



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:16 AM UTC

PDB ID : 2ZVK / pdb_00002zvk
Title : Crystal structure of PCNA in complex with DNA polymerase eta fragment
Authors : Hishiki, A.; Hashimoto, H.; Hanafusa, T.; Kamei, K.; Ohashi, E.; Shimizu, T.; Ohmori, H.; Sato, M.
Deposited on : 2008-11-11
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:

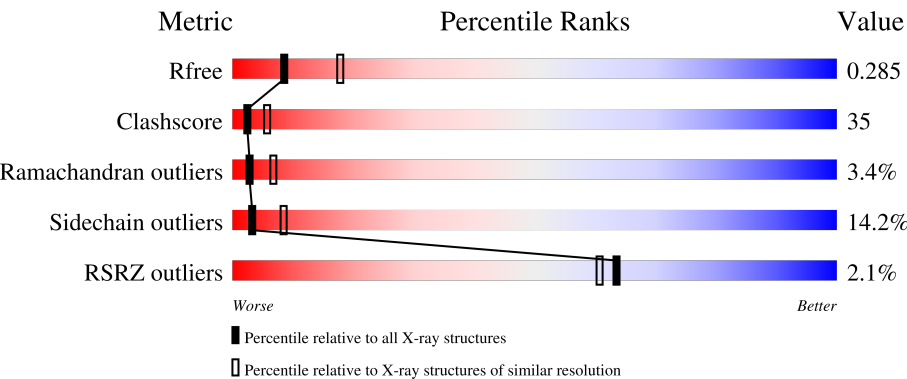
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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))
R_{free}	180053	3538 (2.70-2.70)
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	261	42% 39% 12% • 6%
1	B	261	3% 41% 40% 11% 7%
1	C	261	43% 39% 11% • 5%
2	U	21	5% 48% 38% 10% 5%
2	V	21	5% 29% 19% 52%

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Mol	Chain	Length	Quality of chain
2	W	21	29% 24% 48%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6021 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	89	0	0
			1893	1193	311	373	16			
1	B	243	Total	C	N	O	S	89	0	0
			1873	1180	307	370	16			
1	C	247	Total	C	N	O	S	58	0	0
			1899	1196	311	376	16			

- Molecule 2 is a protein called DNA polymerase eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	20	Total	C	N	O	S	10	0	0
			164	105	29	28	2			
2	V	10	Total	C	N	O	S	0	0	0
			85	57	12	15	1			
2	W	11	Total	C	N	O	S	0	0	0
			89	59	13	16	1			

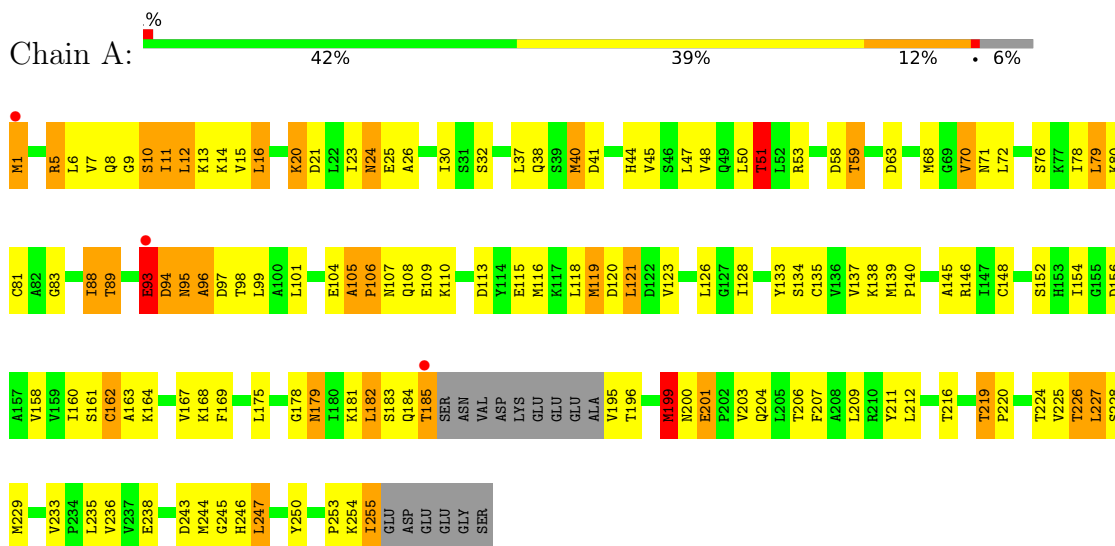
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	6	Total	O	0	0
			6	6		
3	C	4	Total	O	0	0
			4	4		

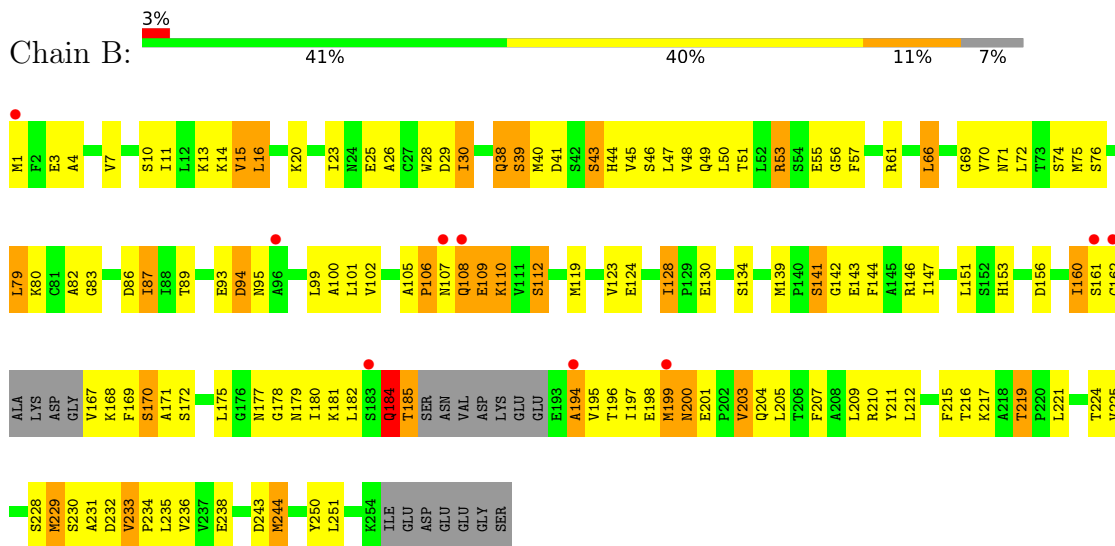
3 Residue-property plots

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.

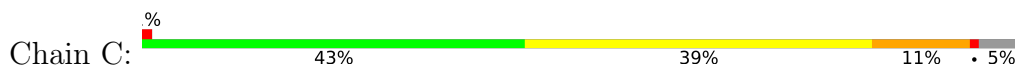
- Molecule 1: Proliferating cell nuclear antigen

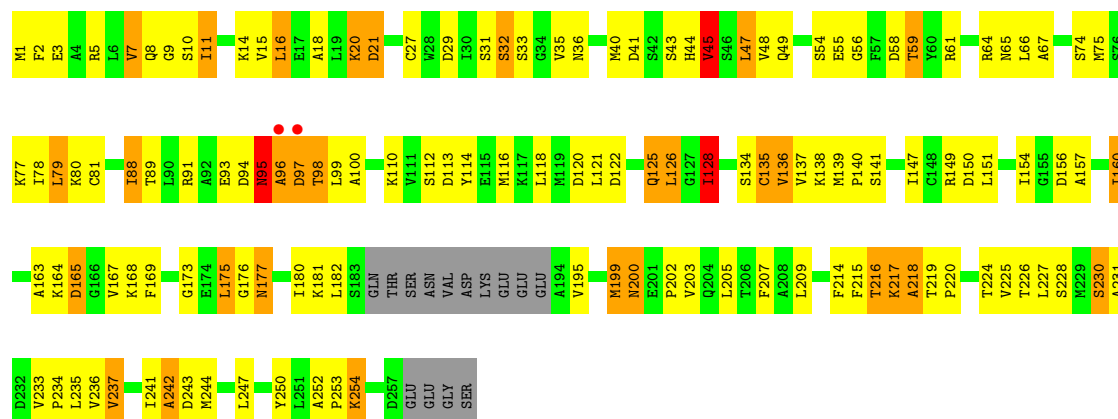


- Molecule 1: Proliferating cell nuclear antigen

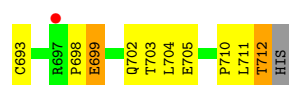


- Molecule 1: Proliferating cell nuclear antigen

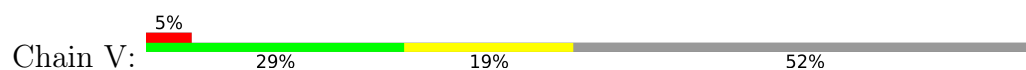




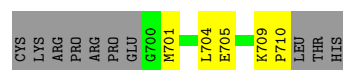
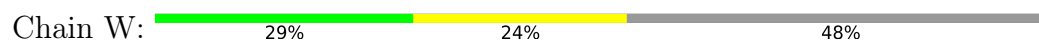
- Molecule 2: DNA polymerase eta



- Molecule 2: DNA polymerase eta



- Molecule 2: DNA polymerase eta



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.03Å 82.03Å 310.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.70) 92.1 (20.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.215 , 0.286 0.222 , 0.285	Depositor DCC
R_{free} test set	1398 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6021	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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](#)

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	1.18	3/1918 (0.2%)	1.29	14/2590 (0.5%)
1	B	1.11	1/1897 (0.1%)	1.20	10/2561 (0.4%)
1	C	1.23	6/1924 (0.3%)	1.28	16/2598 (0.6%)
2	U	1.16	1/168 (0.6%)	1.25	1/224 (0.4%)
2	V	0.87	0/87	1.31	1/115 (0.9%)
2	W	1.12	0/91	1.10	0/120
All	All	1.17	11/6085 (0.2%)	1.26	42/8208 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	699	GLU	CA-CB	-8.12	1.41	1.53
1	C	11	ILE	CA-CB	-6.99	1.46	1.54
1	A	154	ILE	CA-C	-6.02	1.46	1.52
1	B	15	VAL	CA-CB	-5.71	1.47	1.54
1	C	128	ILE	CA-CB	-5.68	1.46	1.54
1	A	179	ASN	N-CA	-5.62	1.39	1.46
1	C	88	ILE	CA-CB	-5.48	1.47	1.54
1	C	147	ILE	CA-CB	-5.21	1.48	1.54
1	C	237	VAL	CA-CB	-5.20	1.47	1.54
1	A	11	ILE	CA-CB	-5.16	1.48	1.54
1	C	45	VAL	CA-CB	-5.02	1.48	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	ILE	N-CA-C	8.64	118.66	110.53
1	B	219	THR	CA-C-N	-8.36	111.01	120.04
1	B	219	THR	C-N-CA	-8.36	111.01	120.04
1	C	154	ILE	CB-CA-C	-8.14	103.48	111.30
1	C	218	ALA	N-CA-C	-7.75	103.97	113.19
1	A	70	VAL	N-CA-C	7.72	119.03	107.75
1	A	154	ILE	N-CA-C	-7.71	105.65	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	GLY	N-CA-C	-7.40	102.60	112.82
1	A	181	LYS	CA-CB-CG	-6.87	100.35	114.10
1	C	95	ASN	N-CA-C	-6.87	96.17	110.80
2	U	699	GLU	CB-CA-C	-6.73	100.16	110.26
1	C	125	GLN	N-CA-C	-6.53	101.33	110.35
1	B	194	ALA	N-CA-C	6.38	118.85	108.63
1	A	11	ILE	N-CA-C	6.27	116.43	110.53
1	C	97	ASP	N-CA-C	-6.16	103.14	110.41
1	C	88	ILE	CB-CA-C	-6.10	101.52	110.62
1	B	195	VAL	CB-CA-C	-6.06	103.11	110.99
2	V	705	GLU	N-CA-C	-5.89	104.58	113.89
1	C	252	ALA	CA-C-N	5.88	125.79	119.85
1	C	252	ALA	C-N-CA	5.88	125.79	119.85
1	A	154	ILE	CB-CA-C	-5.82	105.72	111.30
1	B	39	SER	N-CA-C	5.78	117.19	108.46
1	A	233	VAL	CA-C-N	-5.74	114.06	119.85
1	A	233	VAL	C-N-CA	-5.74	114.06	119.85
1	A	93	GLU	N-CA-C	-5.73	101.92	110.23
1	A	199	MET	N-CA-C	5.70	117.94	108.13
1	B	238	GLU	N-CA-C	5.62	118.25	108.76
1	C	173	GLY	N-CA-C	5.46	119.50	110.55
1	C	160	ILE	CB-CA-C	-5.42	103.55	110.98
1	B	128	ILE	CA-C-N	-5.41	114.76	120.66
1	B	128	ILE	C-N-CA	-5.41	114.76	120.66
1	C	195	VAL	N-CA-C	5.41	115.57	107.51
1	C	195	VAL	CB-CA-C	-5.33	103.84	111.31
1	A	238	GLU	N-CA-C	5.33	118.17	109.59
1	A	115	GLU	N-CA-C	-5.29	99.79	108.41
1	B	87	ILE	CB-CA-C	-5.29	103.83	111.34
1	A	104	GLU	N-CA-C	-5.28	101.67	109.86
1	B	229	MET	N-CA-C	5.16	116.68	108.79
1	C	136	VAL	N-CA-C	5.15	116.08	108.45
1	A	51	THR	N-CA-C	5.03	116.61	108.26
1	C	80	LYS	N-CA-C	-5.00	107.01	113.01
1	C	177	ASN	N-CA-C	5.00	116.67	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1893	0	1912	134	0
1	B	1873	0	1886	115	0
1	C	1899	0	1912	141	0
2	U	164	0	168	21	0
2	V	85	0	83	9	0
2	W	89	0	86	7	0
3	A	8	0	0	1	0
3	B	6	0	0	3	0
3	C	4	0	0	0	0
All	All	6021	0	6047	401	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 35.

All (401) 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:C:128:ILE:HG23	1:C:128:ILE:O	1.39	1.20
2:U:703:THR:HG22	2:U:705:GLU:H	1.05	1.12
1:B:41:ASP:OD1	1:B:43:SER:HB3	1.49	1.10
1:A:105:ALA:HB1	1:A:106:PRO:CD	1.81	1.09
1:B:128:ILE:HD12	2:V:708:PHE:CZ	1.87	1.09
1:C:7:VAL:HB	1:C:58:ASP:OD2	1.53	1.06
1:C:219:THR:CG2	1:C:220:PRO:HD3	1.86	1.06
1:C:95:ASN:H	1:C:95:ASN:ND2	1.56	1.02
1:C:128:ILE:O	1:C:128:ILE:CG2	2.08	1.02
1:C:216:THR:O	1:C:219:THR:HB	1.61	0.99
1:C:5:ARG:HB3	1:C:59:THR:HB	1.40	0.99
1:C:175:LEU:C	1:C:175:LEU:HD12	1.88	0.99
2:U:703:THR:HG22	2:U:705:GLU:N	1.78	0.97
1:B:234:PRO:HD3	2:V:707:PHE:CD2	2.00	0.97
1:C:219:THR:HG22	1:C:220:PRO:HD3	1.46	0.95
1:C:95:ASN:HD22	1:C:95:ASN:N	1.57	0.95
1:A:105:ALA:HB1	1:A:106:PRO:HD3	1.45	0.94
1:C:93:GLU:HB3	1:C:95:ASN:ND2	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASP:O	1:C:95:ASN:O	1.86	0.94
1:C:200:ASN:N	1:C:200:ASN:HD22	1.66	0.93
1:C:199:MET:HG2	1:C:199:MET:O	1.69	0.92
1:A:105:ALA:CB	1:A:106:PRO:CD	2.47	0.92
1:B:184:GLN:HG2	1:B:185:THR:H	1.32	0.92
1:A:30:ILE:HD11	1:A:68:MET:HE2	1.55	0.88
1:C:94:ASP:O	1:C:95:ASN:C	2.21	0.83
1:B:128:ILE:CD1	2:V:708:PHE:CZ	2.62	0.83
1:A:16:LEU:HD22	1:A:79:LEU:HD13	1.60	0.82
1:B:56:GLY:HA3	1:B:244:MET:HE3	1.61	0.82
1:A:105:ALA:CB	1:A:106:PRO:HD2	2.10	0.81
1:A:26:ALA:HB3	1:A:72:LEU:HD11	1.61	0.80
1:B:170:SER:HB2	1:B:179:ASN:HB3	1.63	0.79
1:C:219:THR:HG23	1:C:220:PRO:HD3	1.65	0.79
1:A:95:ASN:CG	1:A:96:ALA:H	1.91	0.79
2:U:703:THR:CG2	2:U:705:GLU:HG3	2.13	0.79
1:C:1:MET:CE	1:C:61:ARG:HE	1.95	0.79
1:A:105:ALA:HB1	1:A:106:PRO:HD2	1.65	0.78
1:B:141:SER:HB2	1:B:219:THR:HG23	1.63	0.78
1:C:40:MET:HE2	2:W:704:LEU:HB2	1.64	0.78
1:B:93:GLU:O	1:B:94:ASP:C	2.27	0.78
1:A:47:LEU:HD23	1:A:48:VAL:N	1.98	0.77
1:C:7:VAL:CB	1:C:58:ASP:OD2	2.32	0.77
1:A:148:CYS:O	1:A:152:SER:HB3	1.85	0.77
1:B:3:GLU:HB3	1:B:61:ARG:HB2	1.68	0.75
1:B:1:MET:HG2	3:B:276:HOH:O	1.87	0.74
1:A:145:ALA:HA	1:A:216:THR:HG21	1.69	0.74
1:A:161:SER:OG	1:A:204:GLN:NE2	2.22	0.73
1:B:184:GLN:HG2	1:B:185:THR:N	2.04	0.73
1:A:12:LEU:HB3	1:A:79:LEU:HD21	1.68	0.73
1:A:7:VAL:HG23	1:A:58:ASP:CG	2.15	0.72
1:B:47:LEU:HD12	1:B:47:LEU:C	2.15	0.72
1:A:16:LEU:HD13	1:A:79:LEU:HD13	1.69	0.71
1:B:83:GLY:O	1:B:86:ASP:HB2	1.91	0.71
1:C:175:LEU:C	1:C:175:LEU:CD1	2.64	0.71
1:C:200:ASN:HD22	1:C:200:ASN:H	1.38	0.71
1:A:37:LEU:C	1:A:37:LEU:HD23	2.16	0.70
2:U:703:THR:CG2	2:U:705:GLU:H	1.95	0.70
1:C:217:LYS:C	1:C:219:THR:H	1.99	0.70
1:B:13:LYS:NZ	1:B:82:ALA:O	2.25	0.70
1:C:200:ASN:N	1:C:200:ASN:ND2	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:ND2	1:A:96:ALA:H	1.90	0.69
1:B:228:SER:HB2	1:B:236:VAL:HG12	1.74	0.69
1:A:168:LYS:HD2	1:A:179:ASN:HD21	1.57	0.69
1:C:40:MET:HE3	1:C:126:LEU:CD2	2.22	0.68
1:B:128:ILE:HD12	2:V:708:PHE:CE2	2.29	0.68
1:C:216:THR:O	1:C:219:THR:CB	2.39	0.68
1:B:23:ILE:HG13	1:B:72:LEU:HD12	1.76	0.68
1:A:185:THR:HG22	1:A:185:THR:O	1.94	0.67
1:C:40:MET:HE3	1:C:126:LEU:HD21	1.74	0.67
1:B:162:CYS:C	1:B:167:VAL:HA	2.20	0.67
1:C:93:GLU:HB3	1:C:95:ASN:HD21	1.60	0.67
1:A:95:ASN:O	1:A:96:ALA:O	2.13	0.67
1:A:107:ASN:O	1:A:109:GLU:N	2.28	0.67
1:B:228:SER:HB2	1:B:236:VAL:CG1	2.25	0.67
1:C:236:VAL:HG22	1:C:250:TYR:CE2	2.30	0.67
2:U:703:THR:CG2	2:U:705:GLU:CG	2.72	0.66
1:C:31:SER:O	1:C:32:SER:C	2.38	0.66
1:C:95:ASN:H	1:C:95:ASN:HD22	0.77	0.66
1:B:13:LYS:HA	1:B:79:LEU:HD23	1.76	0.66
1:A:254:LYS:O	1:A:255:ILE:HB	1.96	0.66
1:C:47:LEU:HD23	1:C:47:LEU:C	2.21	0.65
1:B:147:ILE:HG23	1:B:180:ILE:HD12	1.77	0.65
2:U:703:THR:HG21	2:U:705:GLU:CG	2.26	0.65
1:B:1:MET:CG	3:B:276:HOH:O	2.43	0.65
1:B:29:ASP:C	1:B:30:ILE:HD13	2.22	0.65
1:B:139:MET:SD	1:B:144:PHE:HB2	2.37	0.65
1:C:14:LYS:HE2	1:C:220:PRO:O	1.97	0.64
1:B:204:GLN:O	1:B:204:GLN:HG2	1.97	0.64
1:A:26:ALA:CB	1:A:72:LEU:HD11	2.27	0.64
1:A:175:LEU:HD11	1:C:74:SER:CB	2.27	0.64
1:A:135:CYS:SG	1:A:199:MET:HE2	2.36	0.64
1:C:40:MET:CE	2:W:704:LEU:HB2	2.27	0.64
1:C:43:SER:O	1:C:44:HIS:HB2	1.98	0.64
1:A:139:MET:HE3	1:A:227:LEU:HD11	1.80	0.64
1:B:212:LEU:O	1:B:216:THR:HG23	1.98	0.64
1:A:95:ASN:CG	1:A:96:ALA:N	2.56	0.63
1:C:242:ALA:O	1:C:243:ASP:OD2	2.18	0.62
1:B:30:ILE:HD13	1:B:30:ILE:N	2.15	0.62
1:B:41:ASP:OD1	1:B:43:SER:CB	2.38	0.62
1:B:105:ALA:O	1:B:106:PRO:C	2.42	0.62
1:C:163:ALA:CA	1:C:199:MET:HE1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:VAL:HG12	1:C:49:GLN:N	2.15	0.62
1:B:231:ALA:O	1:B:233:VAL:HG13	1.99	0.61
1:A:1:MET:O	1:A:63:ASP:HB3	1.99	0.61
1:A:9:GLY:HA3	1:A:88:ILE:HG13	1.82	0.61
1:C:214:PHE:O	1:C:217:LYS:HB2	2.01	0.61
1:A:12:LEU:HB3	1:A:79:LEU:CD2	2.30	0.60
1:B:110:LYS:HG2	1:B:110:LYS:O	2.01	0.60
1:A:16:LEU:HD22	1:A:79:LEU:CD1	2.31	0.60
1:C:95:ASN:O	1:C:96:ALA:HB3	2.00	0.60
1:A:224:THR:HG22	1:A:225:VAL:N	2.16	0.60
1:B:185:THR:OG1	1:B:194:ALA:HA	2.02	0.60
1:C:168:LYS:HB2	1:C:181:LYS:HD2	1.82	0.60
1:C:54:SER:C	1:C:56:GLY:H	2.10	0.59
1:A:119:MET:HE2	1:A:121:LEU:HD22	1.84	0.59
1:A:13:LYS:NZ	1:A:79:LEU:O	2.35	0.59
1:A:70:VAL:HG13	1:A:116:MET:HE1	1.84	0.59
1:C:137:VAL:O	1:C:226:THR:HA	2.03	0.59
1:A:37:LEU:HB3	1:A:50:LEU:HB3	1.85	0.58
1:A:168:LYS:HD2	1:A:179:ASN:ND2	2.17	0.58
1:A:195:VAL:HG12	1:A:195:VAL:O	2.00	0.58
1:C:20:LYS:HE3	1:C:21:ASP:OD1	2.03	0.58
1:B:45:VAL:HG12	1:B:251:LEU:HD12	1.85	0.58
1:A:30:ILE:CD1	1:A:68:MET:HE2	2.29	0.58
1:C:175:LEU:HD12	1:C:176:GLY:N	2.18	0.57
1:A:139:MET:HE1	1:A:169:PHE:HZ	1.69	0.57
1:A:185:THR:O	1:A:185:THR:CG2	2.52	0.57
1:A:126:LEU:HA	2:U:710:PRO:HA	1.85	0.57
1:B:107:ASN:O	1:B:108:GLN:C	2.47	0.57
1:C:44:HIS:ND1	2:W:705:GLU:OE2	2.36	0.57
1:A:106:PRO:HG2	1:A:107:ASN:H	1.68	0.57
1:A:40:MET:HA	1:A:47:LEU:HA	1.86	0.57
1:B:93:GLU:O	1:B:95:ASN:N	2.38	0.57
1:A:105:ALA:HB3	1:A:106:PRO:HD2	1.87	0.57
1:B:16:LEU:HD11	1:B:75:MET:HE2	1.84	0.57
1:C:219:THR:N	1:C:220:PRO:CD	2.68	0.57
2:W:709:LYS:O	2:W:710:PRO:C	2.48	0.56
1:A:5:ARG:HB2	1:A:89:THR:HG23	1.87	0.56
1:C:217:LYS:O	1:C:220:PRO:HD2	2.04	0.56
1:A:95:ASN:ND2	1:A:96:ALA:N	2.54	0.56
1:C:16:LEU:HD13	1:C:79:LEU:HD22	1.88	0.56
1:A:47:LEU:HD23	1:A:47:LEU:C	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD13	1:B:79:LEU:HD22	1.87	0.56
1:B:156:ASP:C	1:B:156:ASP:OD1	2.48	0.56
1:A:93:GLU:O	1:A:95:ASN:N	2.29	0.56
1:B:43:SER:OG	1:B:45:VAL:HG23	2.06	0.56
1:C:93:GLU:CB	1:C:95:ASN:ND2	2.65	0.55
1:A:44:HIS:O	2:U:703:THR:HA	2.06	0.55
1:A:59:THR:HG22	1:A:59:THR:O	2.05	0.55
1:A:163:ALA:CA	1:A:199:MET:HE1	2.36	0.55
1:A:182:LEU:HD23	1:C:110:LYS:HG3	1.88	0.55
1:B:112:SER:HB3	1:C:180:ILE:HG12	1.89	0.55
1:A:30:ILE:HD11	1:A:68:MET:CE	2.33	0.55
1:A:99:LEU:HB3	1:A:118:LEU:HD21	1.89	0.55
1:C:16:LEU:HD13	1:C:79:LEU:CD2	2.37	0.55
1:C:7:VAL:N	1:C:58:ASP:OD2	2.40	0.54
1:A:185:THR:HB	1:A:195:VAL:N	2.22	0.54
1:B:143:GLU:OE2	1:B:182:LEU:HD22	2.08	0.54
1:C:200:ASN:H	1:C:200:ASN:ND2	2.04	0.54
1:B:45:VAL:HG12	1:B:45:VAL:O	2.07	0.54
1:A:16:LEU:CD2	1:A:79:LEU:HD13	2.33	0.54
1:B:40:MET:HE2	1:B:44:HIS:HA	1.90	0.54
1:B:56:GLY:HA3	1:B:244:MET:HB2	1.88	0.54
1:C:1:MET:HE1	1:C:61:ARG:HE	1.72	0.54
1:C:215:PHE:O	1:C:217:LYS:N	2.41	0.53
1:C:167:VAL:HG13	1:C:182:LEU:HB2	1.90	0.53
1:A:95:ASN:O	1:A:96:ALA:C	2.52	0.53
1:A:199:MET:O	1:A:199:MET:HG2	2.09	0.53
1:B:167:VAL:HG13	1:B:182:LEU:HB2	1.89	0.53
1:A:37:LEU:HD23	1:A:38:GLN:N	2.22	0.53
1:B:25:GLU:O	1:B:26:ALA:HB2	2.07	0.53
1:B:47:LEU:HD12	1:B:48:VAL:N	2.23	0.53
1:C:236:VAL:CG2	1:C:250:TYR:CE2	2.91	0.53
1:C:236:VAL:HG22	1:C:250:TYR:CD2	2.44	0.53
1:B:204:GLN:O	1:B:204:GLN:CG	2.57	0.53
1:C:163:ALA:HA	1:C:199:MET:HE1	1.90	0.53
1:C:75:MET:CG	1:C:116:MET:HE1	2.39	0.53
1:B:169:PHE:HE1	1:B:182:LEU:CD1	2.22	0.52
1:C:138:LYS:HD3	1:C:224:THR:HG21	1.91	0.52
1:A:53:ARG:NH2	3:A:265:HOH:O	2.42	0.52
1:B:43:SER:O	1:B:44:HIS:HB2	2.07	0.52
1:B:197:ILE:HG22	1:B:198:GLU:N	2.24	0.52
1:A:5:ARG:HB3	1:A:59:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:HD12	1:B:100:ALA:H	1.73	0.52
1:B:107:ASN:O	1:B:109:GLU:N	2.42	0.52
1:A:16:LEU:HD13	1:A:79:LEU:CD1	2.40	0.52
1:C:126:LEU:HD12	2:W:710:PRO:HA	1.91	0.52
1:A:178:GLY:HA2	1:C:113:ASP:O	2.10	0.51
1:C:125:GLN:OE1	1:C:125:GLN:HA	2.09	0.51
1:C:27:CYS:SG	1:C:67:ALA:HB1	2.51	0.51
1:B:69:GLY:HA3	1:B:119:MET:O	2.10	0.51
1:C:54:SER:C	1:C:56:GLY:N	2.68	0.51
1:A:135:CYS:SG	1:A:162:CYS:HB3	2.51	0.51
1:B:105:ALA:O	1:B:106:PRO:O	2.29	0.51
1:A:11:ILE:O	1:A:15:VAL:HG23	2.11	0.51
1:C:156:ASP:OD1	1:C:156:ASP:C	2.54	0.51
1:C:2:PHE:HA	1:C:61:ARG:O	2.11	0.51
1:C:165:ASP:N	1:C:165:ASP:OD1	2.44	0.51
1:A:224:THR:CG2	1:A:225:VAL:N	2.74	0.50
1:A:106:PRO:HG2	1:A:107:ASN:N	2.26	0.50
1:C:18:ALA:HB2	1:C:218:ALA:HA	1.93	0.50
1:A:182:LEU:CD2	1:C:110:LYS:HG3	2.41	0.50
1:A:219:THR:N	1:A:220:PRO:CD	2.73	0.50
1:A:6:LEU:CD2	1:A:12:LEU:HD22	2.41	0.50
1:A:12:LEU:C	1:A:79:LEU:HD22	2.36	0.50
1:B:142:GLY:O	1:B:146:ARG:HG3	2.11	0.50
1:A:23:ILE:HG22	1:A:41:ASP:HA	1.94	0.50
1:A:133:TYR:HB3	1:A:229:MET:O	2.12	0.50
1:B:232:ASP:O	1:B:233:VAL:HG12	2.12	0.50
1:A:10:SER:O	1:A:14:LYS:HG3	2.13	0.49
1:A:175:LEU:CD1	1:C:74:SER:OG	2.60	0.49
2:U:703:THR:HG21	2:U:705:GLU:OE1	2.12	0.49
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.47	0.49
1:A:8:GLN:HA	1:A:8:GLN:OE1	2.11	0.49
1:A:146:ARG:HG3	1:A:146:ARG:HH11	1.78	0.49
1:B:40:MET:HE3	2:V:704:LEU:HB3	1.95	0.49
1:C:140:PRO:O	1:C:141:SER:C	2.54	0.49
2:U:703:THR:HG21	2:U:705:GLU:CD	2.37	0.49
1:B:46:SER:HA	2:V:704:LEU:HD22	1.94	0.49
1:C:254:LYS:HG3	2:W:701:MET:HE3	1.95	0.49
1:B:203:VAL:HG11	1:B:229:MET:HG3	1.95	0.49
1:A:1:MET:HB3	1:A:63:ASP:OD2	2.12	0.49
1:B:172:SER:HA	1:B:177:ASN:HA	1.95	0.49
1:C:233:VAL:HG23	1:C:233:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:PHE:HE1	1:B:182:LEU:HD12	1.78	0.48
1:C:32:SER:OG	1:C:33:SER:N	2.46	0.48
1:C:91:ARG:O	1:C:99:LEU:HD12	2.13	0.48
1:A:203:VAL:HG12	1:A:204:GLN:N	2.27	0.48
1:C:3:GLU:HB3	1:C:61:ARG:HB3	1.96	0.48
1:C:95:ASN:O	1:C:96:ALA:CB	2.62	0.48
1:A:134:SER:HA	1:A:200:ASN:HD22	1.78	0.48
1:C:217:LYS:C	1:C:219:THR:N	2.65	0.48
1:C:242:ALA:O	1:C:243:ASP:C	2.56	0.48
1:A:51:THR:O	1:A:245:GLY:HA3	2.14	0.48
1:A:175:LEU:HD11	1:C:74:SER:OG	2.13	0.48
1:B:160:ILE:HG23	1:B:169:PHE:CD2	2.48	0.48
1:A:6:LEU:HD22	1:A:12:LEU:HD22	1.96	0.48
1:A:20:LYS:HE3	1:A:21:ASP:OD1	2.14	0.48
2:U:702:GLN:OE1	2:U:702:GLN:N	2.47	0.48
1:B:130:GLU:CG	1:B:130:GLU:O	2.61	0.48
2:U:712:THR:O	2:U:712:THR:CG2	2.62	0.47
1:B:161:SER:O	1:B:162:CYS:C	2.56	0.47
1:C:167:VAL:CG1	1:C:182:LEU:HB2	2.44	0.47
1:B:215:PHE:CD1	1:B:215:PHE:N	2.82	0.47
1:C:75:MET:HG3	1:C:116:MET:HE1	1.96	0.47
1:A:113:ASP:O	1:B:178:GLY:HA2	2.15	0.47
1:A:40:MET:HE2	1:A:40:MET:HB3	1.44	0.47
1:A:50:LEU:HD13	1:A:247:LEU:HD13	1.95	0.47
1:A:137:VAL:HG11	1:A:139:MET:HE2	1.96	0.47
1:A:255:ILE:HD12	1:A:255:ILE:HA	1.76	0.47
1:B:234:PRO:HD3	2:V:707:PHE:CE2	2.48	0.47
1:C:31:SER:O	1:C:33:SER:N	2.47	0.47
1:C:78:ILE:O	1:C:81:CYS:HB2	2.13	0.47
1:A:225:VAL:HG22	1:A:226:THR:N	2.28	0.47
1:C:136:VAL:HG22	1:C:228:SER:OG	2.14	0.47
1:C:227:LEU:HD23	1:C:237:VAL:HG13	1.97	0.47
1:A:24:ASN:HD22	1:A:25:GLU:N	2.13	0.47
2:U:703:THR:HG21	2:U:705:GLU:CB	2.45	0.47
1:C:207:PHE:CZ	1:C:235:LEU:HB2	2.50	0.47
1:A:227:LEU:HB3	1:A:235:LEU:HD11	1.96	0.46
1:B:151:LEU:HD22	1:B:171:ALA:HB3	1.97	0.46
1:B:224:THR:HG22	1:B:225:VAL:N	2.29	0.46
1:C:79:LEU:HA	1:C:79:LEU:HD12	1.58	0.46
1:C:233:VAL:O	1:C:234:PRO:C	2.59	0.46
1:A:37:LEU:C	1:A:37:LEU:CD2	2.86	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:O	1:A:164:LYS:C	2.59	0.46
1:B:232:ASP:C	1:B:233:VAL:CG1	2.88	0.46
1:C:15:VAL:O	1:C:15:VAL:HG12	2.16	0.46
1:C:164:LYS:O	1:C:165:ASP:CB	2.63	0.46
1:B:153:HIS:N	1:B:153:HIS:CD2	2.83	0.46
1:C:16:LEU:HD11	1:C:75:MET:HE2	1.97	0.46
1:A:50:LEU:CD1	1:A:247:LEU:HD13	2.46	0.46
1:A:106:PRO:CG	1:A:107:ASN:H	2.27	0.46
1:A:135:CYS:SG	1:A:162:CYS:SG	3.07	0.46
1:A:16:LEU:CD1	1:A:79:LEU:HD13	2.41	0.46
1:B:29:ASP:HA	1:B:66:LEU:O	2.16	0.46
1:C:230:SER:O	1:C:231:ALA:C	2.59	0.46
2:U:703:THR:HG21	2:U:705:GLU:HB2	1.98	0.46
1:B:70:VAL:HG12	1:B:72:LEU:HD23	1.98	0.46
1:B:134:SER:HA	1:B:200:ASN:OD1	2.16	0.46
1:B:40:MET:HE2	1:B:44:HIS:CA	2.46	0.45
1:C:74:SER:O	1:C:78:ILE:HG13	2.16	0.45
1:A:139:MET:HE1	1:A:169:PHE:CZ	2.49	0.45
1:B:7:VAL:HA	1:B:87:ILE:HG23	1.97	0.45
1:C:169:PHE:CD1	1:C:169:PHE:N	2.85	0.45
1:B:38:GLN:O	1:B:39:SER:HB2	2.15	0.45
1:A:96:ALA:O	1:A:98:THR:N	2.44	0.45
1:A:167:VAL:HG13	1:A:167:VAL:O	2.16	0.45
1:C:215:PHE:C	1:C:217:LYS:H	2.25	0.45
1:B:107:ASN:O	1:B:107:ASN:CG	2.59	0.45
1:B:209:LEU:O	1:B:210:ARG:C	2.60	0.45
1:A:246:HIS:C	1:A:246:HIS:CD2	2.94	0.45
1:A:41:ASP:OD2	1:A:41:ASP:C	2.59	0.45
1:A:207:PHE:CZ	1:A:235:LEU:HB2	2.52	0.45
1:B:162:CYS:O	1:B:167:VAL:N	2.50	0.45
1:B:49:GLN:NE2	1:B:49:GLN:C	2.75	0.45
1:C:9:GLY:C	1:C:11:ILE:N	2.70	0.45
1:A:94:ASP:O	1:A:95:ASN:HB3	2.17	0.44
1:A:138:LYS:HB3	1:A:196:THR:HB	1.99	0.44
1:A:207:PHE:CE1	1:A:253:PRO:HA	2.52	0.44
1:C:48:VAL:CG1	1:C:49:GLN:N	2.80	0.44
1:C:95:ASN:ND2	1:C:95:ASN:N	2.30	0.44
1:A:70:VAL:HG13	1:A:116:MET:CE	2.47	0.44
1:B:20:LYS:NZ	1:B:80:LYS:NZ	2.66	0.44
1:B:128:ILE:CD1	1:B:250:TYR:CE2	3.01	0.44
1:B:234:PRO:CD	2:V:707:PHE:CD2	2.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:C	1:C:33:SER:N	2.73	0.44
1:C:138:LYS:HD3	1:C:224:THR:CG2	2.47	0.44
1:C:29:ASP:HA	1:C:66:LEU:O	2.18	0.44
1:A:13:LYS:N	1:A:79:LEU:CD2	2.80	0.44
2:U:703:THR:HG22	2:U:705:GLU:HG3	1.98	0.44
1:B:43:SER:CB	1:B:211:TYR:OH	2.65	0.44
1:A:146:ARG:HG3	1:A:146:ARG:NH1	2.32	0.44
1:B:235:LEU:HG	1:B:236:VAL:N	2.32	0.44
1:A:78:ILE:O	1:A:81:CYS:HB2	2.18	0.44
1:B:45:VAL:O	1:B:45:VAL:CG1	2.65	0.44
1:A:139:MET:HB2	1:A:140:PRO:HD2	2.00	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.78	0.43
1:A:160:ILE:HD12	1:A:207:PHE:CD2	2.52	0.43
1:B:93:GLU:O	1:B:95:ASN:O	2.35	0.43
1:B:128:ILE:HD13	1:B:250:TYR:CE2	2.54	0.43
1:B:55:GLU:O	1:B:56:GLY:C	2.61	0.43
1:B:106:PRO:HB2	1:B:107:ASN:H	1.52	0.43
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.65	0.43
2:U:703:THR:HG22	2:U:704:LEU:N	2.31	0.43
1:C:139:MET:HE1	1:C:227:LEU:HD11	1.99	0.43
1:C:160:ILE:HD12	1:C:207:PHE:CE2	2.52	0.43
1:B:20:LYS:NZ	1:B:80:LYS:HZ1	2.17	0.43
1:A:128:ILE:HD13	1:A:250:TYR:CE2	2.54	0.43
1:A:158:VAL:O	1:A:206:THR:HA	2.19	0.43
1:B:28:TRP:HE1	1:B:72:LEU:HD21	1.84	0.43
1:C:47:LEU:HD23	1:C:48:VAL:N	2.34	0.43
1:C:215:PHE:C	1:C:217:LYS:N	2.76	0.43
1:A:156:ASP:C	1:A:209:LEU:HD12	2.44	0.43
1:B:177:ASN:OD1	1:B:177:ASN:C	2.62	0.43
1:C:79:LEU:C	1:C:81:CYS:N	2.75	0.43
1:A:135:CYS:HG	1:A:162:CYS:CB	2.32	0.42
1:B:47:LEU:C	1:B:47:LEU:CD1	2.85	0.42
1:B:197:ILE:CG2	1:B:198:GLU:N	2.81	0.42
1:C:40:MET:HE3	1:C:126:LEU:HD22	2.00	0.42
1:C:88:ILE:HG22	1:C:89:THR:N	2.29	0.42
2:W:705:GLU:H	2:W:705:GLU:HG3	1.48	0.42
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.72	0.42
1:A:160:ILE:HD12	1:A:207:PHE:HD2	1.84	0.42
1:B:14:LYS:HB2	1:B:221:LEU:HD21	2.01	0.42
1:C:134:SER:O	1:C:135:CYS:HB2	2.19	0.42
1:A:211:TYR:OH	2:U:698:PRO:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD21	1:B:75:MET:HB3	2.00	0.42
1:B:101:LEU:HD12	1:B:101:LEU:N	2.34	0.42
1:C:35:VAL:HG12	1:C:36:ASN:N	2.34	0.42
1:C:241:ILE:O	1:C:242:ALA:C	2.63	0.42
1:B:4:ALA:HB1	1:B:57:PHE:CD2	2.55	0.42
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.84	0.42
1:B:50:LEU:HG	1:B:51:THR:N	2.35	0.42
1:A:163:ALA:C	1:A:199:MET:HE1	2.44	0.42
1:C:95:ASN:HB2	1:C:96:ALA:H	1.47	0.42
1:A:228:SER:HB2	1:A:236:VAL:HB	2.00	0.42
1:C:97:ASP:O	1:C:98:THR:OG1	2.30	0.42
1:A:5:ARG:HA	1:A:89:THR:HA	2.02	0.42
1:C:64:ARG:O	1:C:65:ASN:C	2.62	0.42
2:U:703:THR:CG2	2:U:705:GLU:CB	2.98	0.41
1:C:54:SER:O	1:C:56:GLY:N	2.53	0.41
1:C:219:THR:N	1:C:220:PRO:HD2	2.34	0.41
1:A:134:SER:HB3	1:A:201:GLU:O	2.20	0.41
1:C:112:SER:HB3	1:C:114:TYR:CE1	2.55	0.41
1:A:163:ALA:N	1:A:199:MET:HE1	2.34	0.41
1:B:199:MET:SD	1:B:201:GLU:C	3.03	0.41
1:B:230:SER:O	1:B:231:ALA:C	2.63	0.41
1:A:128:ILE:HD13	1:A:250:TYR:CZ	2.55	0.41
1:B:53:ARG:NH2	3:B:270:HOH:O	2.53	0.41
1:C:202:PRO:C	1:C:203:VAL:CG2	2.93	0.41
1:B:40:MET:HE3	2:V:704:LEU:CB	2.50	0.41
2:U:711:LEU:HD23	2:U:711:LEU:HA	1.72	0.41
1:B:16:LEU:CD2	1:B:75:MET:HB3	2.50	0.41
1:C:205:LEU:HD22	1:C:253:PRO:HB2	2.02	0.41
2:U:712:THR:O	2:U:712:THR:HG23	2.20	0.41
1:C:98:THR:O	1:C:98:THR:HG22	2.19	0.41
1:C:164:LYS:O	1:C:165:ASP:HB3	2.21	0.41
1:C:224:THR:HG22	1:C:225:VAL:N	2.36	0.41
1:A:40:MET:HE1	2:U:704:LEU:HB2	2.02	0.41
1:B:11:ILE:O	1:B:15:VAL:HG23	2.20	0.41
1:B:236:VAL:O	1:B:236:VAL:HG13	2.21	0.41
1:C:98:THR:H	1:C:118:LEU:HD12	1.86	0.41
1:C:99:LEU:HD12	1:C:100:ALA:N	2.35	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.82	0.41
1:C:16:LEU:CD1	1:C:75:MET:HE2	2.51	0.41
1:C:79:LEU:C	1:C:81:CYS:H	2.27	0.41
1:B:71:ASN:OD1	1:B:71:ASN:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:CE1	1:B:235:LEU:HB2	2.56	0.40
1:C:1:MET:HE2	1:C:1:MET:HB3	1.98	0.40
1:A:106:PRO:CG	1:A:107:ASN:N	2.77	0.40
1:B:10:SER:O	1:B:11:ILE:C	2.63	0.40
1:C:14:LYS:CE	1:C:220:PRO:O	2.66	0.40
1:C:157:ALA:N	1:C:209:LEU:HD12	2.37	0.40
1:A:207:PHE:CD1	1:A:253:PRO:HA	2.57	0.40
1:C:45:VAL:O	1:C:45:VAL:HG13	2.21	0.40
1:B:57:PHE:CD1	1:B:57:PHE:N	2.89	0.40
1:A:203:VAL:CG1	1:A:204:GLN:N	2.84	0.40
1:C:45:VAL:O	1:C:45:VAL:CG1	2.66	0.40
1:C:163:ALA:C	1:C:199:MET:HE1	2.47	0.40
1:C:177:ASN:OD1	1:C:177:ASN:C	2.64	0.40
1:C:199:MET:HE2	1:C:202:PRO:HA	2.04	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	242/261 (93%)	220 (91%)	13 (5%)	9 (4%)	2	6
1	B	237/261 (91%)	210 (89%)	21 (9%)	6 (2%)	4	11
1	C	243/261 (93%)	213 (88%)	19 (8%)	11 (4%)	2	4
2	U	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
2	V	8/21 (38%)	8 (100%)	0	0	100	100
2	W	9/21 (43%)	9 (100%)	0	0	100	100
All	All	757/846 (90%)	677 (89%)	54 (7%)	26 (3%)	3	7

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	96	ALA
1	A	105	ALA
1	A	108	GLN
1	B	94	ASP
1	B	106	PRO
1	B	108	GLN
1	C	98	THR
1	C	165	ASP
1	A	106	PRO
1	A	184	GLN
1	C	32	SER
1	C	95	ASN
1	C	96	ALA
1	B	124	GLU
1	B	244	MET
1	C	244	MET
1	A	71	ASN
1	C	150	ASP
1	A	10	SER
1	B	184	GLN
1	C	55	GLU
1	C	135	CYS
1	C	216	THR
1	A	94	ASP
1	C	242	ALA

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	215/228 (94%)	178 (83%)	37 (17%)	2	6
1	B	213/228 (93%)	182 (85%)	31 (15%)	3	8
1	C	215/228 (94%)	189 (88%)	26 (12%)	5	12
2	U	19/20 (95%)	16 (84%)	3 (16%)	2	7
2	V	10/20 (50%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	10/20 (50%)	10 (100%)	0	100	100
All	All	682/744 (92%)	585 (86%)	97 (14%)	3	8

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ARG
1	A	12	LEU
1	A	16	LEU
1	A	20	LYS
1	A	24	ASN
1	A	32	SER
1	A	40	MET
1	A	45	VAL
1	A	51	THR
1	A	59	THR
1	A	76	SER
1	A	79	LEU
1	A	80	LYS
1	A	88	ILE
1	A	89	THR
1	A	93	GLU
1	A	97	ASP
1	A	101	LEU
1	A	110	LYS
1	A	119	MET
1	A	120	ASP
1	A	121	LEU
1	A	123	VAL
1	A	162	CYS
1	A	182	LEU
1	A	183	SER
1	A	185	THR
1	A	199	MET
1	A	201	GLU
1	A	219	THR
1	A	226	THR
1	A	227	LEU
1	A	243	ASP
1	A	244	MET
1	A	247	LEU

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Mol	Chain	Res	Type
1	A	255	ILE
2	U	693	CYS
2	U	699	GLU
2	U	712	THR
1	B	16	LEU
1	B	30	ILE
1	B	38	GLN
1	B	43	SER
1	B	53	ARG
1	B	66	LEU
1	B	74	SER
1	B	76	SER
1	B	79	LEU
1	B	89	THR
1	B	102	VAL
1	B	109	GLU
1	B	110	LYS
1	B	112	SER
1	B	123	VAL
1	B	141	SER
1	B	160	ILE
1	B	168	LYS
1	B	170	SER
1	B	175	LEU
1	B	181	LYS
1	B	184	GLN
1	B	185	THR
1	B	196	THR
1	B	199	MET
1	B	200	ASN
1	B	203	VAL
1	B	205	LEU
1	B	217	LYS
1	B	233	VAL
1	B	243	ASP
1	C	7	VAL
1	C	8	GLN
1	C	10	SER
1	C	16	LEU
1	C	20	LYS
1	C	21	ASP
1	C	41	ASP

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Mol	Chain	Res	Type
1	C	45	VAL
1	C	47	LEU
1	C	59	THR
1	C	77	LYS
1	C	79	LEU
1	C	95	ASN
1	C	120	ASP
1	C	121	LEU
1	C	122	ASP
1	C	126	LEU
1	C	128	ILE
1	C	149	ARG
1	C	175	LEU
1	C	199	MET
1	C	200	ASN
1	C	217	LYS
1	C	230	SER
1	C	247	LEU
1	C	254	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	36	ASN
1	A	65	ASN
1	A	177	ASN
1	A	179	ASN
1	A	200	ASN
1	A	204	GLN
1	B	36	ASN
1	B	44	HIS
1	B	49	GLN
1	B	65	ASN
1	B	179	ASN
1	B	184	GLN
1	B	213	ASN
1	C	49	GLN
1	C	95	ASN
1	C	200	ASN
1	C	246	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	246/261 (94%)	0.04	3 (1%) 76 75	12, 31, 40, 48	21 (8%)
1	B	243/261 (93%)	0.12	9 (3%) 45 41	13, 32, 46, 62	23 (9%)
1	C	247/261 (94%)	-0.02	2 (0%) 82 81	14, 32, 44, 53	15 (6%)
2	U	20/21 (95%)	-0.10	1 (5%) 34 30	2, 8, 27, 35	2 (10%)
2	V	10/21 (47%)	0.76	1 (10%) 12 10	30, 33, 35, 40	0
2	W	11/21 (52%)	-0.41	0 100 100	39, 40, 47, 48	0
All	All	777/846 (91%)	0.04	16 (2%) 63 61	2, 32, 45, 62	61 (7%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.9
1	B	108	GLN	3.4
1	A	93	GLU	3.3
1	B	96	ALA	3.3
1	C	96	ALA	2.8
2	V	710	PRO	2.6
1	C	97	ASP	2.6
1	B	162	CYS	2.5
1	A	185	THR	2.5
2	U	697	ARG	2.5
1	B	107	ASN	2.4
1	B	161	SER	2.3
1	A	1	MET	2.2
1	B	183	SER	2.2
1	B	194	ALA	2.1
1	B	199	MET	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.