



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 09:50 PM UTC

PDB ID : 2ZVL / pdb_00002zvl
Title : Crystal structure of PCNA in complex with DNA polymerase kappa fragment
Authors : Hishiki, A.; Hashimoto, H.; Hanafusa, T.; Kamei, K.; Ohashi, E.; Shimizu, T.; Ohmori, H.; Sato, M.
Deposited on : 2008-11-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

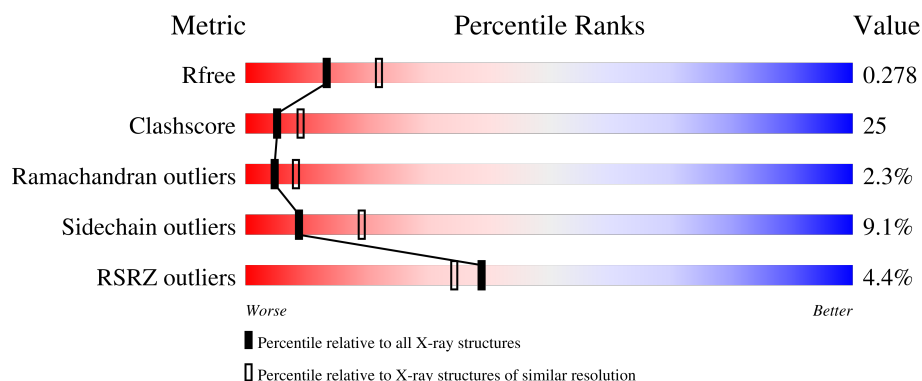
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



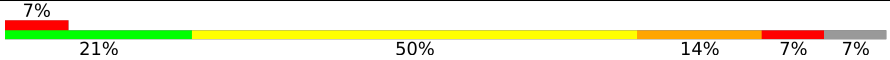
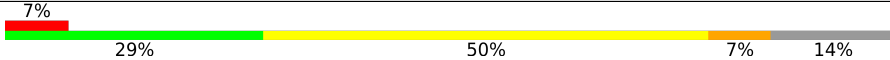
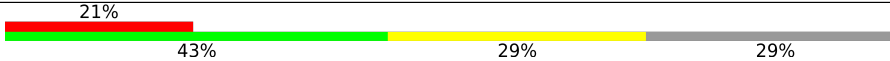
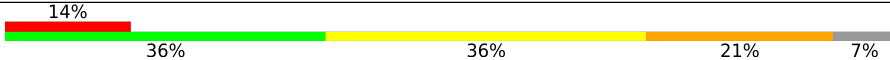
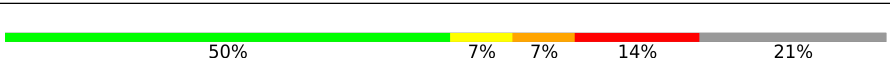
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	 4% 60% 27% 6% • 6%
1	B	261	 3% 58% 28% 8% • 5%
1	C	261	 4% 58% 31% 5% • 5%
1	D	261	 4% 54% 34% 6% • 5%
1	E	261	 2% 61% 27% 5% • 7%

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Mol	Chain	Length	Quality of chain
1	F	261	
2	U	14	
2	V	14	
2	W	14	
2	X	14	
2	Y	14	
2	Z	14	

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
3	SO4	D	262	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12074 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	245	Total	C	N	O	S	89	0	0
			1886	1189	310	371	16			
1	B	247	Total	C	N	O	S	62	0	0
			1898	1196	312	374	16			
1	C	247	Total	C	N	O	S	79	0	0
			1898	1196	312	374	16			
1	D	247	Total	C	N	O	S	61	0	0
			1898	1196	312	374	16			
1	E	244	Total	C	N	O	S	44	0	0
			1875	1184	308	367	16			
1	F	243	Total	C	N	O	S	38	0	0
			1870	1181	307	366	16			

- Molecule 2 is a protein called DNA polymerase kappa.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	11	Total	C	N	O	22	0	0
			96	67	15	14			
2	V	13	Total	C	N	O	7	0	0
			110	76	17	17			
2	W	12	Total	C	N	O	3	0	0
			103	72	16	15			
2	X	10	Total	C	N	O	8	0	0
			88	61	14	13			
2	Y	13	Total	C	N	O	0	0	0
			110	76	17	17			
2	Z	11	Total	C	N	O	4	0	0
			96	67	15	14			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	V	1	Total	Zn	0	0
			1	1		
4	W	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	Y	1	Total	Zn	0	0
			1	1		
4	Z	1	Total	Zn	0	0
			1	1		

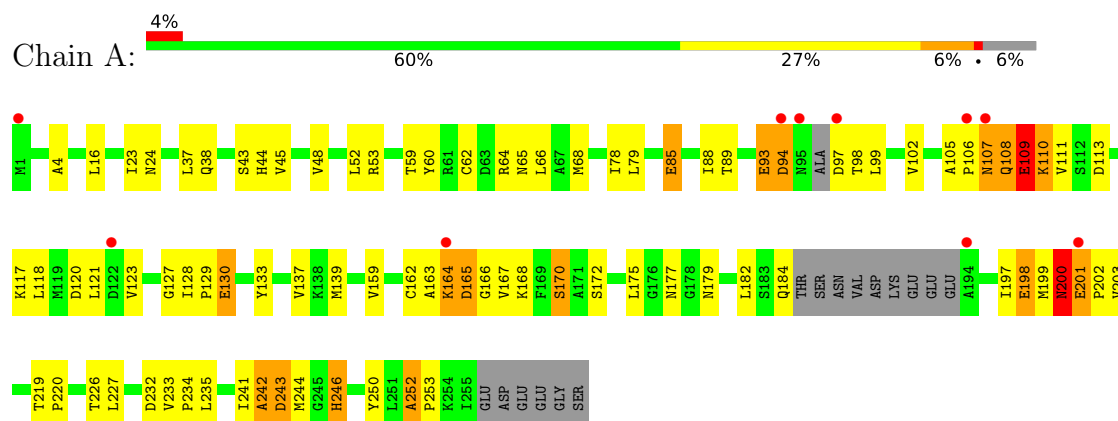
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	U	1	Total 1	O 1	0	0
5	B	26	Total 26	O 26	0	0
5	V	3	Total 3	O 3	0	0
5	C	17	Total 17	O 17	0	0
5	W	3	Total 3	O 3	0	0
5	D	18	Total 18	O 18	0	0
5	X	1	Total 1	O 1	0	0
5	E	17	Total 17	O 17	0	0
5	Y	1	Total 1	O 1	0	0
5	F	21	Total 21	O 21	0	0
5	Z	2	Total 2	O 2	0	0

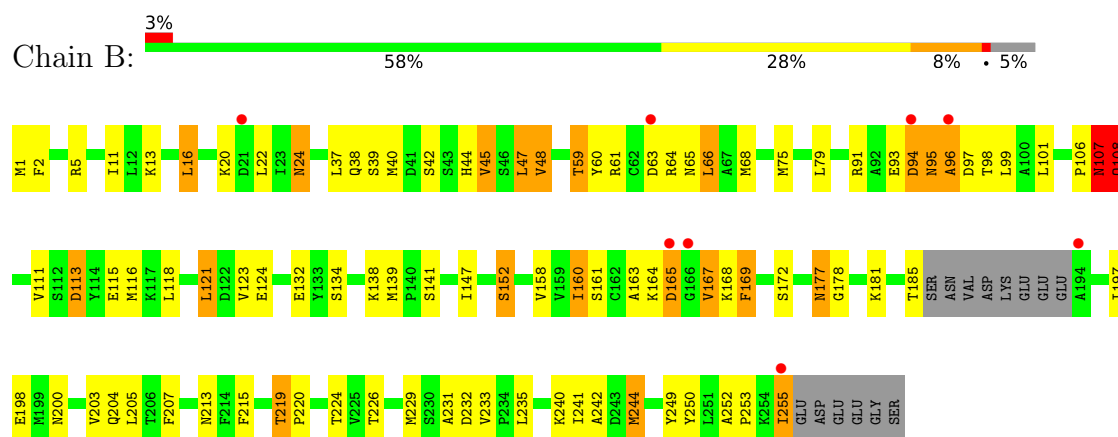
3 Residue-property plots [i](#)

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.

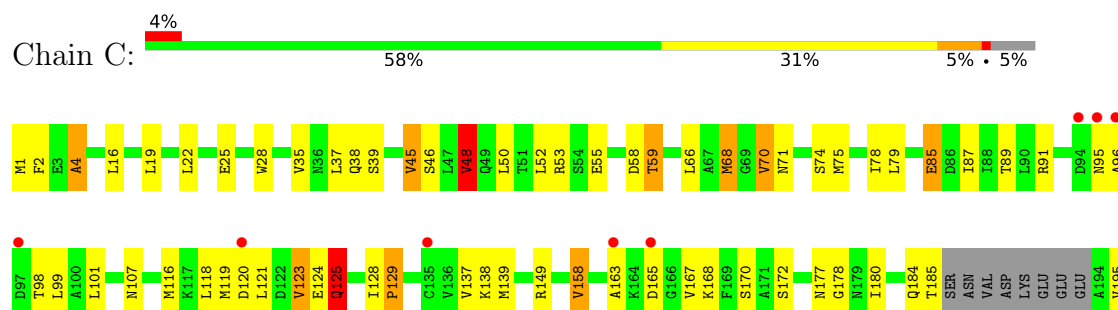
• Molecule 1: Proliferating cell nuclear antigen

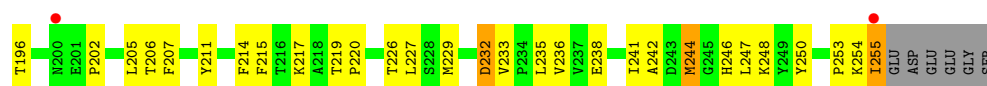


• Molecule 1: Proliferating cell nuclear antigen

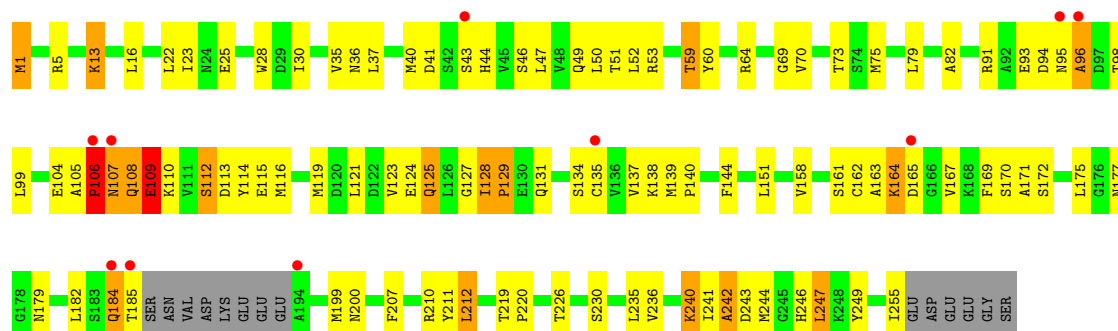


• Molecule 1: Proliferating cell nuclear antigen

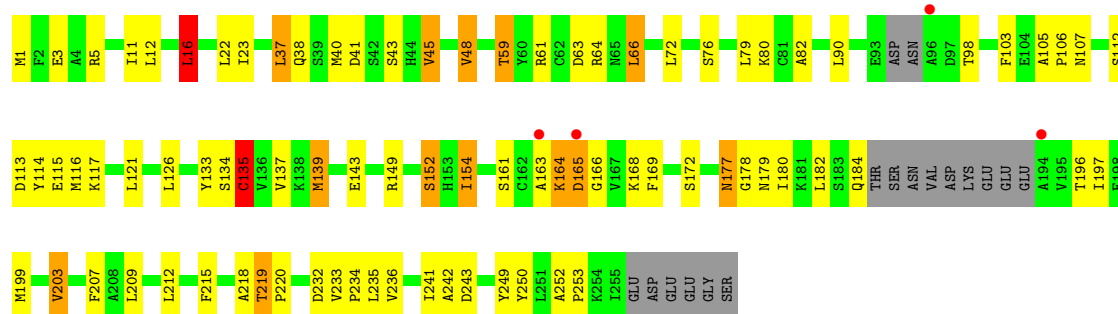




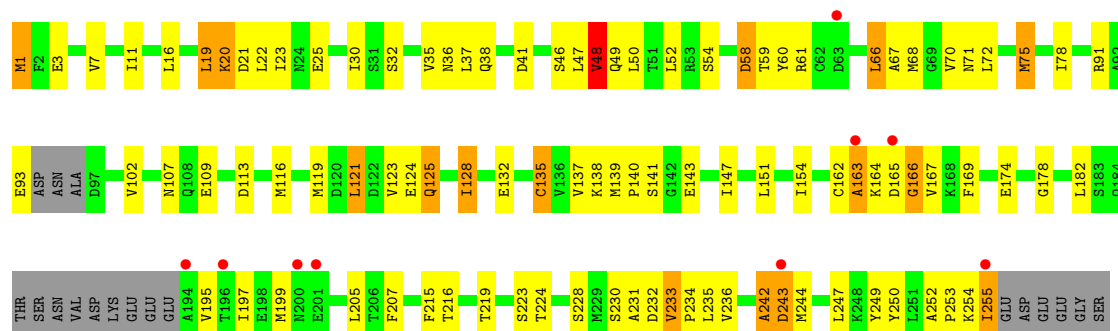
• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen

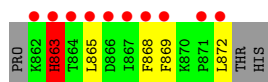


• Molecule 1: Proliferating cell nuclear antigen

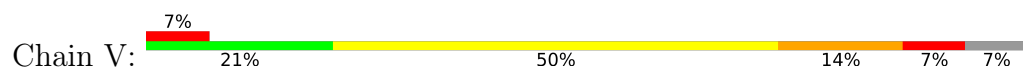


• Molecule 2: DNA polymerase kappa

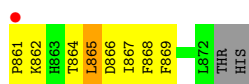




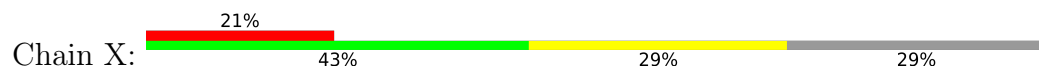
- Molecule 2: DNA polymerase kappa



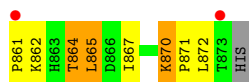
- Molecule 2: DNA polymerase kappa



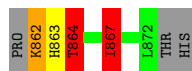
- Molecule 2: DNA polymerase kappa



- Molecule 2: DNA polymerase kappa



- Molecule 2: DNA polymerase kappa



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.77Å 74.71Å 109.05Å 87.25° 77.46° 80.26°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 90.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.225 , 0.289 0.224 , 0.278	Depositor DCC
R_{free} test set	3575 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12074	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.64% 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: SO4, ZN

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	1.07	2/1910 (0.1%)	1.12	8/2577 (0.3%)
1	B	1.23	5/1923 (0.3%)	1.20	7/2597 (0.3%)
1	C	1.19	3/1923 (0.2%)	1.16	2/2597 (0.1%)
1	D	1.11	1/1923 (0.1%)	1.14	2/2597 (0.1%)
1	E	1.24	1/1899 (0.1%)	1.23	9/2562 (0.4%)
1	F	1.27	4/1894 (0.2%)	1.25	10/2555 (0.4%)
2	U	0.76	0/99	0.82	0/132
2	V	1.02	0/114	1.65	2/153 (1.3%)
2	W	1.23	1/107 (0.9%)	1.11	0/143
2	X	0.68	0/91	0.82	0/121
2	Y	1.30	0/114	1.43	2/153 (1.3%)
2	Z	1.47	1/99 (1.0%)	1.52	2/132 (1.5%)
All	All	1.19	18/12096 (0.1%)	1.19	44/16319 (0.3%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	863	HIS	N-CA	7.19	1.55	1.46
1	A	111	VAL	C-O	-6.93	1.17	1.24
1	A	159	VAL	CA-CB	6.79	1.62	1.54
1	C	4	ALA	CA-C	6.57	1.60	1.52
1	F	216	THR	CA-CB	-6.16	1.42	1.53
1	B	111	VAL	C-O	-5.90	1.17	1.24
1	C	70	VAL	CA-CB	-5.67	1.47	1.54
1	C	48	VAL	N-CA	5.59	1.53	1.46
1	F	19	LEU	C-O	-5.46	1.18	1.23
1	E	253	PRO	C-O	-5.45	1.17	1.23
1	F	58	ASP	N-CA	-5.39	1.39	1.46
1	B	219	THR	N-CA	5.38	1.51	1.46
1	B	252	ALA	C-O	-5.23	1.17	1.24
1	F	49	GLN	N-CA	-5.22	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	212	LEU	N-CA	-5.21	1.40	1.46
1	B	253	PRO	C-O	-5.17	1.17	1.23
1	B	244	MET	C-O	-5.16	1.18	1.24
2	W	865	LEU	CA-C	5.01	1.59	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	VAL	CB-CA-C	-11.91	94.19	110.98
1	F	48	VAL	CB-CA-C	-11.56	92.33	110.95
1	A	252	ALA	CA-C-N	10.38	132.82	119.84
1	A	252	ALA	C-N-CA	10.38	132.82	119.84
1	F	128	ILE	CA-C-N	9.09	131.20	119.84
1	F	128	ILE	C-N-CA	9.09	131.20	119.84
1	E	45	VAL	N-CA-C	-8.77	105.38	113.71
1	F	233	VAL	CA-C-N	-7.70	112.08	119.85
1	F	233	VAL	C-N-CA	-7.70	112.08	119.85
1	B	48	VAL	CB-CA-C	-7.35	99.66	110.62
1	E	48	VAL	CB-CA-C	-6.94	99.77	110.95
2	V	871	PRO	N-CA-C	6.62	121.57	114.68
1	B	233	VAL	N-CA-C	6.41	116.25	109.01
1	A	246	HIS	N-CA-C	6.26	117.66	108.14
1	B	45	VAL	N-CA-C	-6.17	106.20	113.42
2	V	867	ILE	CB-CA-C	-6.08	101.32	111.29
1	E	243	ASP	N-CA-C	-6.03	102.68	111.30
1	E	219	THR	CA-C-N	-6.03	113.43	120.12
1	E	219	THR	C-N-CA	-6.03	113.43	120.12
1	A	168	LYS	CG-CD-CE	6.00	125.11	111.30
1	D	110	LYS	N-CA-C	-5.99	98.64	108.76
2	Z	864	THR	N-CA-CB	-5.97	101.30	110.44
2	Z	867	ILE	CB-CA-C	-5.96	102.93	112.16
2	Y	870	LYS	CA-C-N	5.86	125.87	119.90
2	Y	870	LYS	C-N-CA	5.86	125.87	119.90
1	F	164	LYS	CB-CA-C	-5.78	109.92	116.63
1	E	139	MET	N-CA-C	5.63	113.08	108.07
1	F	166	GLY	N-CA-C	5.55	121.27	110.73
1	A	16	LEU	CA-CB-CG	-5.53	96.93	116.30
1	B	95	ASN	N-CA-C	-5.51	106.22	113.17
1	D	109	GLU	N-CA-C	5.41	117.81	107.75
1	E	16	LEU	CA-CB-CG	-5.37	97.49	116.30
1	B	200	ASN	N-CA-C	-5.32	107.80	114.56
1	A	159	VAL	N-CA-C	-5.29	100.76	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	223	SER	CA-C-N	5.29	130.87	122.94
1	F	223	SER	C-N-CA	5.29	130.87	122.94
1	C	39	SER	N-CA-C	5.27	117.09	108.55
1	E	135	CYS	N-CA-C	5.25	118.01	109.24
1	B	16	LEU	CA-CB-CG	-5.23	98.01	116.30
1	E	41	ASP	N-CA-C	-5.22	103.59	110.43
1	A	109	GLU	N-CA-C	5.20	118.09	109.46
1	B	167	VAL	CB-CA-C	-5.10	103.90	111.19
1	A	110	LYS	N-CA-C	-5.08	99.98	110.80
1	F	75	MET	N-CA-C	-5.02	105.70	111.07

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	1886	0	1902	90	0
1	B	1898	0	1915	89	0
1	C	1898	0	1915	93	0
1	D	1898	0	1915	120	0
1	E	1875	0	1897	74	0
1	F	1870	0	1892	92	0
2	U	96	0	101	6	0
2	V	110	0	116	9	0
2	W	103	0	109	11	0
2	X	88	0	90	5	0
2	Y	110	0	116	8	0
2	Z	96	0	101	9	0
3	A	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	5	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	1	0	0	0	0
4	Y	1	0	0	0	0
4	Z	1	0	0	0	0
5	A	10	0	0	1	0
5	B	26	0	0	4	0
5	C	17	0	0	2	0
5	D	18	0	0	2	0
5	E	17	0	0	0	0
5	F	21	0	0	1	0
5	U	1	0	0	0	0
5	V	3	0	0	0	0
5	W	3	0	0	0	0
5	X	1	0	0	0	0
5	Y	1	0	0	0	0
5	Z	2	0	0	0	0
All	All	12074	0	12069	566	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 25.

All (566) 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:163:ALA:O	1:A:199:MET:HE1	1.31	1.28
1:B:40:MET:HE2	1:B:44:HIS:CA	1.75	1.16
1:D:93:GLU:HB2	1:D:96:ALA:HB2	1.14	1.11
1:B:40:MET:HE2	1:B:44:HIS:HA	1.18	1.11
1:C:16:LEU:HD22	1:C:79:LEU:CD1	1.81	1.10
1:D:138:LYS:HG2	1:D:226:THR:CG2	1.81	1.09
1:C:16:LEU:HD22	1:C:79:LEU:HD12	1.32	1.05
1:D:138:LYS:HG2	1:D:226:THR:HG22	1.09	1.04
1:D:40:MET:HE2	1:D:44:HIS:HA	1.40	1.03
1:B:22:LEU:HD23	1:B:48:VAL:CG2	1.90	1.01
1:F:66:LEU:HD23	1:F:67:ALA:H	1.26	1.00
1:E:114:TYR:CE2	1:F:154:ILE:HD11	1.97	1.00
1:C:85:GLU:OE1	1:C:85:GLU:HA	1.63	0.99
1:D:93:GLU:HB2	1:D:96:ALA:CB	1.93	0.99
1:E:172:SER:HB3	1:E:177:ASN:HB3	1.49	0.95
1:E:114:TYR:HE2	1:F:154:ILE:HD11	1.30	0.94
1:A:23:ILE:HG22	1:A:24:ASN:N	1.85	0.91
1:B:16:LEU:HD13	1:B:79:LEU:HD11	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LYS:CG	1:D:226:THR:HG22	1.99	0.91
1:F:123:VAL:HG12	1:F:124:GLU:N	1.84	0.91
1:D:109:GLU:HA	1:D:109:GLU:OE1	1.70	0.90
1:A:43:SER:OG	1:A:45:VAL:HG12	1.72	0.90
1:B:16:LEU:HD13	1:B:79:LEU:CD1	2.02	0.90
1:D:184:GLN:O	1:D:184:GLN:CD	2.18	0.87
1:B:40:MET:HE3	2:V:865:LEU:HB3	1.55	0.85
1:A:163:ALA:C	1:A:199:MET:HE1	2.01	0.85
1:B:138:LYS:HG2	1:B:226:THR:HG22	1.56	0.85
1:D:172:SER:HB3	1:D:177:ASN:HD22	1.42	0.85
1:A:105:ALA:HB3	1:A:108:GLN:O	1.76	0.84
1:B:40:MET:HE2	1:B:44:HIS:CB	2.08	0.84
1:A:163:ALA:O	1:A:199:MET:CE	2.23	0.84
1:A:172:SER:CB	1:A:177:ASN:HD22	1.91	0.84
1:C:50:LEU:HD13	1:C:247:LEU:HD13	1.58	0.84
1:F:123:VAL:HG12	1:F:124:GLU:H	1.40	0.83
1:C:45:VAL:CG2	2:W:861:PRO:O	2.27	0.82
1:E:37:LEU:HD23	1:E:37:LEU:C	2.05	0.82
1:F:66:LEU:CD2	1:F:67:ALA:H	1.92	0.82
1:E:1:MET:HG2	1:E:61:ARG:CZ	2.10	0.81
1:B:255:ILE:CG2	1:B:255:ILE:O	2.27	0.81
2:V:863:HIS:HB3	2:V:866:ASP:OD2	1.78	0.81
1:F:66:LEU:HD23	1:F:67:ALA:N	1.95	0.80
1:F:66:LEU:CD2	1:F:67:ALA:N	2.44	0.80
1:B:22:LEU:HD23	1:B:48:VAL:HG21	1.62	0.80
1:E:98:THR:HB	1:E:116:MET:O	1.82	0.80
1:A:109:GLU:HA	1:A:109:GLU:OE1	1.81	0.79
2:V:867:ILE:O	2:V:867:ILE:HG22	1.83	0.79
1:E:22:LEU:HD23	1:E:48:VAL:CG2	2.13	0.78
5:F:299:HOH:O	2:Z:864:THR:HG21	1.83	0.78
1:D:128:ILE:O	1:D:129:PRO:C	2.26	0.78
1:D:36:ASN:HB3	5:D:294:HOH:O	1.82	0.78
1:A:23:ILE:CG2	1:A:24:ASN:N	2.47	0.77
1:F:22:LEU:HD23	1:F:48:VAL:HG22	1.66	0.77
1:D:172:SER:CB	1:D:177:ASN:HD22	1.98	0.77
1:F:70:VAL:HG13	1:F:116:MET:HE1	1.67	0.77
1:E:114:TYR:HE2	1:F:154:ILE:CD1	1.97	0.77
1:C:139:MET:CE	1:C:227:LEU:HD11	2.15	0.76
1:B:1:MET:HB3	1:B:63:ASP:OD2	1.85	0.76
1:B:205:LEU:HD12	1:B:229:MET:CE	2.16	0.76
1:C:16:LEU:CD2	1:C:79:LEU:HD12	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:CG2	1:A:24:ASN:H	1.99	0.76
1:E:116:MET:HG2	1:E:117:LYS:H	1.49	0.76
1:A:109:GLU:OE1	1:A:109:GLU:CA	2.30	0.75
1:B:40:MET:HE1	1:B:44:HIS:HB3	1.66	0.75
1:F:23:ILE:HG13	1:F:72:LEU:HD12	1.68	0.75
1:B:167:VAL:HG23	1:B:197:ILE:CD1	2.17	0.75
1:D:163:ALA:N	1:D:199:MET:HE1	2.02	0.75
1:D:16:LEU:HD22	1:D:79:LEU:HD12	1.68	0.75
1:B:40:MET:CE	1:B:44:HIS:HB3	2.16	0.75
1:A:172:SER:HB3	1:A:177:ASN:HD22	1.50	0.74
1:E:135:CYS:SG	1:E:199:MET:HG3	2.28	0.74
1:F:166:GLY:HA2	1:F:197:ILE:HD12	1.70	0.74
1:B:39:SER:C	1:B:47:LEU:HD12	2.12	0.74
1:A:166:GLY:HA2	1:A:197:ILE:HD12	1.70	0.74
1:A:200:ASN:O	1:A:201:GLU:HG2	1.87	0.74
1:C:139:MET:HE3	1:C:227:LEU:HD11	1.69	0.74
1:D:16:LEU:HD21	1:D:75:MET:CG	2.19	0.73
2:W:867:ILE:HG22	2:W:867:ILE:O	1.87	0.73
1:B:22:LEU:HD23	1:B:48:VAL:HG22	1.71	0.73
1:B:40:MET:CE	1:B:44:HIS:CA	2.62	0.73
1:F:123:VAL:CG1	1:F:124:GLU:H	2.00	0.73
1:D:40:MET:CE	1:D:44:HIS:HA	2.18	0.73
1:E:1:MET:HB3	1:E:63:ASP:OD1	1.89	0.72
1:F:121:LEU:HD22	1:F:123:VAL:HG23	1.71	0.72
1:A:66:LEU:C	1:A:66:LEU:HD12	2.13	0.72
1:F:123:VAL:CG1	1:F:124:GLU:N	2.52	0.72
1:D:16:LEU:CD2	1:D:75:MET:HG2	2.19	0.72
1:F:123:VAL:O	1:F:124:GLU:HG3	1.90	0.71
1:B:172:SER:HB3	1:B:177:ASN:HB3	1.71	0.71
1:D:16:LEU:HD21	1:D:75:MET:SD	2.30	0.71
1:B:167:VAL:HG23	1:B:197:ILE:HD11	1.71	0.71
1:C:22:LEU:HD23	1:C:48:VAL:HG22	1.71	0.71
1:C:45:VAL:HG23	2:W:861:PRO:O	1.91	0.71
1:C:45:VAL:HG21	2:W:861:PRO:O	1.89	0.71
1:B:255:ILE:O	1:B:255:ILE:HG22	1.91	0.70
1:F:252:ALA:CB	2:Z:864:THR:HG23	2.22	0.70
1:D:36:ASN:ND2	1:D:51:THR:HG22	2.06	0.70
1:D:163:ALA:HA	1:D:199:MET:SD	2.30	0.70
1:F:30:ILE:HG13	1:F:68:MET:HE2	1.74	0.70
1:B:95:ASN:O	1:B:96:ALA:O	2.10	0.70
2:Z:862:LYS:CD	2:Z:862:LYS:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:MET:CE	1:B:44:HIS:CB	2.68	0.69
1:D:184:GLN:N	1:D:184:GLN:OE1	2.25	0.69
1:C:229:MET:HG2	1:C:235:LEU:HD12	1.73	0.69
1:F:166:GLY:HA2	1:F:197:ILE:CD1	2.22	0.69
1:E:166:GLY:HA2	1:E:197:ILE:CD1	2.23	0.69
1:E:172:SER:CB	1:E:177:ASN:HB3	2.23	0.69
1:F:25:GLU:HG2	1:F:119:MET:SD	2.33	0.69
1:F:1:MET:HE3	1:F:3:GLU:HB2	1.74	0.69
1:C:70:VAL:HG13	1:C:116:MET:HE1	1.74	0.69
1:B:22:LEU:CD2	1:B:48:VAL:CG2	2.70	0.68
1:B:93:GLU:OE1	1:B:93:GLU:HA	1.94	0.68
1:D:43:SER:O	1:D:44:HIS:HB2	1.93	0.68
1:F:38:GLN:HE21	1:F:128:ILE:HD11	1.58	0.68
1:D:53:ARG:NH2	3:D:262:SO4:S	2.67	0.68
1:D:107:ASN:O	1:D:108:GLN:C	2.36	0.68
1:A:172:SER:HB2	1:A:177:ASN:ND2	2.09	0.68
1:C:254:LYS:O	1:C:255:ILE:C	2.37	0.67
1:A:127:GLY:O	1:A:129:PRO:HD3	1.94	0.67
1:A:242:ALA:O	1:A:244:MET:N	2.27	0.67
1:D:13:LYS:HE3	1:D:82:ALA:O	1.95	0.67
1:E:64:ARG:O	1:E:66:LEU:HD23	1.95	0.67
1:E:16:LEU:HD13	1:E:79:LEU:HD12	1.77	0.67
1:D:107:ASN:O	1:D:109:GLU:CD	2.38	0.67
1:D:30:ILE:HD12	1:D:35:VAL:HG22	1.74	0.67
1:A:139:MET:CE	1:A:227:LEU:CD1	2.73	0.66
1:A:43:SER:O	1:A:44:HIS:HB2	1.95	0.66
1:A:200:ASN:C	1:A:201:GLU:HG2	2.21	0.66
1:B:24:ASN:ND2	5:B:342:HOH:O	2.29	0.66
1:A:172:SER:HB2	1:A:177:ASN:HD22	1.59	0.66
2:V:867:ILE:O	2:V:867:ILE:CG2	2.43	0.66
1:C:184:GLN:O	1:C:185:THR:HB	1.95	0.66
1:F:107:ASN:OD1	1:F:109:GLU:N	2.21	0.66
1:D:98:THR:HG22	1:D:99:LEU:N	2.09	0.65
1:E:22:LEU:HD23	1:E:48:VAL:HG22	1.77	0.65
1:D:172:SER:CB	1:D:177:ASN:ND2	2.59	0.65
1:D:113:ASP:O	1:E:178:GLY:HA2	1.96	0.65
1:D:184:GLN:O	1:D:184:GLN:OE1	2.15	0.65
1:A:139:MET:CE	1:A:227:LEU:HD12	2.27	0.64
1:D:40:MET:HE2	1:D:44:HIS:CA	2.23	0.64
1:E:116:MET:HG2	1:E:117:LYS:N	2.11	0.64
1:B:205:LEU:HD12	1:B:229:MET:HE3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ALA:HB3	5:B:349:HOH:O	1.96	0.64
1:F:78:ILE:HD12	1:F:116:MET:HG3	1.80	0.64
1:C:45:VAL:HG22	2:W:864:THR:OG1	1.96	0.64
1:B:134:SER:HB2	1:B:203:VAL:HG21	1.80	0.64
1:C:2:PHE:O	1:C:91:ARG:HA	1.98	0.63
1:F:93:GLU:HG3	1:F:93:GLU:O	1.98	0.63
1:C:124:GLU:O	1:C:125:GLN:C	2.41	0.63
1:C:246:HIS:ND1	3:C:262:SO4:O2	2.22	0.63
1:D:163:ALA:CA	1:D:199:MET:HE1	2.28	0.63
2:Z:862:LYS:O	2:Z:862:LYS:HD3	1.99	0.63
1:B:138:LYS:HG2	1:B:226:THR:CG2	2.27	0.63
1:E:16:LEU:HD13	1:E:79:LEU:CD1	2.29	0.63
1:F:16:LEU:CD2	1:F:75:MET:HB3	2.29	0.63
1:B:163:ALA:CB	5:B:349:HOH:O	2.46	0.63
1:D:172:SER:HB2	1:D:177:ASN:ND2	2.14	0.63
1:F:22:LEU:CD2	1:F:48:VAL:HG22	2.29	0.62
1:F:66:LEU:HD22	1:F:67:ALA:N	2.14	0.62
1:A:233:VAL:HB	1:A:234:PRO:HD2	1.82	0.62
1:E:23:ILE:HD12	1:E:72:LEU:HD11	1.80	0.62
1:D:37:LEU:C	1:D:37:LEU:HD23	2.24	0.62
1:D:119:MET:HE2	1:D:121:LEU:HD13	1.82	0.62
1:C:244:MET:O	1:C:244:MET:HG3	1.98	0.62
1:D:98:THR:HG21	1:D:115:GLU:CD	2.25	0.62
1:B:22:LEU:CD2	1:B:48:VAL:HG22	2.29	0.61
1:A:129:PRO:O	1:A:130:GLU:C	2.44	0.61
1:B:169:PHE:N	1:B:169:PHE:CD1	2.68	0.61
1:B:160:ILE:HB	1:B:229:MET:HE1	1.82	0.61
1:E:37:LEU:HD23	1:E:38:GLN:N	2.15	0.61
2:W:867:ILE:O	2:W:867:ILE:CG2	2.48	0.61
1:A:108:GLN:O	1:A:108:GLN:HG3	2.01	0.61
1:A:234:PRO:HD3	2:U:868:PHE:CD1	2.35	0.61
1:D:163:ALA:N	1:D:199:MET:CE	2.64	0.61
1:C:85:GLU:OE1	1:C:85:GLU:CA	2.41	0.61
1:D:99:LEU:HD23	1:D:116:MET:CE	2.30	0.61
1:D:99:LEU:HD23	1:D:116:MET:HE2	1.81	0.61
1:C:137:VAL:CG1	1:C:139:MET:HE2	2.31	0.60
1:C:229:MET:HA	5:C:268:HOH:O	2.00	0.60
1:D:49:GLN:HE22	1:D:51:THR:CG2	2.13	0.60
1:B:39:SER:O	1:B:47:LEU:HD12	2.02	0.60
1:A:163:ALA:C	1:A:199:MET:SD	2.85	0.60
1:F:1:MET:SD	1:F:61:ARG:NH1	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:C	1:A:199:MET:CE	2.73	0.59
1:A:85:GLU:HB2	1:A:106:PRO:HG3	1.83	0.59
1:D:59:THR:CG2	1:D:60:TYR:N	2.65	0.59
1:C:139:MET:CE	1:C:227:LEU:CD1	2.80	0.59
1:E:143:GLU:OE1	1:E:182:LEU:HD11	2.03	0.59
1:B:198:GLU:O	1:B:198:GLU:HG2	2.00	0.59
1:C:16:LEU:HD21	1:C:75:MET:SD	2.43	0.59
1:D:106:PRO:C	1:D:107:ASN:OD1	2.45	0.59
1:D:167:VAL:HG13	1:D:182:LEU:HB2	1.83	0.59
1:E:12:LEU:HD21	1:E:90:LEU:HD11	1.84	0.59
1:E:114:TYR:CE2	1:F:154:ILE:CD1	2.77	0.59
1:A:241:ILE:HG13	1:A:246:HIS:HA	1.84	0.59
1:C:238:GLU:OE1	1:C:248:LYS:HE2	2.03	0.59
1:D:16:LEU:HD22	1:D:79:LEU:CD1	2.32	0.58
1:C:255:ILE:HD13	2:W:861:PRO:HD3	1.85	0.58
1:D:98:THR:CG2	1:D:99:LEU:N	2.65	0.58
1:A:241:ILE:O	1:A:242:ALA:C	2.46	0.58
1:C:16:LEU:HD21	1:C:75:MET:CG	2.33	0.58
1:A:105:ALA:CB	1:A:108:GLN:O	2.52	0.58
2:V:868:PHE:O	2:V:869:PHE:CD1	2.57	0.58
1:B:139:MET:HE1	1:B:169:PHE:HZ	1.69	0.58
1:D:240:LYS:HE2	3:D:262:SO4:O3	2.04	0.58
1:E:23:ILE:HD12	1:E:72:LEU:CD1	2.34	0.58
1:F:11:ILE:HD13	1:F:244:MET:HE3	1.86	0.58
1:B:60:TYR:O	1:B:61:ARG:HG2	2.03	0.57
1:F:11:ILE:CD1	1:F:244:MET:HE3	2.34	0.57
1:C:205:LEU:HD12	1:C:229:MET:CE	2.35	0.57
1:E:22:LEU:CD2	1:E:48:VAL:HG22	2.34	0.57
1:F:38:GLN:HE21	1:F:128:ILE:CD1	2.17	0.57
1:F:254:LYS:CG	1:F:255:ILE:H	2.17	0.57
1:A:170:SER:OG	1:A:179:ASN:HB3	2.04	0.57
1:B:99:LEU:HD23	1:B:116:MET:CE	2.35	0.57
1:F:124:GLU:O	1:F:125:GLN:C	2.46	0.57
2:Y:870:LYS:HB3	2:Y:871:PRO:HD2	1.86	0.57
1:A:23:ILE:HG22	1:A:24:ASN:H	1.53	0.57
1:A:163:ALA:O	1:A:164:LYS:C	2.48	0.57
1:D:16:LEU:CD2	1:D:75:MET:CG	2.81	0.57
1:C:107:ASN:C	1:C:107:ASN:OD1	2.48	0.57
1:C:205:LEU:HD21	1:C:232:ASP:H	1.70	0.57
1:A:164:LYS:O	1:A:165:ASP:C	2.48	0.56
2:V:870:LYS:HB3	2:V:871:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ALA:CB	2:Y:864:THR:HG23	2.35	0.56
1:F:30:ILE:CG1	1:F:68:MET:HE2	2.35	0.56
1:F:50:LEU:HD13	1:F:247:LEU:HD13	1.87	0.56
1:C:78:ILE:CD1	1:C:116:MET:HG3	2.35	0.56
1:B:101:LEU:HD12	1:B:101:LEU:N	2.20	0.56
1:C:205:LEU:HD12	1:C:229:MET:HE2	1.87	0.56
1:A:98:THR:HA	1:A:118:LEU:HD13	1.87	0.56
1:D:95:ASN:O	1:D:96:ALA:O	2.24	0.56
1:A:172:SER:CB	1:A:177:ASN:ND2	2.64	0.56
1:D:163:ALA:C	1:D:199:MET:HE1	2.30	0.56
1:B:241:ILE:O	1:B:242:ALA:C	2.48	0.56
1:E:16:LEU:CD1	1:E:79:LEU:CD1	2.84	0.56
1:B:11:ILE:HD13	1:B:244:MET:HE1	1.88	0.56
1:C:68:MET:HB3	1:C:118:LEU:HD13	1.86	0.56
1:A:93:GLU:O	1:A:94:ASP:C	2.48	0.55
1:B:205:LEU:HD12	1:B:229:MET:HE2	1.86	0.55
1:B:255:ILE:O	1:B:255:ILE:HG23	2.06	0.55
1:C:128:ILE:O	1:C:129:PRO:O	2.24	0.55
1:E:37:LEU:C	1:E:37:LEU:CD2	2.79	0.55
1:F:135:CYS:SG	1:F:199:MET:HG3	2.47	0.55
1:C:95:ASN:CG	1:C:95:ASN:O	2.45	0.55
1:B:5:ARG:HB3	1:B:59:THR:HB	1.88	0.55
1:A:139:MET:HE3	1:A:227:LEU:CD1	2.37	0.55
1:C:206:THR:HG22	1:C:254:LYS:HG3	1.87	0.55
1:D:151:LEU:HD22	1:D:171:ALA:HB3	1.89	0.55
1:E:114:TYR:CD2	1:F:154:ILE:HD11	2.39	0.55
1:A:117:LYS:O	1:A:118:LEU:HD12	2.06	0.55
1:D:49:GLN:HE22	1:D:51:THR:HG23	1.71	0.55
1:D:219:THR:N	1:D:220:PRO:CD	2.70	0.55
1:E:149:ARG:O	1:E:152:SER:HB2	2.07	0.55
1:A:109:GLU:OE1	1:A:109:GLU:N	2.40	0.55
1:C:101:LEU:N	1:C:101:LEU:HD12	2.21	0.54
1:D:184:GLN:CD	1:D:184:GLN:C	2.74	0.54
1:E:166:GLY:HA2	1:E:197:ILE:HD12	1.87	0.54
1:C:128:ILE:O	1:C:129:PRO:C	2.50	0.54
1:D:200:ASN:OD1	1:D:200:ASN:O	2.25	0.54
1:E:207:PHE:CZ	1:E:235:LEU:HB2	2.43	0.54
1:F:19:LEU:O	1:F:20:LYS:C	2.50	0.54
1:F:123:VAL:C	1:F:124:GLU:HG3	2.33	0.54
1:C:207:PHE:CZ	1:C:235:LEU:HB2	2.43	0.54
1:F:254:LYS:HG3	1:F:255:ILE:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HG12	1:B:168:LYS:N	2.23	0.54
1:B:215:PHE:CD1	1:B:249:TYR:CD1	2.96	0.54
1:C:138:LYS:HB3	1:C:196:THR:OG1	2.08	0.54
1:C:172:SER:HB3	1:C:177:ASN:HB2	1.89	0.54
1:A:139:MET:HE1	1:A:227:LEU:CD1	2.38	0.54
1:D:112:SER:HA	1:E:179:ASN:O	2.07	0.54
1:C:236:VAL:HG22	1:C:250:TYR:CE2	2.43	0.54
1:D:163:ALA:O	1:D:164:LYS:C	2.51	0.54
1:D:139:MET:HE2	1:D:144:PHE:N	2.23	0.53
1:F:199:MET:HE2	1:F:199:MET:O	2.08	0.53
1:E:252:ALA:HB3	2:Y:864:THR:HG23	1.91	0.53
1:D:211:TYR:O	1:D:212:LEU:C	2.51	0.53
1:E:5:ARG:HB3	1:E:59:THR:HB	1.90	0.53
1:A:198:GLU:OE1	1:A:198:GLU:HA	2.09	0.53
1:A:43:SER:HG	1:A:45:VAL:HG12	1.74	0.53
1:C:35:VAL:HB	1:C:52:LEU:HB2	1.90	0.53
1:D:255:ILE:HB	2:X:863:HIS:CE1	2.44	0.53
1:C:229:MET:HG2	1:C:235:LEU:CD1	2.37	0.53
1:D:240:LYS:CE	3:D:262:SO4:O3	2.57	0.53
1:A:200:ASN:C	1:A:201:GLU:CG	2.82	0.52
1:D:107:ASN:OD1	1:D:107:ASN:N	2.42	0.52
1:C:28:TRP:CD1	1:C:70:VAL:HG21	2.44	0.52
1:D:105:ALA:O	1:D:106:PRO:C	2.51	0.52
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.44	0.52
1:C:177:ASN:OD1	1:C:177:ASN:C	2.52	0.52
1:F:19:LEU:O	1:F:21:ASP:N	2.42	0.52
1:C:165:ASP:C	5:C:302:HOH:O	2.52	0.52
1:F:140:PRO:HD2	1:F:143:GLU:OE1	2.10	0.52
1:B:106:PRO:O	1:B:107:ASN:C	2.52	0.52
1:D:40:MET:HE1	2:X:865:LEU:HB2	1.92	0.52
1:D:172:SER:HB3	1:D:177:ASN:ND2	2.18	0.52
1:E:219:THR:HB	1:E:220:PRO:HD3	1.90	0.52
1:D:200:ASN:OD1	1:D:200:ASN:C	2.53	0.52
1:B:106:PRO:O	1:B:107:ASN:O	2.27	0.52
1:D:163:ALA:CA	1:D:199:MET:CE	2.88	0.52
1:F:236:VAL:HG22	1:F:250:TYR:CD2	2.45	0.51
1:A:139:MET:HE1	1:A:227:LEU:HD12	1.91	0.51
1:C:16:LEU:HD22	1:C:79:LEU:HD13	1.85	0.51
1:C:137:VAL:HG11	1:C:139:MET:HE2	1.91	0.51
2:W:868:PHE:O	2:W:869:PHE:HD1	1.94	0.51
1:D:50:LEU:HD13	1:D:247:LEU:HD13	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:HD23	1:B:37:LEU:C	2.36	0.51
1:A:37:LEU:C	1:A:37:LEU:HD23	2.36	0.51
1:A:107:ASN:O	1:A:109:GLU:OE1	2.28	0.51
1:D:52:LEU:HD22	1:D:244:MET:HE2	1.93	0.51
1:F:141:SER:HB2	1:F:219:THR:HG23	1.93	0.51
1:D:16:LEU:HD22	1:D:75:MET:HG2	1.93	0.51
1:E:134:SER:HB2	1:E:203:VAL:HG21	1.93	0.51
1:A:164:LYS:O	1:A:165:ASP:O	2.27	0.51
1:E:116:MET:CG	1:E:117:LYS:H	2.21	0.51
1:F:252:ALA:HB3	2:Z:864:THR:CG2	2.41	0.51
1:F:147:ILE:CD1	1:F:182:LEU:HD11	2.40	0.51
1:C:137:VAL:HG12	1:C:139:MET:HE2	1.93	0.50
1:E:76:SER:O	1:E:80:LYS:HG3	2.12	0.50
1:A:219:THR:HB	1:A:220:PRO:HD3	1.93	0.50
1:D:5:ARG:HB3	1:D:59:THR:HB	1.93	0.50
1:D:241:ILE:O	1:D:242:ALA:C	2.54	0.50
2:Z:862:LYS:O	2:Z:862:LYS:CG	2.54	0.50
1:C:37:LEU:HD23	1:C:38:GLN:N	2.27	0.50
1:C:236:VAL:HG22	1:C:250:TYR:CD2	2.46	0.50
1:E:218:ALA:O	1:E:219:THR:C	2.55	0.50
1:F:16:LEU:HD21	1:F:75:MET:HB3	1.93	0.50
1:F:207:PHE:CZ	1:F:235:LEU:HB2	2.46	0.50
1:F:252:ALA:HB3	2:Z:864:THR:HG23	1.92	0.50
1:C:46:SER:HA	2:W:865:LEU:HD22	1.93	0.50
1:D:114:TYR:HE2	1:E:154:ILE:HD13	1.77	0.50
1:B:158:VAL:CG2	1:B:169:PHE:HB3	2.42	0.49
1:E:40:MET:HE3	1:E:126:LEU:HD13	1.93	0.49
1:A:37:LEU:HD23	1:A:38:GLN:N	2.27	0.49
1:A:139:MET:CE	1:A:227:LEU:HD11	2.42	0.49
1:B:11:ILE:HD13	1:B:244:MET:CE	2.42	0.49
1:B:40:MET:CE	2:V:865:LEU:HB3	2.36	0.49
1:B:107:ASN:O	1:B:108:GLN:CB	2.60	0.49
1:C:120:ASP:O	1:C:120:ASP:OD2	2.30	0.49
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.43	0.49
1:E:1:MET:HB3	1:E:63:ASP:CG	2.37	0.49
1:F:169:PHE:HE1	1:F:182:LEU:HD12	1.78	0.49
1:D:210:ARG:NH1	1:D:211:TYR:CE2	2.80	0.49
1:E:163:ALA:O	1:E:165:ASP:N	2.45	0.49
1:B:98:THR:HA	1:B:118:LEU:HG	1.93	0.49
1:C:71:ASN:OD1	1:C:71:ASN:C	2.55	0.49
1:A:137:VAL:O	1:A:226:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLY:CA	1:A:197:ILE:HD12	2.43	0.49
2:V:861:PRO:C	2:V:862:LYS:HG2	2.37	0.49
1:D:167:VAL:CG1	1:D:182:LEU:HB2	2.42	0.49
1:D:246:HIS:ND1	3:D:262:SO4:O4	2.46	0.49
1:E:235:LEU:HD12	1:E:236:VAL:N	2.28	0.49
1:B:66:LEU:CD1	1:B:68:MET:HG3	2.42	0.48
1:C:158:VAL:HA	1:C:170:SER:O	2.13	0.48
1:E:45:VAL:HA	2:Y:864:THR:HG22	1.95	0.48
1:A:166:GLY:HA2	1:A:197:ILE:CD1	2.40	0.48
1:C:139:MET:HE1	1:C:227:LEU:HD11	1.92	0.48
1:A:252:ALA:HB3	2:U:863:HIS:O	2.13	0.48
1:D:5:ARG:NH1	1:D:104:GLU:OE1	2.45	0.48
1:B:99:LEU:HD23	1:B:116:MET:HE2	1.95	0.48
1:D:59:THR:HG22	1:D:60:TYR:N	2.28	0.48
1:D:184:GLN:OE1	1:D:184:GLN:CA	2.61	0.48
1:E:105:ALA:HB1	1:E:106:PRO:HD2	1.95	0.48
1:E:252:ALA:HB2	2:Y:865:LEU:HD23	1.94	0.48
1:A:66:LEU:C	1:A:66:LEU:CD1	2.85	0.48
1:D:40:MET:CE	1:D:44:HIS:CA	2.88	0.48
1:C:66:LEU:HD21	1:C:96:ALA:HB2	1.95	0.48
1:F:107:ASN:OD1	1:F:109:GLU:HB2	2.14	0.48
1:D:53:ARG:NH2	3:D:262:SO4:O2	2.45	0.48
1:E:209:LEU:HD23	1:E:212:LEU:HD12	1.96	0.48
1:D:23:ILE:HG22	1:D:41:ASP:HA	1.96	0.48
1:F:147:ILE:HD11	1:F:182:LEU:HD11	1.95	0.48
1:D:91:ARG:O	1:D:99:LEU:HD12	2.14	0.47
1:C:25:GLU:OE2	1:C:119:MET:SD	2.72	0.47
1:F:1:MET:CE	1:F:3:GLU:HB2	2.42	0.47
1:C:4:ALA:O	1:C:89:THR:HA	2.14	0.47
1:D:124:GLU:O	1:D:125:GLN:C	2.57	0.47
1:F:22:LEU:HD23	1:F:48:VAL:CG2	2.42	0.47
1:A:129:PRO:O	1:A:130:GLU:O	2.32	0.47
1:C:50:LEU:HB2	1:C:247:LEU:CD1	2.44	0.47
1:C:219:THR:N	1:C:220:PRO:CD	2.77	0.47
1:D:158:VAL:HA	1:D:170:SER:O	2.14	0.47
1:A:52:LEU:HB3	1:A:244:MET:HE2	1.96	0.47
1:A:66:LEU:CD1	1:A:68:MET:HG3	2.44	0.47
1:D:107:ASN:O	1:D:109:GLU:OE2	2.31	0.47
1:A:252:ALA:CB	2:U:863:HIS:O	2.63	0.47
1:D:36:ASN:ND2	5:D:294:HOH:O	2.47	0.47
1:D:40:MET:HE2	1:D:40:MET:HB3	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LEU:HD13	2:X:869:PHE:HD2	1.79	0.47
1:E:164:LYS:N	1:E:199:MET:SD	2.78	0.47
1:F:7:VAL:HG23	1:F:58:ASP:HB2	1.96	0.47
1:F:54:SER:HB2	1:F:60:TYR:CD2	2.49	0.47
1:F:242:ALA:O	1:F:243:ASP:C	2.58	0.47
1:C:71:ASN:HB2	1:C:119:MET:HE1	1.95	0.47
1:A:108:GLN:C	1:A:109:GLU:OE1	2.57	0.47
1:B:2:PHE:O	1:B:91:ARG:HA	2.15	0.46
1:C:241:ILE:O	1:C:242:ALA:C	2.57	0.46
1:A:197:ILE:O	1:A:198:GLU:OE1	2.34	0.46
1:E:3:GLU:HA	1:E:90:LEU:O	2.15	0.46
1:F:254:LYS:CG	1:F:255:ILE:N	2.78	0.46
1:B:64:ARG:O	1:B:65:ASN:C	2.55	0.46
1:B:107:ASN:OD1	1:B:107:ASN:N	2.42	0.46
1:C:28:TRP:CD1	1:C:70:VAL:CG2	2.98	0.46
1:D:107:ASN:C	1:D:108:GLN:O	2.55	0.46
1:F:230:SER:O	1:F:231:ALA:C	2.59	0.46
1:E:98:THR:CB	1:E:116:MET:O	2.60	0.46
1:E:163:ALA:O	1:E:164:LYS:C	2.58	0.46
1:E:137:VAL:HG11	1:E:139:MET:HE2	1.97	0.46
1:A:139:MET:HE3	1:A:227:LEU:HD11	1.98	0.46
1:B:134:SER:HB2	1:B:203:VAL:CG2	2.44	0.46
1:F:102:VAL:HG22	1:F:113:ASP:OD1	2.16	0.46
1:B:139:MET:HE1	1:B:169:PHE:CZ	2.51	0.46
1:C:232:ASP:C	1:C:233:VAL:HG13	2.41	0.46
1:F:3:GLU:OE1	1:F:91:ARG:HD2	2.15	0.46
1:F:252:ALA:HB1	2:Z:864:THR:HG23	1.98	0.46
1:F:66:LEU:CD2	1:F:66:LEU:C	2.86	0.46
1:B:95:ASN:O	1:B:96:ALA:C	2.59	0.45
2:V:868:PHE:O	2:V:869:PHE:HD1	1.99	0.45
1:D:22:LEU:HD11	1:D:46:SER:OG	2.16	0.45
1:D:35:VAL:HB	1:D:52:LEU:HB2	1.97	0.45
1:D:16:LEU:HD21	1:D:75:MET:HG2	1.84	0.45
1:F:165:ASP:O	1:F:197:ILE:HD12	2.15	0.45
1:B:40:MET:CE	1:B:44:HIS:HA	2.13	0.45
1:C:206:THR:CG2	1:C:254:LYS:HG3	2.46	0.45
1:F:137:VAL:HG11	1:F:139:MET:CE	2.47	0.45
1:C:255:ILE:H	1:C:255:ILE:HG12	1.55	0.45
1:E:113:ASP:O	1:F:178:GLY:HA2	2.16	0.45
1:F:254:LYS:CG	1:F:255:ILE:HG13	2.47	0.45
1:B:167:VAL:HG23	1:B:197:ILE:HD13	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:THR:O	1:C:59:THR:HG22	2.11	0.45
1:D:98:THR:HG23	1:D:115:GLU:HG3	1.99	0.45
1:D:109:GLU:OE1	1:D:109:GLU:CA	2.54	0.45
1:A:113:ASP:O	1:B:178:GLY:HA2	2.17	0.45
1:A:252:ALA:HA	1:A:253:PRO:HD2	1.78	0.45
1:A:175:LEU:HD22	1:C:74:SER:HB3	1.99	0.45
1:B:113:ASP:O	1:C:178:GLY:HA2	2.16	0.45
1:D:47:LEU:HD13	2:X:869:PHE:CD2	2.52	0.45
1:A:184:GLN:NE2	1:A:197:ILE:H	2.14	0.44
1:A:234:PRO:HD3	2:U:868:PHE:CE1	2.51	0.44
1:C:168:LYS:HA	1:C:180:ILE:O	2.18	0.44
2:W:868:PHE:O	2:W:869:PHE:CD1	2.70	0.44
1:E:1:MET:HG2	1:E:61:ARG:NE	2.31	0.44
1:D:36:ASN:HD22	1:D:51:THR:HG22	1.80	0.44
1:E:23:ILE:CD1	1:E:72:LEU:CD1	2.95	0.44
1:B:205:LEU:CD1	1:B:229:MET:HE3	2.47	0.44
1:D:43:SER:O	1:D:44:HIS:CB	2.63	0.44
1:E:139:MET:HE1	1:E:169:PHE:HZ	1.82	0.44
1:A:59:THR:HG22	1:A:60:TYR:N	2.32	0.44
1:C:50:LEU:CD1	1:C:247:LEU:HD13	2.39	0.44
1:C:211:TYR:O	1:C:214:PHE:HB2	2.17	0.44
1:B:235:LEU:O	1:B:250:TYR:HA	2.18	0.44
1:C:184:GLN:O	1:C:185:THR:CB	2.63	0.44
1:B:138:LYS:CG	1:B:226:THR:HG22	2.37	0.44
1:C:16:LEU:CD2	1:C:75:MET:HG2	2.46	0.44
1:D:169:PHE:O	1:D:179:ASN:HA	2.17	0.44
1:F:234:PRO:HA	1:F:253:PRO:HD3	1.99	0.44
1:A:66:LEU:HD13	1:A:68:MET:HG3	2.00	0.44
1:A:97:ASP:C	1:A:98:THR:CG2	2.91	0.44
1:B:121:LEU:HD12	1:B:121:LEU:HA	1.67	0.44
1:F:38:GLN:NE2	1:F:128:ILE:HD11	2.28	0.44
1:A:99:LEU:HB2	1:A:118:LEU:HD11	1.99	0.44
1:E:16:LEU:CD1	1:E:79:LEU:HD12	2.46	0.44
1:B:40:MET:CE	1:B:44:HIS:C	2.91	0.44
1:F:71:ASN:C	1:F:71:ASN:OD1	2.61	0.44
1:A:97:ASP:C	1:A:98:THR:HG23	2.43	0.43
1:E:168:LYS:HA	1:E:180:ILE:O	2.18	0.43
1:C:1:MET:HE1	1:C:91:ARG:HD3	1.99	0.43
1:C:123:VAL:HG23	1:C:123:VAL:O	2.18	0.43
1:C:163:ALA:HA	1:C:202:PRO:HB3	2.00	0.43
1:A:133:TYR:HE2	5:A:320:HOH:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:O	1:C:125:GLN:O	2.35	0.43
1:C:128:ILE:O	1:C:128:ILE:HG22	2.17	0.43
1:E:116:MET:CG	1:E:117:LYS:N	2.80	0.43
2:Y:865:LEU:HD23	2:Y:865:LEU:HA	1.81	0.43
1:A:4:ALA:O	1:A:89:THR:HA	2.18	0.43
1:F:137:VAL:CG1	1:F:139:MET:HE2	2.48	0.43
1:B:168:LYS:HG3	1:B:181:LYS:HG3	2.00	0.43
1:C:55:GLU:CD	1:C:55:GLU:H	2.26	0.43
1:D:139:MET:HB2	1:D:140:PRO:HD2	2.01	0.43
1:F:35:VAL:HB	1:F:52:LEU:HB2	2.01	0.43
1:B:167:VAL:HG12	1:B:168:LYS:H	1.84	0.43
1:D:1:MET:HE3	1:D:1:MET:HB2	1.94	0.43
1:D:52:LEU:HB3	1:D:244:MET:HE2	1.99	0.43
1:E:103:PHE:HB2	1:E:112:SER:HB2	2.00	0.43
1:F:195:VAL:O	1:F:195:VAL:HG13	2.19	0.43
1:F:37:LEU:C	1:F:37:LEU:HD23	2.43	0.43
1:B:40:MET:HE2	1:B:44:HIS:C	2.39	0.43
1:C:139:MET:HB2	1:C:195:VAL:HG22	2.00	0.43
1:C:229:MET:CG	1:C:235:LEU:HD12	2.44	0.43
1:D:162:CYS:C	1:D:199:MET:HE2	2.44	0.42
1:E:23:ILE:CD1	1:E:72:LEU:HD11	2.47	0.42
1:B:37:LEU:HD23	1:B:38:GLN:N	2.33	0.42
1:C:137:VAL:O	1:C:226:THR:HA	2.19	0.42
1:D:163:ALA:CA	1:D:199:MET:SD	3.04	0.42
1:B:13:LYS:HB3	1:B:13:LYS:HE2	1.83	0.42
1:B:163:ALA:O	1:B:165:ASP:N	2.52	0.42
1:D:137:VAL:O	1:D:226:THR:HA	2.20	0.42
1:E:82:ALA:HB2	1:E:103:PHE:CE2	2.54	0.42
1:F:205:LEU:HD21	1:F:232:ASP:H	1.83	0.42
1:F:215:PHE:CD1	1:F:249:TYR:CD1	3.08	0.42
1:A:59:THR:CG2	1:A:60:TYR:N	2.82	0.42
1:C:98:THR:HG22	1:C:99:LEU:N	2.35	0.42
1:D:127:GLY:O	1:D:129:PRO:HD3	2.18	0.42
1:D:236:VAL:HA	1:D:249:TYR:O	2.20	0.42
1:E:121:LEU:HD12	1:E:121:LEU:HA	1.71	0.42
1:A:246:HIS:ND1	3:A:262:SO4:O2	2.33	0.42
1:B:152:SER:OG	1:B:213:ASN:ND2	2.52	0.42
1:B:16:LEU:HD21	1:B:75:MET:SD	2.60	0.42
1:D:139:MET:HE2	1:D:144:PHE:CA	2.49	0.42
1:E:143:GLU:OE1	1:E:182:LEU:CD1	2.66	0.42
1:E:232:ASP:O	1:E:233:VAL:CG1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:PHE:N	1:C:215:PHE:CD1	2.88	0.42
1:D:49:GLN:NE2	1:D:51:THR:HG23	2.35	0.42
1:F:137:VAL:CG1	1:F:139:MET:CE	2.98	0.42
1:C:16:LEU:HD21	1:C:75:MET:HG2	2.02	0.42
1:C:53:ARG:HB3	1:C:55:GLU:OE1	2.20	0.42
1:E:241:ILE:O	1:E:242:ALA:C	2.62	0.42
1:B:97:ASP:C	1:B:98:THR:HG23	2.44	0.41
1:D:185:THR:O	1:F:109:GLU:OE2	2.37	0.41
1:D:207:PHE:CZ	1:D:235:LEU:HB2	2.54	0.41
1:F:41:ASP:OD2	1:F:46:SER:OG	2.36	0.41
1:F:231:ALA:O	1:F:233:VAL:HG13	2.19	0.41
1:A:242:ALA:C	1:A:244:MET:H	2.28	0.41
1:B:123:VAL:CG2	1:B:124:GLU:N	2.83	0.41
1:F:169:PHE:CD1	1:F:169:PHE:N	2.88	0.41
1:A:88:ILE:HA	1:A:102:VAL:O	2.20	0.41
1:A:166:GLY:CA	1:A:197:ILE:CD1	2.99	0.41
1:B:93:GLU:HB3	1:B:94:ASP:H	1.69	0.41
1:A:64:ARG:O	1:A:65:ASN:C	2.62	0.41
1:A:128:ILE:HA	2:U:869:PHE:CD1	2.55	0.41
1:B:66:LEU:HD12	1:B:68:MET:HG3	2.01	0.41
1:A:53:ARG:NH1	1:A:53:ARG:HB2	2.35	0.41
1:D:28:TRP:CD1	1:D:70:VAL:HG21	2.56	0.41
1:E:235:LEU:O	1:E:250:TYR:HA	2.21	0.41
1:B:219:THR:HB	1:B:220:PRO:HD3	2.02	0.41
1:F:205:LEU:HD11	1:F:230:SER:O	2.21	0.41
1:B:231:ALA:O	1:B:232:ASP:HB2	2.20	0.41
1:C:138:LYS:HB3	1:C:196:THR:HG1	1.84	0.41
2:W:868:PHE:C	2:W:869:PHE:CD1	2.98	0.41
1:C:217:LYS:HA	1:C:217:LYS:HD3	1.86	0.41
1:D:40:MET:CE	2:X:865:LEU:HB2	2.51	0.41
1:E:215:PHE:CD1	1:E:249:TYR:CD1	3.08	0.41
2:Z:867:ILE:O	2:Z:867:ILE:HG22	2.20	0.41
1:D:69:GLY:HA3	1:D:119:MET:O	2.21	0.41
1:D:163:ALA:O	1:D:199:MET:HE1	2.21	0.41
1:D:241:ILE:HG13	1:D:246:HIS:HA	2.03	0.41
1:E:133:TYR:O	1:E:134:SER:C	2.63	0.41
1:E:233:VAL:HB	1:E:234:PRO:CD	2.50	0.41
2:Y:861:PRO:HB2	2:Y:862:LYS:H	1.39	0.41
1:F:138:LYS:O	1:F:195:VAL:HA	2.20	0.41
1:F:162:CYS:O	1:F:163:ALA:HB2	2.19	0.41
1:A:235:LEU:O	1:A:250:TYR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLN:HB2	5:B:307:HOH:O	2.21	0.41
2:U:865:LEU:HD22	2:U:869:PHE:HE2	1.86	0.40
1:F:138:LYS:HE2	1:F:224:THR:CG2	2.51	0.40
1:F:228:SER:HB2	1:F:236:VAL:HB	2.03	0.40
1:F:236:VAL:HG22	1:F:250:TYR:CE2	2.57	0.40
1:A:201:GLU:O	1:A:202:PRO:C	2.64	0.40
1:D:134:SER:HA	1:D:200:ASN:HB3	2.02	0.40
1:A:167:VAL:HG13	1:A:182:LEU:HB2	2.04	0.40
1:B:240:LYS:HB3	1:B:240:LYS:HE2	1.62	0.40
1:D:95:ASN:O	1:D:96:ALA:C	2.64	0.40
1:D:210:ARG:NH1	1:D:211:TYR:CZ	2.90	0.40
1:D:219:THR:N	1:D:220:PRO:HD3	2.36	0.40
1:F:151:LEU:HD23	1:F:154:ILE:HD12	2.03	0.40
1:A:53:ARG:HB2	1:A:53:ARG:HH11	1.86	0.40
1:E:45:VAL:HG22	2:Y:864:THR:CG2	2.52	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	239/261 (92%)	216 (90%)	15 (6%)	8 (3%)	3	4
1	B	243/261 (93%)	227 (93%)	11 (4%)	5 (2%)	5	9
1	C	243/261 (93%)	231 (95%)	9 (4%)	3 (1%)	10	20
1	D	243/261 (93%)	225 (93%)	10 (4%)	8 (3%)	3	4
1	E	238/261 (91%)	228 (96%)	7 (3%)	3 (1%)	9	18
1	F	237/261 (91%)	221 (93%)	11 (5%)	5 (2%)	5	9
2	U	9/14 (64%)	8 (89%)	0	1 (11%)	0	0
2	V	11/14 (79%)	8 (73%)	2 (18%)	1 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	10/14 (71%)	9 (90%)	0	1 (10%)	0	0
2	X	8/14 (57%)	8 (100%)	0	0	100	100
2	Y	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
2	Z	9/14 (64%)	7 (78%)	2 (22%)	0	100	100
All	All	1501/1650 (91%)	1398 (93%)	68 (4%)	35 (2%)	5	8

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	A	243	ASP
2	U	863	HIS
1	B	94	ASP
1	B	96	ALA
1	B	107	ASN
1	B	108	GLN
1	B	164	LYS
1	C	125	GLN
1	D	96	ALA
1	D	106	PRO
1	D	125	GLN
1	E	164	LYS
1	F	20	LYS
1	F	243	ASP
1	A	94	ASP
1	A	130	GLU
1	A	164	LYS
1	A	200	ASN
1	A	242	ALA
2	V	867	ILE
2	W	866	ASP
1	D	94	ASP
1	D	164	LYS
1	D	242	ALA
1	E	107	ASN
1	F	125	GLN
1	A	107	ASN
1	C	129	PRO
1	C	253	PRO
1	D	108	GLN
1	F	163	ALA

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Mol	Chain	Res	Type
1	E	165	ASP
1	F	242	ALA
1	D	129	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	214/228 (94%)	194 (91%)	20 (9%)	8	18
1	B	215/228 (94%)	190 (88%)	25 (12%)	5	11
1	C	215/228 (94%)	199 (93%)	16 (7%)	13	27
1	D	215/228 (94%)	193 (90%)	22 (10%)	7	15
1	E	212/228 (93%)	197 (93%)	15 (7%)	13	29
1	F	212/228 (93%)	199 (94%)	13 (6%)	17	35
2	U	11/14 (79%)	9 (82%)	2 (18%)	2	3
2	V	13/14 (93%)	12 (92%)	1 (8%)	12	25
2	W	12/14 (86%)	11 (92%)	1 (8%)	10	22
2	X	10/14 (71%)	9 (90%)	1 (10%)	7	15
2	Y	13/14 (93%)	9 (69%)	4 (31%)	0	0
2	Z	11/14 (79%)	8 (73%)	3 (27%)	0	1
All	All	1353/1452 (93%)	1230 (91%)	123 (9%)	9	19

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	VAL
1	A	62	CYS
1	A	78	ILE
1	A	79	LEU
1	A	85	GLU
1	A	93	GLU
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	109	GLU
1	A	110	LYS
1	A	120	ASP
1	A	121	LEU
1	A	123	VAL
1	A	162	CYS
1	A	170	SER
1	A	198	GLU
1	A	200	ASN
1	A	201	GLU
1	A	203	VAL
1	A	232	ASP
1	A	243	ASP
2	U	863	HIS
2	U	872	LEU
1	B	20	LYS
1	B	24	ASN
1	B	42	SER
1	B	45	VAL
1	B	47	LEU
1	B	59	THR
1	B	66	LEU
1	B	107	ASN
1	B	108	GLN
1	B	113	ASP
1	B	115	GLU
1	B	121	LEU
1	B	132	GLU
1	B	141	SER
1	B	147	ILE
1	B	152	SER
1	B	160	ILE
1	B	161	SER
1	B	165	ASP
1	B	169	PHE
1	B	177	ASN
1	B	185	THR
1	B	204	GLN
1	B	224	THR
1	B	255	ILE
2	V	862	LYS
1	C	45	VAL

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Mol	Chain	Res	Type
1	C	48	VAL
1	C	58	ASP
1	C	59	THR
1	C	68	MET
1	C	85	GLU
1	C	87	ILE
1	C	121	LEU
1	C	123	VAL
1	C	125	GLN
1	C	149	ARG
1	C	158	VAL
1	C	167	VAL
1	C	232	ASP
1	C	244	MET
1	C	255	ILE
2	W	862	LYS
1	D	1	MET
1	D	13	LYS
1	D	25	GLU
1	D	59	THR
1	D	64	ARG
1	D	73	THR
1	D	106	PRO
1	D	107	ASN
1	D	109	GLU
1	D	112	SER
1	D	123	VAL
1	D	128	ILE
1	D	131	GLN
1	D	135	CYS
1	D	161	SER
1	D	165	ASP
1	D	175	LEU
1	D	184	GLN
1	D	230	SER
1	D	240	LYS
1	D	243	ASP
1	D	247	LEU
2	X	867	ILE
1	E	11	ILE
1	E	16	LEU
1	E	37	LEU

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Mol	Chain	Res	Type
1	E	43	SER
1	E	59	THR
1	E	66	LEU
1	E	115	GLU
1	E	135	CYS
1	E	152	SER
1	E	154	ILE
1	E	161	SER
1	E	177	ASN
1	E	184	GLN
1	E	196	THR
1	E	203	VAL
2	Y	864	THR
2	Y	865	LEU
2	Y	867	ILE
2	Y	872	LEU
1	F	1	MET
1	F	32	SER
1	F	36	ASN
1	F	47	LEU
1	F	48	VAL
1	F	59	THR
1	F	66	LEU
1	F	121	LEU
1	F	132	GLU
1	F	135	CYS
1	F	167	VAL
1	F	174	GLU
1	F	255	ILE
2	Z	862	LYS
2	Z	864	THR
2	Z	867	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	184	GLN
1	A	200	ASN
1	B	8	GLN
1	B	84	ASN
1	B	213	ASN

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	125	GLN
1	C	184	GLN
1	D	36	ASN
1	D	49	GLN
1	D	84	ASN
1	D	177	ASN
2	X	863	HIS
1	E	84	ASN
1	E	107	ASN
1	E	125	GLN
1	E	213	ASN
1	F	49	GLN
1	F	84	ASN
1	F	204	GLN

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 ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	SO4	C	262	-	4,4,4	0.24	0	6,6,6	0.44	0
3	SO4	A	262	-	4,4,4	0.23	0	6,6,6	0.40	0
3	SO4	F	262	-	4,4,4	0.24	0	6,6,6	0.43	0
3	SO4	D	262	-	4,4,4	0.25	0	6,6,6	1.24	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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	262	SO4	1	0
3	A	262	SO4	1	0
3	D	262	SO4	5	0

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	245/261 (93%)	0.38	10 (4%) 41 37	20, 41, 61, 72	25 (10%)
1	B	247/261 (94%)	0.14	8 (3%) 50 46	16, 36, 52, 58	18 (7%)
1	C	247/261 (94%)	0.23	10 (4%) 42 38	16, 36, 55, 60	19 (7%)
1	D	247/261 (94%)	0.24	10 (4%) 42 38	21, 41, 61, 75	16 (6%)
1	E	244/261 (93%)	0.10	4 (1%) 70 67	16, 36, 50, 60	10 (4%)
1	F	243/261 (93%)	0.17	9 (3%) 45 40	18, 37, 55, 65	10 (4%)
2	U	11/14 (78%)	5.05	10 (90%) 0 0	39, 53, 87, 89	5 (45%)
2	V	13/14 (92%)	0.64	1 (7%) 19 17	31, 36, 52, 53	3 (23%)
2	W	12/14 (85%)	0.74	1 (8%) 17 15	30, 37, 47, 48	1 (8%)
2	X	10/14 (71%)	1.59	3 (30%) 1 1	41, 70, 77, 83	2 (20%)
2	Y	13/14 (92%)	0.85	2 (15%) 5 4	28, 41, 50, 54	0
2	Z	11/14 (78%)	0.23	0 100 100	20, 27, 36, 36	1 (9%)
All	All	1543/1650 (93%)	0.27	68 (4%) 39 34	16, 38, 57, 89	110 (7%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	863	HIS	11.4
2	U	864	THR	6.4
2	U	867	ILE	6.1
2	U	862	LYS	5.3
2	U	868	PHE	5.1
2	U	865	LEU	4.1
1	E	165	ASP	4.1
1	B	165	ASP	4.0
1	A	1	MET	4.0
2	U	871	PRO	3.9
2	U	872	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	U	866	ASP	3.8
2	U	869	PHE	3.6
1	D	107	ASN	3.5
1	F	163	ALA	3.5
1	D	184	GLN	3.4
2	Y	873	THR	3.4
1	A	106	PRO	3.2
1	F	201	GLU	3.2
1	C	163	ALA	3.1
1	E	96	ALA	3.1
1	A	95	ASN	3.1
1	C	255	ILE	3.0
1	A	107	ASN	3.0
1	D	185	THR	2.9
1	D	165	ASP	2.9
1	C	96	ALA	2.9
1	A	122	ASP	2.9
1	F	194	ALA	2.9
1	C	165	ASP	2.8
1	C	94	ASP	2.7
1	A	164	LYS	2.7
1	B	194	ALA	2.7
1	C	120	ASP	2.6
2	Y	861	PRO	2.6
2	W	861	PRO	2.6
1	D	95	ASN	2.6
2	V	861	PRO	2.5
1	B	63	ASP	2.5
1	B	94	ASP	2.5
1	B	255	ILE	2.4
1	A	201	GLU	2.4
2	X	871	PRO	2.4
1	C	200	ASN	2.4
1	C	97	ASP	2.4
1	E	163	ALA	2.4
1	B	21	ASP	2.3
1	F	165	ASP	2.3
1	A	97	ASP	2.3
1	D	106	PRO	2.3
1	A	94	ASP	2.2
1	D	194	ALA	2.2
2	X	870	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	200	ASN	2.2
1	D	135	CYS	2.2
1	F	196	THR	2.2
1	B	166	GLY	2.2
1	D	96	ALA	2.2
1	F	255	ILE	2.2
2	X	863	HIS	2.1
1	E	194	ALA	2.1
1	D	43	SER	2.1
1	A	194	ALA	2.1
1	F	243	ASP	2.1
1	C	135	CYS	2.1
1	B	96	ALA	2.0
1	C	95	ASN	2.0
1	F	63	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(Å ²)	Q<0.9
3	SO4	F	262	5/5	0.80	0.16	98,99,101,103	0
3	SO4	D	262	5/5	0.86	0.15	72,73,81,83	0
3	SO4	A	262	5/5	0.87	0.15	94,95,97,97	0
3	SO4	C	262	5/5	0.90	0.13	94,95,96,98	0
4	ZN	B	262	1/1	0.93	0.07	51,51,51,51	0
4	ZN	E	262	1/1	0.95	0.07	54,54,54,54	0
4	ZN	Z	4	1/1	0.95	0.06	47,47,47,47	0
4	ZN	W	2	1/1	0.97	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	Y	3	1/1	0.99	0.03	48,48,48,48	0
4	ZN	V	1	1/1	0.99	0.05	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.