



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:32 AM EDT

PDB ID : 1UL1 / pdb_00001ul1
Title : Crystal structure of the human FEN1-PCNA complex
Authors : Sakurai, S.; Kitano, K.; Yamaguchi, H.; Hamada, K.; Okada, K.; Fukuda, K.;
Uchida, M.; Ohtsuka, E.; Morioka, H.; Hakoshima, T.
Deposited on : 2003-09-05
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

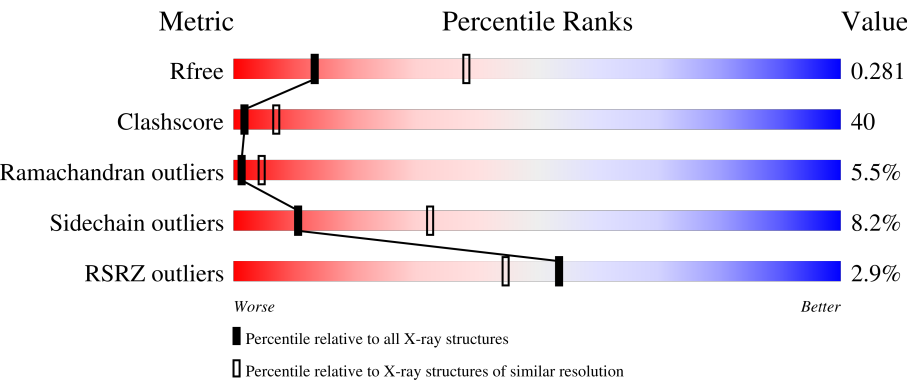
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	379	2% 37% 36% 9% 17%
1	Y	379	3% 32% 42% 7% 18%
1	Z	379	6% 28% 53% 9% 8%
2	A	261	% 48% 44% 6%
2	B	261	3% 44% 44% 11%

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Mol	Chain	Length	Quality of chain
2	C	261	48% 44% 5% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13162 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 Flap endonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	313	Total	C	N	O	S	0	0	0
			2376	1502	410	450	14			
1	Y	312	Total	C	N	O	S	0	0	0
			2335	1468	407	447	13			
1	Z	349	Total	C	N	O	S	0	0	0
			2597	1626	466	491	14			

- Molecule 2 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	256	Total	C	N	O	S	0	0	0
			1960	1230	319	395	16			
2	B	258	Total	C	N	O	S	0	0	0
			1959	1231	318	394	16			
2	C	255	Total	C	N	O	S	0	0	0
			1930	1214	317	383	16			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	2	Total	Mg	0	0
			2	2		
3	Y	2	Total	Mg	0	0
			2	2		

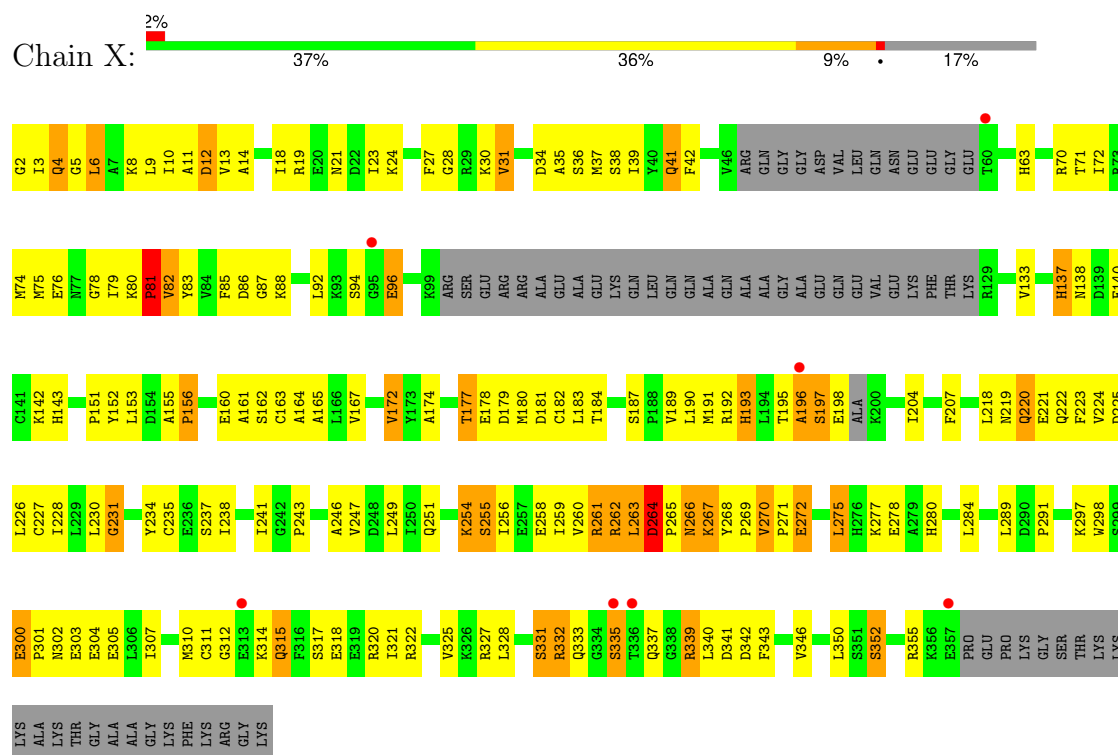
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		

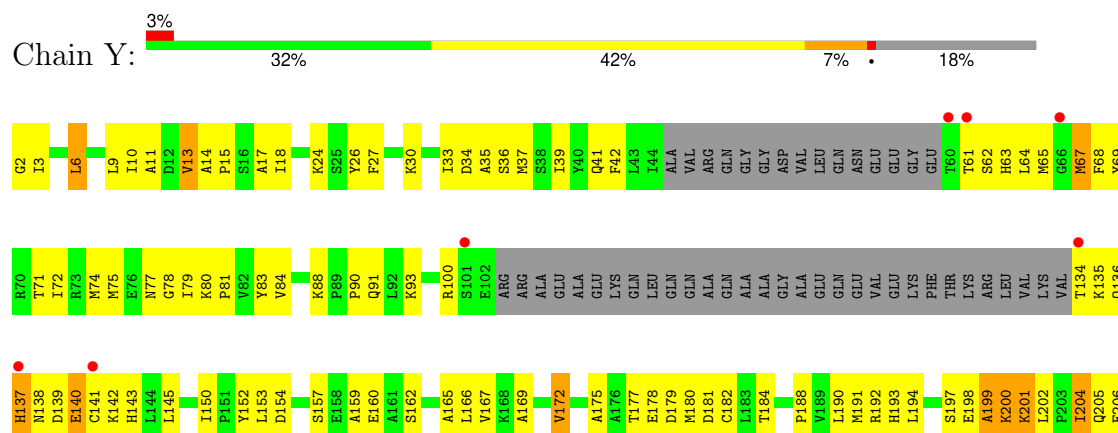
3 Residue-property plots

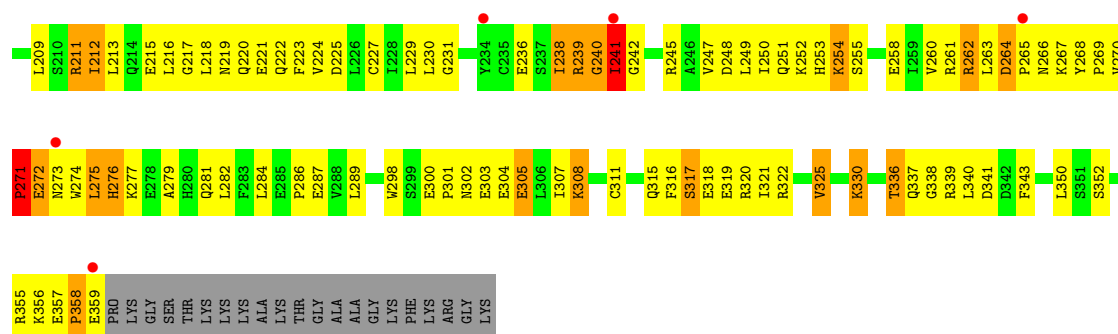
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flap endonuclease-1

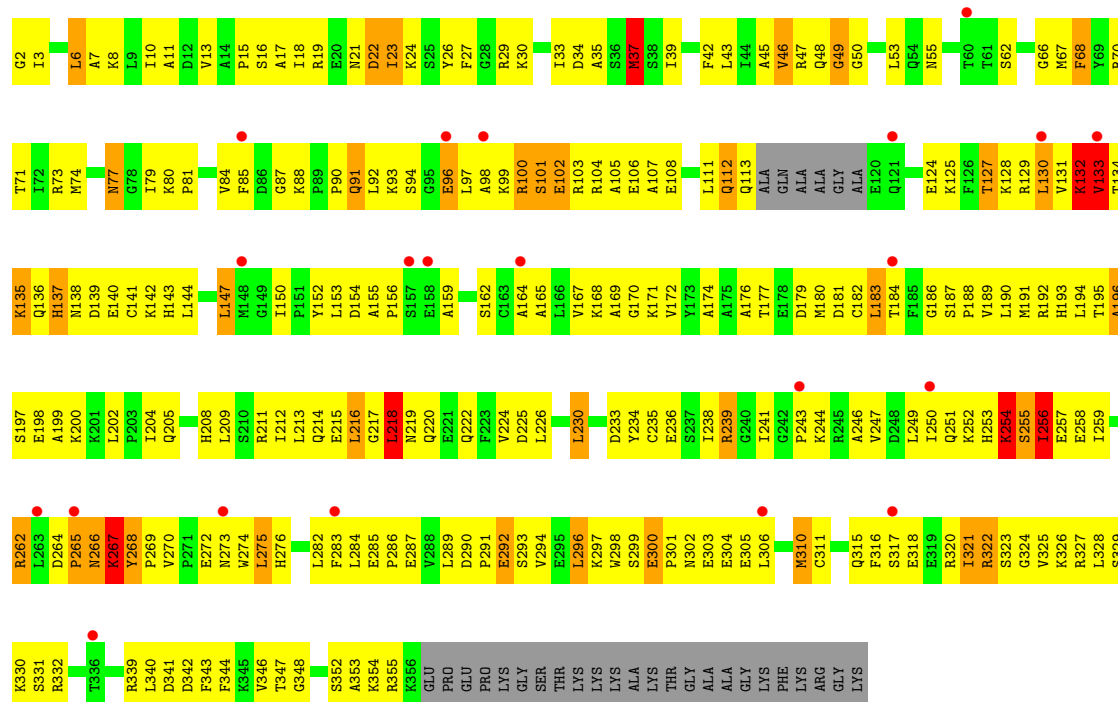


• Molecule 1: Flap endonuclease-1

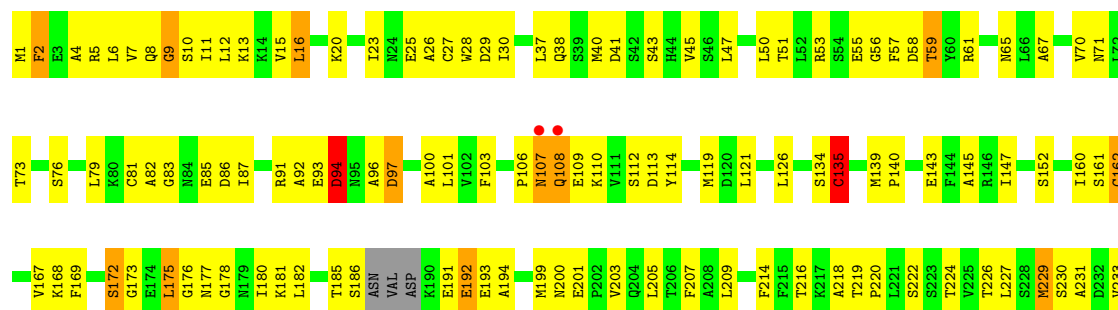


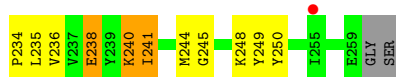


• Molecule 1: Flap endonuclease-1

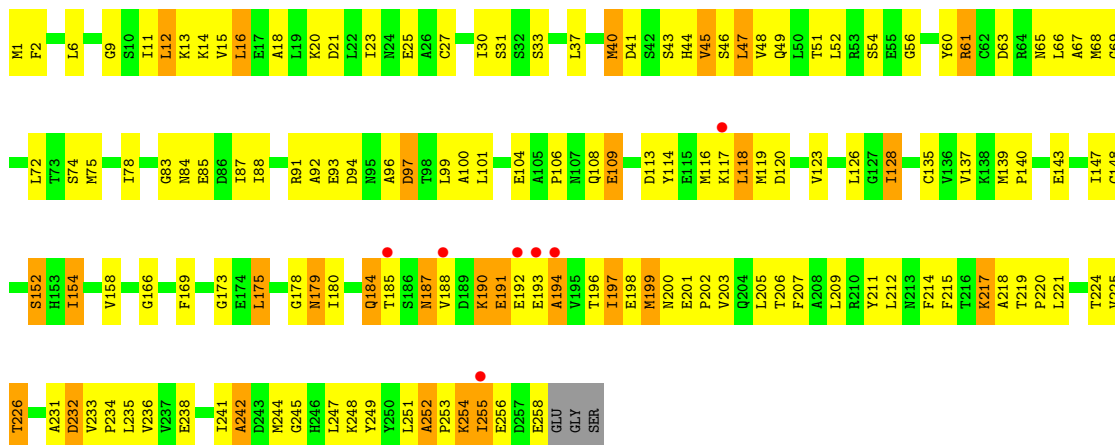


• Molecule 2: Proliferating cell nuclear antigen

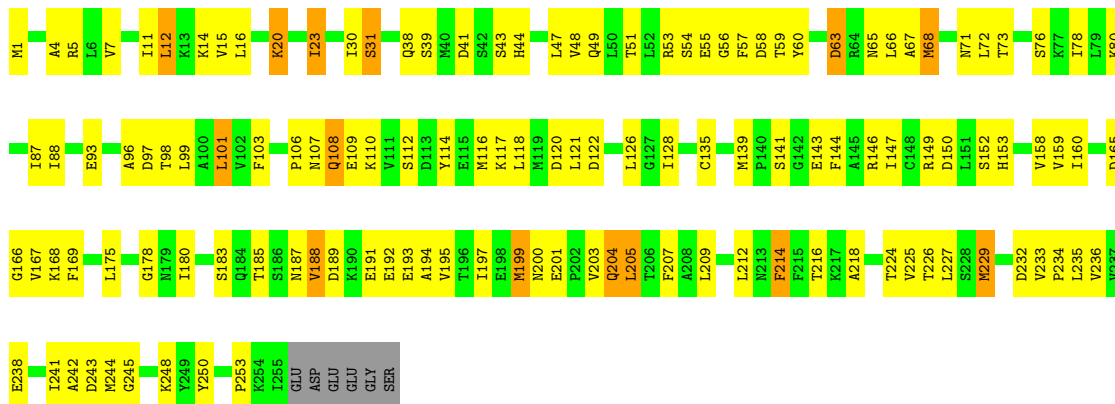




• Molecule 2: Proliferating cell nuclear antigen



• Molecule 2: Proliferating cell nuclear antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.20Å 143.38Å 246.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 85.0 (30.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.284 0.219 , 0.281	Depositor DCC
R_{free} test set	2821 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13162	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: MG

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	X	0.49	0/2418	1.04	12/3264 (0.4%)
1	Y	0.39	0/2376	0.95	7/3212 (0.2%)
1	Z	0.40	0/2640	1.05	23/3565 (0.6%)
2	A	0.56	0/1985	1.01	10/2682 (0.4%)
2	B	0.56	0/1985	1.06	8/2686 (0.3%)
2	C	0.50	0/1956	0.97	3/2649 (0.1%)
All	All	0.48	0/13360	1.02	63/18058 (0.3%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	100	ARG	N-CA-C	-12.64	97.79	113.97
1	Z	132	LYS	N-CA-C	-10.21	100.36	112.92
1	X	137	HIS	N-CA-C	-10.13	99.46	112.23
1	Z	137	HIS	N-CA-C	-10.05	101.01	113.18
1	X	178	GLU	N-CA-C	-9.20	102.18	113.50
2	A	241	ILE	N-CA-C	9.08	115.92	106.21
1	Z	105	ALA	N-CA-C	-7.85	103.72	113.38
1	Z	268	TYR	CA-C-N	7.63	127.56	119.85
1	Z	268	TYR	C-N-CA	7.63	127.56	119.85
2	C	214	PHE	N-CA-C	-7.55	104.20	113.41
1	X	161	ALA	N-CA-C	-7.11	103.22	110.97
1	X	264	ASP	CA-C-N	-7.09	110.98	119.84
1	X	264	ASP	C-N-CA	-7.09	110.98	119.84
1	Y	241	ILE	N-CA-C	6.93	119.42	109.51
1	Z	129	ARG	N-CA-C	-6.72	103.89	111.14
1	X	264	ASP	N-CA-C	6.62	124.43	109.81
1	X	255	SER	N-CA-C	6.53	119.34	109.41
2	A	70	VAL	N-CA-C	6.52	117.51	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	199	MET	N-CA-C	6.45	120.17	109.46
1	Z	124	GLU	N-CA-C	-6.40	105.33	113.01
2	B	198	GLU	N-CA-C	-6.32	98.89	109.07
1	Y	336	THR	N-CA-C	-6.32	106.79	114.75
2	B	123	VAL	N-CA-C	6.28	117.79	107.24
1	Y	266	ASN	N-CA-C	-6.23	106.04	113.21
2	A	238	GLU	N-CA-C	6.20	119.01	108.90
2	A	20	LYS	N-CA-C	6.16	118.53	111.02
1	X	339	ARG	N-CA-C	-6.14	99.69	109.76
1	X	331	SER	N-CA-C	-6.10	104.54	111.07
1	X	277	LYS	N-CA-C	-6.07	104.74	111.36
1	Y	211	ARG	N-CA-C	-6.04	106.04	113.41
2	A	229	MET	N-CA-C	6.03	118.34	109.24
1	Z	18	ILE	N-CA-C	6.02	116.02	106.88
2	A	97	ASP	N-CA-C	-5.99	106.31	113.97
1	Z	300	GLU	CA-C-N	5.99	126.01	119.90
1	Z	300	GLU	C-N-CA	5.99	126.01	119.90
1	Z	101	SER	N-CA-C	-5.93	104.75	112.23
2	B	252	ALA	CA-C-N	5.91	127.23	119.84
2	B	252	ALA	C-N-CA	5.91	127.23	119.84
1	Z	297	LYS	N-CA-C	5.69	116.71	107.32
1	Z	102	GLU	N-CA-C	-5.68	105.84	112.89
2	A	214	PHE	N-CA-C	-5.67	104.49	111.40
1	Z	322	ARG	N-CA-C	-5.63	104.78	111.03
1	Z	103	ARG	N-CA-C	-5.56	105.16	112.72
2	A	41	ASP	N-CA-C	-5.52	102.35	110.52
1	Z	267	LYS	N-CA-C	-5.52	105.75	113.37
2	B	154	ILE	N-CA-C	-5.52	106.32	111.45
1	Z	216	LEU	N-CA-C	-5.51	106.69	113.41
1	Z	183	LEU	N-CA-C	-5.49	106.58	113.28
1	Y	212	ILE	N-CA-C	-5.48	104.99	110.30
2	B	197	ILE	N-CA-C	5.41	115.69	108.11
2	C	199	MET	N-CA-C	5.27	118.02	109.06
1	Z	139	ASP	N-CA-C	-5.26	106.55	112.87
1	Z	88	LYS	CA-C-N	5.26	125.80	120.38
1	Z	88	LYS	C-N-CA	5.26	125.80	120.38
1	X	261	ARG	N-CA-C	-5.22	100.66	108.96
2	A	162	CYS	N-CA-C	5.14	116.80	108.26
1	Y	140	GLU	N-CA-C	-5.13	106.71	112.87
2	B	69	GLY	N-CA-C	-5.12	101.04	113.18
2	C	68	MET	N-CA-C	5.11	116.74	108.41
1	Z	292	GLU	N-CA-C	5.08	116.67	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	ASP	N-CA-C	-5.07	107.08	114.12
1	Y	100	ARG	N-CA-C	-5.04	106.91	113.16
1	X	5	GLY	N-CA-C	5.03	122.06	115.47

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	X	2376	0	2301	174	0
1	Y	2335	0	2231	223	0
1	Z	2597	0	2484	318	0
2	A	1960	0	1945	118	0
2	B	1959	0	1934	140	0
2	C	1930	0	1913	111	0
3	X	2	0	0	0	0
3	Y	2	0	0	0	0
4	C	1	0	0	0	0
All	All	13162	0	12808	1040	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 40.

All (1040) 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:Z:311:CYS:HB3	1:Z:316:PHE:O	1.53	1.08
1:Z:254:LYS:HD3	1:Z:254:LYS:H	1.17	1.08
1:Z:97:LEU:HD23	1:Z:98:ALA:H	1.20	1.06
2:A:175:LEU:H	2:A:175:LEU:HD23	1.18	1.03
1:Z:218:LEU:HD12	1:Z:218:LEU:H	1.26	1.00
1:Y:330:LYS:HE2	1:Y:330:LYS:HA	1.45	0.95
1:Z:218:LEU:HB3	1:Z:222:GLN:HB2	1.47	0.94
2:C:147:ILE:HG23	2:C:180:ILE:HD12	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:238:ILE:HG23	1:Y:241:ILE:HD11	1.51	0.92
1:X:355:ARG:HG2	2:A:96:ALA:O	1.69	0.91
1:Y:71:THR:HG21	1:Y:150:ILE:HD13	1.53	0.90
1:Y:184:THR:HG22	1:Y:227:CYS:SG	2.11	0.89
2:B:175:LEU:HD23	2:B:175:LEU:H	1.37	0.88
1:Z:92:LEU:HB3	1:Z:234:TYR:O	1.74	0.88
1:X:355:ARG:HD2	2:A:97:ASP:HA	1.54	0.87
1:X:142:LYS:HG2	1:X:152:TYR:CE2	2.10	0.86
1:Z:2:GLY:O	1:Z:3:ILE:HD12	1.77	0.84
1:Z:34:ASP:HB2	1:Z:177:THR:OG1	1.78	0.84
2:B:158:VAL:HB	2:B:209:LEU:HD21	1.59	0.84
1:Z:49:GLY:H	1:Z:125:LYS:HD3	1.41	0.84
1:Y:254:LYS:H	1:Y:254:LYS:HD2	1.41	0.84
1:Z:53:LEU:HD23	1:Z:53:LEU:H	1.42	0.84
2:A:175:LEU:H	2:A:175:LEU:CD2	1.92	0.83
1:Z:11:ALA:O	1:Z:15:PRO:HG3	1.80	0.82
2:B:128:ILE:H	2:B:128:ILE:HD12	1.44	0.82
1:Z:2:GLY:C	1:Z:3:ILE:HD12	2.06	0.81
2:B:9:GLY:HA3	2:B:88:ILE:HD13	1.63	0.81
2:C:54:SER:HB2	2:C:60:TYR:CD2	2.16	0.80
2:A:6:LEU:HD21	2:A:11:ILE:HD12	1.61	0.80
2:C:5:ARG:HB3	2:C:59:THR:HB	1.63	0.80
2:C:204:GLN:C	2:C:205:LEU:HD23	2.07	0.80
1:Z:177:THR:HG22	1:Z:179:ASP:H	1.46	0.79
1:Z:97:LEU:HD23	1:Z:98:ALA:N	1.98	0.79
1:Z:3:ILE:HB	1:Z:6:LEU:HD12	1.63	0.79
1:Z:152:TYR:C	1:Z:153:LEU:HD12	2.07	0.79
1:Y:152:TYR:O	1:Y:153:LEU:HD12	1.82	0.78
2:C:175:LEU:HD23	2:C:175:LEU:H	1.47	0.78
1:Y:152:TYR:C	1:Y:153:LEU:HD12	2.08	0.78
2:C:166:GLY:HA2	2:C:197:ILE:HD12	1.66	0.77
1:Z:49:GLY:HA3	1:Z:125:LYS:HB2	1.65	0.77
1:Z:23:ILE:HG23	1:Z:204:ILE:HD11	1.66	0.77
1:Z:67:MET:HB3	1:Z:144:LEU:HD23	1.66	0.77
1:Z:300:GLU:OE2	1:Z:301:PRO:HD2	1.84	0.77
1:Z:99:LYS:HB3	1:Z:102:GLU:HB3	1.67	0.76
1:Z:296:LEU:HD13	1:Z:298:TRP:HZ3	1.50	0.76
1:Z:104:ARG:NE	1:Z:104:ARG:HA	2.00	0.76
2:B:14:LYS:HD3	2:B:220:PRO:HB2	1.65	0.76
1:X:263:LEU:O	1:X:265:PRO:HD3	1.86	0.76
1:X:155:ALA:HA	1:X:289:LEU:HD21	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:166:GLY:HA2	2:C:197:ILE:CD1	2.16	0.76
1:X:264:ASP:O	1:X:265:PRO:C	2.28	0.75
1:X:19:ARG:HD2	1:X:21:ASN:HD21	1.49	0.75
2:C:98:THR:HG22	2:C:117:LYS:HA	1.67	0.75
1:X:340:LEU:HD22	2:A:47:LEU:HB3	1.68	0.75
2:C:7:VAL:HA	2:C:87:ILE:HG23	1.68	0.75
1:X:263:LEU:C	1:X:265:PRO:HD3	2.11	0.75
1:Y:284:LEU:O	1:Y:286:PRO:HD3	1.87	0.75
1:Y:177:THR:HG22	1:Y:178:GLU:H	1.52	0.74
1:Z:218:LEU:H	1:Z:218:LEU:CD1	1.97	0.74
2:A:101:LEU:N	2:A:101:LEU:HD12	2.02	0.74
1:Z:254:LYS:HD3	1:Z:254:LYS:N	1.99	0.74
1:X:255:SER:O	1:X:259:ILE:HG13	1.86	0.74
1:Y:254:LYS:HD2	1:Y:254:LYS:N	2.01	0.74
1:Z:97:LEU:C	1:Z:99:LYS:H	1.95	0.74
2:A:175:LEU:HD23	2:A:175:LEU:N	2.00	0.74
1:Z:252:LYS:HA	1:Z:254:LYS:HE2	1.69	0.74
1:Y:26:TYR:CE2	1:Y:204:ILE:HG12	2.23	0.73
1:X:41:GLN:HE22	1:X:196:ALA:HB1	1.53	0.73
1:X:317:SER:HB3	1:X:320:ARG:HH11	1.53	0.73
1:Z:43:LEU:HD23	1:Z:62:SER:HB2	1.70	0.73
2:B:139:MET:HE1	2:B:169:PHE:HZ	1.52	0.73
1:Z:296:LEU:HD22	1:Z:298:TRP:HH2	1.52	0.73
1:Y:30:LYS:O	1:Y:172:VAL:HG22	1.87	0.73
2:C:66:LEU:HD12	2:C:67:ALA:H	1.54	0.73
1:Y:355:ARG:HH12	2:B:120:ASP:CG	1.96	0.73
1:Z:174:ALA:HB3	1:Z:191:MET:CE	2.19	0.72
2:C:107:ASN:O	2:C:109:GLU:N	2.19	0.72
2:B:233:VAL:HG13	2:B:234:PRO:HD2	1.70	0.72
1:Z:177:THR:HG22	1:Z:179:ASP:N	2.03	0.72
1:Y:221:GLU:HG2	1:Y:284:LEU:HD11	1.71	0.71
1:Z:244:LYS:HA	1:Z:247:VAL:HG23	1.70	0.71
1:Y:350:LEU:HD12	2:B:27:CYS:HB3	1.70	0.71
1:Z:17:ALA:HB2	1:Z:211:ARG:HB3	1.72	0.71
1:Z:150:ILE:HD12	1:Z:150:ILE:H	1.55	0.71
2:B:128:ILE:HD12	2:B:128:ILE:N	2.05	0.71
1:X:70:ARG:HD2	1:X:197:SER:HB3	1.71	0.71
1:X:311:CYS:SG	1:X:318:GLU:HA	2.31	0.71
1:X:265:PRO:O	1:X:267:LYS:N	2.24	0.71
1:Y:272:GLU:HG3	1:Y:273:ASN:H	1.56	0.71
1:Z:266:ASN:C	1:Z:268:TYR:H	1.97	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:282:LEU:C	1:Z:284:LEU:H	1.99	0.70
1:Y:67:MET:HE1	1:Y:83:TYR:CD2	2.26	0.70
1:Z:332:ARG:NH1	1:Z:332:ARG:HB3	2.06	0.70
2:B:217:LYS:NZ	2:B:217:LYS:HB3	2.07	0.70
2:C:146:ARG:NH1	2:C:150:ASP:OD2	2.25	0.70
1:Z:219:ASN:ND2	1:Z:222:GLN:HE21	1.90	0.70
1:Z:6:LEU:HD13	1:Z:180:MET:HB3	1.73	0.70
1:Z:197:SER:HB3	1:Z:200:LYS:HB2	1.73	0.70
2:C:205:LEU:HD12	2:C:207:PHE:HZ	1.57	0.70
1:Y:321:ILE:O	1:Y:325:VAL:HG22	1.93	0.69
2:B:25:GLU:OE2	2:B:119:MET:HE1	1.93	0.69
1:X:174:ALA:HB3	1:X:191:MET:HE3	1.74	0.69
1:Z:164:ALA:CB	1:Z:187:SER:HB2	2.23	0.69
1:Z:19:ARG:NH2	1:Z:21:ASN:HD21	1.90	0.69
1:Z:135:LYS:HD3	1:Z:137:HIS:CE1	2.27	0.69
1:X:271:PRO:O	1:X:272:GLU:O	2.11	0.69
1:Y:2:GLY:HA2	1:Y:181:ASP:OD2	1.92	0.69
1:Y:336:THR:HG23	2:B:255:ILE:O	1.93	0.69
1:Z:96:GLU:O	1:Z:99:LYS:HB2	1.92	0.69
1:Z:226:LEU:HD13	1:Z:250:ILE:HG13	1.74	0.69
1:Y:134:THR:HG22	1:Y:135:LYS:H	1.58	0.69
1:Z:220:GLN:O	1:Z:224:VAL:HG23	1.93	0.68
1:Z:255:SER:C	1:Z:257:GLU:H	2.00	0.68
2:A:7:VAL:HG12	2:A:58:ASP:OD1	1.92	0.68
1:Y:11:ALA:O	1:Y:15:PRO:HG3	1.93	0.68
1:Y:242:GLY:H	1:Y:245:ARG:HB3	1.58	0.68
1:Y:219:ASN:H	1:Y:222:GLN:NE2	1.92	0.68
1:Z:164:ALA:HB1	1:Z:187:SER:HB2	1.76	0.68
1:Z:164:ALA:HB2	1:Z:182:CYS:SG	2.34	0.68
1:Y:63:HIS:O	1:Y:64:LEU:HD23	1.94	0.67
1:Y:141:CYS:C	1:Y:143:HIS:H	2.02	0.67
2:A:2:PHE:CG	2:A:30:ILE:HG21	2.29	0.67
1:Y:264:ASP:N	1:Y:265:PRO:HD2	2.09	0.67
1:Z:355:ARG:HB3	1:Z:355:ARG:HH11	1.58	0.67
1:Y:260:VAL:HG23	1:Y:261:ARG:H	1.59	0.67
1:Z:300:GLU:CD	1:Z:301:PRO:HD2	2.19	0.67
2:A:83:GLY:N	2:A:86:ASP:OD2	2.27	0.67
1:Y:282:LEU:O	1:Y:286:PRO:HG3	1.94	0.67
2:C:141:SER:HA	2:C:225:VAL:HG12	1.77	0.67
1:Y:3:ILE:HG22	1:Y:6:LEU:HB2	1.77	0.67
2:C:226:THR:HG23	2:C:238:GLU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:GLU:O	2:C:96:ALA:HB2	1.95	0.66
2:A:233:VAL:HB	2:A:234:PRO:CD	2.25	0.66
1:Z:85:PHE:CD2	1:Z:142:LYS:HE2	2.30	0.66
1:Z:298:TRP:HE3	1:Z:298:TRP:H	1.44	0.66
1:Z:3:ILE:HG22	1:Z:6:LEU:HB2	1.77	0.66
2:B:199:MET:HE1	2:B:202:PRO:HD3	1.76	0.66
1:Z:26:TYR:O	1:Z:29:ARG:HB2	1.96	0.66
1:Z:125:LYS:C	1:Z:127:THR:H	2.04	0.66
2:B:75:MET:CA	2:B:116:MET:HE1	2.25	0.66
2:B:99:LEU:HD23	2:B:100:ALA:N	2.11	0.66
1:X:34:ASP:HB3	1:X:177:THR:HG23	1.78	0.66
1:Z:183:LEU:HD21	1:Z:190:LEU:HB3	1.78	0.66
1:X:35:ALA:O	1:X:39:ILE:HG13	1.96	0.65
1:Z:219:ASN:CG	1:Z:222:GLN:HE21	2.04	0.65
1:X:23:ILE:HG12	1:X:204:ILE:HD11	1.79	0.65
1:Y:264:ASP:H	1:Y:265:PRO:CD	2.09	0.65
1:Z:24:LYS:H	1:Z:24:LYS:HD2	1.60	0.65
1:Z:39:ILE:HA	1:Z:42:PHE:HD2	1.62	0.65
1:Z:268:TYR:N	1:Z:269:PRO:HD3	2.12	0.65
1:X:219:ASN:HD22	1:X:222:GLN:NE2	1.94	0.65
1:X:196:ALA:O	1:X:198:GLU:HG2	1.96	0.65
1:X:355:ARG:HG3	1:X:355:ARG:HH11	1.61	0.65
2:B:23:ILE:HG13	2:B:72:LEU:HD12	1.79	0.65
1:Y:200:LYS:HB3	1:Y:202:LEU:HD13	1.79	0.65
1:X:261:ARG:O	1:X:262:ARG:HB2	1.96	0.65
1:Z:264:ASP:C	1:Z:266:ASN:H	2.04	0.64
2:B:74:SER:O	2:B:78:ILE:HG13	1.97	0.64
1:X:180:MET:HE2	1:X:183:LEU:HD12	1.80	0.64
1:Z:194:LEU:C	1:Z:196:ALA:H	2.04	0.64
1:Z:249:LEU:CD2	1:Z:259:ILE:HG23	2.27	0.64
2:B:75:MET:HA	2:B:116:MET:HE1	1.79	0.64
1:Y:263:LEU:O	1:Y:263:LEU:HD12	1.98	0.64
1:Y:289:LEU:HD12	1:Y:289:LEU:O	1.97	0.64
1:Z:6:LEU:O	1:Z:10:ILE:HG13	1.98	0.64
2:B:185:THR:C	2:B:187:ASN:H	2.04	0.64
2:C:185:THR:HG23	2:C:188:VAL:HB	1.79	0.64
1:Y:137:HIS:H	1:Y:137:HIS:CD2	2.13	0.64
1:Y:264:ASP:H	1:Y:265:PRO:HD2	1.62	0.64
1:Z:327:ARG:HH11	1:Z:327:ARG:HB2	1.63	0.64
2:B:190:LYS:HG3	2:B:191:GLU:OE1	1.98	0.64
1:X:219:ASN:OD1	1:X:221:GLU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:26:TYR:OH	1:Y:206:GLU:HG3	1.98	0.63
1:Y:350:LEU:HD12	2:B:27:CYS:CB	2.29	0.63
2:A:139:MET:HE3	2:A:227:LEU:HD11	1.80	0.63
1:Z:254:LYS:H	1:Z:254:LYS:CD	1.98	0.63
1:X:238:ILE:HD13	1:X:271:PRO:HD3	1.80	0.63
1:Z:256:ILE:HD12	1:Z:276:HIS:HD2	1.64	0.63
1:Z:300:GLU:OE1	1:Z:332:ARG:HD3	1.98	0.63
2:A:160:ILE:HG21	2:A:229:MET:HE1	1.81	0.63
1:X:307:ILE:HD13	1:X:322:ARG:NH1	2.13	0.63
1:Y:304:GLU:HA	1:Y:307:ILE:HG22	1.81	0.63
1:Z:238:ILE:HD13	1:Z:241:ILE:CB	2.29	0.63
1:Z:24:LYS:HD2	1:Z:24:LYS:N	2.14	0.62
1:Z:53:LEU:H	1:Z:53:LEU:CD2	2.10	0.62
1:X:181:ASP:HA	1:X:184:THR:HG22	1.80	0.62
1:X:321:ILE:O	1:X:325:VAL:HG23	1.99	0.62
1:Z:186:GLY:O	1:Z:209:LEU:HD13	1.98	0.62
1:X:87:GLY:HA3	1:X:156:PRO:O	1.99	0.62
1:Y:162:SER:O	1:Y:165:ALA:HB3	2.00	0.62
1:Z:352:SER:OG	2:C:120:ASP:HA	2.00	0.62
1:Z:292:GLU:C	1:Z:294:VAL:H	2.05	0.62
1:X:343:PHE:CE1	2:A:233:VAL:HA	2.34	0.62
1:Y:26:TYR:HH	1:Y:206:GLU:HG3	1.64	0.62
1:Z:332:ARG:HB3	1:Z:332:ARG:CZ	2.30	0.62
2:A:5:ARG:HB3	2:A:59:THR:HB	1.82	0.62
1:Y:64:LEU:HD11	1:Y:140:GLU:HG2	1.81	0.62
1:Y:135:LYS:HD2	1:Y:135:LYS:C	2.25	0.62
1:Y:159:ALA:O	1:Y:162:SER:N	2.33	0.62
1:X:19:ARG:HD2	1:X:21:ASN:ND2	2.15	0.61
1:Z:24:LYS:HA	1:Z:77:ASN:ND2	2.14	0.61
1:Z:174:ALA:HB3	1:Z:191:MET:HE3	1.81	0.61
1:Z:3:ILE:CB	1:Z:6:LEU:HD12	2.30	0.61
1:Z:97:LEU:C	1:Z:99:LYS:N	2.59	0.61
1:Z:253:HIS:HB3	1:Z:258:GLU:O	2.01	0.61
2:C:152:SER:HA	2:C:209:LEU:HD13	1.82	0.61
1:Z:131:VAL:HA	1:Z:133:VAL:HG22	1.82	0.61
1:Z:321:ILE:O	1:Z:325:VAL:HG23	1.99	0.61
2:B:9:GLY:CA	2:B:88:ILE:HD13	2.30	0.61
2:A:139:MET:HE1	2:A:169:PHE:CZ	2.36	0.61
1:Y:300:GLU:CD	1:Y:301:PRO:HD2	2.25	0.61
1:Z:67:MET:HB3	1:Z:144:LEU:CD2	2.31	0.61
2:A:82:ALA:HB2	2:A:103:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:63:HIS:CD2	1:X:137:HIS:HB3	2.35	0.61
1:Z:256:ILE:HD12	1:Z:276:HIS:CD2	2.36	0.61
2:B:175:LEU:H	2:B:175:LEU:CD2	2.13	0.61
1:Z:267:LYS:C	1:Z:269:PRO:HD3	2.26	0.60
1:Z:301:PRO:HG3	1:Z:328:LEU:CD2	2.31	0.60
1:Z:301:PRO:HG3	1:Z:328:LEU:HD21	1.83	0.60
2:A:23:ILE:CD1	2:A:26:ALA:HB2	2.31	0.60
1:X:6:LEU:HD22	1:X:10:ILE:HD11	1.82	0.60
1:Z:296:LEU:HD22	1:Z:298:TRP:CH2	2.35	0.60
2:B:217:LYS:HB3	2:B:217:LYS:HZ3	1.65	0.60
1:X:192:ARG:O	1:X:193:HIS:HB2	2.01	0.60
1:Z:79:ILE:O	1:Z:81:PRO:HD3	2.01	0.60
2:A:185:THR:HB	2:A:194:ALA:HB1	1.84	0.60
1:Y:9:LEU:O	1:Y:13:VAL:HG13	2.00	0.60
1:Z:29:ARG:HG2	1:Z:29:ARG:HH11	1.66	0.60
2:C:205:LEU:HD12	2:C:207:PHE:CZ	2.37	0.60
1:X:37:MET:HG2	1:X:177:THR:HG22	1.82	0.60
1:Z:91:GLN:C	1:Z:92:LEU:HD22	2.26	0.60
1:X:41:GLN:HE22	1:X:196:ALA:CB	2.14	0.60
1:X:79:ILE:O	1:X:81:PRO:HD3	2.02	0.60
1:Y:330:LYS:HE2	1:Y:330:LYS:CA	2.28	0.60
1:Z:6:LEU:CD2	1:Z:10:ILE:HD11	2.32	0.59
2:B:65:ASN:O	2:B:66:LEU:HD12	2.01	0.59
1:Y:265:PRO:C	1:Y:267:LYS:H	2.07	0.59
1:Z:156:PRO:HB2	1:Z:287:GLU:O	2.02	0.59
1:Z:332:ARG:NH1	1:Z:332:ARG:CB	2.65	0.59
2:A:50:LEU:HD12	2:A:51:THR:H	1.66	0.59
1:X:340:LEU:HD22	2:A:47:LEU:CB	2.32	0.59
1:Z:226:LEU:HB2	1:Z:250:ILE:HG21	1.83	0.59
2:A:191:GLU:HG2	2:A:192:GLU:H	1.67	0.59
1:Y:134:THR:HG22	1:Y:135:LYS:N	2.17	0.59
1:Z:168:LYS:HG2	1:Z:188:PRO:HD3	1.85	0.59
1:Z:296:LEU:HB2	1:Z:298:TRP:CZ3	2.37	0.59
1:Y:218:LEU:HB2	1:Y:222:GLN:HB2	1.83	0.59
1:Y:311:CYS:SG	1:Y:318:GLU:HA	2.42	0.59
1:Y:67:MET:HE1	1:Y:145:LEU:HD11	1.84	0.59
1:X:160:GLU:HA	1:X:163:CYS:HB2	1.85	0.59
2:C:78:ILE:HD12	2:C:116:MET:HB2	1.85	0.59
1:Y:14:ALA:N	1:Y:15:PRO:HD3	2.18	0.59
1:Y:357:GLU:O	1:Y:359:GLU:N	2.35	0.59
2:B:11:ILE:O	2:B:15:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:VAL:CG1	2:B:234:PRO:HD2	2.32	0.59
1:Y:71:THR:HA	1:Y:74:MET:HE3	1.85	0.59
1:Y:270:VAL:HG13	1:Y:271:PRO:HD2	1.84	0.59
1:Z:100:ARG:HG2	1:Z:100:ARG:HH11	1.66	0.59
2:B:78:ILE:HD12	2:B:116:MET:HE3	1.84	0.59
2:A:43:SER:OG	2:A:45:VAL:HG12	2.02	0.58
2:B:47:LEU:HD12	2:B:47:LEU:C	2.28	0.58
2:C:152:SER:CA	2:C:209:LEU:HD13	2.33	0.58
1:Z:267:LYS:HE2	1:Z:267:LYS:HA	1.86	0.58
2:C:11:ILE:O	2:C:15:VAL:HG23	2.03	0.58
1:X:270:VAL:HG13	1:X:271:PRO:HD2	1.85	0.58
1:Z:218:LEU:HD12	1:Z:218:LEU:N	2.08	0.58
2:A:233:VAL:HB	2:A:234:PRO:HD2	1.83	0.58
2:C:47:LEU:HD23	2:C:48:VAL:N	2.19	0.58
1:X:343:PHE:CD1	2:A:234:PRO:HD3	2.37	0.58
1:Y:308:LYS:NZ	1:Y:308:LYS:HB3	2.19	0.58
1:X:355:ARG:CD	2:A:97:ASP:HA	2.31	0.58
1:Z:93:LYS:CB	1:Z:98:ALA:HB2	2.33	0.58
1:Z:290:ASP:O	1:Z:294:VAL:HG23	2.03	0.58
2:B:93:GLU:OE1	2:B:93:GLU:HA	2.04	0.58
1:X:156:PRO:HD3	1:X:289:LEU:CD2	2.34	0.58
1:X:247:VAL:O	1:X:251:GLN:HG2	2.04	0.58
1:X:318:GLU:O	1:X:322:ARG:HG3	2.03	0.58
1:Y:134:THR:C	1:Y:136:GLN:H	2.11	0.58
1:Y:350:LEU:HD11	2:B:67:ALA:HB1	1.85	0.58
2:A:4:ALA:HB1	2:A:57:PHE:CD2	2.38	0.58
1:X:267:LYS:C	1:X:269:PRO:HD3	2.28	0.58
1:Z:104:ARG:NH1	1:Z:106:GLU:HB2	2.19	0.58
2:A:37:LEU:C	2:A:37:LEU:HD23	2.28	0.58
1:X:162:SER:O	1:X:165:ALA:HB3	2.04	0.57
1:Y:241:ILE:HG21	1:Y:249:LEU:HD22	1.85	0.57
1:Z:35:ALA:HB3	1:Z:85:PHE:HA	1.86	0.57
2:B:139:MET:HE1	2:B:169:PHE:CZ	2.37	0.57
2:B:143:GLU:O	2:B:147:ILE:HG12	2.04	0.57
1:X:6:LEU:HD22	1:X:10:ILE:CD1	2.33	0.57
1:X:37:MET:O	1:X:37:MET:HE3	2.04	0.57
1:Z:46:VAL:HG22	1:Z:46:VAL:O	2.04	0.57
1:Z:68:PHE:HD1	1:Z:144:LEU:HD11	1.69	0.57
2:A:87:ILE:N	2:A:87:ILE:HD12	2.19	0.57
1:X:34:ASP:CB	1:X:177:THR:HG23	2.34	0.57
1:X:71:THR:HA	1:X:74:MET:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:8:GLN:O	2:A:9:GLY:C	2.48	0.57
2:A:38:GLN:HE22	2:A:126:LEU:H	1.53	0.57
2:A:56:GLY:O	2:A:244:MET:HE2	2.04	0.57
2:A:139:MET:HE1	2:A:169:PHE:HZ	1.69	0.57
1:Z:45:ALA:C	1:Z:47:ARG:H	2.13	0.57
2:A:176:GLY:HA2	2:C:117:LYS:NZ	2.20	0.57
1:Z:186:GLY:O	1:Z:187:SER:C	2.48	0.57
2:A:82:ALA:HB2	2:A:103:PHE:CE2	2.39	0.57
2:C:234:PRO:HA	2:C:253:PRO:HD3	1.87	0.57
1:X:264:ASP:O	1:X:264:ASP:CG	2.48	0.57
2:C:20:LYS:HG3	2:C:73:THR:HA	1.87	0.57
1:Y:137:HIS:H	1:Y:137:HIS:HD2	1.51	0.57
1:X:263:LEU:HG	1:X:264:ASP:H	1.69	0.56
1:Z:46:VAL:HG11	1:Z:62:SER:OG	2.06	0.56
2:B:6:LEU:HD11	2:B:244:MET:HE1	1.86	0.56
1:Y:194:LEU:HG	1:Y:194:LEU:O	2.04	0.56
1:Y:218:LEU:HB2	1:Y:222:GLN:CB	2.36	0.56
1:Y:307:ILE:HD11	1:Y:311:CYS:SG	2.46	0.56
1:Z:136:GLN:HA	1:Z:136:GLN:OE1	2.04	0.56
2:C:233:VAL:HG13	2:C:234:PRO:HD2	1.87	0.56
1:Y:2:GLY:HA2	1:Y:181:ASP:CG	2.28	0.56
1:Y:27:PHE:CD2	1:Y:78:GLY:HA3	2.41	0.56
1:Y:37:MET:SD	1:Y:177:THR:HG22	2.46	0.56
1:Y:260:VAL:HG23	1:Y:261:ARG:N	2.20	0.56
1:Y:355:ARG:NH1	2:B:120:ASP:OD1	2.38	0.56
1:Z:326:LYS:NZ	1:Z:330:LYS:HE3	2.21	0.56
1:X:30:LYS:O	1:X:172:VAL:HG22	2.06	0.56
1:X:275:LEU:N	1:X:275:LEU:HD22	2.20	0.56
1:Y:225:ASP:O	1:Y:229:LEU:HG	2.06	0.56
1:Y:355:ARG:HG3	1:Y:355:ARG:HH11	1.69	0.56
2:A:25:GLU:OE2	2:A:119:MET:HE1	2.06	0.56
2:B:185:THR:HG22	2:B:187:ASN:HB3	1.88	0.56
1:Y:26:TYR:OH	1:Y:204:ILE:HD11	2.05	0.56
1:Y:322:ARG:O	1:Y:325:VAL:HG23	2.06	0.56
1:X:181:ASP:HA	1:X:184:THR:CG2	2.35	0.56
1:Y:141:CYS:C	1:Y:143:HIS:N	2.63	0.56
1:Y:6:LEU:HD22	1:Y:10:ILE:HD11	1.87	0.56
1:Y:268:TYR:N	1:Y:269:PRO:HD3	2.20	0.56
2:A:30:ILE:N	2:A:30:ILE:HD12	2.20	0.56
2:C:30:ILE:HG22	2:C:31:SER:H	1.70	0.56
1:X:6:LEU:O	1:X:10:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:180:MET:C	1:X:182:CYS:H	2.13	0.55
1:Z:180:MET:C	1:Z:182:CYS:H	2.14	0.55
2:C:135:CYS:SG	2:C:203:VAL:HG13	2.46	0.55
1:Y:71:THR:O	1:Y:75:MET:HG2	2.07	0.55
1:Y:275:LEU:HD22	1:Y:275:LEU:N	2.21	0.55
2:A:218:ALA:HB2	2:A:249:TYR:OH	2.07	0.55
1:X:300:GLU:CD	1:X:300:GLU:H	2.14	0.55
1:Y:199:ALA:O	1:Y:201:LYS:N	2.38	0.55
1:Z:24:LYS:H	1:Z:24:LYS:CD	2.20	0.55
1:Z:93:LYS:HA	1:Z:97:LEU:HB3	1.87	0.55
1:Z:282:LEU:O	1:Z:284:LEU:N	2.39	0.55
1:Z:22:ASP:OD2	1:Z:24:LYS:HB2	2.06	0.55
1:Z:29:ARG:HH22	1:Z:341:ASP:HB2	1.71	0.55
1:X:151:PRO:HG3	1:X:297:LYS:O	2.07	0.55
1:X:267:LYS:O	1:X:269:PRO:HD3	2.07	0.55
1:Y:264:ASP:N	1:Y:265:PRO:CD	2.66	0.55
1:Z:48:GLN:C	1:Z:50:GLY:H	2.14	0.55
1:Z:355:ARG:HB3	1:Z:355:ARG:NH1	2.22	0.55
2:B:6:LEU:HD23	2:B:12:LEU:CD2	2.37	0.55
2:B:241:ILE:O	2:B:242:ALA:C	2.49	0.55
1:X:156:PRO:HD3	1:X:289:LEU:HD23	1.89	0.55
1:X:164:ALA:HB2	1:X:187:SER:HB2	1.88	0.55
1:Z:156:PRO:CB	1:Z:287:GLU:HG2	2.36	0.55
1:Z:265:PRO:C	1:Z:267:LYS:H	2.14	0.55
1:Z:344:PHE:CZ	2:C:128:ILE:HG23	2.42	0.55
2:A:65:ASN:N	2:A:65:ASN:HD22	2.04	0.55
2:B:218:ALA:O	2:B:221:LEU:HB2	2.07	0.55
1:X:261:ARG:O	1:X:262:ARG:CB	2.54	0.54
1:Y:14:ALA:HB1	1:Y:215:GLU:HG3	1.89	0.54
1:Z:85:PHE:CE2	1:Z:142:LYS:HE2	2.42	0.54
1:X:71:THR:O	1:X:75:MET:HG2	2.05	0.54
2:B:40:MET:HE3	2:B:44:HIS:ND1	2.21	0.54
2:B:75:MET:CG	2:B:116:MET:HE1	2.37	0.54
2:B:231:ALA:O	2:B:233:VAL:HG23	2.06	0.54
1:Z:37:MET:HG3	1:Z:177:THR:HG23	1.90	0.54
1:Z:70:ARG:NH1	1:Z:196:ALA:O	2.39	0.54
1:Z:255:SER:O	1:Z:257:GLU:N	2.40	0.54
1:Z:327:ARG:HB2	1:Z:327:ARG:NH1	2.20	0.54
2:B:11:ILE:CD1	2:B:244:MET:HE3	2.37	0.54
1:Y:258:GLU:OE1	1:Y:262:ARG:NH2	2.41	0.54
1:Z:249:LEU:HD21	1:Z:259:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:94:ASP:O	2:A:96:ALA:N	2.37	0.54
2:B:109:GLU:HA	2:C:183:SER:OG	2.07	0.54
1:Z:246:ALA:O	1:Z:250:ILE:HG12	2.08	0.54
1:Z:332:ARG:CB	1:Z:332:ARG:HH11	2.21	0.54
1:Y:33:ILE:HG22	1:Y:34:ASP:N	2.22	0.54
1:Y:69:TYR:O	1:Y:72:ILE:HB	2.08	0.54
1:Z:71:THR:HA	1:Z:74:MET:HE3	1.90	0.54
1:Z:329:SER:C	1:Z:331:SER:H	2.16	0.54
1:X:164:ALA:CB	1:X:187:SER:HB2	2.37	0.54
2:A:91:ARG:NH1	2:A:93:GLU:OE2	2.41	0.54
1:X:219:ASN:ND2	1:X:222:GLN:NE2	2.55	0.54
1:Y:302:ASN:HD22	1:Y:302:ASN:C	2.14	0.54
1:Z:3:ILE:O	1:Z:6:LEU:HB2	2.07	0.54
1:Z:244:LYS:HA	1:Z:247:VAL:CG2	2.37	0.54
2:A:16:LEU:HD13	2:A:79:LEU:CD1	2.37	0.54
1:Y:275:LEU:C	1:Y:277:LYS:H	2.14	0.54
1:Y:308:LYS:HB3	1:Y:308:LYS:HZ3	1.73	0.54
1:Z:299:SER:O	1:Z:332:ARG:NH2	2.40	0.54
2:A:176:GLY:HA2	2:C:117:LYS:HZ3	1.73	0.54
2:B:33:SER:O	2:B:54:SER:HB3	2.08	0.54
1:Z:266:ASN:C	1:Z:268:TYR:N	2.62	0.54
2:B:27:CYS:HA	2:B:68:MET:O	2.08	0.54
2:C:51:THR:O	2:C:245:GLY:HA3	2.08	0.54
2:C:160:ILE:O	2:C:204:GLN:HA	2.08	0.54
1:X:39:ILE:O	1:X:42:PHE:HB2	2.07	0.53
1:X:302:ASN:OD1	1:X:305:GLU:HG2	2.08	0.53
1:Y:263:LEU:HD12	1:Y:263:LEU:C	2.33	0.53
1:Z:17:ALA:CB	1:Z:211:ARG:HB3	2.38	0.53
1:Z:47:ARG:HB2	1:Z:128:LYS:HE2	1.89	0.53
1:Z:169:ALA:C	1:Z:171:LYS:H	2.16	0.53
1:X:6:LEU:HD22	1:X:10:ILE:HG13	1.90	0.53
1:X:8:LYS:O	1:X:11:ALA:HB3	2.08	0.53
1:Y:27:PHE:O	1:Y:339:ARG:HD2	2.07	0.53
2:B:190:LYS:O	2:B:191:GLU:HB2	2.07	0.53
1:Z:177:THR:CG2	1:Z:179:ASP:H	2.20	0.53
2:A:28:TRP:O	2:A:67:ALA:HA	2.07	0.53
2:C:106:PRO:C	2:C:108:GLN:H	2.15	0.53
2:A:238:GLU:HB2	2:A:248:LYS:HG2	1.89	0.53
1:Z:23:ILE:CD1	1:Z:73:ARG:NH1	2.72	0.53
1:Z:251:GLN:O	1:Z:252:LYS:HD3	2.08	0.53
2:B:193:GLU:O	2:B:194:ALA:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:LEU:HD23	2:C:175:LEU:N	2.20	0.53
1:X:70:ARG:NE	1:X:70:ARG:HA	2.24	0.53
1:X:339:ARG:C	1:X:341:ASP:H	2.16	0.53
1:Z:346:VAL:HG12	1:Z:348:GLY:H	1.74	0.53
2:A:147:ILE:HD12	2:A:180:ILE:HG21	1.89	0.53
2:C:23:ILE:CD1	2:C:48:VAL:HG21	2.39	0.53
2:B:68:MET:HE1	2:B:92:ALA:HB2	1.91	0.53
1:Z:218:LEU:HA	1:Z:222:GLN:NE2	2.23	0.53
2:B:23:ILE:HG13	2:B:72:LEU:CD1	2.38	0.53
1:Z:294:VAL:HG12	1:Z:294:VAL:O	2.07	0.53
1:X:265:PRO:O	1:X:266:ASN:C	2.52	0.53
1:Y:74:MET:O	1:Y:79:ILE:HB	2.08	0.53
1:Y:177:THR:HG22	1:Y:178:GLU:N	2.23	0.53
1:Z:70:ARG:HG3	1:Z:70:ARG:HH11	1.74	0.53
1:Z:296:LEU:HD12	1:Z:296:LEU:O	2.08	0.53
2:A:71:ASN:HB2	2:A:119:MET:HE3	1.90	0.53
2:B:154:ILE:O	2:B:173:GLY:HA3	2.09	0.53
2:C:212:LEU:C	2:C:214:PHE:H	2.16	0.53
2:C:241:ILE:O	2:C:242:ALA:C	2.52	0.53
2:A:140:PRO:HG3	2:A:193:GLU:HB3	1.91	0.52
2:B:199:MET:HE1	2:B:202:PRO:CD	2.38	0.52
1:X:320:ARG:NH1	1:X:320:ARG:HB2	2.23	0.52
1:Y:88:LYS:HG3	1:Y:88:LYS:O	2.10	0.52
1:Z:235:CYS:SG	1:Z:236:GLU:N	2.83	0.52
2:C:76:SER:O	2:C:80:LYS:HG3	2.10	0.52
1:X:27:PHE:CE2	1:X:342:ASP:HB3	2.45	0.52
1:Y:27:PHE:CD1	1:Y:27:PHE:C	2.86	0.52
1:Z:292:GLU:HA	1:Z:292:GLU:OE2	2.09	0.52
2:B:68:MET:HE2	2:B:118:LEU:HD21	1.90	0.52
2:B:206:THR:HB	2:B:254:LYS:HB2	1.91	0.52
1:X:339:ARG:C	1:X:341:ASP:N	2.66	0.52
1:Y:273:ASN:O	1:Y:275:LEU:HD22	2.09	0.52
1:Z:49:GLY:H	1:Z:125:LYS:CD	2.17	0.52
2:B:40:MET:HE3	2:B:44:HIS:CG	2.44	0.52
2:C:188:VAL:HG12	2:C:188:VAL:O	2.10	0.52
1:Z:34:ASP:CG	1:Z:37:MET:HB2	2.34	0.52
2:B:2:PHE:CD1	2:B:30:ILE:HG21	2.44	0.52
2:C:43:SER:O	2:C:44:HIS:HB2	2.08	0.52
2:C:199:MET:HG2	2:C:200:ASN:N	2.25	0.52
1:X:219:ASN:O	1:X:220:GLN:C	2.51	0.52
1:Y:181:ASP:O	1:Y:184:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:209:LEU:HD23	1:Z:209:LEU:C	2.35	0.52
1:Z:292:GLU:C	1:Z:294:VAL:N	2.66	0.52
1:Z:282:LEU:C	1:Z:284:LEU:N	2.66	0.52
1:X:263:LEU:HD11	1:X:268:TYR:CE1	2.45	0.51
1:Y:220:GLN:O	1:Y:223:PHE:HB3	2.09	0.51
2:A:23:ILE:HG13	2:A:23:ILE:O	2.06	0.51
2:C:135:CYS:SG	2:C:199:MET:HG3	2.50	0.51
2:A:185:THR:O	2:A:186:SER:HB2	2.10	0.51
2:A:207:PHE:CZ	2:A:235:LEU:HB2	2.45	0.51
1:Y:65:MET:O	1:Y:68:PHE:HB3	2.09	0.51
1:Z:49:GLY:N	1:Z:125:LYS:HD3	2.19	0.51
1:Z:225:ASP:OD1	1:Z:256:ILE:HG12	2.10	0.51
1:Z:255:SER:C	1:Z:257:GLU:N	2.66	0.51
2:A:1:MET:HE1	2:A:61:ARG:NH1	2.26	0.51
2:B:87:ILE:HB	2:B:104:GLU:HB2	1.91	0.51
2:C:30:ILE:O	2:C:31:SER:HB3	2.09	0.51
2:A:178:GLY:HA3	2:C:114:TYR:CD1	2.45	0.51
2:B:78:ILE:CD1	2:B:116:MET:HB2	2.40	0.51
1:X:27:PHE:CD1	1:X:27:PHE:C	2.88	0.51
1:Y:3:ILE:HD12	1:Y:3:ILE:N	2.25	0.51
2:A:185:THR:CB	2:A:194:ALA:HB1	2.41	0.51
1:X:6:LEU:HD22	1:X:10:ILE:CG1	2.41	0.51
2:A:53:ARG:NH1	2:A:245:GLY:HA2	2.26	0.51
1:X:2:GLY:HA2	1:X:179:ASP:OD1	2.09	0.51
1:Z:96:GLU:HB2	1:Z:233:ASP:HB2	1.93	0.51
2:A:175:LEU:CD2	2:A:175:LEU:N	2.69	0.51
2:B:207:PHE:CZ	2:B:235:LEU:HB2	2.46	0.51
1:X:270:VAL:HG12	1:X:271:PRO:O	2.11	0.51
1:Z:48:GLN:O	1:Z:50:GLY:N	2.44	0.51
1:Z:191:MET:HA	1:Z:205:GLN:O	2.11	0.51
2:B:192:GLU:C	2:B:194:ALA:H	2.18	0.51
1:Z:174:ALA:HB1	1:Z:189:VAL:HG12	1.93	0.51
2:C:99:LEU:HB2	2:C:118:LEU:HD21	1.93	0.51
2:C:121:LEU:HD12	2:C:122:ASP:H	1.75	0.51
1:X:195:THR:C	1:X:197:SER:H	2.19	0.51
1:Y:199:ALA:O	1:Y:200:LYS:C	2.54	0.51
1:Y:355:ARG:NH1	2:B:120:ASP:CG	2.67	0.51
1:Z:217:GLY:O	1:Z:218:LEU:O	2.29	0.51
1:Z:238:ILE:HG12	1:Z:239:ARG:N	2.26	0.51
1:Z:326:LYS:HZ3	1:Z:330:LYS:HE3	1.75	0.51
1:Y:209:LEU:HD21	1:Y:220:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:27:PHE:CE2	1:Z:339:ARG:HD3	2.45	0.50
1:Z:236:GLU:HB2	1:Z:274:TRP:CD1	2.46	0.50
1:Y:303:GLU:O	1:Y:307:ILE:HG22	2.11	0.50
2:A:205:LEU:HD12	2:A:205:LEU:N	2.26	0.50
2:B:51:THR:O	2:B:52:LEU:HD23	2.12	0.50
1:Z:22:ASP:OD2	1:Z:24:LYS:N	2.44	0.50
1:Z:219:ASN:OD1	1:Z:222:GLN:HG3	2.10	0.50
1:Z:302:ASN:HB3	1:Z:305:GLU:HB3	1.93	0.50
2:A:222:SER:HB2	2:A:240:LYS:O	2.11	0.50
2:B:140:PRO:HB2	2:B:143:GLU:CB	2.41	0.50
1:Y:275:LEU:HD22	1:Y:275:LEU:H	1.77	0.50
2:A:145:ALA:HA	2:A:216:THR:HG21	1.93	0.50
2:B:199:MET:HG3	2:B:199:MET:O	2.10	0.50
1:Y:215:GLU:C	1:Y:217:GLY:H	2.19	0.50
1:Y:61:THR:HG22	1:Y:61:THR:O	2.12	0.50
1:Z:66:GLY:O	1:Z:70:ARG:HG2	2.12	0.50
1:Y:275:LEU:C	1:Y:277:LYS:N	2.66	0.50
2:B:101:LEU:HD12	2:B:101:LEU:N	2.27	0.50
2:C:185:THR:HB	2:C:195:VAL:H	1.77	0.50
1:Z:296:LEU:HD13	1:Z:298:TRP:CZ3	2.39	0.50
1:Y:321:ILE:O	1:Y:321:ILE:HG22	2.11	0.50
1:Z:99:LYS:HD2	1:Z:102:GLU:HB2	1.93	0.50
2:B:83:GLY:O	2:B:85:GLU:N	2.45	0.50
2:C:54:SER:HB2	2:C:60:TYR:HD2	1.74	0.50
1:Y:134:THR:CG2	1:Y:135:LYS:H	2.21	0.49
1:Z:183:LEU:HD21	1:Z:190:LEU:CB	2.41	0.49
1:Z:222:GLN:O	1:Z:225:ASP:HB2	2.13	0.49
2:A:135:CYS:SG	2:A:162:CYS:HB3	2.51	0.49
2:A:11:ILE:O	2:A:15:VAL:HG23	2.12	0.49
2:A:23:ILE:HD11	2:A:26:ALA:HB2	1.94	0.49
2:B:199:MET:HE3	2:B:200:ASN:C	2.37	0.49
2:B:200:ASN:HB3	2:B:201:GLU:OE2	2.12	0.49
1:X:167:VAL:HA	1:X:172:VAL:HG12	1.95	0.49
1:X:256:ILE:O	1:X:260:VAL:HG23	2.11	0.49
1:Z:7:ALA:HA	1:Z:180:MET:HE2	1.93	0.49
1:Z:189:VAL:HG22	1:Z:208:HIS:HD1	1.76	0.49
2:A:47:LEU:HD13	2:A:126:LEU:HD12	1.93	0.49
1:X:220:GLN:O	1:X:224:VAL:HG23	2.12	0.49
1:Y:339:ARG:NH2	1:Y:341:ASP:OD2	2.43	0.49
1:Z:29:ARG:NH2	1:Z:341:ASP:OD2	2.46	0.49
1:Z:156:PRO:HB3	1:Z:287:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:168:LYS:HG3	2:A:181:LYS:HG3	1.95	0.49
2:B:23:ILE:HD13	2:B:48:VAL:HG21	1.94	0.49
2:C:47:LEU:HD23	2:C:47:LEU:C	2.38	0.49
1:X:4:GLN:HB2	1:X:231:GLY:HA3	1.94	0.49
1:X:30:LYS:HA	1:X:80:LYS:O	2.12	0.49
1:X:192:ARG:O	1:X:193:HIS:CB	2.60	0.49
1:Z:135:LYS:HG3	1:Z:136:GLN:N	2.27	0.49
1:Z:346:VAL:HA	2:C:126:LEU:HD23	1.95	0.49
1:X:94:SER:C	1:X:96:GLU:H	2.20	0.49
1:X:140:GLU:O	1:X:143:HIS:HB3	2.12	0.49
1:Y:26:TYR:CZ	1:Y:204:ILE:HG12	2.48	0.49
1:Y:330:LYS:HA	1:Y:330:LYS:CE	2.32	0.49
1:Z:174:ALA:CB	1:Z:189:VAL:HG12	2.43	0.49
1:Z:343:PHE:HE1	2:C:232:ASP:O	1.96	0.49
2:B:68:MET:CE	2:B:92:ALA:HB2	2.43	0.49
1:Y:63:HIS:C	1:Y:64:LEU:HD23	2.38	0.49
2:C:101:LEU:N	2:C:101:LEU:HD12	2.28	0.49
1:X:301:PRO:HG2	1:X:328:LEU:HG	1.95	0.49
1:Z:29:ARG:HG2	1:Z:29:ARG:NH1	2.27	0.49
2:B:68:MET:HE3	2:B:92:ALA:CB	2.43	0.49
2:B:205:LEU:HD21	2:B:232:ASP:H	1.78	0.49
1:X:63:HIS:HD2	1:X:137:HIS:HB3	1.76	0.49
1:Z:19:ARG:CZ	1:Z:21:ASN:HD21	2.26	0.49
2:B:37:LEU:HD23	2:B:37:LEU:C	2.38	0.49
1:X:237:SER:O	1:X:271:PRO:HG3	2.13	0.49
1:Z:251:GLN:HB3	1:Z:252:LYS:NZ	2.28	0.49
1:Z:272:GLU:O	1:Z:273:ASN:C	2.56	0.49
2:A:200:ASN:HB3	2:A:201:GLU:OE2	2.12	0.49
2:B:106:PRO:C	2:B:108:GLN:H	2.21	0.49
2:B:185:THR:C	2:B:187:ASN:N	2.70	0.49
1:Y:221:GLU:HA	1:Y:224:VAL:HG23	1.95	0.48
1:Z:73:ARG:HD3	1:Z:198:GLU:CB	2.43	0.48
1:Z:130:LEU:C	1:Z:130:LEU:HD23	2.38	0.48
2:A:134:SER:HB2	2:A:201:GLU:HB2	1.94	0.48
2:C:98:THR:HA	2:C:118:LEU:HG	1.95	0.48
1:X:272:GLU:OE1	1:X:272:GLU:HA	2.13	0.48
1:Z:162:SER:O	1:Z:165:ALA:HB3	2.13	0.48
1:Z:209:LEU:O	1:Z:212:ILE:HB	2.12	0.48
1:Z:249:LEU:HD23	1:Z:249:LEU:O	2.13	0.48
2:B:140:PRO:HB2	2:B:143:GLU:HB3	1.93	0.48
2:C:203:VAL:HG21	2:C:229:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:67:MET:CE	1:Y:145:LEU:HD21	2.44	0.48
2:C:103:PHE:HB2	2:C:112:SER:HB2	1.95	0.48
1:X:280:HIS:CE1	1:X:284:LEU:HD22	2.48	0.48
1:Z:292:GLU:O	1:Z:294:VAL:N	2.46	0.48
2:A:56:GLY:HA3	2:A:244:MET:HG3	1.96	0.48
1:X:12:ASP:O	1:X:14:ALA:N	2.46	0.48
1:X:321:ILE:HD12	1:X:321:ILE:N	2.29	0.48
2:A:241:ILE:O	2:A:241:ILE:HG22	2.14	0.48
1:Y:10:ILE:HG22	1:Y:18:ILE:HD11	1.95	0.48
1:Y:167:VAL:HG12	1:Y:188:PRO:CG	2.44	0.48
1:Z:290:ASP:OD1	1:Z:292:GLU:HG2	2.13	0.48
2:A:1:MET:SD	2:A:1:MET:C	2.97	0.48
2:B:187:ASN:OD1	2:B:190:LYS:HD3	2.14	0.48
1:X:355:ARG:HG3	1:X:355:ARG:NH1	2.28	0.48
1:Z:8:LYS:O	1:Z:11:ALA:HB3	2.13	0.48
1:Z:97:LEU:O	1:Z:98:ALA:HB3	2.14	0.48
1:Z:275:LEU:N	1:Z:275:LEU:HD22	2.28	0.48
1:Z:192:ARG:NE	1:Z:205:GLN:OE1	2.46	0.48
2:B:56:GLY:HA3	2:B:244:MET:HB2	1.96	0.48
1:X:18:ILE:HG12	1:X:207:PHE:CE1	2.48	0.47
1:X:224:VAL:O	1:X:228:ILE:HG13	2.14	0.47
1:Y:80:LYS:HB3	1:Y:298:TRP:CE2	2.49	0.47
1:Y:245:ARG:HG2	1:Y:245:ARG:HH11	1.78	0.47
1:Z:22:ASP:OD1	1:Z:24:LYS:HD3	2.14	0.47
2:C:149:ARG:O	2:C:152:SER:OG	2.29	0.47
1:X:275:LEU:HB3	1:X:278:GLU:HB2	1.96	0.47
1:Z:3:ILE:CG2	1:Z:6:LEU:HD12	2.43	0.47
2:C:41:ASP:OD2	2:C:43:SER:OG	2.29	0.47
2:C:88:ILE:HG23	2:C:103:PHE:CE1	2.49	0.47
1:Y:167:VAL:HG12	1:Y:188:PRO:HG2	1.97	0.47
1:Y:316:PHE:HD2	1:Y:317:SER:H	1.61	0.47
1:Z:169:ALA:O	1:Z:171:LYS:N	2.47	0.47
1:Z:329:SER:HA	1:Z:332:ARG:HG3	1.96	0.47
2:A:13:LYS:HE3	2:A:79:LEU:O	2.14	0.47
2:A:113:ASP:OD2	2:B:179:ASN:ND2	2.47	0.47
2:B:78:ILE:HD12	2:B:116:MET:HB2	1.96	0.47
1:X:180:MET:HE2	1:X:183:LEU:CD1	2.44	0.47
1:X:350:LEU:HD23	2:A:27:CYS:HB3	1.95	0.47
1:Y:135:LYS:HA	1:Y:138:ASN:HB3	1.96	0.47
1:Z:143:HIS:O	1:Z:147:LEU:HG	2.13	0.47
1:Z:164:ALA:O	1:Z:168:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:221:GLU:CD	1:X:284:LEU:HD21	2.40	0.47
1:X:310:MET:O	1:X:314:LYS:O	2.31	0.47
1:Y:24:LYS:HA	1:Y:77:ASN:HD22	1.79	0.47
1:Y:30:LYS:C	1:Y:172:VAL:HG22	2.38	0.47
1:Z:138:ASN:O	1:Z:142:LYS:HG3	2.14	0.47
1:Z:303:GLU:HG3	1:Z:304:GLU:N	2.29	0.47
1:Z:332:ARG:HH11	1:Z:332:ARG:HB2	1.78	0.47
2:B:20:LYS:HG3	2:B:21:ASP:N	2.29	0.47
1:X:298:TRP:CE3	1:X:298:TRP:N	2.82	0.47
1:Y:202:LEU:N	1:Y:202:LEU:HD12	2.29	0.47
1:Z:192:ARG:O	1:Z:193:HIS:HB2	2.14	0.47
1:Z:329:SER:C	1:Z:331:SER:N	2.71	0.47
2:A:85:GLU:HB3	2:A:106:PRO:HG2	1.96	0.47
1:X:180:MET:C	1:X:182:CYS:N	2.72	0.47
1:X:195:THR:O	1:X:197:SER:N	2.48	0.47
1:X:219:ASN:HD21	1:X:222:GLN:HG3	1.78	0.47
1:Y:175:ALA:O	1:Y:190:LEU:HD12	2.14	0.47
1:Y:251:GLN:O	1:Y:254:LYS:NZ	2.43	0.47
1:Z:104:ARG:HH11	1:Z:107:ALA:HB2	1.79	0.47
1:Z:174:ALA:HB3	1:Z:191:MET:HE2	1.92	0.47
1:Z:244:LYS:C	1:Z:246:ALA:H	2.22	0.47
2:C:216:THR:C	2:C:218:ALA:H	2.23	0.47
1:X:280:HIS:HE1	1:X:284:LEU:HD22	1.80	0.47
1:Z:181:ASP:HA	1:Z:184:THR:HG23	1.97	0.47
2:A:191:GLU:HG2	2:A:192:GLU:N	2.30	0.47
2:B:16:LEU:HG	2:B:75:MET:HB3	1.96	0.47
1:Y:30:LYS:HA	1:Y:80:LYS:O	2.14	0.47
1:Z:127:THR:O	1:Z:131:VAL:HG23	2.14	0.47
2:B:238:GLU:HG3	2:B:248:LYS:HG2	1.97	0.47
2:C:175:LEU:HG	2:C:175:LEU:O	2.15	0.47
1:X:218:LEU:HD22	1:X:222:GLN:HB3	1.97	0.47
1:X:225:ASP:OD1	1:X:280:HIS:HD2	1.97	0.47
2:B:148:CYS:O	2:B:152:SER:HB3	2.14	0.47
2:C:152:SER:N	2:C:209:LEU:HD13	2.30	0.47
1:X:331:SER:O	1:X:332:ARG:C	2.58	0.46
1:Y:338:GLY:O	2:B:45:VAL:HG12	2.15	0.46
1:Z:253:HIS:N	1:Z:254:LYS:HD3	2.30	0.46
1:Z:253:HIS:O	1:Z:255:SER:N	2.48	0.46
2:A:1:MET:HA	2:A:92:ALA:O	2.14	0.46
2:C:38:GLN:O	2:C:39:SER:HB2	2.15	0.46
1:X:76:GLU:OE2	1:X:327:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:137:HIS:O	1:X:140:GLU:N	2.49	0.46
1:X:340:LEU:CD2	2:A:47:LEU:HB3	2.43	0.46
1:Y:352:SER:HA	2:B:67:ALA:O	2.14	0.46
1:Z:35:ALA:HB3	1:Z:85:PHE:CA	2.45	0.46
1:Z:131:VAL:HG12	1:Z:131:VAL:O	2.15	0.46
1:Z:264:ASP:O	1:Z:266:ASN:N	2.49	0.46
1:X:75:MET:HE3	1:X:75:MET:HA	1.97	0.46
1:Z:3:ILE:HG22	1:Z:3:ILE:O	2.15	0.46
1:Z:320:ARG:O	1:Z:324:GLY:N	2.48	0.46
1:Y:64:LEU:HA	1:Y:67:MET:HB2	1.96	0.46
1:X:258:GLU:O	1:X:261:ARG:O	2.34	0.46
1:Y:71:THR:HG21	1:Y:150:ILE:CD1	2.36	0.46
1:Y:298:TRP:HE3	1:Y:298:TRP:H	1.64	0.46
2:B:211:TYR:O	2:B:214:PHE:HB2	2.15	0.46
1:X:137:HIS:O	1:X:138:ASN:C	2.57	0.46
1:X:352:SER:HB3	2:A:121:LEU:H	1.81	0.46
1:Y:3:ILE:N	1:Y:3:ILE:CD1	2.79	0.46
1:Y:26:TYR:HH	1:Y:206:GLU:CG	2.29	0.46
1:Z:155:ALA:HB1	1:Z:162:SER:OG	2.15	0.46
1:Z:257:GLU:C	1:Z:259:ILE:H	2.22	0.46
1:Z:291:PRO:O	1:Z:294:VAL:HB	2.16	0.46
1:Z:292:GLU:OE2	1:Z:292:GLU:CA	2.64	0.46
2:B:175:LEU:HD23	2:B:175:LEU:N	2.19	0.46
2:B:212:LEU:HA	2:B:215:PHE:CD2	2.51	0.46
2:B:219:THR:C	2:B:221:LEU:H	2.24	0.46
2:C:56:GLY:HA3	2:C:244:MET:HB2	1.96	0.46
2:C:65:ASN:N	2:C:65:ASN:HD22	2.14	0.46
1:X:218:LEU:HD23	1:X:222:GLN:OE1	2.15	0.46
1:X:219:ASN:ND2	1:X:222:GLN:HG3	2.31	0.46
1:X:241:ILE:HD13	1:X:249:LEU:CD1	2.45	0.46
2:B:65:ASN:N	2:B:65:ASN:HD22	2.13	0.46
2:C:78:ILE:CD1	2:C:116:MET:HB2	2.44	0.46
1:Y:63:HIS:CD2	1:Y:137:HIS:HB2	2.50	0.46
1:Y:74:MET:HE1	1:Y:83:TYR:OH	2.16	0.46
1:Y:239:ARG:HG3	1:Y:239:ARG:HH11	1.80	0.46
1:Z:10:ILE:HD13	1:Z:212:ILE:CD1	2.46	0.46
1:Z:252:LYS:O	1:Z:253:HIS:HB2	2.16	0.46
2:A:101:LEU:N	2:A:101:LEU:CD1	2.74	0.46
2:A:135:CYS:SG	2:A:162:CYS:SG	3.12	0.46
2:C:165:ASP:CG	2:C:166:GLY:N	2.73	0.46
1:X:243:PRO:O	1:X:246:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:219:ASN:CB	1:Y:222:GLN:HE21	2.29	0.46
1:Z:194:LEU:C	1:Z:196:ALA:N	2.71	0.46
1:Z:285:GLU:N	1:Z:286:PRO:CD	2.79	0.46
2:C:187:ASN:C	2:C:189:ASP:H	2.24	0.46
1:X:184:THR:HB	1:X:227:CYS:SG	2.56	0.45
1:Y:238:ILE:HG23	1:Y:241:ILE:CD1	2.35	0.45
1:Z:147:LEU:HA	1:Z:302:ASN:HD22	1.80	0.45
1:Z:235:CYS:HG	1:Z:236:GLU:N	2.13	0.45
1:Z:320:ARG:HA	1:Z:323:SER:HB3	1.98	0.45
2:B:6:LEU:CD1	2:B:244:MET:HE1	2.46	0.45
2:C:14:LYS:O	2:C:15:VAL:C	2.59	0.45
1:X:314:LYS:O	1:X:315:GLN:C	2.59	0.45
1:Y:6:LEU:HD22	1:Y:10:ILE:CD1	2.47	0.45
1:Y:337:GLN:OE1	2:B:254:LYS:HE2	2.17	0.45
2:B:68:MET:HE1	2:B:99:LEU:HG	1.98	0.45
2:C:12:LEU:HD12	2:C:12:LEU:HA	1.76	0.45
2:C:216:THR:C	2:C:218:ALA:N	2.74	0.45
1:X:31:VAL:HA	1:X:172:VAL:HG22	1.97	0.45
1:Y:3:ILE:HG12	1:Y:227:CYS:HB3	1.97	0.45
1:Y:139:ASP:C	1:Y:141:CYS:H	2.25	0.45
1:Y:167:VAL:HG12	1:Y:188:PRO:HD2	1.98	0.45
1:Y:200:LYS:C	1:Y:202:LEU:H	2.24	0.45
1:Y:302:ASN:C	1:Y:302:ASN:ND2	2.74	0.45
1:Y:350:LEU:CD1	2:B:67:ALA:HB1	2.46	0.45
1:Z:197:SER:O	1:Z:198:GLU:C	2.59	0.45
2:B:31:SER:OG	2:B:33:SER:HB3	2.17	0.45
2:C:11:ILE:CD1	2:C:244:MET:HE3	2.46	0.45
2:C:233:VAL:CG1	2:C:234:PRO:HD2	2.45	0.45
1:X:18:ILE:HG22	1:X:19:ARG:N	2.31	0.45
1:Y:91:GLN:HA	1:Y:91:GLN:OE1	2.16	0.45
1:Y:180:MET:O	1:Y:181:ASP:C	2.60	0.45
1:Z:155:ALA:HA	1:Z:289:LEU:HD23	1.99	0.45
1:X:350:LEU:HD23	2:A:27:CYS:CB	2.47	0.45
1:Z:84:VAL:HG12	1:Z:159:ALA:HB1	1.98	0.45
1:Z:264:ASP:C	1:Z:266:ASN:N	2.74	0.45
2:B:225:VAL:HG22	2:B:226:THR:N	2.30	0.45
1:X:80:LYS:HB3	1:X:298:TRP:CE2	2.52	0.45
1:X:83:TYR:O	1:X:152:TYR:HA	2.17	0.45
1:X:263:LEU:CG	1:X:264:ASP:H	2.26	0.45
1:Y:352:SER:OG	2:B:120:ASP:HA	2.17	0.45
1:Y:355:ARG:HD2	2:B:97:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:153:LEU:HD21	1:Z:294:VAL:HG13	1.98	0.45
1:Z:252:LYS:O	1:Z:253:HIS:CB	2.64	0.45
1:Z:270:VAL:HG13	1:Z:274:TRP:CE3	2.51	0.45
2:A:172:SER:HB2	2:A:177:ASN:HB3	1.98	0.45
1:X:275:LEU:HA	1:X:278:GLU:OE2	2.16	0.45
1:Y:37:MET:HE1	1:Y:179:ASP:OD2	2.17	0.45
1:Y:139:ASP:C	1:Y:141:CYS:N	2.73	0.45
1:Z:249:LEU:HD22	1:Z:259:ILE:HG23	1.98	0.45
2:A:40:MET:HG3	2:A:47:LEU:HD12	1.97	0.45
1:Y:35:ALA:HB3	1:Y:84:VAL:O	2.17	0.45
1:Y:62:SER:C	1:Y:64:LEU:N	2.75	0.45
1:Z:104:ARG:CZ	1:Z:106:GLU:HB2	2.46	0.45
1:Z:167:VAL:HG12	1:Z:188:PRO:HG2	1.99	0.45
1:X:23:ILE:HG12	1:X:204:ILE:CD1	2.45	0.45
1:X:335:SER:C	1:X:337:GLN:N	2.73	0.45
1:Y:166:LEU:O	1:Y:169:ALA:N	2.50	0.45
1:Z:130:LEU:HD23	1:Z:130:LEU:O	2.16	0.45
2:A:169:PHE:N	2:A:169:PHE:CD1	2.85	0.45
2:C:185:THR:CB	2:C:195:VAL:H	2.29	0.45
1:Y:204:ILE:HD12	1:Y:205:GLN:N	2.32	0.44
1:Z:23:ILE:HG23	1:Z:204:ILE:CD1	2.43	0.44
1:Z:219:ASN:ND2	1:Z:222:GLN:NE2	2.61	0.44
2:B:25:GLU:HA	2:B:72:LEU:HG	1.99	0.44
1:X:23:ILE:O	1:X:24:LYS:C	2.61	0.44
1:Y:10:ILE:HD13	1:Y:212:ILE:HD11	1.99	0.44
1:Y:134:THR:C	1:Y:136:GLN:N	2.70	0.44
1:Y:239:ARG:HG3	1:Y:239:ARG:NH1	2.33	0.44
1:Z:204:ILE:HG22	1:Z:205:GLN:N	2.33	0.44
2:A:91:ARG:HH11	2:A:91:ARG:HG2	1.81	0.44
2:A:143:GLU:O	2:A:147:ILE:HG12	2.16	0.44
2:B:252:ALA:HA	2:B:253:PRO:HD3	1.72	0.44
2:C:54:SER:C	2:C:56:GLY:N	2.74	0.44
2:C:143:GLU:O	2:C:147:ILE:HG13	2.17	0.44
1:X:263:LEU:C	1:X:265:PRO:CD	2.87	0.44
2:A:134:SER:O	2:A:201:GLU:O	2.35	0.44
2:A:172:SER:HA	2:A:177:ASN:HA	1.99	0.44
1:Y:200:LYS:CB	1:Y:202:LEU:HD13	2.47	0.44
1:Y:238:ILE:O	1:Y:240:GLY:N	2.50	0.44
2:C:4:ALA:HB1	2:C:57:PHE:CD2	2.53	0.44
1:X:92:LEU:C	1:X:92:LEU:HD12	2.43	0.44
1:X:263:LEU:HG	1:X:264:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:303:GLU:O	1:X:304:GLU:C	2.59	0.44
1:Y:220:GLN:O	1:Y:224:VAL:HG23	2.18	0.44
1:Y:316:PHE:O	1:Y:317:SER:C	2.61	0.44
1:Z:262:ARG:HE	1:Z:262:ARG:HA	1.82	0.44
2:B:83:GLY:C	2:B:85:GLU:N	2.76	0.44
2:C:23:ILE:HD13	2:C:48:VAL:HG21	1.98	0.44
1:Y:318:GLU:O	1:Y:319:GLU:C	2.61	0.44
1:Y:343:PHE:HE1	2:B:232:ASP:O	2.01	0.44
1:Z:34:ASP:HB3	1:Z:37:MET:HB2	2.00	0.44
1:Z:80:LYS:HB3	1:Z:298:TRP:CZ2	2.53	0.44
2:C:54:SER:CB	2:C:60:TYR:CD2	2.94	0.44
1:Z:181:ASP:C	1:Z:181:ASP:OD1	2.61	0.44
2:C:167:VAL:CG2	2:C:168:LYS:N	2.80	0.44
1:X:35:ALA:O	1:X:38:SER:HB3	2.17	0.44
1:X:82:VAL:HG13	1:X:151:PRO:HB2	2.00	0.44
1:Z:238:ILE:HG23	1:Z:241:ILE:O	2.18	0.44
1:Z:256:ILE:CD1	1:Z:276:HIS:HD2	2.28	0.44
2:C:144:PHE:CE1	2:C:227:LEU:HD11	2.53	0.44
1:X:222:GLN:NE2	1:X:254:LYS:HD3	2.33	0.44
1:Y:135:LYS:HD2	1:Y:135:LYS:O	2.17	0.44
1:Y:198:GLU:CD	1:Y:198:GLU:H	2.26	0.44
1:Z:22:ASP:OD2	1:Z:22:ASP:C	2.58	0.44
1:Z:111:LEU:O	1:Z:113:GLN:N	2.47	0.44
1:Z:135:LYS:HG2	1:Z:137:HIS:CD2	2.52	0.44
2:B:60:TYR:O	2:B:61:ARG:HB2	2.18	0.44
2:C:63:ASP:OD2	2:C:63:ASP:N	2.50	0.44
2:C:204:GLN:O	2:C:205:LEU:HD23	2.18	0.44
1:X:37:MET:HE2	1:X:41:GLN:HG3	2.00	0.43
1:X:223:PHE:O	1:X:226:LEU:HB3	2.18	0.43
1:Y:204:ILE:HD11	1:Y:206:GLU:HG3	1.99	0.43
1:Y:279:ALA:C	1:Y:281:GLN:N	2.75	0.43
1:Z:179:ASP:OD1	1:Z:181:ASP:CG	2.61	0.43
1:Z:197:SER:C	1:Z:199:ALA:N	2.72	0.43
2:B:93:GLU:O	2:B:96:ALA:HB2	2.16	0.43
2:B:219:THR:C	2:B:221:LEU:N	2.76	0.43
1:Y:143:HIS:C	1:Y:145:LEU:N	2.75	0.43
1:Y:218:LEU:HD12	1:Y:218:LEU:O	2.19	0.43
1:Y:304:GLU:O	1:Y:305:GLU:C	2.61	0.43
1:Z:33:ILE:HG12	1:Z:176:ALA:HB3	2.00	0.43
2:B:12:LEU:O	2:B:13:LYS:C	2.61	0.43
1:X:70:ARG:O	1:X:74:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:263:LEU:HD11	1:X:268:TYR:CD1	2.54	0.43
1:X:318:GLU:HG2	1:X:322:ARG:HG3	2.00	0.43
1:Y:134:THR:O	1:Y:137:HIS:CD2	2.71	0.43
1:Z:218:LEU:CD1	1:Z:218:LEU:N	2.74	0.43
2:A:167:VAL:CG1	2:A:182:LEU:HB2	2.47	0.43
1:Y:225:ASP:HB3	1:Y:250:ILE:HD11	2.01	0.43
1:Z:197:SER:O	1:Z:200:LYS:N	2.51	0.43
2:B:114:TYR:CD1	2:C:178:GLY:HA3	2.53	0.43
1:X:243:PRO:O	1:X:247:VAL:HG23	2.19	0.43
1:Y:253:HIS:C	1:Y:255:SER:H	2.26	0.43
1:Z:87:GLY:HA3	1:Z:156:PRO:O	2.19	0.43
1:Z:92:LEU:HD22	1:Z:92:LEU:N	2.33	0.43
2:A:134:SER:O	2:A:135:CYS:HB2	2.19	0.43
1:X:37:MET:CE	1:X:41:GLN:HG3	2.48	0.43
1:X:340:LEU:HD21	2:A:250:TYR:HB2	1.99	0.43
1:Y:190:LEU:HD12	1:Y:191:MET:N	2.34	0.43
1:Z:135:LYS:CG	1:Z:136:GLN:H	2.31	0.43
2:B:128:ILE:H	2:B:128:ILE:CD1	2.22	0.43
2:C:167:VAL:HG22	2:C:168:LYS:N	2.34	0.43
1:Y:289:LEU:HD12	1:Y:289:LEU:C	2.43	0.43
1:Y:357:GLU:HB3	1:Y:358:PRO:HD2	2.00	0.43
1:Z:134:THR:O	1:Z:135:LYS:C	2.62	0.43
1:Z:142:LYS:NZ	1:Z:154:ASP:OD2	2.52	0.43
1:Z:180:MET:C	1:Z:182:CYS:N	2.73	0.43
2:A:23:ILE:HD12	2:A:26:ALA:HB2	2.01	0.43
2:A:100:ALA:C	2:A:101:LEU:HD12	2.43	0.43
2:B:1:MET:HB3	2:B:63:ASP:OD1	2.19	0.43
1:Y:181:ASP:O	1:Y:182:CYS:C	2.60	0.43
2:A:87:ILE:N	2:A:87:ILE:CD1	2.82	0.43
2:A:203:VAL:HB	2:A:205:LEU:CD1	2.49	0.43
2:B:101:LEU:O	2:B:113:ASP:HA	2.18	0.43
2:B:166:GLY:HA2	2:B:197:ILE:CD1	2.49	0.43
2:C:158:VAL:HG22	2:C:159:VAL:N	2.33	0.43
1:Y:284:LEU:C	1:Y:286:PRO:HD3	2.42	0.43
1:Y:340:LEU:HD11	2:B:46:SER:HA	2.01	0.43
1:Z:10:ILE:HD13	1:Z:212:ILE:HD11	2.01	0.43
1:Z:265:PRO:C	1:Z:267:LYS:N	2.75	0.43
1:Z:267:LYS:HE2	1:Z:267:LYS:CA	2.48	0.43
2:A:147:ILE:HD11	2:C:110:LYS:HE3	2.01	0.43
2:A:152:SER:HA	2:A:209:LEU:HD13	2.01	0.43
1:Y:67:MET:HE1	1:Y:145:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:197:SER:HB3	1:Y:200:LYS:HG2	2.01	0.43
1:Z:265:PRO:O	1:Z:267:LYS:N	2.52	0.42
1:Z:344:PHE:HB2	2:C:126:LEU:HD13	2.01	0.42
2:A:94:ASP:C	2:A:96:ALA:N	2.77	0.42
2:B:99:LEU:HB2	2:B:118:LEU:HD11	2.00	0.42
2:C:53:ARG:HB3	2:C:55:GLU:OE1	2.18	0.42
2:C:236:VAL:HG22	2:C:250:TYR:CD2	2.54	0.42
1:X:265:PRO:C	1:X:267:LYS:N	2.77	0.42
1:Y:236:GLU:HG3	1:Y:271:PRO:HB3	2.00	0.42
2:B:137:VAL:HG11	2:B:139:MET:HE2	2.00	0.42
2:C:71:ASN:O	2:C:72:LEU:C	2.59	0.42
2:C:139:MET:SD	2:C:144:PHE:HB2	2.59	0.42
1:Z:266:ASN:O	1:Z:269:PRO:HG3	2.19	0.42
1:Z:275:LEU:HD22	1:Z:275:LEU:H	1.83	0.42
2:A:173:GLY:N	2:A:176:GLY:O	2.48	0.42
2:B:219:THR:N	2:B:220:PRO:HD2	2.33	0.42
1:X:270:VAL:HG13	1:X:271:PRO:CD	2.49	0.42
1:Y:10:ILE:CG2	1:Y:18:ILE:HD11	2.49	0.42
1:Y:62:SER:C	1:Y:64:LEU:H	2.26	0.42
1:Y:139:ASP:HA	1:Y:142:LYS:HD3	2.01	0.42
1:Y:194:LEU:O	1:Y:194:LEU:CG	2.67	0.42
1:Y:254:LYS:O	1:Y:255:SER:HB3	2.18	0.42
1:Z:226:LEU:O	1:Z:230:LEU:HB2	2.20	0.42
2:A:55:GLU:H	2:A:55:GLU:CD	2.27	0.42
2:B:99:LEU:HD23	2:B:99:LEU:C	2.44	0.42
2:C:126:LEU:HD23	2:C:126:LEU:HA	1.86	0.42
1:X:9:LEU:HD22	1:X:230:LEU:HD21	2.01	0.42
1:X:39:ILE:HD11	1:X:85:PHE:HE1	1.85	0.42
1:Y:63:HIS:HD2	1:Y:137:HIS:O	2.03	0.42
1:Y:236:GLU:CD	1:Y:236:GLU:H	2.27	0.42
1:Y:238:ILE:O	1:Y:238:ILE:HG12	2.19	0.42
1:Z:253:HIS:CE1	1:Z:262:ARG:HB3	2.55	0.42
2:A:219:THR:N	2:A:220:PRO:HD2	2.34	0.42
1:X:221:GLU:O	1:X:222:GLN:C	2.63	0.42
1:X:289:LEU:O	1:X:291:PRO:HD3	2.19	0.42
1:Y:192:ARG:O	1:Y:193:HIS:HB2	2.19	0.42
1:Z:67:MET:HE2	1:Z:141:CYS:HB3	2.02	0.42
1:Z:316:PHE:HB3	1:Z:321:ILE:HD13	2.01	0.42
1:Z:355:ARG:HG2	2:C:97:ASP:OD1	2.19	0.42
2:A:65:ASN:N	2:A:65:ASN:ND2	2.68	0.42
2:A:167:VAL:HG12	2:A:182:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:MET:HE1	2:C:169:PHE:CZ	2.54	0.42
1:X:234:TYR:O	1:X:235:CYS:HB3	2.19	0.42
1:Y:215:GLU:C	1:Y:217:GLY:N	2.78	0.42
1:Z:353:ALA:O	1:Z:354:LYS:C	2.63	0.42
1:Y:9:LEU:HD11	1:Y:247:VAL:HG21	2.02	0.42
1:Y:137:HIS:CD2	1:Y:137:HIS:N	2.84	0.42
1:Y:248:ASP:O	1:Y:251:GLN:HB2	2.20	0.42
1:Y:263:LEU:HD13	1:Y:268:TYR:CB	2.50	0.42
1:Y:320:ARG:C	1:Y:322:ARG:H	2.28	0.42
1:Z:138:ASN:C	1:Z:140:GLU:N	2.75	0.42
1:Z:311:CYS:HA	1:Z:316:PHE:H	1.85	0.42
1:Z:30:LYS:HB3	1:Z:172:VAL:HG23	2.02	0.42
1:Z:132:LYS:NZ	1:Z:134:THR:CG2	2.83	0.42
1:Z:150:ILE:H	1:Z:150:ILE:CD1	2.29	0.42
1:Z:256:ILE:HG12	1:Z:256:ILE:H	1.57	0.42
1:Z:311:CYS:SG	1:Z:318:GLU:HA	2.59	0.42
2:A:113:ASP:OD2	2:A:113:ASP:C	2.63	0.42
2:B:18:ALA:HB1	2:B:249:TYR:OH	2.20	0.42
2:B:41:ASP:OD2	2:B:43:SER:HB3	2.19	0.42
2:B:75:MET:HG2	2:B:116:MET:HE1	2.02	0.42
1:X:339:ARG:O	1:X:341:ASP:N	2.53	0.41
1:Y:252:LYS:HD3	1:Y:252:LYS:HA	1.92	0.41
1:Z:24:LYS:HA	1:Z:77:ASN:HD22	1.80	0.41
1:Z:251:GLN:C	1:Z:254:LYS:HD2	2.45	0.41
1:Z:320:ARG:HE	1:Z:320:ARG:HB2	1.56	0.41
2:A:7:VAL:HA	2:A:87:ILE:HG23	2.01	0.41
2:A:114:TYR:CD1	2:B:178:GLY:HA3	2.55	0.41
2:B:6:LEU:HD23	2:B:12:LEU:HD22	2.02	0.41
2:B:40:MET:HB3	2:B:46:SER:O	2.19	0.41
1:X:335:SER:C	1:X:337:GLN:H	2.28	0.41
1:Y:192:ARG:O	1:Y:193:HIS:CB	2.68	0.41
1:Z:90:PRO:C	1:Z:92:LEU:H	2.27	0.41
1:Z:304:GLU:C	1:Z:306:LEU:N	2.78	0.41
2:A:110:LYS:HE3	2:B:180:ILE:HG21	2.02	0.41
2:C:30:ILE:HG13	2:C:68:MET:CE	2.50	0.41
1:X:195:THR:C	1:X:197:SER:N	2.75	0.41
1:X:355:ARG:HH11	1:X:355:ARG:CG	2.30	0.41
1:Y:202:LEU:N	1:Y:202:LEU:CD1	2.84	0.41
2:B:68:MET:CE	2:B:92:ALA:CB	2.98	0.41
2:C:212:LEU:C	2:C:214:PHE:N	2.77	0.41
1:X:28:GLY:N	1:X:78:GLY:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:275:LEU:O	1:Y:277:LYS:N	2.52	0.41
1:Z:45:ALA:C	1:Z:47:ARG:N	2.78	0.41
1:Z:100:ARG:HH11	1:Z:100:ARG:CG	2.33	0.41
1:Z:212:ILE:O	1:Z:215:GLU:N	2.53	0.41
2:A:2:PHE:CD1	2:A:30:ILE:HG21	2.54	0.41
2:C:1:MET:SD	2:C:1:MET:C	3.04	0.41
2:C:226:THR:CG2	2:C:238:GLU:HB3	2.46	0.41
1:Z:167:VAL:HG12	1:Z:188:PRO:CG	2.50	0.41
2:B:200:ASN:N	2:B:200:ASN:ND2	2.69	0.41
2:C:72:LEU:HD13	2:C:72:LEU:HA	1.86	0.41
2:C:150:ASP:O	2:C:153:HIS:N	2.44	0.41
1:X:36:SER:HB2	1:X:86:ASP:OD2	2.20	0.41
1:Y:79:ILE:O	1:Y:81:PRO:HD3	2.21	0.41
1:Y:159:ALA:O	1:Y:160:GLU:C	2.64	0.41
1:Y:308:LYS:NZ	1:Y:308:LYS:CB	2.83	0.41
1:Z:23:ILE:O	1:Z:24:LYS:C	2.63	0.41
2:A:106:PRO:O	2:A:108:GLN:N	2.54	0.41
2:B:2:PHE:O	2:B:91:ARG:HA	2.20	0.41
2:B:192:GLU:C	2:B:194:ALA:N	2.76	0.41
2:C:238:GLU:HG3	2:C:248:LYS:HG2	2.03	0.41
1:Y:258:GLU:O	1:Y:262:ARG:HG2	2.20	0.41
1:Y:272:GLU:HG3	1:Y:273:ASN:N	2.31	0.41
1:Z:222:GLN:O	1:Z:225:ASP:N	2.52	0.41
1:Z:310:MET:HB3	1:Z:321:ILE:HG12	2.02	0.41
2:B:51:THR:O	2:B:245:GLY:HA3	2.21	0.41
2:B:185:THR:HG22	2:B:187:ASN:CB	2.50	0.41
2:C:7:VAL:HG12	2:C:58:ASP:OD1	2.20	0.41
2:C:192:GLU:C	2:C:194:ALA:H	2.28	0.41
2:C:229:MET:HE3	2:C:235:LEU:HD13	2.01	0.41
1:X:320:ARG:HH11	1:X:320:ARG:HB2	1.86	0.41
1:Y:316:PHE:CD2	1:Y:317:SER:N	2.88	0.41
1:Z:104:ARG:HA	1:Z:104:ARG:HE	1.80	0.41
1:Z:112:GLN:O	1:Z:113:GLN:C	2.63	0.41
2:A:37:LEU:HB3	2:A:50:LEU:HB3	2.03	0.41
1:X:343:PHE:CE1	2:A:234:PRO:HD3	2.56	0.41
1:Y:141:CYS:O	1:Y:143:HIS:N	2.54	0.41
1:Y:166:LEU:O	1:Y:167:VAL:C	2.64	0.41
1:Y:212:ILE:HG22	1:Y:213:LEU:N	2.35	0.41
1:Y:311:CYS:SG	1:Y:321:ILE:HB	2.60	0.41
1:Z:48:GLN:C	1:Z:50:GLY:N	2.74	0.41
1:Z:73:ARG:CZ	1:Z:198:GLU:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:101:SER:O	1:Z:104:ARG:HB2	2.21	0.41
1:Z:135:LYS:CG	1:Z:136:GLN:N	2.84	0.41
1:Z:169:ALA:C	1:Z:171:LYS:N	2.76	0.41
1:Z:216:LEU:HB3	1:Z:218:LEU:HD13	2.03	0.41
2:A:73:THR:O	2:A:76:SER:HB3	2.20	0.41
2:A:79:LEU:C	2:A:81:CYS:H	2.28	0.41
2:B:46:SER:HB3	2:B:251:LEU:HD12	2.02	0.41
2:B:191:GLU:HB3	2:B:192:GLU:H	1.60	0.41
2:B:215:PHE:CD1	2:B:249:TYR:CD1	3.09	0.41
2:B:219:THR:O	2:B:221:LEU:N	2.54	0.41
2:C:235:LEU:O	2:C:250:TYR:HA	2.20	0.41
1:X:72:ILE:O	1:X:75:MET:HB2	2.21	0.41
1:Y:142:LYS:NZ	1:Y:154:ASP:OD2	2.53	0.41
1:Z:16:SER:OG	1:Z:211:ARG:NH1	2.54	0.41
1:Z:212:ILE:O	1:Z:214:GLN:N	2.54	0.41
2:A:107:ASN:O	2:A:109:GLU:N	2.54	0.41
2:B:184:GLN:HG3	2:B:196:THR:HA	2.03	0.41
1:X:3:ILE:O	1:X:4:GLN:C	2.63	0.40
1:Y:274:TRP:CE3	1:Y:276:HIS:HB3	2.56	0.40
1:Y:320:ARG:C	1:Y:322:ARG:N	2.79	0.40
1:Z:153:LEU:HD12	1:Z:153:LEU:N	2.35	0.40
1:Z:298:TRP:CE3	1:Z:298:TRP:N	2.84	0.40
2:B:200:ASN:N	2:B:200:ASN:HD22	2.17	0.40
1:X:350:LEU:CD2	2:A:27:CYS:HB3	2.50	0.40
1:Y:241:ILE:HD12	1:Y:241:ILE:O	2.21	0.40
1:Z:67:MET:CE	1:Z:141:CYS:HB3	2.52	0.40
1:Z:142:LYS:NZ	1:Z:154:ASP:OD1	2.51	0.40
2:B:166:GLY:HA2	2:B:197:ILE:HD11	2.02	0.40
2:C:11:ILE:HD13	2:C:244:MET:HE3	2.02	0.40
2:C:47:LEU:HD12	2:C:126:LEU:HD12	2.02	0.40
1:Y:3:ILE:CG2	1:Y:6:LEU:HB2	2.48	0.40
1:Y:39:ILE:HA	1:Y:42:PHE:HD2	1.86	0.40
1:Z:91:GLN:HA	1:Z:91:GLN:NE2	2.37	0.40
1:Z:347:THR:O	1:Z:347:THR:HG22	2.20	0.40
2:A:8:GLN:O	2:A:10:SER:N	2.54	0.40
2:C:88:ILE:HG23	2:C:103:PHE:CD1	2.56	0.40
1:X:75:MET:HG3	1:X:328:LEU:HD13	2.04	0.40
1:Z:135:LYS:CG	1:Z:137:HIS:CD2	3.04	0.40
1:Z:341:ASP:C	1:Z:343:PHE:H	2.29	0.40
2:A:40:MET:HA	2:A:47:LEU:HA	2.02	0.40
2:B:21:ASP:OD2	2:B:217:LYS:HE3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:17:ALA:HB2	1:Y:211:ARG:CG	2.52	0.40
1:Y:213:LEU:HD21	1:Y:220:GLN:HA	2.02	0.40
1:Y:302:ASN:CG	1:Y:305:GLU:HB3	2.46	0.40
1:Z:212:ILE:C	1:Z:214:GLN:N	2.80	0.40
1:Z:322:ARG:C	1:Z:324:GLY:N	2.79	0.40
2:A:93:GLU:O	2:A:96:ALA:HB2	2.21	0.40
2:B:247:LEU:HD12	2:B:247:LEU:HA	1.90	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	X	305/379 (80%)	239 (78%)	44 (14%)	22 (7%)	1	2
1	Y	306/379 (81%)	219 (72%)	66 (22%)	21 (7%)	1	2
1	Z	345/379 (91%)	239 (69%)	79 (23%)	27 (8%)	1	2
2	A	252/261 (97%)	222 (88%)	23 (9%)	7 (3%)	4	15
2	B	256/261 (98%)	223 (87%)	23 (9%)	10 (4%)	2	10
2	C	253/261 (97%)	221 (87%)	25 (10%)	7 (3%)	4	15
All	All	1717/1920 (89%)	1363 (79%)	260 (15%)	94 (6%)	1	4

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	13	VAL
1	X	254	LYS
1	X	262	ARG
1	X	263	LEU
1	X	264	ASP

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Mol	Chain	Res	Type
1	X	266	ASN
1	X	272	GLU
1	Y	93	LYS
1	Y	271	PRO
1	Y	272	GLU
1	Y	315	GLN
1	Z	68	PHE
1	Z	196	ALA
1	Z	218	LEU
1	Z	243	PRO
1	Z	254	LYS
1	Z	256	ILE
2	A	94	ASP
2	A	108	GLN
2	A	192	GLU
2	A	231	ALA
2	B	194	ALA
2	C	108	GLN
1	X	12	ASP
1	X	193	HIS
1	X	196	ALA
1	Y	157	SER
1	Y	200	LYS
1	Y	239	ARG
1	Y	254	LYS
1	Y	356	LYS
1	Y	358	PRO
1	Z	46	VAL
1	Z	49	GLY
1	Z	94	SER
1	Z	133	VAL
1	Z	170	GLY
1	Z	255	SER
1	Z	266	ASN
1	Z	283	PHE
1	Z	293	SER
1	Z	310	MET
1	Z	342	ASP
2	A	9	GLY
2	A	135	CYS
2	B	84	ASN
2	B	188	VAL

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Mol	Chain	Res	Type
2	B	232	ASP
2	C	188	VAL
2	C	191	GLU
1	X	81	PRO
1	X	96	GLU
1	X	156	PRO
1	X	231	GLY
1	X	333	GLN
1	X	335	SER
1	Y	201	LYS
1	Y	264	ASP
1	Z	135	LYS
1	Z	213	LEU
1	Z	317	SER
2	B	61	ARG
2	B	191	GLU
2	B	242	ALA
2	C	20	LYS
2	C	31	SER
2	C	193	GLU
1	X	315	GLN
1	X	332	ARG
1	Y	36	SER
1	Y	199	ALA
1	Y	240	GLY
1	Y	262	ARG
1	Y	305	GLU
1	Y	317	SER
1	Z	37	MET
1	Z	55	ASN
1	Z	195	THR
2	B	94	ASP
2	C	204	GLN
1	X	133	VAL
1	X	197	SER
1	X	220	GLN
1	Z	96	GLU
1	Z	315	GLN
2	A	107	ASN
2	B	187	ASN
1	X	312	GLY
1	Y	216	LEU

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Mol	Chain	Res	Type
1	Z	265	PRO
1	Z	13	VAL
2	B	255	ILE
1	Y	90	PRO
1	Y	231	GLY

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	X	247/321 (77%)	228 (92%)	19 (8%)	12	35
1	Y	238/321 (74%)	221 (93%)	17 (7%)	13	40
1	Z	259/321 (81%)	234 (90%)	25 (10%)	8	25
2	A	220/228 (96%)	204 (93%)	16 (7%)	13	38
2	B	218/228 (96%)	192 (88%)	26 (12%)	5	16
2	C	214/228 (94%)	203 (95%)	11 (5%)	21	53
All	All	1396/1647 (85%)	1282 (92%)	114 (8%)	10	32

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	4	GLN
1	X	6	LEU
1	X	31	VAL
1	X	41	GLN
1	X	81	PRO
1	X	82	VAL
1	X	88	LYS
1	X	153	LEU
1	X	172	VAL
1	X	177	THR
1	X	189	VAL
1	X	190	LEU
1	X	264	ASP

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Mol	Chain	Res	Type
1	X	267	LYS
1	X	270	VAL
1	X	275	LEU
1	X	300	GLU
1	X	346	VAL
1	X	352	SER
1	Y	6	LEU
1	Y	13	VAL
1	Y	41	GLN
1	Y	67	MET
1	Y	137	HIS
1	Y	172	VAL
1	Y	204	ILE
1	Y	230	LEU
1	Y	238	ILE
1	Y	241	ILE
1	Y	271	PRO
1	Y	275	LEU
1	Y	276	HIS
1	Y	287	GLU
1	Y	308	LYS
1	Y	325	VAL
1	Y	330	LYS
1	Z	6	LEU
1	Z	22	ASP
1	Z	23	ILE
1	Z	37	MET
1	Z	77	ASN
1	Z	91	GLN
1	Z	108	GLU
1	Z	112	GLN
1	Z	127	THR
1	Z	130	LEU
1	Z	132	LYS
1	Z	133	VAL
1	Z	147	LEU
1	Z	202	LEU
1	Z	218	LEU
1	Z	230	LEU
1	Z	239	ARG
1	Z	254	LYS
1	Z	256	ILE

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Mol	Chain	Res	Type
1	Z	262	ARG
1	Z	267	LYS
1	Z	275	LEU
1	Z	296	LEU
1	Z	321	ILE
1	Z	340	LEU
2	A	2	PHE
2	A	12	LEU
2	A	16	LEU
2	A	29	ASP
2	A	59	THR
2	A	94	ASP
2	A	112	SER
2	A	135	CYS
2	A	161	SER
2	A	172	SER
2	A	175	LEU
2	A	224	THR
2	A	226	THR
2	A	230	SER
2	A	236	VAL
2	A	240	LYS
2	B	12	LEU
2	B	16	LEU
2	B	40	MET
2	B	45	VAL
2	B	47	LEU
2	B	49	GLN
2	B	109	GLU
2	B	117	LYS
2	B	118	LEU
2	B	126	LEU
2	B	128	ILE
2	B	135	CYS
2	B	152	SER
2	B	175	LEU
2	B	179	ASN
2	B	184	GLN
2	B	190	LYS
2	B	199	MET
2	B	203	VAL
2	B	217	LYS

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Mol	Chain	Res	Type
2	B	224	THR
2	B	226	THR
2	B	236	VAL
2	B	254	LYS
2	B	256	GLU
2	B	258	GLU
2	C	12	LEU
2	C	16	LEU
2	C	23	ILE
2	C	49	GLN
2	C	63	ASP
2	C	101	LEU
2	C	201	GLU
2	C	205	LEU
2	C	224	THR
2	C	229	MET
2	C	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	91	GLN
1	X	137	HIS
1	X	219	ASN
1	X	276	HIS
1	X	280	HIS
1	X	333	GLN
1	Y	4	GLN
1	Y	21	ASN
1	Y	63	HIS
1	Y	77	ASN
1	Y	137	HIS
1	Y	138	ASN
1	Y	193	HIS
1	Y	222	GLN
1	Y	253	HIS
1	Y	273	ASN
1	Y	302	ASN
1	Z	21	ASN
1	Z	48	GLN
1	Z	54	GLN
1	Z	91	GLN

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Mol	Chain	Res	Type
1	Z	112	GLN
1	Z	137	HIS
1	Z	214	GLN
1	Z	222	GLN
1	Z	276	HIS
1	Z	302	ASN
2	A	38	GLN
2	A	65	ASN
2	A	125	GLN
2	B	65	ASN
2	B	177	ASN
2	B	200	ASN
2	B	204	GLN
2	C	49	GLN
2	C	65	ASN
2	C	84	ASN
2	C	153	HIS
2	C	184	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	X	313/379 (82%)	-0.20	7 (2%) 62 53	15, 46, 114, 176	0
1	Y	312/379 (82%)	0.18	12 (3%) 44 36	28, 74, 131, 181	0
1	Z	349/379 (92%)	0.51	21 (6%) 27 21	30, 82, 136, 175	0
2	A	256/261 (98%)	-0.68	3 (1%) 76 69	9, 29, 94, 151	0
2	B	258/261 (98%)	-0.49	7 (2%) 56 47	10, 33, 98, 174	0
2	C	255/261 (97%)	-0.53	0 100 100	12, 41, 95, 176	0
All	All	1743/1920 (90%)	-0.15	50 (2%) 53 45	9, 51, 123, 181	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	193	GLU	7.7
1	Z	121	GLN	6.9
1	Z	273	ASN	5.0
2	B	192	GLU	4.2
1	Z	317	SER	4.0
1	Z	130	LEU	4.0
1	Z	158	GLU	3.9
1	Z	243	PRO	3.8
1	Z	148	MET	3.8
2	B	185	THR	3.8
2	A	107	ASN	3.8
1	Y	61	THR	3.7
1	Z	265	PRO	3.2
1	Z	250	ILE	3.2
2	B	194	ALA	3.1
1	X	357	GLU	3.1
1	Y	359	GLU	3.0
2	B	117	LYS	3.0
2	B	188	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	255	ILE	2.9
1	X	313	GLU	2.9
1	Z	283	PHE	2.9
1	Z	98	ALA	2.8
1	Z	306	LEU	2.8
1	X	336	THR	2.8
2	A	108	GLN	2.7
1	Y	60	THR	2.7
1	X	95	GLY	2.7
1	Z	133	VAL	2.7
1	X	60	THR	2.7
1	Z	263	LEU	2.6
1	X	196	ALA	2.6
1	Y	234	TYR	2.4
1	Y	137	HIS	2.4
1	Y	241	ILE	2.4
1	Y	141	CYS	2.4
1	Z	184	THR	2.4
1	Z	336	THR	2.4
1	X	335	SER	2.3
1	Y	265	PRO	2.3
1	Y	101	SER	2.2
1	Z	157	SER	2.2
2	A	255	ILE	2.2
1	Z	60	THR	2.2
1	Z	96	GLU	2.2
1	Z	164	ALA	2.2
1	Y	134	THR	2.1
1	Y	273	ASN	2.0
1	Y	66	GLY	2.0
1	Z	85	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	Y	1003	1/1	0.89	0.10	56,56,56,56	0
3	MG	Y	1004	1/1	0.89	0.08	55,55,55,55	0
3	MG	X	1002	1/1	0.95	0.13	48,48,48,48	0
3	MG	X	1001	1/1	0.96	0.07	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.