETION	UNP P07700

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P07700
A	?	-	HIS	DELETION	UNP P07700
A	?	-	GLN	DELETION	UNP P07700
A	?	-	PRO	DELETION	UNP P07700
A	?	-	ILE	DELETION	UNP P07700
A	?	-	LEU	DELETION	UNP P07700
A	?	-	GLY	DELETION	UNP P07700
A	?	-	ASN	DELETION	UNP P07700
A	?	-	GLY	DELETION	UNP P07700
A	?	-	THR	DELETION	UNP P07700
A	?	-	SER	DELETION	UNP P07700
A	282	LEU	ALA	CONFLICT	UNP P07700
A	327	ALA	PHE	CONFLICT	UNP P07700
A	338	MET	PHE	CONFLICT	UNP P07700
A	358	ALA	CYS	CONFLICT	UNP P07700
A	369	HIS	-	EXPRESSION TAG	UNP P07700
A	370	HIS	-	EXPRESSION TAG	UNP P07700
A	371	HIS	-	EXPRESSION TAG	UNP P07700
A	372	HIS	-	EXPRESSION TAG	UNP P07700
A	373	HIS	-	EXPRESSION TAG	UNP P07700
B	31	MET	VAL	CONFLICT	UNP P07700
B	32	GLY	SER	CONFLICT	UNP P07700
B	68	SER	ARG	CONFLICT	UNP P07700
B	90	VAL	MET	CONFLICT	UNP P07700
B	116	LEU	CYS	CONFLICT	UNP P07700
B	227	ALA	TYR	CONFLICT	UNP P07700
B	?	-	ARG	DELETION	UNP P07700
B	?	-	CYS	DELETION	UNP P07700
B	?	-	GLU	DELETION	UNP P07700
B	?	-	GLY	DELETION	UNP P07700
B	?	-	ARG	DELETION	UNP P07700
B	?	-	PHE	DELETION	UNP P07700
B	?	-	TYR	DELETION	UNP P07700
B	?	-	GLY	DELETION	UNP P07700
B	?	-	SER	DELETION	UNP P07700
B	?	-	GLN	DELETION	UNP P07700
B	?	-	GLU	DELETION	UNP P07700
B	?	-	GLN	DELETION	UNP P07700
B	?	-	PRO	DELETION	UNP P07700
B	?	-	GLN	DELETION	UNP P07700
B	?	-	PRO	DELETION	UNP P07700
B	?	-	PRO	DELETION	UNP P07700

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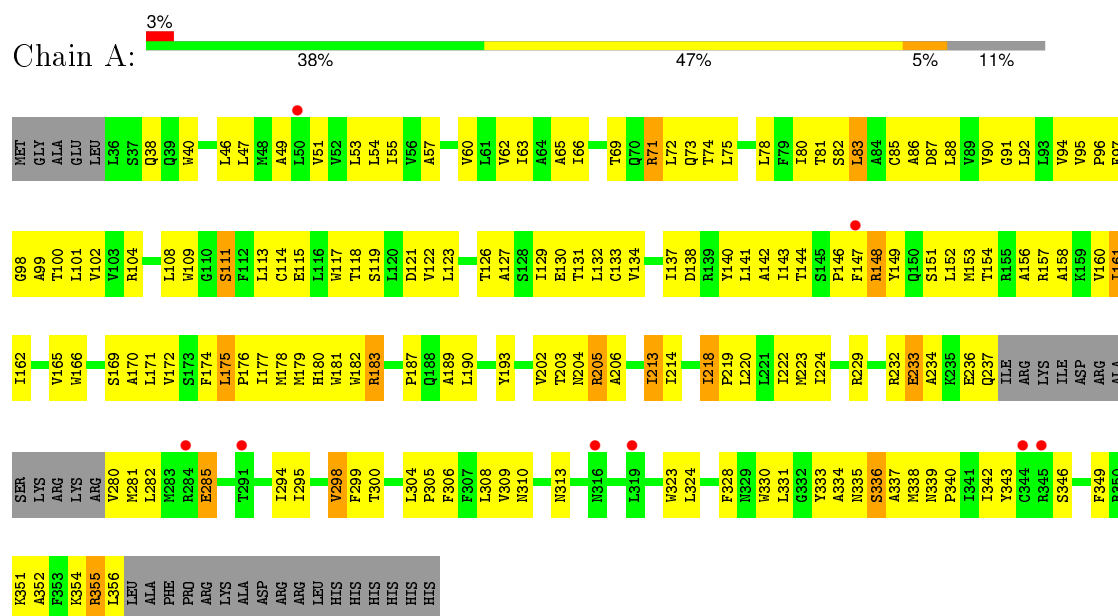
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	DELETION	UNP P07700
B	?	-	LEU	DELETION	UNP P07700
B	?	-	PRO	DELETION	UNP P07700
B	?	-	GLN	DELETION	UNP P07700
B	?	-	HIS	DELETION	UNP P07700
B	?	-	GLN	DELETION	UNP P07700
B	?	-	PRO	DELETION	UNP P07700
B	?	-	ILE	DELETION	UNP P07700
B	?	-	LEU	DELETION	UNP P07700
B	?	-	GLY	DELETION	UNP P07700
B	?	-	ASN	DELETION	UNP P07700
B	?	-	GLY	DELETION	UNP P07700
B	?	-	THR	DELETION	UNP P07700
B	?	-	SER	DELETION	UNP P07700
B	282	LEU	ALA	CONFLICT	UNP P07700
B	327	ALA	PHE	CONFLICT	UNP P07700
B	338	MET	PHE	CONFLICT	UNP P07700
B	358	ALA	CYS	CONFLICT	UNP P07700
B	369	HIS	-	EXPRESSION TAG	UNP P07700
B	370	HIS	-	EXPRESSION TAG	UNP P07700
B	371	HIS	-	EXPRESSION TAG	UNP P07700
B	372	HIS	-	EXPRESSION TAG	UNP P07700
B	373	HIS	-	EXPRESSION TAG	UNP P07700

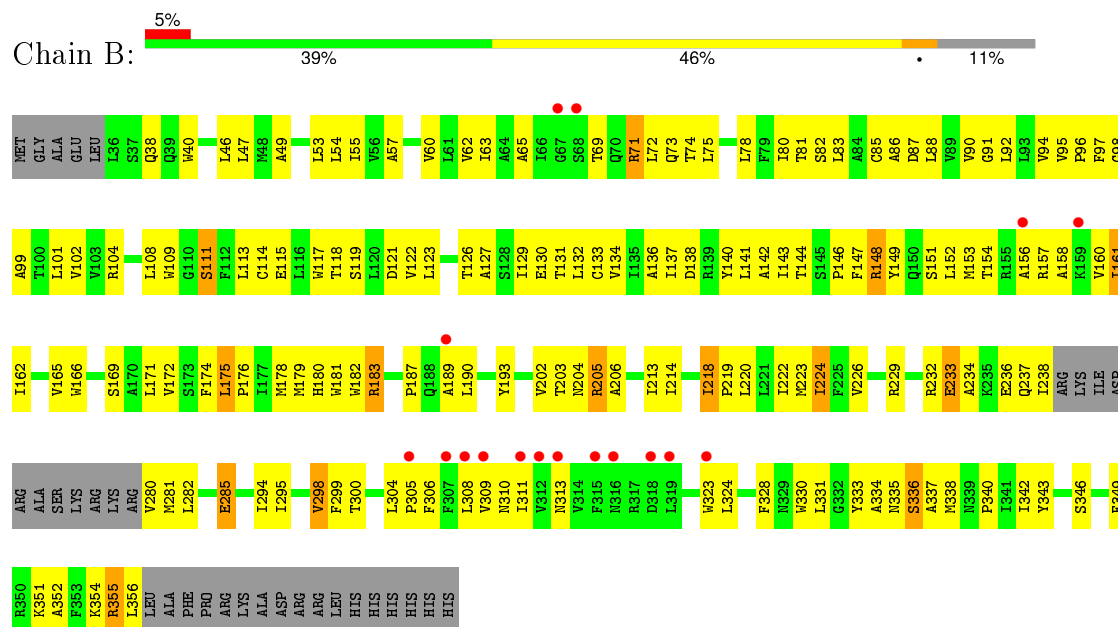
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Beta-1 adrenergic receptor



• Molecule 1: Beta-1 adrenergic receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.66 Å 79.59 Å 69.04 Å 90.00° 101.83° 90.00°	Depositor
Resolution (Å)	29.78 – 3.50 67.57 – 3.35	Depositor EDS
% Data completeness (in resolution range)	83.6 (29.78-3.50) 76.5 (67.57-3.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.64 (at 3.33 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.310 , 0.355 0.305 , 0.336	Depositor DCC
R_{free} test set	639 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 60.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	5 of 13587 reflections (0.037%)	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	4442	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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

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	0.35	0/2271	0.56	0/3097
1	B	0.34	0/2279	0.55	0/3108
All	All	0.34	0/4550	0.56	0/6205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2217	0	2293	151	0
1	B	2225	0	2304	146	0
All	All	4442	0	4597	285	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 32.

All (285) 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:182:TRP:HB2	1:A:203:THR:HG22	1.42	1.01
1:B:182:TRP:HB2	1:B:203:THR:HG22	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TRP:HB3	1:A:113:LEU:HD23	1.59	0.83
1:B:130:GLU:O	1:B:134:VAL:HG23	1.80	0.81
1:B:237:GLN:HG3	1:B:238:ILE:H	1.45	0.81
1:A:126:THR:HG22	1:A:130:GLU:OE1	1.80	0.81
1:B:109:TRP:HB3	1:B:113:LEU:HD23	1.64	0.79
1:A:53:LEU:HD13	1:B:53:LEU:HD13	1.62	0.79
1:B:126:THR:HG22	1:B:130:GLU:OE1	1.83	0.78
1:A:92:LEU:O	1:A:96:PRO:HG3	1.83	0.78
1:B:92:LEU:O	1:B:96:PRO:HG3	1.83	0.77
1:A:130:GLU:O	1:A:134:VAL:HG23	1.86	0.75
1:B:237:GLN:HG3	1:B:238:ILE:HG12	1.68	0.75
1:B:180:HIS:O	1:B:183:ARG:HG3	1.86	0.75
1:B:123:LEU:CD1	1:B:169:SER:HB3	2.17	0.74
1:A:94:VAL:HG21	1:A:121:ASP:HA	1.70	0.74
1:B:237:GLN:HG3	1:B:238:ILE:N	2.02	0.74
1:A:180:HIS:O	1:A:183:ARG:HG3	1.87	0.74
1:B:294:ILE:O	1:B:298:VAL:HG12	1.89	0.72
1:B:82:SER:O	1:B:85:CYS:HB2	1.89	0.71
1:B:94:VAL:HG21	1:B:121:ASP:HA	1.71	0.71
1:A:352:ALA:O	1:A:356:LEU:HB2	1.91	0.71
1:A:294:ILE:O	1:A:298:VAL:HG12	1.90	0.70
1:A:306:PHE:HB2	1:A:328:PHE:HB3	1.74	0.70
1:B:352:ALA:O	1:B:356:LEU:HB2	1.92	0.70
1:A:123:LEU:CD1	1:A:169:SER:HB3	2.21	0.70
1:A:82:SER:O	1:A:85:CYS:HB2	1.92	0.69
1:B:126:THR:O	1:B:130:GLU:HB2	1.93	0.69
1:A:82:SER:HB2	1:A:162:ILE:HG21	1.75	0.69
1:B:306:PHE:HB2	1:B:328:PHE:HB3	1.73	0.69
1:B:343:TYR:HB3	1:B:349:PHE:CD2	2.28	0.69
1:A:343:TYR:HB3	1:A:349:PHE:CD2	2.27	0.68
1:A:213:ILE:HG22	1:A:214:ILE:N	2.08	0.68
1:B:161:ILE:O	1:B:165:VAL:HG23	1.93	0.68
1:B:82:SER:HB2	1:B:162:ILE:HG21	1.75	0.68
1:B:213:ILE:HG22	1:B:214:ILE:N	2.09	0.68
1:B:205:ARG:HG2	1:B:206:ALA:N	2.10	0.67
1:A:80:ILE:HD12	1:A:343:TYR:OH	1.94	0.67
1:A:205:ARG:HG2	1:A:206:ALA:N	2.09	0.67
1:A:62:VAL:HA	1:A:349:PHE:HZ	1.60	0.66
1:A:126:THR:O	1:A:130:GLU:HB2	1.94	0.66
1:B:65:ALA:HB3	1:B:349:PHE:CE1	2.31	0.65
1:A:62:VAL:HA	1:A:349:PHE:CZ	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:O	1:B:313:ASN:HB3	1.97	0.65
1:A:161:ILE:O	1:A:165:VAL:HG23	1.97	0.64
1:B:62:VAL:HA	1:B:349:PHE:HZ	1.61	0.64
1:A:181:TRP:O	1:A:204:ASN:ND2	2.24	0.64
1:B:65:ALA:HB3	1:B:349:PHE:HE1	1.63	0.63
1:B:80:ILE:HD12	1:B:343:TYR:OH	1.98	0.63
1:A:75:LEU:HD12	1:A:75:LEU:H	1.63	0.63
1:A:282:LEU:O	1:A:285:GLU:HB3	1.99	0.63
1:B:62:VAL:HA	1:B:349:PHE:CZ	2.34	0.63
1:A:310:ASN:O	1:A:313:ASN:HB3	1.98	0.63
1:A:65:ALA:HB3	1:A:349:PHE:CE1	2.33	0.62
1:B:75:LEU:H	1:B:75:LEU:HD12	1.64	0.62
1:B:183:ARG:HA	1:B:193:TYR:CE2	2.35	0.61
1:B:304:LEU:N	1:B:305:PRO:HD2	2.15	0.61
1:B:87:ASP:O	1:B:90:VAL:HB	2.01	0.61
1:A:218:ILE:HG22	1:A:219:PRO:HD3	1.83	0.61
1:B:181:TRP:O	1:B:204:ASN:ND2	2.30	0.60
1:A:304:LEU:N	1:A:305:PRO:HD2	2.16	0.60
1:A:65:ALA:HB3	1:A:349:PHE:HE1	1.65	0.60
1:A:183:ARG:HA	1:A:193:TYR:CE2	2.36	0.60
1:B:55:ILE:HG21	1:B:91:GLY:HA3	1.83	0.60
1:B:330:TRP:HA	1:B:333:TYR:HD2	1.67	0.59
1:A:99:ALA:O	1:A:102:VAL:N	2.34	0.59
1:B:282:LEU:O	1:B:285:GLU:HB3	2.02	0.59
1:B:99:ALA:O	1:B:102:VAL:N	2.35	0.59
1:B:354:LYS:HG3	1:B:355:ARG:H	1.68	0.59
1:B:142:ALA:HB2	1:B:149:TYR:HE1	1.68	0.58
1:A:87:ASP:O	1:A:90:VAL:HB	2.02	0.58
1:A:330:TRP:HA	1:A:333:TYR:HD2	1.68	0.58
1:A:343:TYR:HB3	1:A:349:PHE:HD2	1.69	0.57
1:A:142:ALA:HB2	1:A:149:TYR:HE1	1.70	0.57
1:A:193:TYR:CE1	1:A:202:VAL:HG13	2.39	0.57
1:B:140:TYR:HE2	1:B:229:ARG:HD3	1.70	0.57
1:B:175:LEU:CB	1:B:176:PRO:HD3	2.35	0.57
1:A:95:VAL:N	1:A:96:PRO:HD2	2.20	0.57
1:A:55:ILE:HG21	1:A:91:GLY:HA3	1.87	0.57
1:B:218:ILE:HG22	1:B:219:PRO:HD3	1.85	0.56
1:A:354:LYS:HG3	1:A:355:ARG:H	1.69	0.56
1:A:205:ARG:HG2	1:A:206:ALA:H	1.70	0.56
1:A:53:LEU:CD1	1:B:53:LEU:HD22	2.36	0.56
1:B:330:TRP:HA	1:B:333:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CB	1:A:176:PRO:HD3	2.36	0.56
1:A:179:MET:HB3	1:A:181:TRP:CD1	2.41	0.56
1:B:351:LYS:O	1:B:355:ARG:HG3	2.06	0.56
1:B:134:VAL:O	1:B:137:ILE:HG22	2.05	0.55
1:A:351:LYS:O	1:A:355:ARG:HG3	2.06	0.55
1:A:140:TYR:HE2	1:A:229:ARG:HD3	1.71	0.55
1:B:193:TYR:CE1	1:B:202:VAL:HG13	2.41	0.55
1:A:330:TRP:HA	1:A:333:TYR:CD2	2.41	0.55
1:A:134:VAL:O	1:A:137:ILE:HG22	2.07	0.55
1:B:95:VAL:N	1:B:96:PRO:HD2	2.20	0.55
1:B:87:ASP:O	1:B:336:SER:OG	2.24	0.55
1:A:343:TYR:HB3	1:A:349:PHE:CE2	2.42	0.55
1:B:343:TYR:HB3	1:B:349:PHE:HD2	1.72	0.55
1:B:205:ARG:HG2	1:B:206:ALA:H	1.72	0.54
1:B:343:TYR:HB3	1:B:349:PHE:CE2	2.42	0.54
1:B:138:ASP:O	1:B:141:LEU:HB2	2.07	0.54
1:B:295:ILE:HD13	1:B:342:ILE:HD12	1.89	0.54
1:B:111:SER:HA	1:B:114:CYS:CB	2.36	0.54
1:B:340:PRO:HA	1:B:343:TYR:HD2	1.73	0.53
1:B:334:ALA:O	1:B:338:MET:HG3	2.08	0.53
1:B:80:ILE:HG23	1:B:343:TYR:OH	2.08	0.53
1:B:179:MET:HB3	1:B:181:TRP:CD1	2.43	0.53
1:A:111:SER:HA	1:A:114:CYS:CB	2.39	0.53
1:A:53:LEU:HD22	1:B:53:LEU:CD1	2.39	0.52
1:A:295:ILE:HD13	1:A:342:ILE:HD12	1.91	0.52
1:A:300:THR:O	1:A:304:LEU:CB	2.57	0.52
1:A:182:TRP:HB2	1:A:203:THR:CG2	2.27	0.52
1:B:331:LEU:HD23	1:B:331:LEU:O	2.10	0.52
1:A:331:LEU:HD23	1:A:331:LEU:O	2.10	0.52
1:B:62:VAL:HG21	1:B:340:PRO:HA	1.90	0.52
1:A:138:ASP:O	1:A:141:LEU:HB2	2.09	0.52
1:A:69:THR:HB	1:A:72:LEU:HD12	1.92	0.52
1:B:300:THR:O	1:B:304:LEU:CB	2.58	0.52
1:B:299:PHE:HD2	1:B:335:ASN:OD1	1.93	0.52
1:A:334:ALA:O	1:A:338:MET:HG3	2.10	0.51
1:A:62:VAL:HG21	1:A:340:PRO:HA	1.91	0.51
1:A:300:THR:O	1:A:304:LEU:HB2	2.10	0.51
1:A:55:ILE:HG12	1:A:337:ALA:HB2	1.92	0.51
1:A:340:PRO:HA	1:A:343:TYR:HD2	1.76	0.51
1:A:80:ILE:HG23	1:A:343:TYR:OH	2.10	0.51
1:A:87:ASP:O	1:A:336:SER:OG	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:O	1:A:330:TRP:HZ2	1.93	0.51
1:B:98:GLY:O	1:B:330:TRP:HZ2	1.93	0.51
1:A:53:LEU:HD11	1:B:53:LEU:HD22	1.93	0.51
1:B:69:THR:HB	1:B:72:LEU:HD12	1.92	0.51
1:A:305:PRO:O	1:A:309:VAL:HG23	2.11	0.51
1:A:47:LEU:HD23	1:A:47:LEU:C	2.31	0.51
1:A:299:PHE:HD2	1:A:335:ASN:OD1	1.94	0.51
1:B:129:ILE:O	1:B:132:LEU:HB2	2.11	0.51
1:A:53:LEU:HD22	1:B:53:LEU:HD11	1.93	0.51
1:B:57:ALA:O	1:B:60:VAL:HG12	2.11	0.51
1:A:187:PRO:HA	1:A:190:LEU:CB	2.41	0.51
1:B:47:LEU:HD23	1:B:47:LEU:C	2.31	0.51
1:B:305:PRO:O	1:B:309:VAL:HG23	2.12	0.50
1:A:62:VAL:HG22	1:A:349:PHE:CE2	2.46	0.50
1:B:129:ILE:HG23	1:B:130:GLU:N	2.27	0.50
1:B:86:ALA:O	1:B:90:VAL:HG23	2.10	0.50
1:B:55:ILE:HG12	1:B:337:ALA:HB2	1.93	0.50
1:A:86:ALA:O	1:A:90:VAL:HG23	2.12	0.50
1:B:78:LEU:O	1:B:81:THR:HB	2.12	0.50
1:A:129:ILE:O	1:A:132:LEU:HB2	2.11	0.50
1:B:62:VAL:HG22	1:B:349:PHE:CE2	2.47	0.49
1:A:118:THR:O	1:A:122:VAL:HG23	2.12	0.49
1:B:300:THR:O	1:B:304:LEU:HB2	2.12	0.49
1:B:189:ALA:HB2	1:B:202:VAL:HG21	1.95	0.49
1:B:111:SER:HA	1:B:114:CYS:HB3	1.93	0.49
1:A:57:ALA:O	1:A:60:VAL:HG12	2.12	0.49
1:A:189:ALA:HB2	1:A:202:VAL:HG21	1.94	0.49
1:A:160:VAL:CG1	1:A:161:ILE:N	2.76	0.49
1:A:97:PHE:HB2	1:A:117:TRP:CD1	2.48	0.49
1:A:46:LEU:HA	1:B:49:ALA:HB2	1.94	0.49
1:A:78:LEU:O	1:A:81:THR:HB	2.13	0.48
1:B:97:PHE:HB2	1:B:117:TRP:CD1	2.49	0.48
1:A:220:LEU:HD12	1:A:224:ILE:HD13	1.95	0.48
1:B:187:PRO:HA	1:B:190:LEU:CB	2.43	0.48
1:B:140:TYR:CE2	1:B:229:ARG:HD3	2.49	0.48
1:B:118:THR:O	1:B:122:VAL:HG23	2.14	0.48
1:B:182:TRP:HB2	1:B:203:THR:CG2	2.31	0.48
1:A:129:ILE:HG23	1:A:130:GLU:N	2.28	0.48
1:B:171:LEU:O	1:B:175:LEU:HB2	2.13	0.48
1:B:160:VAL:CG1	1:B:161:ILE:N	2.77	0.48
1:A:115:GLU:OE2	1:A:180:HIS:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:O	1:B:123:LEU:HD12	2.13	0.47
1:A:94:VAL:HG21	1:A:121:ASP:CA	2.42	0.47
1:A:140:TYR:CE2	1:A:229:ARG:HD3	2.49	0.47
1:B:115:GLU:OE2	1:B:180:HIS:NE2	2.47	0.47
1:B:234:ALA:O	1:B:237:GLN:HG2	2.15	0.47
1:A:62:VAL:HG12	1:A:63:ILE:N	2.30	0.47
1:A:69:THR:O	1:A:73:GLN:HG3	2.13	0.47
1:B:331:LEU:O	1:B:334:ALA:HB3	2.14	0.47
1:A:143:ILE:HG21	1:A:233:GLU:HB3	1.97	0.47
1:B:146:PRO:HD2	1:B:147:PHE:CD2	2.50	0.47
1:A:111:SER:HA	1:A:114:CYS:HB3	1.95	0.47
1:B:143:ILE:CG2	1:B:233:GLU:HG2	2.45	0.47
1:B:123:LEU:HD12	1:B:169:SER:HB3	1.93	0.47
1:B:69:THR:O	1:B:73:GLN:HG3	2.15	0.47
1:B:111:SER:HA	1:B:114:CYS:HB2	1.97	0.46
1:A:331:LEU:O	1:A:334:ALA:HB3	2.15	0.46
1:B:71:ARG:HD2	1:B:71:ARG:H	1.80	0.46
1:A:161:ILE:HD13	1:A:161:ILE:HA	1.66	0.46
1:B:143:ILE:HG21	1:B:233:GLU:HB3	1.97	0.46
1:A:182:TRP:O	1:A:203:THR:HA	2.15	0.46
1:A:187:PRO:HA	1:A:190:LEU:HB2	1.98	0.46
1:A:104:ARG:HE	1:B:38:GLN:NE2	2.14	0.46
1:B:72:LEU:HD21	1:B:349:PHE:N	2.31	0.46
1:A:218:ILE:O	1:A:222:ILE:HG12	2.16	0.46
1:A:143:ILE:CG2	1:A:233:GLU:HG2	2.46	0.46
1:A:154:THR:C	1:A:156:ALA:N	2.68	0.45
1:B:148:ARG:HG3	1:B:148:ARG:O	2.16	0.45
1:A:54:LEU:HB3	1:A:337:ALA:HB1	1.98	0.45
1:B:111:SER:O	1:B:114:CYS:HB3	2.15	0.45
1:B:55:ILE:CG2	1:B:91:GLY:HA3	2.45	0.45
1:A:152:LEU:O	1:A:157:ARG:HD2	2.17	0.45
1:A:123:LEU:HD12	1:A:169:SER:HB3	1.96	0.45
1:B:218:ILE:O	1:B:222:ILE:HG12	2.16	0.45
1:A:71:ARG:H	1:A:71:ARG:HD2	1.80	0.45
1:A:146:PRO:HD2	1:A:147:PHE:CD2	2.52	0.45
1:B:54:LEU:HB3	1:B:337:ALA:HB1	1.99	0.45
1:A:234:ALA:O	1:A:237:GLN:HG2	2.17	0.45
1:B:280:VAL:HG12	1:B:281:MET:HG2	1.99	0.44
1:B:152:LEU:O	1:B:157:ARG:HD2	2.17	0.44
1:B:306:PHE:C	1:B:306:PHE:CD1	2.90	0.44
1:B:193:TYR:HE1	1:B:202:VAL:HG13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD12	1:A:123:LEU:O	2.17	0.44
1:A:72:LEU:HD21	1:A:349:PHE:N	2.33	0.44
1:A:158:ALA:O	1:A:162:ILE:HG13	2.17	0.44
1:B:62:VAL:HG12	1:B:63:ILE:N	2.32	0.44
1:A:171:LEU:O	1:A:175:LEU:HB2	2.17	0.44
1:A:148:ARG:O	1:A:148:ARG:HG3	2.18	0.44
1:A:280:VAL:HG12	1:A:281:MET:HG2	1.99	0.44
1:A:193:TYR:HE1	1:A:202:VAL:HG13	1.80	0.44
1:B:134:VAL:HG11	1:B:161:ILE:CG2	2.48	0.44
1:B:158:ALA:O	1:B:162:ILE:HG13	2.18	0.44
1:B:75:LEU:CD2	1:B:153:MET:HB3	2.48	0.44
1:A:111:SER:O	1:A:114:CYS:HB3	2.18	0.44
1:B:65:ALA:CB	1:B:349:PHE:HE1	2.31	0.43
1:A:62:VAL:O	1:A:66:ILE:HG13	2.18	0.43
1:B:154:THR:C	1:B:156:ALA:N	2.69	0.43
1:A:119:SER:OG	1:A:177:ILE:HD12	2.18	0.43
1:B:94:VAL:HG21	1:B:121:ASP:CA	2.43	0.43
1:A:75:LEU:CD2	1:A:153:MET:HB3	2.48	0.43
1:B:175:LEU:HA	1:B:175:LEU:HD22	1.80	0.43
1:B:175:LEU:HB3	1:B:176:PRO:HD3	2.00	0.43
1:B:157:ARG:O	1:B:160:VAL:HG12	2.18	0.43
1:A:162:ILE:O	1:A:166:TRP:HD1	2.01	0.43
1:B:133:CYS:SG	1:B:223:MET:HB3	2.59	0.43
1:A:49:ALA:HB2	1:B:46:LEU:HA	2.00	0.43
1:A:87:ASP:OD2	1:A:339:ASN:ND2	2.52	0.43
1:A:127:ALA:O	1:A:131:THR:HB	2.19	0.43
1:A:183:ARG:HD2	1:A:183:ARG:O	2.18	0.43
1:A:172:VAL:O	1:A:176:PRO:HD2	2.18	0.43
1:A:304:LEU:O	1:A:308:LEU:N	2.51	0.42
1:A:55:ILE:CG2	1:A:91:GLY:HA3	2.49	0.42
1:B:311:ILE:HD13	1:B:311:ILE:HA	1.77	0.42
1:B:295:ILE:CD1	1:B:342:ILE:HD12	2.49	0.42
1:A:83:LEU:HD23	1:A:339:ASN:ND2	2.34	0.42
1:A:111:SER:HA	1:A:114:CYS:HB2	2.00	0.42
1:B:220:LEU:HD12	1:B:224:ILE:HD13	2.01	0.42
1:B:154:THR:O	1:B:157:ARG:N	2.53	0.42
1:A:98:GLY:HA2	1:A:117:TRP:CZ2	2.55	0.42
1:A:99:ALA:O	1:A:101:LEU:N	2.52	0.42
1:A:187:PRO:HA	1:A:190:LEU:HB3	2.01	0.42
1:B:182:TRP:O	1:B:203:THR:HA	2.20	0.42
1:A:154:THR:O	1:A:157:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:O	1:A:149:TYR:C	2.58	0.42
1:A:133:CYS:SG	1:A:223:MET:HB3	2.60	0.42
1:A:180:HIS:C	1:A:182:TRP:N	2.73	0.42
1:A:306:PHE:CD1	1:A:306:PHE:C	2.93	0.42
1:B:187:PRO:HA	1:B:190:LEU:HB2	2.01	0.42
1:A:157:ARG:O	1:A:160:VAL:HG12	2.20	0.42
1:A:53:LEU:HD13	1:B:53:LEU:HD22	2.01	0.42
1:A:100:THR:CB	1:A:109:TRP:HE1	2.33	0.41
1:B:99:ALA:O	1:B:101:LEU:N	2.53	0.41
1:A:134:VAL:HG11	1:A:161:ILE:CG2	2.50	0.41
1:A:180:HIS:C	1:A:182:TRP:H	2.23	0.41
1:A:92:LEU:O	1:A:96:PRO:CG	2.61	0.41
1:B:127:ALA:O	1:B:131:THR:HB	2.20	0.41
1:B:172:VAL:O	1:B:176:PRO:HD2	2.20	0.41
1:A:53:LEU:HD13	1:B:53:LEU:CD1	2.41	0.41
1:B:304:LEU:O	1:B:308:LEU:N	2.52	0.41
1:A:38:GLN:NE2	1:B:104:ARG:HE	2.18	0.41
1:A:294:ILE:HG22	1:A:342:ILE:HD13	2.01	0.41
1:B:148:ARG:O	1:B:149:TYR:C	2.59	0.41
1:A:170:ALA:O	1:A:174:PHE:HB2	2.21	0.41
1:A:134:VAL:HG11	1:A:161:ILE:HG21	2.03	0.41
1:B:119:SER:HB2	1:B:174:PHE:CE2	2.56	0.41
1:A:175:LEU:HB3	1:A:176:PRO:HD3	2.02	0.41
1:B:187:PRO:HA	1:B:190:LEU:HB3	2.02	0.41
1:B:162:ILE:O	1:B:166:TRP:HD1	2.04	0.41
1:A:51:VAL:O	1:A:55:ILE:HG13	2.21	0.41
1:A:148:ARG:O	1:A:148:ARG:CG	2.69	0.41
1:A:119:SER:HB2	1:A:174:PHE:CE2	2.56	0.41
1:A:53:LEU:CD1	1:B:53:LEU:HD13	2.43	0.40
1:B:294:ILE:HG22	1:B:342:ILE:HD13	2.02	0.40
1:B:98:GLY:HA2	1:B:117:TRP:CZ2	2.55	0.40
1:B:136:ALA:O	1:B:226:VAL:HG12	2.21	0.40
1:B:144:THR:O	1:B:144:THR:HG22	2.22	0.40
1:B:183:ARG:O	1:B:183:ARG:HD2	2.21	0.40
1:B:205:ARG:CG	1:B:206:ALA:N	2.83	0.40
1:A:144:THR:O	1:A:144:THR:HG22	2.22	0.40
1:A:343:TYR:CB	1:A:349:PHE:CE2	3.05	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	275/313 (88%)	262 (95%)	13 (5%)	0	100	100
1	B	276/313 (88%)	261 (95%)	15 (5%)	0	100	100
All	All	551/626 (88%)	523 (95%)	28 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	242/271 (89%)	216 (89%)	26 (11%)	8	37
1	B	243/271 (90%)	217 (89%)	26 (11%)	8	37
All	All	485/542 (90%)	433 (89%)	52 (11%)	8	37

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	TRP
1	A	71	ARG
1	A	74	THR
1	A	83	LEU
1	A	88	LEU
1	A	108	LEU
1	A	111	SER
1	A	148	ARG

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Mol	Chain	Res	Type
1	A	151	SER
1	A	161	ILE
1	A	175	LEU
1	A	178	MET
1	A	183	ARG
1	A	205	ARG
1	A	213	ILE
1	A	218	ILE
1	A	232	ARG
1	A	233	GLU
1	A	236	GLU
1	A	285	GLU
1	A	298	VAL
1	A	323	TRP
1	A	324	LEU
1	A	336	SER
1	A	346	SER
1	A	355	ARG
1	B	40	TRP
1	B	71	ARG
1	B	74	THR
1	B	83	LEU
1	B	88	LEU
1	B	108	LEU
1	B	111	SER
1	B	148	ARG
1	B	151	SER
1	B	161	ILE
1	B	175	LEU
1	B	178	MET
1	B	183	ARG
1	B	205	ARG
1	B	218	ILE
1	B	224	ILE
1	B	232	ARG
1	B	233	GLU
1	B	236	GLU
1	B	285	GLU
1	B	298	VAL
1	B	323	TRP
1	B	324	LEU
1	B	336	SER

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Mol	Chain	Res	Type
1	B	346	SER
1	B	355	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	B	286	HIS

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 ⓘ

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	279/313 (89%)	-0.16	8 (2%) 55 45	8, 72, 138, 169	0
1	B	280/313 (89%)	-0.12	17 (6%) 25 19	14, 73, 142, 170	0
All	All	559/626 (89%)	-0.14	25 (4%) 37 29	8, 72, 142, 170	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ASN	4.9
1	B	318	ASP	4.8
1	A	319	LEU	4.8
1	B	319	LEU	3.9
1	A	344	CYS	3.8
1	A	345	ARG	3.3
1	A	316	ASN	3.2
1	B	311	ILE	3.1
1	A	284	ARG	3.1
1	B	315	PHE	2.9
1	B	67	GLY	2.8
1	B	305	PRO	2.6
1	A	50	LEU	2.5
1	B	159	LYS	2.4
1	A	147	PHE	2.4
1	B	156	ALA	2.4
1	B	323	TRP	2.3
1	B	307	PHE	2.3
1	B	68	SER	2.3
1	B	189	ALA	2.3
1	B	312	VAL	2.2
1	B	309	VAL	2.2
1	B	308	LEU	2.2
1	B	313	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	291	THR	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.