



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:51 AM UTC

PDB ID : 2C1W / pdb_00002c1w
Title : The structure of XendoU: a splicing independent snoRNA processing endoribonuclease
Authors : Renzi, F.; Caffarelli, E.; Laneve, P.; Bozzoni, I.; Brunori, M.; Vallone, B.
Deposited on : 2005-09-21
Resolution : 2.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

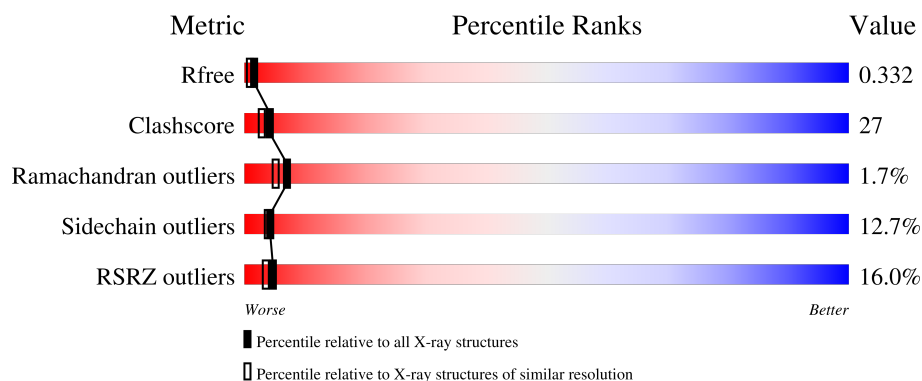
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	292	
1	B	292	
1	C	292	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1290	-	-	X	-

2 Entry composition [i](#)

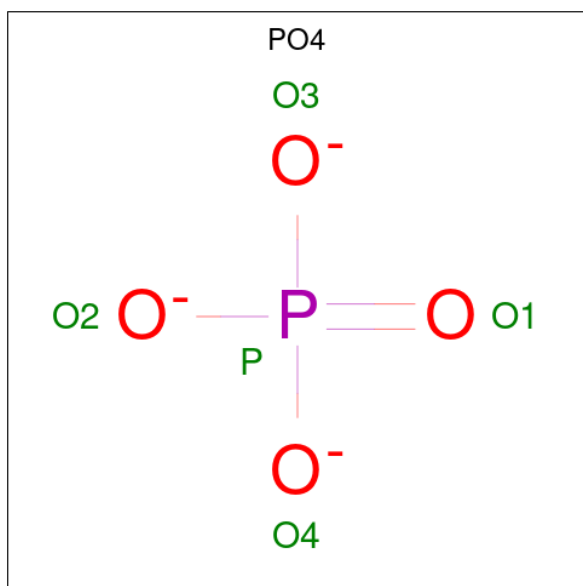
There are 3 unique types of molecules in this entry. The entry contains 7368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOU PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	7	0
			2293	1466	396	421	10			
1	B	276	Total	C	N	O	S	0	7	0
			2317	1479	401	428	9			
1	C	271	Total	C	N	O	S	0	12	0
			2305	1475	396	425	9			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

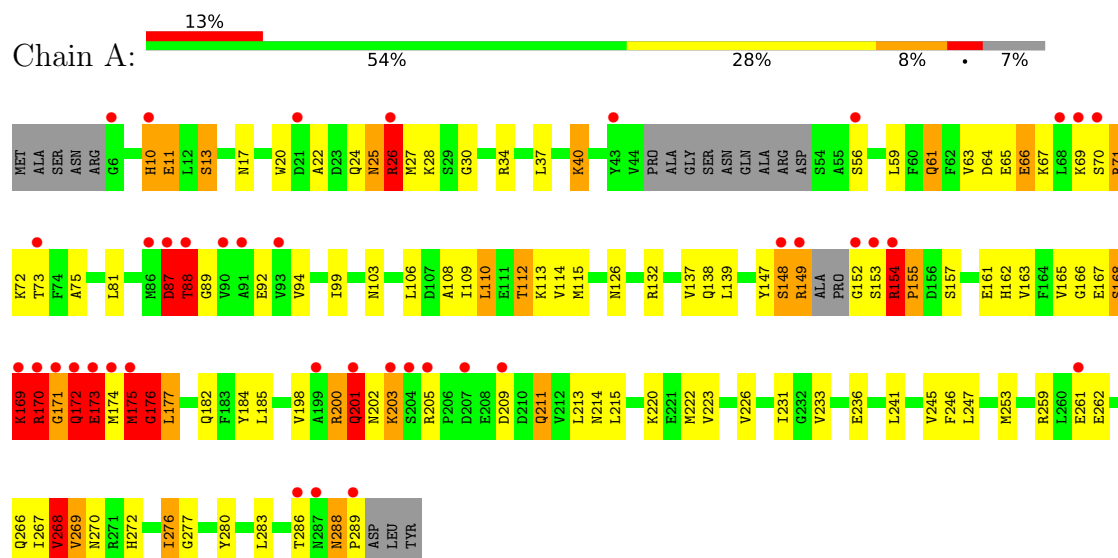
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	167	Total 167	O 167	0	0
3	C	110	Total 110	O 110	0	0

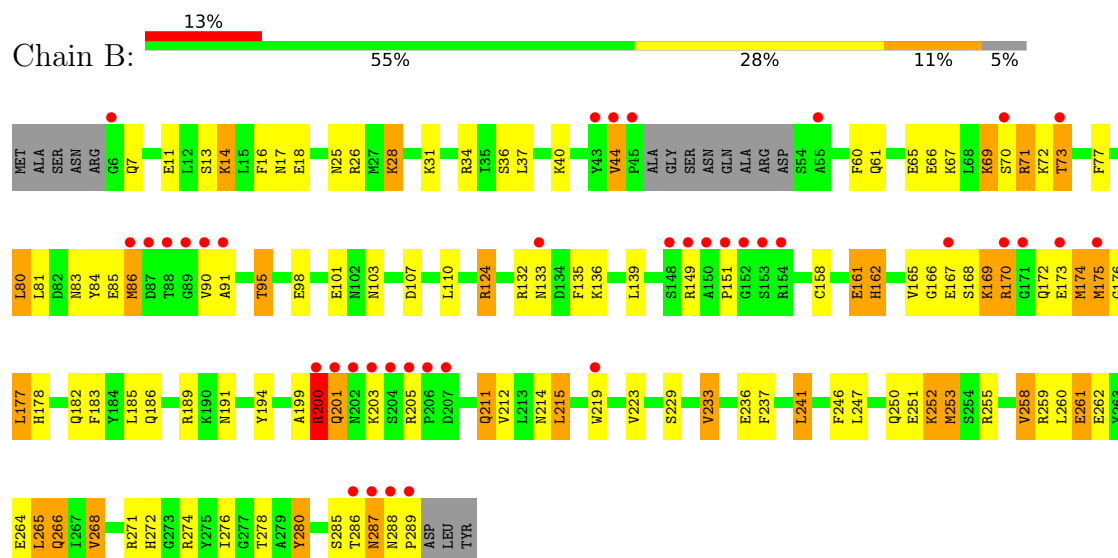
3 Residue-property plots

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: ENDOU PROTEIN

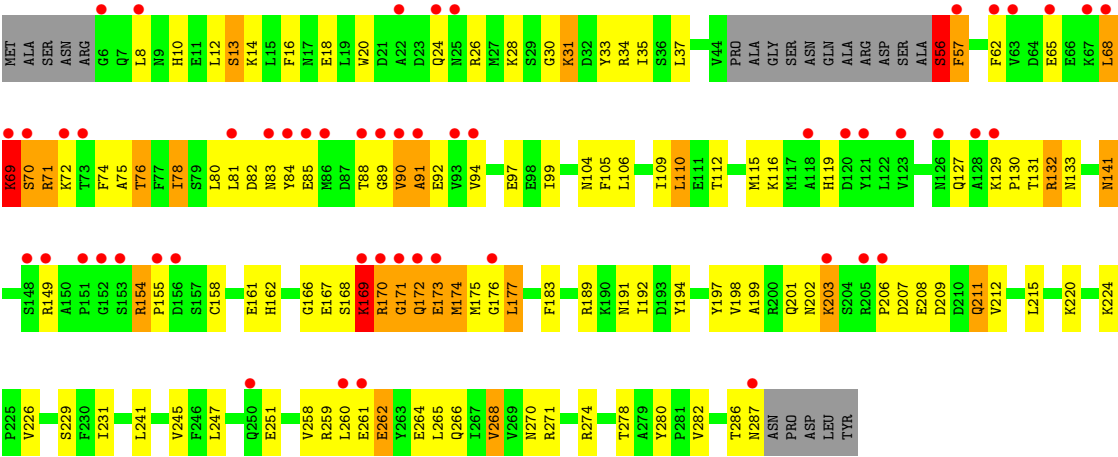


• Molecule 1: ENDOU PROTEIN



• Molecule 1: ENDOU PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.45Å 53.20Å 133.47Å 90.00° 121.86° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.20) 96.7 (20.00-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.277 0.269 , 0.332	Depositor DCC
R_{free} test set	2466 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7368	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.92	0/2363	1.32	21/3176 (0.7%)
1	B	0.93	0/2388	1.17	13/3218 (0.4%)
1	C	0.97	4/2391 (0.2%)	1.16	10/3219 (0.3%)
All	All	0.94	4/7142 (0.1%)	1.22	44/9613 (0.5%)

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	16
1	B	0	2
1	C	1	9
All	All	1	27

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133[A]	ASN	C-N	-17.83	1.11	1.33
1	C	133[B]	ASN	C-N	-17.83	1.11	1.33
1	C	264	GLU	C-N	-7.19	1.23	1.33
1	C	132	ARG	C-N	-5.21	1.26	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CB-CA-C	-17.69	81.07	110.79
1	C	70	SER	N-CA-C	17.59	139.99	113.61
1	A	169	LYS	N-CA-C	17.20	132.39	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	SER	N-CA-CB	-14.52	89.17	110.80
1	B	69	LYS	CB-CA-C	-14.16	86.58	110.22
1	B	70	SER	CB-CA-C	-13.45	90.69	110.06
1	A	170[A]	ARG	CA-C-O	13.21	134.94	118.43
1	A	170[B]	ARG	CA-C-O	13.21	134.94	118.43
1	A	88	THR	N-CA-C	-13.07	90.63	110.10
1	A	170[A]	ARG	N-CA-C	-12.91	95.01	114.64
1	A	170[B]	ARG	N-CA-C	-12.91	95.01	114.64
1	A	172	GLN	CB-CA-C	-11.82	90.25	109.75
1	B	71	ARG	N-CA-C	-10.28	88.90	110.80
1	A	173	GLU	N-CA-CB	-9.34	96.41	110.71
1	C	69	LYS	CB-CA-C	9.05	125.32	110.92
1	C	69	LYS	N-CA-C	8.82	121.78	111.02
1	B	287	ASN	N-CA-C	8.45	120.80	110.91
1	C	133[A]	ASN	O-C-N	-8.09	111.71	122.23
1	C	133[B]	ASN	O-C-N	-8.09	111.71	122.23
1	C	92	GLU	N-CA-C	7.48	122.21	110.32
1	A	89	GLY	N-CA-C	7.10	130.55	110.68
1	A	172	GLN	N-CA-C	6.91	120.50	109.24
1	B	175	MET	N-CA-C	6.72	120.62	109.46
1	A	176	GLY	N-CA-C	6.55	132.29	113.30
1	A	56	SER	CB-CA-C	6.44	123.24	110.42
1	B	280	TYR	CA-C-N	-6.44	113.90	120.85
1	B	280	TYR	C-N-CA	-6.44	113.90	120.85
1	A	173	GLU	N-CA-C	-6.00	97.17	107.61
1	C	57	PHE	N-CA-C	-5.98	96.60	109.81
1	A	205	ARG	N-CA-C	5.95	118.30	110.08
1	B	201	GLN	N-CA-C	5.86	117.34	111.07
1	A	163	VAL	N-CA-C	5.77	115.96	110.53
1	A	103	ASN	N-CA-C	5.65	117.11	111.07
1	A	280	TYR	N-CA-C	5.54	113.12	108.13
1	A	148	SER	N-CA-C	5.49	117.76	109.41
1	A	88	THR	CB-CA-C	5.46	118.42	109.90
1	C	224	LYS	N-CA-C	5.45	114.41	108.14
1	C	202	ASN	N-CA-C	-5.40	107.25	112.97
1	B	261	GLU	N-CA-CB	5.38	119.58	110.49
1	B	44	VAL	N-CA-C	5.33	114.17	108.95
1	B	161	GLU	N-CA-C	5.16	116.71	111.14
1	B	71	ARG	N-CA-CB	5.11	119.12	110.49
1	A	268	VAL	N-CA-C	5.11	115.93	108.58
1	B	287	ASN	CB-CA-C	-5.08	103.37	112.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	69	LYS	CA

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLY	Peptide
1	A	168	SER	Peptide
1	A	169	LYS	Peptide
1	A	170[A]	ARG	Peptide
1	A	170[B]	ARG	Peptide
1	A	171	GLY	Peptide
1	A	173	GLU	Peptide
1	A	175	MET	Peptide
1	A	176	GLY	Peptide
1	A	201[A]	GLN	Peptide
1	A	201[B]	GLN	Peptide
1	A	25	ASN	Peptide
1	A	26	ARG	Peptide
1	A	87	ASP	Peptide
1	B	174	MET	Peptide
1	B	200	ARG	Peptide
1	C	169[A]	LYS	Peptide
1	C	169[B]	LYS	Peptide
1	C	171	GLY	Peptide
1	C	286	THR	Peptide
1	C	56	SER	Peptide
1	C	68	LEU	Peptide
1	C	69	LYS	Peptide
1	C	91	ALA	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	2293	0	2270	133	0
1	B	2317	0	2282	145	0
1	C	2305	0	2290	114	0
2	A	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	161	0	0	12	0
3	B	167	0	0	14	0
3	C	110	0	0	7	0
All	All	7368	0	6842	376	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 27.

All (376) 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:170[A]:ARG:H	1:A:171:GLY:N	1.36	1.24
1:B:169:LYS:HG3	1:B:172:GLN:CG	1.73	1.17
1:A:201[A]:GLN:CG	1:B:274:ARG:HE	1.57	1.16
1:C:170:ARG:HG3	1:C:171:GLY:N	1.52	1.14
1:A:109:ILE:HD12	1:A:115:MET:HE2	1.30	1.13
1:C:170:ARG:CG	1:C:171:GLY:H	1.61	1.12
1:B:169:LYS:HG3	1:B:172:GLN:HG3	1.11	1.11
1:B:95:THR:HG22	1:B:98:GLU:H	1.17	1.07
1:B:288:ASN:HB3	1:B:289:PRO:HD2	1.06	1.06
1:A:201[A]:GLN:HG2	1:B:274:ARG:HE	0.88	1.05
1:B:288:ASN:CB	1:B:289:PRO:HD2	1.85	1.04
1:C:71:ARG:HG3	1:C:72:LYS:HG3	1.38	1.04
1:B:169:LYS:CG	1:B:172:GLN:HG3	1.88	1.03
1:A:201[A]:GLN:HG2	1:B:274:ARG:NE	1.73	1.02
1:B:251[B]:GLU:HB2	3:B:2147:HOH:O	1.63	0.98
1:B:170[B]:ARG:HH11	1:B:170[B]:ARG:CG	1.75	0.98
1:B:170[B]:ARG:HH11	1:B:170[B]:ARG:HG3	1.26	0.97
1:B:288:ASN:HB3	1:B:289:PRO:CD	1.97	0.95
1:B:169:LYS:HG3	1:B:172:GLN:CB	1.98	0.92
1:A:153:SER:O	1:A:154:ARG:HB2	1.70	0.91
1:B:286:THR:HG23	1:B:287:ASN:ND2	1.86	0.90
1:A:253:MET:HE3	1:A:270:ASN:HD21	1.34	0.90
1:A:166:GLY:O	1:A:176:GLY:HA3	1.70	0.89
1:A:112:THR:HG22	1:A:115:MET:H	1.38	0.88
1:B:168:SER:OG	1:B:169:LYS:HE2	1.75	0.88
1:A:201[A]:GLN:CG	1:B:274:ARG:NE	2.33	0.87
1:A:169:LYS:HB2	1:A:171:GLY:H	1.38	0.87
1:C:30:GLY:HA2	1:C:34:ARG:HE	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149[B]:ARG:HG3	1:B:272:HIS:ND1	1.90	0.85
1:B:169:LYS:HG3	1:B:172:GLN:HB2	1.59	0.85
1:A:26:ARG:HE	1:A:28:LYS:HE3	1.41	0.84
1:C:69:LYS:HD2	1:C:69:LYS:O	1.78	0.83
1:C:170:ARG:HG3	1:C:171:GLY:H	0.72	0.83
1:B:175:MET:HB3	1:B:177:LEU:HB2	1.61	0.82
1:C:70:SER:HA	1:C:75:ALA:HB2	1.61	0.82
1:C:278:THR:CG2	3:C:2051:HOH:O	2.29	0.80
1:B:278:THR:HG23	3:B:2105:HOH:O	1.80	0.80
1:B:168:SER:HG	1:B:169:LYS:HE2	1.45	0.80
1:B:200:ARG:NH1	1:B:203:LYS:HB3	1.96	0.80
1:B:200:ARG:HD3	1:B:203:LYS:HD3	1.63	0.79
1:C:174:MET:O	1:C:175:MET:HG2	1.83	0.79
1:A:17:ASN:HD21	1:A:261:GLU:H	1.32	0.78
1:A:167:GLU:OE2	1:A:172:GLN:HB3	1.84	0.78
1:A:109:ILE:O	1:A:112:THR:HB	1.83	0.77
1:A:223:VAL:HG11	1:B:136:LYS:HZ2	1.50	0.77
1:C:129[B]:LYS:HE3	1:C:130:PRO:HD2	1.67	0.77
1:B:170[B]:ARG:HG3	1:B:170[B]:ARG:NH1	1.97	0.76
1:B:251[A]:GLU:HB2	3:B:2147:HOH:O	1.84	0.76
1:C:91:ALA:HB2	1:C:154:ARG:HE	1.48	0.76
1:C:194:TYR:CD2	3:C:2063:HOH:O	2.38	0.76
1:C:194:TYR:HD2	3:C:2063:HOH:O	1.69	0.76
1:A:223:VAL:HG12	1:B:103:ASN:OD1	1.85	0.75
1:B:71:ARG:HD3	1:B:72:LYS:HG3	1.68	0.75
1:B:169:LYS:CG	1:B:172:GLN:HB2	2.16	0.75
1:B:135:PHE:O	1:B:139:LEU:HD13	1.87	0.75
1:C:170:ARG:CG	1:C:171:GLY:N	2.28	0.75
1:B:286:THR:HG23	1:B:287:ASN:HD22	1.52	0.73
1:A:201[B]:GLN:HA	1:A:201[B]:GLN:OE1	1.89	0.73
1:C:172[B]:GLN:OE1	1:C:174:MET:HA	1.89	0.73
1:B:28[A]:LYS:NZ	1:B:28[A]:LYS:HB3	2.04	0.72
1:B:194:TYR:HE1	1:B:215:LEU:HD12	1.54	0.72
1:C:278:THR:HG22	3:C:2051:HOH:O	1.89	0.71
1:B:95:THR:HG22	1:B:98:GLU:N	2.00	0.71
1:C:91:ALA:CB	1:C:154:ARG:HE	2.02	0.71
1:A:170[A]:ARG:H	1:A:171:GLY:H	1.38	0.71
1:B:288:ASN:CB	1:B:289:PRO:CD	2.61	0.71
1:A:170[A]:ARG:H	1:A:171:GLY:CA	2.04	0.70
1:B:34:ARG:NH2	3:B:2030:HOH:O	2.24	0.70
1:A:22:ALA:HB1	1:A:113:LYS:HE2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:HB2	3:A:2061:HOH:O	1.90	0.70
1:A:109:ILE:CD1	1:A:115:MET:HE2	2.16	0.70
1:B:199:ALA:O	1:C:274:ARG:NH2	2.25	0.69
1:B:255:ARG:NH2	1:C:91:ALA:O	2.25	0.69
1:C:166:GLY:O	1:C:176:GLY:N	2.24	0.69
1:A:34:ARG:HD3	1:A:61:GLN:OE1	1.92	0.69
1:A:66:GLU:HG3	1:A:67:LYS:N	2.06	0.69
1:C:91:ALA:CB	1:C:154:ARG:NE	2.56	0.68
1:C:129[B]:LYS:CE	1:C:130:PRO:HD2	2.22	0.68
1:A:26:ARG:HE	1:A:28:LYS:CE	2.06	0.68
1:B:83:ASN:ND2	1:B:101:GLU:OE1	2.26	0.68
1:A:157:SER:OG	1:A:162:HIS:CE1	2.48	0.67
1:A:157:SER:OG	1:A:162:HIS:HE1	1.77	0.67
1:B:211:GLN:HG3	3:B:2158:HOH:O	1.94	0.67
1:A:148:SER:HB3	1:A:155:PRO:HA	1.75	0.67
1:C:28:LYS:HB2	1:C:31:LYS:HD2	1.75	0.67
1:A:34:ARG:HB3	1:A:61:GLN:HG3	1.77	0.67
1:C:91:ALA:HB2	1:C:154:ARG:NE	2.10	0.66
1:B:203:LYS:HB2	3:B:2167:HOH:O	1.94	0.66
1:A:253:MET:HE3	1:A:270:ASN:ND2	2.06	0.65
1:A:174[B]:MET:SD	1:A:222:MET:HG2	2.36	0.65
1:A:201[A]:GLN:HG3	1:B:274:ARG:NE	2.11	0.65
1:B:80:LEU:CD1	1:B:101:GLU:HB3	2.26	0.65
1:B:177:LEU:HD21	1:B:182:GLN:HG3	1.77	0.65
1:C:167:GLU:HB2	1:C:173:GLU:HB2	1.79	0.65
1:B:194:TYR:CE1	1:B:215:LEU:HD12	2.31	0.64
1:B:167:GLU:HG3	1:B:169:LYS:H	1.63	0.64
1:C:167:GLU:OE2	1:C:173:GLU:N	2.31	0.64
1:B:169:LYS:CD	1:B:172:GLN:HG3	2.28	0.63
1:C:169[B]:LYS:HA	1:C:170:ARG:HB3	1.80	0.63
1:A:10[B]:HIS:CD2	3:A:2007:HOH:O	2.50	0.63
1:C:112:THR:O	1:C:116:LYS:HG3	1.99	0.62
1:C:197:TYR:CE2	1:C:206:PRO:HD3	2.34	0.62
1:B:177:LEU:HD21	1:B:182:GLN:CG	2.30	0.62
1:C:169[A]:LYS:HA	1:C:170:ARG:HB3	1.81	0.62
1:B:161:GLU:HG2	1:B:167:GLU:O	1.98	0.61
1:A:170[A]:ARG:CA	1:A:171:GLY:N	2.42	0.61
1:B:28[A]:LYS:HB3	1:B:28[A]:LYS:HZ3	1.65	0.61
1:B:149[A]:ARG:NH2	1:B:168:SER:HB2	2.16	0.61
1:A:112:THR:CG2	1:A:115:MET:H	2.14	0.61
1:C:241:LEU:O	1:C:245:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:HB3	1:A:155:PRO:CA	2.31	0.60
3:A:2117:HOH:O	1:B:274:ARG:HD3	2.00	0.60
1:A:87:ASP:O	1:A:88:THR:C	2.44	0.60
1:B:80:LEU:HD12	1:B:101:GLU:HB3	1.82	0.60
1:C:183:PHE:HA	1:C:192:ILE:CD1	2.32	0.60
1:A:70:SER:HA	1:A:75:ALA:HB2	1.83	0.60
1:C:261:GLU:HB2	3:C:2099:HOH:O	2.02	0.59
1:A:245:VAL:HG21	1:A:267:ILE:CG2	2.33	0.59
1:A:20:TRP:HH2	1:A:211:GLN:HB3	1.66	0.59
1:C:106:LEU:O	1:C:110:LEU:HD23	2.03	0.59
1:A:177:LEU:C	1:A:177:LEU:HD12	2.28	0.58
1:B:25:ASN:HD22	1:B:72:LYS:HD3	1.68	0.58
1:B:26:ARG:NH1	3:B:2021:HOH:O	2.35	0.58
1:C:76:THR:HG23	1:C:105:PHE:HA	1.86	0.58
1:A:65:GLU:O	1:A:69:LYS:HB2	2.03	0.58
1:A:26:ARG:NE	1:A:28:LYS:HE3	2.16	0.58
1:B:13:SER:HA	1:B:258:VAL:HG22	1.86	0.58
1:B:166:GLY:O	1:B:176:GLY:N	2.35	0.58
1:C:10:HIS:O	1:C:14[A]:LYS:HD3	2.03	0.58
1:A:168:SER:OG	1:A:169:LYS:HE2	2.05	0.57
1:A:10[B]:HIS:CD2	1:A:11:GLU:H	2.22	0.57
1:B:84:TYR:CD1	1:B:165:VAL:HG21	2.39	0.57
1:C:141:ASN:N	1:C:141:ASN:HD22	2.03	0.57
1:B:158:CYS:O	1:B:162:HIS:CD2	2.58	0.57
1:C:199:ALA:HB1	1:C:203:LYS:HB3	1.86	0.57
1:B:167:GLU:CD	1:B:168:SER:H	2.13	0.56
1:C:266:GLN:HB3	1:C:282:VAL:HB	1.87	0.56
1:B:252:LYS:HA	1:B:271:ARG:HB2	1.88	0.56
1:A:148:SER:HB3	1:A:154:ARG:C	2.29	0.56
1:A:223:VAL:CG1	1:B:136:LYS:HZ2	2.17	0.56
1:B:85:GLU:OE2	1:B:186:GLN:NE2	2.28	0.56
1:B:16:PHE:CD2	1:B:241:LEU:HD22	2.41	0.56
1:A:22:ALA:CB	1:A:113:LYS:HE2	2.36	0.55
1:A:223:VAL:HG11	1:B:136:LYS:NZ	2.20	0.55
1:A:201[B]:GLN:HB2	1:B:274:ARG:HE	1.70	0.55
1:B:28[B]:LYS:HE3	1:B:31:LYS:HD3	1.88	0.55
1:C:201:GLN:OE1	1:C:201:GLN:HA	2.07	0.55
1:A:26:ARG:NH2	3:A:2021:HOH:O	2.40	0.54
1:C:90:VAL:HG13	1:C:91:ALA:H	1.71	0.54
1:A:214:ASN:HD21	1:A:283:LEU:HB3	1.72	0.54
1:B:135:PHE:CZ	1:B:139:LEU:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:O	1:B:261:GLU:HG2	2.07	0.54
1:C:191:ASN:OD1	1:C:220:LYS:HE2	2.06	0.54
1:A:112:THR:HG21	1:A:236:GLU:HG3	1.88	0.54
1:A:25:ASN:HB2	1:A:236:GLU:OE1	2.07	0.54
1:A:276:ILE:HG13	1:A:277:GLY:N	2.23	0.54
1:B:253:MET:HE1	1:B:255:ARG:HH11	1.71	0.54
1:A:170[B]:ARG:H	1:A:171:GLY:CA	2.05	0.54
1:C:28:LYS:HD2	1:C:31:LYS:HD2	1.90	0.54
1:A:148:SER:HB3	1:A:155:PRO:N	2.22	0.54
1:A:223:VAL:CG1	1:B:136:LYS:NZ	2.72	0.53
1:A:173:GLU:HA	1:A:174[A]:MET:HB3	1.90	0.53
1:A:26:ARG:HG3	1:A:28:LYS:HG2	1.89	0.53
1:A:161:GLU:HA	1:A:165:VAL:HB	1.90	0.53
1:A:288:ASN:H	1:A:289:PRO:HD3	1.73	0.53
1:B:44:VAL:HG12	1:C:129[A]:LYS:HE2	1.91	0.53
1:C:127:GLN:HE21	1:C:247:LEU:HB3	1.74	0.53
1:B:14:LYS:HE2	1:B:18:GLU:OE2	2.09	0.53
1:C:262:GLU:O	1:C:287:ASN:HB2	2.09	0.53
1:A:174[B]:MET:HE2	3:A:2058:HOH:O	2.08	0.52
1:C:162:HIS:CE1	1:C:168:SER:HB3	2.44	0.52
1:A:147:TYR:HE1	1:A:149[B]:ARG:HH12	1.57	0.52
1:A:213:LEU:HD12	1:A:231:ILE:HD12	1.90	0.52
1:A:63:VAL:HG11	1:A:184:TYR:CZ	2.44	0.52
1:C:91:ALA:HB2	1:C:154:ARG:HH21	1.73	0.52
1:C:268:VAL:HG11	1:C:280:TYR:CE2	2.44	0.52
1:B:169:LYS:CG	1:B:172:GLN:CB	2.76	0.52
1:C:69:LYS:HD2	1:C:69:LYS:C	2.34	0.52
1:B:287:ASN:ND2	3:B:2167:HOH:O	2.41	0.51
1:C:13:SER:HA	1:C:258:VAL:HG13	1.92	0.51
1:B:73:THR:O	1:B:73:THR:OG1	2.27	0.51
1:C:91:ALA:HB1	1:C:154:ARG:NE	2.26	0.51
1:A:223:VAL:HG12	1:B:103:ASN:CG	2.35	0.51
1:B:200:ARG:O	1:B:203:LYS:HG2	2.10	0.51
1:C:70:SER:CA	1:C:75:ALA:HB2	2.36	0.51
1:C:158:CYS:O	1:C:162:HIS:HD2	1.93	0.51
1:B:170[B]:ARG:HH11	1:B:170[B]:ARG:HG2	1.66	0.51
1:A:166:GLY:O	1:A:175:MET:HA	2.10	0.51
1:A:26:ARG:HH21	1:A:28:LYS:HE3	1.75	0.51
1:B:73:THR:HG21	1:B:236:GLU:OE2	2.11	0.50
1:B:253:MET:HE1	1:B:255:ARG:NH1	2.26	0.50
1:A:269:VAL:HB	1:A:276:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40[B]:LYS:HE3	1:A:40[B]:LYS:H	1.77	0.50
1:B:31:LYS:NZ	3:B:2027:HOH:O	2.30	0.50
1:B:85:GLU:HG2	1:B:189:ARG:HH11	1.77	0.50
1:A:24:GLN:HB3	3:A:2019:HOH:O	2.12	0.50
1:B:200:ARG:HH11	1:B:286:THR:HG22	1.77	0.50
1:C:268:VAL:HG13	1:C:280:TYR:O	2.11	0.50
1:A:198:VAL:HG21	1:A:226:VAL:HG11	1.92	0.50
1:A:162:HIS:HD2	2:A:1290:PO4:O2	1.94	0.49
1:B:175:MET:HB3	1:B:177:LEU:CB	2.38	0.49
1:C:71:ARG:CG	1:C:72:LYS:HG3	2.25	0.49
1:A:200:ARG:O	1:A:202:ASN:O	2.30	0.49
1:C:245:VAL:O	1:C:271:ARG:NH2	2.44	0.49
1:B:167:GLU:OE2	1:B:169:LYS:HG2	2.12	0.49
1:C:74:PHE:O	1:C:78:ILE:HG23	2.12	0.49
1:C:168:SER:OG	1:C:173:GLU:OE1	2.25	0.49
1:B:178:HIS:CD2	1:B:280:TYR:HB3	2.48	0.49
1:B:212:VAL:HG11	1:B:265:LEU:HD21	1.95	0.49
1:C:91:ALA:HB2	1:C:154:ARG:NH2	2.27	0.49
1:B:191:ASN:HB3	1:B:219:TRP:CZ3	2.48	0.49
1:C:76:THR:CG2	1:C:105:PHE:HA	2.42	0.49
1:B:107:ASP:OD1	1:B:136:LYS:HE2	2.13	0.49
1:C:278:THR:HG21	3:C:2051:HOH:O	2.02	0.49
1:A:149[B]:ARG:NH2	1:A:272:HIS:CE1	2.81	0.49
1:C:80:LEU:HD11	1:C:105:PHE:HB2	1.95	0.48
1:B:133:ASN:HB2	3:B:2093:HOH:O	2.12	0.48
1:A:245:VAL:HG21	1:A:267:ILE:HG21	1.94	0.48
1:A:201[A]:GLN:HG3	1:A:201[A]:GLN:H	1.42	0.48
1:A:169:LYS:HB2	1:A:171:GLY:N	2.18	0.48
1:B:236:GLU:OE1	1:B:236:GLU:N	2.38	0.48
1:C:94:VAL:CG2	1:C:99:ILE:HD11	2.44	0.48
1:A:13:SER:HB3	1:A:259:ARG:H	1.78	0.48
1:B:172:GLN:O	1:B:174:MET:HG2	2.14	0.48
1:C:261:GLU:HG3	1:C:262:GLU:H	1.78	0.48
1:A:200:ARG:NH1	1:A:203[B]:LYS:HE3	2.29	0.48
1:B:71:ARG:HD3	1:B:72:LYS:CG	2.40	0.48
1:A:172:GLN:NE2	1:A:220:LYS:NZ	2.62	0.47
1:A:200:ARG:HD3	1:A:203[B]:LYS:HD3	1.96	0.47
1:B:169:LYS:CG	1:B:172:GLN:CG	2.64	0.47
1:B:266:GLN:OE1	1:C:154:ARG:HG2	2.15	0.47
1:A:20:TRP:CH2	1:A:211:GLN:HB3	2.48	0.47
1:C:65[A]:GLU:HA	1:C:68:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:PHE:O	1:C:78:ILE:CG2	2.62	0.47
1:A:65:GLU:OE1	1:A:184:TYR:OH	2.29	0.47
1:B:203:LYS:CB	3:B:2167:HOH:O	2.59	0.47
1:C:70:SER:O	1:C:71:ARG:C	2.57	0.47
1:A:40[B]:LYS:H	1:A:40[B]:LYS:CE	2.27	0.47
1:A:87:ASP:HB2	1:A:170[A]:ARG:HE	1.79	0.47
1:B:149[A]:ARG:HG2	1:B:272:HIS:ND1	2.29	0.47
1:B:169:LYS:HG2	1:B:172:GLN:HB2	1.96	0.47
1:C:65[B]:GLU:HA	1:C:68:LEU:HD12	1.96	0.47
1:C:169[A]:LYS:HB2	1:C:173:GLU:HG3	1.96	0.47
1:C:212:VAL:HG11	1:C:265:LEU:HD21	1.97	0.47
1:A:73:THR:HG22	1:A:108:ALA:HB1	1.96	0.47
1:A:266:GLN:NE2	3:A:2152:HOH:O	2.47	0.47
1:B:36:SER:HB3	1:B:61:GLN:NE2	2.29	0.47
1:B:67:LYS:HA	1:B:71:ARG:HB3	1.96	0.47
1:A:162:HIS:CD2	2:A:1290:PO4:O2	2.68	0.47
1:A:59:LEU:HD22	1:A:215:LEU:HD13	1.96	0.46
1:B:177:LEU:CD2	1:B:182:GLN:HG2	2.45	0.46
1:A:30:GLY:HA2	3:A:2026:HOH:O	2.14	0.46
1:B:149[A]:ARG:HD3	1:B:272:HIS:CE1	2.51	0.46
1:A:67:LYS:HZ2	1:A:71:ARG:NH2	2.14	0.46
1:A:211:GLN:HG3	1:A:231:ILE:O	2.15	0.46
1:A:174[A]:MET:HE1	1:A:222:MET:HE3	1.97	0.46
1:C:209:ASP:O	1:C:211:GLN:NE2	2.48	0.46
1:B:162:HIS:CD2	1:B:162:HIS:H	2.33	0.46
1:C:259:ARG:HH11	1:C:259:ARG:HG2	1.81	0.46
1:C:169[A]:LYS:HB3	1:C:171:GLY:O	2.15	0.46
1:B:66:GLU:O	1:B:69:LYS:O	2.34	0.46
1:B:158:CYS:O	1:B:162:HIS:HD2	1.98	0.46
1:B:233:VAL:HG13	1:B:237:PHE:HB3	1.97	0.46
1:C:197:TYR:CD2	1:C:197:TYR:C	2.94	0.46
1:B:167:GLU:OE1	1:B:174:MET:O	2.33	0.46
1:C:132:ARG:O	1:C:132:ARG:HG2	2.15	0.46
1:B:167:GLU:OE2	1:B:168:SER:N	2.46	0.46
1:A:132:ARG:CZ	3:A:2081:HOH:O	2.64	0.46
1:A:175:MET:HA	1:A:176:GLY:HA3	1.74	0.46
1:A:137:VAL:O	1:A:138:GLN:C	2.59	0.45
1:B:71:ARG:HG3	3:B:2045:HOH:O	2.15	0.45
1:A:10[B]:HIS:HD2	1:A:11:GLU:HG2	1.81	0.45
1:C:251:GLU:O	1:C:271:ARG:HD2	2.15	0.45
1:B:67:LYS:HA	1:B:71:ARG:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLU:O	1:A:288:ASN:HB2	2.15	0.45
1:A:71:ARG:HG3	1:A:72:LYS:HG3	1.98	0.45
1:C:149[B]:ARG:NH2	1:C:168:SER:OG	2.50	0.45
1:A:288:ASN:H	1:A:289:PRO:CD	2.30	0.45
1:C:20:TRP:O	1:C:26:ARG:NH2	2.50	0.45
1:A:94:VAL:HG22	1:A:99:ILE:HD11	1.98	0.45
1:A:174[B]:MET:HE1	3:A:2130:HOH:O	2.16	0.45
1:C:65[A]:GLU:OE1	1:C:69:LYS:HB2	2.17	0.45
1:A:63:VAL:CG1	1:A:184:TYR:CZ	3.01	0.44
1:A:288:ASN:N	1:A:289:PRO:CD	2.81	0.44
1:B:65:GLU:O	1:B:69:LYS:HE3	2.17	0.44
1:B:151:PRO:HD2	3:B:2100:HOH:O	2.16	0.44
1:B:170[B]:ARG:CG	1:B:170[B]:ARG:NH1	2.46	0.44
1:B:203:LYS:HD2	1:B:286:THR:HG21	1.99	0.44
1:C:167:GLU:OE2	1:C:172[B]:GLN:HA	2.17	0.44
1:C:198:VAL:HB	1:C:226:VAL:HG21	1.99	0.44
1:C:229:SER:O	1:C:231:ILE:HD12	2.18	0.44
1:C:35:ILE:HD12	1:C:37:LEU:HD22	2.00	0.44
1:C:177:LEU:C	1:C:177:LEU:HD12	2.42	0.44
1:B:185:LEU:O	1:B:189:ARG:HG2	2.18	0.44
1:C:80:LEU:HD11	1:C:105:PHE:CB	2.48	0.44
1:C:91:ALA:HB2	1:C:154:ARG:CZ	2.48	0.44
1:C:94:VAL:HG22	1:C:99:ILE:HD11	2.00	0.43
1:B:201:GLN:C	1:B:203:LYS:H	2.26	0.43
1:B:17:ASN:HD21	1:B:261:GLU:N	2.17	0.43
1:B:246:PHE:HB2	1:B:276:ILE:HD12	2.00	0.43
1:B:77:PHE:CE2	1:B:81:LEU:HD11	2.53	0.43
1:C:191:ASN:CG	1:C:220:LYS:HE2	2.43	0.43
1:B:178:HIS:CD2	1:B:280:TYR:CB	3.02	0.43
1:A:214:ASN:ND2	1:A:283:LEU:HB3	2.32	0.43
1:B:34:ARG:HB3	1:B:61:GLN:HB2	2.01	0.43
1:A:148:SER:CB	1:A:154:ARG:C	2.92	0.43
1:B:261:GLU:HG3	1:B:262:GLU:H	1.84	0.43
1:B:172:GLN:O	1:B:173:GLU:HG2	2.18	0.43
1:C:33:TYR:CD1	1:C:33:TYR:C	2.97	0.43
1:B:31:LYS:HB3	1:B:31:LYS:HE2	1.85	0.43
1:B:11:GLU:OE2	1:B:124:ARG:NH2	2.52	0.43
1:A:203[B]:LYS:CE	1:A:286:THR:H	2.32	0.42
1:C:167:GLU:OE2	1:C:172[A]:GLN:HA	2.19	0.42
1:B:28[B]:LYS:CE	1:B:31:LYS:HD3	2.48	0.42
1:B:67:LYS:HG2	3:B:2045:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PHE:CD2	1:C:241:LEU:HD22	2.54	0.42
1:A:81:LEU:HD22	1:A:182:GLN:CD	2.44	0.42
1:B:212:VAL:HA	1:B:229:SER:O	2.20	0.42
1:B:16:PHE:CE2	1:B:241:LEU:HD22	2.55	0.42
1:C:109:ILE:O	1:C:115:MET:HB2	2.20	0.42
1:C:174:MET:O	1:C:175:MET:CG	2.63	0.42
1:A:81:LEU:HD13	1:A:185:LEU:HD12	2.02	0.42
1:A:94:VAL:CG2	1:A:99:ILE:HD11	2.49	0.42
1:B:162:HIS:CD2	1:B:162:HIS:N	2.88	0.42
1:A:253:MET:HE2	1:A:268:VAL:HG21	2.02	0.42
1:B:86:MET:O	1:B:170[B]:ARG:NH2	2.53	0.42
1:C:109:ILE:HD12	1:C:115:MET:HE2	2.00	0.42
1:A:174[B]:MET:CE	3:A:2058:HOH:O	2.67	0.42
1:A:37:LEU:HD21	1:A:213:LEU:HD13	2.01	0.41
1:B:268:VAL:HG21	1:B:280:TYR:CZ	2.55	0.41
1:C:14[B]:LYS:HG2	1:C:18:GLU:OE2	2.20	0.41
1:B:37:LEU:HA	1:B:37:LEU:HD12	1.84	0.41
1:C:56:SER:HB2	3:C:2017:HOH:O	2.19	0.41
1:A:114:VAL:HG23	3:A:2017:HOH:O	2.20	0.41
1:A:246:PHE:HB2	1:A:276:ILE:HD13	2.01	0.41
1:C:20:TRP:CE3	1:C:260:LEU:HD21	2.56	0.41
1:A:126:ASN:O	1:A:126:ASN:CG	2.63	0.41
1:A:213:LEU:HD12	1:A:231:ILE:CD1	2.50	0.41
1:B:60:PHE:HE2	1:B:183:PHE:CD2	2.38	0.41
1:A:167:GLU:CD	1:A:172:GLN:HB3	2.45	0.41
1:A:262:GLU:HB2	1:A:286:THR:O	2.21	0.41
1:A:106:LEU:O	1:A:110:LEU:HD22	2.20	0.41
1:A:172:GLN:H	1:A:172:GLN:HG2	1.45	0.41
1:B:90:VAL:HG22	1:B:91:ALA:H	1.86	0.41
1:C:8:LEU:HD11	1:C:259:ARG:HB2	2.03	0.41
1:B:203:LYS:HD2	1:B:286:THR:CG2	2.51	0.41
1:B:149[B]:ARG:HD2	1:B:149[B]:ARG:HA	1.98	0.40
1:C:69:LYS:O	1:C:75:ALA:CB	2.69	0.40
1:B:73:THR:HG21	1:B:236:GLU:CD	2.46	0.40
1:C:84:TYR:CE2	1:C:161:GLU:HG2	2.56	0.40
1:C:189:ARG:HD3	1:C:189:ARG:N	2.37	0.40
1:B:200:ARG:HE	1:B:200:ARG:HB2	1.63	0.40
1:B:288:ASN:O	1:B:289:PRO:C	2.64	0.40
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.99	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	273/292 (94%)	231 (85%)	32 (12%)	10 (4%)	2	1
1	B	279/292 (96%)	245 (88%)	32 (12%)	2 (1%)	18	19
1	C	279/292 (96%)	250 (90%)	25 (9%)	4 (1%)	9	7
All	All	831/876 (95%)	726 (87%)	89 (11%)	16 (2%)	7	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	175	MET
1	A	203[A]	LYS
1	A	203[B]	LYS
1	A	10[A]	HIS
1	A	10[B]	HIS
1	A	64	ASP
1	B	73	THR
1	C	90	VAL
1	B	200	ARG
1	C	173	GLU
1	A	154	ARG
1	C	89	GLY
1	A	288	ASN
1	C	155	PRO
1	A	155	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/259 (97%)	219 (87%)	33 (13%)	4	3
1	B	254/259 (98%)	219 (86%)	35 (14%)	3	3
1	C	255/259 (98%)	219 (86%)	36 (14%)	3	3
All	All	761/777 (98%)	657 (86%)	104 (14%)	4	3

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	13	SER
1	A	27	MET
1	A	40[A]	LYS
1	A	40[B]	LYS
1	A	61	GLN
1	A	66	GLU
1	A	71	ARG
1	A	87	ASP
1	A	88	THR
1	A	110	LEU
1	A	112	THR
1	A	139	LEU
1	A	149[A]	ARG
1	A	149[B]	ARG
1	A	154	ARG
1	A	169	LYS
1	A	170[A]	ARG
1	A	170[B]	ARG
1	A	172	GLN
1	A	175	MET
1	A	177	LEU
1	A	200	ARG
1	A	201[A]	GLN
1	A	201[B]	GLN
1	A	209	ASP
1	A	211	GLN
1	A	233	VAL
1	A	241	LEU
1	A	247	LEU
1	A	268	VAL
1	A	269	VAL

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Mol	Chain	Res	Type
1	A	276	ILE
1	B	7	GLN
1	B	14	LYS
1	B	28[A]	LYS
1	B	28[B]	LYS
1	B	40	LYS
1	B	80	LEU
1	B	86	MET
1	B	95	THR
1	B	110	LEU
1	B	124	ARG
1	B	132	ARG
1	B	162	HIS
1	B	169	LYS
1	B	170[A]	ARG
1	B	170[B]	ARG
1	B	177	LEU
1	B	200	ARG
1	B	205	ARG
1	B	211	GLN
1	B	214	ASN
1	B	215	LEU
1	B	223	VAL
1	B	233	VAL
1	B	241	LEU
1	B	247	LEU
1	B	250	GLN
1	B	252	LYS
1	B	253	MET
1	B	258	VAL
1	B	259	ARG
1	B	264	GLU
1	B	265	LEU
1	B	266	GLN
1	B	268	VAL
1	B	285	SER
1	C	12	LEU
1	C	13	SER
1	C	24	GLN
1	C	31	LYS
1	C	56	SER
1	C	57	PHE

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Mol	Chain	Res	Type
1	C	62	PHE
1	C	71	ARG
1	C	76	THR
1	C	78	ILE
1	C	82[A]	ASP
1	C	82[B]	ASP
1	C	88	THR
1	C	97	GLU
1	C	104[A]	ASN
1	C	104[B]	ASN
1	C	110	LEU
1	C	131	THR
1	C	141	ASN
1	C	154	ARG
1	C	169[A]	LYS
1	C	169[B]	LYS
1	C	170	ARG
1	C	172[A]	GLN
1	C	172[B]	GLN
1	C	174	MET
1	C	177	LEU
1	C	203	LYS
1	C	207	ASP
1	C	208	GLU
1	C	211	GLN
1	C	215	LEU
1	C	262	GLU
1	C	268	VAL
1	C	270[A]	ASN
1	C	270[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	127	GLN
1	A	145	GLN
1	A	162	HIS
1	A	172	GLN
1	A	211	GLN
1	A	214	ASN
1	A	216	GLN

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Mol	Chain	Res	Type
1	A	218	ASN
1	A	270	ASN
1	A	287	ASN
1	B	17	ASN
1	B	25	ASN
1	B	102	ASN
1	B	127	GLN
1	B	133	ASN
1	B	138	GLN
1	B	141	ASN
1	B	162	HIS
1	B	202	ASN
1	B	214	ASN
1	B	216	GLN
1	B	218	ASN
1	B	270	ASN
1	B	287	ASN
1	C	25	ASN
1	C	83	ASN
1	C	119	HIS
1	C	141	ASN
1	C	211	GLN
1	C	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	1290	-	4,4,4	1.29	0	6,6,6	1.08	0
2	PO4	C	1288	-	4,4,4	1.14	0	6,6,6	0.36	0
2	PO4	B	1290	-	4,4,4	0.77	0	6,6,6	0.68	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1290	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	133:ASN	C	134:ASP	N	1.11

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	273/292 (93%)	0.91	39 (14%) 6 4	12, 31, 66, 83	7 (2%)
1	B	276/292 (94%)	0.80	39 (14%) 6 4	12, 30, 75, 89	8 (2%)
1	C	271/292 (92%)	1.25	53 (19%) 3 2	16, 39, 76, 100	12 (4%)
All	All	820/876 (93%)	0.98	131 (15%) 5 3	12, 33, 74, 100	27 (3%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	SER	7.4
1	A	203[A]	LYS	6.2
1	B	70	SER	5.8
1	C	90	VAL	5.7
1	C	69	LYS	4.7
1	C	205[A]	ARG	4.6
1	C	88	THR	4.5
1	C	170	ARG	4.5
1	A	152	GLY	4.4
1	B	152	GLY	4.3
1	B	203	LYS	4.3
1	B	201	GLN	4.2
1	A	169	LYS	4.1
1	C	250[A]	GLN	4.0
1	A	174[A]	MET	4.0
1	A	289	PRO	3.9
1	C	151	PRO	3.9
1	A	148	SER	3.9
1	B	170[A]	ARG	3.9
1	A	171	GLY	3.8
1	C	89	GLY	3.8
1	B	44	VAL	3.8
1	B	88	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	88	THR	3.7
1	B	89	GLY	3.7
1	C	94	VAL	3.7
1	A	10[A]	HIS	3.7
1	C	68	LEU	3.5
1	A	90	VAL	3.5
1	B	150	ALA	3.4
1	C	86	MET	3.4
1	B	153	SER	3.4
1	C	84	TYR	3.3
1	B	289	PRO	3.3
1	A	91	ALA	3.3
1	C	172[A]	GLN	3.3
1	C	93	VAL	3.3
1	C	91	ALA	3.2
1	A	73	THR	3.2
1	C	73	THR	3.2
1	C	176	GLY	3.1
1	A	201[A]	GLN	3.1
1	A	170[A]	ARG	3.1
1	A	205	ARG	3.1
1	A	86	MET	3.1
1	A	153	SER	3.1
1	C	8	LEU	3.1
1	B	90	VAL	3.0
1	A	21	ASP	3.0
1	A	149[A]	ARG	3.0
1	B	288	ASN	3.0
1	C	63	VAL	3.0
1	B	200	ARG	3.0
1	C	148	SER	3.0
1	B	73	THR	2.9
1	A	70	SER	2.9
1	C	83	ASN	2.9
1	B	91	ALA	2.9
1	C	152	GLY	2.9
1	C	287	ASN	2.9
1	C	22	ALA	2.9
1	C	261	GLU	2.9
1	C	121	TYR	2.8
1	C	57	PHE	2.8
1	B	175	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	202	ASN	2.8
1	B	206	PRO	2.8
1	C	173	GLU	2.8
1	B	154[A]	ARG	2.8
1	A	286	THR	2.7
1	B	287	ASN	2.7
1	A	87	ASP	2.7
1	C	62	PHE	2.7
1	C	123	VAL	2.7
1	B	45	PRO	2.7
1	B	86	MET	2.7
1	C	120	ASP	2.6
1	C	81	LEU	2.6
1	A	172	GLN	2.6
1	A	6	GLY	2.6
1	B	43	TYR	2.6
1	B	55	ALA	2.6
1	B	171	GLY	2.6
1	B	204	SER	2.6
1	B	286	THR	2.5
1	C	171	GLY	2.5
1	A	175	MET	2.5
1	C	260	LEU	2.5
1	B	6	GLY	2.4
1	B	219	TRP	2.4
1	B	173	GLU	2.4
1	C	85	GLU	2.4
1	A	199	ALA	2.4
1	B	151	PRO	2.4
1	C	169[A]	LYS	2.4
1	C	24	GLN	2.4
1	B	167	GLU	2.4
1	C	206	PRO	2.4
1	A	93	VAL	2.4
1	C	126	ASN	2.3
1	C	118	ALA	2.3
1	C	156	ASP	2.3
1	A	204	SER	2.3
1	B	148	SER	2.3
1	A	69	LYS	2.3
1	A	287	ASN	2.3
1	C	6	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	149[A]	ARG	2.3
1	A	68	LEU	2.3
1	B	207[A]	ASP	2.3
1	A	173	GLU	2.3
1	C	129[A]	LYS	2.3
1	A	26	ARG	2.2
1	A	56	SER	2.2
1	C	203	LYS	2.2
1	A	43	TYR	2.2
1	B	149[A]	ARG	2.2
1	B	205	ARG	2.2
1	B	133	ASN	2.2
1	C	155	PRO	2.2
1	C	72	LYS	2.2
1	B	87	ASP	2.1
1	C	65[A]	GLU	2.1
1	A	261	GLU	2.1
1	C	25	ASN	2.1
1	C	128	ALA	2.1
1	C	67	LYS	2.1
1	A	207	ASP	2.0
1	A	154	ARG	2.0
1	C	153	SER	2.0
1	A	209	ASP	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	PO4	B	1290	5/5	0.86	0.12	48,49,50,50	0
2	PO4	C	1288	5/5	0.91	0.10	46,47,47,49	0
2	PO4	A	1290	5/5	0.97	0.07	37,38,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.