



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:00 PM UTC

PDB ID : 1SS8 / pdb_00001ss8
Title : GroEL
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : 2004-03-23
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

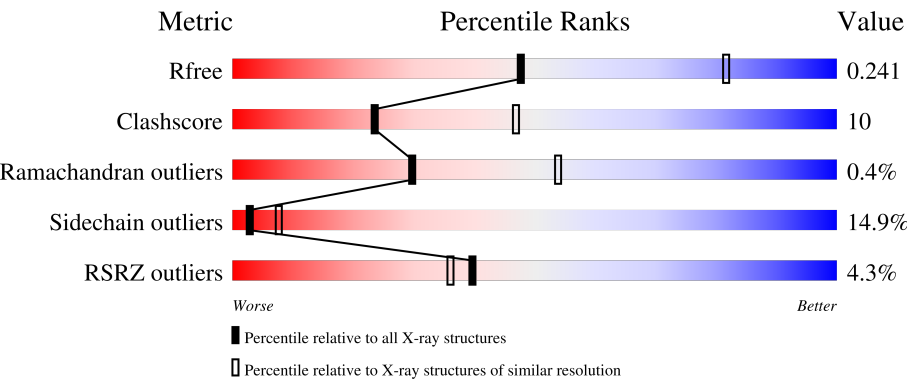
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	524	3% 68% 25% 7% .
1	B	524	5% 70% 22% 7% .
1	C	524	4% 71% 24% . .
1	D	524	3% 70% 24% 6% .
1	E	524	2% 70% 25% 5% .

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Mol	Chain	Length	Quality of chain
1	F	524	12% 71% 25% . .
1	G	524	2% 69% 25% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27064 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	B	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	C	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	D	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	E	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	F	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			
1	G	524	Total	C	N	O	S	0	0	0
			3851	2395	662	774	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
A	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
B	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
B	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
C	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
C	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
D	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
D	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
E	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
E	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
F	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
F	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5
G	13	GLY	ARG	SEE REMARK 999	UNP P0A6F5
G	126	VAL	ALA	SEE REMARK 999	UNP P0A6F5

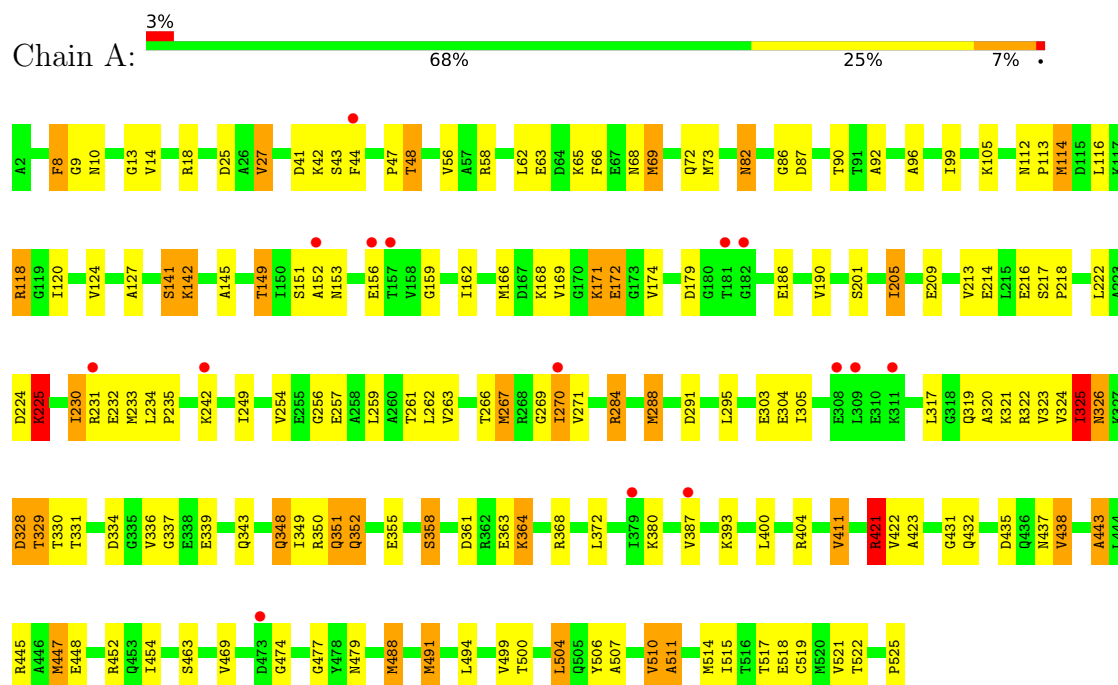
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total 18	O 18	0	0
2	B	21	Total 21	O 21	0	0
2	C	15	Total 15	O 15	0	0
2	D	16	Total 16	O 16	0	0
2	E	17	Total 17	O 17	0	0
2	F	7	Total 7	O 7	0	0
2	G	13	Total 13	O 13	0	0

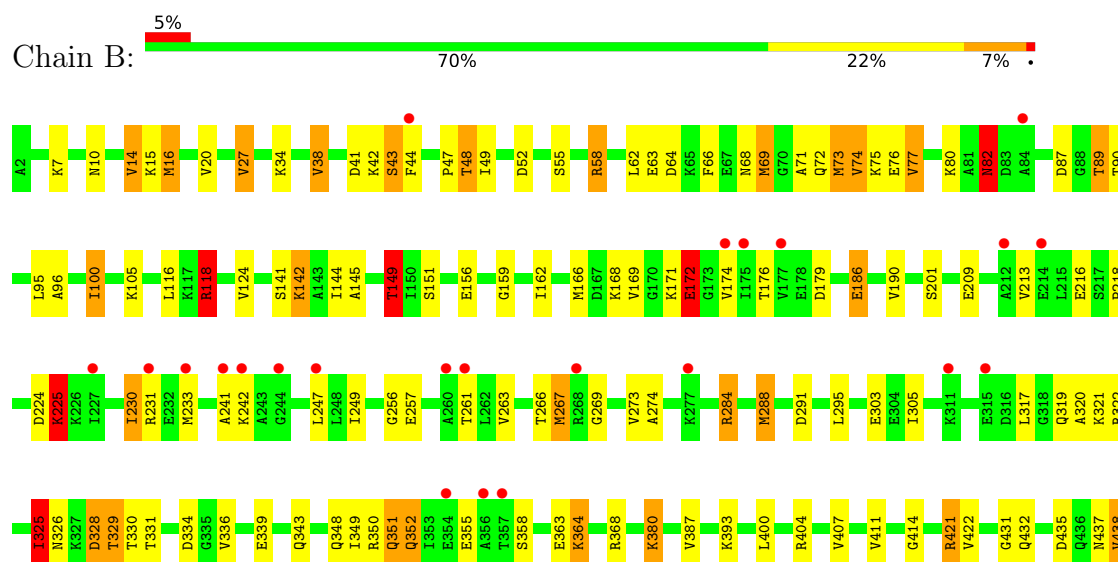
3 Residue-property plots

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: groEL protein

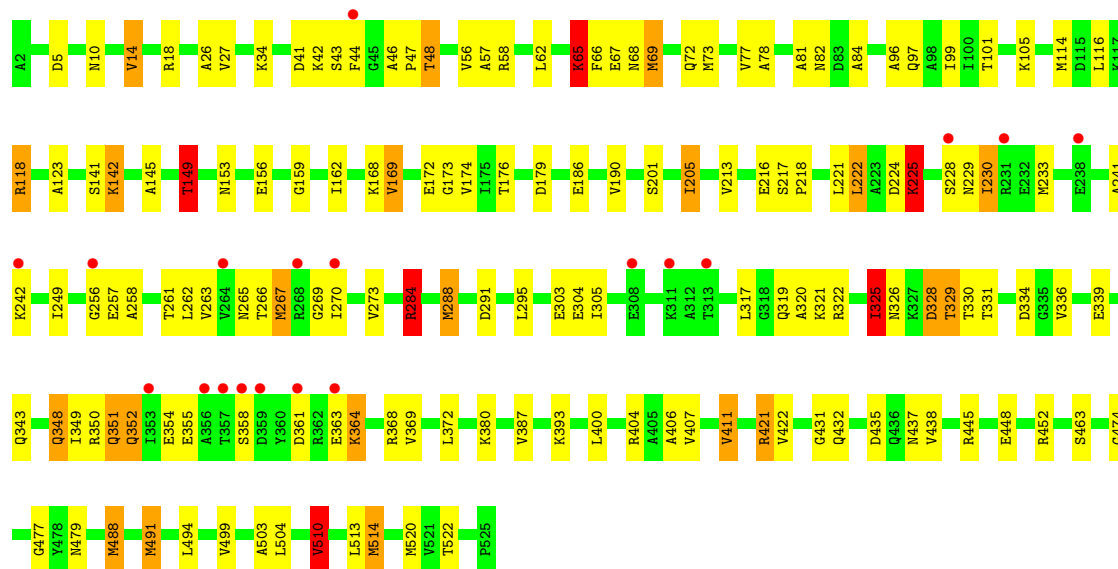


• Molecule 1: groEL protein

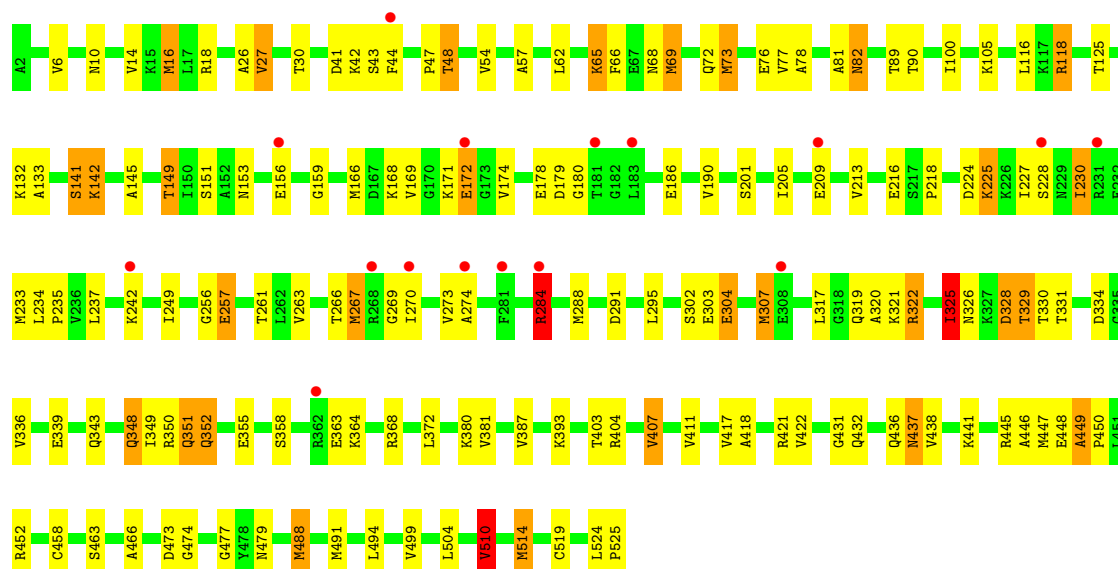




• Molecule 1: groEL protein

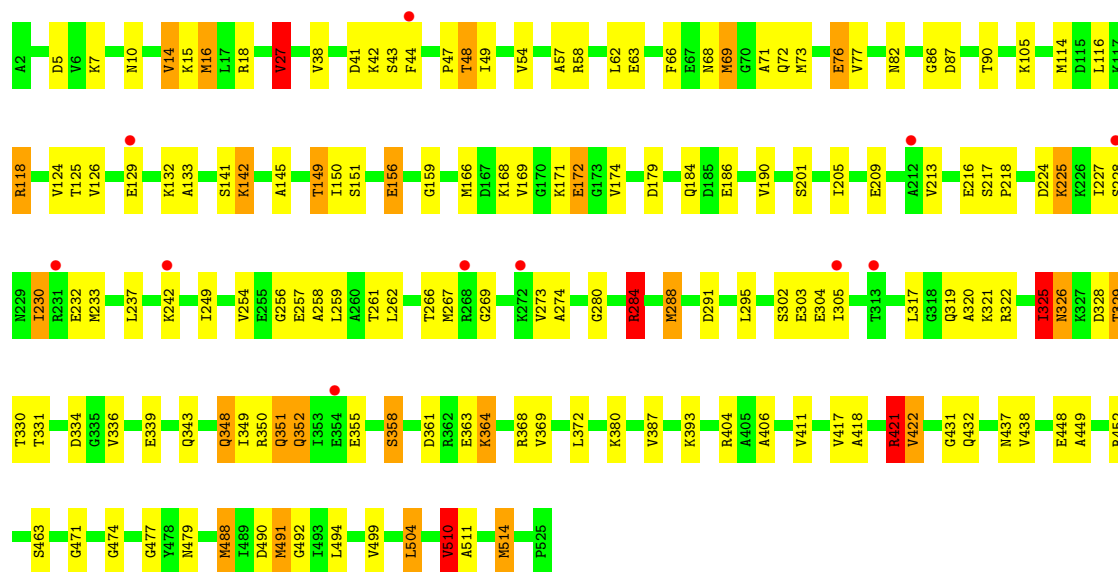


• Molecule 1: groEL protein



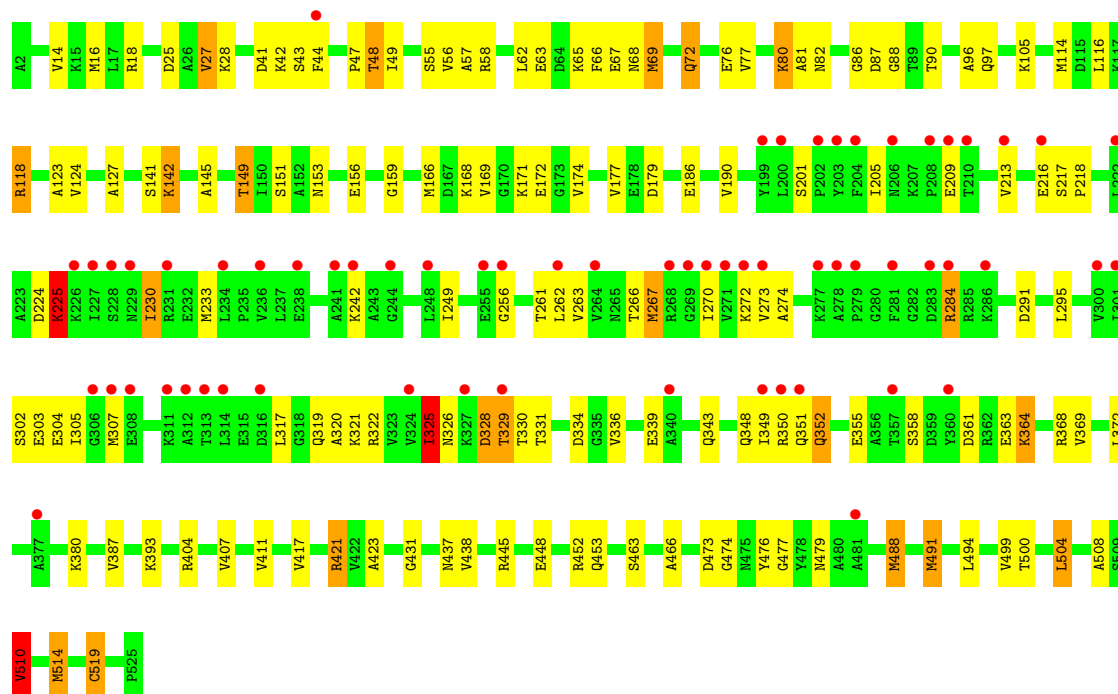
• Molecule 1: groEL protein





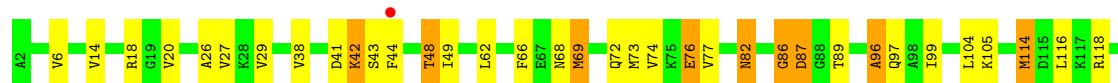
• Molecule 1: groEL protein

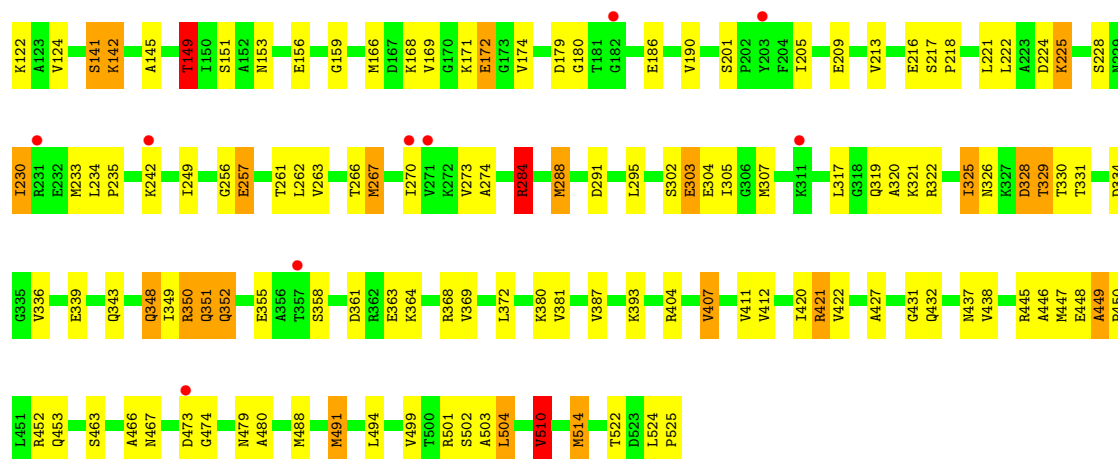
Chain F: 12% 71% 25%



• Molecule 1: groEL protein

Chain G: 2% 69% 25% 6%





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	178.38Å 204.98Å 280.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 83.8 (30.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.68Å)	Xtriage
Refinement program	REFMAC refmac_5.1.19	Depositor
R, R_{free}	0.215 , 0.249 0.209 , 0.241	Depositor DCC
R_{free} test set	2966 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27064	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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 ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.52	43/3879 (1.1%)	1.35	18/5237 (0.3%)
1	B	1.55	47/3879 (1.2%)	1.42	17/5237 (0.3%)
1	C	1.46	40/3879 (1.0%)	1.34	12/5237 (0.2%)
1	D	1.45	30/3879 (0.8%)	1.36	12/5237 (0.2%)
1	E	1.55	38/3879 (1.0%)	1.41	16/5237 (0.3%)
1	F	1.36	26/3879 (0.7%)	1.33	14/5237 (0.3%)
1	G	1.49	39/3879 (1.0%)	1.35	7/5237 (0.1%)
All	All	1.49	263/27153 (1.0%)	1.37	96/36659 (0.3%)

All (263) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	MET	SD-CE	19.55	2.28	1.79
1	F	69	MET	SD-CE	-16.27	1.38	1.79
1	B	69	MET	SD-CE	-14.79	1.42	1.79
1	G	288	MET	SD-CE	13.49	2.13	1.79
1	C	69	MET	SD-CE	-12.43	1.48	1.79
1	D	69	MET	SD-CE	-12.12	1.49	1.79
1	E	69	MET	SD-CE	-11.63	1.50	1.79
1	C	491	MET	SD-CE	11.29	2.07	1.79
1	E	118	ARG	NE-CZ	10.83	1.45	1.33
1	F	491	MET	SD-CE	10.76	2.06	1.79
1	B	118	ARG	NE-CZ	10.20	1.44	1.33
1	C	488	MET	SD-CE	-10.10	1.54	1.79
1	B	44	PHE	CA-C	10.02	1.66	1.52
1	F	488	MET	SD-CE	-9.95	1.54	1.79
1	E	288	MET	SD-CE	9.78	2.04	1.79
1	A	118	ARG	NE-CZ	9.73	1.43	1.33
1	G	69	MET	SD-CE	-9.59	1.55	1.79
1	A	288	MET	SD-CE	9.56	2.03	1.79
1	B	466	ALA	CA-CB	-9.52	1.38	1.53
1	C	118	ARG	NE-CZ	9.35	1.43	1.33
1	A	447	MET	SD-CE	-9.24	1.56	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	GLU	CD-OE2	9.23	1.42	1.25
1	C	288	MET	SD-CE	9.21	2.02	1.79
1	E	129	GLU	CD-OE1	9.13	1.42	1.25
1	B	473	ASP	CB-CG	9.13	1.74	1.52
1	C	81	ALA	CA-CB	-8.81	1.39	1.53
1	G	114	MET	SD-CE	8.80	2.01	1.79
1	A	127	ALA	CA-CB	-8.77	1.39	1.53
1	B	489	ILE	CG1-CD1	8.57	1.85	1.51
1	B	44	PHE	CA-CB	8.49	1.66	1.53
1	B	16	MET	SD-CE	8.25	2.00	1.79
1	D	6	VAL	C-O	-8.22	1.15	1.24
1	E	488	MET	SD-CE	-8.22	1.59	1.79
1	B	491	MET	SD-CE	7.99	1.99	1.79
1	G	44	PHE	CA-CB	7.99	1.65	1.53
1	A	488	MET	SD-CE	-7.90	1.59	1.79
1	A	69	MET	SD-CE	-7.86	1.59	1.79
1	F	466	ALA	CA-CB	-7.85	1.41	1.53
1	G	118	ARG	NE-CZ	7.83	1.41	1.33
1	B	432	GLN	CG-CD	7.82	1.71	1.52
1	F	114	MET	SD-CE	7.79	1.99	1.79
1	D	432	GLN	CG-CD	7.74	1.71	1.52
1	B	100	ILE	CA-CB	-7.67	1.44	1.54
1	C	114	MET	SD-CE	7.67	1.98	1.79
1	E	71	ALA	CA-CB	-7.66	1.41	1.53
1	A	491	MET	SD-CE	7.65	1.98	1.79
1	D	447	MET	SD-CE	-7.49	1.60	1.79
1	D	44	PHE	CA-CB	7.46	1.65	1.53
1	A	44	PHE	CD1-CE1	7.41	1.60	1.38
1	G	488	MET	SD-CE	-7.39	1.61	1.79
1	A	92	ALA	CA-CB	-7.35	1.41	1.53
1	A	432	GLN	CG-CD	7.31	1.70	1.52
1	C	514	MET	SD-CE	7.24	1.97	1.79
1	A	96	ALA	CA-CB	-7.23	1.42	1.53
1	A	152	ALA	CA-CB	-7.16	1.43	1.53
1	D	30	THR	C-O	-7.15	1.14	1.24
1	C	96	ALA	CA-CB	-7.13	1.42	1.53
1	B	490	ASP	CA-C	-7.10	1.43	1.52
1	B	414	GLY	C-O	7.09	1.30	1.23
1	F	127	ALA	CA-CB	-7.09	1.42	1.53
1	B	10	ASN	CB-CG	7.05	1.69	1.52
1	E	10	ASN	CB-CG	6.99	1.69	1.52
1	A	284	ARG	NE-CZ	6.97	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	VAL	CA-CB	-6.97	1.46	1.54
1	F	123	ALA	CA-CB	-6.95	1.42	1.53
1	F	81	ALA	CA-C	6.92	1.61	1.52
1	C	514	MET	CG-SD	6.91	1.98	1.80
1	B	52	ASP	CA-CB	-6.89	1.44	1.53
1	G	447	MET	SD-CE	-6.88	1.62	1.79
1	B	490	ASP	CA-CB	-6.87	1.42	1.53
1	B	82	ASN	CG-OD1	6.84	1.36	1.23
1	B	44	PHE	CD2-CE2	6.82	1.59	1.38
1	G	491	MET	SD-CE	6.80	1.96	1.79
1	F	118	ARG	NE-CZ	6.76	1.40	1.33
1	B	43	SER	N-CA	6.70	1.54	1.46
1	C	432	GLN	CA-C	6.68	1.62	1.52
1	E	406	ALA	CA-CB	-6.68	1.41	1.53
1	C	520	MET	SD-CE	6.67	1.96	1.79
1	G	466	ALA	CA-CB	-6.67	1.43	1.53
1	F	49	ILE	C-O	-6.65	1.17	1.24
1	F	508	ALA	CA-CB	-6.65	1.42	1.53
1	G	96	ALA	CA-CB	-6.64	1.43	1.53
1	E	156	GLU	CD-OE2	6.59	1.37	1.25
1	C	445	ARG	CG-CD	6.57	1.72	1.52
1	B	58	ARG	CZ-NH1	6.57	1.42	1.32
1	E	76	GLU	CD-OE1	6.54	1.37	1.25
1	C	10	ASN	CB-CG	6.54	1.68	1.52
1	B	490	ASP	CG-OD1	6.51	1.37	1.25
1	A	511	ALA	CA-C	6.50	1.61	1.52
1	E	44	PHE	CA-CB	6.49	1.63	1.53
1	C	44	PHE	CD1-CE1	6.44	1.57	1.38
1	A	500	THR	CA-CB	-6.42	1.43	1.53
1	E	44	PHE	CD1-CE1	6.41	1.57	1.38
1	B	288	MET	SD-CE	6.38	1.95	1.79
1	D	441	LYS	C-O	-6.37	1.16	1.24
1	A	18	ARG	CG-CD	6.36	1.71	1.52
1	F	514	MET	CG-SD	6.35	1.96	1.80
1	B	71	ALA	CA-CB	-6.34	1.43	1.53
1	E	58	ARG	NE-CZ	6.33	1.40	1.33
1	C	44	PHE	CA-CB	6.30	1.63	1.53
1	A	270	ILE	CA-CB	6.29	1.61	1.54
1	E	114	MET	CG-SD	6.28	1.96	1.80
1	C	58	ARG	NE-CZ	6.28	1.40	1.33
1	E	44	PHE	CD2-CE2	6.28	1.57	1.38
1	A	44	PHE	CA-CB	6.28	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	44	PHE	CA-CB	6.27	1.63	1.53
1	C	57	ALA	CA-CB	-6.25	1.43	1.53
1	D	81	ALA	CA-CB	-6.25	1.43	1.53
1	F	44	PHE	CD1-CE1	6.24	1.57	1.38
1	D	458	CYS	C-O	-6.23	1.15	1.24
1	C	18	ARG	CZ-NH2	6.21	1.41	1.33
1	C	118	ARG	CD-NE	6.21	1.54	1.46
1	C	18	ARG	NE-CZ	6.20	1.39	1.33
1	D	473	ASP	CB-CG	6.20	1.67	1.52
1	D	18	ARG	CG-CD	6.19	1.71	1.52
1	F	58	ARG	NE-CZ	6.16	1.39	1.33
1	C	58	ARG	CZ-NH1	6.16	1.41	1.32
1	G	270	ILE	CA-CB	6.12	1.61	1.54
1	G	432	GLN	CG-CD	6.08	1.67	1.52
1	C	97	GLN	C-O	6.08	1.31	1.24
1	D	118	ARG	NE-CZ	6.07	1.39	1.33
1	A	454	ILE	CA-CB	-6.06	1.47	1.54
1	G	74	VAL	CA-C	6.04	1.60	1.52
1	B	438	VAL	C-O	-6.04	1.16	1.24
1	D	57	ALA	CA-CB	-6.04	1.43	1.53
1	D	445	ARG	CG-CD	6.03	1.70	1.52
1	E	18	ARG	CZ-NH2	6.03	1.41	1.33
1	A	118	ARG	CZ-NH2	5.98	1.41	1.33
1	G	514	MET	C-O	-5.97	1.16	1.24
1	E	54	VAL	CA-CB	5.93	1.61	1.54
1	G	44	PHE	CA-C	5.91	1.60	1.52
1	G	445	ARG	CG-CD	5.91	1.70	1.52
1	D	418	ALA	CA-CB	-5.89	1.44	1.53
1	E	18	ARG	NE-CZ	5.89	1.39	1.33
1	F	270	ILE	CA-CB	5.88	1.61	1.54
1	A	10	ASN	C-O	5.87	1.30	1.24
1	A	44	PHE	CD2-CE2	5.86	1.56	1.38
1	G	445	ARG	NE-CZ	5.86	1.39	1.33
1	F	423	ALA	CA-CB	-5.86	1.44	1.53
1	G	427	ALA	CA-CB	-5.84	1.43	1.53
1	E	133	ALA	C-O	-5.84	1.16	1.24
1	D	488	MET	SD-CE	-5.84	1.65	1.79
1	E	491	MET	SD-CE	5.83	1.94	1.79
1	B	74	VAL	CA-C	5.82	1.60	1.52
1	B	44	PHE	CD1-CE1	5.82	1.56	1.38
1	F	16	MET	SD-CE	5.80	1.94	1.79
1	A	120	ILE	CA-C	5.78	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	473	ASP	CG-OD2	5.78	1.36	1.25
1	D	16	MET	SD-CE	5.77	1.94	1.79
1	B	76	GLU	CD-OE1	5.76	1.36	1.25
1	E	284	ARG	NE-CZ	5.76	1.39	1.33
1	A	13	GLY	C-O	5.75	1.30	1.23
1	D	514	MET	CG-SD	5.73	1.95	1.80
1	C	26	ALA	CA-CB	-5.72	1.44	1.53
1	F	476	TYR	CA-C	5.72	1.60	1.52
1	F	284	ARG	NE-CZ	5.72	1.39	1.33
1	E	118	ARG	CZ-NH1	5.70	1.40	1.32
1	E	129	GLU	C-O	-5.67	1.17	1.24
1	C	78	ALA	CA-CB	-5.66	1.44	1.53
1	F	177	VAL	CA-CB	5.66	1.61	1.54
1	C	149	THR	CA-CB	5.65	1.62	1.53
1	B	490	ASP	CB-CG	-5.64	1.38	1.52
1	C	284	ARG	CA-C	5.64	1.60	1.52
1	G	44	PHE	CD2-CE2	5.63	1.55	1.38
1	A	58	ARG	CG-CD	5.63	1.69	1.52
1	G	44	PHE	CD1-CE1	5.62	1.55	1.38
1	F	25	ASP	C-O	-5.62	1.17	1.24
1	G	44	PHE	CB-CG	5.62	1.63	1.50
1	A	118	ARG	CZ-NH1	5.61	1.40	1.32
1	E	126	VAL	C-O	5.61	1.30	1.24
1	D	89	THR	CA-C	-5.59	1.45	1.52
1	B	20	VAL	CA-CB	-5.58	1.47	1.54
1	G	26	ALA	CA-C	5.58	1.60	1.52
1	B	95	LEU	C-O	5.56	1.30	1.24
1	A	8	PHE	C-O	-5.55	1.16	1.23
1	E	118	ARG	CZ-NH2	5.54	1.40	1.33
1	A	443	ALA	CA-CB	-5.54	1.44	1.53
1	E	494	LEU	C-O	-5.54	1.17	1.23
1	A	25	ASP	C-O	-5.52	1.17	1.24
1	C	14	VAL	CA-CB	5.52	1.62	1.54
1	D	284	ARG	CG-CD	5.50	1.69	1.52
1	G	49	ILE	C-O	-5.50	1.18	1.24
1	B	118	ARG	CZ-NH2	5.50	1.40	1.33
1	G	18	ARG	CZ-NH2	5.50	1.40	1.33
1	C	44	PHE	CD2-CE2	5.48	1.55	1.38
1	A	18	ARG	CZ-NH2	5.48	1.40	1.33
1	B	49	ILE	C-O	-5.48	1.18	1.24
1	G	446	ALA	CA-CB	-5.44	1.44	1.53
1	A	82	ASN	N-CA	5.44	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	TYR	CA-C	-5.44	1.46	1.52
1	A	438	VAL	CA-CB	5.44	1.61	1.54
1	E	449	ALA	CA-CB	-5.43	1.46	1.53
1	G	149	THR	CA-CB	5.42	1.62	1.53
1	A	87	ASP	C-O	5.42	1.29	1.23
1	B	473	ASP	CG-OD1	5.41	1.35	1.25
1	D	78	ALA	CA-CB	-5.40	1.44	1.53
1	G	480	ALA	CA-CB	-5.39	1.44	1.53
1	B	445	ARG	CD-NE	5.39	1.53	1.46
1	D	437	ASN	CA-C	-5.38	1.45	1.52
1	G	412	VAL	C-O	-5.38	1.18	1.23
1	G	501	ARG	NE-CZ	5.37	1.39	1.33
1	B	144	ILE	C-O	5.37	1.30	1.24
1	B	80	LYS	C-O	5.36	1.30	1.24
1	D	26	ALA	CA-CB	-5.35	1.44	1.53
1	C	270	ILE	CA-CB	5.33	1.60	1.54
1	D	449	ALA	CA-CB	-5.33	1.46	1.53
1	G	449	ALA	N-CA	5.33	1.51	1.46
1	B	38	VAL	CA-CB	-5.32	1.48	1.54
1	C	123	ALA	CA-CB	-5.31	1.45	1.53
1	G	473	ASP	CG-OD1	5.31	1.35	1.25
1	F	519	CYS	C-O	-5.30	1.17	1.23
1	G	514	MET	CG-SD	5.29	1.94	1.80
1	D	446	ALA	CA-CB	-5.29	1.44	1.53
1	D	54	VAL	CA-CB	5.29	1.61	1.54
1	G	6	VAL	C-O	-5.29	1.18	1.24
1	A	521	VAL	C-O	-5.29	1.18	1.24
1	C	44	PHE	CA-C	5.28	1.59	1.52
1	E	44	PHE	CA-C	5.28	1.59	1.52
1	G	76	GLU	CD-OE2	5.28	1.35	1.25
1	G	467	ASN	N-CA	-5.26	1.40	1.46
1	A	56	VAL	N-CA	-5.25	1.40	1.46
1	E	514	MET	SD-CE	5.24	1.92	1.79
1	G	87	ASP	CA-C	5.24	1.59	1.52
1	G	453	GLN	C-O	5.24	1.30	1.24
1	E	27	VAL	CA-C	5.23	1.60	1.52
1	A	445	ARG	CD-NE	5.21	1.53	1.46
1	E	150	ILE	CA-CB	5.21	1.61	1.54
1	C	513	LEU	C-O	5.21	1.30	1.24
1	D	44	PHE	CD1-CE1	5.21	1.54	1.38
1	B	87	ASP	C-O	5.21	1.29	1.23
1	B	172	GLU	CA-CB	5.20	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	ARG	CD-NE	5.20	1.53	1.46
1	G	284	ARG	CA-C	5.20	1.60	1.52
1	E	57	ALA	CA-CB	-5.20	1.45	1.53
1	E	49	ILE	C-O	-5.17	1.18	1.24
1	C	101	THR	CA-CB	-5.14	1.45	1.53
1	C	10	ASN	CG-ND2	5.14	1.44	1.33
1	C	84	ALA	CA-C	5.14	1.59	1.52
1	A	92	ALA	N-CA	-5.14	1.40	1.46
1	B	14	VAL	CA-CB	5.14	1.60	1.54
1	A	44	PHE	CG-CD2	5.13	1.49	1.38
1	B	44	PHE	CB-CG	5.13	1.62	1.50
1	A	58	ARG	CZ-NH1	5.13	1.40	1.32
1	B	447	MET	SD-CE	-5.12	1.66	1.79
1	E	16	MET	CG-SD	5.11	1.93	1.80
1	F	445	ARG	CG-CD	5.11	1.67	1.52
1	B	149	THR	CA-CB	5.10	1.61	1.53
1	A	44	PHE	CB-CG	5.09	1.62	1.50
1	B	514	MET	CG-SD	5.09	1.93	1.80
1	A	96	ALA	N-CA	-5.08	1.40	1.46
1	E	432	GLN	CD-OE1	5.07	1.33	1.23
1	C	284	ARG	CG-CD	5.07	1.67	1.52
1	A	423	ALA	C-O	-5.07	1.18	1.24
1	C	406	ALA	CA-CB	-5.06	1.44	1.53
1	D	133	ALA	C-O	-5.06	1.17	1.24
1	E	14	VAL	CA-CB	5.06	1.61	1.54
1	F	18	ARG	CZ-NH2	5.06	1.40	1.33
1	G	447	MET	C-O	-5.04	1.17	1.24
1	D	270	ILE	CA-CB	5.03	1.60	1.54
1	B	58	ARG	CZ-NH2	5.03	1.40	1.33
1	D	18	ARG	CZ-NH1	5.02	1.39	1.32
1	C	432	GLN	CD-OE1	5.00	1.33	1.23
1	F	57	ALA	CA-CB	-5.00	1.45	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	VAL	CB-CA-C	-10.88	97.45	112.14
1	F	510	VAL	CB-CA-C	-10.80	97.56	112.14
1	B	490	ASP	N-CA-C	10.64	122.88	111.28
1	G	510	VAL	CB-CA-C	-10.00	99.18	111.97
1	C	510	VAL	CB-CA-C	-9.82	98.88	112.14
1	B	510	VAL	CB-CA-C	-9.75	98.97	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	510	VAL	CB-CA-C	-9.46	99.86	111.97
1	B	490	ASP	CB-CA-C	-9.27	95.41	110.79
1	G	510	VAL	N-CA-CB	8.97	121.05	110.55
1	D	510	VAL	CB-CA-C	-8.89	100.14	112.14
1	E	132	LYS	N-CA-C	-8.74	101.75	111.28
1	B	491	MET	CG-SD-CE	-8.67	81.84	100.90
1	C	99	ILE	N-CA-C	-8.49	101.75	111.00
1	F	417	VAL	N-CA-C	7.95	118.05	110.42
1	A	87	ASP	CA-C-N	-7.86	114.28	123.08
1	A	87	ASP	C-N-CA	-7.86	114.28	123.08
1	C	65	LYS	N-CA-C	7.86	119.84	111.28
1	A	63	GLU	N-CA-C	7.41	119.44	111.36
1	B	77	VAL	N-CA-C	-7.31	103.03	111.00
1	F	81	ALA	N-CA-C	6.84	118.43	110.97
1	G	29	VAL	N-CA-C	-6.74	104.24	113.00
1	F	56	VAL	N-CA-C	-6.44	104.48	110.53
1	A	510	VAL	N-CA-CB	6.42	119.27	110.54
1	E	491	MET	CG-SD-CE	-6.40	86.83	100.90
1	C	118	ARG	CA-C-N	6.31	126.95	119.94
1	C	118	ARG	C-N-CA	6.31	126.95	119.94
1	C	46	ALA	N-CA-C	-6.18	102.28	110.07
1	D	10	ASN	N-CA-C	6.07	117.90	111.28
1	C	5	ASP	N-CA-C	-6.06	99.02	108.90
1	E	417	VAL	N-CA-C	6.04	116.21	110.53
1	A	99	ILE	N-CA-C	-6.01	104.65	110.42
1	B	494	LEU	N-CA-C	5.98	118.26	109.24
1	A	9	GLY	N-CA-C	5.97	122.20	111.34
1	E	326	ASN	CB-CA-C	-5.94	99.73	111.60
1	D	417	VAL	N-CA-C	5.90	116.08	110.53
1	E	63	GLU	N-CA-C	5.90	117.39	111.07
1	D	73	MET	N-CA-C	-5.88	104.78	111.07
1	B	73	MET	N-CA-C	-5.82	104.85	111.14
1	B	489	ILE	N-CA-C	5.81	116.59	110.72
1	D	466	ALA	N-CA-C	-5.79	105.05	111.36
1	F	80	LYS	N-CA-C	-5.79	104.94	112.23
1	E	491	MET	N-CA-C	-5.78	106.20	113.20
1	D	82	ASN	N-CA-C	-5.77	104.99	111.28
1	E	5	ASP	CA-C-N	-5.76	115.59	123.14
1	E	5	ASP	C-N-CA	-5.76	115.59	123.14
1	A	469	VAL	CB-CA-C	-5.73	104.55	111.88
1	D	436	GLN	N-CA-C	-5.69	105.06	112.23
1	E	421	ARG	NE-CZ-NH2	-5.68	114.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	172	GLU	CA-CB-CG	5.66	125.43	114.10
1	D	325	ILE	N-CA-C	5.65	116.61	108.48
1	F	86	GLY	N-CA-C	-5.57	107.63	115.32
1	F	48	THR	OG1-CB-CG2	-5.57	98.17	109.30
1	E	125	THR	OG1-CB-CG2	-5.56	98.18	109.30
1	A	171	LYS	N-CA-C	5.46	117.24	111.28
1	F	72	GLN	N-CA-C	5.44	117.29	111.36
1	F	325	ILE	N-CA-C	5.44	116.31	108.48
1	F	67	GLU	N-CA-C	-5.35	105.45	111.28
1	B	443	ALA	N-CA-C	-5.34	105.37	111.14
1	G	86	GLY	N-CA-C	-5.33	107.96	115.32
1	G	20	VAL	N-CA-C	-5.33	105.33	110.72
1	D	510	VAL	N-CA-CB	5.31	117.76	110.54
1	C	325	ILE	N-CA-C	5.30	116.12	108.48
1	A	325	ILE	N-CA-C	5.30	116.11	108.48
1	A	114	MET	N-CA-C	-5.29	105.59	111.36
1	F	63	GLU	N-CA-C	5.28	117.12	111.36
1	E	510	VAL	N-CA-CB	5.28	116.73	110.55
1	D	141	SER	N-CA-C	5.26	117.70	111.33
1	D	125	THR	OG1-CB-CG2	-5.25	98.79	109.30
1	A	411	VAL	N-CA-CB	-5.24	102.13	111.92
1	B	63	GLU	N-CA-C	5.23	116.67	111.07
1	E	227	ILE	N-CA-C	5.22	114.81	106.88
1	A	141	SER	N-CA-C	5.22	117.64	111.33
1	B	432	GLN	CA-CB-CG	5.21	124.51	114.10
1	C	435	ASP	N-CA-C	-5.19	105.70	111.36
1	C	369	VAL	N-CA-CB	5.18	117.59	110.54
1	A	86	GLY	N-CA-C	-5.17	108.18	115.32
1	E	471	GLY	N-CA-C	-5.17	108.54	115.32
1	A	435	ASP	N-CA-C	-5.15	105.74	111.36
1	G	99	ILE	N-CA-C	-5.14	105.53	110.72
1	F	500	THR	OG1-CB-CG2	-5.14	99.02	109.30
1	B	452	ARG	CB-CG-CD	5.13	123.11	111.30
1	C	503	ALA	N-CA-C	-5.12	105.59	111.07
1	A	421	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	B	480	ALA	N-CA-C	5.10	117.74	111.82
1	B	486	GLY	CA-C-O	-5.09	116.80	121.63
1	F	510	VAL	N-CA-CB	5.07	117.44	110.54
1	E	325	ILE	N-CA-C	5.06	115.77	108.48
1	B	325	ILE	N-CA-C	5.06	115.77	108.48
1	D	227	ILE	N-CA-C	5.04	114.55	106.88
1	F	369	VAL	N-CA-CB	5.04	116.45	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ASN	CB-CA-C	-5.04	101.53	111.60
1	B	435	ASP	N-CA-C	-5.03	105.88	111.36
1	C	411	VAL	N-CA-CB	-5.03	102.63	111.93
1	A	58	ARG	N-CA-C	-5.02	106.41	112.54
1	B	445	ARG	N-CA-C	-5.01	105.92	112.23
1	G	141	SER	N-CA-C	5.01	117.39	111.33

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	3851	0	3970	83	0
1	B	3851	0	3970	90	0
1	C	3851	0	3970	81	1
1	D	3851	0	3970	82	0
1	E	3851	0	3970	84	0
1	F	3851	0	3970	74	0
1	G	3851	0	3970	84	1
2	A	18	0	0	1	0
2	B	21	0	0	4	0
2	C	15	0	0	0	0
2	D	16	0	0	0	0
2	E	17	0	0	0	0
2	F	7	0	0	1	0
2	G	13	0	0	1	0
All	All	27064	0	27790	559	1

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 10.

All (559) 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:B:473:ASP:CG	1:B:473:ASP:CB	1.74	1.56
1:B:489:ILE:CD1	1:B:489:ILE:CG1	1.85	1.52
1:A:288:MET:CE	1:A:288:MET:SD	2.03	1.47
1:G:114:MET:SD	1:G:114:MET:CE	2.01	1.46
1:C:288:MET:SD	1:C:288:MET:CE	2.02	1.46
1:E:288:MET:SD	1:E:288:MET:CE	2.04	1.46
1:F:491:MET:SD	1:F:491:MET:CE	2.06	1.44
1:C:491:MET:CE	1:C:491:MET:SD	2.07	1.43
1:G:288:MET:SD	1:G:288:MET:CE	2.13	1.36
1:A:114:MET:SD	1:A:114:MET:CE	2.28	1.22
1:G:142:LYS:H	1:G:142:LYS:HD3	1.08	1.12
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.40	1.04
1:B:142:LYS:H	1:B:142:LYS:HD3	1.25	0.98
1:G:142:LYS:HD3	1:G:142:LYS:N	1.77	0.98
1:E:142:LYS:HD3	1:E:142:LYS:H	1.29	0.97
1:B:142:LYS:HD3	1:B:142:LYS:N	1.81	0.95
1:B:473:ASP:OD1	2:B:528:HOH:O	1.84	0.94
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.48	0.94
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.48	0.94
1:C:142:LYS:H	1:C:142:LYS:HD3	1.32	0.93
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.48	0.93
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.48	0.93
1:F:142:LYS:H	1:F:142:LYS:HD3	1.34	0.92
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.50	0.91
1:C:62:LEU:H	1:C:68:ASN:HD22	1.16	0.91
1:D:142:LYS:H	1:D:142:LYS:HD3	1.33	0.91
1:A:62:LEU:H	1:A:68:ASN:HD22	1.13	0.91
1:E:142:LYS:HD3	1:E:142:LYS:N	1.89	0.88
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.53	0.87
1:G:149:THR:HG22	1:G:159:GLY:HA3	1.57	0.86
1:C:142:LYS:HD3	1:C:142:LYS:N	1.91	0.85
1:C:421:ARG:HD2	1:C:474:GLY:O	1.76	0.85
1:B:149:THR:HG22	1:B:159:GLY:HA3	1.57	0.85
1:A:62:LEU:H	1:A:68:ASN:ND2	1.75	0.84
1:A:142:LYS:H	1:A:142:LYS:HD3	1.41	0.84
1:B:490:ASP:OD2	2:B:536:HOH:O	1.95	0.84
1:C:149:THR:HG22	1:C:159:GLY:HA3	1.58	0.83
1:D:142:LYS:HD3	1:D:142:LYS:N	1.93	0.83
1:D:149:THR:HG22	1:D:159:GLY:HA3	1.58	0.83
1:A:42:LYS:HE2	1:A:48:THR:HG23	1.60	0.82
1:A:142:LYS:HD3	1:A:142:LYS:N	1.94	0.81
1:B:62:LEU:H	1:B:68:ASN:ND2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:HD2	1:A:474:GLY:O	1.79	0.81
1:C:62:LEU:H	1:C:68:ASN:ND2	1.79	0.80
1:G:213:VAL:HB	1:G:325:ILE:CG1	2.12	0.80
1:D:421:ARG:HD2	1:D:474:GLY:O	1.82	0.79
1:C:42:LYS:HE2	1:C:48:THR:HG23	1.64	0.79
1:D:62:LEU:H	1:D:68:ASN:ND2	1.80	0.79
1:E:145:ALA:O	1:E:149:THR:CG2	2.31	0.79
1:D:145:ALA:O	1:D:149:THR:HG23	1.83	0.78
1:F:62:LEU:H	1:F:68:ASN:HD22	1.30	0.78
1:F:142:LYS:HD3	1:F:142:LYS:N	1.97	0.78
1:A:149:THR:HG22	1:A:159:GLY:HA3	1.64	0.78
1:E:145:ALA:O	1:E:149:THR:HG23	1.82	0.78
1:A:452:ARG:NH2	1:A:463:SER:HB3	1.98	0.78
1:D:213:VAL:HB	1:D:325:ILE:CG1	2.14	0.77
1:B:62:LEU:H	1:B:68:ASN:HD22	1.32	0.77
1:B:494:LEU:O	1:B:494:LEU:HD12	1.85	0.77
1:F:149:THR:HG22	1:F:159:GLY:HA3	1.64	0.77
1:F:452:ARG:NH2	1:F:463:SER:HB3	2.00	0.77
1:C:494:LEU:HD12	1:C:494:LEU:O	1.85	0.76
1:G:142:LYS:H	1:G:142:LYS:CD	1.95	0.76
1:D:42:LYS:HE2	1:D:48:THR:HG23	1.66	0.76
1:B:213:VAL:HB	1:B:325:ILE:CG1	2.16	0.76
1:A:145:ALA:O	1:A:149:THR:HG23	1.85	0.76
1:F:421:ARG:HD2	1:F:474:GLY:O	1.86	0.76
1:B:448:GLU:OE1	1:B:452:ARG:NH1	2.19	0.75
1:G:62:LEU:H	1:G:68:ASN:ND2	1.84	0.75
1:G:62:LEU:H	1:G:68:ASN:HD22	1.34	0.75
1:F:213:VAL:HB	1:F:325:ILE:CG1	2.17	0.74
1:D:62:LEU:H	1:D:68:ASN:HD22	1.35	0.74
1:C:213:VAL:HB	1:C:325:ILE:CG1	2.17	0.74
1:D:431:GLY:H	1:D:437:ASN:HD21	1.36	0.74
1:E:213:VAL:HB	1:E:325:ILE:CG1	2.17	0.74
1:F:473:ASP:OD1	2:F:527:HOH:O	2.05	0.74
1:D:452:ARG:NH2	1:D:463:SER:HB3	2.02	0.73
1:A:213:VAL:HB	1:A:325:ILE:CG1	2.18	0.73
1:A:231:ARG:NH1	1:B:241:ALA:HB1	2.03	0.73
1:F:62:LEU:H	1:F:68:ASN:ND2	1.88	0.72
1:E:431:GLY:H	1:E:437:ASN:HD21	1.35	0.72
1:D:77:VAL:HG21	1:D:510:VAL:HG13	1.71	0.72
1:F:145:ALA:O	1:F:149:THR:HG23	1.90	0.72
1:E:166:MET:HG2	1:E:171:LYS:HA	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:431:GLY:H	1:G:437:ASN:HD21	1.35	0.71
1:A:319:GLN:HB3	1:A:336:VAL:HG21	1.73	0.71
1:G:291:ASP:OD2	1:G:368:ARG:HD2	1.91	0.71
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.90	0.71
1:B:291:ASP:OD2	1:B:368:ARG:HD2	1.90	0.70
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.73	0.70
1:C:431:GLY:H	1:C:437:ASN:ND2	1.90	0.70
1:F:179:ASP:OD1	1:F:393:LYS:HE3	1.91	0.70
1:C:42:LYS:HE2	1:C:48:THR:CG2	2.20	0.70
1:B:431:GLY:H	1:B:437:ASN:HD21	1.38	0.70
1:E:431:GLY:H	1:E:437:ASN:ND2	1.90	0.70
1:C:479:ASN:HD22	1:C:491:MET:HE2	1.57	0.70
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.74	0.69
1:A:448:GLU:OE1	1:A:452:ARG:NH1	2.25	0.69
1:G:421:ARG:HD2	1:G:474:GLY:O	1.93	0.69
1:C:431:GLY:H	1:C:437:ASN:HD21	1.40	0.69
1:A:291:ASP:OD2	1:A:368:ARG:HD2	1.92	0.69
1:G:145:ALA:O	1:G:149:THR:HG23	1.94	0.68
1:A:42:LYS:HE2	1:A:48:THR:CG2	2.23	0.68
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.76	0.68
1:B:42:LYS:HE2	1:B:48:THR:HG23	1.76	0.67
1:A:269:GLY:HA3	1:G:257:GLU:HG3	1.77	0.67
1:G:41:ASP:O	1:G:42:LYS:HD3	1.95	0.67
1:E:149:THR:HG22	1:E:159:GLY:HA3	1.75	0.67
1:B:166:MET:HG2	1:B:171:LYS:HA	1.76	0.67
1:A:231:ARG:CZ	1:B:241:ALA:HB1	2.24	0.66
1:F:42:LYS:HE2	1:F:48:THR:HG23	1.75	0.66
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.77	0.66
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.76	0.66
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.76	0.66
1:A:431:GLY:H	1:A:437:ASN:HD21	1.43	0.66
1:E:326:ASN:HD22	1:E:329:THR:HB	1.61	0.66
1:A:145:ALA:O	1:A:149:THR:CG2	2.44	0.66
1:D:145:ALA:O	1:D:149:THR:CG2	2.43	0.66
1:B:145:ALA:O	1:B:149:THR:HG23	1.95	0.65
1:D:494:LEU:HD12	1:D:494:LEU:O	1.97	0.65
1:D:73:MET:HE2	1:D:514:MET:HE2	1.78	0.65
1:E:62:LEU:H	1:E:68:ASN:HD22	1.43	0.65
1:E:291:ASP:OD2	1:E:368:ARG:HD2	1.96	0.65
1:B:431:GLY:H	1:B:437:ASN:ND2	1.95	0.65
1:E:142:LYS:H	1:E:142:LYS:CD	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:H	1:E:68:ASN:ND2	1.95	0.65
1:B:479:ASN:HD22	1:B:491:MET:HE2	1.61	0.64
1:C:321:LYS:HG3	1:C:334:ASP:HB3	1.80	0.64
1:A:66:PHE:HA	1:A:69:MET:HE3	1.77	0.64
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.28	0.64
1:G:42:LYS:HE2	1:G:48:THR:HG23	1.80	0.64
1:C:291:ASP:OD2	1:C:368:ARG:HD2	1.98	0.64
1:D:431:GLY:H	1:D:437:ASN:ND2	1.95	0.64
1:C:145:ALA:O	1:C:149:THR:HG23	1.98	0.63
1:B:224:ASP:O	1:B:225:LYS:HB3	1.99	0.63
1:B:494:LEU:HD12	1:B:494:LEU:C	2.23	0.63
1:D:421:ARG:CD	1:D:474:GLY:O	2.47	0.63
1:E:421:ARG:HD2	1:E:474:GLY:O	1.98	0.63
1:F:68:ASN:ND2	1:F:72:GLN:HE21	1.97	0.63
1:D:257:GLU:HG3	1:E:269:GLY:O	1.98	0.63
1:E:452:ARG:NH2	1:E:463:SER:HB3	2.14	0.63
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.80	0.62
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.99	0.62
1:F:321:LYS:HG3	1:F:334:ASP:HB3	1.81	0.62
1:G:452:ARG:NH2	1:G:463:SER:HB3	2.13	0.62
1:F:41:ASP:O	1:F:42:LYS:HD3	1.99	0.62
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.82	0.62
1:E:68:ASN:HD21	1:E:72:GLN:HE21	1.47	0.62
1:C:229:ASN:OD1	1:D:269:GLY:O	2.18	0.62
1:E:321:LYS:HG3	1:E:334:ASP:HB3	1.81	0.62
1:F:145:ALA:O	1:F:149:THR:CG2	2.47	0.62
1:G:166:MET:HG2	1:G:171:LYS:HA	1.82	0.62
1:B:179:ASP:OD1	1:B:393:LYS:HE3	2.00	0.62
1:B:326:ASN:HD22	1:B:329:THR:HB	1.65	0.61
1:G:73:MET:HE2	1:G:514:MET:HE2	1.82	0.61
1:D:321:LYS:HG3	1:D:334:ASP:HB3	1.81	0.61
1:F:431:GLY:H	1:F:437:ASN:ND2	1.97	0.61
1:C:224:ASP:O	1:C:225:LYS:HB3	2.00	0.61
1:E:77:VAL:HG21	1:E:510:VAL:HG13	1.81	0.61
1:C:77:VAL:HG21	1:C:510:VAL:HG13	1.82	0.61
1:D:142:LYS:H	1:D:142:LYS:CD	2.11	0.61
1:F:224:ASP:O	1:F:225:LYS:HB3	2.01	0.61
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.83	0.61
1:C:179:ASP:OD1	1:C:393:LYS:HE3	2.01	0.61
1:D:319:GLN:HB3	1:D:336:VAL:HG21	1.83	0.60
1:D:42:LYS:HE2	1:D:48:THR:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASN:HD22	1:A:329:THR:HB	1.66	0.60
1:E:42:LYS:CE	1:E:48:THR:HG23	2.31	0.60
1:B:142:LYS:H	1:B:142:LYS:CD	2.06	0.60
1:E:477:GLY:C	1:E:488:MET:HE3	2.27	0.60
1:D:166:MET:HG2	1:D:171:LYS:HA	1.84	0.60
1:E:27:VAL:HG13	1:E:90:THR:HG23	1.82	0.60
1:C:142:LYS:H	1:C:142:LYS:CD	2.13	0.60
1:C:491:MET:CE	1:C:491:MET:CG	2.79	0.60
1:F:42:LYS:CE	1:F:48:THR:HG23	2.32	0.60
1:G:77:VAL:HG21	1:G:510:VAL:HG13	1.83	0.60
1:F:68:ASN:HD21	1:F:72:GLN:HE21	1.48	0.59
1:E:179:ASP:OD1	1:E:393:LYS:HE3	2.02	0.59
1:C:145:ALA:O	1:C:149:THR:CG2	2.50	0.59
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.83	0.59
1:D:42:LYS:CE	1:D:48:THR:CG2	2.81	0.59
1:A:224:ASP:O	1:A:225:LYS:HB3	2.03	0.58
1:C:494:LEU:HD12	1:C:494:LEU:C	2.28	0.58
1:G:326:ASN:HD22	1:G:329:THR:HB	1.69	0.58
1:D:494:LEU:HD12	1:D:494:LEU:C	2.28	0.58
1:E:66:PHE:HA	1:E:69:MET:HE3	1.86	0.58
1:E:68:ASN:ND2	1:E:72:GLN:HE21	2.00	0.58
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.84	0.58
1:C:421:ARG:CD	1:C:474:GLY:O	2.50	0.58
1:D:66:PHE:HA	1:D:69:MET:HE3	1.84	0.58
1:B:142:LYS:N	1:B:142:LYS:CD	2.63	0.57
1:D:477:GLY:C	1:D:488:MET:HE3	2.29	0.57
1:E:42:LYS:HE2	1:E:48:THR:HG23	1.87	0.57
1:E:233:MET:HE1	1:E:249:ILE:CD1	2.34	0.57
1:D:42:LYS:HE3	1:D:48:THR:HG21	1.86	0.57
1:G:68:ASN:O	1:G:72:GLN:HG2	2.04	0.57
1:F:27:VAL:HG13	1:F:90:THR:HG23	1.85	0.57
1:C:452:ARG:NH2	1:C:463:SER:HB3	2.20	0.57
1:B:7:LYS:HE3	1:B:15:LYS:HE3	1.86	0.57
1:C:284:ARG:O	1:C:288:MET:HG3	2.03	0.57
1:G:66:PHE:HA	1:G:69:MET:HE3	1.86	0.57
1:B:257:GLU:HG3	1:C:269:GLY:HA3	1.86	0.57
1:B:145:ALA:O	1:B:149:THR:CG2	2.52	0.56
1:C:448:GLU:OE1	1:C:452:ARG:NH1	2.34	0.56
1:A:42:LYS:CE	1:A:48:THR:CG2	2.84	0.56
1:E:42:LYS:HE3	1:E:48:THR:CG2	2.35	0.56
1:E:145:ALA:O	1:E:149:THR:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:MET:CE	1:G:514:MET:HE2	2.34	0.56
1:D:179:ASP:OD1	1:D:393:LYS:HE3	2.05	0.56
1:C:326:ASN:HD22	1:C:329:THR:HB	1.70	0.56
1:G:421:ARG:CD	1:G:474:GLY:O	2.53	0.56
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.86	0.56
1:A:321:LYS:HG3	1:A:334:ASP:HB3	1.87	0.56
1:C:42:LYS:CE	1:C:48:THR:CG2	2.84	0.56
1:B:68:ASN:O	1:B:72:GLN:HG2	2.05	0.56
1:G:431:GLY:H	1:G:437:ASN:ND2	2.02	0.56
1:A:47:PRO:HG2	1:G:73:MET:HG3	1.86	0.55
1:A:288:MET:CE	1:A:288:MET:CG	2.83	0.55
1:F:491:MET:CE	1:F:491:MET:CG	2.84	0.55
1:A:431:GLY:H	1:A:437:ASN:ND2	2.04	0.55
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.37	0.55
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.88	0.55
1:B:27:VAL:HG13	1:B:90:THR:HG23	1.88	0.55
1:D:326:ASN:HB3	1:D:328:ASP:H	1.72	0.55
1:E:224:ASP:O	1:E:225:LYS:HB3	2.07	0.55
1:B:172:GLU:OE1	1:B:172:GLU:HA	2.07	0.54
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.88	0.54
1:A:166:MET:HG2	1:A:171:LYS:HA	1.89	0.54
1:F:326:ASN:HD22	1:F:329:THR:HB	1.72	0.54
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.89	0.54
1:G:233:MET:HE1	1:G:249:ILE:CD1	2.37	0.54
1:D:326:ASN:HD22	1:D:329:THR:HB	1.72	0.54
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.88	0.54
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.90	0.54
1:A:325:ILE:HG22	1:A:330:THR:OG1	2.08	0.54
1:B:473:ASP:CG	1:B:473:ASP:CA	2.74	0.54
1:D:218:PRO:HD2	1:D:320:ALA:O	2.07	0.54
1:E:358:SER:HB3	1:E:361:ASP:OD1	2.08	0.54
1:F:68:ASN:O	1:F:72:GLN:HG2	2.07	0.54
1:G:479:ASN:HD22	1:G:491:MET:HE2	1.72	0.53
1:F:218:PRO:HD2	1:F:320:ALA:O	2.08	0.53
1:F:325:ILE:HG22	1:F:330:THR:OG1	2.08	0.53
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.91	0.53
1:C:448:GLU:O	1:C:452:ARG:HG3	2.08	0.53
1:D:73:MET:HG3	1:E:47:PRO:HG2	1.90	0.53
1:E:73:MET:HE2	1:E:514:MET:HE2	1.90	0.53
1:A:233:MET:HE1	1:A:249:ILE:CD1	2.39	0.53
1:A:494:LEU:HD12	1:A:494:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:H	1:A:142:LYS:CD	2.18	0.53
1:C:69:MET:HE1	1:C:522:THR:HB	1.91	0.53
1:G:145:ALA:O	1:G:149:THR:CG2	2.55	0.53
1:G:224:ASP:O	1:G:225:LYS:HB3	2.08	0.53
1:D:73:MET:CE	1:D:514:MET:HE2	2.38	0.53
1:A:257:GLU:HG3	1:B:269:GLY:HA3	1.91	0.53
1:B:118:ARG:HH22	1:C:34:LYS:HE2	1.74	0.53
1:C:69:MET:CE	1:C:522:THR:HB	2.39	0.53
1:E:233:MET:HE1	1:E:249:ILE:HD12	1.91	0.53
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.89	0.52
1:A:179:ASP:OD1	1:A:393:LYS:HE3	2.09	0.52
1:F:42:LYS:HE3	1:F:48:THR:HG21	1.91	0.52
1:E:326:ASN:HB3	1:E:328:ASP:H	1.74	0.52
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.39	0.52
1:A:218:PRO:HD2	1:A:320:ALA:O	2.10	0.52
1:F:42:LYS:HE3	1:F:48:THR:CG2	2.39	0.52
1:G:448:GLU:HB3	1:G:452:ARG:HD2	1.91	0.52
1:D:325:ILE:HG22	1:D:330:THR:OG1	2.10	0.52
1:F:448:GLU:OE1	1:F:452:ARG:NH1	2.42	0.52
1:B:172:GLU:OE1	1:B:172:GLU:CA	2.58	0.51
1:F:233:MET:HE1	1:F:249:ILE:CD1	2.40	0.51
1:G:349:ILE:CG2	1:G:369:VAL:HG13	2.40	0.51
1:C:218:PRO:HD2	1:C:320:ALA:O	2.10	0.51
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.92	0.51
1:C:233:MET:HE1	1:C:249:ILE:HD12	1.92	0.51
1:B:162:ILE:HD12	1:B:400:LEU:HA	1.92	0.51
1:C:477:GLY:C	1:C:488:MET:HE3	2.35	0.51
1:A:62:LEU:N	1:A:68:ASN:HD22	1.96	0.51
1:C:319:GLN:HB3	1:C:336:VAL:HG21	1.93	0.51
1:C:479:ASN:HD22	1:C:491:MET:CE	2.21	0.51
1:C:358:SER:HB3	1:C:361:ASP:OD1	2.10	0.51
1:E:218:PRO:HD2	1:E:320:ALA:O	2.11	0.51
1:F:326:ASN:HB3	1:F:328:ASP:H	1.76	0.51
1:B:319:GLN:HB3	1:B:336:VAL:CG2	2.41	0.50
1:F:494:LEU:HD12	1:F:494:LEU:O	2.11	0.50
1:C:73:MET:HG3	1:D:47:PRO:HG2	1.93	0.50
1:C:263:VAL:O	1:C:267:MET:HB2	2.12	0.50
1:B:233:MET:HE1	1:B:249:ILE:CD1	2.42	0.50
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.40	0.50
1:F:42:LYS:CE	1:F:48:THR:CG2	2.89	0.50
1:D:180:GLY:HA3	1:D:381:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:431:GLY:H	1:F:437:ASN:HD21	1.57	0.50
1:G:321:LYS:HG3	1:G:334:ASP:HB3	1.93	0.50
1:G:448:GLU:OE1	1:G:452:ARG:NH1	2.40	0.50
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.92	0.50
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.11	0.50
1:E:288:MET:CE	1:E:288:MET:CG	2.89	0.50
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.12	0.50
1:D:224:ASP:O	1:D:225:LYS:HB3	2.11	0.49
1:G:233:MET:HE1	1:G:249:ILE:HD12	1.92	0.49
1:D:302:SER:H	1:D:307:MET:HE3	1.77	0.49
1:B:421:ARG:HD2	1:B:474:GLY:O	2.12	0.49
1:E:16:MET:SD	1:E:514:MET:HG3	2.52	0.49
1:D:266:THR:CG2	1:D:273:VAL:H	2.25	0.49
1:D:519:CYS:HB3	1:E:38:VAL:HG22	1.92	0.49
1:G:142:LYS:N	1:G:142:LYS:CD	2.62	0.49
1:F:96:ALA:O	1:F:97:GLN:C	2.55	0.49
1:G:179:ASP:OD1	1:G:393:LYS:HE3	2.13	0.49
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.93	0.49
1:D:16:MET:SD	1:D:514:MET:HG3	2.53	0.49
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.95	0.49
1:B:479:ASN:HD22	1:B:491:MET:CE	2.25	0.49
1:F:358:SER:HB3	1:F:361:ASP:OD1	2.13	0.49
1:B:73:MET:HG3	1:C:47:PRO:HG2	1.94	0.49
1:B:218:PRO:HD2	1:B:320:ALA:O	2.12	0.49
1:D:68:ASN:ND2	1:D:72:GLN:HE21	2.11	0.49
1:B:77:VAL:HG21	1:B:510:VAL:HG13	1.94	0.49
1:G:351:GLN:HE21	1:G:351:GLN:HB3	1.40	0.48
1:B:66:PHE:HA	1:B:69:MET:HE3	1.95	0.48
1:B:247:LEU:HD21	1:B:249:ILE:HD11	1.95	0.48
1:G:62:LEU:N	1:G:68:ASN:HD22	2.06	0.48
1:B:321:LYS:HG3	1:B:334:ASP:HB3	1.96	0.48
1:D:77:VAL:CG2	1:D:510:VAL:HG13	2.42	0.48
1:F:305:ILE:O	1:F:305:ILE:HG22	2.14	0.48
1:A:443:ALA:O	1:A:447:MET:HG3	2.13	0.48
1:C:65:LYS:HB3	1:C:65:LYS:HE2	1.60	0.48
1:G:452:ARG:NH2	1:G:463:SER:CB	2.76	0.48
1:G:284:ARG:O	1:G:288:MET:HG3	2.12	0.48
1:B:494:LEU:C	1:B:494:LEU:CD1	2.86	0.48
1:D:524:LEU:O	1:D:525:PRO:C	2.57	0.48
1:F:477:GLY:C	1:F:488:MET:HE3	2.39	0.48
1:C:348:GLN:O	1:C:351:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:ARG:NH2	1:D:463:SER:CB	2.74	0.48
1:F:262:LEU:O	1:F:266:THR:HG23	2.14	0.48
1:D:351:GLN:HE21	1:D:351:GLN:HB3	1.48	0.48
1:D:448:GLU:OE1	1:D:452:ARG:NH1	2.42	0.48
1:G:218:PRO:HD2	1:G:320:ALA:O	2.14	0.48
1:E:284:ARG:O	1:E:288:MET:HG3	2.14	0.47
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.97	0.47
1:E:42:LYS:HE3	1:E:48:THR:HG21	1.96	0.47
1:E:479:ASN:HD22	1:E:491:MET:HE2	1.78	0.47
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.96	0.47
1:E:280:GLY:HA2	1:E:284:ARG:HH21	1.79	0.47
1:F:263:VAL:O	1:F:267:MET:HB2	2.14	0.47
1:A:325:ILE:HG22	1:A:330:THR:HA	1.95	0.47
1:B:16:MET:SD	1:B:514:MET:HG3	2.54	0.47
1:B:41:ASP:O	1:B:42:LYS:HD3	2.15	0.47
1:C:42:LYS:CE	1:C:48:THR:HG21	2.44	0.47
1:C:266:THR:CG2	1:C:273:VAL:H	2.26	0.47
1:D:42:LYS:HE3	1:D:48:THR:CG2	2.44	0.47
1:D:452:ARG:HH21	1:D:463:SER:HB3	1.79	0.47
1:E:325:ILE:HG22	1:E:330:THR:HA	1.97	0.47
1:F:479:ASN:HD22	1:F:491:MET:HE2	1.78	0.47
1:A:348:GLN:O	1:A:351:GLN:HB2	2.15	0.47
1:D:233:MET:HE1	1:D:249:ILE:CD1	2.44	0.47
1:G:502:SER:O	1:G:503:ALA:C	2.55	0.47
1:A:494:LEU:HD12	1:A:494:LEU:C	2.40	0.47
1:B:273:VAL:HG12	1:B:274:ALA:N	2.30	0.47
1:C:66:PHE:HA	1:C:69:MET:HE3	1.96	0.47
1:E:448:GLU:OE1	1:E:452:ARG:NH1	2.35	0.47
1:C:233:MET:HE1	1:C:249:ILE:CD1	2.44	0.47
1:D:27:VAL:HG13	1:D:90:THR:HG23	1.97	0.47
1:D:448:GLU:O	1:D:452:ARG:HG3	2.15	0.47
1:E:41:ASP:O	1:E:42:LYS:HD3	2.15	0.47
1:G:348:GLN:O	1:G:351:GLN:HB2	2.14	0.47
1:B:466:ALA:O	1:B:470:LYS:HG3	2.16	0.46
1:D:348:GLN:O	1:D:351:GLN:HB2	2.15	0.46
1:A:326:ASN:HB3	1:A:328:ASP:H	1.80	0.46
1:B:42:LYS:CE	1:B:48:THR:HG23	2.45	0.46
1:D:273:VAL:HG12	1:D:274:ALA:N	2.31	0.46
1:E:349:ILE:CG2	1:E:369:VAL:HG13	2.46	0.46
1:C:326:ASN:HB3	1:C:328:ASP:H	1.81	0.46
1:E:86:GLY:O	1:E:87:ASP:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:494:LEU:HD12	1:F:494:LEU:C	2.41	0.46
1:D:68:ASN:HD21	1:D:72:GLN:HE21	1.63	0.46
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.96	0.46
1:F:166:MET:HG2	1:F:171:LYS:HA	1.98	0.46
1:G:305:ILE:HG22	1:G:305:ILE:O	2.15	0.46
1:A:477:GLY:C	1:A:488:MET:HE3	2.40	0.46
1:D:284:ARG:O	1:D:288:MET:HG3	2.15	0.46
1:D:479:ASN:HD22	1:D:491:MET:HE2	1.80	0.46
1:F:233:MET:HE1	1:F:249:ILE:HD12	1.97	0.46
1:A:358:SER:HB3	1:A:361:ASP:OD1	2.16	0.46
1:B:34:LYS:O	1:B:457:ASN:HB3	2.16	0.46
1:F:452:ARG:HH22	1:F:463:SER:HB3	1.77	0.46
1:B:514:MET:HE3	1:B:514:MET:HB2	1.86	0.46
1:B:233:MET:HE1	1:B:249:ILE:HD12	1.98	0.46
1:B:490:ASP:CB	2:B:536:HOH:O	2.64	0.46
1:B:263:VAL:O	1:B:267:MET:HB2	2.16	0.45
1:B:326:ASN:HB3	1:B:328:ASP:H	1.82	0.45
1:E:224:ASP:HB3	1:E:302:SER:HB3	1.98	0.45
1:F:421:ARG:CD	1:F:474:GLY:O	2.59	0.45
1:A:41:ASP:O	1:A:42:LYS:HD3	2.17	0.45
1:D:178:GLU:HG2	1:D:322:ARG:CZ	2.46	0.45
1:E:217:SER:N	1:E:218:PRO:CD	2.78	0.45
1:C:62:LEU:N	1:C:68:ASN:HD22	1.99	0.45
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.97	0.45
1:A:68:ASN:O	1:A:72:GLN:HG2	2.16	0.45
1:A:525:PRO:O	2:A:537:HOH:O	2.21	0.45
1:C:66:PHE:O	1:C:67:GLU:C	2.60	0.45
1:D:234:LEU:N	1:D:235:PRO:HD2	2.32	0.45
1:F:519:CYS:HB3	1:G:38:VAL:HG22	1.97	0.45
1:B:305:ILE:HG22	1:B:305:ILE:O	2.17	0.45
1:D:68:ASN:O	1:D:72:GLN:HG2	2.16	0.45
1:C:65:LYS:H	1:C:65:LYS:HG2	1.67	0.45
1:E:510:VAL:O	1:E:511:ALA:C	2.59	0.45
1:G:42:LYS:CE	1:G:48:THR:HG23	2.44	0.45
1:G:288:MET:CE	1:G:288:MET:CG	2.94	0.45
1:E:68:ASN:O	1:E:72:GLN:HG2	2.16	0.45
1:F:87:ASP:OD1	1:F:88:GLY:N	2.46	0.45
1:G:302:SER:H	1:G:307:MET:HE3	1.82	0.45
1:A:233:MET:HE1	1:A:249:ILE:HD12	1.98	0.45
1:B:490:ASP:HB3	2:B:536:HOH:O	2.16	0.45
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLN:HB3	1:A:336:VAL:CG2	2.43	0.44
1:C:305:ILE:HG22	1:C:305:ILE:O	2.17	0.44
1:E:233:MET:HE1	1:E:249:ILE:HD11	1.99	0.44
1:D:228:SER:O	1:D:257:GLU:HB3	2.16	0.44
1:A:69:MET:CE	1:A:522:THR:HB	2.47	0.44
1:A:364:LYS:HD3	1:A:364:LYS:HA	1.81	0.44
1:A:233:MET:HE1	1:A:249:ILE:HD11	2.00	0.44
1:A:479:ASN:HD22	1:A:491:MET:CE	2.31	0.44
1:D:237:LEU:HA	1:D:237:LEU:HD23	1.86	0.44
1:E:273:VAL:HG12	1:E:274:ALA:N	2.32	0.44
1:G:494:LEU:O	1:G:494:LEU:HD12	2.17	0.44
1:A:336:VAL:O	1:A:337:GLY:C	2.61	0.44
1:B:42:LYS:CE	1:B:48:THR:CG2	2.95	0.44
1:B:351:GLN:HE21	1:B:351:GLN:HB3	1.36	0.44
1:C:479:ASN:ND2	1:C:491:MET:HE2	2.29	0.44
1:C:41:ASP:O	1:C:42:LYS:HD3	2.17	0.44
1:D:403:THR:O	1:D:407:VAL:HG13	2.18	0.44
1:F:364:LYS:HD3	1:F:364:LYS:HA	1.86	0.44
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.98	0.44
1:A:479:ASN:HD22	1:A:491:MET:HE2	1.81	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:E:364:LYS:HD3	1:E:364:LYS:HA	1.70	0.44
1:F:28:LYS:HB2	1:F:453:GLN:HG2	2.00	0.44
1:A:305:ILE:O	1:A:305:ILE:HG22	2.18	0.43
1:B:68:ASN:ND2	1:B:72:GLN:HE21	2.15	0.43
1:C:364:LYS:HD3	1:C:364:LYS:HA	1.86	0.43
1:G:263:VAL:O	1:G:267:MET:HB2	2.18	0.43
1:B:42:LYS:HE2	1:B:48:THR:CG2	2.46	0.43
1:B:266:THR:CG2	1:B:273:VAL:H	2.31	0.43
1:D:42:LYS:CE	1:D:48:THR:HG21	2.47	0.43
1:G:326:ASN:HB3	1:G:328:ASP:H	1.83	0.43
1:A:162:ILE:HD12	1:A:400:LEU:HA	2.00	0.43
1:A:172:GLU:CA	1:A:172:GLU:OE1	2.66	0.43
1:D:479:ASN:HD22	1:D:491:MET:CE	2.31	0.43
1:E:421:ARG:CD	1:E:474:GLY:O	2.65	0.43
1:G:86:GLY:O	1:G:87:ASP:HB2	2.17	0.43
1:A:73:MET:HG3	1:B:47:PRO:HG2	1.99	0.43
1:D:263:VAL:O	1:D:267:MET:HB2	2.18	0.43
1:A:42:LYS:HE3	1:A:48:THR:HG21	2.00	0.43
1:G:234:LEU:N	1:G:235:PRO:HD2	2.34	0.43
1:G:524:LEU:O	1:G:525:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:O	1:A:266:THR:HG23	2.18	0.43
1:G:452:ARG:HH21	1:G:463:SER:HB3	1.82	0.43
1:C:288:MET:CE	1:C:288:MET:CG	2.93	0.43
1:E:228:SER:O	1:E:257:GLU:HB3	2.18	0.43
1:E:325:ILE:HD13	1:E:325:ILE:HG23	1.74	0.43
1:B:171:LYS:HB3	1:B:407:VAL:HG21	2.01	0.43
1:B:479:ASN:ND2	1:B:493:ILE:HD11	2.34	0.43
1:D:233:MET:HE1	1:D:249:ILE:HD12	1.99	0.43
1:F:171:LYS:HB3	1:F:407:VAL:HG21	2.01	0.43
1:A:511:ALA:O	1:A:515:ILE:HD12	2.19	0.42
1:B:96:ALA:O	1:B:100:ILE:HD12	2.19	0.42
1:E:266:THR:CG2	1:E:273:VAL:H	2.31	0.42
1:F:319:GLN:HB3	1:F:336:VAL:CG2	2.48	0.42
1:G:180:GLY:HA3	1:G:381:VAL:O	2.18	0.42
1:B:524:LEU:O	1:B:525:PRO:C	2.63	0.42
1:A:214:GLU:HG3	1:A:324:VAL:HG22	2.01	0.42
1:B:68:ASN:HD21	1:B:72:GLN:HE21	1.67	0.42
1:C:325:ILE:HG22	1:C:330:THR:HA	2.01	0.42
1:E:73:MET:HG3	1:F:47:PRO:HG2	2.00	0.42
1:G:217:SER:N	1:G:218:PRO:CD	2.82	0.42
1:B:186:GLU:HB2	1:B:380:LYS:HG3	2.01	0.42
1:D:41:ASP:O	1:D:42:LYS:HD3	2.18	0.42
1:E:452:ARG:HH22	1:E:463:SER:HB3	1.83	0.42
1:G:262:LEU:O	1:G:266:THR:HG23	2.19	0.42
1:C:217:SER:N	1:C:218:PRO:CD	2.83	0.42
1:D:449:ALA:N	1:D:450:PRO:CD	2.83	0.42
1:F:217:SER:N	1:F:218:PRO:HD3	2.34	0.42
1:G:171:LYS:HB3	1:G:407:VAL:HG21	2.02	0.42
1:A:263:VAL:O	1:A:267:MET:HB2	2.19	0.42
1:A:452:ARG:HH22	1:A:463:SER:HB3	1.80	0.42
1:C:162:ILE:HD12	1:C:400:LEU:HA	2.02	0.42
1:F:514:MET:HE3	1:F:514:MET:HB2	1.88	0.42
1:A:270:ILE:HG22	1:A:271:VAL:HG23	2.01	0.42
1:C:221:LEU:HD12	1:C:222:LEU:N	2.35	0.42
1:A:234:LEU:N	1:A:235:PRO:HD2	2.35	0.42
1:E:418:ALA:O	1:E:422:VAL:HG13	2.19	0.42
1:F:66:PHE:HA	1:F:69:MET:HE3	2.00	0.42
1:G:96:ALA:O	1:G:97:GLN:C	2.62	0.42
1:G:273:VAL:HG12	1:G:274:ALA:N	2.34	0.42
1:B:62:LEU:N	1:B:68:ASN:HD22	2.09	0.41
1:E:254:VAL:HG12	1:E:259:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ILE:HG21	1:E:325:ILE:HD12	1.78	0.41
1:E:348:GLN:O	1:E:351:GLN:HB2	2.20	0.41
1:F:273:VAL:HG12	1:F:274:ALA:N	2.35	0.41
1:G:217:SER:N	1:G:218:PRO:HD3	2.34	0.41
1:E:205:ILE:HA	1:E:213:VAL:HG22	2.02	0.41
1:E:228:SER:HB3	1:F:272:LYS:NZ	2.34	0.41
1:E:258:ALA:O	1:E:262:LEU:HG	2.20	0.41
1:F:62:LEU:N	1:F:68:ASN:HD22	2.06	0.41
1:G:69:MET:CE	1:G:522:THR:HB	2.50	0.41
1:B:325:ILE:HG22	1:B:330:THR:HA	2.02	0.41
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.86	0.41
1:C:228:SER:O	1:C:257:GLU:HB3	2.20	0.41
1:D:266:THR:HG21	1:D:273:VAL:H	1.85	0.41
1:D:325:ILE:HG22	1:D:330:THR:HA	2.01	0.41
1:G:228:SER:O	1:G:257:GLU:HB3	2.20	0.41
1:G:349:ILE:HG21	1:G:369:VAL:HG13	2.02	0.41
1:A:506:TYR:O	1:A:507:ALA:C	2.61	0.41
1:C:266:THR:HG21	1:C:273:VAL:H	1.85	0.41
1:C:325:ILE:HG22	1:C:330:THR:OG1	2.20	0.41
1:E:490:ASP:C	1:E:492:GLY:H	2.27	0.41
1:F:77:VAL:HG21	1:F:510:VAL:HG13	2.02	0.41
1:G:221:LEU:HD12	1:G:222:LEU:N	2.34	0.41
1:A:112:ASN:HA	1:A:113:PRO:HD3	1.95	0.41
1:G:172:GLU:OE1	1:G:172:GLU:HA	2.20	0.41
1:A:217:SER:N	1:A:218:PRO:CD	2.84	0.41
1:D:304:GLU:H	1:D:304:GLU:HG3	1.75	0.41
1:G:225:LYS:HD3	1:G:303:GLU:CD	2.45	0.41
1:G:325:ILE:HG22	1:G:330:THR:OG1	2.20	0.41
1:A:8:PHE:HA	1:A:518:GLU:O	2.21	0.41
1:E:351:GLN:HE21	1:E:351:GLN:HB3	1.43	0.41
1:G:494:LEU:HD12	1:G:494:LEU:C	2.46	0.41
1:B:284:ARG:O	1:B:288:MET:HG3	2.20	0.41
1:C:68:ASN:ND2	1:C:72:GLN:HE21	2.19	0.41
1:C:265:ASN:HD22	1:C:265:ASN:HA	1.68	0.41
1:E:7:LYS:HE3	1:E:15:LYS:HE3	2.03	0.41
1:E:68:ASN:HD21	1:E:72:GLN:NE2	2.17	0.41
1:E:305:ILE:HG22	1:E:305:ILE:O	2.20	0.41
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.21	0.41
1:G:104:LEU:HD23	1:G:104:LEU:HA	1.87	0.41
1:B:448:GLU:HB3	1:B:452:ARG:HD2	2.02	0.41
1:C:42:LYS:HE3	1:C:48:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ILE:HA	1:C:213:VAL:HG22	2.03	0.41
1:E:237:LEU:HA	1:E:237:LEU:HD23	1.88	0.41
1:G:122:LYS:NZ	2:G:528:HOH:O	2.44	0.41
1:G:172:GLU:OE1	1:G:172:GLU:CA	2.69	0.41
1:F:302:SER:H	1:F:307:MET:HE3	1.85	0.41
1:B:489:ILE:CD1	1:B:489:ILE:HA	2.52	0.40
1:E:77:VAL:CG2	1:E:510:VAL:HG13	2.50	0.40
1:F:217:SER:N	1:F:218:PRO:CD	2.84	0.40
1:A:519:CYS:HB3	1:B:38:VAL:HG22	2.04	0.40
1:C:68:ASN:O	1:C:72:GLN:HG2	2.20	0.40
1:F:77:VAL:O	1:F:80:LYS:HB2	2.22	0.40
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.21	0.40
1:B:231:ARG:NH1	1:C:241:ALA:HB1	2.35	0.40
1:A:514:MET:HE3	1:A:514:MET:HB2	1.86	0.40
1:B:74:VAL:O	1:B:75:LYS:C	2.64	0.40
1:C:258:ALA:O	1:C:262:LEU:HG	2.21	0.40
1:F:452:ARG:NH2	1:F:463:SER:CB	2.80	0.40
1:G:358:SER:HB3	1:G:361:ASP:OD1	2.21	0.40
1:B:455:VAL:HG13	1:B:460:GLU:HB2	2.04	0.40
1:C:169:VAL:HG13	1:C:173:GLY:HA3	2.03	0.40
1:C:514:MET:HE3	1:C:514:MET:HB2	1.86	0.40
1:D:65:LYS:HE2	1:D:65:LYS:HB3	1.84	0.40
1:E:184:GLN:OE1	1:E:184:GLN:HA	2.21	0.40
1:F:68:ASN:HD21	1:F:72:GLN:NE2	2.17	0.40
1:F:205:ILE:HA	1:F:213:VAL:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLU:OE1	1:G:350:ARG:NH1[5_455]	2.05	0.15

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	522/524 (100%)	507 (97%)	12 (2%)	3 (1%)	21	44
1	B	522/524 (100%)	505 (97%)	15 (3%)	2 (0%)	30	54
1	C	522/524 (100%)	506 (97%)	13 (2%)	3 (1%)	21	44
1	D	522/524 (100%)	507 (97%)	13 (2%)	2 (0%)	30	54
1	E	522/524 (100%)	504 (97%)	17 (3%)	1 (0%)	43	68
1	F	522/524 (100%)	506 (97%)	14 (3%)	2 (0%)	30	54
1	G	522/524 (100%)	504 (97%)	15 (3%)	3 (1%)	21	44
All	All	3654/3668 (100%)	3539 (97%)	99 (3%)	16 (0%)	30	54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLY
1	B	256	GLY
1	C	256	GLY
1	D	256	GLY
1	E	256	GLY
1	F	256	GLY
1	G	256	GLY
1	A	225	LYS
1	D	257	GLU
1	F	225	LYS
1	G	257	GLU
1	B	225	LYS
1	C	225	LYS
1	A	205	ILE
1	G	205	ILE
1	C	205	ILE

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	404/404 (100%)	341 (84%)	63 (16%)	2	7
1	B	404/404 (100%)	344 (85%)	60 (15%)	3	8
1	C	404/404 (100%)	345 (85%)	59 (15%)	3	8
1	D	404/404 (100%)	341 (84%)	63 (16%)	2	7
1	E	404/404 (100%)	346 (86%)	58 (14%)	3	8
1	F	404/404 (100%)	346 (86%)	58 (14%)	3	8
1	G	404/404 (100%)	345 (85%)	59 (15%)	3	8
All	All	2828/2828 (100%)	2408 (85%)	420 (15%)	3	8

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	27	VAL
1	A	43	SER
1	A	48	THR
1	A	65	LYS
1	A	82	ASN
1	A	105	LYS
1	A	116	LEU
1	A	118	ARG
1	A	141	SER
1	A	142	LYS
1	A	149	THR
1	A	151	SER
1	A	153	ASN
1	A	156	GLU
1	A	168	LYS
1	A	169	VAL
1	A	172	GLU
1	A	174	VAL
1	A	186	GLU
1	A	190	VAL
1	A	201	SER
1	A	209	GLU
1	A	216	GLU
1	A	222	LEU
1	A	225	LYS
1	A	230	ILE
1	A	232	GLU
1	A	242	LYS

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Mol	Chain	Res	Type
1	A	267	MET
1	A	284	ARG
1	A	295	LEU
1	A	303	GLU
1	A	304	GLU
1	A	317	LEU
1	A	322	ARG
1	A	323	VAL
1	A	325	ILE
1	A	328	ASP
1	A	329	THR
1	A	331	THR
1	A	339	GLU
1	A	343	GLN
1	A	348	GLN
1	A	350	ARG
1	A	351	GLN
1	A	352	GLN
1	A	355	GLU
1	A	358	SER
1	A	363	GLU
1	A	364	LYS
1	A	372	LEU
1	A	380	LYS
1	A	387	VAL
1	A	404	ARG
1	A	411	VAL
1	A	421	ARG
1	A	422	VAL
1	A	438	VAL
1	A	499	VAL
1	A	504	LEU
1	A	510	VAL
1	A	517	THR
1	B	14	VAL
1	B	27	VAL
1	B	43	SER
1	B	48	THR
1	B	55	SER
1	B	58	ARG
1	B	64	ASP
1	B	82	ASN

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Mol	Chain	Res	Type
1	B	89	THR
1	B	105	LYS
1	B	116	LEU
1	B	118	ARG
1	B	141	SER
1	B	142	LYS
1	B	149	THR
1	B	151	SER
1	B	156	GLU
1	B	168	LYS
1	B	169	VAL
1	B	172	GLU
1	B	174	VAL
1	B	176	THR
1	B	186	GLU
1	B	190	VAL
1	B	201	SER
1	B	209	GLU
1	B	216	GLU
1	B	225	LYS
1	B	230	ILE
1	B	242	LYS
1	B	267	MET
1	B	284	ARG
1	B	295	LEU
1	B	303	GLU
1	B	317	LEU
1	B	322	ARG
1	B	325	ILE
1	B	328	ASP
1	B	329	THR
1	B	331	THR
1	B	339	GLU
1	B	343	GLN
1	B	348	GLN
1	B	350	ARG
1	B	351	GLN
1	B	352	GLN
1	B	355	GLU
1	B	358	SER
1	B	363	GLU
1	B	364	LYS

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Mol	Chain	Res	Type
1	B	380	LYS
1	B	387	VAL
1	B	404	ARG
1	B	411	VAL
1	B	421	ARG
1	B	422	VAL
1	B	438	VAL
1	B	499	VAL
1	B	504	LEU
1	B	510	VAL
1	C	14	VAL
1	C	27	VAL
1	C	43	SER
1	C	48	THR
1	C	65	LYS
1	C	82	ASN
1	C	105	LYS
1	C	116	LEU
1	C	118	ARG
1	C	141	SER
1	C	142	LYS
1	C	149	THR
1	C	153	ASN
1	C	156	GLU
1	C	168	LYS
1	C	169	VAL
1	C	172	GLU
1	C	174	VAL
1	C	176	THR
1	C	186	GLU
1	C	190	VAL
1	C	201	SER
1	C	216	GLU
1	C	222	LEU
1	C	225	LYS
1	C	230	ILE
1	C	242	LYS
1	C	267	MET
1	C	284	ARG
1	C	295	LEU
1	C	303	GLU
1	C	304	GLU

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Mol	Chain	Res	Type
1	C	317	LEU
1	C	322	ARG
1	C	325	ILE
1	C	328	ASP
1	C	329	THR
1	C	331	THR
1	C	339	GLU
1	C	343	GLN
1	C	348	GLN
1	C	350	ARG
1	C	351	GLN
1	C	352	GLN
1	C	355	GLU
1	C	363	GLU
1	C	364	LYS
1	C	372	LEU
1	C	380	LYS
1	C	387	VAL
1	C	404	ARG
1	C	407	VAL
1	C	411	VAL
1	C	421	ARG
1	C	422	VAL
1	C	438	VAL
1	C	499	VAL
1	C	504	LEU
1	C	510	VAL
1	D	14	VAL
1	D	27	VAL
1	D	43	SER
1	D	48	THR
1	D	65	LYS
1	D	76	GLU
1	D	82	ASN
1	D	100	ILE
1	D	105	LYS
1	D	116	LEU
1	D	118	ARG
1	D	132	LYS
1	D	141	SER
1	D	142	LYS
1	D	149	THR

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Mol	Chain	Res	Type
1	D	151	SER
1	D	153	ASN
1	D	156	GLU
1	D	168	LYS
1	D	169	VAL
1	D	172	GLU
1	D	174	VAL
1	D	186	GLU
1	D	190	VAL
1	D	201	SER
1	D	209	GLU
1	D	216	GLU
1	D	225	LYS
1	D	230	ILE
1	D	242	LYS
1	D	267	MET
1	D	284	ARG
1	D	295	LEU
1	D	303	GLU
1	D	304	GLU
1	D	307	MET
1	D	317	LEU
1	D	322	ARG
1	D	325	ILE
1	D	328	ASP
1	D	329	THR
1	D	331	THR
1	D	339	GLU
1	D	343	GLN
1	D	348	GLN
1	D	350	ARG
1	D	351	GLN
1	D	352	GLN
1	D	355	GLU
1	D	358	SER
1	D	363	GLU
1	D	364	LYS
1	D	372	LEU
1	D	380	LYS
1	D	387	VAL
1	D	404	ARG
1	D	407	VAL

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Mol	Chain	Res	Type
1	D	411	VAL
1	D	422	VAL
1	D	438	VAL
1	D	499	VAL
1	D	504	LEU
1	D	510	VAL
1	E	14	VAL
1	E	27	VAL
1	E	43	SER
1	E	48	THR
1	E	76	GLU
1	E	82	ASN
1	E	105	LYS
1	E	116	LEU
1	E	118	ARG
1	E	141	SER
1	E	142	LYS
1	E	149	THR
1	E	151	SER
1	E	156	GLU
1	E	168	LYS
1	E	169	VAL
1	E	172	GLU
1	E	174	VAL
1	E	186	GLU
1	E	190	VAL
1	E	201	SER
1	E	209	GLU
1	E	216	GLU
1	E	225	LYS
1	E	230	ILE
1	E	232	GLU
1	E	242	LYS
1	E	267	MET
1	E	284	ARG
1	E	295	LEU
1	E	303	GLU
1	E	304	GLU
1	E	317	LEU
1	E	322	ARG
1	E	325	ILE
1	E	329	THR

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Mol	Chain	Res	Type
1	E	331	THR
1	E	339	GLU
1	E	343	GLN
1	E	348	GLN
1	E	350	ARG
1	E	351	GLN
1	E	352	GLN
1	E	355	GLU
1	E	358	SER
1	E	363	GLU
1	E	364	LYS
1	E	372	LEU
1	E	380	LYS
1	E	387	VAL
1	E	404	ARG
1	E	411	VAL
1	E	421	ARG
1	E	422	VAL
1	E	438	VAL
1	E	499	VAL
1	E	504	LEU
1	E	510	VAL
1	F	14	VAL
1	F	27	VAL
1	F	43	SER
1	F	55	SER
1	F	65	LYS
1	F	76	GLU
1	F	82	ASN
1	F	105	LYS
1	F	116	LEU
1	F	118	ARG
1	F	141	SER
1	F	142	LYS
1	F	149	THR
1	F	151	SER
1	F	153	ASN
1	F	156	GLU
1	F	168	LYS
1	F	169	VAL
1	F	172	GLU
1	F	174	VAL

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Mol	Chain	Res	Type
1	F	186	GLU
1	F	190	VAL
1	F	201	SER
1	F	209	GLU
1	F	216	GLU
1	F	225	LYS
1	F	230	ILE
1	F	242	LYS
1	F	267	MET
1	F	284	ARG
1	F	295	LEU
1	F	303	GLU
1	F	304	GLU
1	F	317	LEU
1	F	322	ARG
1	F	325	ILE
1	F	328	ASP
1	F	329	THR
1	F	331	THR
1	F	339	GLU
1	F	343	GLN
1	F	348	GLN
1	F	350	ARG
1	F	351	GLN
1	F	352	GLN
1	F	355	GLU
1	F	363	GLU
1	F	364	LYS
1	F	372	LEU
1	F	380	LYS
1	F	387	VAL
1	F	404	ARG
1	F	411	VAL
1	F	421	ARG
1	F	438	VAL
1	F	499	VAL
1	F	504	LEU
1	F	510	VAL
1	G	14	VAL
1	G	27	VAL
1	G	42	LYS
1	G	43	SER

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Mol	Chain	Res	Type
1	G	48	THR
1	G	76	GLU
1	G	82	ASN
1	G	105	LYS
1	G	116	LEU
1	G	141	SER
1	G	142	LYS
1	G	149	THR
1	G	151	SER
1	G	153	ASN
1	G	156	GLU
1	G	168	LYS
1	G	169	VAL
1	G	172	GLU
1	G	174	VAL
1	G	186	GLU
1	G	190	VAL
1	G	201	SER
1	G	209	GLU
1	G	216	GLU
1	G	225	LYS
1	G	230	ILE
1	G	242	LYS
1	G	267	MET
1	G	284	ARG
1	G	295	LEU
1	G	303	GLU
1	G	304	GLU
1	G	317	LEU
1	G	322	ARG
1	G	325	ILE
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	339	GLU
1	G	343	GLN
1	G	348	GLN
1	G	350	ARG
1	G	351	GLN
1	G	352	GLN
1	G	355	GLU
1	G	363	GLU

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Mol	Chain	Res	Type
1	G	364	LYS
1	G	372	LEU
1	G	380	LYS
1	G	387	VAL
1	G	404	ARG
1	G	407	VAL
1	G	411	VAL
1	G	421	ARG
1	G	422	VAL
1	G	438	VAL
1	G	499	VAL
1	G	504	LEU
1	G	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	68	ASN
1	A	97	GLN
1	A	265	ASN
1	A	351	GLN
1	A	437	ASN
1	B	68	ASN
1	B	265	ASN
1	B	290	GLN
1	B	351	GLN
1	B	437	ASN
1	C	68	ASN
1	C	229	ASN
1	C	265	ASN
1	C	351	GLN
1	C	437	ASN
1	C	453	GLN
1	D	10	ASN
1	D	68	ASN
1	D	265	ASN
1	D	351	GLN
1	D	437	ASN
1	E	68	ASN
1	E	265	ASN
1	E	351	GLN

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Mol	Chain	Res	Type
1	E	437	ASN
1	E	453	GLN
1	F	68	ASN
1	F	265	ASN
1	F	351	GLN
1	F	437	ASN
1	F	453	GLN
1	G	68	ASN
1	G	229	ASN
1	G	265	ASN
1	G	351	GLN
1	G	437	ASN
1	G	453	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	524/524 (100%)	-0.11	15 (2%)	53	50	2, 2, 4, 6	0
1	B	524/524 (100%)	0.04	24 (4%)	37	34	2, 2, 4, 6	0
1	C	524/524 (100%)	-0.10	19 (3%)	46	42	2, 2, 4, 6	0
1	D	524/524 (100%)	-0.13	16 (3%)	51	48	2, 2, 4, 6	0
1	E	524/524 (100%)	-0.28	11 (2%)	63	61	2, 2, 4, 6	0
1	F	524/524 (100%)	0.40	63 (12%)	9	7	2, 2, 4, 6	0
1	G	524/524 (100%)	-0.21	10 (1%)	66	63	2, 2, 4, 6	0
All	All	3668/3668 (100%)	-0.06	158 (4%)	40	36	2, 2, 4, 6	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	231	ARG	9.2
1	F	268	ARG	8.9
1	F	242	LYS	6.0
1	F	270	ILE	5.6
1	F	203	TYR	5.6
1	F	256	GLY	5.1
1	C	242	LYS	5.1
1	F	311	LYS	5.0
1	F	272	LYS	4.6
1	B	231	ARG	4.5
1	G	231	ARG	4.5
1	F	264	VAL	4.5
1	F	327	LYS	4.4
1	G	44	PHE	4.4
1	F	238	GLU	4.3
1	B	44	PHE	4.2
1	D	44	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	308	GLU	4.2
1	B	268	ARG	4.0
1	F	244	GLY	3.9
1	C	311	LYS	3.9
1	C	44	PHE	3.8
1	F	273	VAL	3.8
1	C	231	ARG	3.8
1	A	242	LYS	3.8
1	C	357	THR	3.6
1	G	270	ILE	3.6
1	E	354	GLU	3.6
1	F	200	LEU	3.5
1	F	314	LEU	3.5
1	C	270	ILE	3.5
1	D	242	LYS	3.5
1	F	306	GLY	3.4
1	F	269	GLY	3.4
1	A	182	GLY	3.4
1	F	234	LEU	3.4
1	G	473	ASP	3.4
1	B	242	LYS	3.3
1	A	44	PHE	3.3
1	F	283	ASP	3.3
1	C	268	ARG	3.3
1	E	44	PHE	3.3
1	F	229	ASN	3.3
1	F	213	VAL	3.2
1	B	174	VAL	3.2
1	E	268	ARG	3.2
1	A	387	VAL	3.1
1	F	44	PHE	3.1
1	F	222	LEU	3.1
1	B	84	ALA	3.1
1	B	175	ILE	3.1
1	A	181	THR	3.1
1	F	357	THR	3.1
1	F	255	GLU	3.1
1	B	357	THR	3.0
1	C	256	GLY	3.0
1	F	227	ILE	2.9
1	B	214	GLU	2.8
1	F	301	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	281	PHE	2.8
1	D	308	GLU	2.8
1	F	313	THR	2.8
1	A	231	ARG	2.7
1	B	311	LYS	2.7
1	B	261	THR	2.7
1	F	204	PHE	2.7
1	F	208	PRO	2.7
1	F	316	ASP	2.7
1	F	199	TYR	2.6
1	E	129	GLU	2.6
1	C	359	ASP	2.6
1	B	233	MET	2.6
1	E	231	ARG	2.6
1	F	271	VAL	2.6
1	F	278	ALA	2.6
1	F	481	ALA	2.6
1	C	358	SER	2.5
1	B	247	LEU	2.5
1	G	311	LYS	2.5
1	F	236	VAL	2.5
1	F	340	ALA	2.5
1	F	284	ARG	2.5
1	C	313	THR	2.5
1	C	228	SER	2.5
1	F	377	ALA	2.5
1	E	242	LYS	2.4
1	B	489	ILE	2.4
1	C	361	ASP	2.4
1	A	308	GLU	2.4
1	C	238	GLU	2.4
1	F	307	MET	2.4
1	C	264	VAL	2.4
1	F	228	SER	2.4
1	B	244	GLY	2.4
1	G	242	LYS	2.4
1	F	210	THR	2.4
1	G	182	GLY	2.4
1	F	281	PHE	2.4
1	G	203	TYR	2.4
1	F	349	ILE	2.4
1	C	363	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	272	LYS	2.4
1	D	362	ARG	2.4
1	F	300	VAL	2.4
1	F	324	VAL	2.4
1	B	212	ALA	2.4
1	B	260	ALA	2.4
1	B	356	ALA	2.4
1	E	313	THR	2.3
1	D	284	ARG	2.3
1	A	270	ILE	2.3
1	A	379	ILE	2.3
1	F	216	GLU	2.3
1	F	226	LYS	2.3
1	F	286	LYS	2.3
1	D	228	SER	2.3
1	G	271	VAL	2.3
1	A	157	THR	2.3
1	D	183	LEU	2.3
1	D	274	ALA	2.3
1	F	279	PRO	2.3
1	F	350	ARG	2.3
1	B	177	VAL	2.3
1	E	212	ALA	2.2
1	G	357	THR	2.2
1	B	315	GLU	2.2
1	A	311	LYS	2.2
1	F	241	ALA	2.2
1	F	360	TYR	2.2
1	F	262	LEU	2.2
1	B	241	ALA	2.2
1	C	308	GLU	2.2
1	F	329	THR	2.2
1	D	268	ARG	2.2
1	F	206	ASN	2.2
1	F	351	GLN	2.2
1	B	227	ILE	2.2
1	B	277	LYS	2.2
1	F	209	GLU	2.1
1	D	181	THR	2.1
1	F	248	LEU	2.1
1	A	156	GLU	2.1
1	A	152	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	202	PRO	2.1
1	A	473	ASP	2.1
1	B	354	GLU	2.1
1	D	156	GLU	2.1
1	D	209	GLU	2.1
1	D	231	ARG	2.0
1	E	228	SER	2.0
1	F	312	ALA	2.0
1	F	277	LYS	2.0
1	D	172	GLU	2.0
1	C	356	ALA	2.0
1	A	309	LEU	2.0
1	C	353	ILE	2.0
1	D	270	ILE	2.0
1	E	305	ILE	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.