



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:03 AM UTC

PDB ID : 1ZQV / pdb_00001zqv
Title : DNA POLYMERASE BETA (POL B) (E.C.2.7.7.7), 31-KD DOMAIN;
SOAKED IN THE PRESENCE OF CACL2 (150 MILLIMOLAR)
Authors : Pelletier, H.; Sawaya, M.R.
Deposited on : 1996-04-19
Resolution : 2.70 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

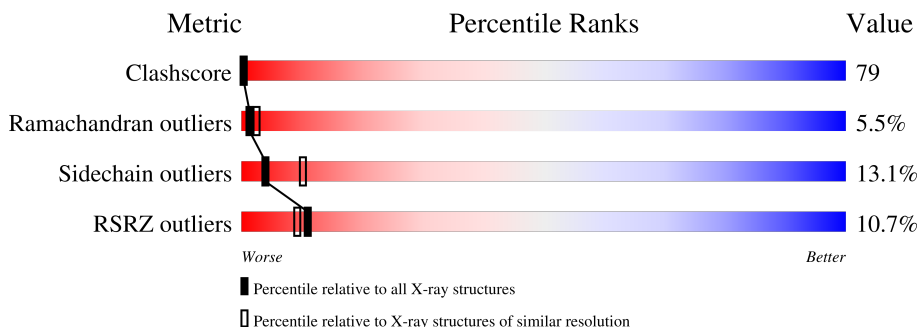
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	248	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2046 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 DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1939	1221	343	367	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

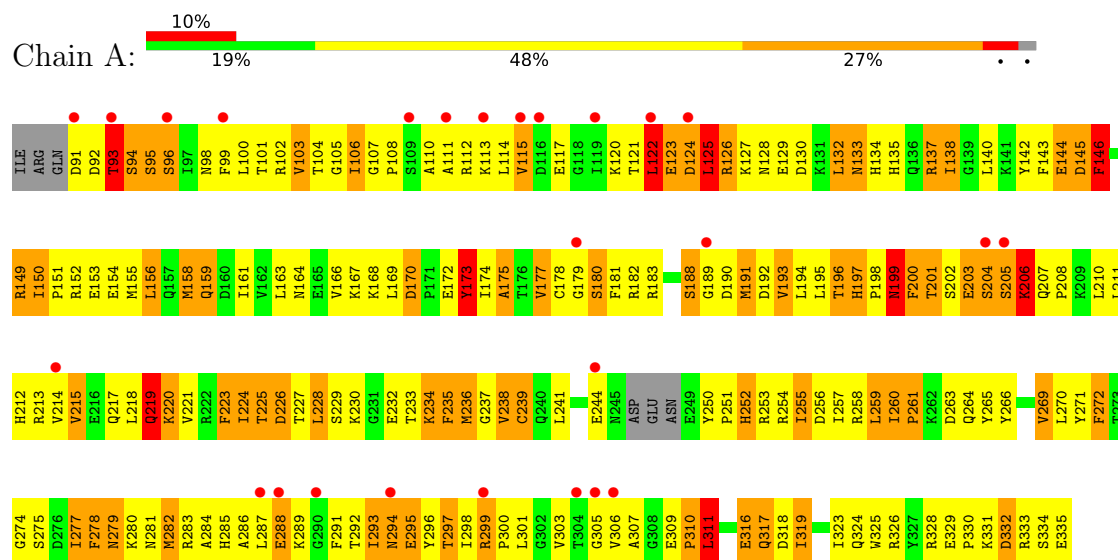
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

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: DNA POLYMERASE BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.77Å 63.35Å 35.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-2.70) 81.8 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.41Å)	Xtriage
Refinement program	TNT 5-D	Depositor
R, R_{free}	(Not available) , (Not available) 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	1.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 135.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2046	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.52	16/1977 (0.8%)	2.10	83/2666 (3.1%)

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	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	LEU	C-N	-6.60	1.25	1.33
1	A	201	THR	CA-C	-6.15	1.44	1.52
1	A	150	ILE	N-CA	-5.99	1.41	1.46
1	A	316	GLU	CD-OE1	5.93	1.36	1.25
1	A	229	SER	CA-CB	-5.82	1.44	1.53
1	A	197	HIS	CA-C	-5.67	1.46	1.52
1	A	192	ASP	CG-OD1	5.56	1.35	1.25
1	A	152	ARG	CA-C	-5.52	1.45	1.52
1	A	200	PHE	CA-C	-5.37	1.46	1.52
1	A	326	ARG	N-CA	-5.35	1.39	1.46
1	A	239	CYS	C-N	5.24	1.41	1.33
1	A	177	VAL	C-N	-5.21	1.28	1.33
1	A	178	CYS	CA-C	-5.17	1.47	1.53
1	A	235	PHE	CA-CB	5.16	1.61	1.53
1	A	236	MET	N-CA	5.16	1.52	1.46
1	A	150	ILE	CA-C	-5.07	1.48	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	SER	N-CA-C	-8.81	101.79	112.54
1	A	220	LYS	N-CA-C	-8.79	101.70	111.28
1	A	319	ILE	CB-CA-C	-8.75	100.32	112.14
1	A	224	ILE	N-CA-C	-8.38	100.92	110.05
1	A	150	ILE	O-C-N	8.27	127.91	121.46
1	A	214	VAL	CB-CA-C	8.20	124.88	112.16
1	A	219	GLN	N-CA-C	-8.16	103.11	113.23
1	A	152	ARG	N-CA-C	7.86	120.94	111.82
1	A	170	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	316	GLU	N-CA-C	-7.59	102.36	111.69
1	A	153	GLU	N-CA-C	-7.46	101.92	111.02
1	A	137	ARG	N-CA-CB	7.34	120.72	110.07
1	A	297	THR	N-CA-C	7.28	117.88	108.34
1	A	150	ILE	CA-C-N	7.21	127.20	119.78
1	A	150	ILE	C-N-CA	7.21	127.20	119.78
1	A	253	ARG	N-CA-C	7.07	120.00	108.26
1	A	229	SER	CA-CB-OG	-6.92	97.26	111.10
1	A	236	MET	CA-C-N	-6.88	107.93	121.41
1	A	236	MET	C-N-CA	-6.88	107.93	121.41
1	A	152	ARG	N-CA-CB	6.84	120.89	110.28
1	A	197	HIS	CB-CA-C	-6.80	99.59	109.45
1	A	235	PHE	CA-CB-CG	-6.63	107.17	113.80
1	A	226	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	253	ARG	CB-CA-C	-6.51	100.11	110.14
1	A	173	TYR	CB-CA-C	-6.41	99.90	109.90
1	A	234	LYS	CB-CA-C	-6.38	103.35	111.70
1	A	278	PHE	N-CA-CB	6.37	119.25	110.01
1	A	150	ILE	N-CA-C	6.25	114.77	107.77
1	A	235	PHE	CA-C-O	-6.25	114.16	121.16
1	A	124	ASP	N-CA-C	-6.20	104.60	111.36
1	A	266	TYR	CB-CA-C	6.18	120.48	110.96
1	A	282	MET	N-CA-CB	6.17	118.91	109.91
1	A	95	SER	N-CA-C	-6.12	104.61	111.28
1	A	138	ILE	N-CA-CB	6.10	118.83	110.54
1	A	96	SER	CB-CA-C	6.09	120.34	110.96
1	A	132	LEU	N-CA-C	6.07	119.71	109.76
1	A	96	SER	N-CA-CB	6.06	118.76	109.91
1	A	225	THR	N-CA-CB	6.01	120.38	111.01
1	A	260	ILE	CB-CA-C	-6.01	100.43	111.36
1	A	279	ASN	CA-CB-CG	-5.97	106.63	112.60
1	A	224	ILE	CA-C-O	-5.97	114.75	121.98
1	A	192	ASP	CA-CB-CG	-5.95	106.65	112.60
1	A	122	LEU	N-CA-CB	5.95	119.47	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	161	ILE	CA-C-O	-5.89	115.29	121.41
1	A	272	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	206	LYS	N-CA-CB	-5.74	100.79	110.49
1	A	149	ARG	CA-C-N	-5.72	117.07	123.02
1	A	149	ARG	C-N-CA	-5.72	117.07	123.02
1	A	152	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	A	164	ASN	N-CA-CB	5.67	118.44	109.82
1	A	226	ASP	N-CA-CB	5.67	120.18	111.56
1	A	261	PRO	N-CA-CB	5.66	108.28	103.35
1	A	228	LEU	CB-CA-C	5.57	119.54	110.24
1	A	199	ASN	N-CA-C	5.54	119.13	112.38
1	A	191	MET	CA-C-N	-5.49	115.31	123.11
1	A	191	MET	C-N-CA	-5.49	115.31	123.11
1	A	214	VAL	CA-CB-CG1	5.47	119.71	110.40
1	A	244	GLU	N-CA-C	-5.45	107.18	113.88
1	A	293	ILE	N-CA-C	5.45	117.74	108.86
1	A	192	ASP	N-CA-CB	5.44	119.50	110.47
1	A	252	HIS	CA-C-O	-5.39	115.27	121.47
1	A	223	PHE	N-CA-CB	5.38	117.97	110.07
1	A	318	ASP	N-CA-CB	5.33	117.89	109.94
1	A	218	LEU	N-CA-C	5.32	117.99	111.82
1	A	226	ASP	CA-C-N	-5.28	113.94	122.81
1	A	226	ASP	C-N-CA	-5.28	113.94	122.81
1	A	103	VAL	CB-CA-C	-5.25	103.51	111.33
1	A	175	ALA	N-CA-C	5.21	116.81	107.80
1	A	152	ARG	CA-C-O	-5.20	113.99	119.97
1	A	234	LYS	N-CA-C	5.20	115.89	107.32
1	A	146	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	318	ASP	CA-C-O	-5.16	115.38	120.90
1	A	193	VAL	N-CA-C	5.14	115.98	108.53
1	A	199	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	93	THR	N-CA-C	-5.13	107.15	113.41
1	A	177	VAL	CB-CA-C	-5.12	104.56	110.91
1	A	319	ILE	O-C-N	5.08	126.80	121.87
1	A	269	VAL	N-CA-CB	5.07	117.43	110.54
1	A	164	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	123	GLU	N-CA-C	-5.04	105.92	111.71
1	A	177	VAL	CA-C-N	-5.01	113.56	123.99
1	A	177	VAL	C-N-CA	-5.01	113.56	123.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ASP	Sidechain
1	A	199	ASN	Sidechain

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	1939	0	1875	303	1
2	A	1	0	0	0	0
3	A	106	0	0	23	1
All	All	2046	0	1875	303	2

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 79.

All (303) 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:103:VAL:HB	1:A:106:ILE:HD13	1.19	1.10
1:A:270:LEU:HD21	1:A:282:MET:HE3	1.30	1.08
1:A:278:PHE:HE1	1:A:282:MET:HE2	1.15	1.04
1:A:317:GLN:H	1:A:317:GLN:NE2	1.59	1.00
1:A:278:PHE:HE2	1:A:328:ARG:HD2	1.21	1.00
1:A:317:GLN:N	1:A:317:GLN:HE21	1.61	0.97
1:A:133:ASN:ND2	1:A:135:HIS:H	1.63	0.96
1:A:135:HIS:CE1	1:A:228:LEU:HB3	2.05	0.91
1:A:289:LYS:NZ	1:A:324:GLN:HG3	1.85	0.91
1:A:133:ASN:HD22	1:A:135:HIS:H	1.12	0.90
1:A:278:PHE:CE1	1:A:282:MET:HE2	2.06	0.90
1:A:277:ILE:HD13	1:A:277:ILE:H	1.36	0.89
1:A:158:MET:HB2	1:A:191:MET:HE1	1.53	0.88
1:A:278:PHE:CE2	1:A:328:ARG:HD2	2.08	0.87
1:A:125:LEU:HB3	1:A:140:LEU:HD22	1.54	0.85
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:HH11	1.40	0.85
1:A:317:GLN:H	1:A:317:GLN:HE21	0.88	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD21	1:A:282:MET:CE	2.10	0.82
1:A:113:LYS:HG3	1:A:114:LEU:HD12	1.60	0.82
1:A:197:HIS:ND1	1:A:199:ASN:HB2	1.95	0.81
1:A:286:ALA:HB2	1:A:323:ILE:HG21	1.63	0.78
1:A:138:ILE:HB	1:A:228:LEU:HD21	1.66	0.77
1:A:158:MET:HB2	1:A:191:MET:CE	2.14	0.77
1:A:217:GLN:O	1:A:221:VAL:HG22	1.84	0.77
1:A:158:MET:HG2	1:A:241:LEU:HD11	1.67	0.76
1:A:234:LYS:HE3	1:A:236:MET:HG3	1.68	0.76
1:A:143:PHE:HB3	1:A:144:GLU:OE1	1.85	0.75
1:A:138:ILE:HB	1:A:228:LEU:CD2	2.17	0.74
1:A:274:GLY:HA2	1:A:279:ASN:OD1	1.86	0.74
1:A:158:MET:CE	1:A:191:MET:HE3	2.18	0.74
1:A:103:VAL:CB	1:A:106:ILE:HD13	2.10	0.73
1:A:204:SER:CA	1:A:206:LYS:HE2	2.18	0.73
1:A:299[A]:ARG:HG2	1:A:310:PRO:HA	1.72	0.72
1:A:331:LYS:HG3	1:A:332:ASP:OD1	1.89	0.72
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.25	0.72
1:A:200:PHE:CE2	1:A:259:LEU:HD23	2.25	0.71
1:A:294:ASN:ND2	1:A:297:THR:H	1.88	0.71
1:A:159:GLN:HG3	1:A:177:VAL:CG2	2.21	0.71
1:A:135:HIS:ND1	1:A:228:LEU:HB3	2.06	0.71
1:A:270:LEU:HD11	1:A:282:MET:HE1	1.71	0.71
1:A:292:THR:HG22	1:A:301:LEU:HD11	1.72	0.71
1:A:133:ASN:HD22	1:A:135:HIS:N	1.87	0.70
1:A:277:ILE:HD13	1:A:277:ILE:N	2.05	0.70
1:A:260:ILE:HG22	1:A:261:PRO:O	1.91	0.70
1:A:292:THR:HG22	1:A:301:LEU:CD1	2.20	0.70
1:A:277:ILE:HG12	1:A:335:GLU:HA	1.72	0.70
1:A:155:MET:SD	1:A:158:MET:HE2	2.32	0.70
1:A:329:GLU:HB3	3:A:429:HOH:O	1.93	0.69
1:A:224:ILE:HD13	1:A:235:PHE:CE1	2.27	0.69
1:A:104:THR:HG22	3:A:435:HOH:O	1.93	0.68
1:A:175:ALA:HB2	1:A:195:LEU:HD12	1.76	0.68
1:A:133:ASN:ND2	1:A:135:HIS:N	2.39	0.68
1:A:278:PHE:HB2	1:A:333:ARG:O	1.94	0.68
1:A:159:GLN:HG2	1:A:159:GLN:O	1.92	0.68
1:A:103:VAL:HB	1:A:106:ILE:CD1	2.12	0.68
1:A:108:PRO:O	1:A:112:ARG:HG3	1.94	0.67
1:A:287:LEU:HD12	1:A:287:LEU:O	1.95	0.67
1:A:299[A]:ARG:HG3	1:A:299[A]:ARG:NH1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PRO:HD3	1:A:311:LEU:CD2	2.25	0.67
1:A:145:ASP:CG	1:A:252:HIS:H	2.03	0.66
1:A:158:MET:C	1:A:191:MET:HE1	2.20	0.66
1:A:213:ARG:HD3	3:A:444:HOH:O	1.94	0.66
1:A:144:GLU:OE1	1:A:144:GLU:N	2.29	0.66
1:A:289:LYS:HZ3	1:A:324:GLN:HG3	1.59	0.66
1:A:292:THR:CB	1:A:301:LEU:HD11	2.26	0.66
1:A:137:ARG:NE	3:A:445:HOH:O	2.29	0.65
1:A:204:SER:HA	1:A:206:LYS:HE2	1.78	0.65
1:A:212:HIS:CD2	1:A:230:LYS:HE3	2.32	0.65
1:A:92:ASP:O	1:A:95:SER:HB3	1.95	0.65
1:A:167:LYS:HA	3:A:406:HOH:O	1.97	0.65
1:A:172:GLU:HG2	1:A:198:PRO:HG3	1.80	0.64
1:A:277:ILE:HD11	1:A:334:SER:O	1.98	0.64
1:A:172:GLU:CG	1:A:198:PRO:HG3	2.28	0.64
1:A:289:LYS:HD2	1:A:323:ILE:O	1.97	0.64
1:A:295:GLU:CD	1:A:295:GLU:H	2.06	0.64
1:A:106:ILE:HG22	1:A:111:ALA:HB2	1.80	0.64
1:A:177:VAL:HG23	3:A:424:HOH:O	1.97	0.64
1:A:292:THR:CG2	1:A:301:LEU:HD11	2.27	0.63
1:A:286:ALA:CB	1:A:323:ILE:HG21	2.28	0.63
1:A:281:ASN:O	1:A:284:ALA:HB3	1.99	0.63
1:A:142:TYR:O	1:A:146:PHE:HB2	1.98	0.63
1:A:175:ALA:HB2	1:A:195:LEU:CD1	2.28	0.63
1:A:197:HIS:ND1	1:A:198:PRO:HD2	2.13	0.63
1:A:114:LEU:HD12	1:A:114:LEU:N	2.15	0.62
1:A:289:LYS:HZ2	1:A:324:GLN:HG3	1.63	0.62
1:A:125:LEU:O	1:A:128:ASN:N	2.32	0.62
1:A:158:MET:HE2	1:A:191:MET:HE3	1.81	0.62
1:A:159:GLN:NE2	3:A:514:HOH:O	2.30	0.62
1:A:158:MET:HE3	1:A:191:MET:HE3	1.80	0.62
1:A:158:MET:CB	1:A:191:MET:HE1	2.26	0.61
1:A:98:ASN:O	1:A:101:THR:HG22	2.00	0.61
1:A:170:ASP:O	1:A:173:TYR:HB2	2.00	0.61
1:A:106:ILE:HD12	1:A:106:ILE:N	2.14	0.61
1:A:155:MET:HB3	1:A:181:PHE:CE2	2.35	0.61
1:A:104:THR:O	1:A:106:ILE:HD12	2.01	0.61
1:A:294:ASN:HD22	1:A:297:THR:H	1.48	0.61
1:A:154:GLU:HG2	1:A:250:TYR:HE2	1.65	0.60
1:A:122:LEU:O	1:A:125:LEU:HB2	2.01	0.60
1:A:200:PHE:HD1	1:A:204:SER:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HE1	1:A:282:MET:CE	2.03	0.60
1:A:150:ILE:HD11	3:A:411:HOH:O	2.00	0.60
1:A:208:PRO:HB3	1:A:232:GLU:HA	1.84	0.59
1:A:100:LEU:O	1:A:103:VAL:HG23	2.03	0.58
1:A:223:PHE:CE1	1:A:239:CYS:HB2	2.37	0.58
1:A:323:ILE:C	1:A:324:GLN:HG2	2.28	0.58
1:A:280:LYS:O	1:A:284:ALA:HB2	2.03	0.58
1:A:331:LYS:O	1:A:333:ARG:N	2.36	0.57
1:A:100:LEU:HD11	1:A:120:LYS:O	2.04	0.57
1:A:212:HIS:HD2	1:A:230:LYS:HE3	1.69	0.57
1:A:137:ARG:HD3	3:A:434:HOH:O	2.03	0.57
1:A:159:GLN:N	1:A:191:MET:HE1	2.19	0.57
1:A:293:ILE:HD11	1:A:298:ILE:HD12	1.87	0.56
1:A:106:ILE:CG2	1:A:111:ALA:HB2	2.35	0.56
1:A:211:LEU:O	1:A:215:VAL:HG23	2.05	0.56
1:A:277:ILE:H	1:A:277:ILE:CD1	2.13	0.56
1:A:271:TYR:HB2	3:A:403:HOH:O	2.05	0.56
1:A:283:ARG:NE	1:A:293:ILE:O	2.38	0.56
1:A:303:VAL:C	1:A:305:GLY:H	2.14	0.56
1:A:328:ARG:HD3	1:A:332:ASP:O	2.06	0.56
1:A:172:GLU:HG2	1:A:198:PRO:CG	2.35	0.56
1:A:194:LEU:HD21	1:A:272:PHE:CD2	2.40	0.56
1:A:260:ILE:HG21	1:A:265:TYR:HA	1.88	0.56
1:A:291:PHE:CA	1:A:301:LEU:HD13	2.37	0.55
1:A:263:ASP:N	1:A:263:ASP:OD1	2.36	0.55
1:A:332:ASP:OD1	1:A:332:ASP:N	2.38	0.55
1:A:110:ALA:O	1:A:113:LYS:HG2	2.06	0.55
1:A:125:LEU:CB	1:A:140:LEU:HD22	2.31	0.54
1:A:122:LEU:HD12	1:A:123:GLU:N	2.22	0.54
1:A:200:PHE:CD1	1:A:204:SER:HB2	2.42	0.54
1:A:99:PHE:O	1:A:102:ARG:HB2	2.08	0.54
1:A:132:LEU:HA	3:A:471:HOH:O	2.07	0.54
1:A:188:SER:HB3	3:A:501:HOH:O	2.06	0.54
1:A:264:GLN:HG2	3:A:504:HOH:O	2.07	0.54
1:A:239:CYS:SG	1:A:255:ILE:HB	2.48	0.54
1:A:285:HIS:O	1:A:288:GLU:N	2.35	0.54
1:A:92:ASP:HA	1:A:95:SER:HB2	1.90	0.53
1:A:196:THR:OG1	1:A:260:ILE:O	2.22	0.53
1:A:113:LYS:HG3	1:A:114:LEU:CD1	2.35	0.53
1:A:135:HIS:HE1	1:A:228:LEU:HB3	1.68	0.53
1:A:127:LYS:HD3	1:A:127:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:HA	1:A:301:LEU:HD13	1.91	0.53
1:A:170:ASP:OD2	1:A:197:HIS:NE2	2.27	0.53
1:A:193:VAL:O	1:A:194:LEU:HD12	2.08	0.53
1:A:291:PHE:HD1	1:A:300:PRO:HA	1.73	0.53
1:A:183:ARG:HD2	1:A:333:ARG:HB2	1.91	0.53
1:A:196:THR:HG23	1:A:197:HIS:N	2.23	0.53
1:A:292:THR:HB	1:A:301:LEU:HD11	1.90	0.53
1:A:285:HIS:CD2	1:A:325:TRP:NE1	2.78	0.52
1:A:296:TYR:C	1:A:297:THR:HG23	2.34	0.52
1:A:301:LEU:HD12	1:A:301:LEU:N	2.23	0.52
1:A:159:GLN:HG3	1:A:177:VAL:HG21	1.90	0.52
1:A:223:PHE:CZ	1:A:239:CYS:HB2	2.45	0.51
1:A:300:PRO:HD3	1:A:311:LEU:HD22	1.92	0.51
1:A:158:MET:HE3	1:A:191:MET:CE	2.39	0.51
1:A:163:LEU:HD13	3:A:506:HOH:O	2.09	0.51
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.75	0.51
1:A:137:ARG:HB2	3:A:434:HOH:O	2.09	0.51
1:A:142:TYR:CE1	1:A:252:HIS:CG	2.98	0.51
1:A:135:HIS:HD1	1:A:228:LEU:HB3	1.72	0.51
1:A:300:PRO:HD3	1:A:311:LEU:HD21	1.92	0.51
1:A:129:GLU:HA	1:A:132:LEU:HD12	1.92	0.51
1:A:207:GLN:O	1:A:210:LEU:HB2	2.11	0.51
1:A:292:THR:N	1:A:301:LEU:HD11	2.25	0.51
1:A:110:ALA:HA	1:A:113:LYS:HE3	1.91	0.51
1:A:174:ILE:HA	3:A:427:HOH:O	2.10	0.51
1:A:91:ASP:C	1:A:93:THR:H	2.17	0.51
1:A:155:MET:HE1	1:A:190:ASP:O	2.11	0.51
1:A:201:THR:C	1:A:203:GLU:H	2.19	0.51
1:A:133:ASN:HD22	1:A:134:HIS:N	2.09	0.50
1:A:232:GLU:C	1:A:233:THR:HG23	2.36	0.50
1:A:120:LYS:N	1:A:124:ASP:OD2	2.35	0.50
1:A:133:ASN:N	3:A:471:HOH:O	2.45	0.50
1:A:154:GLU:HG2	1:A:250:TYR:CE2	2.47	0.50
1:A:156:LEU:HD12	1:A:181:PHE:CZ	2.47	0.50
1:A:183:ARG:NH1	1:A:275:SER:HA	2.26	0.50
1:A:285:HIS:O	1:A:288:GLU:HB2	2.12	0.50
1:A:204:SER:HB3	1:A:207:GLN:HE21	1.77	0.50
1:A:254:ARG:NH1	1:A:256:ASP:OD1	2.45	0.49
1:A:133:ASN:HD22	1:A:133:ASN:C	2.19	0.49
1:A:110:ALA:O	1:A:114:LEU:HD13	2.12	0.49
1:A:142:TYR:CE1	1:A:252:HIS:ND1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:HB2	1:A:177:VAL:HG21	1.94	0.49
1:A:189:GLY:O	1:A:190:ASP:HB3	2.12	0.49
1:A:299[A]:ARG:HG2	1:A:310:PRO:CA	2.42	0.49
1:A:292:THR:HG22	1:A:301:LEU:HD12	1.93	0.49
1:A:285:HIS:CE1	1:A:289:LYS:HG3	2.48	0.49
1:A:172:GLU:HG3	1:A:198:PRO:HG3	1.95	0.49
1:A:291:PHE:CD1	1:A:300:PRO:HA	2.48	0.49
1:A:299[B]:ARG:HG2	1:A:310:PRO:HA	1.95	0.49
1:A:204:SER:C	1:A:206:LYS:HE2	2.38	0.48
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.95	0.48
1:A:138:ILE:HB	1:A:228:LEU:HD23	1.96	0.48
1:A:235:PHE:CE1	1:A:237:GLY:HA3	2.48	0.48
1:A:96:SER:O	1:A:99:PHE:N	2.46	0.48
1:A:254:ARG:NH2	1:A:256:ASP:OD1	2.44	0.48
1:A:227:THR:HG22	1:A:228:LEU:N	2.28	0.48
1:A:183:ARG:NH1	1:A:275:SER:CA	2.77	0.48
1:A:133:ASN:HD21	1:A:135:HIS:CB	2.26	0.48
1:A:193:VAL:C	1:A:194:LEU:HD12	2.39	0.48
1:A:159:GLN:HG3	1:A:177:VAL:HG23	1.94	0.48
1:A:224:ILE:HD13	1:A:235:PHE:CZ	2.47	0.48
1:A:319:ILE:HG21	1:A:319:ILE:HD13	1.50	0.47
1:A:250:TYR:HB3	1:A:251:PRO:HD2	1.97	0.47
1:A:180:SER:OG	1:A:181:PHE:N	2.47	0.47
1:A:197:HIS:ND1	1:A:198:PRO:CD	2.77	0.47
1:A:215:VAL:HG11	1:A:235:PHE:CD2	2.50	0.47
1:A:223:PHE:CZ	1:A:239:CYS:CB	2.98	0.47
1:A:197:HIS:CG	1:A:199:ASN:HB2	2.49	0.47
1:A:234:LYS:HE3	1:A:236:MET:CG	2.40	0.47
1:A:299[B]:ARG:HG2	1:A:310:PRO:N	2.29	0.47
1:A:328:ARG:HG3	3:A:430:HOH:O	2.14	0.47
1:A:278:PHE:HE2	1:A:328:ARG:CD	2.09	0.47
1:A:212:HIS:CD2	1:A:230:LYS:CE	2.98	0.47
1:A:91:ASP:O	1:A:94:SER:N	2.48	0.46
1:A:300:PRO:C	1:A:301:LEU:HD12	2.40	0.46
1:A:181:PHE:CD1	1:A:181:PHE:C	2.93	0.46
1:A:330:PRO:HA	1:A:333:ARG:NE	2.30	0.46
1:A:150:ILE:HA	1:A:151:PRO:HD2	1.69	0.46
1:A:183:ARG:HH12	1:A:275:SER:HA	1.79	0.46
1:A:114:LEU:N	1:A:114:LEU:CD1	2.79	0.46
1:A:331:LYS:HG2	3:A:429:HOH:O	2.14	0.46
1:A:208:PRO:HB3	1:A:232:GLU:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:HB2	1:A:295:GLU:OE2	2.15	0.46
1:A:279:ASN:O	1:A:283:ARG:HG2	2.16	0.45
1:A:292:THR:N	1:A:301:LEU:CD1	2.78	0.45
1:A:271:TYR:N	3:A:403:HOH:O	2.50	0.45
1:A:300:PRO:HD3	1:A:311:LEU:CD1	2.46	0.45
1:A:91:ASP:O	1:A:94:SER:HB3	2.17	0.45
1:A:285:HIS:NE2	1:A:289:LYS:HD2	2.31	0.45
1:A:289:LYS:CE	1:A:324:GLN:HG3	2.46	0.45
1:A:149:ARG:HE	1:A:149:ARG:HB3	1.53	0.45
1:A:204:SER:O	1:A:205:SER:HB2	2.17	0.45
1:A:323:ILE:O	1:A:324:GLN:HG2	2.17	0.45
1:A:163:LEU:CD2	1:A:175:ALA:HB3	2.47	0.45
1:A:163:LEU:HD21	1:A:175:ALA:HB3	1.99	0.45
1:A:179:GLY:O	1:A:182:ARG:N	2.44	0.45
1:A:227:THR:CG2	1:A:228:LEU:N	2.80	0.45
1:A:228:LEU:N	1:A:236:MET:O	2.43	0.45
1:A:254:ARG:HH22	1:A:256:ASP:CG	2.23	0.45
1:A:257:ILE:C	1:A:258:ARG:HG3	2.42	0.45
1:A:120:LYS:H	1:A:124:ASP:CG	2.22	0.44
1:A:121:THR:O	1:A:124:ASP:HB2	2.17	0.44
1:A:234:LYS:O	1:A:234:LYS:HG2	2.12	0.44
1:A:122:LEU:O	1:A:125:LEU:N	2.50	0.44
1:A:201:THR:C	1:A:203:GLU:N	2.75	0.44
1:A:113:LYS:O	1:A:117:GLU:HG2	2.17	0.44
1:A:104:THR:O	1:A:106:ILE:N	2.50	0.44
1:A:207:GLN:N	1:A:208:PRO:HD3	2.33	0.44
1:A:208:PRO:O	1:A:212:HIS:ND1	2.50	0.44
1:A:306:VAL:O	1:A:307:ALA:HB2	2.16	0.44
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.54	0.43
1:A:316:GLU:O	1:A:319:ILE:HB	2.18	0.43
1:A:111:ALA:O	1:A:115:VAL:HG23	2.18	0.43
1:A:127:LYS:O	1:A:128:ASN:ND2	2.52	0.43
1:A:156:LEU:HD12	1:A:181:PHE:HZ	1.83	0.43
1:A:207:GLN:HB2	1:A:210:LEU:HD12	2.01	0.43
1:A:289:LYS:HD3	1:A:324:GLN:CG	2.49	0.43
1:A:237:GLY:C	1:A:238:VAL:HG23	2.44	0.43
1:A:138:ILE:HD12	1:A:226:ASP:OD2	2.19	0.42
1:A:146:PHE:N	1:A:146:PHE:HD1	2.18	0.42
1:A:205:SER:O	1:A:206:LYS:HB3	2.19	0.42
1:A:278:PHE:CD1	1:A:278:PHE:C	2.97	0.42
1:A:99:PHE:CD1	1:A:99:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLY:O	1:A:111:ALA:N	2.44	0.42
1:A:159:GLN:CG	1:A:177:VAL:HG21	2.49	0.42
1:A:145:ASP:CB	1:A:252:HIS:H	2.32	0.42
1:A:142:TYR:CD1	1:A:252:HIS:HB2	2.54	0.42
1:A:154:GLU:CG	1:A:250:TYR:HE2	2.31	0.42
1:A:200:PHE:CD2	1:A:259:LEU:HD23	2.53	0.42
1:A:105:GLY:HA2	1:A:135:HIS:HD2	1.85	0.42
1:A:250:TYR:N	1:A:250:TYR:CD1	2.86	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.94	0.42
1:A:206:LYS:C	1:A:207:GLN:HG3	2.44	0.42
1:A:291:PHE:C	1:A:301:LEU:HD13	2.45	0.42
1:A:194:LEU:HB3	1:A:265:TYR:HE1	1.85	0.42
1:A:311:LEU:CD1	1:A:311:LEU:N	2.82	0.42
1:A:169:LEU:HD21	1:A:217:GLN:HE21	1.85	0.41
1:A:204:SER:HA	1:A:206:LYS:CE	2.47	0.41
1:A:225:THR:O	1:A:226:ASP:OD1	2.38	0.41
1:A:146:PHE:N	1:A:146:PHE:CD1	2.88	0.41
1:A:299[B]:ARG:HG2	1:A:310:PRO:CA	2.50	0.41
1:A:122:LEU:O	1:A:126:ARG:HG3	2.20	0.41
1:A:163:LEU:HD21	1:A:175:ALA:O	2.20	0.41
1:A:92:ASP:C	1:A:95:SER:HB3	2.44	0.41
1:A:127:LYS:C	1:A:128:ASN:ND2	2.79	0.41
1:A:193:VAL:HG12	1:A:194:LEU:N	2.34	0.41
1:A:112:ARG:O	1:A:115:VAL:HG23	2.20	0.41
1:A:207:GLN:HA	3:A:473:HOH:O	2.20	0.41
1:A:215:VAL:O	1:A:219:GLN:HG2	2.21	0.41
1:A:271:TYR:CD1	1:A:271:TYR:C	2.98	0.41
1:A:114:LEU:HD12	1:A:114:LEU:H	1.86	0.41
1:A:91:ASP:C	1:A:93:THR:N	2.79	0.41
1:A:271:TYR:CG	1:A:295:GLU:HB3	2.56	0.41
1:A:299[B]:ARG:HD2	3:A:459:HOH:O	2.21	0.41
1:A:104:THR:N	3:A:435:HOH:O	2.27	0.40
1:A:217:GLN:O	1:A:220:LYS:HB3	2.21	0.40
1:A:285:HIS:HE2	1:A:289:LYS:HD2	1.86	0.40
1:A:104:THR:C	1:A:106:ILE:H	2.28	0.40
1:A:254:ARG:CZ	1:A:254:ARG:HB3	2.50	0.40
1:A:166:VAL:CG1	1:A:173:TYR:HB3	2.52	0.40
1:A:274:GLY:HA3	1:A:275:SER:HA	1.91	0.40
1:A:158:MET:CA	1:A:191:MET:HE1	2.51	0.40
1:A:270:LEU:CD1	1:A:282:MET:HE1	2.48	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:477:HOH:O	3:A:477:HOH:O[2_555]	0.85	1.35
1:A:206:LYS:NZ	1:A:206:LYS:NZ[2_555]	1.92	0.28

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	239/248 (96%)	191 (80%)	35 (15%)	13 (5%)	1 2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLU
1	A	204	SER
1	A	206	LYS
1	A	309	GLU
1	A	146	PHE
1	A	205	SER
1	A	180	SER
1	A	310	PRO
1	A	145	ASP
1	A	202	SER
1	A	125	LEU
1	A	126	ARG
1	A	238	VAL

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	207/226 (92%)	179 (86%)	28 (14%)	4 9

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	106	ILE
1	A	115	VAL
1	A	122	LEU
1	A	125	LEU
1	A	133	ASN
1	A	156	LEU
1	A	158	MET
1	A	159	GLN
1	A	168	LYS
1	A	173	TYR
1	A	188	SER
1	A	196	THR
1	A	203	GLU
1	A	215	VAL
1	A	219	GLN
1	A	255	ILE
1	A	259	LEU
1	A	269	VAL
1	A	277	ILE
1	A	288	GLU
1	A	294	ASN
1	A	295	GLU
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	311	LEU
1	A	317	GLN
1	A	332	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	135	HIS
1	A	136	GLN
1	A	159	GLN
1	A	207	GLN
1	A	217	GLN
1	A	264	GLN
1	A	279	ASN
1	A	281	ASN
1	A	294	ASN
1	A	317	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	242/248 (97%)	0.75	26 (10%) 11 9	10, 39, 87, 100	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	SER	5.3
1	A	306	VAL	4.2
1	A	111	ALA	3.9
1	A	304	THR	3.7
1	A	93	THR	3.4
1	A	91	ASP	3.4
1	A	124	ASP	3.1
1	A	119	ILE	3.0
1	A	299[A]	ARG	3.0
1	A	179	GLY	2.9
1	A	115	VAL	2.8
1	A	305	GLY	2.8
1	A	109	SER	2.7
1	A	204	SER	2.6
1	A	122	LEU	2.4
1	A	288	GLU	2.2
1	A	294	ASN	2.2
1	A	189	GLY	2.2
1	A	290	GLY	2.2
1	A	287	LEU	2.1
1	A	96	SER	2.1
1	A	244	GLU	2.1
1	A	113	LYS	2.1
1	A	214	VAL	2.1
1	A	116	ASP	2.0
1	A	99	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	340	1/1	0.69	0.09	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.