Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 05:26 PM EDT

PDB ID	:	2ZVL
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:

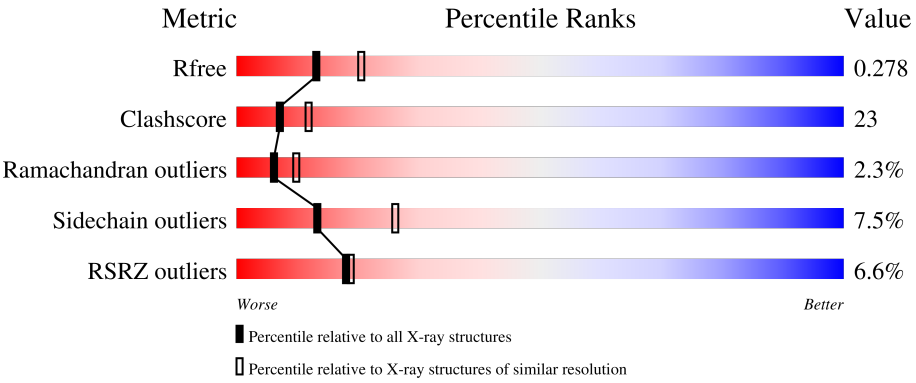
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	8% 63% 25% 5% 6%
1	B	261	5% 59% 30% 5% • 5%
1	C	261	3% 60% 31% • 5%
1	D	261	8% 56% 34% 5% 5%
1	E	261	5% 64% 26% • • 7%

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Mol	Chain	Length	Quality of chain
1	F	261	5% 59% 30% 7%
2	U	14	14% 36% 36% 7% 21%
2	V	14	21% 21% 50% 14% 7% 7%
2	W	14	21% 36% 50% 14%
2	X	14	7% 43% 29% 29%
2	Y	14	14% 43% 29% 21% 7%
2	Z	14	7% 50% 14% 14% 21%

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 (i)

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.

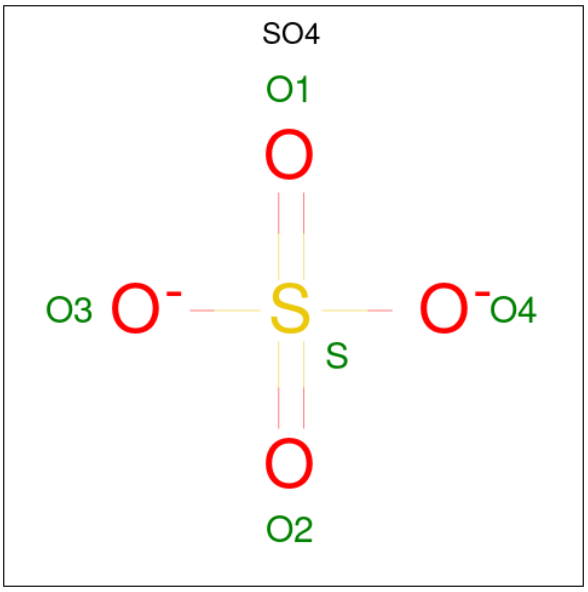
- Molecule 1 is a protein called Proliferating cell nuclear antigen.

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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

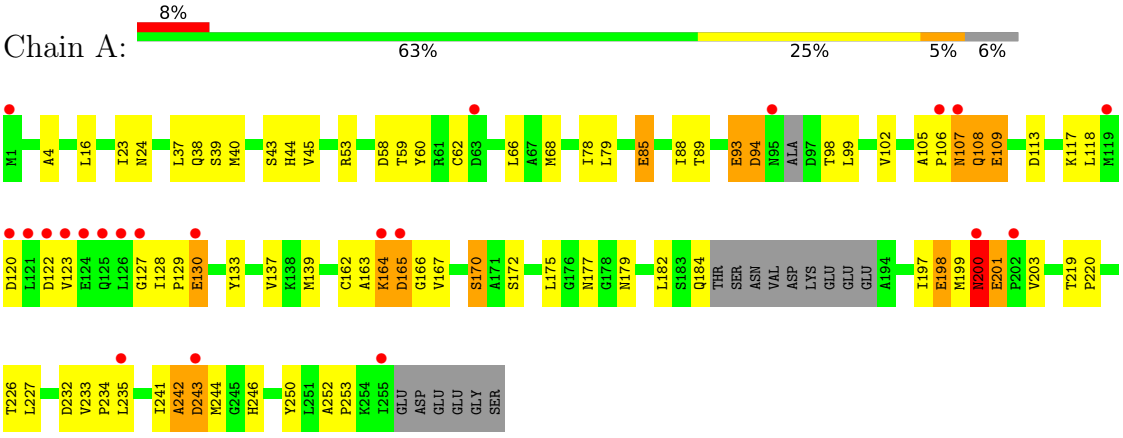
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	U	1	Total O 1 1	0	0
5	B	26	Total O 26 26	0	0
5	V	3	Total O 3 3	0	0
5	C	17	Total O 17 17	0	0
5	W	3	Total O 3 3	0	0
5	D	18	Total O 18 18	0	0
5	X	1	Total O 1 1	0	0
5	E	17	Total O 17 17	0	0
5	Y	1	Total O 1 1	0	0
5	F	21	Total O 21 21	0	0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

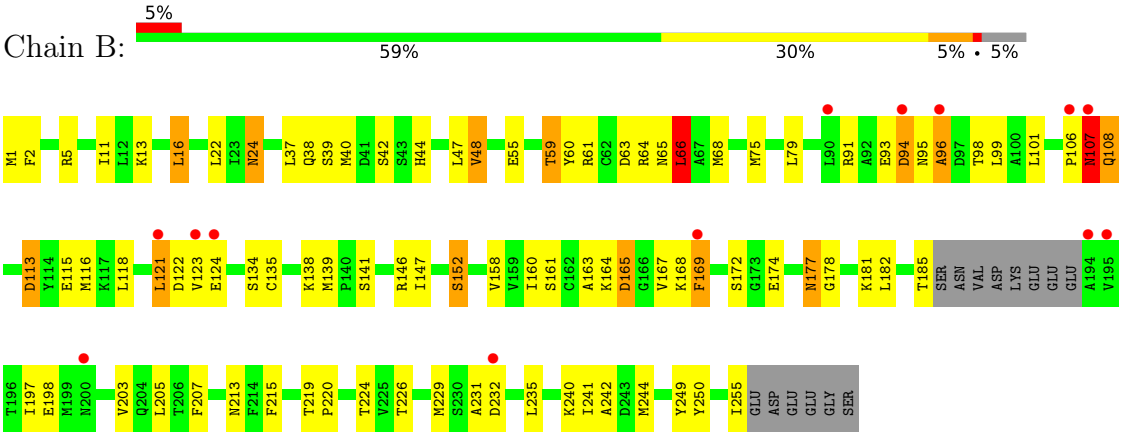
• Molecule 1: Proliferating cell nuclear antigen

Chain A:



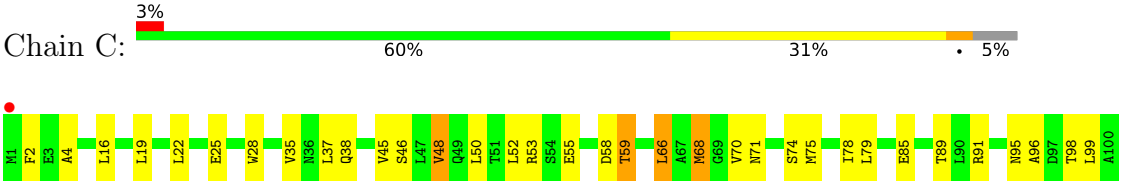
• Molecule 1: Proliferating cell nuclear antigen

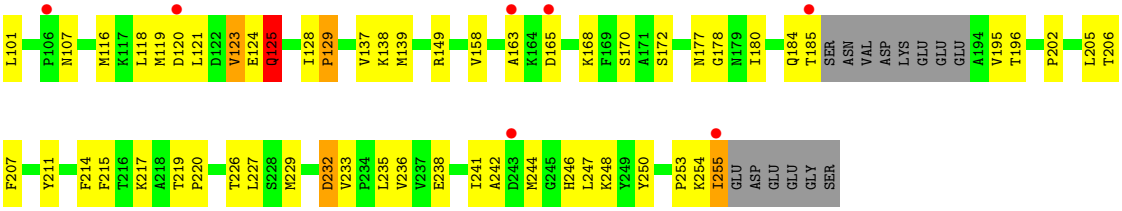
Chain B:



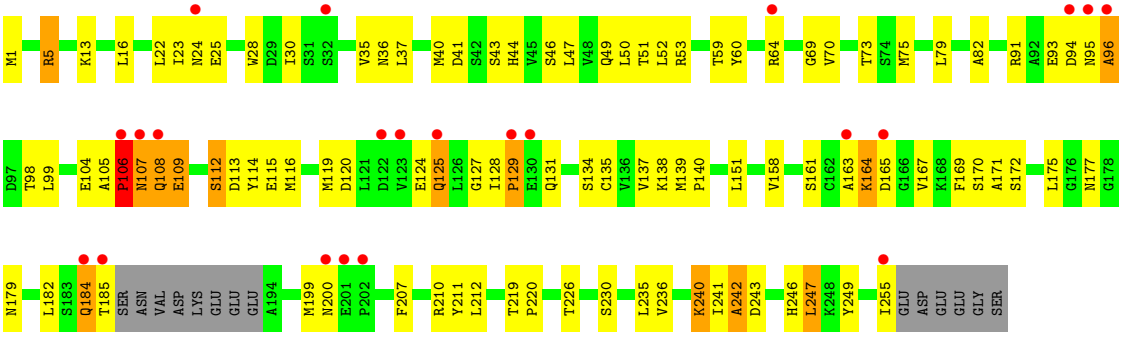
• Molecule 1: Proliferating cell nuclear antigen

Chain C:

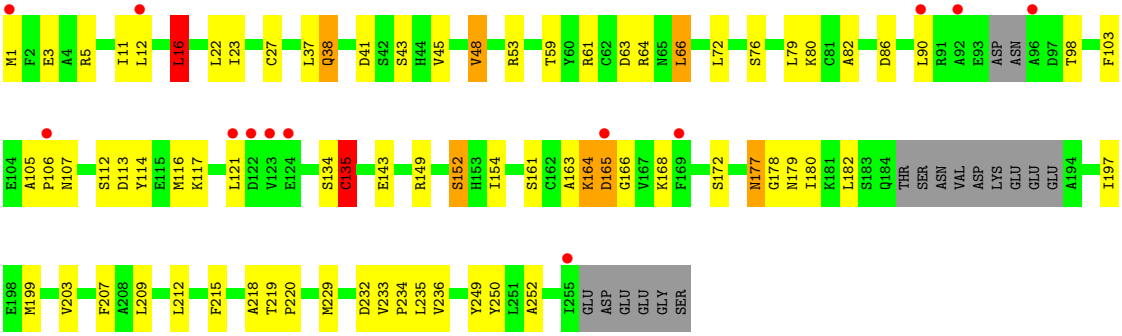




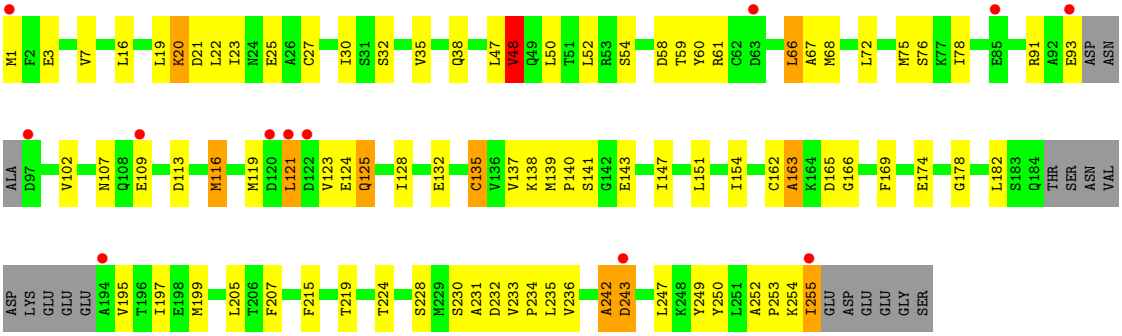
• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen

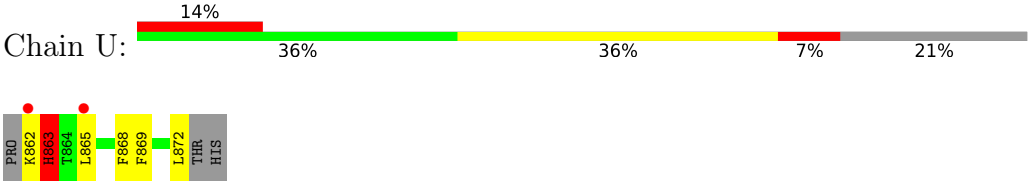


• Molecule 1: Proliferating cell nuclear antigen



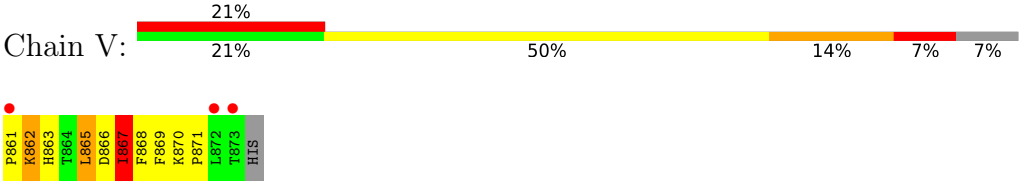
• Molecule 2: DNA polymerase kappa

Chain U:



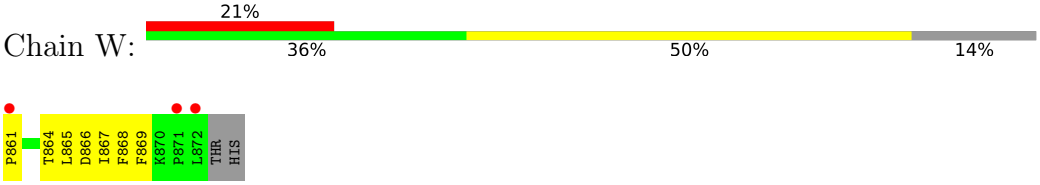
• Molecule 2: DNA polymerase kappa

Chain V:



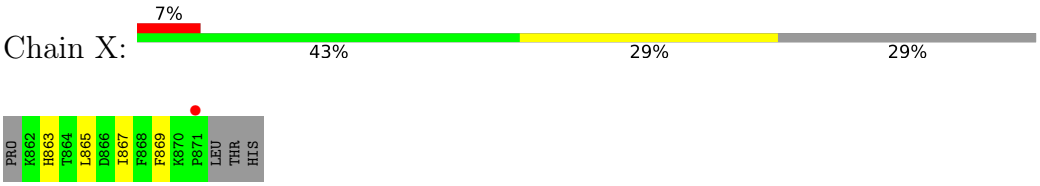
• Molecule 2: DNA polymerase kappa

Chain W:



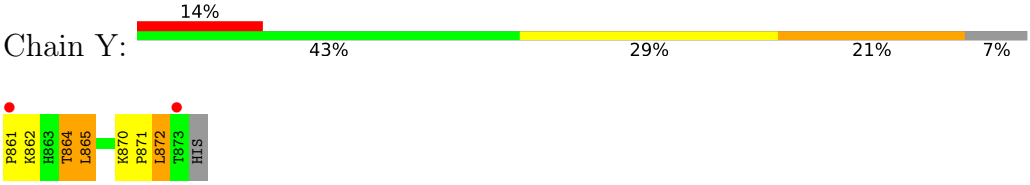
• Molecule 2: DNA polymerase kappa

Chain X:



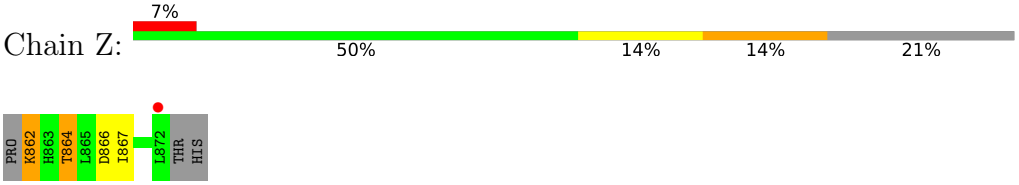
• Molecule 2: DNA polymerase kappa

Chain Y:



• Molecule 2: DNA polymerase kappa

Chain Z:



4 Data and refinement statistics (i)

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 19.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 90.4 (19.51-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.35 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, SO4

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	0.85	0/1910	0.87	2/2577 (0.1%)
1	B	0.94	3/1923 (0.2%)	0.91	4/2597 (0.2%)
1	C	0.91	0/1923	0.90	1/2597 (0.0%)
1	D	0.87	0/1923	0.87	1/2597 (0.0%)
1	E	0.98	1/1899 (0.1%)	0.94	4/2562 (0.2%)
1	F	1.00	1/1894 (0.1%)	0.96	1/2555 (0.0%)
2	U	0.52	0/99	0.62	0/132
2	V	0.83	0/114	1.12	2/153 (1.3%)
2	W	0.85	0/107	0.84	0/143
2	X	0.53	0/91	0.72	0/121
2	Y	1.04	0/114	1.04	1/153 (0.7%)
2	Z	1.15	0/99	1.37	1/132 (0.8%)
All	All	0.92	5/12096 (0.0%)	0.91	17/16319 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	135	CYS	CB-SG	-5.58	1.72	1.81
1	F	27	CYS	CB-SG	-5.53	1.72	1.81
1	B	55	GLU	CB-CG	-5.40	1.41	1.52
1	B	174	GLU	CG-CD	5.31	1.59	1.51
1	B	135	CYS	CB-SG	5.29	1.91	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	48	VAL	CB-CA-C	-10.04	92.33	111.40
1	C	48	VAL	CB-CA-C	-9.06	94.19	111.40
1	A	58	ASP	CB-CG-OD1	-8.24	110.88	118.30
1	A	16	LEU	CA-CB-CG	-7.99	96.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	16	LEU	CA-CB-CG	-7.74	97.49	115.30
2	Z	866	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	16	LEU	CA-CB-CG	-7.52	98.01	115.30
1	B	66	LEU	CA-CB-CG	6.67	130.64	115.30
1	B	48	VAL	CB-CA-C	-6.18	99.66	111.40
1	E	48	VAL	CB-CA-C	-6.12	99.77	111.40
1	E	53	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	146	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	E	86	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	V	865	LEU	CB-CG-CD2	5.45	120.26	111.00
2	V	867	ILE	CB-CA-C	-5.14	101.32	111.60
1	D	5	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	Y	872	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	84	0
1	B	1898	0	1915	84	0
1	C	1898	0	1915	85	0
1	D	1898	0	1915	111	0
1	E	1875	0	1897	69	0
1	F	1870	0	1892	84	0
2	U	96	0	101	6	0
2	V	110	0	116	9	0
2	W	103	0	109	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	V	1	0	0	0	0
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	2	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	524	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 23.

All (524) 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	1.26
1:D:93:GLU:HB2	1:D:96:ALA:HB2	1.14	1.11
1:B:40:MET:HE2	1:B:44:HIS:CB	1.80	1.11
1:C:16:LEU:HD22	1:C:79:LEU:CD1	1.81	1.10
1:B:40:MET:HE2	1:B:44:HIS:CA	1.83	1.09
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: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:C:139:MET:HE3	1:C:227:LEU:HD11	1.42	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:B:40:MET:HE2	1:B:44:HIS:HA	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:SER:HB3	1:E:177:ASN:HB3	1.49	0.95
1:D:40:MET:HE2	1:D:44:HIS:HA	1.50	0.94
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
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:B:40:MET:HE2	1:B:44:HIS:HB3	1.53	0.89
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: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:D:184:GLN:O	1:D:184:GLN:CD	2.18	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:B:205:LEU:HD12	1:B:229:MET:HE2	1.64	0.78
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:36:ASN:HB3	5:D:294:HOH:O	1.82	0.78
1:E:37:LEU:HD23	1:E:37:LEU:C	2.05	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:E:114:TYR:HE2	1:F:154:ILE:CD1	1.97	0.77
1:B:1:MET:HB3	1:B:63:ASP:OD2	1.85	0.76
1:B:40:MET:CE	1:B:44:HIS:HA	2.13	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:23:ILE:HG13	1:F:72:LEU:HD12	1.68	0.75
1:B:40:MET:CE	1:B:44:HIS:CA	2.62	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: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:D:128:ILE:O	1:D:129:PRO:C	2.26	0.73
1:A:163:ALA:C	1:A:199:MET:HE1	2.09	0.73
1:D:16:LEU:HD21	1:D:75:MET:CG	2.19	0.73
1:C:139:MET:CE	1:C:227:LEU:HD11	2.15	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: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: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:B:95:ASN:O	1:B:96:ALA:O	2.10	0.70
1:B:39:SER:C	1:B:47:LEU:HD12	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:862:LYS:CD	2:Z:862:LYS:O	2.40	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: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:99:LEU:HD23	1:D:116:MET:HE2	1.76	0.68
1:A:172:SER:HB2	1:A:177:ASN:ND2	2.09	0.68
1:A:66:LEU:C	1:A:66:LEU:HD12	2.13	0.68
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: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: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:A:139:MET:HE3	1:A:227:LEU:CD1	2.26	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:E:116:MET:HG2	1:E:117:LYS:N	2.11	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:GLU:HG3	1:F:93:GLU:O	1.98	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:D:107:ASN:O	1:D:108:GLN:C	2.36	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:C:254:LYS:O	1:C:255:ILE:C	2.37	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:A:139:MET:HE3	1:A:227:LEU:HD11	1.80	0.62
1:E:23:ILE:HD12	1:E:72:LEU:HD11	1.80	0.62
1:E:37:LEU:HD23	1:E:38:GLN:N	2.15	0.62
1:D:107:ASN:O	1:D:109:GLU:CD	2.38	0.62
1:C:244:MET:O	1:C:244:MET:HG3	1.98	0.62
1:B:22:LEU:CD2	1:B:48:VAL:HG22	2.29	0.61
1:B:169:PHE:N	1:B:169:PHE:CD1	2.68	0.61
1:A:200:ASN:C	1:A:201:GLU:HG2	2.21	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: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:F:1:MET:SD	1:F:61:ARG:NH1	2.74	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HG13	1:A:246:HIS:HA	1.84	0.59
1:C:124:GLU:O	1:C:125:GLN:C	2.41	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: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: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:B:60:TYR:O	1:B:61:ARG:HG2	2.03	0.57
1:F:1:MET:HE3	1:F:3:GLU:HB2	1.85	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:D:37:LEU:C	1:D:37:LEU:HD23	2.24	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
2:Y:870:LYS:HB3	2:Y:871:PRO:HD2	1.86	0.57
1:D:98:THR:HG21	1:D:115:GLU:CD	2.25	0.57
1:A:23:ILE:HG22	1:A:24:ASN:H	1.53	0.57
1:D:16:LEU:CD2	1:D:75:MET:CG	2.81	0.57
1:A:129:PRO:O	1:A:130:GLU:C	2.44	0.57
1:C:205:LEU:HD21	1:C:232:ASP:H	1.70	0.57
2:V:870:LYS:HB3	2:V:871:PRO:HD2	1.87	0.56
1:E:252:ALA:CB	2:Y:864:THR:HG23	2.35	0.56
1:F:50:LEU:HD13	1:F:247:LEU:HD13	1.87	0.56
1:B:40:MET:CE	2:V:865:LEU:HB3	2.36	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: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:A:163:ALA:C	1:A:199:MET:CE	2.73	0.56
1:E:16:LEU:CD1	1:E:79:LEU:CD1	2.84	0.56
1:C:68:MET:HB3	1:C:118:LEU:HD13	1.86	0.56
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:F:135:CYS:SG	1:F:199:MET:HG3	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:C	1:A:199:MET:SD	2.85	0.55
1:B:5:ARG:HB3	1:B:59:THR:HB	1.88	0.55
1:B:40:MET:HE3	2:V:865:LEU:HB3	1.89	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:B:160:ILE:HB	1:B:229:MET:HE1	1.87	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:106:PRO:C	1:D:107:ASN:OD1	2.45	0.54
1:E:166:GLY:HA2	1:E:197:ILE:HD12	1.87	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: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
1:B:99:LEU:HD23	1:B:116:MET:HE2	1.90	0.54
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: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:B:40:MET:HE2	1:B:44:HIS:CG	2.41	0.53
1:A:241:ILE:O	1:A:242:ALA:C	2.46	0.53
1:E:252:ALA:HB3	2:Y:864:THR:HG23	1.91	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: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:D:107:ASN:OD1	1:D:107:ASN:N	2.42	0.52
1:F:124:GLU:O	1:F:125:GLN:C	2.46	0.52
1:C:28:TRP:CD1	1:C:70:VAL:HG21	2.44	0.52
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.44	0.52
1:F:19:LEU:O	1:F:21:ASP:N	2.42	0.52
1:A:163:ALA:O	1:A:164:LYS:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:PRO:HD2	1:F:143:GLU:OE1	2.10	0.52
1:C:107:ASN:C	1:C:107:ASN:OD1	2.48	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:A:164:LYS:O	1:A:165:ASP:C	2.48	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:D:163:ALA:C	1:D:199:MET:HE1	2.30	0.51
1:F:236:VAL:HG22	1:F:250:TYR:CD2	2.45	0.51
1:C:16:LEU:HD22	1:C:79:LEU:HD13	1.85	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
1:A:107:ASN:O	1:A:109:GLU:OE1	2.28	0.51
1:B:241:ILE:O	1:B:242:ALA:C	2.48	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:93:GLU:O	1:A:94:ASP:C	2.48	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:95:ASN:CG	1:C:95:ASN:O	2.45	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:C:205:LEU:HD12	1:C:229:MET:HE3	1.93	0.50
1:D:5:ARG:HB3	1:D:59:THR:HB	1.93	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: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:C:128:ILE:O	1:C:129:PRO:C	2.50	0.49
1:F:19:LEU:O	1:F:20:LYS:C	2.50	0.49
1:F:123:VAL:C	1:F:124:GLU:HG3	2.33	0.49
1:A:37:LEU:HD23	1:A:38:GLN:N	2.27	0.49
1:B:11:ILE:HD13	1:B:244:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:40:MET:HE2	1:A:44:HIS:HA	1.93	0.49
1:A:139:MET:HE1	1:A:227:LEU:HD12	1.94	0.49
1:B:98:THR:HA	1:B:118:LEU:HG	1.93	0.49
1:F:1:MET:CE	1:F:3:GLU:HB2	2.42	0.49
1:A:137:VAL:O	1:A:226:THR:HA	2.13	0.49
1:D:163:ALA:O	1:D:164:LYS:C	2.51	0.49
1:A:166:GLY:CA	1:A:197:ILE:HD12	2.43	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:D:107:ASN:O	1:D:109:GLU:OE2	2.31	0.48
1:A:43:SER:HG	1:A:45:VAL:HG12	1.74	0.48
1:A:166:GLY:HA2	1:A:197:ILE:CD1	2.40	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: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:D:211:TYR:O	1:D:212:LEU:C	2.51	0.48
1:E:37:LEU:C	1:E:37:LEU:CD2	2.79	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: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:A:200:ASN:C	1:A:201:GLU:CG	2.82	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:C:165:ASP:C	5:C:302:HOH:O	2.52	0.48
1:D:105:ALA:O	1:D:106:PRO:C	2.51	0.48
1:C:177:ASN:OD1	1:C:177:ASN:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:O	1:D:99:LEU:HD12	2.14	0.47
1:F:1:MET:HE1	5:F:358:HOH:O	2.13	0.47
1:C:25:GLU:OE2	1:C:119:MET:SD	2.72	0.47
1:B:106:PRO:O	1:B:107:ASN:C	2.52	0.47
1:C:4:ALA:O	1:C:89:THR:HA	2.14	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:D:200:ASN:OD1	1:D:200:ASN:C	2.53	0.47
1:A:66:LEU:CD1	1:A:68:MET:HG3	2.44	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: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:B:2:PHE:O	1:B:91:ARG:HA	2.15	0.46
1:B:37:LEU:HD23	1:B:37:LEU:C	2.36	0.46
1:A:37:LEU:HD23	1:A:37:LEU:C	2.36	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: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:A:139:MET:CE	1:A:227:LEU:HD11	2.42	0.46
1:E:98:THR:CB	1:E:116:MET:O	2.60	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: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
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:D:241:ILE:O	1:D:242:ALA:C	2.54	0.45
1:F:165:ASP:O	1:F:197:ILE:HD12	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ALA:O	1:E:219:THR:C	2.55	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
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:C:124:GLU:O	1:C:125:GLN:O	2.35	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:E:1:MET:HB3	1:E:63:ASP:CG	2.37	0.44
1:D:36:ASN:HD22	1:D:51:THR:HG22	1.80	0.44
1:D:184:GLN:CD	1:D:184:GLN:C	2.74	0.44
1:E:23:ILE:CD1	1:E:72:LEU:CD1	2.95	0.44
1:C:71:ASN:OD1	1:C:71:ASN:C	2.55	0.44
1:D:43:SER:O	1:D:44:HIS:CB	2.63	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
2:V:861:PRO:C	2:V:862:LYS:HG2	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: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:E:168:LYS:HA	1:E:180:ILE:O	2.18	0.43
1:C:123:VAL:HG23	1:C:123:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:128:ILE:O	1:C:128:ILE:HG22	2.17	0.43
1:D:40:MET:HE2	1:D:40:MET:HB3	1.63	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:B:64:ARG:O	1:B:65:ASN:C	2.55	0.43
1:B:168:LYS:HG3	1:B:181:LYS:HG3	2.00	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:C:205:LEU:HD12	1:C:229:MET:HE2	2.01	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: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:124:GLU:O	1:D:125:GLN:C	2.57	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:B:139:MET:HE1	1:B:182:LEU:CD1	2.49	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:A:108:GLN:C	1:A:109:GLU:OE1	2.57	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:F:162:CYS:O	1:F:163:ALA:HB2	2.19	0.42
1:F:242:ALA:O	1:F:243:ASP:C	2.58	0.42
1:A:66:LEU:C	1:A:66:LEU:CD1	2.85	0.42
1:B:16:LEU:HD21	1:B:75:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:241:ILE:O	1:C:242:ALA:C	2.57	0.42
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:231:ALA:O	1:F:233:VAL:HG13	2.19	0.41
1:B:123:VAL:CG2	1:B:124:GLU:N	2.83	0.41
1:B:139:MET:HE1	1:B:182:LEU:HD12	2.02	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:D:107:ASN:C	1:D:108:GLN:O	2.55	0.41
1:E:163:ALA:O	1:E:164:LYS:C	2.58	0.41
1:F:230:SER:O	1:F:231:ALA:C	2.59	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:F:30:ILE:HG13	1:F:68:MET:HE1	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:D:40:MET:CE	2:X:865:LEU:HB2	2.51	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:C:232:ASP:C	1:C:233:VAL:HG13	2.41	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:217:LYS:HA	1:C:217:LYS:HD3	1.86	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:B:11:ILE:HD13	1:B:244:MET:HE1	2.03	0.41
1:B:95:ASN:O	1:B:96:ALA:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:LYS:O	1:F:195:VAL:HA	2.20	0.41
1:A:235:LEU:O	1:A:250:TYR:HA	2.21	0.41
1:B:38:GLN:HB2	5:B:307:HOH:O	2.21	0.41
1:D:40:MET:HE1	2:X:865:LEU:HB2	2.03	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:D:134:SER:HA	1:D:200:ASN:HB3	2.02	0.40
1:F:30:ILE:HG13	1:F:68:MET:CE	2.51	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: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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	239/261 (92%)	216 (90%)	15 (6%)	8 (3%)	4 5
1	B	243/261 (93%)	227 (93%)	11 (4%)	5 (2%)	7 11
1	C	243/261 (93%)	231 (95%)	9 (4%)	3 (1%)	13 24
1	D	243/261 (93%)	225 (93%)	10 (4%)	8 (3%)	4 5
1	E	238/261 (91%)	228 (96%)	7 (3%)	3 (1%)	12 21
1	F	237/261 (91%)	221 (93%)	11 (5%)	5 (2%)	7 11
2	U	9/14 (64%)	8 (89%)	0	1 (11%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	V	11/14 (79%)	8 (73%)	2 (18%)	1 (9%)	1 0
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%)	6 10

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

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Mol	Chain	Res	Type
1	D	108	GLN
1	F	163	ALA
1	E	165	ASP
1	F	242	ALA
1	D	129	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	214/228 (94%)	195 (91%)	19 (9%)	9 19
1	B	215/228 (94%)	197 (92%)	18 (8%)	11 21
1	C	215/228 (94%)	205 (95%)	10 (5%)	26 49
1	D	215/228 (94%)	195 (91%)	20 (9%)	9 17
1	E	212/228 (93%)	200 (94%)	12 (6%)	20 39
1	F	212/228 (93%)	200 (94%)	12 (6%)	20 39
2	U	11/14 (79%)	8 (73%)	3 (27%)	0 0
2	V	13/14 (93%)	12 (92%)	1 (8%)	13 25
2	W	12/14 (86%)	12 (100%)	0	100 100
2	X	10/14 (71%)	9 (90%)	1 (10%)	7 15
2	Y	13/14 (93%)	10 (77%)	3 (23%)	1 1
2	Z	11/14 (79%)	9 (82%)	2 (18%)	1 3
All	All	1353/1452 (93%)	1252 (92%)	101 (8%)	13 26

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	62	CYS
1	A	78	ILE
1	A	79	LEU
1	A	85	GLU

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Mol	Chain	Res	Type
1	A	93	GLU
1	A	108	GLN
1	A	109	GLU
1	A	120	ASP
1	A	122	ASP
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	862	LYS
2	U	863	HIS
2	U	872	LEU
1	B	24	ASN
1	B	42	SER
1	B	59	THR
1	B	66	LEU
1	B	107	ASN
1	B	113	ASP
1	B	115	GLU
1	B	121	LEU
1	B	122	ASP
1	B	141	SER
1	B	147	ILE
1	B	152	SER
1	B	161	SER
1	B	165	ASP
1	B	169	PHE
1	B	177	ASN
1	B	185	THR
1	B	224	THR
2	V	862	LYS
1	C	58	ASP
1	C	59	THR
1	C	66	LEU
1	C	68	MET
1	C	121	LEU
1	C	123	VAL

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Mol	Chain	Res	Type
1	C	125	GLN
1	C	149	ARG
1	C	232	ASP
1	C	255	ILE
1	D	1	MET
1	D	24	ASN
1	D	25	GLU
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	120	ASP
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	27	CYS
1	E	38	GLN
1	E	41	ASP
1	E	43	SER
1	E	66	LEU
1	E	135	CYS
1	E	152	SER
1	E	161	SER
1	E	177	ASN
1	E	229	MET
2	Y	864	THR
2	Y	865	LEU
2	Y	872	LEU
1	F	32	SER
1	F	47	LEU

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Mol	Chain	Res	Type
1	F	48	VAL
1	F	59	THR
1	F	66	LEU
1	F	76	SER
1	F	116	MET
1	F	121	LEU
1	F	132	GLU
1	F	135	CYS
1	F	174	GLU
1	F	255	ILE
2	Z	862	LYS
2	Z	864	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	213	ASN
1	C	49	GLN
1	C	84	ASN
1	C	125	GLN
1	C	184	GLN
1	D	36	ASN
1	D	49	GLN
1	D	65	ASN
1	D	177	ASN
2	X	863	HIS
1	E	125	GLN
1	F	49	GLN
1	F	84	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	0.13	0	6,6,6	0.48	0
3	SO4	D	262	-	4,4,4	0.17	0	6,6,6	1.27	0
3	SO4	A	262	-	4,4,4	0.12	0	6,6,6	0.45	0
3	SO4	F	262	-	4,4,4	0.13	0	6,6,6	0.44	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	D	262	SO4	5	0
3	A	262	SO4	1	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, 95^{th} 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%)	0.50	22 (8%) 9 9	31, 43, 66, 74	25 (10%)
1	B	247/261 (94%)	0.29	13 (5%) 26 28	25, 37, 54, 58	18 (7%)
1	C	247/261 (94%)	0.20	8 (3%) 47 51	27, 36, 57, 60	19 (7%)
1	D	247/261 (94%)	0.43	22 (8%) 9 9	29, 42, 64, 75	16 (6%)
1	E	244/261 (93%)	0.27	13 (5%) 26 28	23, 37, 50, 60	10 (4%)
1	F	243/261 (93%)	0.32	12 (4%) 29 31	25, 38, 56, 65	10 (4%)
2	U	11/14 (78%)	1.14	2 (18%) 1 1	81, 85, 89, 89	5 (45%)
2	V	13/14 (92%)	0.76	3 (23%) 0 0	33, 41, 53, 55	3 (23%)
2	W	12/14 (85%)	1.13	3 (25%) 0 0	30, 40, 48, 50	1 (8%)
2	X	10/14 (71%)	0.78	1 (10%) 7 6	68, 74, 81, 83	2 (20%)
2	Y	13/14 (92%)	0.62	2 (15%) 2 1	28, 41, 50, 54	0
2	Z	11/14 (78%)	0.45	1 (9%) 9 9	22, 28, 36, 41	1 (9%)
All	All	1543/1650 (93%)	0.36	102 (6%) 18 19	22, 39, 60, 89	110 (7%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	185	THR	7.7
1	A	122	ASP	6.8
1	A	107	ASN	5.5
1	F	255	ILE	5.2
1	C	255	ILE	5.2
2	W	861	PRO	5.0
1	D	107	ASN	5.0
1	D	106	PRO	4.8
1	D	96	ALA	4.8
1	A	1	MET	4.8
1	D	165	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
2	V	861	PRO	4.6
1	A	121	LEU	4.5
1	D	122	ASP	4.5
1	A	125	GLN	4.1
1	A	165	ASP	4.1
1	F	120	ASP	4.0
1	C	120	ASP	4.0
1	A	106	PRO	4.0
1	C	163	ALA	3.9
1	A	127	GLY	3.9
1	B	94	ASP	3.8
2	Y	873	THR	3.8
2	Z	872	LEU	3.7
1	D	130	GLU	3.7
1	B	106	PRO	3.7
1	E	124	GLU	3.6
1	F	194	ALA	3.6
1	D	184	GLN	3.5
1	F	122	ASP	3.4
1	E	106	PRO	3.4
1	D	200	ASN	3.3
1	D	202	PRO	3.2
1	F	121	LEU	3.2
2	U	865	LEU	3.2
1	F	1	MET	3.2
1	D	125	GLN	3.2
1	A	164	LYS	3.1
2	Y	861	PRO	3.1
2	W	872	LEU	3.1
1	A	120	ASP	3.1
1	D	64	ARG	3.1
1	D	95	ASN	3.1
1	D	108	GLN	3.0
1	E	255	ILE	3.0
1	E	1	MET	3.0
1	A	243	ASP	3.0
1	B	90	LEU	3.0
1	A	126	LEU	2.9
1	C	185	THR	2.9
2	V	873	THR	2.9
1	E	123	VAL	2.9
1	E	165	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASN	2.9
1	A	63	ASP	2.8
1	B	194	ALA	2.8
1	B	124	GLU	2.8
2	X	871	PRO	2.8
1	F	63	ASP	2.8
1	E	90	LEU	2.8
1	B	96	ALA	2.8
1	C	243	ASP	2.8
1	B	123	VAL	2.7
1	A	255	ILE	2.7
2	U	862	LYS	2.7
1	B	107	ASN	2.7
1	D	255	ILE	2.7
1	E	121	LEU	2.7
1	A	119	MET	2.6
1	E	96	ALA	2.6
1	B	200	ASN	2.6
1	E	92	ALA	2.6
2	W	871	PRO	2.6
1	A	123	VAL	2.5
1	B	121	LEU	2.5
1	C	1	MET	2.5
1	C	106	PRO	2.5
1	A	200	ASN	2.5
1	C	165	ASP	2.4
1	F	243	ASP	2.4
1	A	202	PRO	2.4
2	V	872	LEU	2.3
1	D	32	SER	2.3
1	B	232	ASP	2.2
1	B	195	VAL	2.2
1	B	169	PHE	2.2
1	D	24	ASN	2.2
1	D	94	ASP	2.2
1	E	122	ASP	2.2
1	E	169	PHE	2.2
1	D	163	ALA	2.1
1	E	12	LEU	2.1
1	F	93	GLU	2.1
1	F	85	GLU	2.1
1	D	201	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	109	GLU	2.1
1	D	129	PRO	2.1
1	F	97	ASP	2.0
1	A	124	GLU	2.0
1	D	123	VAL	2.0
1	A	235	LEU	2.0
1	A	130	GLU	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 monosaccharides 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, 95^{th} 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	0.89	0.21	98,99,101,103	0
3	SO4	D	262	5/5	0.92	0.20	72,73,81,83	0
3	SO4	A	262	5/5	0.92	0.22	94,95,97,97	0
3	SO4	C	262	5/5	0.94	0.16	94,95,96,98	0
4	ZN	B	262	1/1	0.96	0.09	51,51,51,51	0
4	ZN	W	2	1/1	0.96	0.10	45,45,45,45	0
4	ZN	Z	4	1/1	0.96	0.09	47,47,47,47	0
4	ZN	E	262	1/1	0.97	0.09	54,54,54,54	0
4	ZN	Y	3	1/1	0.99	0.09	48,48,48,48	0
4	ZN	V	1	1/1	0.99	0.10	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.