



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:13 PM UTC

PDB ID : 2OZK / pdb_00002ozk
Title : Structure of an N-Terminal Truncated Form of Nendou (NSP15) From SARS-CORONAVIRUS
Authors : Saikatendu, K.; Joseph, J.; Subramanian, V.; Neuman, B.; Buchmeier, M.; Stevens, R.C.; Kuhn, P.
Deposited on : 2007-02-26
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

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

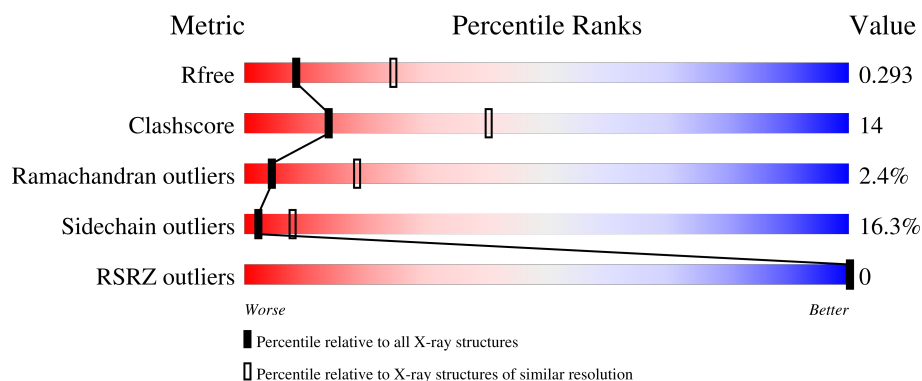
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 ≥ 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	346	 58% 26% 5% 12%
1	B	346	 59% 25% 5% 12%
1	C	346	 53% 24% 5% 16%
1	D	346	 49% 30% 6% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9402 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.

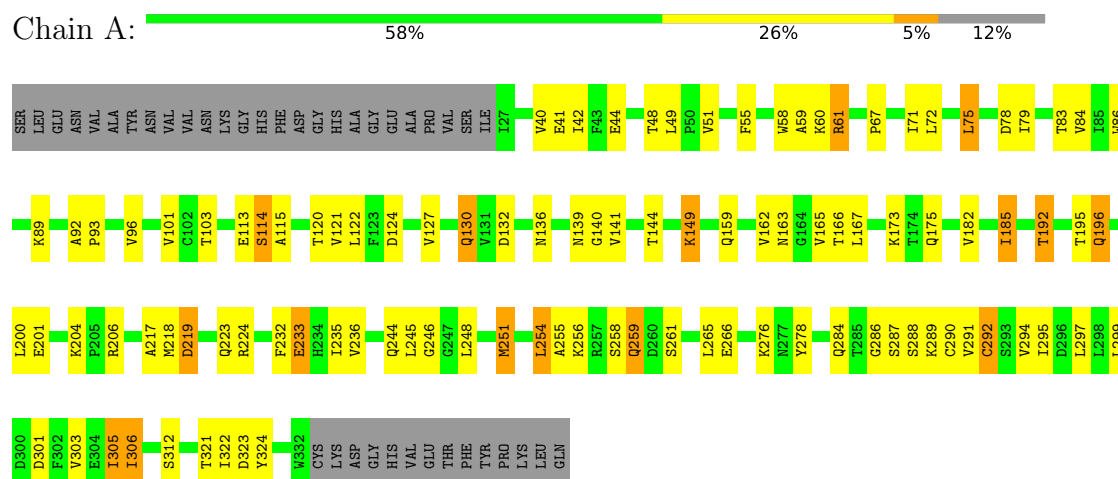
- Molecule 1 is a protein called Uridylate-specific endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2402	1538	391	463	10			
1	B	305	Total	C	N	O	S	0	0	0
			2394	1532	390	462	10			
1	C	291	Total	C	N	O	S	0	0	0
			2294	1473	371	440	10			
1	D	296	Total	C	N	O	S	0	0	0
			2312	1485	374	443	10			

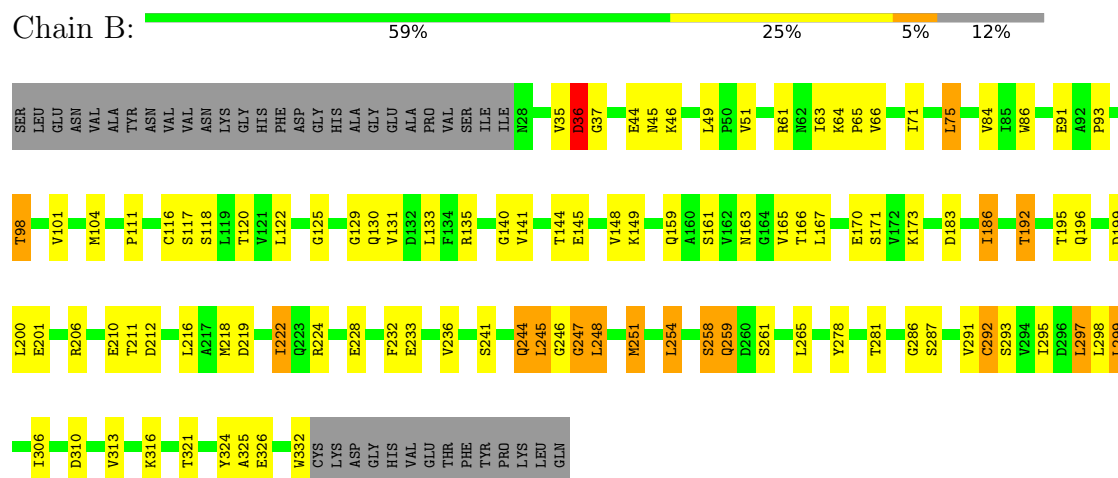
3 Residue-property plots

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: Uridylate-specific endoribonuclease

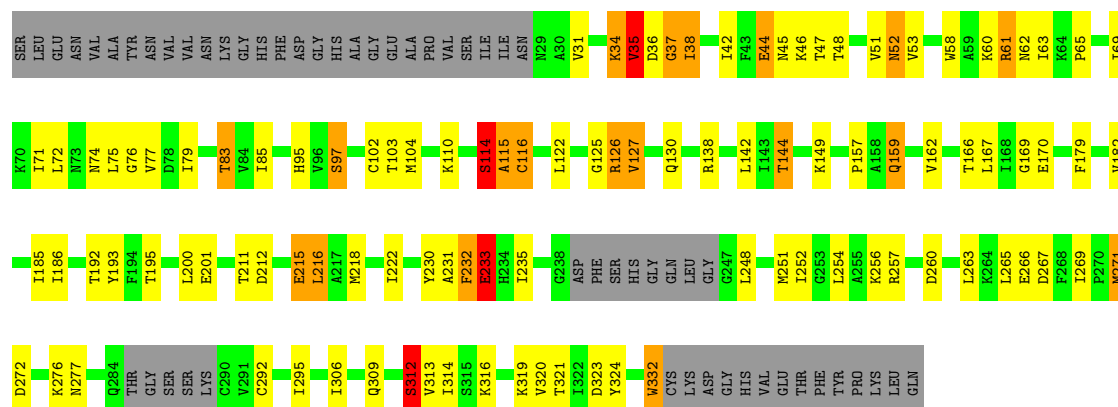


• Molecule 1: Uridylate-specific endoribonuclease

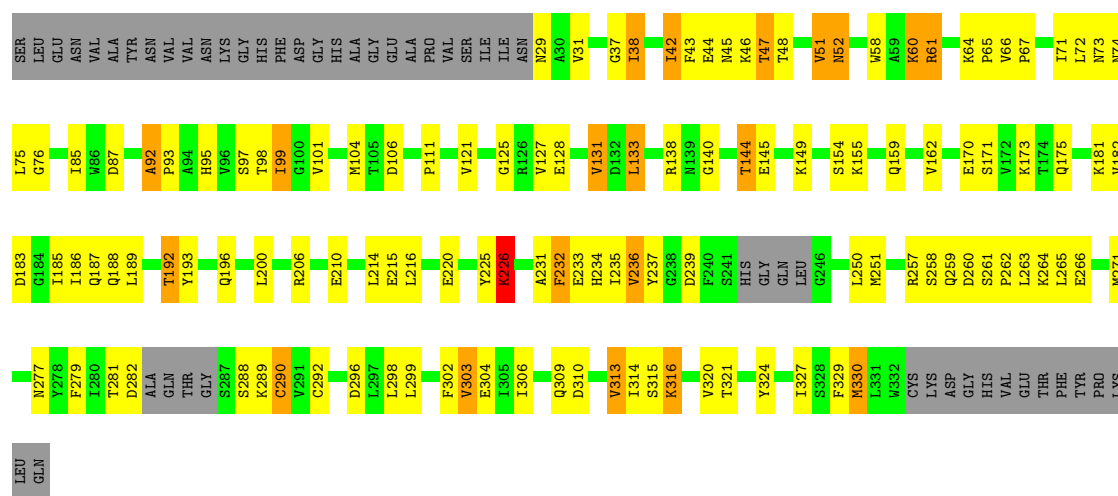


• Molecule 1: Uridylate-specific endoribonuclease





• Molecule 1: Uridylate-specific endoribonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	98.97Å 98.97Å 214.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.75 – 2.90 85.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.75-2.90) 97.8 (85.71-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.301 0.237 , 0.293	Depositor DCC
R_{free} test set	2601 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.448 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9402	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/2447	1.00	7/3316 (0.2%)
1	B	0.71	0/2439	1.00	3/3305 (0.1%)
1	C	0.65	0/2335	0.95	4/3163 (0.1%)
1	D	0.69	0/2354	1.00	3/3190 (0.1%)
All	All	0.69	0/9575	0.99	17/12974 (0.1%)

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	C	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	140	GLY	N-CA-C	6.64	120.82	111.19
1	D	232	PHE	N-CA-C	6.34	124.31	110.80
1	A	185	ILE	N-CA-C	6.24	117.29	108.36
1	C	232	PHE	N-CA-C	5.84	123.25	110.80
1	A	162	VAL	N-CA-C	5.80	114.95	106.55
1	A	235	ILE	N-CA-C	5.24	115.51	110.74
1	B	98	THR	N-CA-C	5.16	117.70	109.81
1	A	140	GLY	N-CA-C	5.14	118.09	110.63
1	C	312	SER	CA-C-N	5.14	130.94	121.70
1	C	312	SER	C-N-CA	5.14	130.94	121.70
1	D	237	TYR	N-CA-C	5.10	120.36	114.04
1	D	92	ALA	N-CA-C	5.07	112.58	108.07
1	A	290	CYS	N-CA-C	5.05	116.96	109.69
1	C	169	GLY	N-CA-C	5.03	118.07	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LYS	CA-C-N	5.01	125.30	119.93
1	A	204	LYS	C-N-CA	5.01	125.30	119.93
1	B	170	GLU	N-CA-C	-5.00	107.30	113.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	35	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2402	0	2410	59	0
1	B	2394	0	2401	57	0
1	C	2294	0	2308	65	0
1	D	2312	0	2311	96	0
All	All	9402	0	9430	271	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 14.

All (271) 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:D:281:THR:HA	1:D:282:ASP:CB	1.80	1.10
1:D:281:THR:HA	1:D:282:ASP:HB2	1.12	1.05
1:D:281:THR:CA	1:D:282:ASP:HB2	1.94	0.96
1:D:192:THR:HG21	1:D:324:TYR:H	1.31	0.96
1:D:315:SER:HB3	1:D:330:MET:HE1	1.51	0.93
1:B:192:THR:HG21	1:B:324:TYR:H	1.31	0.92
1:C:192:THR:HG21	1:C:324:TYR:H	1.34	0.91
1:C:45:ASN:O	1:C:47:THR:N	2.03	0.91
1:D:98:THR:CG2	1:D:101:VAL:HB	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:O	1:B:36:ASP:HB3	1.73	0.89
1:A:200:LEU:HD13	1:A:251:MET:HE2	1.56	0.87
1:B:200:LEU:HD13	1:B:251:MET:HE2	1.56	0.86
1:D:234:HIS:CE1	1:D:239:ASP:HB3	2.10	0.86
1:D:234:HIS:HE1	1:D:239:ASP:HB3	1.41	0.85
1:B:36:ASP:OD1	1:B:37:GLY:N	2.08	0.85
1:D:98:THR:HG23	1:D:101:VAL:HB	1.55	0.84
1:D:188:GLN:O	1:D:189:LEU:HG	1.79	0.83
1:C:159:GLN:H	1:C:159:GLN:HE21	1.23	0.82
1:A:124:ASP:H	1:A:130:GLN:NE2	1.77	0.81
1:A:301:ASP:O	1:A:305:ILE:HG23	1.82	0.79
1:D:31:VAL:HG22	1:D:52:ASN:HB2	1.66	0.78
1:D:44:GLU:CB	1:D:45:ASN:HA	2.14	0.77
1:C:309:GLN:HE21	1:C:316:LYS:HD3	1.49	0.77
1:C:312:SER:HB2	1:C:313:VAL:C	2.09	0.76
1:C:312:SER:HB2	1:C:314:ILE:N	2.02	0.75
1:A:192:THR:HG21	1:A:324:TYR:H	1.52	0.74
1:D:192:THR:HG23	1:D:321:THR:HG22	1.69	0.73
1:C:312:SER:HB2	1:C:313:VAL:CA	2.18	0.73
1:B:61:ARG:NH1	1:B:163:ASN:ND2	2.36	0.73
1:B:61:ARG:HH12	1:B:163:ASN:ND2	1.86	0.73
1:D:314:ILE:O	1:D:316:LYS:NZ	2.22	0.72
1:D:98:THR:HG22	1:D:106:ASP:HB3	1.70	0.72
1:C:192:THR:HG22	1:C:193:TYR:O	1.90	0.72
1:B:61:ARG:NH1	1:B:163:ASN:HD21	1.89	0.70
1:B:192:THR:CG2	1:B:324:TYR:H	2.04	0.70
1:B:291:VAL:O	1:B:292:CYS:HB3	1.91	0.70
1:A:58:TRP:O	1:A:61:ARG:HG3	1.91	0.70
1:C:45:ASN:C	1:C:47:THR:H	1.96	0.70
1:C:44:GLU:HB3	1:C:45:ASN:O	1.93	0.69
1:A:61:ARG:HG2	1:A:86:TRP:HB2	1.73	0.69
1:C:277:ASN:HA	1:C:292:CYS:O	1.93	0.68
1:B:61:ARG:HH12	1:B:163:ASN:HD21	1.40	0.68
1:D:281:THR:CA	1:D:282:ASP:CB	2.64	0.68
1:D:316:LYS:NZ	1:D:316:LYS:HB2	2.08	0.68
1:C:51:VAL:HG23	1:C:52:ASN:H	1.59	0.67
1:C:312:SER:HB3	1:C:316:LYS:NZ	2.11	0.65
1:D:98:THR:HG21	1:D:101:VAL:HB	1.78	0.65
1:B:259:GLN:HA	1:B:259:GLN:OE1	1.96	0.65
1:D:234:HIS:HE1	1:D:239:ASP:CB	2.08	0.65
1:B:192:THR:HG21	1:B:324:TYR:N	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLN:OE1	1:B:63:ILE:HG12	1.96	0.64
1:D:309:GLN:HB3	1:D:316:LYS:HD3	1.78	0.64
1:B:295:ILE:HG12	1:B:297:LEU:HD23	1.78	0.64
1:C:65:PRO:HB3	1:C:162:VAL:HG22	1.80	0.64
1:C:127:VAL:HG23	1:C:130:GLN:HG3	1.79	0.64
1:B:218:MET:HE2	1:B:233:GLU:HB2	1.79	0.63
1:A:276:LYS:HB3	1:A:278:TYR:CE1	2.34	0.63
1:D:235:ILE:HD11	1:D:302:PHE:HZ	1.64	0.63
1:D:289:LYS:H	1:D:290:CYS:HA	1.64	0.63
1:B:245:LEU:HD23	1:D:329:PHE:HA	1.80	0.62
1:B:196:GLN:HE21	1:B:206:ARG:HD2	1.64	0.61
1:A:127:VAL:CG2	1:A:130:GLN:HG3	2.30	0.61
1:D:303:VAL:HA	1:D:306:ILE:HD12	1.81	0.61
1:B:111:PRO:HD2	1:B:133:LEU:HD22	1.83	0.61
1:D:37:GLY:HA2	1:D:38:ILE:O	2.00	0.61
1:D:44:GLU:HB3	1:D:45:ASN:CA	2.31	0.61
1:D:192:THR:CG2	1:D:324:TYR:H	2.11	0.60
1:C:65:PRO:O	1:C:126:ARG:NH2	2.33	0.60
1:D:192:THR:HG22	1:D:193:TYR:O	2.01	0.60
1:C:212:ASP:HB3	1:C:216:LEU:HD23	1.83	0.60
1:D:44:GLU:CB	1:D:45:ASN:CA	2.80	0.60
1:D:95:HIS:HD2	1:D:97:SER:O	1.83	0.60
1:A:192:THR:HG21	1:A:324:TYR:N	2.16	0.60
1:C:159:GLN:H	1:C:159:GLN:NE2	1.98	0.60
1:D:196:GLN:HE21	1:D:206:ARG:HH11	1.48	0.60
1:C:257:ARG:O	1:C:260:ASP:O	2.20	0.59
1:A:259:GLN:HE21	1:A:259:GLN:N	2.00	0.59
1:C:71:ILE:CD1	1:C:157:PRO:HG2	2.32	0.59
1:C:65:PRO:HB3	1:C:162:VAL:CG2	2.32	0.59
1:D:186:ILE:HD12	1:D:186:ILE:H	1.68	0.59
1:B:218:MET:HE1	1:B:232:PHE:HD2	1.67	0.58
1:D:125:GLY:HA2	1:D:131:VAL:HG22	1.86	0.58
1:A:127:VAL:HG23	1:A:130:GLN:HG3	1.86	0.58
1:A:259:GLN:HE21	1:A:259:GLN:H	1.51	0.58
1:D:51:VAL:HG23	1:D:52:ASN:H	1.69	0.58
1:D:65:PRO:HB3	1:D:162:VAL:HG22	1.85	0.57
1:B:129:GLY:O	1:B:133:LEU:HD12	2.05	0.57
1:B:241:SER:HB3	1:B:248:LEU:HB2	1.87	0.57
1:D:37:GLY:HA2	1:D:38:ILE:HG13	1.84	0.57
1:D:44:GLU:HB3	1:D:45:ASN:C	2.29	0.57
1:A:196:GLN:HG3	1:A:206:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ILE:HG12	1:B:297:LEU:CD2	2.34	0.57
1:C:58:TRP:O	1:C:61:ARG:HB3	2.04	0.56
1:C:31:VAL:HG22	1:C:52:ASN:HB2	1.86	0.56
1:D:315:SER:HB3	1:D:330:MET:CE	2.29	0.56
1:C:69:ILE:HA	1:C:72:LEU:HD12	1.88	0.55
1:A:61:ARG:NH1	1:A:163:ASN:ND2	2.54	0.55
1:C:51:VAL:HG23	1:C:52:ASN:N	2.21	0.55
1:C:231:ALA:O	1:C:233:GLU:N	2.39	0.55
1:C:312:SER:HB2	1:C:313:VAL:HA	1.87	0.55
1:A:124:ASP:H	1:A:130:GLN:HE22	1.55	0.55
1:A:124:ASP:N	1:A:130:GLN:HE21	2.04	0.55
1:B:196:GLN:HE21	1:B:206:ARG:HH11	1.55	0.55
1:D:231:ALA:O	1:D:233:GLU:N	2.34	0.54
1:B:254:LEU:O	1:B:258:SER:HB2	2.07	0.54
1:C:142:LEU:HD21	1:C:144:THR:HG23	1.90	0.54
1:C:312:SER:HB3	1:C:316:LYS:HZ2	1.71	0.54
1:D:196:GLN:HE21	1:D:206:ARG:NH1	2.06	0.54
1:A:124:ASP:N	1:A:130:GLN:NE2	2.50	0.53
1:B:244:GLN:CD	1:B:244:GLN:H	2.16	0.53
1:C:142:LEU:C	1:C:142:LEU:HD23	2.32	0.53
1:D:235:ILE:HD11	1:D:302:PHE:CZ	2.43	0.53
1:D:309:GLN:HE21	1:D:316:LYS:HG2	1.72	0.53
1:A:41:GLU:OE2	1:A:44:GLU:HB2	2.08	0.53
1:A:265:LEU:HD23	1:A:278:TYR:CG	2.44	0.53
1:A:192:THR:HG21	1:A:324:TYR:HA	1.91	0.52
1:D:316:LYS:HB2	1:D:316:LYS:HZ3	1.73	0.52
1:D:42:ILE:O	1:D:51:VAL:HG22	2.10	0.52
1:D:277:ASN:HA	1:D:292:CYS:O	2.10	0.52
1:D:66:VAL:HB	1:D:67:PRO:HD2	1.91	0.52
1:D:258:SER:HB2	1:D:263:LEU:H	1.75	0.52
1:D:44:GLU:HB2	1:D:45:ASN:HA	1.90	0.52
1:B:130:GLN:HA	1:B:133:LEU:HD12	1.92	0.52
1:D:47:THR:O	1:D:48:THR:HB	2.09	0.52
1:D:170:GLU:HG2	1:D:171:SER:N	2.25	0.52
1:D:196:GLN:HB2	1:D:296:ASP:OD1	2.09	0.52
1:D:183:ASP:C	1:D:185:ILE:H	2.17	0.52
1:D:200:LEU:HD23	1:D:265:LEU:HD22	1.91	0.52
1:A:79:ILE:HG23	1:A:121:VAL:HG22	1.91	0.52
1:C:230:TYR:O	1:C:313:VAL:HG23	2.09	0.52
1:A:139:ASN:OD1	1:A:182:VAL:O	2.28	0.51
1:D:155:LYS:HE2	1:D:175:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:NH1	1:A:163:ASN:HD21	2.09	0.51
1:D:74:ASN:C	1:D:76:GLY:H	2.19	0.51
1:B:244:GLN:HG3	1:B:248:LEU:HG	1.92	0.51
1:D:210:GLU:HG2	1:D:299:LEU:HB2	1.93	0.50
1:D:92:ALA:HB1	1:D:93:PRO:CD	2.42	0.50
1:D:95:HIS:CD2	1:D:97:SER:O	2.64	0.50
1:D:288:SER:HB2	1:D:290:CYS:HB3	1.93	0.50
1:A:86:TRP:CZ3	1:A:93:PRO:HD3	2.46	0.50
1:C:271:MET:CG	1:C:272:ASP:H	2.24	0.50
1:B:286:GLY:O	1:B:287:SER:C	2.55	0.49
1:C:312:SER:CB	1:C:313:VAL:HA	2.42	0.49
1:B:212:ASP:O	1:B:216:LEU:HG	2.12	0.49
1:D:125:GLY:HA3	1:D:144:THR:HG23	1.94	0.49
1:A:58:TRP:C	1:A:60:LYS:H	2.21	0.49
1:C:211:THR:O	1:C:215:GLU:HG2	2.13	0.49
1:A:113:GLU:O	1:A:114:SER:C	2.56	0.49
1:A:67:PRO:HG2	1:A:72:LEU:HD11	1.93	0.49
1:A:165:VAL:HG21	1:B:201:GLU:HB2	1.96	0.48
1:A:201:GLU:HB3	1:B:165:VAL:HG21	1.95	0.48
1:A:265:LEU:HD23	1:A:278:TYR:CD2	2.48	0.48
1:B:219:ASP:HA	1:B:222:ILE:HG12	1.95	0.48
1:D:265:LEU:HA	1:D:279:PHE:O	2.13	0.48
1:B:246:GLY:HA3	1:B:292:CYS:HA	1.94	0.48
1:D:44:GLU:HB3	1:D:46:LYS:N	2.29	0.48
1:D:99:ILE:HA	1:D:106:ASP:HB2	1.96	0.48
1:A:286:GLY:O	1:A:287:SER:C	2.56	0.48
1:B:125:GLY:HA3	1:B:144:THR:HG22	1.94	0.48
1:C:195:THR:OG1	1:C:323:ASP:OD2	2.23	0.48
1:D:182:VAL:HG23	1:D:187:GLN:HG3	1.96	0.47
1:B:145:GLU:HB2	1:B:173:LYS:HD2	1.97	0.47
1:D:60:LYS:HE3	1:D:101:VAL:O	2.15	0.47
1:A:124:ASP:H	1:A:130:GLN:HE21	1.52	0.47
1:C:248:LEU:HD21	1:C:295:ILE:HG22	1.96	0.47
1:A:60:LYS:HD3	1:A:101:VAL:HG13	1.96	0.47
1:A:61:ARG:HH11	1:A:163:ASN:ND2	2.13	0.47
1:D:289:LYS:N	1:D:290:CYS:HA	2.30	0.47
1:B:116:CYS:C	1:B:118:SER:H	2.24	0.46
1:D:251:MET:HE3	1:D:251:MET:HA	1.96	0.46
1:D:58:TRP:O	1:D:61:ARG:HB3	2.15	0.46
1:A:217:ALA:O	1:A:218:MET:C	2.59	0.46
1:A:255:ALA:O	1:A:258:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ASP:OD1	1:D:87:ASP:C	2.58	0.46
1:C:72:LEU:O	1:C:77:VAL:HG23	2.16	0.46
1:D:236:VAL:HG22	1:D:250:LEU:HD21	1.96	0.46
1:A:79:ILE:CG2	1:A:121:VAL:HG22	2.46	0.46
1:B:216:LEU:HD11	1:B:224:ARG:NH2	2.31	0.46
1:B:310:ASP:O	1:B:313:VAL:HG22	2.15	0.46
1:C:34:LYS:O	1:C:35:VAL:C	2.59	0.46
1:C:125:GLY:HA3	1:C:144:THR:HG22	1.96	0.46
1:C:45:ASN:C	1:C:47:THR:N	2.64	0.46
1:C:114:SER:O	1:C:116:CYS:N	2.49	0.46
1:C:218:MET:O	1:C:222:ILE:HG13	2.16	0.46
1:D:85:ILE:H	1:D:95:HIS:CE1	2.34	0.46
1:C:44:GLU:HB3	1:C:45:ASN:CA	2.46	0.46
1:C:79:ILE:HG23	1:C:95:HIS:CD2	2.52	0.45
1:C:142:LEU:HD22	1:C:179:PHE:CD1	2.51	0.45
1:D:67:PRO:HG2	1:D:72:LEU:HD21	1.98	0.45
1:B:61:ARG:NH1	1:B:63:ILE:HG22	2.31	0.45
1:B:84:VAL:HG23	1:B:101:VAL:HG11	1.98	0.45
1:A:113:GLU:O	1:A:115:ALA:N	2.50	0.45
1:C:312:SER:CB	1:C:313:VAL:CA	2.91	0.45
1:A:192:THR:HG21	1:A:324:TYR:CA	2.47	0.45
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.77	0.45
1:B:196:GLN:NE2	1:B:206:ARG:HH11	2.15	0.45
1:C:95:HIS:HD2	1:C:97:SER:O	2.00	0.45
1:D:263:LEU:HD23	1:D:282:ASP:HA	1.99	0.45
1:C:44:GLU:HB3	1:C:45:ASN:C	2.42	0.45
1:C:212:ASP:HB3	1:C:216:LEU:CD2	2.47	0.45
1:D:144:THR:HG22	1:D:145:GLU:OE2	2.16	0.45
1:B:332:TRP:HZ3	1:D:271:MET:HG3	1.82	0.44
1:C:159:GLN:HE21	1:C:159:GLN:N	2.04	0.44
1:D:261:SER:N	1:D:262:PRO:HD3	2.32	0.44
1:D:316:LYS:N	1:D:330:MET:HE1	2.32	0.44
1:A:75:LEU:HD13	1:A:75:LEU:HA	1.88	0.44
1:D:281:THR:HA	1:D:282:ASP:HB3	1.88	0.44
1:A:83:THR:OG1	1:A:84:VAL:N	2.51	0.44
1:C:51:VAL:CG2	1:C:52:ASN:H	2.27	0.44
1:A:71:ILE:HG22	1:A:75:LEU:HD23	2.00	0.43
1:D:309:GLN:HB3	1:D:316:LYS:CD	2.45	0.43
1:A:132:ASP:O	1:A:136:ASN:ND2	2.51	0.43
1:D:258:SER:C	1:D:260:ASP:N	2.76	0.43
1:D:92:ALA:HB1	1:D:93:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:TYR:O	1:D:226:LYS:C	2.61	0.43
1:A:58:TRP:O	1:A:60:LYS:N	2.52	0.43
1:A:92:ALA:HB1	1:A:93:PRO:HD2	2.00	0.43
1:C:62:ASN:HD22	1:C:83:THR:HG21	1.83	0.43
1:A:232:PHE:O	1:A:233:GLU:C	2.60	0.43
1:B:86:TRP:CZ3	1:B:93:PRO:HD3	2.53	0.43
1:B:210:GLU:HG2	1:B:299:LEU:HB2	2.00	0.43
1:A:149:LYS:O	1:A:149:LYS:HG2	2.19	0.43
1:C:37:GLY:HA2	1:C:38:ILE:HA	1.67	0.43
1:C:71:ILE:HD12	1:C:157:PRO:HG2	2.00	0.43
1:C:74:ASN:C	1:C:76:GLY:H	2.27	0.43
1:C:231:ALA:HB1	1:C:332:TRP:HA	2.01	0.43
1:B:316:LYS:H	1:D:73:ASN:HD22	1.67	0.43
1:D:216:LEU:HD23	1:D:220:GLU:HB3	2.00	0.43
1:A:278:TYR:O	1:A:291:VAL:HA	2.19	0.42
1:B:75:LEU:HD12	1:B:75:LEU:HA	1.66	0.42
1:C:85:ILE:H	1:C:95:HIS:HE1	1.67	0.42
1:A:301:ASP:O	1:A:305:ILE:CG2	2.62	0.42
1:D:258:SER:HB2	1:D:263:LEU:N	2.33	0.42
1:D:320:VAL:HG22	1:D:321:THR:N	2.35	0.42
1:C:85:ILE:H	1:C:95:HIS:CE1	2.37	0.42
1:D:48:THR:HG22	1:D:48:THR:O	2.19	0.42
1:D:264:LYS:HB3	1:D:281:THR:O	2.19	0.42
1:B:278:TYR:O	1:B:291:VAL:HA	2.20	0.42
1:D:43:PHE:O	1:D:51:VAL:HG13	2.20	0.42
1:D:111:PRO:HG2	1:D:133:LEU:HD23	2.01	0.42
1:A:294:VAL:HG12	1:A:295:ILE:N	2.35	0.42
1:B:321:THR:HA	1:B:325:ALA:O	2.20	0.42
1:D:214:LEU:HG	1:D:259:GLN:HE22	1.85	0.42
1:B:61:ARG:NH1	1:B:63:ILE:CG2	2.83	0.42
1:D:121:VAL:H	1:D:140:GLY:HA2	1.85	0.42
1:D:154:SER:HB2	1:D:189:LEU:HD13	2.02	0.42
1:C:313:VAL:HG22	1:C:313:VAL:O	2.20	0.41
1:C:48:THR:O	1:C:48:THR:HG22	2.19	0.41
1:A:322:ILE:O	1:A:323:ASP:HB2	2.20	0.41
1:A:60:LYS:O	1:A:61:ARG:C	2.63	0.41
1:A:246:GLY:HA3	1:A:292:CYS:HA	2.02	0.41
1:B:186:ILE:HD13	1:B:186:ILE:HA	1.91	0.41
1:B:247:GLY:N	1:B:292:CYS:HB2	2.35	0.41
1:C:216:LEU:O	1:C:256:LYS:NZ	2.51	0.41
1:D:258:SER:C	1:D:260:ASP:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLU:HB3	1:C:45:ASN:HA	2.02	0.41
1:A:256:LYS:O	1:A:259:GLN:NE2	2.51	0.41
1:A:42:ILE:HD12	1:A:55:PHE:HE1	1.86	0.41
1:B:232:PHE:O	1:B:233:GLU:C	2.63	0.41
1:D:258:SER:HB3	1:D:263:LEU:HD12	2.02	0.41
1:B:135:ARG:NH2	1:B:149:LYS:O	2.49	0.41
1:B:258:SER:O	1:B:259:GLN:C	2.63	0.41
1:C:312:SER:HB3	1:C:316:LYS:HZ3	1.86	0.41
1:C:71:ILE:CD1	1:C:157:PRO:CG	2.97	0.40
1:A:219:ASP:O	1:A:223:GLN:HB2	2.21	0.40
1:A:303:VAL:HA	1:A:306:ILE:HG23	2.01	0.40
1:B:64:LYS:HB3	1:B:65:PRO:CD	2.51	0.40
1:B:195:THR:C	1:B:196:GLN:O	2.65	0.40
1:B:91:GLU:O	1:B:91:GLU:HG3	2.21	0.40
1:C:114:SER:HB2	1:C:115:ALA:H	1.62	0.40
1:D:98:THR:HG22	1:D:106:ASP:CB	2.46	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	304/346 (88%)	267 (88%)	34 (11%)	3 (1%)	12	39
1	B	303/346 (88%)	271 (89%)	27 (9%)	5 (2%)	7	26
1	C	285/346 (82%)	240 (84%)	32 (11%)	13 (5%)	2	7
1	D	290/346 (84%)	247 (85%)	36 (12%)	7 (2%)	4	18
All	All	1182/1384 (85%)	1025 (87%)	129 (11%)	28 (2%)	4	18

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	46	LYS
1	C	115	ALA
1	C	232	PHE
1	D	52	ASN
1	D	232	PHE
1	D	310	ASP
1	D	313	VAL
1	A	59	ALA
1	A	61	ARG
1	A	114	SER
1	B	247	GLY
1	C	35	VAL
1	C	36	ASP
1	C	114	SER
1	C	116	CYS
1	C	312	SER
1	D	38	ILE
1	D	226	LYS
1	C	37	GLY
1	C	52	ASN
1	C	233	GLU
1	D	149	LYS
1	B	36	ASP
1	B	171	SER
1	B	292	CYS
1	B	117	SER
1	C	38	ILE
1	C	126	ARG

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	270/303 (89%)	225 (83%)	45 (17%)	2	7
1	B	269/303 (89%)	225 (84%)	44 (16%)	2	8
1	C	258/303 (85%)	209 (81%)	49 (19%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	258/303 (85%)	224 (87%)	34 (13%)	4 13
All	All	1055/1212 (87%)	883 (84%)	172 (16%)	2 8

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	48	THR
1	A	49	LEU
1	A	51	VAL
1	A	75	LEU
1	A	78	ASP
1	A	89	LYS
1	A	96	VAL
1	A	103	THR
1	A	120	THR
1	A	122	LEU
1	A	130	GLN
1	A	141	VAL
1	A	144	THR
1	A	149	LYS
1	A	159	GLN
1	A	166	THR
1	A	167	LEU
1	A	173	LYS
1	A	175	GLN
1	A	185	ILE
1	A	192	THR
1	A	195	THR
1	A	196	GLN
1	A	219	ASP
1	A	224	ARG
1	A	233	GLU
1	A	236	VAL
1	A	244	GLN
1	A	245	LEU
1	A	248	LEU
1	A	251	MET
1	A	254	LEU
1	A	259	GLN
1	A	261	SER
1	A	266	GLU

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Mol	Chain	Res	Type
1	A	288	SER
1	A	289	LYS
1	A	292	CYS
1	A	297	LEU
1	A	299	LEU
1	A	305	ILE
1	A	306	ILE
1	A	312	SER
1	A	321	THR
1	B	36	ASP
1	B	44	GLU
1	B	45	ASN
1	B	46	LYS
1	B	49	LEU
1	B	51	VAL
1	B	66	VAL
1	B	71	ILE
1	B	75	LEU
1	B	98	THR
1	B	104	MET
1	B	120	THR
1	B	122	LEU
1	B	131	VAL
1	B	141	VAL
1	B	148	VAL
1	B	159	GLN
1	B	161	SER
1	B	166	THR
1	B	167	LEU
1	B	183	ASP
1	B	186	ILE
1	B	192	THR
1	B	199	ASP
1	B	211	THR
1	B	222	ILE
1	B	228	GLU
1	B	236	VAL
1	B	244	GLN
1	B	245	LEU
1	B	248	LEU
1	B	251	MET
1	B	254	LEU

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Mol	Chain	Res	Type
1	B	258	SER
1	B	259	GLN
1	B	261	SER
1	B	265	LEU
1	B	281	THR
1	B	293	SER
1	B	297	LEU
1	B	298	LEU
1	B	299	LEU
1	B	306	ILE
1	B	326	GLU
1	C	34	LYS
1	C	42	ILE
1	C	44	GLU
1	C	53	VAL
1	C	60	LYS
1	C	61	ARG
1	C	63	ILE
1	C	75	LEU
1	C	83	THR
1	C	97	SER
1	C	102	CYS
1	C	103	THR
1	C	104	MET
1	C	110	LYS
1	C	114	SER
1	C	122	LEU
1	C	127	VAL
1	C	138	ARG
1	C	144	THR
1	C	149	LYS
1	C	159	GLN
1	C	166	THR
1	C	167	LEU
1	C	170	GLU
1	C	182	VAL
1	C	185	ILE
1	C	186	ILE
1	C	200	LEU
1	C	201	GLU
1	C	215	GLU
1	C	216	LEU

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Mol	Chain	Res	Type
1	C	233	GLU
1	C	235	ILE
1	C	251	MET
1	C	252	ILE
1	C	254	LEU
1	C	263	LEU
1	C	265	LEU
1	C	266	GLU
1	C	267	ASP
1	C	269	ILE
1	C	271	MET
1	C	276	LYS
1	C	306	ILE
1	C	312	SER
1	C	319	LYS
1	C	320	VAL
1	C	321	THR
1	C	332	TRP
1	D	29	ASN
1	D	42	ILE
1	D	47	THR
1	D	51	VAL
1	D	60	LYS
1	D	61	ARG
1	D	64	LYS
1	D	71	ILE
1	D	75	LEU
1	D	99	ILE
1	D	104	MET
1	D	127	VAL
1	D	128	GLU
1	D	131	VAL
1	D	133	LEU
1	D	138	ARG
1	D	144	THR
1	D	159	GLN
1	D	173	LYS
1	D	181	LYS
1	D	192	THR
1	D	215	GLU
1	D	226	LYS
1	D	236	VAL

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Mol	Chain	Res	Type
1	D	257	ARG
1	D	266	GLU
1	D	290	CYS
1	D	298	LEU
1	D	303	VAL
1	D	304	GLU
1	D	313	VAL
1	D	316	LYS
1	D	327	ILE
1	D	330	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	82	ASN
1	A	130	GLN
1	A	139	ASN
1	A	159	GLN
1	A	163	ASN
1	A	175	GLN
1	A	187	GLN
1	A	208	GLN
1	A	242	HIS
1	A	259	GLN
1	B	163	ASN
1	B	175	GLN
1	B	187	GLN
1	B	196	GLN
1	B	208	GLN
1	B	223	GLN
1	B	234	HIS
1	B	277	ASN
1	C	52	ASN
1	C	62	ASN
1	C	73	ASN
1	C	95	HIS
1	C	130	GLN
1	C	159	GLN
1	C	187	GLN
1	C	249	HIS
1	C	259	GLN

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Mol	Chain	Res	Type
1	C	309	GLN
1	D	29	ASN
1	D	82	ASN
1	D	95	HIS
1	D	130	GLN
1	D	196	GLN
1	D	234	HIS
1	D	259	GLN
1	D	309	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](#)

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	306/346 (88%)	-1.28	0 100 100	48, 63, 79, 86	0
1	B	305/346 (88%)	-1.26	0 100 100	47, 63, 79, 82	0
1	C	291/346 (84%)	-1.16	0 100 100	50, 78, 95, 103	0
1	D	296/346 (85%)	-1.13	0 100 100	55, 77, 95, 104	0
All	All	1198/1384 (86%)	-1.21	0 100 100	47, 70, 92, 104	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.