



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 AM UTC

PDB ID : 1ZCF / pdb_00001zcf
Title : L-asparaginase from Erwinia carotovora
Authors : Kuranova, I.P.; Kislizin, Y.A.; Kravchenko, O.V.; Nikonov, S.V.
Deposited on : 2005-04-12
Resolution : 3.00 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:

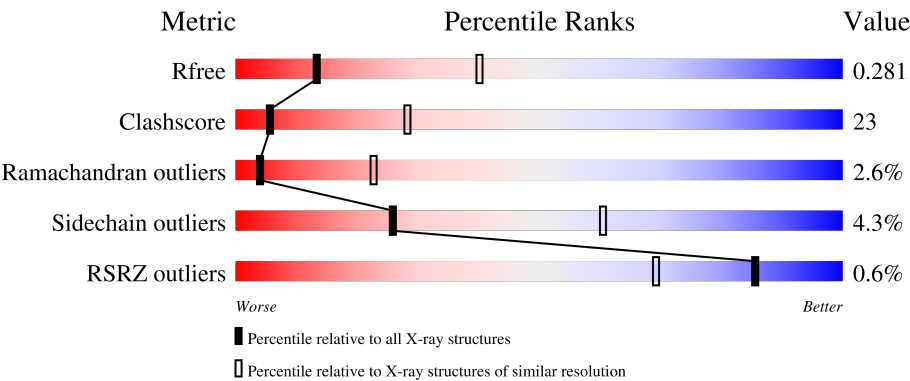
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	327	60%35%..
1	B	327	62%33%5%.
1	C	327	% 59%36%..
1	D	327	% 49%43%7%.
1	E	327	% 63%34%..

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Mol	Chain	Length	Quality of chain
1	F	327	54%38%7% %
1	G	327	48%43%9% %
1	H	327	54%39%6% %

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19296 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.

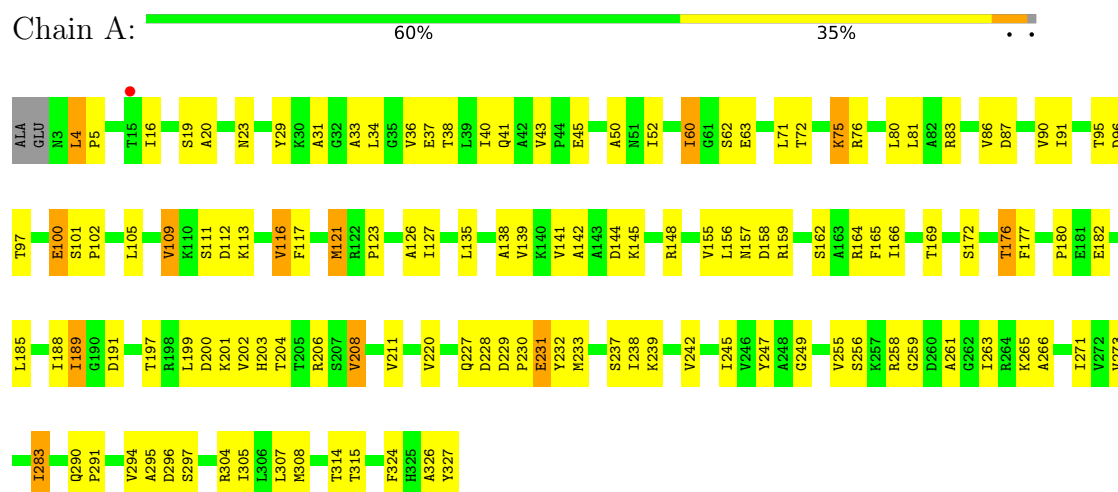
- Molecule 1 is a protein called L-asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	B	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	C	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	D	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	E	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	F	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	G	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			
1	H	325	Total	C	N	O	S	0	0	0
			2412	1519	415	472	6			

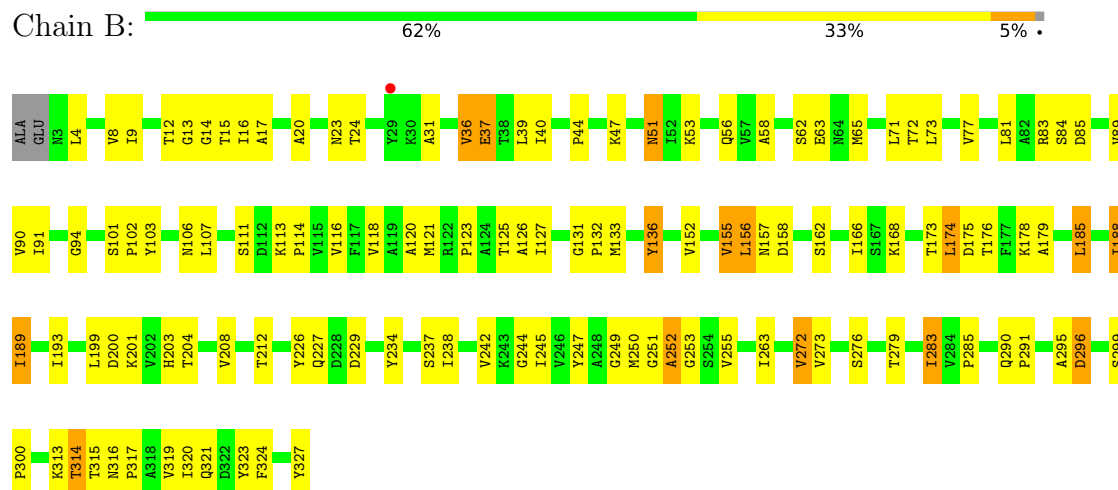
3 Residue-property plots

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: L-asparaginase

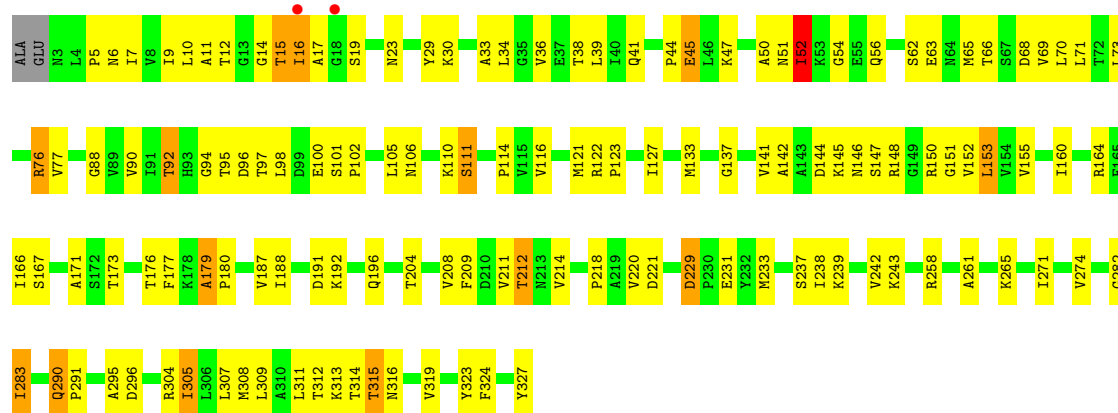


• Molecule 1: L-asparaginase

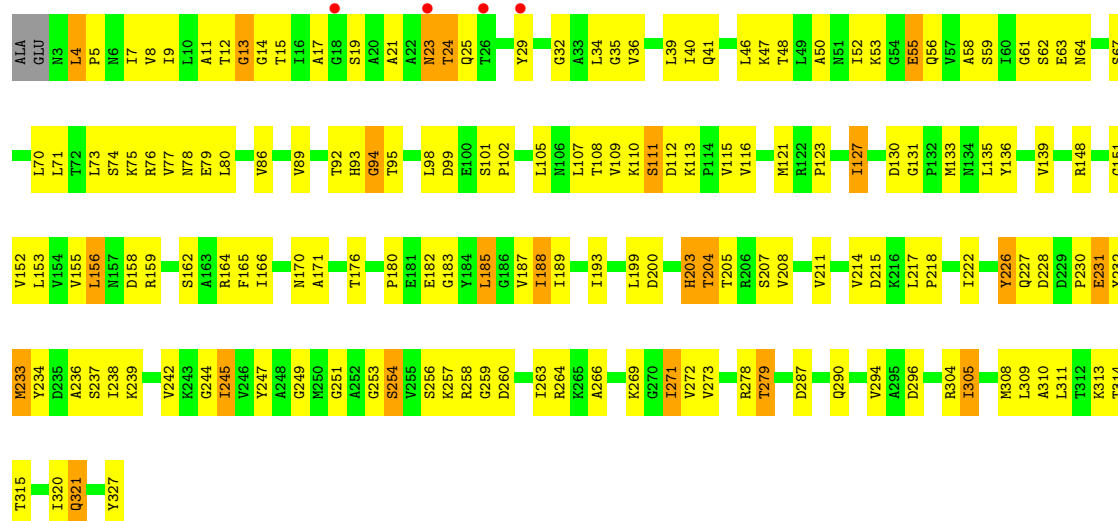


• Molecule 1: L-asparaginase

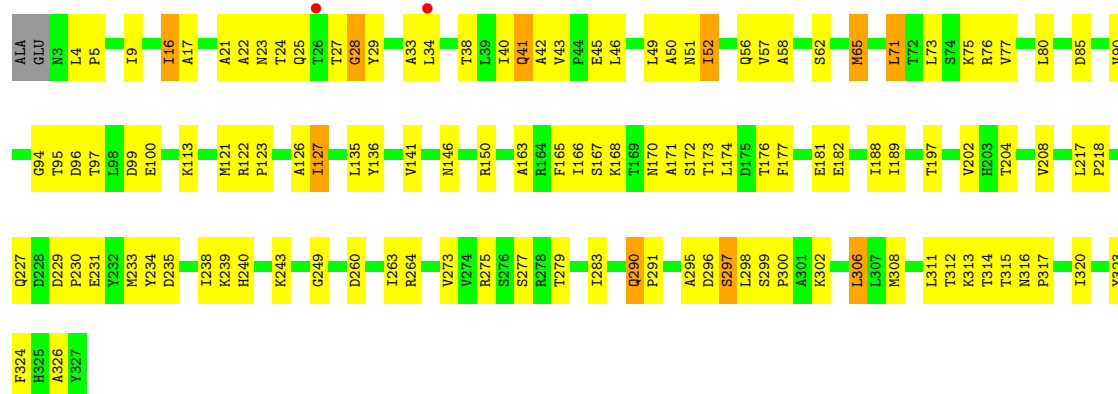




• Molecule 1: L-asparaginase

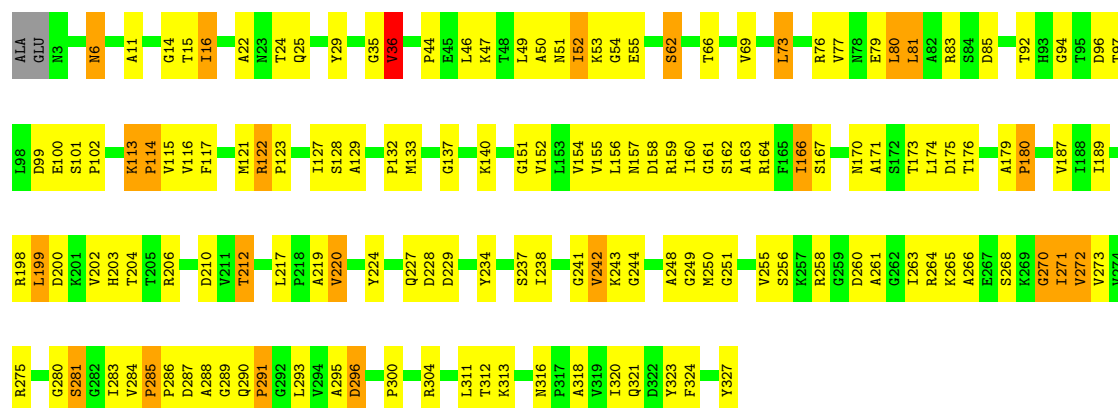


• Molecule 1: L-asparaginase

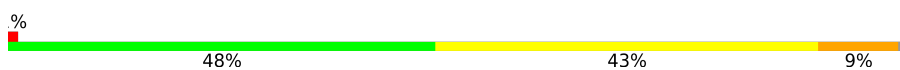


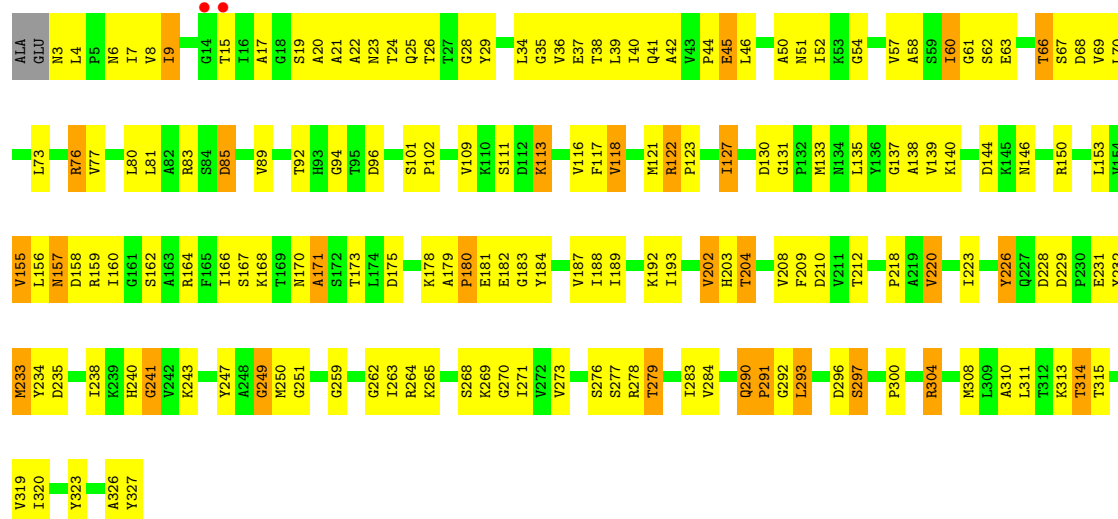
• Molecule 1: L-asparaginase

Chain F:  54% 38% 7% .



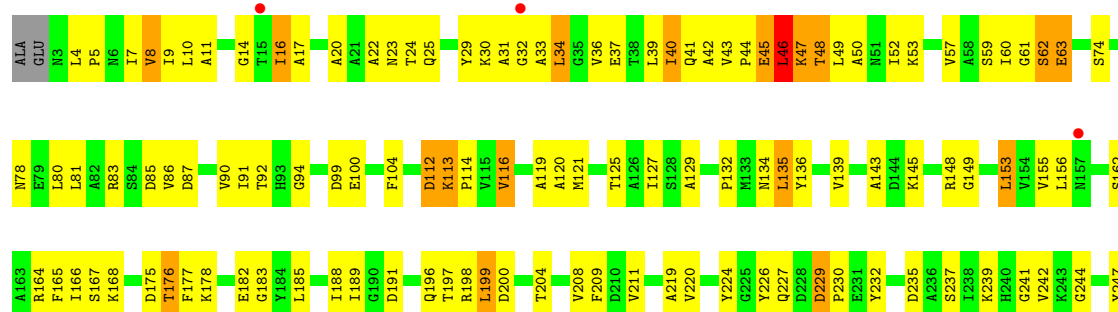
• Molecule 1: L-asparaginase

Chain G:  48% 43% 9% .



• Molecule 1: L-asparaginase

Chain H:  54% 39% 6% .



A248	G249	M250	G251	A252	G253	S254	V255		R258		R264		P285	P296		Q290	P291	G292	L293		D296	S297	L298		R304		M308		T315	N316	P317	A318	V319	I320	Q321	D322	Y323		Y327
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.64Å 141.99Å 260.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.97-3.00) 98.0 (19.97-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.282 0.203 , 0.281	Depositor DCC
R_{free} test set	2786 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19296	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0693e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.53	0/2448	1.09	17/3324 (0.5%)
1	B	0.52	0/2448	1.09	22/3324 (0.7%)
1	C	0.51	0/2448	1.08	14/3324 (0.4%)
1	D	0.47	0/2448	1.07	18/3324 (0.5%)
1	E	0.51	0/2448	1.09	16/3324 (0.5%)
1	F	0.54	0/2448	1.18	30/3324 (0.9%)
1	G	0.48	0/2448	1.10	22/3324 (0.7%)
1	H	0.51	0/2448	1.08	20/3324 (0.6%)
All	All	0.51	0/19584	1.10	159/26592 (0.6%)

There are no bond length outliers.

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	285	PRO	N-CA-C	10.15	120.21	110.47
1	F	249	GLY	N-CA-C	9.18	122.48	111.93
1	F	81	LEU	N-CA-C	-8.85	102.50	113.38
1	F	80	LEU	N-CA-C	-8.50	103.76	114.56
1	H	113	LYS	CA-C-N	8.38	130.31	119.84
1	H	113	LYS	C-N-CA	8.38	130.31	119.84
1	E	227	GLN	N-CA-C	8.24	119.89	111.07
1	E	113	LYS	CA-C-N	8.19	130.07	119.84
1	E	113	LYS	C-N-CA	8.19	130.07	119.84
1	B	252	ALA	N-CA-C	-8.04	102.26	113.20
1	F	227	GLN	N-CA-C	7.95	120.65	111.11
1	G	66	THR	N-CA-C	7.94	120.97	109.14
1	A	229	ASP	CA-C-N	7.61	127.53	119.85
1	A	229	ASP	C-N-CA	7.61	127.53	119.85
1	E	171	ALA	N-CA-C	7.55	119.15	111.07
1	E	229	ASP	CA-C-N	7.30	128.38	120.13
1	E	229	ASP	C-N-CA	7.30	128.38	120.13
1	A	176	THR	N-CA-C	7.27	119.00	111.14
1	A	52	ILE	N-CA-C	7.27	119.94	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	116	VAL	N-CA-C	7.10	118.11	108.17
1	F	116	VAL	N-CA-C	7.06	118.05	108.17
1	H	176	THR	N-CA-C	6.97	118.88	111.28
1	C	282	GLY	N-CA-C	6.92	120.56	111.70
1	D	203	HIS	N-CA-C	6.92	117.37	108.24
1	A	43	VAL	CA-C-N	6.88	126.69	119.05
1	A	43	VAL	C-N-CA	6.88	126.69	119.05
1	D	4	LEU	CA-C-N	6.84	127.77	120.11
1	D	4	LEU	C-N-CA	6.84	127.77	120.11
1	F	122	ARG	CA-C-N	6.80	128.34	119.84
1	F	122	ARG	C-N-CA	6.80	128.34	119.84
1	C	179	ALA	CA-C-N	6.79	128.33	119.84
1	C	179	ALA	C-N-CA	6.79	128.33	119.84
1	C	290	GLN	CA-C-N	6.75	126.72	120.03
1	C	290	GLN	C-N-CA	6.75	126.72	120.03
1	G	155	VAL	N-CA-C	6.73	117.80	107.78
1	G	229	ASP	CA-C-N	6.71	127.24	119.99
1	G	229	ASP	C-N-CA	6.71	127.24	119.99
1	D	233	MET	N-CA-C	-6.69	103.98	111.28
1	D	290	GLN	CA-C-N	6.64	127.55	120.11
1	D	290	GLN	C-N-CA	6.64	127.55	120.11
1	A	295	ALA	N-CA-C	-6.64	102.25	110.41
1	C	52	ILE	N-CA-C	6.62	118.36	108.96
1	G	113	LYS	CA-C-N	6.57	128.06	119.84
1	G	113	LYS	C-N-CA	6.57	128.06	119.84
1	D	227	GLN	N-CA-C	6.54	120.36	112.38
1	D	50	ALA	N-CA-C	6.53	116.48	107.73
1	H	63	GLU	N-CA-C	6.46	120.42	112.54
1	F	113	LYS	CA-C-N	6.45	126.80	119.83
1	F	113	LYS	C-N-CA	6.45	126.80	119.83
1	E	172	SER	N-CA-C	6.44	121.06	112.30
1	H	285	PRO	N-CA-C	6.38	118.49	110.70
1	B	116	VAL	N-CA-C	6.37	117.06	107.75
1	H	290	GLN	CA-C-N	6.33	127.75	119.84
1	H	290	GLN	C-N-CA	6.33	127.75	119.84
1	D	94	GLY	N-CA-C	-6.33	102.92	112.60
1	B	188	ILE	N-CA-C	6.29	115.78	106.85
1	F	52	ILE	N-CA-C	6.28	116.89	110.05
1	F	272	VAL	N-CA-C	6.24	117.56	108.58
1	B	229	ASP	N-CA-C	6.23	116.76	109.60
1	A	249	GLY	N-CA-C	6.20	120.13	112.14
1	H	40	ILE	N-CA-C	-6.18	106.93	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	260	ASP	N-CA-C	-6.13	104.51	111.07
1	D	189	ILE	N-CA-C	6.13	117.02	107.28
1	D	279	THR	N-CA-C	6.06	117.97	111.36
1	E	290	GLN	CA-C-N	5.99	127.39	120.98
1	E	290	GLN	C-N-CA	5.99	127.39	120.98
1	B	189	ILE	N-CA-C	5.98	116.48	107.75
1	C	171	ALA	N-CA-C	5.93	118.70	111.82
1	D	41	GLN	N-CA-C	-5.93	104.72	111.07
1	C	155	VAL	N-CA-C	5.92	116.39	107.75
1	B	166	ILE	N-CA-C	5.91	117.20	109.58
1	E	312	THR	N-CA-C	-5.89	105.92	113.23
1	A	326	ALA	N-CA-C	5.83	120.67	113.50
1	A	155	VAL	N-CA-C	5.82	116.38	107.77
1	B	175	ASP	N-CA-C	-5.80	104.60	112.26
1	H	112	ASP	N-CA-C	-5.80	106.02	112.57
1	E	181	GLU	N-CA-C	5.79	117.67	111.36
1	B	290	GLN	CA-C-N	5.77	125.75	120.21
1	B	290	GLN	C-N-CA	5.77	125.75	120.21
1	E	297	SER	N-CA-C	-5.72	103.66	111.56
1	C	295	ALA	N-CA-C	-5.72	102.43	110.50
1	C	176	THR	N-CA-C	5.71	118.23	111.33
1	A	116	VAL	N-CA-C	5.68	116.67	108.48
1	G	290	GLN	CA-C-N	5.67	126.92	119.84
1	G	290	GLN	C-N-CA	5.67	126.92	119.84
1	F	290	GLN	CA-C-N	5.66	126.92	119.84
1	F	290	GLN	C-N-CA	5.66	126.92	119.84
1	H	104	PHE	N-CA-C	-5.65	105.04	111.14
1	B	113	LYS	CA-C-N	5.65	125.58	119.76
1	B	113	LYS	C-N-CA	5.65	125.58	119.76
1	H	47	LYS	N-CA-C	-5.64	106.38	113.20
1	F	100	GLU	N-CA-C	5.64	120.17	113.12
1	A	229	ASP	N-CA-C	5.62	116.97	109.83
1	B	179	ALA	CA-C-N	5.59	126.83	119.84
1	B	179	ALA	C-N-CA	5.59	126.83	119.84
1	B	295	ALA	N-CA-C	-5.57	101.47	110.32
1	E	249	GLY	N-CA-C	5.52	121.96	112.51
1	G	89	VAL	N-CA-C	5.52	115.94	107.77
1	H	229	ASP	CA-C-N	5.49	128.53	120.46
1	H	229	ASP	C-N-CA	5.49	128.53	120.46
1	B	176	THR	N-CA-C	5.49	117.27	111.28
1	F	155	VAL	N-CA-C	5.48	116.00	107.99
1	B	114	PRO	N-CA-C	5.46	119.66	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	96	ASP	N-CA-C	5.46	118.15	111.82
1	H	285	PRO	CA-C-N	5.46	126.94	120.23
1	H	285	PRO	C-N-CA	5.46	126.94	120.23
1	F	160	ILE	CB-CA-C	-5.45	103.61	111.19
1	G	122	ARG	CA-C-N	5.44	125.44	119.89
1	G	122	ARG	C-N-CA	5.44	125.44	119.89
1	F	175	ASP	N-CA-C	-5.43	104.91	112.03
1	F	166	ILE	N-CA-C	5.43	117.02	109.80
1	B	283	ILE	N-CA-C	5.42	115.69	108.11
1	G	130	ASP	N-CA-C	5.39	118.08	111.82
1	B	314	THR	N-CA-C	5.39	115.48	107.88
1	D	245	ILE	N-CA-C	5.37	115.44	108.35
1	A	290	GLN	CA-C-N	5.37	125.37	120.21
1	A	290	GLN	C-N-CA	5.37	125.37	120.21
1	D	9	ILE	N-CA-C	5.37	114.47	106.85
1	F	171	ALA	N-CA-C	5.34	117.52	111.11
1	H	48	THR	N-CA-C	-5.33	106.36	112.92
1	C	114	PRO	N-CA-C	5.30	118.83	110.50
1	D	148	ARG	N-CA-C	5.28	118.00	110.24
1	G	171	ALA	N-CA-C	5.28	119.77	113.23
1	B	188	ILE	CB-CA-C	-5.26	104.69	111.53
1	G	284	VAL	N-CA-C	-5.26	101.97	107.60
1	H	155	VAL	N-CA-C	5.25	115.60	107.78
1	F	312	THR	N-CA-C	-5.23	106.74	113.23
1	F	176	THR	N-CA-C	5.22	118.75	112.38
1	D	166	ILE	N-CA-C	5.22	117.15	109.63
1	F	179	ALA	CA-C-N	5.20	126.34	119.84
1	F	179	ALA	C-N-CA	5.20	126.34	119.84
1	D	247	TYR	N-CA-C	5.19	117.89	107.41
1	B	212	THR	N-CA-C	5.16	119.05	112.34
1	F	284	VAL	CA-C-N	5.16	123.42	119.66
1	F	284	VAL	C-N-CA	5.16	123.42	119.66
1	G	38	THR	N-CA-C	5.16	116.59	110.97
1	B	203	HIS	N-CA-C	5.15	115.97	108.14
1	C	315	THR	N-CA-C	-5.14	106.93	114.39
1	D	188	ILE	N-CA-C	5.14	115.02	107.15
1	E	52	ILE	N-CA-C	5.13	117.22	108.86
1	H	227	GLN	N-CA-C	5.11	119.81	111.37
1	G	249	GLY	N-CA-C	5.09	120.94	112.89
1	E	65	MET	N-CA-C	-5.09	102.75	110.28
1	G	131	GLY	CA-C-N	5.09	124.53	119.24
1	G	131	GLY	C-N-CA	5.09	124.53	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	297	SER	N-CA-C	-5.08	104.37	110.88
1	B	155	VAL	N-CA-C	5.07	115.27	108.17
1	H	149	GLY	N-CA-C	-5.06	108.62	115.36
1	A	231	GLU	N-CA-C	-5.05	107.25	113.41
1	F	217	LEU	CA-C-N	5.04	124.97	119.78
1	F	217	LEU	C-N-CA	5.04	124.97	119.78
1	G	229	ASP	N-CA-C	5.04	116.18	109.93
1	G	283	ILE	N-CA-C	5.04	116.22	108.71
1	A	297	SER	N-CA-C	-5.03	105.44	112.03
1	A	189	ILE	N-CA-C	5.03	115.09	107.75
1	C	229	ASP	CA-C-N	5.01	124.92	119.85
1	C	229	ASP	C-N-CA	5.01	124.92	119.85
1	G	51	ASN	N-CA-C	-5.00	101.72	109.72
1	F	114	PRO	N-CA-C	5.00	118.73	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2468	103	0
1	B	2412	0	2468	91	0
1	C	2412	0	2468	133	0
1	D	2412	0	2468	138	0
1	E	2412	0	2468	97	0
1	F	2412	0	2468	116	0
1	G	2412	0	2468	153	0
1	H	2412	0	2468	138	0
All	All	19296	0	19744	915	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 (915) 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:G:17:ALA:HB1	1:G:34:LEU:HB3	1.19	1.12
1:H:62:SER:HB3	1:H:94:GLY:HA3	1.34	1.08
1:C:62:SER:HB2	1:C:94:GLY:HA3	1.35	1.06
1:F:283:ILE:HG22	1:F:285:PRO:HD3	1.36	1.05
1:B:174:LEU:H	1:B:174:LEU:HD23	1.20	1.04
1:E:170:ASN:HB3	1:E:176:THR:HG22	1.40	1.01
1:C:164:ARG:HD3	1:C:164:ARG:O	1.62	1.00
1:E:17:ALA:HA	1:E:34:LEU:HD12	1.45	0.99
1:A:228:ASP:HA	1:A:258:ARG:HH12	1.25	0.98
1:A:283:ILE:HD11	1:E:189:ILE:HG21	1.47	0.95
1:A:4:LEU:HD12	1:A:50:ALA:HA	1.48	0.95
1:C:19:SER:HB2	1:C:30:LYS:HB3	1.46	0.95
1:D:217:LEU:HD13	1:D:308:MET:HE3	1.47	0.95
1:E:17:ALA:HB1	1:E:34:LEU:HB2	1.46	0.95
1:A:164:ARG:O	1:A:164:ARG:HD3	1.67	0.94
1:E:218:PRO:HB3	1:E:243:LYS:HG3	1.49	0.94
1:A:4:LEU:HD23	1:A:4:LEU:H	1.32	0.94
1:F:16:ILE:HD13	1:F:16:ILE:O	1.67	0.94
1:C:160:ILE:HD11	1:C:188:ILE:HD11	1.50	0.93
1:E:62:SER:HB3	1:E:94:GLY:HA3	1.48	0.92
1:H:9:ILE:HG22	1:H:90:VAL:HB	1.49	0.92
1:H:226:TYR:HA	1:H:250:MET:HE3	1.51	0.91
1:C:314:THR:HG22	1:C:316:ASN:H	1.33	0.90
1:F:62:SER:HB2	1:F:94:GLY:HA3	1.55	0.89
1:C:283:ILE:H	1:C:283:ILE:CD1	1.87	0.88
1:G:188:ILE:HD13	1:G:193:ILE:HG12	1.55	0.88
1:A:189:ILE:HB	1:E:283:ILE:HD11	1.53	0.88
1:B:174:LEU:H	1:B:174:LEU:CD2	1.86	0.88
1:D:164:ARG:O	1:D:164:ARG:HD3	1.72	0.87
1:A:63:GLU:HA	1:F:250:MET:CE	2.05	0.87
1:A:63:GLU:HA	1:F:250:MET:HE1	1.56	0.87
1:A:245:ILE:HB	1:A:273:VAL:HG22	1.56	0.87
1:G:21:ALA:HB3	1:G:25:GLN:HE22	1.37	0.86
1:D:321:GLN:HE21	1:D:321:GLN:HA	1.42	0.85
1:H:164:ARG:HD3	1:H:164:ARG:O	1.76	0.85
1:B:62:SER:HB2	1:B:94:GLY:HA3	1.57	0.85
1:C:23:ASN:HB3	1:C:127:ILE:HG12	1.59	0.85
1:B:121:MET:HE1	1:B:168:LYS:NZ	1.92	0.84
1:C:52:ILE:HD13	1:C:52:ILE:H	1.40	0.84
1:E:22:ALA:HB3	1:E:25:GLN:HB2	1.59	0.83
1:C:229:ASP:H	1:C:258:ARG:HH21	1.25	0.83
1:E:73:LEU:O	1:E:77:VAL:HG23	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ILE:HD11	1:G:189:ILE:HG13	1.61	0.81
1:G:60:ILE:HD13	1:G:60:ILE:H	1.43	0.81
1:F:121:MET:HB2	1:F:174:LEU:HD12	1.59	0.81
1:D:188:ILE:HG12	1:D:193:ILE:HD13	1.62	0.81
1:C:11:ALA:HB3	1:C:56:GLN:HA	1.62	0.81
1:H:16:ILE:HD13	1:H:16:ILE:O	1.79	0.80
1:G:116:VAL:HG12	1:G:153:LEU:HB2	1.62	0.80
1:C:283:ILE:H	1:C:283:ILE:HD13	1.45	0.80
1:D:8:VAL:HG22	1:D:53:LYS:HB3	1.63	0.80
1:H:165:PHE:CG	1:H:182:GLU:HG2	2.18	0.79
1:D:17:ALA:HB2	1:D:39:LEU:HD11	1.64	0.79
1:D:263:ILE:HG23	1:D:273:VAL:HG11	1.63	0.79
1:B:250:MET:HE2	1:E:97:THR:HG22	1.64	0.78
1:B:249:GLY:HA3	1:B:253:GLY:HA2	1.66	0.77
1:E:188:ILE:C	1:E:189:ILE:HD12	2.10	0.77
1:C:97:THR:HG22	1:H:250:MET:HE2	1.67	0.77
1:B:73:LEU:O	1:B:77:VAL:HG22	1.85	0.77
1:E:9:ILE:HD13	1:E:90:VAL:HB	1.67	0.76
1:F:77:VAL:O	1:F:81:LEU:HD13	1.86	0.76
1:C:101:SER:HB2	1:C:102:PRO:HD3	1.65	0.76
1:C:36:VAL:HG11	1:C:54:GLY:HA3	1.68	0.76
1:A:4:LEU:H	1:A:4:LEU:CD2	1.98	0.75
1:D:63:GLU:HB2	1:G:250:MET:HE3	1.68	0.75
1:D:251:GLY:HA3	1:G:96:ASP:OD1	1.87	0.74
1:F:243:LYS:HG3	1:F:311:LEU:HD23	1.69	0.74
1:G:73:LEU:O	1:G:77:VAL:HG23	1.87	0.74
1:G:22:ALA:HB3	1:G:25:GLN:HB3	1.69	0.74
1:H:320:ILE:HA	1:H:323:TYR:HD1	1.52	0.74
1:H:220:VAL:CG2	1:H:304:ARG:HG3	2.18	0.74
1:E:263:ILE:HD12	1:E:273:VAL:HG11	1.68	0.73
1:G:127:ILE:HD13	1:G:127:ILE:H	1.53	0.73
1:C:160:ILE:HD11	1:C:188:ILE:CD1	2.19	0.73
1:E:163:ALA:O	1:E:302:LYS:HE2	1.89	0.73
1:A:4:LEU:HD12	1:A:50:ALA:CA	2.18	0.73
1:B:237:SER:HB3	1:B:242:VAL:HG21	1.69	0.72
1:B:276:SER:OG	1:B:300:PRO:HD3	1.89	0.72
1:A:19:SER:O	1:A:29:TYR:HB2	1.88	0.72
1:D:304:ARG:NH2	1:G:228:ASP:HB2	2.03	0.72
1:C:283:ILE:CD1	1:G:189:ILE:HG13	2.18	0.72
1:A:4:LEU:HD23	1:A:4:LEU:N	2.04	0.72
1:A:80:LEU:O	1:A:86:VAL:HG11	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:THR:HG22	1:F:127:ILE:HD11	1.70	0.72
1:G:62:SER:HB3	1:G:94:GLY:HA3	1.72	0.72
1:B:226:TYR:HA	1:B:250:MET:HE3	1.73	0.71
1:G:9:ILE:N	1:G:9:ILE:HD12	2.05	0.71
1:G:218:PRO:HB3	1:G:243:LYS:HG3	1.71	0.71
1:A:230:PRO:HB3	1:A:232:TYR:CE2	2.25	0.71
1:E:235:ASP:HA	1:E:238:ILE:HD12	1.71	0.71
1:H:316:ASN:HD21	1:H:318:ALA:HB3	1.55	0.70
1:C:221:ASP:OD2	1:C:242:VAL:HG11	1.91	0.70
1:F:199:LEU:HD22	1:F:200:ASP:N	2.07	0.70
1:D:217:LEU:HD23	1:D:218:PRO:HD2	1.74	0.70
1:H:235:ASP:O	1:H:239:LYS:HG2	1.91	0.70
1:D:21:ALA:HB3	1:D:25:GLN:OE1	1.92	0.70
1:D:200:ASP:OD1	1:H:198:ARG:HD2	1.91	0.69
1:D:237:SER:HB3	1:D:242:VAL:HG21	1.74	0.69
1:A:97:THR:HG23	1:F:250:MET:HE3	1.72	0.69
1:H:121:MET:HE1	1:H:168:LYS:NZ	2.07	0.69
1:F:263:ILE:HG23	1:F:273:VAL:HG11	1.74	0.69
1:B:8:VAL:HG22	1:B:53:LYS:HD3	1.75	0.69
1:G:133:MET:HE2	1:H:127:ILE:HB	1.73	0.69
1:F:219:ALA:O	1:F:242:VAL:HG23	1.93	0.69
1:G:42:ALA:C	1:G:44:PRO:HD3	2.17	0.69
1:E:17:ALA:CA	1:E:34:LEU:HD12	2.23	0.68
1:D:93:HIS:HB3	1:D:98:LEU:HD23	1.75	0.68
1:A:238:ILE:HD11	1:A:266:ALA:HB2	1.75	0.68
1:A:45:GLU:H	1:A:45:GLU:CD	2.02	0.68
1:E:234:TYR:O	1:E:238:ILE:HG13	1.94	0.68
1:D:75:LYS:HD2	1:D:75:LYS:C	2.18	0.68
1:G:202:VAL:HG22	1:G:326:ALA:O	1.94	0.68
1:G:60:ILE:HD13	1:G:60:ILE:N	2.09	0.68
1:A:239:LYS:HG2	1:A:239:LYS:O	1.93	0.67
1:D:19:SER:O	1:D:29:TYR:HB2	1.94	0.67
1:H:316:ASN:ND2	1:H:318:ALA:HB3	2.09	0.67
1:C:71:LEU:HD12	1:C:211:VAL:HG11	1.75	0.67
1:H:220:VAL:HG23	1:H:304:ARG:HG3	1.76	0.67
1:C:98:LEU:HD12	1:C:177:PHE:CE1	2.29	0.67
1:H:116:VAL:HG22	1:H:153:LEU:HD21	1.75	0.67
1:H:320:ILE:HA	1:H:323:TYR:CD1	2.29	0.67
1:F:170:ASN:HB3	1:F:173:THR:HG22	1.75	0.67
1:A:188:ILE:C	1:A:189:ILE:HD12	2.20	0.67
1:A:283:ILE:HD11	1:E:189:ILE:CG2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLU:HB3	1:C:305:ILE:HD11	1.75	0.66
1:D:116:VAL:HG12	1:D:153:LEU:HB2	1.76	0.66
1:G:9:ILE:HD13	1:G:52:ILE:HG23	1.76	0.66
1:G:36:VAL:HG21	1:G:54:GLY:HA3	1.77	0.66
1:A:228:ASP:HA	1:A:258:ARG:NH1	2.06	0.66
1:B:121:MET:HE1	1:B:168:LYS:HZ1	1.59	0.66
1:F:55:GLU:CD	1:F:76:ARG:HH21	2.04	0.66
1:F:73:LEU:O	1:F:77:VAL:HG13	1.95	0.66
1:C:76:ARG:O	1:C:76:ARG:HD3	1.96	0.65
1:G:127:ILE:HD13	1:G:127:ILE:N	2.10	0.65
1:B:283:ILE:HD12	1:F:189:ILE:HD12	1.78	0.65
1:F:157:ASN:O	1:F:158:ASP:HB2	1.97	0.65
1:A:127:ILE:HB	1:B:133:MET:HE2	1.78	0.65
1:B:174:LEU:HD23	1:B:174:LEU:N	2.01	0.65
1:D:230:PRO:HB2	1:D:232:TYR:CE2	2.31	0.64
1:F:6:ASN:HB3	1:F:51:ASN:HB2	1.79	0.64
1:B:251:GLY:C	1:B:253:GLY:H	2.03	0.64
1:C:52:ILE:HD13	1:C:52:ILE:N	2.11	0.64
1:H:165:PHE:CD1	1:H:182:GLU:HG2	2.32	0.64
1:C:98:LEU:HD13	1:C:98:LEU:O	1.98	0.64
1:D:17:ALA:C	1:D:34:LEU:HD22	2.23	0.64
1:G:76:ARG:HE	1:G:80:LEU:HG	1.63	0.64
1:C:62:SER:CB	1:C:94:GLY:HA3	2.21	0.64
1:F:244:GLY:H	1:F:271:ILE:CD1	2.10	0.64
1:C:73:LEU:O	1:C:77:VAL:HG23	1.98	0.64
1:C:16:ILE:HG23	1:C:17:ALA:H	1.62	0.64
1:C:44:PRO:O	1:C:47:LYS:HG2	1.97	0.64
1:H:304:ARG:O	1:H:308:MET:HG3	1.98	0.63
1:B:250:MET:CE	1:E:97:THR:HG22	2.28	0.63
1:C:314:THR:HG22	1:C:316:ASN:N	2.10	0.63
1:C:97:THR:HG22	1:H:250:MET:CE	2.28	0.63
1:D:158:ASP:O	1:D:187:VAL:HG23	1.96	0.63
1:E:173:THR:O	1:E:176:THR:HG23	1.97	0.63
1:F:238:ILE:HD11	1:F:266:ALA:HB2	1.79	0.63
1:G:9:ILE:CD1	1:G:52:ILE:HG23	2.28	0.63
1:G:157:ASN:O	1:G:159:ARG:HG2	1.99	0.63
1:H:17:ALA:HA	1:H:39:LEU:HD11	1.79	0.63
1:H:24:THR:HG22	1:H:127:ILE:HD11	1.79	0.63
1:C:65:MET:SD	1:C:69:VAL:HG11	2.39	0.63
1:E:306:LEU:HD13	1:E:324:PHE:CE1	2.33	0.63
1:F:46:LEU:HB3	1:F:52:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:GLN:HG2	1:G:26:THR:N	2.14	0.63
1:B:17:ALA:HB2	1:B:39:LEU:HD11	1.80	0.62
1:B:36:VAL:HG13	1:B:37:GLU:H	1.63	0.62
1:F:206:ARG:HH11	1:F:206:ARG:HG2	1.64	0.62
1:F:244:GLY:H	1:F:271:ILE:HD11	1.64	0.62
1:D:108:THR:HG21	1:D:211:VAL:HG21	1.82	0.62
1:A:101:SER:HB2	1:A:102:PRO:HD3	1.81	0.62
1:D:182:GLU:O	1:H:183:GLY:HA3	1.98	0.62
1:B:242:VAL:HG12	1:B:244:GLY:H	1.64	0.62
1:E:4:LEU:HD22	1:E:49:LEU:O	1.99	0.62
1:E:76:ARG:O	1:E:80:LEU:HD12	1.99	0.62
1:E:165:PHE:CD1	1:E:182:GLU:HG2	2.35	0.61
1:G:21:ALA:HB3	1:G:25:GLN:NE2	2.12	0.61
1:D:13:GLY:N	1:D:59:SER:HA	2.15	0.61
1:A:197:THR:HG23	1:E:197:THR:OG1	1.99	0.61
1:G:170:ASN:HB3	1:G:173:THR:HG22	1.82	0.61
1:D:230:PRO:HB2	1:D:232:TYR:CD2	2.36	0.61
1:G:188:ILE:HD12	1:G:192:LYS:O	1.99	0.61
1:G:223:ILE:HG21	1:G:234:TYR:HE1	1.64	0.61
1:A:5:PRO:O	1:A:50:ALA:HB1	2.00	0.61
1:C:283:ILE:CD1	1:C:283:ILE:N	2.60	0.61
1:H:90:VAL:O	1:H:91:ILE:HD12	2.01	0.61
1:F:280:GLY:O	1:F:281:SER:HB3	2.01	0.61
1:D:311:LEU:C	1:D:313:LYS:H	2.09	0.61
1:B:174:LEU:CD2	1:B:174:LEU:N	2.60	0.61
1:D:98:LEU:HD13	1:D:98:LEU:O	2.01	0.61
1:F:187:VAL:HG12	1:F:189:ILE:HG13	1.84	0.60
1:B:101:SER:HB2	1:B:102:PRO:HD3	1.83	0.60
1:G:77:VAL:O	1:G:81:LEU:HD13	2.01	0.60
1:F:44:PRO:O	1:F:47:LYS:HG2	2.02	0.60
1:B:189:ILE:HD12	1:F:283:ILE:HD12	1.83	0.60
1:G:310:ALA:HB1	1:G:320:ILE:CD1	2.31	0.60
1:F:229:ASP:O	1:F:258:ARG:NE	2.34	0.60
1:B:63:GLU:CD	1:B:63:GLU:H	2.09	0.60
1:G:276:SER:OG	1:G:300:PRO:HG3	2.01	0.60
1:A:304:ARG:NH2	1:F:228:ASP:HB2	2.17	0.60
1:F:283:ILE:HG22	1:F:285:PRO:CD	2.24	0.60
1:G:17:ALA:CB	1:G:34:LEU:HB3	2.12	0.60
1:H:46:LEU:HG	1:H:52:ILE:HD11	1.83	0.60
1:H:237:SER:O	1:H:242:VAL:HG23	2.02	0.60
1:F:83:ARG:HB3	1:F:85:ASP:OD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ALA:HA	1:H:34:LEU:HD23	1.84	0.59
1:C:66:THR:O	1:C:69:VAL:HG12	2.01	0.59
1:E:166:ILE:HG22	1:E:167:SER:N	2.17	0.59
1:E:275:ARG:HH12	1:E:290:GLN:HB2	1.67	0.59
1:E:283:ILE:HG22	1:E:297:SER:HB3	1.83	0.59
1:G:24:THR:HG21	1:H:136:TYR:CE1	2.37	0.59
1:G:162:SER:O	1:G:166:ILE:HG12	2.02	0.59
1:B:162:SER:HB2	1:B:185:LEU:HD21	1.83	0.59
1:C:314:THR:HG22	1:C:315:THR:N	2.17	0.59
1:D:71:LEU:HD11	1:D:217:LEU:CD1	2.32	0.59
1:A:97:THR:CG2	1:F:250:MET:HE3	2.32	0.59
1:C:45:GLU:H	1:C:45:GLU:CD	2.11	0.59
1:A:123:PRO:HD2	1:A:126:ALA:HB2	1.85	0.59
1:C:191:ASP:O	1:C:192:LYS:HG3	2.03	0.59
1:A:60:ILE:HD13	1:A:60:ILE:H	1.67	0.59
1:C:34:LEU:HD12	1:C:34:LEU:H	1.67	0.59
1:B:51:ASN:N	1:B:51:ASN:HD22	1.99	0.58
1:A:189:ILE:HD12	1:A:189:ILE:N	2.17	0.58
1:C:7:ILE:HG23	1:C:88:GLY:O	2.03	0.58
1:E:43:VAL:HG12	1:E:46:LEU:HG	1.84	0.58
1:G:36:VAL:HG13	1:G:37:GLU:H	1.68	0.58
1:D:24:THR:HG22	1:D:127:ILE:HD11	1.84	0.58
1:H:81:LEU:HD11	1:H:113:LYS:CB	2.33	0.58
1:H:208:VAL:HG23	1:H:209:PHE:N	2.17	0.58
1:C:133:MET:HE2	1:D:127:ILE:HB	1.84	0.58
1:D:80:LEU:O	1:D:86:VAL:HG21	2.03	0.58
1:F:199:LEU:HD22	1:F:200:ASP:H	1.66	0.58
1:B:279:THR:HG22	1:E:168:LYS:O	2.04	0.58
1:C:283:ILE:HD13	1:C:283:ILE:N	2.13	0.58
1:D:249:GLY:O	1:D:278:ARG:HG2	2.04	0.58
1:E:260:ASP:O	1:E:264:ARG:HG3	2.03	0.58
1:G:310:ALA:HB1	1:G:320:ILE:HD12	1.86	0.58
1:A:169:THR:HB	1:A:176:THR:O	2.04	0.58
1:F:11:ALA:HA	1:F:92:THR:OG1	2.03	0.57
1:G:243:LYS:HB3	1:G:311:LEU:HD13	1.86	0.57
1:A:172:SER:HB2	1:B:189:ILE:HD13	1.87	0.57
1:E:217:LEU:HD13	1:E:308:MET:HE3	1.85	0.57
1:A:105:LEU:O	1:A:109:VAL:HG13	2.04	0.57
1:C:45:GLU:CD	1:C:45:GLU:N	2.63	0.57
1:F:243:LYS:HZ2	1:F:271:ILE:HA	1.68	0.57
1:F:115:VAL:HG11	1:F:152:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:C	1:C:41:GLN:H	2.11	0.57
1:H:34:LEU:HD23	1:H:39:LEU:HD11	1.87	0.57
1:D:304:ARG:HH22	1:G:228:ASP:HB2	1.68	0.57
1:F:243:LYS:NZ	1:F:271:ILE:HA	2.20	0.57
1:H:37:GLU:OE1	1:H:40:ILE:HG13	2.04	0.57
1:G:140:LYS:HG3	1:G:193:ILE:HD11	1.86	0.57
1:H:211:VAL:O	1:H:211:VAL:HG22	2.03	0.57
1:C:296:ASP:HB2	1:C:324:PHE:O	2.05	0.57
1:D:238:ILE:HD11	1:D:269:LYS:CG	2.34	0.57
1:G:243:LYS:O	1:G:271:ILE:HG23	2.04	0.57
1:A:71:LEU:HD11	1:A:211:VAL:HB	1.86	0.56
1:B:9:ILE:HG13	1:B:9:ILE:O	2.05	0.56
1:D:233:MET:O	1:D:236:ALA:HB3	2.05	0.56
1:H:220:VAL:HG21	1:H:304:ARG:HG3	1.85	0.56
1:C:145:LYS:HD3	1:C:148:ARG:NH1	2.20	0.56
1:D:315:THR:O	1:D:315:THR:HG22	2.05	0.56
1:A:208:VAL:HG13	1:A:208:VAL:O	2.04	0.56
1:C:36:VAL:HG11	1:C:54:GLY:CA	2.34	0.56
1:D:32:GLY:HA2	1:D:59:SER:HB3	1.85	0.56
1:D:238:ILE:HD11	1:D:269:LYS:HG2	1.87	0.56
1:F:52:ILE:HG22	1:F:53:LYS:N	2.21	0.56
1:F:244:GLY:N	1:F:271:ILE:HG13	2.21	0.56
1:G:262:GLY:O	1:G:265:LYS:HB3	2.05	0.56
1:H:5:PRO:O	1:H:50:ALA:HB1	2.05	0.56
1:G:223:ILE:HG21	1:G:234:TYR:CE1	2.40	0.56
1:G:234:TYR:O	1:G:238:ILE:HG13	2.06	0.56
1:H:42:ALA:O	1:H:44:PRO:HD3	2.05	0.56
1:E:76:ARG:NE	1:E:80:LEU:HD11	2.20	0.56
1:E:97:THR:C	1:E:99:ASP:H	2.13	0.56
1:D:321:GLN:HE21	1:D:321:GLN:CA	2.12	0.56
1:A:283:ILE:HD13	1:A:283:ILE:O	2.06	0.56
1:D:151:GLY:HA2	1:D:204:THR:HG23	1.88	0.56
1:B:20:ALA:HB3	1:B:125:THR:OG1	2.06	0.56
1:E:62:SER:CB	1:E:94:GLY:HA3	2.29	0.56
1:H:188:ILE:O	1:H:189:ILE:HD13	2.05	0.56
1:A:83:ARG:HB2	1:A:86:VAL:HG12	1.88	0.55
1:F:62:SER:HB3	1:F:96:ASP:HB2	1.88	0.55
1:H:90:VAL:C	1:H:91:ILE:HD12	2.31	0.55
1:A:95:THR:HG21	1:A:121:MET:HE3	1.86	0.55
1:B:106:ASN:HA	1:B:152:VAL:HG23	1.88	0.55
1:B:199:LEU:HD11	1:B:201:LYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HD3	1:C:76:ARG:C	2.31	0.55
1:F:36:VAL:HG21	1:F:54:GLY:HA3	1.88	0.55
1:G:45:GLU:N	1:G:45:GLU:OE1	2.39	0.55
1:H:153:LEU:HD23	1:H:153:LEU:O	2.06	0.55
1:G:166:ILE:HG22	1:G:167:SER:N	2.21	0.55
1:G:118:VAL:HG22	1:G:138:ALA:CB	2.37	0.55
1:H:81:LEU:HD11	1:H:113:LYS:HB3	1.88	0.55
1:B:4:LEU:HB2	1:B:51:ASN:HD21	1.71	0.55
1:G:66:THR:OG1	1:G:67:SER:N	2.40	0.55
1:B:15:THR:HB	1:B:120:ALA:O	2.07	0.55
1:A:157:ASN:O	1:A:158:ASP:HB2	2.05	0.55
1:C:147:SER:HA	1:C:150:ARG:HD2	1.88	0.55
1:D:121:MET:HA	1:D:121:MET:HE2	1.89	0.55
1:G:17:ALA:HA	1:G:34:LEU:HD23	1.88	0.55
1:C:127:ILE:O	1:D:133:MET:HE2	2.07	0.55
1:H:52:ILE:HG22	1:H:53:LYS:N	2.22	0.54
1:B:247:TYR:CE2	1:B:255:VAL:HG12	2.41	0.54
1:C:209:PHE:HZ	1:C:323:TYR:CD2	2.25	0.54
1:E:314:THR:OG1	1:E:315:THR:N	2.37	0.54
1:B:263:ILE:HG21	1:B:291:PRO:HB2	1.90	0.54
1:G:127:ILE:H	1:G:127:ILE:CD1	2.19	0.54
1:G:268:SER:C	1:G:270:GLY:H	2.14	0.54
1:H:316:ASN:O	1:H:319:VAL:HG22	2.06	0.54
1:A:36:VAL:O	1:A:40:ILE:HG13	2.08	0.54
1:H:119:ALA:O	1:H:156:LEU:HD21	2.07	0.54
1:H:46:LEU:HD12	1:H:139:VAL:HG21	1.88	0.54
1:H:134:ASN:CG	1:H:156:LEU:HD23	2.32	0.54
1:E:218:PRO:HB3	1:E:243:LYS:CG	2.28	0.54
1:H:45:GLU:O	1:H:48:THR:HG23	2.08	0.54
1:H:22:ALA:HB3	1:H:25:GLN:HG2	1.90	0.54
1:B:242:VAL:HG11	1:B:245:ILE:HD13	1.90	0.54
1:E:316:ASN:O	1:E:320:ILE:HG12	2.08	0.54
1:F:293:LEU:N	1:F:293:LEU:HD12	2.22	0.54
1:C:283:ILE:HG12	1:G:189:ILE:HG21	1.89	0.54
1:B:227:GLN:HE21	1:E:65:MET:HB3	1.73	0.53
1:C:305:ILE:HA	1:C:308:MET:HE2	1.90	0.53
1:G:36:VAL:HG13	1:G:37:GLU:N	2.23	0.53
1:E:57:VAL:O	1:E:58:ALA:HB2	2.08	0.53
1:A:304:ARG:HH22	1:F:228:ASP:HB2	1.72	0.53
1:B:81:LEU:HD13	1:B:111:SER:HB3	1.90	0.53
1:C:63:GLU:CD	1:C:63:GLU:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:GLY:HA2	1:F:272:VAL:O	2.09	0.53
1:H:11:ALA:O	1:H:57:VAL:HG12	2.08	0.53
1:B:155:VAL:O	1:B:156:LEU:HG	2.08	0.53
1:C:211:VAL:HG13	1:C:214:VAL:HB	1.90	0.53
1:E:127:ILE:HG22	1:F:133:MET:HB2	1.91	0.53
1:G:76:ARG:HD3	1:G:76:ARG:C	2.33	0.53
1:G:175:ASP:O	1:G:178:LYS:HE3	2.09	0.53
1:G:81:LEU:O	1:G:113:LYS:NZ	2.42	0.53
1:A:159:ARG:NH2	1:B:173:THR:HG21	2.23	0.53
1:D:40:ILE:CG2	1:D:47:LYS:HE3	2.39	0.53
1:G:101:SER:HB2	1:G:102:PRO:HD3	1.89	0.53
1:A:141:VAL:HG23	1:A:142:ALA:N	2.23	0.53
1:D:95:THR:HG21	1:D:121:MET:HE3	1.90	0.53
1:C:164:ARG:HD3	1:C:164:ARG:C	2.31	0.53
1:D:234:TYR:O	1:D:238:ILE:HG22	2.08	0.53
1:E:208:VAL:HG13	1:E:313:LYS:NZ	2.24	0.53
1:F:80:LEU:HD12	1:F:83:ARG:HD3	1.90	0.53
1:H:11:ALA:HA	1:H:92:THR:OG1	2.09	0.53
1:B:12:THR:HG23	1:B:58:ALA:HB3	1.90	0.53
1:D:71:LEU:HD11	1:D:217:LEU:HD11	1.90	0.53
1:E:38:THR:O	1:E:41:GLN:HG2	2.08	0.53
1:F:316:ASN:O	1:F:320:ILE:HG13	2.09	0.53
1:A:86:VAL:HG13	1:A:86:VAL:O	2.08	0.52
1:C:12:THR:CG2	1:C:65:MET:HE1	2.39	0.52
1:C:133:MET:CE	1:D:127:ILE:HB	2.38	0.52
1:D:110:LYS:HE2	1:D:207:SER:O	2.08	0.52
1:G:67:SER:HA	1:G:70:LEU:HB2	1.91	0.52
1:C:69:VAL:HG13	1:C:70:LEU:N	2.23	0.52
1:D:35:GLY:HA2	1:D:56:GLN:OE1	2.09	0.52
1:E:235:ASP:O	1:E:239:LYS:HG3	2.08	0.52
1:F:234:TYR:O	1:F:238:ILE:HG13	2.09	0.52
1:C:141:VAL:HG23	1:C:142:ALA:N	2.24	0.52
1:G:259:GLY:O	1:G:263:ILE:HG12	2.09	0.52
1:C:191:ASP:C	1:C:192:LYS:HG3	2.35	0.52
1:D:188:ILE:HG12	1:D:193:ILE:CD1	2.36	0.52
1:F:275:ARG:HB2	1:F:293:LEU:O	2.09	0.52
1:A:90:VAL:O	1:A:91:ILE:HD13	2.09	0.52
1:C:23:ASN:HB3	1:C:127:ILE:CG1	2.34	0.52
1:D:15:THR:HG23	1:D:29:TYR:HE2	1.73	0.52
1:D:217:LEU:CD2	1:D:218:PRO:HD2	2.39	0.52
1:G:314:THR:OG1	1:G:315:THR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:ASP:O	1:H:178:LYS:HE3	2.09	0.52
1:C:208:VAL:HG12	1:C:327:TYR:OH	2.09	0.52
1:D:76:ARG:HG3	1:D:76:ARG:HH11	1.75	0.52
1:H:229:ASP:OD1	1:H:258:ARG:NH2	2.41	0.52
1:D:23:ASN:O	1:D:25:GLN:N	2.42	0.52
1:E:17:ALA:CB	1:E:34:LEU:HB2	2.30	0.52
1:E:146:ASN:O	1:E:150:ARG:NH1	2.42	0.52
1:E:146:ASN:ND2	1:E:150:ARG:HH12	2.08	0.52
1:A:4:LEU:CD1	1:A:50:ALA:HA	2.32	0.52
1:E:27:THR:HG22	1:E:28:GLY:N	2.25	0.52
1:H:316:ASN:HB3	1:H:319:VAL:HG22	1.91	0.52
1:H:41:GLN:O	1:H:44:PRO:HG3	2.10	0.52
1:B:103:TYR:O	1:B:107:LEU:HD13	2.10	0.51
1:F:210:ASP:OD1	1:F:212:THR:HB	2.10	0.51
1:B:123:PRO:HD2	1:B:126:ALA:HB2	1.92	0.51
1:E:76:ARG:HG3	1:E:80:LEU:HD11	1.92	0.51
1:G:17:ALA:HB2	1:G:39:LEU:HD11	1.92	0.51
1:G:155:VAL:HG22	1:G:160:ILE:HD13	1.93	0.51
1:H:316:ASN:O	1:H:320:ILE:HG13	2.11	0.51
1:A:62:SER:HB3	1:A:97:THR:H	1.74	0.51
1:G:9:ILE:N	1:G:9:ILE:CD1	2.72	0.51
1:H:20:ALA:HB3	1:H:125:THR:OG1	2.10	0.51
1:C:19:SER:OG	1:C:33:ALA:HB3	2.11	0.51
1:B:251:GLY:C	1:B:253:GLY:N	2.68	0.51
1:G:220:VAL:CG2	1:G:308:MET:HG2	2.41	0.51
1:B:208:VAL:HG22	1:B:327:TYR:OH	2.10	0.51
1:D:237:SER:C	1:D:239:LYS:H	2.17	0.51
1:H:46:LEU:O	1:H:49:LEU:HB2	2.10	0.51
1:A:38:THR:HA	1:A:41:GLN:HG2	1.93	0.51
1:C:209:PHE:HZ	1:C:323:TYR:HD2	1.59	0.51
1:E:5:PRO:O	1:E:50:ALA:HB1	2.10	0.51
1:F:237:SER:O	1:F:242:VAL:HG12	2.10	0.51
1:E:45:GLU:OE1	1:E:45:GLU:N	2.33	0.51
1:A:261:ALA:O	1:A:265:LYS:HB2	2.10	0.51
1:G:203:HIS:CD2	1:G:204:THR:OG1	2.64	0.51
1:G:231:GLU:C	1:G:233:MET:H	2.19	0.51
1:G:277:SER:HB2	1:G:279:THR:HG23	1.91	0.51
1:E:230:PRO:HG2	1:E:233:MET:HB2	1.93	0.50
1:F:255:VAL:HG12	1:F:256:SER:O	2.11	0.50
1:G:3:ASN:C	1:G:4:LEU:HD23	2.36	0.50
1:H:46:LEU:HB2	1:H:49:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:VAL:HG12	1:D:115:VAL:HG22	1.94	0.50
1:D:101:SER:HB2	1:D:102:PRO:HD3	1.94	0.50
1:H:7:ILE:HD11	1:H:143:ALA:HA	1.92	0.50
1:H:43:VAL:O	1:H:46:LEU:CD2	2.59	0.50
1:H:166:ILE:HG22	1:H:167:SER:N	2.26	0.50
1:C:19:SER:CB	1:C:30:LYS:HB3	2.32	0.50
1:C:208:VAL:HG22	1:C:313:LYS:HE2	1.93	0.50
1:C:229:ASP:N	1:C:258:ARG:HH21	2.01	0.50
1:F:6:ASN:CB	1:F:51:ASN:HB2	2.42	0.50
1:G:62:SER:HB3	1:G:94:GLY:CA	2.40	0.50
1:G:181:GLU:HB3	1:G:182:GLU:OE2	2.11	0.50
1:G:264:ARG:HG2	1:G:264:ARG:HH11	1.76	0.50
1:A:81:LEU:HD22	1:A:113:LYS:HB2	1.93	0.50
1:B:323:TYR:HD2	1:B:327:TYR:HE2	1.60	0.50
1:C:305:ILE:O	1:C:308:MET:HB3	2.11	0.50
1:A:16:ILE:HG12	1:A:16:ILE:O	2.10	0.50
1:A:263:ILE:HD12	1:A:273:VAL:HG11	1.94	0.50
1:E:23:ASN:O	1:E:127:ILE:N	2.44	0.50
1:E:33:ALA:O	1:E:34:LEU:HD23	2.12	0.50
1:D:203:HIS:HD2	1:D:204:THR:HG23	1.76	0.50
1:H:264:ARG:NE	1:H:291:PRO:HG3	2.27	0.50
1:D:78:ASN:O	1:D:80:LEU:N	2.41	0.50
1:D:111:SER:N	1:D:205:THR:HG22	2.27	0.50
1:G:37:GLU:O	1:G:41:GLN:HG2	2.12	0.50
1:H:226:TYR:CA	1:H:250:MET:HE3	2.31	0.50
1:A:237:SER:HB3	1:A:242:VAL:HG21	1.94	0.50
1:F:264:ARG:CZ	1:F:291:PRO:HG3	2.42	0.50
1:H:320:ILE:C	1:H:322:ASP:H	2.18	0.50
1:C:166:ILE:HG22	1:C:167:SER:N	2.26	0.49
1:D:152:VAL:O	1:D:153:LEU:HD23	2.12	0.49
1:A:96:ASP:OD1	1:F:251:GLY:HA3	2.13	0.49
1:C:187:VAL:HG22	1:C:188:ILE:N	2.27	0.49
1:F:101:SER:HB2	1:F:102:PRO:HD3	1.94	0.49
1:H:36:VAL:HG22	1:H:36:VAL:O	2.12	0.49
1:B:121:MET:HE1	1:B:168:LYS:HZ2	1.74	0.49
1:D:12:THR:HA	1:D:58:ALA:O	2.12	0.49
1:C:261:ALA:O	1:C:265:LYS:HG3	2.11	0.49
1:D:230:PRO:CB	1:D:232:TYR:CE2	2.94	0.49
1:A:45:GLU:CD	1:A:45:GLU:N	2.70	0.49
1:B:8:VAL:CG2	1:B:53:LYS:HD3	2.42	0.49
1:D:183:GLY:HA3	1:H:182:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:THR:OG1	1:D:315:THR:N	2.46	0.49
1:H:63:GLU:CD	1:H:63:GLU:H	2.21	0.49
1:E:238:ILE:C	1:E:240:HIS:H	2.20	0.49
1:G:23:ASN:HD22	1:H:45:GLU:HG2	1.77	0.49
1:G:29:TYR:CE2	1:G:123:PRO:HG3	2.48	0.49
1:H:60:ILE:HG22	1:H:61:GLY:H	1.78	0.49
1:B:188:ILE:HG12	1:B:193:ILE:CD1	2.43	0.49
1:B:314:THR:OG1	1:B:315:THR:N	2.46	0.49
1:C:71:LEU:HD12	1:C:211:VAL:CG1	2.43	0.49
1:E:167:SER:O	1:E:177:PHE:HA	2.12	0.49
1:G:42:ALA:O	1:G:44:PRO:HD3	2.12	0.49
1:G:118:VAL:HG22	1:G:138:ALA:HB2	1.94	0.49
1:B:315:THR:O	1:B:315:THR:HG22	2.11	0.49
1:D:75:LYS:HD2	1:D:76:ARG:N	2.27	0.49
1:G:209:PHE:HZ	1:G:323:TYR:CD2	2.31	0.49
1:A:23:ASN:ND2	1:A:127:ILE:HG12	2.28	0.49
1:B:188:ILE:HG12	1:B:193:ILE:HD13	1.95	0.49
1:C:15:THR:HG23	1:C:29:TYR:OH	2.12	0.49
1:D:89:VAL:CG1	1:D:115:VAL:HG22	2.43	0.49
1:D:93:HIS:CD2	1:D:98:LEU:HD23	2.48	0.49
1:D:111:SER:C	1:D:113:LYS:H	2.21	0.49
1:H:85:ASP:OD1	1:H:86:VAL:HG23	2.13	0.49
1:H:321:GLN:HG3	1:H:321:GLN:O	2.13	0.49
1:A:189:ILE:CB	1:E:283:ILE:HD11	2.35	0.48
1:E:43:VAL:CG1	1:E:46:LEU:HG	2.43	0.48
1:E:38:THR:O	1:E:41:GLN:N	2.47	0.48
1:B:24:THR:HG22	1:B:127:ILE:HD11	1.95	0.48
1:D:24:THR:HG22	1:D:127:ILE:CD1	2.43	0.48
1:D:155:VAL:O	1:D:156:LEU:HB2	2.13	0.48
1:E:24:THR:HG22	1:E:127:ILE:HB	1.96	0.48
1:H:319:VAL:HG23	1:H:320:ILE:N	2.28	0.48
1:C:144:ASP:OD1	1:C:146:ASN:N	2.46	0.48
1:D:73:LEU:O	1:D:77:VAL:HG22	2.13	0.48
1:D:244:GLY:C	1:D:245:ILE:HG13	2.38	0.48
1:F:320:ILE:HA	1:F:323:TYR:HD2	1.78	0.48
1:A:63:GLU:HA	1:F:250:MET:HE2	1.93	0.48
1:D:258:ARG:HG3	1:D:258:ARG:HH11	1.78	0.48
1:F:15:THR:HG22	1:F:15:THR:O	2.14	0.48
1:C:116:VAL:HG12	1:C:153:LEU:HB2	1.95	0.48
1:D:228:ASP:HB2	1:G:304:ARG:HH12	1.79	0.48
1:G:15:THR:C	1:G:17:ALA:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:PRO:HD2	1:H:45:GLU:OE1	2.14	0.48
1:H:285:PRO:HA	1:H:286:PRO:HD3	1.70	0.48
1:B:44:PRO:O	1:B:47:LYS:HG2	2.13	0.48
1:C:314:THR:HG22	1:C:315:THR:H	1.79	0.48
1:E:306:LEU:HD13	1:E:324:PHE:CD1	2.49	0.48
1:H:16:ILE:HG12	1:H:120:ALA:HB2	1.96	0.48
1:A:76:ARG:O	1:A:80:LEU:HB2	2.14	0.48
1:A:199:LEU:HD23	1:A:203:HIS:CD2	2.49	0.48
1:A:231:GLU:C	1:A:233:MET:H	2.22	0.48
1:C:166:ILE:HD13	1:C:179:ALA:HB2	1.95	0.48
1:D:110:LYS:NZ	1:D:207:SER:O	2.45	0.48
1:F:66:THR:OG1	1:F:69:VAL:HG23	2.14	0.48
1:G:15:THR:C	1:G:17:ALA:N	2.70	0.48
1:A:162:SER:HB2	1:A:185:LEU:HD11	1.96	0.48
1:B:314:THR:HG23	1:B:320:ILE:HD11	1.96	0.48
1:G:63:GLU:CD	1:G:63:GLU:H	2.20	0.48
1:H:319:VAL:O	1:H:322:ASP:HB2	2.14	0.48
1:C:68:ASP:O	1:C:71:LEU:HB3	2.13	0.48
1:D:271:ILE:HD13	1:D:272:VAL:N	2.29	0.48
1:D:310:ALA:HB1	1:D:320:ILE:CD1	2.44	0.48
1:E:275:ARG:NH1	1:E:290:GLN:HB2	2.27	0.48
1:H:224:TYR:HA	1:H:248:ALA:HB3	1.96	0.48
1:C:173:THR:HG21	1:D:159:ARG:CZ	2.44	0.47
1:D:25:GLN:O	1:D:123:PRO:HG2	2.13	0.47
1:H:219:ALA:O	1:H:242:VAL:HG12	2.14	0.47
1:A:305:ILE:HA	1:A:308:MET:HE2	1.95	0.47
1:B:37:GLU:O	1:B:40:ILE:HB	2.13	0.47
1:B:136:TYR:CD1	1:B:136:TYR:C	2.91	0.47
1:C:141:VAL:O	1:C:144:ASP:HB3	2.14	0.47
1:D:8:VAL:O	1:D:89:VAL:HG23	2.14	0.47
1:D:310:ALA:HB1	1:D:320:ILE:HD13	1.96	0.47
1:G:6:ASN:C	1:G:7:ILE:HD12	2.40	0.47
1:A:145:LYS:O	1:A:148:ARG:HD3	2.15	0.47
1:C:229:ASP:OD1	1:C:258:ARG:NH2	2.47	0.47
1:C:283:ILE:H	1:C:283:ILE:HD12	1.75	0.47
1:E:97:THR:C	1:E:99:ASP:N	2.72	0.47
1:G:158:ASP:O	1:G:187:VAL:HG23	2.14	0.47
1:H:8:VAL:HG11	1:H:80:LEU:HD21	1.95	0.47
1:H:60:ILE:HG22	1:H:61:GLY:N	2.30	0.47
1:H:185:LEU:HD23	1:H:197:THR:OG1	2.15	0.47
1:B:91:ILE:O	1:B:118:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASN:HD22	1:C:51:ASN:HB2	1.79	0.47
1:C:52:ILE:N	1:C:52:ILE:CD1	2.77	0.47
1:C:316:ASN:CG	1:C:319:VAL:HG23	2.40	0.47
1:F:102:PRO:HG3	1:F:117:PHE:CD2	2.50	0.47
1:B:83:ARG:C	1:B:85:ASP:H	2.23	0.47
1:D:170:ASN:OD1	1:D:171:ALA:N	2.48	0.47
1:F:321:GLN:HG3	1:F:321:GLN:O	2.15	0.47
1:G:249:GLY:O	1:G:278:ARG:HG2	2.15	0.47
1:D:271:ILE:HD13	1:D:271:ILE:C	2.39	0.47
1:F:115:VAL:CG1	1:F:152:VAL:HG22	2.44	0.47
1:A:230:PRO:HB3	1:A:232:TYR:CZ	2.48	0.47
1:G:264:ARG:O	1:G:265:LYS:C	2.57	0.47
1:H:46:LEU:HG	1:H:52:ILE:CD1	2.45	0.47
1:C:305:ILE:O	1:C:309:LEU:HD23	2.15	0.47
1:C:311:LEU:C	1:C:313:LYS:H	2.22	0.47
1:D:46:LEU:HD21	1:D:136:TYR:HA	1.97	0.47
1:F:14:GLY:C	1:F:16:ILE:H	2.23	0.47
1:F:115:VAL:HG13	1:F:115:VAL:O	2.15	0.47
1:F:137:GLY:O	1:F:140:LYS:HB3	2.15	0.47
1:F:296:ASP:HB2	1:F:324:PHE:O	2.14	0.47
1:H:230:PRO:HB3	1:H:232:TYR:CE2	2.50	0.47
1:C:15:THR:HG21	1:C:95:THR:OG1	2.15	0.46
1:C:220:VAL:O	1:C:304:ARG:HD2	2.16	0.46
1:C:239:LYS:O	1:C:239:LYS:HG3	2.15	0.46
1:D:231:GLU:HB3	1:D:258:ARG:HB3	1.96	0.46
1:F:154:VAL:O	1:F:154:VAL:HG13	2.15	0.46
1:G:231:GLU:O	1:G:233:MET:N	2.48	0.46
1:B:36:VAL:HG12	1:B:56:GLN:HG3	1.97	0.46
1:E:121:MET:HB2	1:E:174:LEU:HD23	1.97	0.46
1:A:238:ILE:HD11	1:A:266:ALA:CB	2.44	0.46
1:B:200:ASP:OD1	1:F:198:ARG:HD2	2.15	0.46
1:F:154:VAL:HG12	1:F:161:GLY:O	2.16	0.46
1:F:164:ARG:NH1	1:F:327:TYR:OXT	2.48	0.46
1:G:17:ALA:HA	1:G:34:LEU:CD2	2.45	0.46
1:C:96:ASP:OD1	1:H:251:GLY:HA3	2.15	0.46
1:D:78:ASN:C	1:D:80:LEU:H	2.22	0.46
1:H:176:THR:HG23	1:H:177:PHE:CD1	2.50	0.46
1:A:87:ASP:O	1:A:113:LYS:HD2	2.16	0.46
1:B:123:PRO:C	1:B:125:THR:H	2.23	0.46
1:B:157:ASN:O	1:B:158:ASP:HB2	2.16	0.46
1:B:237:SER:HB3	1:B:242:VAL:CG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:THR:HG21	1:D:211:VAL:CG2	2.43	0.46
1:D:162:SER:C	1:D:164:ARG:H	2.22	0.46
1:E:29:TYR:CE2	1:E:123:PRO:HG3	2.51	0.46
1:E:123:PRO:HD2	1:E:126:ALA:HB2	1.98	0.46
1:F:264:ARG:NE	1:F:291:PRO:HG3	2.30	0.46
1:G:102:PRO:HG3	1:G:117:PHE:CD2	2.49	0.46
1:H:320:ILE:C	1:H:322:ASP:N	2.74	0.46
1:C:208:VAL:HG13	1:C:208:VAL:O	2.13	0.46
1:D:109:VAL:O	1:D:109:VAL:HG12	2.16	0.46
1:D:162:SER:HB2	1:D:185:LEU:HD21	1.97	0.46
1:F:129:ALA:O	1:F:132:PRO:HD2	2.16	0.46
1:A:165:PHE:CD1	1:A:182:GLU:HG2	2.50	0.46
1:B:234:TYR:O	1:B:238:ILE:HG13	2.15	0.46
1:E:16:ILE:HD11	1:E:135:LEU:HD22	1.97	0.46
1:E:208:VAL:C	1:E:313:LYS:HZ1	2.24	0.46
1:G:144:ASP:OD1	1:G:146:ASN:HB2	2.16	0.46
1:H:23:ASN:C	1:H:25:GLN:H	2.23	0.46
1:C:19:SER:O	1:C:29:TYR:HB2	2.16	0.46
1:E:17:ALA:HB1	1:E:34:LEU:CB	2.32	0.46
1:E:166:ILE:CG2	1:E:167:SER:N	2.79	0.46
1:C:12:THR:HB	1:C:92:THR:O	2.15	0.46
1:D:61:GLY:O	1:D:63:GLU:N	2.49	0.46
1:D:151:GLY:HA2	1:D:204:THR:CG2	2.46	0.46
1:D:36:VAL:HG11	1:D:55:GLU:H	1.81	0.46
1:F:287:ASP:O	1:F:289:GLY:N	2.49	0.46
1:G:118:VAL:CG2	1:G:138:ALA:CB	2.94	0.46
1:H:135:LEU:O	1:H:136:TYR:C	2.59	0.46
1:B:296:ASP:HB2	1:B:324:PHE:O	2.16	0.45
1:D:226:TYR:N	1:D:226:TYR:CD1	2.84	0.45
1:F:242:VAL:O	1:F:271:ILE:HD12	2.16	0.45
1:H:220:VAL:HG12	1:H:244:GLY:HA3	1.98	0.45
1:D:76:ARG:HG3	1:D:76:ARG:NH1	2.30	0.45
1:F:166:ILE:HG22	1:F:167:SER:N	2.30	0.45
1:C:9:ILE:O	1:C:10:LEU:HD23	2.16	0.45
1:C:290:GLN:HA	1:C:291:PRO:HD3	1.77	0.45
1:E:76:ARG:HG3	1:E:80:LEU:CD1	2.45	0.45
1:F:22:ALA:HB3	1:F:25:GLN:HG3	1.97	0.45
1:H:249:GLY:HA3	1:H:253:GLY:HA2	1.98	0.45
1:H:319:VAL:HG23	1:H:320:ILE:H	1.81	0.45
1:G:8:VAL:C	1:G:9:ILE:HD12	2.40	0.45
1:B:199:LEU:HD12	1:B:200:ASP:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:THR:HG23	1:F:29:TYR:CE1	2.51	0.45
1:G:135:LEU:C	1:G:137:GLY:N	2.72	0.45
1:D:237:SER:C	1:D:239:LYS:N	2.73	0.45
1:E:51:ASN:OD1	1:E:51:ASN:N	2.50	0.45
1:H:29:TYR:CD1	1:H:30:LYS:N	2.85	0.45
1:H:33:ALA:O	1:H:34:LEU:HB2	2.17	0.45
1:H:229:ASP:OD1	1:H:258:ARG:NE	2.50	0.45
1:A:20:ALA:HB2	1:A:29:TYR:HB3	1.99	0.45
1:A:90:VAL:HG22	1:A:116:VAL:CG2	2.47	0.45
1:A:138:ALA:O	1:A:141:VAL:HG22	2.17	0.45
1:D:71:LEU:HD11	1:D:217:LEU:HD12	1.99	0.45
1:E:71:LEU:O	1:E:75:LYS:HG3	2.16	0.45
1:E:320:ILE:O	1:E:323:TYR:HB2	2.16	0.45
1:A:31:ALA:C	1:A:33:ALA:H	2.25	0.45
1:D:23:ASN:HD21	1:D:127:ILE:HG12	1.81	0.45
1:D:237:SER:CB	1:D:242:VAL:HG21	2.46	0.45
1:H:59:SER:C	1:H:60:ILE:HG13	2.40	0.45
1:H:293:LEU:HD12	1:H:293:LEU:N	2.32	0.45
1:B:226:TYR:CD1	1:B:226:TYR:N	2.85	0.45
1:E:277:SER:OG	1:E:279:THR:HG23	2.16	0.45
1:E:298:LEU:CD1	1:E:306:LEU:HD12	2.47	0.45
1:A:75:LYS:NZ	1:A:75:LYS:HB3	2.32	0.45
1:B:323:TYR:HD2	1:B:327:TYR:CE2	2.35	0.45
1:C:34:LEU:HD12	1:C:34:LEU:N	2.30	0.45
1:D:116:VAL:HG23	1:D:116:VAL:O	2.17	0.45
1:F:29:TYR:CD2	1:F:123:PRO:HG3	2.52	0.45
1:A:263:ILE:HG21	1:A:291:PRO:HB2	1.99	0.44
1:D:294:VAL:HG23	1:D:294:VAL:O	2.17	0.44
1:F:73:LEU:O	1:F:73:LEU:HD12	2.16	0.44
1:G:22:ALA:HB3	1:G:25:GLN:CB	2.43	0.44
1:G:44:PRO:C	1:G:46:LEU:H	2.25	0.44
1:G:187:VAL:HG22	1:G:188:ILE:N	2.32	0.44
1:A:72:THR:O	1:A:75:LYS:HG2	2.18	0.44
1:F:62:SER:CB	1:F:96:ASP:HB2	2.47	0.44
1:F:202:VAL:HG12	1:F:203:HIS:N	2.32	0.44
1:F:266:ALA:O	1:F:271:ILE:CG2	2.65	0.44
1:H:121:MET:HE1	1:H:168:LYS:HZ1	1.81	0.44
1:B:162:SER:HB2	1:B:185:LEU:CD2	2.47	0.44
1:C:39:LEU:C	1:C:41:GLN:N	2.73	0.44
1:E:238:ILE:HG13	1:E:238:ILE:H	1.63	0.44
1:G:296:ASP:HB3	1:G:297:SER:H	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LEU:HD21	1:H:39:LEU:HD21	1.99	0.44
1:H:45:GLU:OE1	1:H:45:GLU:N	2.51	0.44
1:A:247:TYR:CE2	1:A:255:VAL:HG12	2.52	0.44
1:D:264:ARG:C	1:D:266:ALA:N	2.74	0.44
1:G:7:ILE:HD12	1:G:7:ILE:N	2.33	0.44
1:A:245:ILE:HG12	1:A:271:ILE:CD1	2.47	0.44
1:E:40:ILE:HD12	1:E:52:ILE:HD11	1.99	0.44
1:E:56:GLN:NE2	1:E:58:ALA:O	2.50	0.44
1:G:178:LYS:O	1:G:180:PRO:HD3	2.17	0.44
1:G:231:GLU:C	1:G:233:MET:N	2.75	0.44
1:H:4:LEU:HB3	1:H:50:ALA:HA	1.99	0.44
1:H:121:MET:HE1	1:H:168:LYS:HZ2	1.78	0.44
1:A:314:THR:OG1	1:A:315:THR:N	2.51	0.44
1:B:315:THR:O	1:B:317:PRO:HD3	2.18	0.44
1:C:211:VAL:O	1:C:212:THR:C	2.60	0.44
1:C:220:VAL:HG11	1:C:307:LEU:HD23	2.00	0.44
1:D:214:VAL:HG12	1:D:215:ASP:N	2.32	0.44
1:F:287:ASP:C	1:F:289:GLY:N	2.76	0.44
1:G:202:VAL:HG23	1:G:327:TYR:HA	2.00	0.44
1:H:17:ALA:HB1	1:H:34:LEU:HB3	2.00	0.44
1:A:185:LEU:CD2	1:A:197:THR:HG22	2.48	0.44
1:D:266:ALA:HB1	1:D:271:ILE:HG23	2.00	0.44
1:G:61:GLY:HA3	1:G:63:GLU:OE2	2.17	0.44
1:D:40:ILE:HG21	1:D:47:LYS:HE3	1.99	0.44
1:G:28:GLY:O	1:G:29:TYR:HB3	2.18	0.44
1:G:85:ASP:OD1	1:G:85:ASP:N	2.44	0.44
1:C:11:ALA:HB2	1:C:36:VAL:HG23	2.00	0.44
1:D:256:SER:O	1:D:259:GLY:N	2.51	0.44
1:H:164:ARG:NH2	1:H:298:LEU:HG	2.33	0.44
1:A:296:ASP:HB2	1:A:324:PHE:O	2.18	0.43
1:F:46:LEU:HB3	1:F:52:ILE:CD1	2.45	0.43
1:F:49:LEU:O	1:F:50:ALA:HB2	2.18	0.43
1:F:243:LYS:NZ	1:F:270:GLY:O	2.48	0.43
1:H:83:ARG:HD3	1:H:86:VAL:HG21	1.99	0.43
1:C:98:LEU:HD12	1:C:177:PHE:CZ	2.53	0.43
1:C:151:GLY:O	1:C:153:LEU:HD13	2.18	0.43
1:E:170:ASN:O	1:E:176:THR:HG21	2.17	0.43
1:F:283:ILE:O	1:F:285:PRO:HD2	2.17	0.43
1:G:40:ILE:HD12	1:G:52:ILE:HG21	2.00	0.43
1:G:76:ARG:NE	1:G:80:LEU:HG	2.30	0.43
1:H:315:THR:O	1:H:317:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PRO:O	1:C:50:ALA:HB1	2.18	0.43
1:C:218:PRO:HD3	1:C:312:THR:HG22	2.00	0.43
1:C:283:ILE:CG1	1:G:189:ILE:HG21	2.48	0.43
1:D:21:ALA:HB3	1:D:25:GLN:CD	2.42	0.43
1:D:253:GLY:O	1:D:254:SER:C	2.62	0.43
1:F:287:ASP:C	1:F:289:GLY:H	2.25	0.43
1:F:313:LYS:HE3	1:F:313:LYS:HB3	1.87	0.43
1:F:321:GLN:O	1:F:321:GLN:NE2	2.48	0.43
1:G:77:VAL:HG12	1:G:81:LEU:HD13	2.00	0.43
1:A:105:LEU:HD12	1:A:117:PHE:CZ	2.53	0.43
1:B:36:VAL:O	1:B:37:GLU:C	2.61	0.43
1:D:165:PHE:CG	1:D:182:GLU:HG2	2.53	0.43
1:D:238:ILE:HD11	1:D:269:LYS:HG3	1.99	0.43
1:F:224:TYR:HA	1:F:248:ALA:HB3	2.01	0.43
1:G:29:TYR:CZ	1:G:123:PRO:HG3	2.54	0.43
1:G:127:ILE:HG12	1:G:127:ILE:O	2.18	0.43
1:A:256:SER:HB2	1:A:258:ARG:HH21	1.84	0.43
1:E:231:GLU:O	1:E:234:TYR:HB2	2.19	0.43
1:F:35:GLY:O	1:F:36:VAL:C	2.61	0.43
1:G:220:VAL:HG23	1:G:308:MET:HG2	2.00	0.43
1:H:113:LYS:HA	1:H:114:PRO:HD2	1.65	0.43
1:A:259:GLY:O	1:A:263:ILE:HG12	2.18	0.43
1:B:252:ALA:HB1	1:B:285:PRO:HD2	2.00	0.43
1:G:164:ARG:NH1	1:G:327:TYR:OXT	2.52	0.43
1:G:220:VAL:O	1:G:304:ARG:HD2	2.18	0.43
1:G:269:LYS:O	1:G:269:LYS:HG3	2.19	0.43
1:G:319:VAL:O	1:G:323:TYR:CD1	2.72	0.43
1:H:74:SER:O	1:H:78:ASN:ND2	2.51	0.43
1:H:196:GLN:HE21	1:H:196:GLN:HB2	1.68	0.43
1:D:256:SER:O	1:D:257:LYS:C	2.62	0.43
1:F:285:PRO:HA	1:F:286:PRO:HD2	1.77	0.43
1:G:3:ASN:O	1:G:4:LEU:HD23	2.19	0.43
1:H:162:SER:O	1:H:166:ILE:HG12	2.19	0.43
1:H:230:PRO:HB3	1:H:232:TYR:CZ	2.54	0.43
1:C:110:LYS:O	1:C:111:SER:HB2	2.19	0.43
1:D:7:ILE:HD11	1:D:139:VAL:HG13	1.99	0.43
1:G:179:ALA:HB3	1:G:183:GLY:O	2.18	0.43
1:G:268:SER:C	1:G:270:GLY:N	2.76	0.43
1:B:89:VAL:HG12	1:B:90:VAL:N	2.34	0.43
1:C:283:ILE:HG13	1:G:189:ILE:HB	2.01	0.43
1:D:305:ILE:O	1:D:309:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:VAL:CG1	1:F:304:ARG:HG3	2.49	0.43
1:C:243:LYS:C	1:C:271:ILE:HG23	2.44	0.42
1:D:4:LEU:HA	1:D:5:PRO:HD3	1.76	0.42
1:D:34:LEU:N	1:D:34:LEU:HD12	2.34	0.42
1:D:105:LEU:C	1:D:107:LEU:N	2.77	0.42
1:G:20:ALA:HA	1:G:29:TYR:HB3	2.01	0.42
1:A:294:VAL:O	1:A:294:VAL:HG23	2.17	0.42
1:D:266:ALA:O	1:D:271:ILE:HG22	2.20	0.42
1:E:295:ALA:HA	1:E:324:PHE:CD2	2.53	0.42
1:G:188:ILE:HG23	1:G:188:ILE:O	2.19	0.42
1:G:290:GLN:HA	1:G:291:PRO:HD3	1.87	0.42
1:H:43:VAL:O	1:H:46:LEU:HD22	2.19	0.42
1:H:99:ASP:OD2	1:H:167:SER:HB2	2.19	0.42
1:H:153:LEU:N	1:H:153:LEU:CD2	2.82	0.42
1:B:12:THR:O	1:B:12:THR:HG22	2.18	0.42
1:F:52:ILE:CG2	1:F:53:LYS:N	2.82	0.42
1:F:295:ALA:HA	1:F:324:PHE:CD2	2.54	0.42
1:H:52:ILE:HG22	1:H:53:LYS:H	1.83	0.42
1:H:237:SER:HB3	1:H:242:VAL:HG21	2.00	0.42
1:B:321:GLN:HA	1:B:321:GLN:NE2	2.35	0.42
1:D:67:SER:O	1:D:70:LEU:HB2	2.20	0.42
1:D:74:SER:O	1:D:78:ASN:ND2	2.52	0.42
1:D:208:VAL:HG22	1:D:327:TYR:OH	2.19	0.42
1:F:164:ARG:HD2	1:F:164:ARG:O	2.19	0.42
1:B:36:VAL:HG13	1:B:37:GLU:N	2.33	0.42
1:C:208:VAL:HG22	1:C:208:VAL:O	2.19	0.42
1:D:260:ASP:O	1:D:264:ARG:HG3	2.19	0.42
1:E:243:LYS:HB3	1:E:311:LEU:HD13	2.00	0.42
1:F:122:ARG:HA	1:F:123:PRO:HD3	1.92	0.42
1:G:34:LEU:HD23	1:G:39:LEU:HD21	2.02	0.42
1:A:202:VAL:HG23	1:A:327:TYR:CD2	2.54	0.42
1:B:244:GLY:HA2	1:B:272:VAL:O	2.19	0.42
1:C:90:VAL:HG22	1:C:116:VAL:CG2	2.49	0.42
1:C:211:VAL:O	1:C:211:VAL:HG12	2.19	0.42
1:C:237:SER:O	1:C:238:ILE:C	2.62	0.42
1:D:238:ILE:HD12	1:D:266:ALA:HA	2.02	0.42
1:G:57:VAL:O	1:G:58:ALA:HB2	2.19	0.42
1:A:189:ILE:HD13	1:E:283:ILE:HD11	2.02	0.42
1:B:227:GLN:OE1	1:E:100:GLU:HB2	2.19	0.42
1:B:245:ILE:O	1:B:273:VAL:HG13	2.19	0.42
1:E:121:MET:HE2	1:E:173:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:316:ASN:HD22	1:H:319:VAL:HG13	1.85	0.42
1:B:16:ILE:O	1:B:16:ILE:HG12	2.19	0.42
1:B:123:PRO:C	1:B:125:THR:N	2.76	0.42
1:D:11:ALA:HA	1:D:92:THR:OG1	2.19	0.42
1:D:46:LEU:HB3	1:D:52:ILE:HD11	2.01	0.42
1:E:136:TYR:CD1	1:E:136:TYR:C	2.97	0.42
1:F:151:GLY:HA2	1:F:203:HIS:CD2	2.54	0.42
1:G:251:GLY:O	1:G:277:SER:HB2	2.19	0.42
1:H:208:VAL:CG2	1:H:209:PHE:N	2.81	0.42
1:A:83:ARG:HB2	1:A:86:VAL:CG1	2.49	0.42
1:A:200:ASP:O	1:A:201:LYS:HG2	2.20	0.42
1:C:14:GLY:C	1:C:16:ILE:H	2.28	0.42
1:D:71:LEU:N	1:D:71:LEU:HD12	2.34	0.42
1:D:135:LEU:O	1:D:139:VAL:HG23	2.19	0.42
1:E:165:PHE:CE1	1:E:182:GLU:HG2	2.55	0.42
1:E:299:SER:O	1:E:300:PRO:C	2.62	0.42
1:G:170:ASN:OD1	1:G:171:ALA:N	2.52	0.42
1:G:234:TYR:N	1:G:234:TYR:CD1	2.88	0.42
1:G:263:ILE:HD12	1:G:273:VAL:HG11	2.01	0.42
1:H:29:TYR:HE1	1:H:31:ALA:HB2	1.84	0.42
1:A:100:GLU:O	1:A:101:SER:C	2.62	0.42
1:D:110:LYS:CE	1:D:207:SER:O	2.66	0.42
1:D:130:ASP:O	1:D:131:GLY:C	2.63	0.42
1:F:159:ARG:HG2	1:F:159:ARG:HH11	1.84	0.42
1:G:122:ARG:HA	1:G:123:PRO:HD3	1.84	0.42
1:G:208:VAL:O	1:G:313:LYS:HE3	2.20	0.42
1:H:46:LEU:HA	1:H:49:LEU:HD12	2.02	0.42
1:C:311:LEU:C	1:C:313:LYS:N	2.78	0.41
1:D:78:ASN:C	1:D:80:LEU:N	2.78	0.41
1:D:222:ILE:HB	1:G:226:TYR:CE2	2.55	0.41
1:E:260:ASP:OD1	1:E:264:ARG:NH1	2.52	0.41
1:F:6:ASN:N	1:F:6:ASN:ND2	2.68	0.41
1:G:139:VAL:O	1:G:140:LYS:C	2.62	0.41
1:H:145:LYS:O	1:H:148:ARG:HG3	2.20	0.41
1:A:228:ASP:CA	1:A:258:ARG:HH12	2.13	0.41
1:C:16:ILE:HG23	1:C:17:ALA:N	2.31	0.41
1:F:321:GLN:O	1:F:321:GLN:CG	2.68	0.41
1:H:134:ASN:ND2	1:H:156:LEU:CD2	2.83	0.41
1:H:255:VAL:HG22	1:H:290:GLN:HE21	1.85	0.41
1:A:176:THR:HG23	1:A:177:PHE:CD2	2.55	0.41
1:C:315:THR:HG22	1:C:315:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:VAL:HG22	1:E:326:ALA:O	2.20	0.41
1:A:144:ASP:OD1	1:A:145:LYS:N	2.54	0.41
1:A:220:VAL:HG11	1:A:307:LEU:HD23	2.03	0.41
1:C:16:ILE:HD13	1:C:92:THR:HG23	2.03	0.41
1:C:19:SER:OG	1:C:33:ALA:CB	2.68	0.41
1:C:34:LEU:HB3	1:C:38:THR:OG1	2.19	0.41
1:C:231:GLU:C	1:C:233:MET:H	2.28	0.41
1:D:61:GLY:O	1:D:64:ASN:N	2.43	0.41
1:E:188:ILE:O	1:E:189:ILE:HD12	2.20	0.41
1:E:275:ARG:NH1	1:E:290:GLN:CB	2.83	0.41
1:G:166:ILE:CG2	1:G:167:SER:N	2.84	0.41
1:G:235:ASP:O	1:G:238:ILE:N	2.53	0.41
1:B:106:ASN:HA	1:B:152:VAL:CG2	2.51	0.41
1:C:106:ASN:OD1	1:C:152:VAL:HG23	2.21	0.41
1:F:113:LYS:HA	1:F:114:PRO:HD3	1.86	0.41
1:G:109:VAL:HG12	1:G:111:SER:H	1.85	0.41
1:H:29:TYR:HD1	1:H:30:LYS:N	2.18	0.41
1:H:112:ASP:OD1	1:H:112:ASP:N	2.52	0.41
1:G:293:LEU:N	1:G:293:LEU:HD23	2.36	0.41
1:B:131:GLY:N	1:B:132:PRO:CD	2.83	0.41
1:C:11:ALA:HB2	1:C:36:VAL:CG2	2.51	0.41
1:C:122:ARG:HA	1:C:123:PRO:HD3	1.93	0.41
1:D:46:LEU:O	1:D:48:THR:N	2.45	0.41
1:G:247:TYR:CE2	1:G:249:GLY:HA3	2.56	0.41
1:H:81:LEU:HD21	1:H:113:LYS:HB2	2.02	0.41
1:A:135:LEU:O	1:A:139:VAL:HG23	2.21	0.41
1:A:202:VAL:HG23	1:A:327:TYR:CE2	2.56	0.41
1:A:231:GLU:C	1:A:233:MET:N	2.79	0.41
1:B:71:LEU:O	1:B:72:THR:C	2.63	0.41
1:B:299:SER:O	1:B:300:PRO:C	2.63	0.41
1:C:12:THR:HG21	1:C:65:MET:HE1	2.02	0.41
1:C:45:GLU:HG2	1:D:23:ASN:HD22	1.86	0.41
1:C:105:LEU:HD12	1:C:105:LEU:N	2.35	0.41
1:C:229:ASP:O	1:C:258:ARG:NE	2.52	0.41
1:C:304:ARG:O	1:C:305:ILE:C	2.64	0.41
1:D:14:GLY:HA2	1:D:94:GLY:CA	2.51	0.41
1:D:21:ALA:HB3	1:D:25:GLN:HE22	1.86	0.41
1:E:127:ILE:HD13	1:E:127:ILE:HA	1.88	0.41
1:F:122:ARG:NH1	1:F:128:SER:HB2	2.35	0.41
1:F:162:SER:C	1:F:164:ARG:H	2.28	0.41
1:F:241:GLY:O	1:F:242:VAL:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:ALA:O	1:F:265:LYS:HG3	2.21	0.41
1:G:210:ASP:OD2	1:G:212:THR:HG23	2.20	0.41
1:H:116:VAL:HG22	1:H:153:LEU:CD2	2.46	0.41
1:A:37:GLU:O	1:A:41:GLN:HG2	2.20	0.41
1:B:14:GLY:O	1:B:31:ALA:HB1	2.20	0.41
1:C:137:GLY:O	1:C:141:VAL:HG13	2.21	0.41
1:C:187:VAL:CG2	1:C:188:ILE:N	2.84	0.41
1:F:15:THR:HG23	1:F:29:TYR:CZ	2.55	0.41
1:F:295:ALA:HA	1:F:324:PHE:HD2	1.86	0.41
1:F:316:ASN:OD1	1:F:318:ALA:HB3	2.21	0.41
1:G:44:PRO:C	1:G:46:LEU:N	2.77	0.41
1:H:83:ARG:HB3	1:H:85:ASP:OD1	2.21	0.41
1:H:129:ALA:O	1:H:132:PRO:HD2	2.21	0.41
1:B:65:MET:HE3	1:B:65:MET:HB2	1.99	0.40
1:C:29:TYR:CD2	1:C:123:PRO:HG3	2.56	0.40
1:E:43:VAL:HG12	1:E:43:VAL:O	2.21	0.40
1:G:220:VAL:HB	1:G:304:ARG:HG2	2.03	0.40
1:G:226:TYR:CD2	1:G:226:TYR:N	2.89	0.40
1:G:234:TYR:N	1:G:234:TYR:HD1	2.19	0.40
1:H:5:PRO:HA	1:H:87:ASP:OD1	2.21	0.40
1:H:45:GLU:O	1:H:47:LYS:N	2.53	0.40
1:A:111:SER:OG	1:A:112:ASP:N	2.49	0.40
1:B:316:ASN:ND2	1:B:319:VAL:HG23	2.37	0.40
1:C:196:GLN:NE2	1:G:182:GLU:HG3	2.36	0.40
1:C:319:VAL:HG12	1:C:323:TYR:CE1	2.57	0.40
1:D:321:GLN:CA	1:D:321:GLN:NE2	2.83	0.40
1:F:83:ARG:HG2	1:F:83:ARG:HH11	1.85	0.40
1:G:62:SER:CB	1:G:94:GLY:HA3	2.46	0.40
1:G:109:VAL:HG12	1:G:111:SER:N	2.36	0.40
1:H:46:LEU:HD23	1:H:47:LYS:N	2.35	0.40
1:H:291:PRO:O	1:H:292:GLY:O	2.39	0.40
1:A:90:VAL:C	1:A:91:ILE:HD13	2.46	0.40
1:A:202:VAL:HG23	1:A:202:VAL:O	2.19	0.40
1:F:97:THR:C	1:F:99:ASP:H	2.30	0.40
1:F:121:MET:HE2	1:F:173:THR:O	2.21	0.40
1:F:268:SER:C	1:F:270:GLY:H	2.29	0.40
1:G:264:ARG:CZ	1:G:291:PRO:HG3	2.52	0.40
1:H:14:GLY:H	1:H:32:GLY:HA2	1.86	0.40
1:H:199:LEU:HD23	1:H:200:ASP:H	1.87	0.40
1:H:293:LEU:N	1:H:293:LEU:CD1	2.85	0.40
1:E:264:ARG:NH1	1:E:291:PRO:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:GLY:O	1:G:62:SER:C	2.65	0.40
1:G:133:MET:CE	1:H:127:ILE:HB	2.46	0.40
1:G:240:HIS:CD2	1:G:240:HIS:N	2.87	0.40
1:H:320:ILE:O	1:H:322:ASP:N	2.54	0.40
1:A:34:LEU:N	1:A:34:LEU:CD1	2.85	0.40
1:A:71:LEU:CD1	1:A:211:VAL:HB	2.50	0.40
1:B:23:ASN:C	1:B:23:ASN:HD22	2.30	0.40
1:D:279:THR:HG22	1:G:168:LYS:O	2.22	0.40
1:E:4:LEU:HD13	1:E:50:ALA:HA	2.04	0.40
1:G:178:LYS:HB3	1:G:184:TYR:OH	2.22	0.40
1:G:238:ILE:O	1:G:241:GLY:N	2.52	0.40
1:H:247:TYR:HE2	1:H:254:SER:O	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/327 (99%)	286 (88%)	32 (10%)	5 (2%)	8	35
1	B	323/327 (99%)	282 (87%)	36 (11%)	5 (2%)	8	35
1	C	323/327 (99%)	285 (88%)	32 (10%)	6 (2%)	6	30
1	D	323/327 (99%)	260 (80%)	49 (15%)	14 (4%)	2	12
1	E	323/327 (99%)	285 (88%)	32 (10%)	6 (2%)	6	30
1	F	323/327 (99%)	281 (87%)	31 (10%)	11 (3%)	3	17
1	G	323/327 (99%)	264 (82%)	48 (15%)	11 (3%)	3	17
1	H	323/327 (99%)	264 (82%)	50 (16%)	9 (3%)	4	21
All	All	2584/2616 (99%)	2207 (85%)	310 (12%)	67 (3%)	4	23

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	296	ASP
1	H	62	SER
1	H	296	ASP
1	A	204	THR
1	A	206	ARG
1	B	13	GLY
1	B	84	SER
1	B	296	ASP
1	C	204	THR
1	D	62	SER
1	D	111	SER
1	D	112	ASP
1	D	204	THR
1	D	254	SER
1	D	296	ASP
1	E	28	GLY
1	E	42	ALA
1	E	204	THR
1	F	163	ALA
1	F	242	VAL
1	F	288	ALA
1	F	291	PRO
1	G	35	GLY
1	G	232	TYR
1	G	291	PRO
1	G	292	GLY
1	H	46	LEU
1	H	292	GLY
1	C	15	THR
1	D	24	THR
1	D	55	GLU
1	D	176	THR
1	D	287	ASP
1	E	296	ASP
1	F	36	VAL
1	F	62	SER
1	F	281	SER
1	G	83	ARG
1	G	204	THR
1	H	34	LEU
1	A	227	GLN
1	B	37	GLU
1	C	111	SER

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Mol	Chain	Res	Type
1	C	212	THR
1	G	19	SER
1	H	191	ASP
1	H	321	GLN
1	A	100	GLU
1	A	180	PRO
1	D	13	GLY
1	D	127	ILE
1	D	180	PRO
1	E	21	ALA
1	E	41	GLN
1	F	180	PRO
1	G	157	ASN
1	H	204	THR
1	H	241	GLY
1	B	204	THR
1	D	23	ASN
1	F	204	THR
1	F	270	GLY
1	G	50	ALA
1	C	305	ILE
1	G	180	PRO
1	G	241	GLY
1	C	180	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/261 (100%)	250 (96%)	10 (4%)	29	63
1	B	260/261 (100%)	251 (96%)	9 (4%)	32	65
1	C	260/261 (100%)	251 (96%)	9 (4%)	32	65
1	D	260/261 (100%)	250 (96%)	10 (4%)	29	63
1	E	260/261 (100%)	251 (96%)	9 (4%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	260/261 (100%)	248 (95%)	12 (5%)	24	58
1	G	260/261 (100%)	239 (92%)	21 (8%)	11	38
1	H	260/261 (100%)	251 (96%)	9 (4%)	32	65
All	All	2080/2088 (100%)	1991 (96%)	89 (4%)	26	60

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	60	ILE
1	A	75	LYS
1	A	109	VAL
1	A	121	MET
1	A	156	LEU
1	A	166	ILE
1	A	191	ASP
1	A	208	VAL
1	A	283	ILE
1	B	36	VAL
1	B	51	ASN
1	B	136	TYR
1	B	156	LEU
1	B	174	LEU
1	B	178	LYS
1	B	185	LEU
1	B	272	VAL
1	B	313	LYS
1	C	16	ILE
1	C	45	GLU
1	C	52	ILE
1	C	76	ARG
1	C	92	THR
1	C	121	MET
1	C	153	LEU
1	C	274	VAL
1	C	283	ILE
1	D	79	GLU
1	D	99	ASP
1	D	156	LEU
1	D	185	LEU
1	D	199	LEU

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Mol	Chain	Res	Type
1	D	226	TYR
1	D	231	GLU
1	D	271	ILE
1	D	305	ILE
1	D	321	GLN
1	E	16	ILE
1	E	71	LEU
1	E	85	ASP
1	E	95	THR
1	E	122	ARG
1	E	127	ILE
1	E	141	VAL
1	E	306	LEU
1	E	317	PRO
1	F	6	ASN
1	F	16	ILE
1	F	36	VAL
1	F	73	LEU
1	F	79	GLU
1	F	156	LEU
1	F	180	PRO
1	F	199	LEU
1	F	212	THR
1	F	220	VAL
1	F	271	ILE
1	F	300	PRO
1	G	9	ILE
1	G	45	GLU
1	G	60	ILE
1	G	68	ASP
1	G	69	VAL
1	G	76	ARG
1	G	85	ASP
1	G	92	THR
1	G	118	VAL
1	G	121	MET
1	G	127	ILE
1	G	150	ARG
1	G	156	LEU
1	G	202	VAL
1	G	220	VAL
1	G	226	TYR

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Mol	Chain	Res	Type
1	G	233	MET
1	G	279	THR
1	G	293	LEU
1	G	304	ARG
1	G	314	THR
1	H	8	VAL
1	H	10	LEU
1	H	16	ILE
1	H	45	GLU
1	H	46	LEU
1	H	100	GLU
1	H	135	LEU
1	H	153	LEU
1	H	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	25	GLN
1	A	64	ASN
1	A	93	HIS
1	A	146	ASN
1	A	213	ASN
1	A	240	HIS
1	B	51	ASN
1	B	146	ASN
1	B	157	ASN
1	B	203	HIS
1	B	227	GLN
1	C	6	ASN
1	C	51	ASN
1	C	196	GLN
1	C	203	HIS
1	D	3	ASN
1	D	23	ASN
1	D	56	GLN
1	D	93	HIS
1	D	203	HIS
1	D	321	GLN
1	E	146	ASN
1	E	203	HIS

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Mol	Chain	Res	Type
1	F	6	ASN
1	F	51	ASN
1	F	157	ASN
1	F	196	GLN
1	F	203	HIS
1	F	321	GLN
1	G	23	ASN
1	G	25	GLN
1	G	56	GLN
1	G	134	ASN
1	G	146	ASN
1	G	203	HIS
1	H	3	ASN
1	H	157	ASN
1	H	196	GLN
1	H	290	GLN
1	H	316	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	325/327 (99%)	-0.74	1 (0%) 90 79	8, 34, 75, 128	0
1	B	325/327 (99%)	-0.61	1 (0%) 90 79	5, 34, 95, 151	0
1	C	325/327 (99%)	-0.60	2 (0%) 85 69	8, 41, 83, 130	0
1	D	325/327 (99%)	-0.38	4 (1%) 76 55	12, 48, 142, 198	0
1	E	325/327 (99%)	-0.62	2 (0%) 85 69	10, 33, 114, 192	0
1	F	325/327 (99%)	-0.72	0 100 100	2, 30, 71, 125	0
1	G	325/327 (99%)	-0.47	2 (0%) 85 69	10, 44, 127, 200	0
1	H	325/327 (99%)	-0.46	3 (0%) 81 61	9, 41, 125, 182	0
All	All	2600/2616 (99%)	-0.57	15 (0%) 85 69	2, 38, 101, 200	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	GLY	3.4
1	G	15	THR	3.4
1	H	157	ASN	3.2
1	H	15	THR	2.9
1	D	23	ASN	2.6
1	H	32	GLY	2.5
1	G	14	GLY	2.5
1	C	16	ILE	2.4
1	D	29	TYR	2.3
1	D	26	THR	2.3
1	E	26	THR	2.2
1	E	34	LEU	2.2
1	B	29	TYR	2.1
1	C	18	GLY	2.1
1	A	15	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.