



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 AM UTC

PDB ID : 2GHO / pdb_00002gho
Title : Recombinant *Thermus aquaticus* RNA polymerase for Structural Studies
Authors : Lamour, V.; Darst, S.A.
Deposited on : 2006-03-27
Resolution : 5.00 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

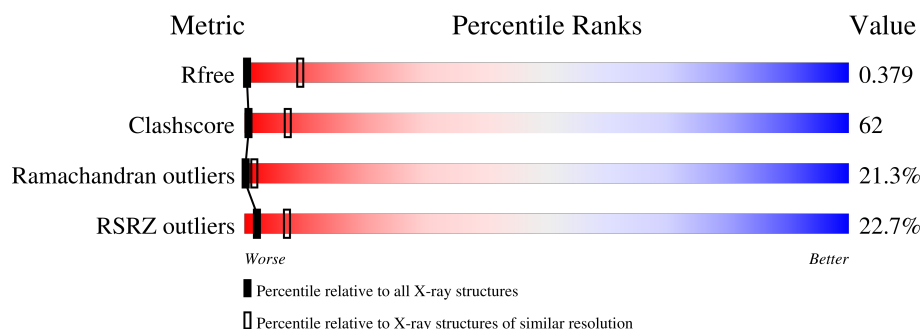
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
RSRZ outliers	180081	1004 (6.02-3.98)

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	314	
1	B	314	
2	C	1119	
3	D	1233	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11060 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	0	0	0
			920	460	230	230			
1	B	225	Total	C	N	O	0	0	0
			900	450	225	225			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	0	0	0
			4456	2228	1114	1114			

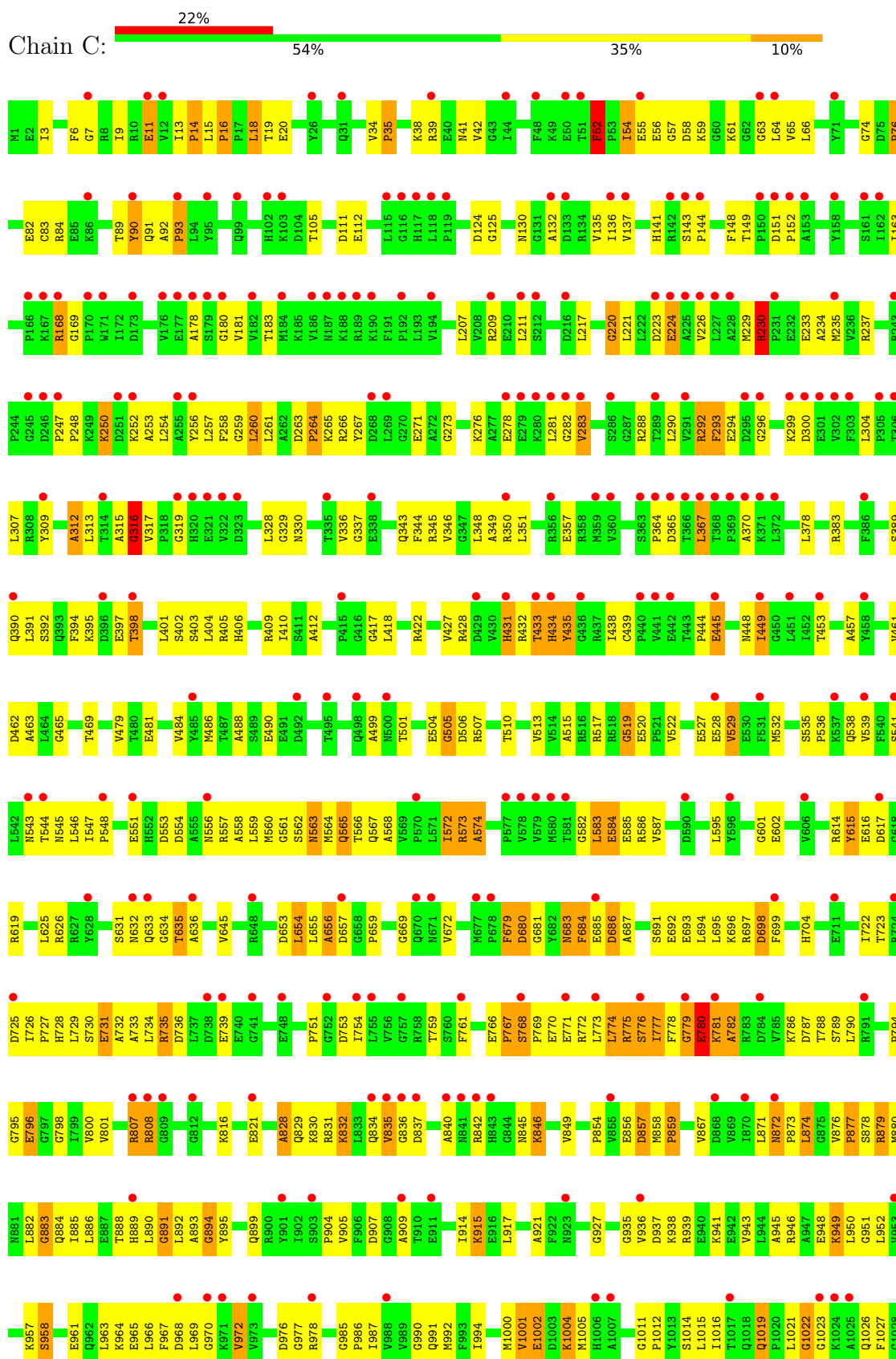
- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta',DNA-directed RNA polymerase subunit beta'.

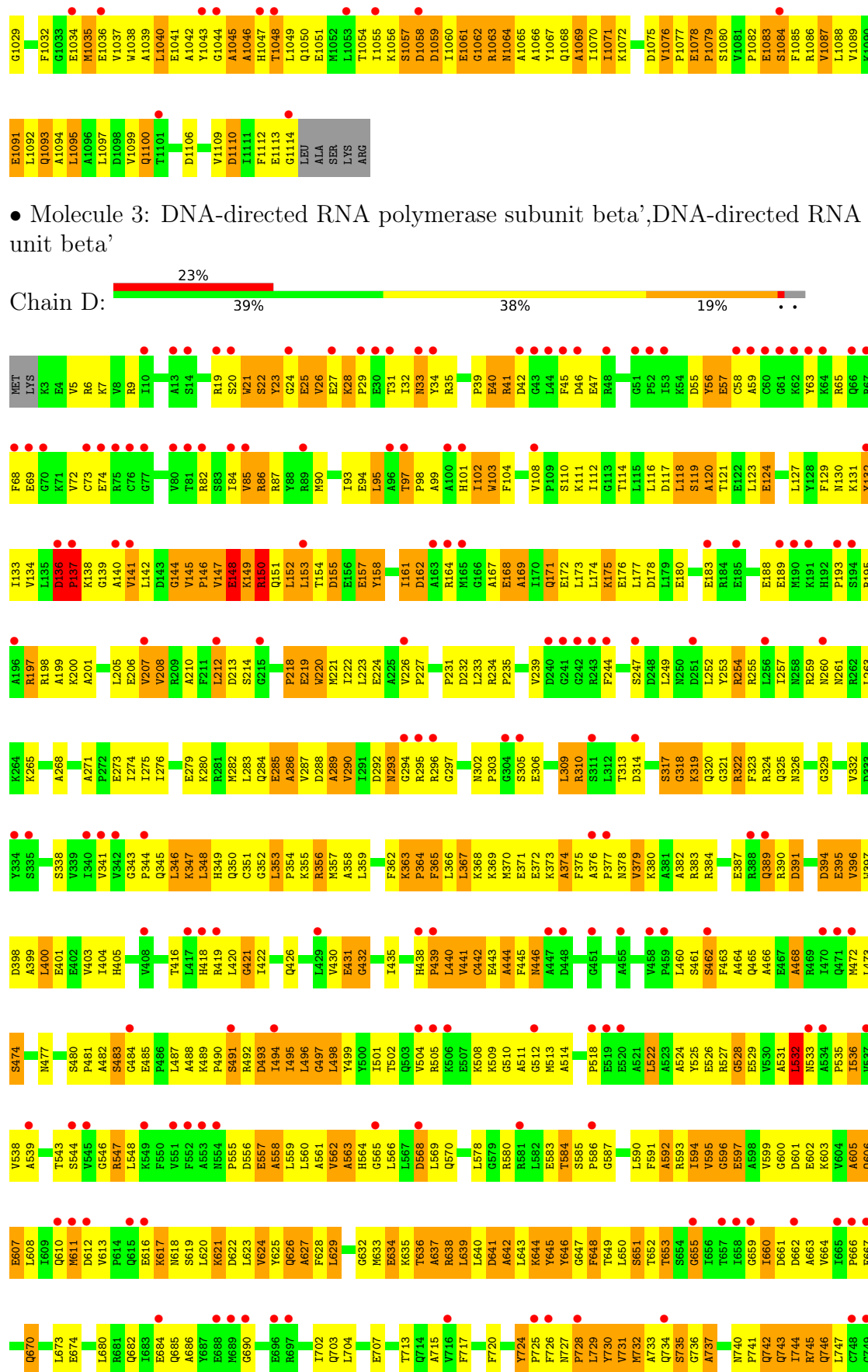
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	1196	Total	C	N	O	0	0	0
			4784	2392	1196	1196			

There are 2 discrepancies between the modelled and reference sequences:

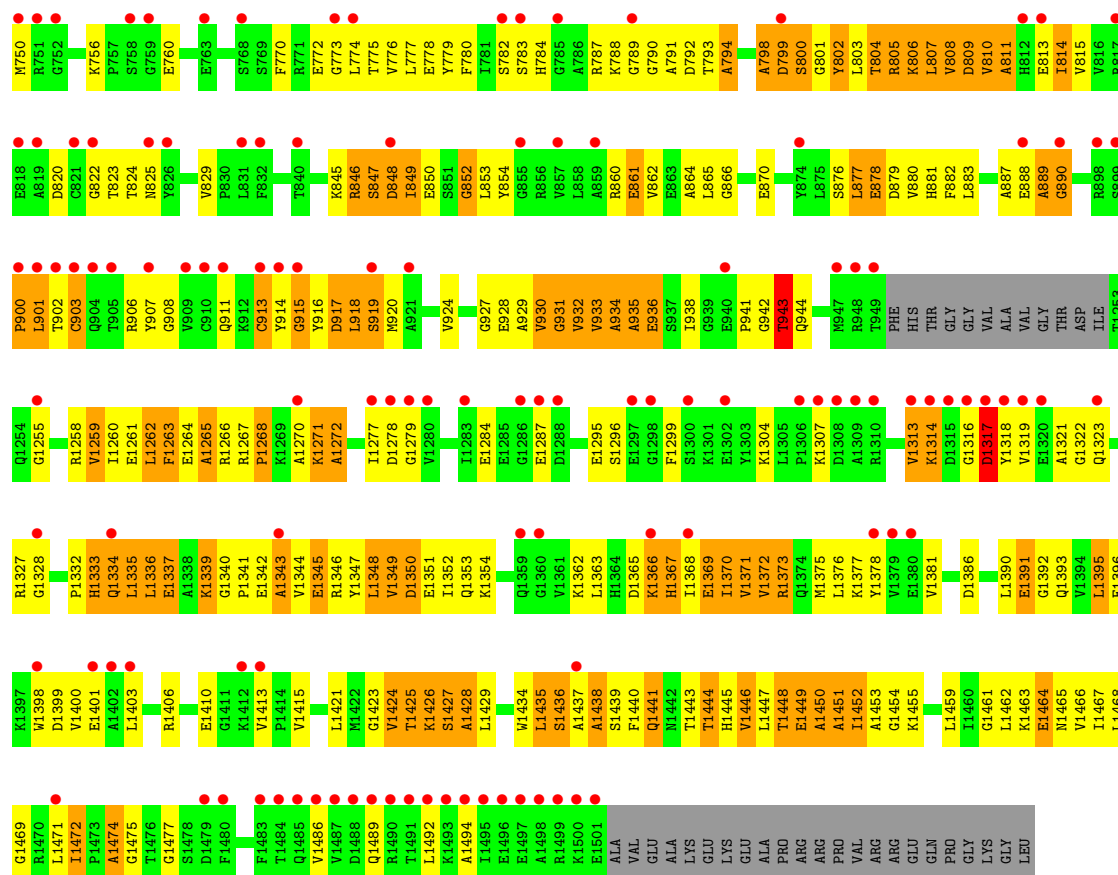
Chain	Residue	Modelled	Actual	Comment	Reference
D	159	GLY	-	linker	UNP Q9KWU6
D	160	GLY	-	linker	UNP Q9KWU6

● Molecule 2: DNA-directed RNA polymerase subunit beta





● Molecule 3: DNA-directed RNA polymerase subunit beta', DNA-directed RNA polymerase subunit beta'



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	202.80Å 202.80Å 326.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 5.00 25.00 – 5.00	Depositor EDS
% Data completeness (in resolution range)	87.1 (25.00-5.00) 86.3 (25.00-5.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 4.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.336 , 0.337 0.385 , 0.379	Depositor DCC
R_{free} test set	3069 reflections (7.06%)	wwPDB-VP
Wilson B-factor (Å ²)	138.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 999.0	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	0.81	EDS
Total number of atoms	11060	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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	0.62	0/919	1.43	19/1147 (1.7%)
1	B	0.67	0/899	1.46	17/1122 (1.5%)
2	C	0.95	11/4455 (0.2%)	1.69	131/5567 (2.4%)
3	D	0.94	21/4782 (0.4%)	1.68	140/5974 (2.3%)
All	All	0.90	32/11055 (0.3%)	1.65	307/13810 (2.2%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	704	HIS	C-N	20.58	1.60	1.33
3	D	943	THR	C-N	-16.07	1.11	1.33
2	C	828	ALA	C-N	12.53	1.51	1.33
3	D	1435	LEU	C-N	-10.68	1.18	1.33
2	C	1057	SER	C-N	10.48	1.48	1.33
3	D	138	LYS	CA-C	-10.31	1.39	1.52
2	C	141	HIS	C-N	9.88	1.47	1.33
3	D	137	PRO	N-CA	-9.68	1.34	1.47
2	C	768	SER	N-CA	8.32	1.57	1.46
3	D	138	LYS	N-CA	-8.29	1.34	1.46
3	D	322	ARG	C-N	-8.18	1.23	1.33
3	D	142	LEU	N-CA	8.14	1.56	1.46
2	C	769	PRO	N-CA	7.53	1.56	1.47
2	C	777	ILE	N-CA	-7.37	1.37	1.46
3	D	141	VAL	CA-C	7.35	1.62	1.52
3	D	134	VAL	N-CA	-7.14	1.38	1.46
2	C	130	ASN	C-N	-7.02	1.23	1.33
2	C	773	LEU	N-CA	-7.02	1.38	1.46
3	D	144	GLY	C-N	6.90	1.41	1.33
3	D	145	VAL	N-CA	6.80	1.54	1.46
3	D	138	LYS	C-N	-6.72	1.23	1.33
3	D	137	PRO	CA-C	-6.67	1.43	1.52
3	D	152	LEU	N-CA	-6.58	1.37	1.46
3	D	133	ILE	CA-C	-6.12	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1278	ASP	CA-C	5.98	1.59	1.52
3	D	139	GLY	N-CA	-5.94	1.36	1.45
2	C	781	LYS	N-CA	-5.84	1.38	1.46
3	D	141	VAL	N-CA	5.66	1.53	1.46
2	C	364	PRO	CA-C	5.61	1.57	1.52
3	D	148	GLU	CA-C	5.45	1.60	1.52
3	D	145	VAL	CA-C	5.07	1.58	1.52
3	D	152	LEU	C-N	-5.06	1.26	1.33

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	207	VAL	N-CA-C	-13.50	99.95	111.56
3	D	140	ALA	CA-C-N	12.71	144.84	121.97
3	D	140	ALA	C-N-CA	12.71	144.84	121.97
3	D	141	VAL	N-CA-C	12.54	135.41	109.34
3	D	918	LEU	N-CA-C	-12.32	99.04	113.21
3	D	137	PRO	CA-C-N	12.24	140.20	122.09
3	D	137	PRO	C-N-CA	12.24	140.20	122.09
2	C	781	LYS	CA-C-N	-12.16	98.32	121.54
2	C	781	LYS	C-N-CA	-12.16	98.32	121.54
3	D	137	PRO	O-C-N	12.15	139.04	122.64
3	D	888	GLU	N-CA-C	-12.07	98.12	111.28
3	D	446	ASN	N-CA-C	-11.37	95.30	111.56
2	C	312	ALA	N-CA-C	-11.00	100.18	112.72
2	C	345	ARG	N-CA-C	-10.96	99.57	113.16
2	C	777	ILE	N-CA-C	-10.96	99.06	111.00
2	C	383	ARG	N-CA-C	-10.91	100.51	114.04
2	C	163	ILE	N-CA-C	10.70	117.29	107.56
2	C	329	GLY	N-CA-C	-10.02	103.65	114.67
2	C	1027	PHE	N-CA-C	9.85	123.17	109.18
2	C	484	VAL	N-CA-C	9.84	122.16	106.32
2	C	3	ILE	N-CA-C	9.53	121.90	107.99
3	D	686	ALA	N-CA-C	-9.50	101.81	113.97
2	C	773	LEU	N-CA-C	-9.48	100.58	112.72
2	C	528	GLU	N-CA-C	-9.48	102.31	112.93
1	B	139	TYR	N-CA-C	-9.39	98.14	110.53
3	D	1319	VAL	N-CA-C	9.35	128.79	109.34
3	D	462	SER	N-CA-C	-9.27	100.29	112.34
3	D	788	LYS	N-CA-C	-9.19	102.06	113.18
3	D	943	THR	O-C-N	-9.16	110.40	122.59
3	D	319	LYS	N-CA-C	-9.09	99.90	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	562	SER	N-CA-C	-8.93	101.54	111.28
3	D	1393	GLN	N-CA-C	8.91	122.06	108.52
3	D	28	LYS	CA-C-N	8.85	130.90	119.84
3	D	28	LYS	C-N-CA	8.85	130.90	119.84
3	D	137	PRO	CA-C-O	8.85	136.70	120.60
3	D	150	ARG	CA-C-N	-8.78	104.78	121.54
3	D	150	ARG	C-N-CA	-8.78	104.78	121.54
2	C	52	PHE	CA-C-N	-8.73	108.92	119.84
2	C	52	PHE	C-N-CA	-8.73	108.92	119.84
2	C	412	ALA	N-CA-C	-8.65	103.24	113.88
3	D	157	GLU	N-CA-C	-8.64	99.77	110.65
3	D	224	GLU	N-CA-C	-8.63	102.29	113.17
2	C	780	GLU	N-CA-C	-8.62	92.44	110.80
2	C	307	LEU	N-CA-C	-8.57	102.88	112.57
2	C	343	GLN	N-CA-C	-8.57	102.89	112.57
2	C	481	GLU	N-CA-C	-8.51	103.49	114.04
2	C	633	GLN	N-CA-C	-8.50	101.77	112.90
2	C	207	LEU	N-CA-C	-8.29	103.36	113.97
3	D	183	GLU	N-CA-C	-8.23	103.22	113.18
3	D	1459	LEU	O-C-N	-8.18	111.69	122.40
3	D	1494	ALA	N-CA-C	-8.16	101.38	113.61
3	D	234	ARG	CA-C-N	8.03	129.87	119.84
3	D	234	ARG	C-N-CA	8.03	129.87	119.84
2	C	253	ALA	N-CA-C	-7.99	104.06	113.88
2	C	247	PRO	N-CA-C	7.98	120.44	110.70
2	C	1076	VAL	N-CA-C	7.97	126.09	108.88
1	B	165	ILE	N-CA-C	7.97	116.57	107.89
3	D	943	THR	CA-C-N	7.96	136.75	121.54
3	D	943	THR	C-N-CA	7.96	136.75	121.54
1	B	91	ASP	CA-C-N	7.96	129.79	119.84
1	B	91	ASP	C-N-CA	7.96	129.79	119.84
1	A	151	VAL	CA-C-N	7.89	129.71	119.84
1	A	151	VAL	C-N-CA	7.89	129.71	119.84
3	D	198	ARG	N-CA-C	-7.88	104.10	112.93
3	D	147	VAL	CA-C-N	7.85	136.54	121.54
3	D	147	VAL	C-N-CA	7.85	136.54	121.54
3	D	1340	GLY	CA-C-N	7.82	129.61	119.84
3	D	1340	GLY	C-N-CA	7.82	129.61	119.84
2	C	237	ARG	N-CA-C	-7.77	103.39	113.17
3	D	1321	ALA	N-CA-C	7.75	127.30	110.80
3	D	1313	VAL	N-CA-C	-7.69	93.35	109.34
2	C	234	ALA	N-CA-C	-7.68	104.33	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	555	PRO	N-CA-C	-7.66	103.54	113.57
3	D	1362	LYS	N-CA-C	-7.64	97.68	109.52
2	C	698	ASP	N-CA-C	-7.57	101.56	111.02
3	D	586	PRO	N-CA-C	-7.50	103.53	113.65
2	C	1091	GLU	N-CA-C	-7.42	103.48	112.54
3	D	1400	VAL	N-CA-C	-7.37	103.77	112.98
2	C	830	LYS	N-CA-C	-7.36	99.62	110.52
3	D	1323	GLN	N-CA-C	7.36	114.84	108.22
3	D	151	GLN	O-C-N	7.35	132.36	122.59
3	D	73	CYS	N-CA-C	7.27	117.57	108.19
3	D	488	ALA	N-CA-C	-7.27	104.85	113.21
2	C	772	ARG	O-C-N	7.26	132.25	122.59
1	A	95	ALA	N-CA-C	-7.25	103.31	111.14
1	A	184	THR	N-CA-C	7.25	120.95	109.50
2	C	529	VAL	N-CA-C	7.16	118.60	108.36
3	D	1461	GLY	N-CA-C	7.15	123.54	112.60
3	D	913	CYS	N-CA-C	-7.04	98.26	109.59
3	D	151	GLN	CA-C-O	7.02	130.54	120.51
2	C	872	ASN	CA-C-N	7.00	128.59	119.84
2	C	872	ASN	C-N-CA	7.00	128.59	119.84
3	D	1314	LYS	N-CA-C	6.97	125.64	110.80
3	D	59	ALA	N-CA-C	-6.94	104.33	114.39
2	C	501	THR	N-CA-C	6.89	118.05	109.57
2	C	828	ALA	O-C-N	-6.87	113.46	122.59
2	C	316	GLY	N-CA-C	6.85	129.40	113.18
3	D	1459	LEU	CA-C-N	6.84	131.53	120.30
3	D	1459	LEU	C-N-CA	6.84	131.53	120.30
3	D	124	GLU	N-CA-C	-6.83	103.76	111.07
3	D	811	ALA	N-CA-C	6.83	121.27	113.15
3	D	791	ALA	N-CA-C	-6.79	103.68	112.23
2	C	169	GLY	CA-C-N	6.74	126.70	120.03
2	C	169	GLY	C-N-CA	6.74	126.70	120.03
2	C	217	LEU	N-CA-C	-6.73	104.97	113.72
3	D	322	ARG	O-C-N	-6.72	113.65	122.59
2	C	344	PHE	N-CA-C	-6.71	106.05	114.56
2	C	899	GLN	N-CA-C	6.69	116.69	107.73
2	C	35	PRO	CA-C-N	6.66	128.17	119.84
2	C	35	PRO	C-N-CA	6.66	128.17	119.84
2	C	263	ASP	N-CA-C	-6.64	104.61	113.25
2	C	357	GLU	N-CA-C	-6.62	104.79	114.39
2	C	776	SER	N-CA-C	-6.61	105.08	113.01
2	C	392	SER	CA-C-N	6.60	131.31	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	392	SER	C-N-CA	6.60	131.31	120.94
2	C	211	LEU	N-CA-C	6.58	120.53	111.71
2	C	265	LYS	N-CA-C	6.58	120.03	110.42
3	D	136	ASP	CA-C-N	-6.56	111.64	119.84
3	D	136	ASP	C-N-CA	-6.56	111.64	119.84
2	C	224	GLU	N-CA-C	-6.55	96.85	110.80
2	C	1019	GLN	CA-C-N	6.54	128.01	119.84
2	C	1019	GLN	C-N-CA	6.54	128.01	119.84
3	D	351	CYS	N-CA-C	6.54	118.47	108.07
3	D	302	ASN	N-CA-C	-6.51	100.10	109.48
3	D	223	LEU	N-CA-C	6.50	119.30	108.96
3	D	86	ARG	N-CA-C	-6.49	105.22	113.01
3	D	162	ASP	N-CA-C	-6.48	102.72	111.54
3	D	1403	LEU	N-CA-C	-6.46	102.64	111.56
3	D	222	ILE	N-CA-C	-6.44	99.30	108.58
2	C	507	ARG	N-CA-C	6.42	115.88	108.49
2	C	250	LYS	N-CA-C	-6.42	102.56	111.81
3	D	188	GLU	N-CA-C	-6.40	106.68	114.75
2	C	367	LEU	N-CA-C	6.38	119.64	109.24
3	D	543	THR	N-CA-C	6.38	118.25	108.42
2	C	1004	LYS	N-CA-C	-6.38	100.13	109.63
3	D	474	SER	N-CA-C	-6.38	103.61	111.33
2	C	431	HIS	N-CA-C	6.34	119.79	109.59
2	C	221	LEU	N-CA-C	-6.32	105.53	113.18
1	B	159	LYS	N-CA-C	6.32	118.19	109.54
2	C	499	ALA	N-CA-C	-6.30	105.41	113.23
1	A	8	ALA	CA-C-N	6.29	126.24	119.76
1	A	8	ALA	C-N-CA	6.29	126.24	119.76
3	D	775	THR	N-CA-C	6.25	118.59	110.53
3	D	31	THR	N-CA-C	6.24	118.61	108.26
3	D	522	LEU	N-CA-C	-6.19	104.45	112.68
3	D	673	LEU	N-CA-C	-6.16	105.73	113.18
3	D	829	VAL	N-CA-C	6.16	113.92	108.63
3	D	707	GLU	N-CA-C	-6.15	104.50	111.14
2	C	149	THR	CA-C-N	6.13	127.50	119.84
2	C	149	THR	C-N-CA	6.13	127.50	119.84
2	C	782	ALA	N-CA-C	6.12	123.84	110.80
2	C	346	VAL	N-CA-C	-6.12	107.53	113.53
3	D	789	GLY	N-CA-C	-6.09	105.21	115.80
1	B	64	GLU	N-CA-C	-6.08	104.96	112.38
3	D	322	ARG	CA-C-N	6.08	132.93	121.81
3	D	322	ARG	C-N-CA	6.08	132.93	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	PHE	N-CA-C	6.05	118.58	108.73
2	C	469	THR	CA-C-N	6.04	126.35	119.83
2	C	469	THR	C-N-CA	6.04	126.35	119.83
2	C	1110	ASP	N-CA-C	-6.03	97.97	110.80
2	C	1040	LEU	N-CA-C	-6.02	101.44	111.37
2	C	313	LEU	N-CA-C	-5.99	106.58	114.31
2	C	378	LEU	N-CA-C	-5.99	106.30	113.97
2	C	857	ASP	N-CA-C	-5.98	98.05	110.80
1	B	127	LEU	N-CA-C	-5.98	98.07	110.80
2	C	1026	GLN	N-CA-C	-5.97	101.63	110.46
2	C	786	LYS	N-CA-C	5.97	119.67	110.42
3	D	1381	VAL	N-CA-C	5.96	118.47	108.81
3	D	138	LYS	CA-C-N	-5.95	109.75	121.41
3	D	138	LYS	C-N-CA	-5.95	109.75	121.41
2	C	679	PHE	N-CA-C	-5.95	101.13	109.69
3	D	145	VAL	CA-C-N	-5.94	112.42	119.84
3	D	145	VAL	C-N-CA	-5.94	112.42	119.84
2	C	151	ASP	CA-C-N	5.92	127.24	119.84
2	C	151	ASP	C-N-CA	5.92	127.24	119.84
3	D	611	MET	N-CA-C	5.91	123.39	110.80
2	C	563	ASN	N-CA-C	-5.91	102.19	110.35
1	B	100	ILE	N-CA-C	5.91	116.11	106.72
3	D	664	VAL	N-CA-C	5.90	119.11	109.78
2	C	317	VAL	CA-C-N	5.89	125.80	119.85
2	C	317	VAL	C-N-CA	5.89	125.80	119.85
2	C	915	LYS	N-CA-C	-5.89	104.20	111.33
2	C	230	ARG	CA-C-N	5.88	127.19	119.84
2	C	230	ARG	C-N-CA	5.88	127.19	119.84
1	B	62	LEU	N-CA-C	-5.87	100.62	109.95
3	D	142	LEU	N-CA-C	5.82	118.30	107.99
2	C	952	LEU	N-CA-C	-5.82	105.28	112.90
3	D	532	LEU	N-CA-C	5.80	123.16	110.80
2	C	695	LEU	N-CA-C	-5.79	105.05	111.36
1	A	12	THR	N-CA-C	5.79	118.16	108.73
3	D	234	ARG	N-CA-C	-5.78	100.54	109.79
2	C	565	GLN	N-CA-C	-5.77	105.34	112.38
1	B	222	LEU	N-CA-C	-5.77	106.89	114.04
2	C	520	GLU	CA-C-N	5.76	127.05	119.84
2	C	520	GLU	C-N-CA	5.76	127.05	119.84
3	D	1271	LYS	N-CA-C	5.76	123.08	110.80
2	C	461	VAL	N-CA-C	-5.76	100.04	108.97
2	C	759	THR	N-CA-C	5.75	118.10	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASN	CA-C-N	5.74	127.02	119.84
1	A	227	ASN	C-N-CA	5.74	127.02	119.84
1	A	48	ILE	CA-C-N	5.74	127.01	119.84
1	A	48	ILE	C-N-CA	5.74	127.01	119.84
2	C	1064	ASN	N-CA-C	-5.74	102.14	111.04
3	D	685	GLN	N-CA-C	-5.74	105.94	113.17
3	D	132	TYR	CA-C-N	-5.74	115.14	123.06
3	D	132	TYR	C-N-CA	-5.74	115.14	123.06
3	D	824	THR	N-CA-C	-5.72	104.50	112.45
3	D	1436	SER	N-CA-C	-5.72	104.42	111.40
1	A	9	PRO	N-CA-C	5.71	120.05	111.14
2	C	726	ILE	CA-C-N	5.71	126.98	119.84
2	C	726	ILE	C-N-CA	5.71	126.98	119.84
2	C	539	VAL	N-CA-C	5.70	117.62	111.58
2	C	319	GLY	N-CA-C	-5.69	106.86	114.25
3	D	416	THR	N-CA-C	-5.69	102.98	110.43
2	C	632	ASN	N-CA-C	-5.67	107.35	114.56
3	D	919	SER	N-CA-C	-5.67	98.72	110.80
3	D	226	VAL	CA-C-N	5.67	126.93	119.84
3	D	226	VAL	C-N-CA	5.67	126.93	119.84
2	C	879	ARG	N-CA-C	-5.66	101.64	110.42
3	D	862	VAL	N-CA-C	5.66	116.89	108.46
3	D	384	ARG	N-CA-C	5.65	118.37	111.82
2	C	59	LYS	N-CA-C	5.63	118.56	107.98
3	D	353	LEU	CA-C-N	5.62	125.39	119.76
3	D	353	LEU	C-N-CA	5.62	125.39	119.76
2	C	828	ALA	CA-C-N	5.62	132.28	121.54
2	C	828	ALA	C-N-CA	5.62	132.28	121.54
2	C	252	LYS	N-CA-C	-5.60	104.69	112.30
3	D	244	PHE	N-CA-C	5.59	118.52	109.86
3	D	653	THR	N-CA-C	-5.58	105.19	111.28
3	D	95	LEU	N-CA-C	5.57	117.52	110.33
2	C	840	ALA	N-CA-C	5.57	115.90	108.38
3	D	268	ALA	N-CA-C	-5.57	105.36	111.82
3	D	568	ASP	N-CA-C	5.57	117.17	109.54
3	D	138	LYS	CA-C-O	5.56	127.32	120.92
2	C	143	SER	CA-C-N	5.54	126.77	119.84
2	C	143	SER	C-N-CA	5.54	126.77	119.84
3	D	180	GLU	N-CA-C	5.54	117.32	111.28
1	A	177	VAL	N-CA-C	5.54	115.85	108.27
1	A	169	ALA	N-CA-C	5.51	117.72	108.96
3	D	153	LEU	N-CA-C	-5.51	99.06	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1421	LEU	N-CA-C	5.51	117.39	108.41
2	C	299	LYS	N-CA-C	5.50	117.47	109.71
3	D	74	GLU	N-CA-C	-5.50	102.51	111.04
3	D	782	SER	N-CA-C	-5.50	106.57	113.28
2	C	1075	ASP	N-CA-C	-5.49	105.29	111.28
3	D	168	GLU	N-CA-C	-5.49	102.31	111.37
2	C	76	PRO	N-CA-C	5.47	117.37	110.70
3	D	257	ILE	N-CA-C	-5.47	105.78	111.58
3	D	889	ALA	N-CA-C	-5.46	106.46	113.02
3	D	684	GLU	N-CA-C	-5.45	106.77	113.41
1	A	145	ASP	N-CA-C	5.44	117.46	109.24
3	D	1279	GLY	N-CA-C	5.44	126.08	113.18
2	C	1093	GLN	N-CA-C	-5.43	104.76	111.33
2	C	479	VAL	N-CA-C	5.41	115.85	107.78
3	D	1304	LYS	N-CA-C	5.41	117.07	110.41
1	B	124	ASN	CA-C-N	5.38	126.56	119.84
1	B	124	ASN	C-N-CA	5.38	126.56	119.84
2	C	230	ARG	N-CA-C	5.38	121.69	109.81
2	C	655	LEU	N-CA-C	-5.36	106.78	113.15
2	C	220	GLY	N-CA-C	-5.35	100.51	113.18
3	D	1318	TYR	N-CA-C	5.32	117.85	108.75
1	A	148	VAL	N-CA-C	5.32	115.55	108.11
2	C	6	PHE	N-CA-C	5.31	117.72	110.55
3	D	1492	LEU	N-CA-C	-5.27	106.63	114.64
3	D	99	ALA	N-CA-C	5.25	116.26	108.60
1	A	183	ASP	N-CA-C	-5.24	103.57	110.43
3	D	151	GLN	N-CA-C	5.24	121.96	110.80
3	D	1486	VAL	N-CA-C	5.24	115.80	108.89
2	C	486	MET	N-CA-C	5.24	117.21	108.99
3	D	1295	GLU	N-CA-C	5.23	117.47	107.75
2	C	657	ASP	N-CA-C	5.22	116.67	110.19
2	C	772	ARG	CA-C-O	5.21	127.97	120.51
1	B	132	LEU	N-CA-C	5.20	118.05	109.72
2	C	595	LEU	N-CA-C	5.20	117.21	108.73
2	C	779	GLY	CA-C-N	5.20	131.47	121.54
2	C	779	GLY	C-N-CA	5.20	131.47	121.54
3	D	878	GLU	N-CA-C	-5.20	102.85	111.37
2	C	1011	GLY	CA-C-N	5.19	126.33	119.84
2	C	1011	GLY	C-N-CA	5.19	126.33	119.84
3	D	197	ARG	N-CA-C	-5.18	105.70	113.89
3	D	823	THR	N-CA-C	5.16	117.92	110.28
3	D	1317	ASP	N-CA-C	5.16	121.79	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1051	GLU	N-CA-C	-5.16	106.82	113.01
3	D	306	GLU	N-CA-C	-5.16	105.28	112.30
1	B	122	ILE	N-CA-C	-5.15	102.86	109.30
3	D	528	GLY	N-CA-C	-5.15	109.00	114.67
3	D	563	ALA	N-CA-C	-5.15	105.75	111.36
3	D	1474	ALA	N-CA-C	5.15	117.64	109.50
3	D	1284	GLU	N-CA-C	5.14	117.74	108.48
1	A	74	ASP	N-CA-C	-5.13	99.87	110.80
2	C	754	ILE	N-CA-C	5.12	116.61	109.80
3	D	97	THR	N-CA-C	5.11	121.11	109.81
2	C	226	VAL	N-CA-C	-5.11	107.86	113.43
2	C	348	LEU	N-CA-C	-5.10	106.65	112.92
2	C	513	VAL	N-CA-C	5.10	115.65	108.36
1	B	182	GLU	N-CA-C	-5.09	103.67	110.55
1	A	84	GLU	N-CA-C	5.09	116.52	111.07
2	C	927	GLY	N-CA-C	-5.08	106.58	113.24
1	B	145	ASP	N-CA-C	5.08	117.88	109.85
3	D	877	LEU	N-CA-C	-5.07	103.06	111.37
3	D	189	GLU	N-CA-C	-5.06	106.42	112.59
2	C	1015	LEU	N-CA-C	-5.05	107.80	114.31
3	D	1299	PHE	N-CA-C	5.05	116.87	107.99
3	D	505	ARG	N-CA-C	5.04	117.56	110.14
2	C	501	THR	CA-C-N	5.03	126.13	119.84
2	C	501	THR	C-N-CA	5.03	126.13	119.84
3	D	347	LYS	N-CA-C	-5.02	103.06	110.48

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	920	0	246	47	0
1	B	900	0	242	41	0
2	C	4456	0	1247	271	0
3	D	4784	0	1312	517	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11060	0	3047	873	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 62.

All (873) 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)
3:D:145:VAL:O	3:D:146:PRO:O	1.56	1.19
2:C:775:ARG:O	2:C:778:PHE:N	1.88	1.05
3:D:1438:ALA:O	3:D:1440:PHE:N	1.98	0.94
2:C:775:ARG:O	2:C:779:GLY:N	2.00	0.94
3:D:917:ASP:C	3:D:919:SER:H	1.68	0.90
3:D:918:LEU:C	3:D:920:MET:H	1.76	0.89
2:C:52:PHE:C	2:C:54:ILE:H	1.84	0.85
3:D:145:VAL:C	3:D:146:PRO:O	2.19	0.85
2:C:554:ASP:N	2:C:880:MET:O	2.09	0.84
3:D:650:LEU:C	3:D:652:THR:H	1.86	0.84
3:D:101:HIS:O	3:D:103:TRP:N	2.11	0.84
3:D:1423:GLY:O	3:D:1425:THR:N	2.14	0.81
3:D:798:ALA:O	3:D:800:SER:N	2.13	0.80
2:C:74:GLY:HA3	2:C:93:PRO:O	1.80	0.80
3:D:22:SER:O	3:D:24:GLY:N	2.12	0.80
2:C:1039:ALA:O	2:C:1042:ALA:N	2.14	0.80
3:D:887:ALA:C	3:D:890:GLY:H	1.90	0.79
3:D:218:PRO:O	3:D:220:TRP:N	2.14	0.79
3:D:420:LEU:O	3:D:422:ILE:N	2.15	0.79
3:D:801:GLY:O	3:D:804:THR:N	2.17	0.78
3:D:1270:ALA:O	3:D:1272:ALA:N	2.17	0.78
2:C:734:LEU:O	2:C:736:ASP:N	2.18	0.77
3:D:26:VAL:C	3:D:28:LYS:H	1.92	0.77
3:D:401:GLU:C	3:D:403:VAL:H	1.89	0.77
2:C:349:ALA:C	2:C:351:LEU:H	1.93	0.76
3:D:318:GLY:C	3:D:321:GLY:H	1.93	0.76
3:D:420:LEU:C	3:D:422:ILE:H	1.93	0.75
2:C:18:LEU:C	2:C:20:GLU:H	1.95	0.75
2:C:18:LEU:O	2:C:20:GLU:N	2.20	0.74
3:D:461:SER:C	3:D:463:PHE:N	2.39	0.74
3:D:495:ILE:O	3:D:496:LEU:C	2.30	0.74
3:D:622:ASP:O	3:D:623:LEU:C	2.30	0.74
2:C:257:LEU:O	2:C:259:GLY:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:900:PRO:O	3:D:902:THR:N	2.21	0.73
2:C:566:THR:C	2:C:568:ALA:H	1.96	0.73
3:D:145:VAL:O	3:D:146:PRO:C	2.29	0.72
3:D:887:ALA:O	3:D:890:GLY:N	2.22	0.72
3:D:930:VAL:O	3:D:931:GLY:C	2.30	0.72
3:D:212:LEU:O	3:D:214:SER:N	2.21	0.72
2:C:775:ARG:C	2:C:778:PHE:H	1.97	0.72
2:C:312:ALA:O	2:C:316:GLY:HA3	1.90	0.71
2:C:1093:GLN:C	2:C:1095:LEU:H	1.98	0.71
3:D:1376:LEU:O	3:D:1378:TYR:N	2.23	0.71
3:D:84:ILE:O	3:D:86:ARG:N	2.24	0.71
3:D:401:GLU:C	3:D:403:VAL:N	2.47	0.71
3:D:468:ALA:O	3:D:472:MET:N	2.20	0.71
3:D:231:PRO:C	3:D:233:LEU:H	1.99	0.70
3:D:487:LEU:C	3:D:489:LYS:H	1.98	0.70
2:C:254:LEU:C	2:C:256:TYR:H	1.99	0.70
2:C:1039:ALA:O	2:C:1040:LEU:C	2.35	0.70
3:D:119:SER:O	3:D:121:THR:N	2.24	0.70
2:C:679:PHE:O	2:C:681:GLY:N	2.25	0.70
3:D:650:LEU:O	3:D:652:THR:N	2.24	0.70
3:D:1443:THR:O	3:D:1444:THR:C	2.34	0.70
2:C:1043:TYR:C	2:C:1045:ALA:H	1.99	0.70
1:A:89:PHE:O	1:A:91:ASP:N	2.25	0.69
3:D:847:SER:O	3:D:848:ASP:C	2.36	0.69
3:D:167:ALA:O	3:D:168:GLU:C	2.35	0.69
3:D:112:ILE:C	3:D:114:THR:H	2.01	0.69
3:D:397:TRP:O	3:D:398:ASP:C	2.35	0.69
3:D:639:LEU:O	3:D:640:LEU:C	2.35	0.69
3:D:642:ALA:O	3:D:643:LEU:C	2.36	0.69
3:D:394:ASP:O	3:D:396:VAL:N	2.26	0.69
1:B:112:GLY:C	1:B:114:PHE:H	2.01	0.69
3:D:418:HIS:O	3:D:421:GLY:N	2.25	0.68
2:C:774:LEU:O	2:C:776:SER:N	2.27	0.68
3:D:934:ALA:O	3:D:935:ALA:C	2.36	0.68
2:C:52:PHE:O	2:C:54:ILE:N	2.27	0.67
3:D:1423:GLY:O	3:D:1424:VAL:C	2.37	0.67
3:D:932:VAL:O	3:D:933:VAL:C	2.37	0.67
3:D:1262:LEU:O	3:D:1263:PHE:C	2.37	0.67
3:D:929:ALA:O	3:D:930:VAL:C	2.37	0.67
3:D:1372:VAL:O	3:D:1375:MET:N	2.25	0.67
3:D:730:TYR:O	3:D:731:VAL:C	2.37	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:PRO:C	2:C:18:LEU:H	2.03	0.67
1:B:37:GLY:O	1:B:40:LEU:N	2.27	0.67
3:D:431:GLU:O	3:D:432:GLY:O	2.13	0.67
3:D:626:GLN:O	3:D:629:LEU:N	2.28	0.67
3:D:461:SER:C	3:D:463:PHE:H	2.01	0.67
3:D:917:ASP:C	3:D:919:SER:N	2.39	0.67
3:D:702:ILE:C	3:D:704:LEU:H	2.01	0.66
2:C:543:ASN:C	2:C:545:ASN:H	2.03	0.66
1:A:121:GLU:O	1:A:123:MET:N	2.28	0.66
3:D:643:LEU:O	3:D:644:LYS:C	2.38	0.66
3:D:620:LEU:O	3:D:621:LYS:C	2.38	0.66
3:D:63:TYR:C	3:D:65:ARG:H	2.03	0.66
3:D:45:PHE:O	3:D:46:ASP:C	2.39	0.66
3:D:526:GLU:O	3:D:529:GLU:N	2.23	0.66
2:C:795:GLY:O	2:C:796:GLU:O	2.14	0.65
3:D:1427:SER:O	3:D:1428:ALA:C	2.38	0.65
3:D:605:ALA:O	3:D:607:GLU:N	2.29	0.65
3:D:935:ALA:O	3:D:936:GLU:C	2.40	0.65
3:D:399:ALA:O	3:D:401:GLU:N	2.29	0.65
2:C:1014:SER:N	2:C:1019:GLN:O	2.20	0.65
3:D:801:GLY:O	3:D:802:TYR:C	2.40	0.65
3:D:439:PRO:O	3:D:441:VAL:N	2.29	0.65
2:C:267:TYR:O	2:C:273:GLY:HA3	1.97	0.65
2:C:845:ASN:O	2:C:846:LYS:C	2.38	0.65
2:C:1034:GLU:O	2:C:1035:MET:C	2.38	0.64
3:D:641:ASP:O	3:D:644:LYS:N	2.29	0.64
3:D:900:PRO:C	3:D:902:THR:N	2.55	0.64
1:A:74:ASP:O	1:A:75:VAL:C	2.41	0.64
3:D:853:LEU:O	3:D:854:TYR:C	2.40	0.64
3:D:641:ASP:O	3:D:642:ALA:C	2.41	0.64
3:D:1335:LEU:O	3:D:1336:LEU:C	2.41	0.64
3:D:1427:SER:O	3:D:1429:LEU:N	2.31	0.64
1:B:172:SER:O	1:B:174:VAL:N	2.31	0.64
2:C:774:LEU:O	2:C:777:ILE:N	2.25	0.63
3:D:355:LYS:O	3:D:356:ARG:C	2.41	0.63
3:D:362:PHE:O	3:D:363:LYS:C	2.41	0.63
3:D:918:LEU:C	3:D:920:MET:N	2.48	0.63
3:D:1434:TRP:O	3:D:1437:ALA:N	2.31	0.63
3:D:546:GLY:O	3:D:548:LEU:N	2.32	0.63
3:D:309:LEU:O	3:D:310:ARG:O	2.17	0.63
3:D:941:PRO:C	3:D:943:THR:N	2.55	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:563:ASN:C	2:C:565:GLN:H	2.06	0.63
3:D:801:GLY:O	3:D:803:LEU:N	2.31	0.63
1:A:75:VAL:O	1:A:79:ILE:N	2.28	0.63
2:C:877:PRO:O	2:C:879:ARG:O	2.16	0.63
2:C:1054:THR:C	2:C:1056:LYS:H	2.07	0.63
3:D:157:GLU:O	3:D:158:TYR:O	2.17	0.63
3:D:363:LYS:O	3:D:364:PRO:O	2.16	0.63
3:D:364:PRO:O	3:D:366:LEU:N	2.32	0.63
3:D:40:GLU:O	3:D:41:ARG:C	2.42	0.62
2:C:1045:ALA:O	2:C:1046:ALA:C	2.42	0.62
2:C:1047:HIS:O	2:C:1049:LEU:N	2.32	0.62
1:A:110:ARG:O	1:A:112:GLY:N	2.32	0.62
2:C:1001:VAL:O	2:C:1004:LYS:N	2.33	0.62
3:D:877:LEU:O	3:D:878:GLU:C	2.42	0.62
2:C:858:MET:O	2:C:859:PRO:C	2.42	0.62
2:C:948:GLU:O	2:C:951:GLY:N	2.21	0.62
2:C:582:GLY:O	2:C:584:GLU:N	2.32	0.62
2:C:1066:ALA:O	2:C:1067:TYR:C	2.42	0.61
3:D:495:ILE:O	3:D:497:GLY:N	2.32	0.61
2:C:723:THR:C	2:C:725:ASP:H	2.08	0.61
3:D:1262:LEU:O	3:D:1265:ALA:N	2.32	0.61
3:D:1316:GLY:O	3:D:1317:ASP:O	2.19	0.61
1:B:37:GLY:O	1:B:38:ASN:C	2.43	0.61
2:C:1041:GLU:O	2:C:1042:ALA:C	2.43	0.61
3:D:171:GLN:C	3:D:173:LEU:N	2.55	0.61
3:D:1344:VAL:O	3:D:1345:GLU:C	2.43	0.61
3:D:1450:ALA:O	3:D:1451:ALA:C	2.43	0.61
1:B:224:TYR:C	1:B:226:ALA:H	2.08	0.61
2:C:1000:MET:O	2:C:1002:GLU:N	2.33	0.61
1:B:209:GLU:O	1:B:210:ALA:C	2.42	0.61
2:C:504:GLU:O	2:C:506:ASP:N	2.34	0.61
3:D:623:LEU:O	3:D:627:ALA:N	2.34	0.61
3:D:635:LYS:O	3:D:636:THR:C	2.42	0.61
2:C:1058:ASP:O	2:C:1060:ILE:N	2.34	0.61
3:D:493:ASP:O	3:D:494:ILE:C	2.44	0.61
1:A:171:PHE:O	1:A:172:SER:C	2.44	0.60
2:C:1093:GLN:C	2:C:1095:LEU:N	2.58	0.60
3:D:659:GLY:O	3:D:661:ASP:N	2.34	0.60
3:D:805:ARG:O	3:D:806:LYS:C	2.43	0.60
1:A:208:LEU:O	1:A:209:GLU:C	2.44	0.60
3:D:620:LEU:O	3:D:623:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:623:LEU:O	3:D:624:VAL:C	2.44	0.60
3:D:1390:LEU:O	3:D:1391:GLU:C	2.43	0.60
1:A:209:GLU:O	1:A:210:ALA:C	2.45	0.60
3:D:1261:GLU:O	3:D:1265:ALA:N	2.33	0.60
3:D:102:ILE:C	3:D:104:PHE:H	2.09	0.60
3:D:743:GLN:O	3:D:744:ILE:C	2.45	0.60
3:D:876:SER:O	3:D:877:LEU:C	2.44	0.60
3:D:324:ARG:O	3:D:326:ASN:N	2.34	0.60
3:D:1365:ASP:O	3:D:1366:LYS:C	2.44	0.60
1:A:218:LEU:O	1:A:219:LYS:C	2.44	0.60
3:D:441:VAL:O	3:D:442:CYS:C	2.44	0.60
2:C:349:ALA:O	2:C:351:LEU:N	2.34	0.60
2:C:1032:PHE:O	3:D:329:GLY:HA2	2.02	0.60
2:C:1047:HIS:C	2:C:1049:LEU:N	2.58	0.60
3:D:1466:VAL:C	3:D:1468:LEU:N	2.57	0.60
3:D:321:GLY:O	3:D:323:PHE:N	2.27	0.60
3:D:171:GLN:C	3:D:173:LEU:H	2.09	0.59
3:D:592:ALA:O	3:D:595:VAL:N	2.35	0.59
3:D:637:ALA:O	3:D:638:ARG:C	2.44	0.59
3:D:1425:THR:O	3:D:1426:LYS:C	2.44	0.59
3:D:174:LEU:O	3:D:175:LYS:C	2.46	0.59
3:D:289:ALA:O	3:D:293:ASN:N	2.35	0.59
3:D:508:LYS:O	3:D:510:GLY:N	2.32	0.59
3:D:626:GLN:O	3:D:627:ALA:C	2.44	0.59
3:D:648:PHE:O	3:D:649:THR:C	2.44	0.59
3:D:1350:ASP:O	3:D:1351:GLU:C	2.45	0.59
2:C:891:GLY:O	2:C:892:LEU:C	2.45	0.59
3:D:171:GLN:O	3:D:173:LEU:N	2.36	0.59
3:D:592:ALA:O	3:D:593:ARG:C	2.46	0.59
3:D:799:ASP:O	3:D:800:SER:C	2.46	0.59
3:D:1349:VAL:O	3:D:1350:ASP:C	2.45	0.59
3:D:292:ASP:O	3:D:293:ASN:C	2.46	0.59
3:D:371:GLU:C	3:D:373:LYS:H	2.08	0.59
3:D:511:ALA:O	3:D:513:MET:N	2.36	0.59
3:D:373:LYS:O	3:D:375:PHE:N	2.36	0.59
3:D:1341:PRO:O	3:D:1342:GLU:C	2.45	0.59
2:C:798:GLY:HA3	2:C:828:ALA:O	2.02	0.59
2:C:1038:TRP:O	2:C:1042:ALA:N	2.35	0.59
3:D:637:ALA:O	3:D:640:LEU:N	2.35	0.59
2:C:82:GLU:C	2:C:84:ARG:H	2.09	0.59
3:D:583:GLU:O	3:D:584:THR:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1426:LYS:O	3:D:1427:SER:O	2.20	0.59
2:C:561:GLY:HA3	2:C:842:ARG:O	2.03	0.58
2:C:527:GLU:C	2:C:529:VAL:H	2.09	0.58
2:C:683:ASN:O	2:C:687:ALA:N	2.33	0.58
3:D:876:SER:O	3:D:879:ASP:N	2.36	0.58
2:C:556:ASN:C	2:C:558:ALA:H	2.10	0.58
3:D:275:ILE:O	3:D:276:ILE:C	2.47	0.58
3:D:1447:LEU:O	3:D:1448:THR:C	2.46	0.58
1:A:44:LEU:O	1:A:46:SER:N	2.35	0.58
2:C:948:GLU:C	2:C:950:LEU:N	2.59	0.58
3:D:622:ASP:O	3:D:626:GLN:N	2.33	0.58
3:D:1466:VAL:O	3:D:1469:GLY:N	2.36	0.58
3:D:219:GLU:O	3:D:221:MET:N	2.36	0.58
3:D:849:ILE:O	3:D:852:GLY:N	2.36	0.58
3:D:933:VAL:O	3:D:934:ALA:C	2.46	0.58
2:C:543:ASN:C	2:C:545:ASN:N	2.60	0.58
2:C:1070:ILE:C	2:C:1072:LYS:N	2.61	0.58
3:D:596:GLY:O	3:D:599:VAL:N	2.32	0.58
3:D:742:GLN:O	3:D:743:GLN:C	2.46	0.58
3:D:916:TYR:O	3:D:918:LEU:N	2.37	0.57
3:D:1448:THR:O	3:D:1449:GLU:C	2.47	0.57
2:C:775:ARG:O	2:C:778:PHE:CA	2.51	0.57
3:D:730:TYR:O	3:D:732:MET:N	2.37	0.57
3:D:702:ILE:C	3:D:704:LEU:N	2.61	0.57
1:B:34:VAL:O	1:B:35:THR:C	2.47	0.57
2:C:680:ASP:O	2:C:681:GLY:C	2.47	0.57
3:D:231:PRO:O	3:D:233:LEU:N	2.37	0.57
3:D:1399:ASP:C	3:D:1401:GLU:H	2.12	0.57
2:C:1047:HIS:O	2:C:1048:THR:C	2.45	0.57
2:C:52:PHE:C	2:C:54:ILE:N	2.50	0.57
2:C:1088:LEU:O	2:C:1089:VAL:C	2.47	0.57
3:D:1471:LEU:O	3:D:1472:ILE:O	2.23	0.57
3:D:121:THR:C	3:D:123:LEU:H	2.12	0.57
2:C:410:ILE:N	2:C:453:THR:O	2.37	0.57
2:C:775:ARG:C	2:C:777:ILE:N	2.59	0.57
3:D:118:LEU:O	3:D:119:SER:C	2.48	0.57
3:D:205:LEU:O	3:D:208:VAL:N	2.37	0.57
2:C:18:LEU:C	2:C:20:GLU:N	2.59	0.57
2:C:349:ALA:C	2:C:351:LEU:N	2.62	0.57
2:C:563:ASN:O	2:C:565:GLN:N	2.28	0.57
3:D:252:LEU:C	3:D:254:ARG:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:633:MET:O	3:D:634:GLU:C	2.48	0.57
3:D:1371:VAL:O	3:D:1372:VAL:C	2.47	0.57
3:D:357:MET:O	3:D:359:LEU:N	2.38	0.57
3:D:860:ARG:O	3:D:861:GLU:O	2.22	0.57
3:D:55:ASP:O	3:D:57:GLU:N	2.38	0.56
3:D:524:ALA:O	3:D:525:TYR:C	2.46	0.56
1:A:208:LEU:O	1:A:211:LEU:N	2.39	0.56
2:C:731:GLU:C	2:C:733:ALA:N	2.61	0.56
2:C:1000:MET:O	2:C:1001:VAL:C	2.48	0.56
3:D:26:VAL:C	3:D:28:LYS:N	2.57	0.56
3:D:287:VAL:O	3:D:288:ASP:C	2.48	0.56
3:D:620:LEU:O	3:D:624:VAL:N	2.38	0.56
3:D:647:GLY:O	3:D:651:SER:N	2.22	0.56
3:D:1466:VAL:O	3:D:1467:ILE:C	2.48	0.56
1:A:74:ASP:O	1:A:77:GLU:N	2.39	0.56
2:C:292:ARG:O	2:C:294:GLU:N	2.38	0.56
2:C:751:PRO:C	2:C:753:ASP:H	2.13	0.56
3:D:25:GLU:O	3:D:27:GLU:N	2.34	0.56
3:D:546:GLY:C	3:D:548:LEU:N	2.62	0.56
2:C:566:THR:C	2:C:568:ALA:N	2.64	0.56
2:C:634:GLY:O	2:C:635:THR:C	2.48	0.56
3:D:728:PRO:O	3:D:729:LEU:C	2.48	0.56
3:D:1336:LEU:O	3:D:1337:GLU:C	2.48	0.56
1:A:164:ALA:O	1:A:165:ILE:C	2.48	0.56
2:C:968:ASP:C	2:C:970:GLY:H	2.11	0.56
2:C:941:LYS:O	2:C:945:ALA:N	2.36	0.56
3:D:441:VAL:O	3:D:443:GLU:N	2.39	0.56
2:C:82:GLU:C	2:C:84:ARG:N	2.63	0.56
3:D:119:SER:O	3:D:121:THR:O	2.24	0.56
3:D:396:VAL:O	3:D:399:ALA:N	2.38	0.56
3:D:729:LEU:O	3:D:730:TYR:C	2.48	0.56
2:C:431:HIS:O	2:C:433:THR:N	2.39	0.56
2:C:558:ALA:O	2:C:561:GLY:N	2.38	0.56
2:C:882:LEU:O	2:C:884:GLN:N	2.38	0.56
3:D:736:GLY:O	3:D:737:ALA:C	2.47	0.56
2:C:1093:GLN:O	2:C:1095:LEU:N	2.30	0.56
3:D:401:GLU:O	3:D:403:VAL:N	2.38	0.56
1:A:74:ASP:O	1:A:76:VAL:N	2.39	0.56
2:C:582:GLY:C	2:C:584:GLU:N	2.64	0.56
3:D:1367:HIS:O	3:D:1368:ILE:C	2.49	0.56
2:C:563:ASN:C	2:C:565:GLN:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:399:ALA:O	3:D:400:LEU:C	2.49	0.55
3:D:499:TYR:O	3:D:502:THR:N	2.29	0.55
2:C:964:LYS:O	2:C:965:GLU:C	2.49	0.55
3:D:366:LEU:O	3:D:367:LEU:C	2.49	0.55
3:D:371:GLU:C	3:D:373:LYS:N	2.64	0.55
3:D:792:ASP:C	3:D:794:ALA:N	2.61	0.55
2:C:561:GLY:O	2:C:563:ASN:O	2.24	0.55
2:C:882:LEU:O	2:C:885:ILE:N	2.36	0.55
3:D:231:PRO:C	3:D:233:LEU:N	2.65	0.55
3:D:396:VAL:O	3:D:397:TRP:C	2.50	0.55
2:C:582:GLY:O	2:C:583:LEU:C	2.50	0.55
3:D:617:LYS:O	3:D:618:ASN:C	2.49	0.55
3:D:1395:LEU:O	3:D:1398:TRP:N	2.39	0.55
2:C:82:GLU:O	2:C:84:ARG:N	2.39	0.55
2:C:1070:ILE:O	2:C:1072:LYS:N	2.40	0.55
2:C:1044:GLY:C	2:C:1046:ALA:H	2.14	0.55
3:D:284:GLN:O	3:D:286:ALA:N	2.40	0.55
3:D:364:PRO:O	3:D:365:PHE:C	2.48	0.55
3:D:715:ALA:C	3:D:717:PHE:N	2.64	0.55
3:D:440:LEU:O	3:D:441:VAL:C	2.50	0.55
3:D:444:ALA:C	3:D:446:ASN:H	2.14	0.55
3:D:559:LEU:C	3:D:561:ALA:N	2.62	0.55
1:A:127:LEU:O	1:A:128:HIS:C	2.50	0.55
2:C:402:SER:O	2:C:403:SER:C	2.50	0.55
2:C:966:LEU:O	2:C:969:LEU:N	2.40	0.55
3:D:259:ARG:C	3:D:261:ASN:H	2.14	0.55
3:D:102:ILE:O	3:D:104:PHE:N	2.40	0.55
3:D:259:ARG:O	3:D:261:ASN:N	2.40	0.55
3:D:645:TYR:O	3:D:648:PHE:N	2.40	0.55
3:D:849:ILE:O	3:D:850:GLU:C	2.48	0.55
3:D:1342:GLU:O	3:D:1345:GLU:N	2.40	0.55
2:C:1054:THR:O	2:C:1056:LYS:N	2.41	0.54
3:D:590:LEU:O	3:D:591:PHE:C	2.49	0.54
3:D:932:VAL:O	3:D:935:ALA:N	2.40	0.54
1:B:152:PRO:C	1:B:154:GLU:H	2.15	0.54
2:C:1060:ILE:O	2:C:1061:GLU:C	2.51	0.54
3:D:439:PRO:O	3:D:440:LEU:C	2.51	0.54
3:D:632:GLY:O	3:D:633:MET:C	2.51	0.54
3:D:1348:LEU:O	3:D:1349:VAL:C	2.51	0.54
3:D:1462:LEU:C	3:D:1464:GLU:N	2.63	0.54
2:C:653:ASP:O	2:C:654:LEU:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:697:ARG:O	2:C:698:ASP:C	2.51	0.54
2:C:1047:HIS:O	2:C:1050:GLN:N	2.40	0.54
1:B:112:GLY:O	1:B:114:PHE:N	2.41	0.54
3:D:364:PRO:O	3:D:367:LEU:N	2.39	0.54
3:D:557:GLU:O	3:D:558:ALA:C	2.51	0.54
2:C:572:ILE:C	2:C:574:ALA:H	2.15	0.54
3:D:129:PHE:O	3:D:131:LYS:N	2.41	0.54
3:D:367:LEU:O	3:D:370:MET:N	2.40	0.54
3:D:418:HIS:O	3:D:419:ARG:C	2.51	0.54
3:D:811:ALA:C	3:D:813:GLU:H	2.14	0.54
3:D:1449:GLU:O	3:D:1450:ALA:C	2.49	0.54
3:D:219:GLU:C	3:D:221:MET:N	2.65	0.54
3:D:564:HIS:O	3:D:566:LEU:N	2.40	0.54
3:D:941:PRO:O	3:D:943:THR:N	2.40	0.53
1:A:209:GLU:O	1:A:212:ASN:N	2.41	0.53
2:C:92:ALA:O	2:C:93:PRO:C	2.51	0.53
3:D:348:LEU:O	3:D:350:GLN:N	2.41	0.53
3:D:743:GLN:O	3:D:745:ARG:N	2.41	0.53
3:D:900:PRO:C	3:D:902:THR:H	2.15	0.53
2:C:89:THR:O	2:C:90:TYR:C	2.50	0.53
2:C:1043:TYR:C	2:C:1045:ALA:N	2.66	0.53
3:D:792:ASP:O	3:D:794:ALA:N	2.42	0.53
3:D:813:GLU:O	3:D:814:ILE:C	2.51	0.53
3:D:815:VAL:H	3:D:908:GLY:HA2	1.72	0.53
1:B:41:ARG:C	1:B:43:ILE:H	2.16	0.53
2:C:254:LEU:C	2:C:256:TYR:N	2.67	0.53
2:C:1035:MET:O	2:C:1036:GLU:C	2.50	0.53
3:D:420:LEU:C	3:D:422:ILE:N	2.53	0.53
3:D:480:SER:O	3:D:481:PRO:C	2.51	0.53
3:D:650:LEU:C	3:D:652:THR:N	2.54	0.53
2:C:876:VAL:O	2:C:879:ARG:O	2.26	0.53
3:D:399:ALA:C	3:D:401:GLU:N	2.65	0.53
3:D:559:LEU:O	3:D:561:ALA:N	2.42	0.53
3:D:880:VAL:O	3:D:881:HIS:C	2.52	0.53
3:D:887:ALA:C	3:D:890:GLY:N	2.65	0.53
3:D:1266:ARG:O	3:D:1268:PRO:N	2.42	0.53
3:D:318:GLY:CA	3:D:321:GLY:H	2.21	0.53
2:C:517:ARG:O	2:C:519:GLY:N	2.42	0.53
2:C:834:GLN:O	2:C:835:VAL:C	2.49	0.53
3:D:33:ASN:O	3:D:35:ARG:N	2.42	0.53
3:D:1434:TRP:O	3:D:1435:LEU:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1444:THR:O	3:D:1445:HIS:C	2.52	0.53
2:C:448:ASN:O	2:C:449:ILE:C	2.51	0.53
2:C:462:ASP:O	2:C:463:ALA:C	2.51	0.53
3:D:84:ILE:C	3:D:86:ARG:H	2.17	0.53
3:D:493:ASP:C	3:D:495:ILE:N	2.62	0.53
3:D:811:ALA:O	3:D:931:GLY:HA3	2.09	0.53
3:D:205:LEU:O	3:D:207:VAL:N	2.42	0.53
3:D:1347:TYR:O	3:D:1348:LEU:C	2.52	0.53
2:C:13:ILE:O	2:C:14:PRO:O	2.27	0.52
3:D:461:SER:O	3:D:462:SER:C	2.50	0.52
3:D:1445:HIS:O	3:D:1446:VAL:C	2.51	0.52
2:C:775:ARG:O	2:C:778:PHE:C	2.52	0.52
2:C:831:ARG:O	2:C:832:LYS:C	2.52	0.52
2:C:1068:GLN:O	2:C:1071:ILE:N	2.43	0.52
3:D:605:ALA:C	3:D:607:GLU:N	2.66	0.52
2:C:775:ARG:C	2:C:778:PHE:N	2.59	0.52
3:D:680:LEU:C	3:D:682:GLN:H	2.17	0.52
3:D:792:ASP:C	3:D:794:ALA:H	2.17	0.52
1:B:114:PHE:O	1:B:115:THR:C	2.52	0.52
2:C:433:THR:O	2:C:435:TYR:N	2.43	0.52
2:C:74:GLY:CA	2:C:93:PRO:O	2.57	0.52
2:C:551:GLU:O	3:D:773:GLY:HA2	2.10	0.52
3:D:397:TRP:O	3:D:400:LEU:N	2.43	0.52
3:D:1369:GLU:O	3:D:1370:ILE:C	2.52	0.52
3:D:1425:THR:O	3:D:1427:SER:N	2.43	0.52
1:A:156:HIS:O	1:A:157:GLY:O	2.28	0.52
3:D:805:ARG:O	3:D:808:VAL:N	2.43	0.52
2:C:780:GLU:O	2:C:782:ALA:N	2.43	0.52
2:C:1064:ASN:O	2:C:1065:ALA:C	2.52	0.52
1:B:37:GLY:O	1:B:39:PRO:N	2.43	0.52
3:D:605:ALA:O	3:D:606:GLN:C	2.52	0.52
2:C:684:PHE:O	2:C:686:ASP:N	2.37	0.52
3:D:596:GLY:O	3:D:597:GLU:C	2.53	0.52
3:D:21:TRP:C	3:D:23:TYR:H	2.17	0.51
3:D:431:GLU:C	3:D:432:GLY:O	2.53	0.51
3:D:783:SER:O	3:D:784:HIS:C	2.50	0.51
3:D:787:ARG:C	3:D:790:GLY:H	2.18	0.51
2:C:16:PRO:O	2:C:18:LEU:N	2.42	0.51
3:D:368:LYS:O	3:D:369:LYS:C	2.52	0.51
3:D:715:ALA:C	3:D:717:PHE:H	2.18	0.51
1:A:229:GLU:O	1:A:230:ALA:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:948:GLU:C	2:C:950:LEU:H	2.16	0.51
2:C:1062:GLY:O	2:C:1066:ALA:N	2.38	0.51
3:D:773:GLY:O	3:D:774:LEU:C	2.53	0.51
3:D:900:PRO:O	3:D:901:LEU:C	2.53	0.51
2:C:948:GLU:O	2:C:950:LEU:N	2.44	0.51
3:D:136:ASP:O	3:D:137:PRO:O	2.29	0.51
3:D:745:ARG:O	3:D:747:LEU:N	2.44	0.51
3:D:811:ALA:C	3:D:813:GLU:N	2.66	0.51
1:A:219:LYS:O	1:A:220:GLU:C	2.52	0.51
3:D:347:LYS:O	3:D:348:LEU:C	2.53	0.51
3:D:379:VAL:O	3:D:382:ALA:N	2.42	0.51
3:D:474:SER:O	3:D:477:ASN:O	2.28	0.51
1:B:225:PHE:O	1:B:226:ALA:O	2.29	0.51
3:D:597:GLU:O	3:D:600:GLY:N	2.44	0.51
3:D:916:TYR:H	3:D:924:VAL:H	1.58	0.51
3:D:941:PRO:O	3:D:942:GLY:C	2.52	0.51
3:D:559:LEU:O	3:D:560:LEU:C	2.52	0.51
3:D:929:ALA:O	3:D:932:VAL:N	2.44	0.51
3:D:1258:ARG:O	3:D:1259:VAL:C	2.54	0.51
2:C:733:ALA:O	2:C:734:LEU:C	2.52	0.51
3:D:124:GLU:O	3:D:127:LEU:N	2.36	0.51
3:D:593:ARG:O	3:D:594:ILE:C	2.53	0.51
3:D:637:ALA:O	3:D:639:LEU:N	2.43	0.51
2:C:1037:VAL:O	2:C:1041:GLU:N	2.30	0.50
3:D:148:GLU:O	3:D:149:LYS:C	2.54	0.50
3:D:820:ASP:C	3:D:822:GLY:N	2.69	0.50
3:D:491:SER:O	3:D:493:ASP:N	2.44	0.50
2:C:13:ILE:C	2:C:14:PRO:O	2.54	0.50
3:D:148:GLU:O	3:D:150:ARG:N	2.44	0.50
3:D:745:ARG:O	3:D:746:GLN:C	2.54	0.50
1:B:172:SER:O	1:B:173:PRO:C	2.54	0.50
2:C:888:THR:O	2:C:990:GLY:HA3	2.11	0.50
3:D:318:GLY:O	3:D:321:GLY:N	2.44	0.50
3:D:1451:ALA:O	3:D:1452:ILE:C	2.54	0.50
3:D:461:SER:O	3:D:463:PHE:N	2.43	0.50
3:D:777:LEU:O	3:D:780:PHE:N	2.45	0.50
1:A:110:ARG:O	1:A:111:ALA:C	2.55	0.50
2:C:1086:ARG:O	2:C:1087:VAL:C	2.55	0.50
3:D:628:PHE:O	3:D:629:LEU:C	2.55	0.50
2:C:961:GLU:C	2:C:963:LEU:N	2.66	0.50
3:D:625:TYR:O	3:D:626:GLN:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:ASN:C	2:C:547:ILE:N	2.69	0.50
2:C:727:PRO:C	2:C:729:LEU:H	2.20	0.50
3:D:483:SER:O	3:D:485:GLU:N	2.45	0.50
3:D:916:TYR:N	3:D:924:VAL:H	2.10	0.50
3:D:63:TYR:C	3:D:65:ARG:N	2.69	0.49
3:D:284:GLN:C	3:D:286:ALA:N	2.69	0.49
3:D:807:LEU:O	3:D:808:VAL:C	2.54	0.49
1:B:211:LEU:O	1:B:212:ASN:C	2.55	0.49
3:D:117:ASP:O	3:D:118:LEU:C	2.54	0.49
3:D:850:GLU:C	3:D:852:GLY:H	2.20	0.49
2:C:515:ALA:O	2:C:522:VAL:O	2.30	0.49
3:D:394:ASP:O	3:D:395:GLU:C	2.55	0.49
3:D:1260:ILE:O	3:D:1261:GLU:C	2.54	0.49
2:C:556:ASN:O	2:C:558:ALA:N	2.46	0.49
2:C:733:ALA:C	2:C:735:ARG:N	2.69	0.49
3:D:730:TYR:O	3:D:733:ALA:N	2.45	0.49
1:A:219:LYS:O	1:A:222:LEU:N	2.45	0.49
1:B:116:PRO:O	1:B:117:SER:O	2.31	0.49
2:C:389:SER:O	2:C:391:LEU:N	2.46	0.49
2:C:766:GLU:O	2:C:767:PRO:O	2.29	0.49
3:D:1336:LEU:O	3:D:1339:LYS:N	2.46	0.49
3:D:1446:VAL:O	3:D:1447:LEU:C	2.55	0.49
3:D:1466:VAL:O	3:D:1468:LEU:N	2.45	0.49
2:C:397:GLU:O	2:C:398:THR:C	2.55	0.49
3:D:259:ARG:C	3:D:261:ASN:N	2.71	0.49
3:D:397:TRP:O	3:D:399:ALA:N	2.45	0.49
1:B:83:LYS:C	1:B:85:LEU:N	2.70	0.49
2:C:543:ASN:O	2:C:545:ASN:N	2.45	0.49
2:C:694:LEU:O	2:C:698:ASP:N	2.45	0.49
2:C:1088:LEU:O	2:C:1091:GLU:N	2.46	0.49
3:D:317:SER:O	3:D:318:GLY:C	2.56	0.49
1:A:217:ILE:O	1:A:218:LEU:C	2.54	0.49
3:D:154:THR:O	3:D:157:GLU:N	2.44	0.49
3:D:808:VAL:O	3:D:810:VAL:N	2.46	0.49
3:D:1462:LEU:O	3:D:1463:LYS:C	2.55	0.49
1:A:34:VAL:C	1:A:36:LEU:N	2.68	0.49
3:D:480:SER:C	3:D:482:ALA:N	2.65	0.49
3:D:535:PRO:O	3:D:536:ILE:C	2.56	0.49
1:B:219:LYS:O	1:B:220:GLU:C	2.56	0.49
2:C:282:GLY:O	2:C:283:VAL:O	2.31	0.49
2:C:572:ILE:O	2:C:574:ALA:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1345:GLU:O	3:D:1346:ARG:C	2.55	0.48
1:B:32:PHE:O	1:B:33:GLY:C	2.55	0.48
2:C:427:VAL:O	2:C:428:ARG:C	2.55	0.48
2:C:564:MET:C	2:C:566:THR:N	2.69	0.48
2:C:831:ARG:O	2:C:832:LYS:O	2.31	0.48
3:D:473:LEU:O	3:D:474:SER:C	2.56	0.48
3:D:546:GLY:C	3:D:548:LEU:H	2.20	0.48
1:B:112:GLY:C	1:B:114:PHE:N	2.66	0.48
2:C:731:GLU:O	2:C:733:ALA:N	2.46	0.48
2:C:1054:THR:C	2:C:1056:LYS:N	2.71	0.48
3:D:1440:PHE:O	3:D:1441:GLN:C	2.56	0.48
1:A:122:ILE:O	1:A:123:MET:C	2.56	0.48
2:C:684:PHE:C	2:C:686:ASP:H	2.20	0.48
2:C:1044:GLY:O	2:C:1046:ALA:N	2.42	0.48
3:D:934:ALA:O	3:D:935:ALA:O	2.31	0.48
2:C:787:ASP:O	2:C:789:SER:N	2.46	0.48
3:D:569:LEU:O	3:D:587:GLY:N	2.42	0.48
3:D:659:GLY:O	3:D:660:ILE:C	2.56	0.48
2:C:401:LEU:O	2:C:402:SER:C	2.56	0.48
2:C:1070:ILE:C	2:C:1072:LYS:H	2.21	0.48
3:D:642:ALA:O	3:D:646:TYR:N	2.45	0.48
3:D:941:PRO:C	3:D:943:THR:H	2.21	0.48
1:B:152:PRO:C	1:B:154:GLU:N	2.67	0.48
3:D:1438:ALA:C	3:D:1440:PHE:H	2.08	0.48
2:C:731:GLU:C	2:C:733:ALA:H	2.21	0.48
3:D:627:ALA:O	3:D:628:PHE:C	2.57	0.48
1:B:105:GLY:HA2	1:B:135:GLY:HA2	1.96	0.48
1:A:44:LEU:C	1:A:46:SER:H	2.22	0.48
2:C:1066:ALA:O	2:C:1069:ALA:N	2.47	0.48
2:C:1083:GLU:O	2:C:1085:PHE:N	2.47	0.48
3:D:119:SER:O	3:D:120:ALA:C	2.57	0.48
3:D:592:ALA:O	3:D:596:GLY:N	2.46	0.48
3:D:1424:VAL:O	3:D:1425:THR:O	2.32	0.48
2:C:1043:TYR:O	2:C:1045:ALA:N	2.45	0.47
3:D:680:LEU:C	3:D:682:GLN:N	2.68	0.47
1:A:34:VAL:C	1:A:36:LEU:H	2.22	0.47
2:C:168:ARG:O	2:C:264:PRO:O	2.32	0.47
2:C:404:LEU:O	2:C:405:ARG:C	2.54	0.47
3:D:289:ALA:O	3:D:290:VAL:C	2.57	0.47
3:D:624:VAL:O	3:D:625:TYR:C	2.56	0.47
1:A:104:GLU:O	1:A:105:GLY:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:557:GLU:O	3:D:560:LEU:N	2.47	0.47
3:D:645:TYR:O	3:D:646:TYR:C	2.57	0.47
2:C:135:VAL:O	2:C:137:VAL:N	2.47	0.47
2:C:545:ASN:C	2:C:547:ILE:H	2.21	0.47
2:C:1037:VAL:O	2:C:1038:TRP:C	2.55	0.47
3:D:167:ALA:C	3:D:169:ALA:N	2.71	0.47
3:D:557:GLU:C	3:D:559:LEU:N	2.72	0.47
3:D:724:TYR:C	3:D:726:PHE:H	2.21	0.47
3:D:1351:GLU:O	3:D:1352:ILE:C	2.56	0.47
3:D:1462:LEU:O	3:D:1464:GLU:N	2.47	0.47
3:D:318:GLY:HA2	3:D:321:GLY:H	1.79	0.47
3:D:430:VAL:O	3:D:431:GLU:O	2.32	0.47
3:D:444:ALA:C	3:D:446:ASN:N	2.70	0.47
1:A:82:LEU:O	1:A:83:LYS:C	2.58	0.47
2:C:914:ILE:O	2:C:915:LYS:C	2.57	0.47
3:D:56:TYR:O	3:D:57:GLU:O	2.33	0.47
3:D:101:HIS:O	3:D:102:ILE:C	2.58	0.47
3:D:252:LEU:O	3:D:253:TYR:C	2.57	0.47
3:D:371:GLU:O	3:D:373:LYS:N	2.48	0.47
2:C:448:ASN:O	2:C:449:ILE:O	2.33	0.47
2:C:731:GLU:O	2:C:732:ALA:C	2.55	0.47
2:C:1058:ASP:O	2:C:1059:ASP:C	2.58	0.47
3:D:642:ALA:O	3:D:645:TYR:N	2.47	0.47
3:D:648:PHE:O	3:D:651:SER:N	2.48	0.47
2:C:365:ASP:C	2:C:367:LEU:H	2.22	0.47
2:C:545:ASN:O	2:C:547:ILE:N	2.47	0.47
2:C:614:ARG:O	2:C:615:TYR:O	2.33	0.47
2:C:775:ARG:C	2:C:777:ILE:H	2.21	0.47
3:D:21:TRP:O	3:D:23:TYR:N	2.48	0.47
3:D:247:SER:C	3:D:249:LEU:H	2.23	0.47
3:D:557:GLU:O	3:D:559:LEU:N	2.48	0.47
1:A:206:THR:O	1:A:207:PRO:C	2.58	0.46
1:B:224:TYR:C	1:B:226:ALA:N	2.71	0.46
2:C:891:GLY:O	2:C:893:ALA:N	2.48	0.46
3:D:522:LEU:C	3:D:524:ALA:N	2.72	0.46
3:D:845:LYS:O	3:D:846:ARG:C	2.57	0.46
1:A:76:VAL:O	1:A:77:GLU:C	2.56	0.46
3:D:378:ASN:O	3:D:379:VAL:C	2.59	0.46
3:D:1342:GLU:O	3:D:1343:ALA:C	2.58	0.46
1:A:75:VAL:O	1:A:76:VAL:C	2.58	0.46
2:C:1062:GLY:O	2:C:1065:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:318:GLY:C	3:D:320:GLN:N	2.66	0.46
3:D:805:ARG:O	3:D:807:LEU:N	2.48	0.46
2:C:233:GLU:C	2:C:235:MET:H	2.22	0.46
2:C:873:PRO:O	2:C:874:LEU:C	2.59	0.46
3:D:286:ALA:O	3:D:287:VAL:C	2.58	0.46
3:D:806:LYS:O	3:D:807:LEU:C	2.58	0.46
3:D:1261:GLU:O	3:D:1265:ALA:CA	2.63	0.46
2:C:836:GLY:N	2:C:849:VAL:O	2.49	0.46
3:D:635:LYS:O	3:D:637:ALA:N	2.49	0.46
3:D:736:GLY:O	3:D:737:ALA:O	2.34	0.46
3:D:1366:LYS:O	3:D:1367:HIS:C	2.57	0.46
3:D:1395:LEU:O	3:D:1396:GLU:C	2.58	0.46
3:D:1434:TRP:O	3:D:1438:ALA:N	2.45	0.46
2:C:56:GLU:O	2:C:57:GLY:C	2.59	0.46
2:C:276:LYS:C	2:C:278:GLU:H	2.23	0.46
2:C:434:HIS:O	2:C:435:TYR:C	2.57	0.46
2:C:937:ASP:O	2:C:938:LYS:C	2.59	0.46
3:D:808:VAL:O	3:D:809:ASP:C	2.57	0.46
3:D:1369:GLU:O	3:D:1372:VAL:N	2.48	0.46
3:D:1372:VAL:O	3:D:1373:ARG:C	2.58	0.46
1:B:207:PRO:O	1:B:208:LEU:C	2.59	0.46
2:C:696:LYS:C	2:C:698:ASP:H	2.23	0.46
3:D:1472:ILE:C	3:D:1474:ALA:H	2.24	0.46
2:C:889:HIS:O	2:C:890:LEU:C	2.59	0.46
2:C:1070:ILE:O	2:C:1071:ILE:C	2.59	0.46
3:D:25:GLU:C	3:D:27:GLU:H	2.19	0.46
3:D:84:ILE:C	3:D:86:ARG:N	2.70	0.46
3:D:313:THR:O	3:D:314:ASP:C	2.59	0.46
3:D:1428:ALA:O	3:D:1429:LEU:C	2.58	0.46
2:C:586:ARG:O	2:C:587:VAL:C	2.57	0.46
2:C:601:GLY:HA3	2:C:615:TYR:CA	2.46	0.46
2:C:1062:GLY:O	2:C:1063:ARG:C	2.58	0.46
2:C:1100:GLN:N	3:D:9:ARG:O	2.49	0.46
3:D:1399:ASP:C	3:D:1401:GLU:N	2.70	0.46
1:B:215:VAL:O	1:B:216:ALA:C	2.59	0.46
2:C:444:PRO:O	2:C:445:GLU:C	2.59	0.46
2:C:730:SER:O	2:C:733:ALA:N	2.36	0.46
3:D:114:THR:C	3:D:116:LEU:N	2.71	0.46
3:D:345:GLN:O	3:D:346:LEU:C	2.59	0.46
3:D:878:GLU:O	3:D:879:ASP:C	2.59	0.46
3:D:882:PHE:O	3:D:883:LEU:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:GLY:O	2:C:986:PRO:C	2.58	0.45
3:D:45:PHE:O	3:D:47:GLU:N	2.49	0.45
3:D:263:LEU:C	3:D:265:LYS:N	2.70	0.45
3:D:354:PRO:O	3:D:355:LYS:C	2.58	0.45
3:D:906:ARG:O	3:D:908:GLY:N	2.44	0.45
1:A:224:TYR:C	1:A:226:ALA:H	2.24	0.45
2:C:938:LYS:O	2:C:939:ARG:C	2.60	0.45
3:D:93:ILE:O	3:D:94:GLU:C	2.59	0.45
2:C:917:LEU:O	2:C:921:ALA:N	2.49	0.45
3:D:460:LEU:O	3:D:461:SER:C	2.59	0.45
3:D:546:GLY:O	3:D:547:ARG:C	2.60	0.45
2:C:558:ALA:O	2:C:559:LEU:C	2.59	0.45
3:D:529:GLU:C	3:D:531:ALA:H	2.23	0.45
2:C:972:VAL:O	2:C:987:ILE:N	2.43	0.45
3:D:219:GLU:C	3:D:221:MET:H	2.23	0.45
3:D:343:GLY:O	3:D:344:PRO:C	2.58	0.45
3:D:702:ILE:O	3:D:704:LEU:N	2.50	0.45
3:D:777:LEU:O	3:D:779:TYR:N	2.50	0.45
3:D:889:ALA:O	3:D:890:GLY:C	2.59	0.45
1:A:40:LEU:O	1:A:41:ARG:C	2.60	0.45
1:B:58:ILE:O	1:B:59:GLU:C	2.59	0.45
1:B:83:LYS:O	1:B:84:GLU:C	2.60	0.45
2:C:669:GLY:HA3	2:C:994:ILE:O	2.16	0.45
2:C:854:PRO:C	2:C:856:GLU:H	2.25	0.45
2:C:1083:GLU:O	2:C:1084:SER:C	2.60	0.45
3:D:487:LEU:C	3:D:489:LYS:N	2.65	0.45
3:D:1453:ALA:O	3:D:1454:GLY:C	2.59	0.45
2:C:16:PRO:C	2:C:18:LEU:N	2.71	0.45
2:C:976:ASP:O	2:C:978:ARG:N	2.50	0.45
3:D:641:ASP:O	3:D:643:LEU:N	2.49	0.45
2:C:566:THR:O	2:C:568:ALA:N	2.49	0.45
2:C:943:VAL:C	2:C:945:ALA:N	2.72	0.45
3:D:397:TRP:C	3:D:399:ALA:N	2.73	0.45
3:D:493:ASP:O	3:D:495:ILE:N	2.50	0.45
3:D:497:GLY:O	3:D:498:LEU:C	2.60	0.45
3:D:526:GLU:C	3:D:528:GLY:N	2.73	0.45
1:A:210:ALA:O	1:A:211:LEU:C	2.59	0.45
2:C:836:GLY:O	2:C:837:ASP:C	2.60	0.45
2:C:1039:ALA:C	2:C:1041:GLU:N	2.73	0.45
3:D:522:LEU:C	3:D:524:ALA:H	2.24	0.45
3:D:732:MET:O	3:D:733:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:734:GLN:C	3:D:735:SER:O	2.58	0.45
3:D:848:ASP:O	3:D:849:ILE:C	2.59	0.45
2:C:882:LEU:O	2:C:883:GLY:C	2.60	0.44
2:C:1041:GLU:O	2:C:1043:TYR:O	2.35	0.44
2:C:1078:GLU:O	2:C:1079:PRO:C	2.60	0.44
3:D:161:ILE:O	3:D:162:ASP:C	2.60	0.44
3:D:804:THR:O	3:D:805:ARG:C	2.60	0.44
3:D:1369:GLU:O	3:D:1371:VAL:N	2.50	0.44
2:C:401:LEU:O	2:C:404:LEU:N	2.49	0.44
2:C:488:ALA:C	2:C:490:GLU:N	2.75	0.44
3:D:489:LYS:O	3:D:490:PRO:C	2.60	0.44
1:A:26:GLU:O	1:A:193:ASP:O	2.35	0.44
2:C:556:ASN:C	2:C:558:ALA:N	2.73	0.44
3:D:438:HIS:O	3:D:439:PRO:O	2.35	0.44
3:D:597:GLU:C	3:D:599:VAL:H	2.25	0.44
1:B:105:GLY:HA2	1:B:136:GLY:H	1.82	0.44
2:C:672:VAL:O	2:C:992:MET:N	2.46	0.44
3:D:197:ARG:C	3:D:199:ALA:H	2.25	0.44
2:C:405:ARG:O	2:C:406:HIS:C	2.60	0.44
2:C:691:SER:C	2:C:693:GLU:N	2.71	0.44
3:D:913:CYS:O	3:D:915:GLY:N	2.51	0.44
2:C:1034:GLU:O	2:C:1037:VAL:N	2.50	0.44
3:D:208:VAL:C	3:D:210:ALA:N	2.72	0.44
3:D:850:GLU:O	3:D:854:TYR:N	2.40	0.44
3:D:889:ALA:O	3:D:890:GLY:O	2.34	0.44
1:B:31:GLY:O	1:B:32:PHE:C	2.61	0.44
2:C:433:THR:O	2:C:434:HIS:C	2.60	0.44
2:C:694:LEU:O	2:C:699:PHE:N	2.47	0.44
3:D:25:GLU:C	3:D:27:GLU:N	2.76	0.44
3:D:357:MET:C	3:D:359:LEU:N	2.75	0.44
1:B:105:GLY:HA2	1:B:135:GLY:CA	2.47	0.44
3:D:1437:ALA:O	3:D:1438:ALA:O	2.35	0.44
3:D:404:ILE:O	3:D:405:HIS:C	2.60	0.44
3:D:597:GLU:C	3:D:599:VAL:N	2.75	0.44
3:D:715:ALA:O	3:D:717:PHE:N	2.51	0.44
3:D:729:LEU:O	3:D:730:TYR:O	2.36	0.44
3:D:864:ALA:O	3:D:866:GLY:N	2.51	0.44
1:A:109:VAL:N	1:A:130:ALA:O	2.44	0.43
1:A:223:ASN:O	1:A:224:TYR:C	2.60	0.43
1:B:29:GLU:O	1:B:30:ARG:C	2.61	0.43
2:C:248:PRO:C	2:C:250:LYS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:121:THR:C	3:D:123:LEU:N	2.76	0.43
3:D:129:PHE:C	3:D:131:LYS:N	2.76	0.43
3:D:314:ASP:O	3:D:317:SER:N	2.51	0.43
3:D:442:CYS:O	3:D:443:GLU:C	2.60	0.43
3:D:595:VAL:O	3:D:596:GLY:C	2.60	0.43
2:C:15:LEU:O	2:C:16:PRO:C	2.61	0.43
3:D:22:SER:O	3:D:90:MET:O	2.36	0.43
3:D:529:GLU:C	3:D:531:ALA:N	2.75	0.43
2:C:691:SER:O	2:C:692:GLU:C	2.61	0.43
3:D:280:LYS:C	3:D:282:MET:N	2.75	0.43
3:D:324:ARG:C	3:D:326:ASN:N	2.76	0.43
1:A:202:ASP:O	1:A:204:SER:N	2.52	0.43
2:C:583:LEU:O	2:C:586:ARG:N	2.52	0.43
2:C:845:ASN:O	2:C:846:LYS:O	2.37	0.43
3:D:112:ILE:C	3:D:114:THR:N	2.68	0.43
3:D:601:ASP:C	3:D:603:LYS:H	2.27	0.43
3:D:887:ALA:C	3:D:889:ALA:N	2.70	0.43
2:C:891:GLY:HA3	2:C:991:GLN:H	1.84	0.43
2:C:1092:LEU:O	2:C:1093:GLN:C	2.61	0.43
3:D:19:ARG:O	3:D:20:SER:C	2.62	0.43
3:D:279:GLU:O	3:D:280:LYS:C	2.60	0.43
3:D:670:GLN:O	3:D:674:GLU:N	2.50	0.43
1:B:211:LEU:O	1:B:214:ALA:N	2.51	0.43
2:C:488:ALA:C	2:C:490:GLU:H	2.26	0.43
2:C:1092:LEU:O	2:C:1095:LEU:N	2.52	0.43
3:D:112:ILE:O	3:D:114:THR:N	2.50	0.43
3:D:481:PRO:C	3:D:483:SER:N	2.76	0.43
3:D:544:SER:O	3:D:547:ARG:N	2.52	0.43
2:C:229:MET:O	2:C:230:ARG:O	2.37	0.43
2:C:625:LEU:O	2:C:626:ARG:C	2.61	0.43
2:C:1112:PHE:O	2:C:1114:GLY:N	2.52	0.43
3:D:136:ASP:O	3:D:137:PRO:C	2.56	0.43
3:D:444:ALA:O	3:D:446:ASN:N	2.51	0.43
3:D:496:LEU:O	3:D:497:GLY:C	2.62	0.43
3:D:1333:HIS:O	3:D:1334:GLN:C	2.61	0.43
3:D:1466:VAL:C	3:D:1469:GLY:H	2.27	0.43
1:B:63:HIS:C	1:B:65:PHE:N	2.75	0.43
2:C:696:LYS:C	2:C:698:ASP:N	2.75	0.43
2:C:963:LEU:O	2:C:964:LYS:C	2.61	0.43
2:C:1092:LEU:C	2:C:1094:ALA:N	2.74	0.43
3:D:155:ASP:C	3:D:157:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:254:ARG:O	3:D:255:ARG:C	2.61	0.43
3:D:341:VAL:N	3:D:435:ILE:O	2.51	0.43
3:D:363:LYS:O	3:D:364:PRO:C	2.62	0.43
3:D:526:GLU:O	3:D:527:ARG:C	2.61	0.43
3:D:616:GLU:O	3:D:617:LYS:C	2.61	0.43
3:D:1352:ILE:O	3:D:1353:GLN:C	2.62	0.43
3:D:1474:ALA:O	3:D:1477:GLY:N	2.48	0.43
2:C:178:ALA:C	2:C:180:GLY:H	2.27	0.43
2:C:891:GLY:O	2:C:894:GLY:N	2.52	0.43
3:D:379:VAL:O	3:D:380:LYS:C	2.61	0.43
2:C:948:GLU:O	2:C:949:LYS:C	2.62	0.42
3:D:318:GLY:O	3:D:319:LYS:C	2.60	0.42
3:D:621:LYS:O	3:D:622:ASP:C	2.61	0.42
3:D:927:GLY:O	3:D:928:GLU:C	2.62	0.42
2:C:1001:VAL:O	2:C:1002:GLU:C	2.61	0.42
3:D:175:LYS:O	3:D:177:LEU:N	2.53	0.42
3:D:902:THR:O	3:D:903:CYS:C	2.61	0.42
1:B:192:LEU:O	1:B:193:ASP:C	2.62	0.42
2:C:723:THR:C	2:C:725:ASP:N	2.76	0.42
3:D:653:THR:C	3:D:655:GLY:H	2.27	0.42
2:C:1040:LEU:O	2:C:1043:TYR:O	2.37	0.42
3:D:168:GLU:O	3:D:169:ALA:C	2.62	0.42
3:D:666:PRO:O	3:D:667:GLU:C	2.63	0.42
2:C:328:LEU:C	2:C:330:ASN:N	2.76	0.42
2:C:564:MET:C	2:C:566:THR:H	2.27	0.42
3:D:362:PHE:O	3:D:364:PRO:N	2.52	0.42
3:D:917:ASP:O	3:D:919:SER:N	2.51	0.42
1:A:164:ALA:O	1:A:166:PRO:N	2.52	0.42
2:C:730:SER:O	2:C:731:GLU:C	2.63	0.42
3:D:594:ILE:O	3:D:595:VAL:C	2.62	0.42
3:D:727:ASN:O	3:D:728:PRO:C	2.61	0.42
3:D:1425:THR:C	3:D:1427:SER:N	2.76	0.42
3:D:1466:VAL:C	3:D:1468:LEU:H	2.27	0.42
2:C:968:ASP:C	2:C:970:GLY:N	2.77	0.42
2:C:1082:PRO:O	2:C:1083:GLU:O	2.38	0.42
3:D:93:ILE:O	3:D:95:LEU:N	2.52	0.42
3:D:585:SER:C	3:D:587:GLY:N	2.74	0.42
3:D:756:LYS:N	3:D:760:GLU:O	2.36	0.42
3:D:811:ALA:O	3:D:813:GLU:N	2.52	0.42
1:A:206:THR:C	1:A:208:LEU:N	2.77	0.42
2:C:572:ILE:C	2:C:574:ALA:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LEU:O	2:C:584:GLU:C	2.63	0.42
2:C:943:VAL:O	2:C:946:ARG:N	2.50	0.42
2:C:966:LEU:O	2:C:967:PHE:C	2.62	0.42
3:D:568:ASP:O	3:D:570:GLN:N	2.41	0.42
3:D:717:PHE:O	3:D:720:PHE:N	2.53	0.42
3:D:770:PHE:C	3:D:772:GLU:N	2.75	0.42
3:D:814:ILE:CA	3:D:908:GLY:HA2	2.50	0.42
3:D:860:ARG:O	3:D:861:GLU:C	2.62	0.42
3:D:1262:LEU:O	3:D:1264:GLU:N	2.51	0.42
2:C:11:GLU:C	2:C:13:ILE:N	2.77	0.42
2:C:259:GLY:O	2:C:260:LEU:O	2.37	0.42
2:C:905:VAL:C	2:C:907:ASP:N	2.78	0.42
3:D:616:GLU:O	3:D:617:LYS:O	2.38	0.42
3:D:640:LEU:O	3:D:641:ASP:O	2.37	0.42
1:B:43:ILE:O	1:B:44:LEU:C	2.61	0.42
2:C:807:ARG:O	2:C:808:ARG:C	2.62	0.42
3:D:489:LYS:C	3:D:490:PRO:O	2.60	0.42
3:D:528:GLY:O	3:D:532:LEU:O	2.38	0.42
3:D:610:GLN:O	3:D:612:ASP:N	2.53	0.42
3:D:1344:VAL:O	3:D:1347:TYR:N	2.52	0.42
3:D:252:LEU:O	3:D:254:ARG:N	2.52	0.41
3:D:501:ILE:O	3:D:587:GLY:C	2.63	0.41
3:D:282:MET:O	3:D:283:LEU:C	2.61	0.41
3:D:284:GLN:O	3:D:285:GLU:C	2.62	0.41
3:D:365:PHE:O	3:D:366:LEU:C	2.63	0.41
3:D:480:SER:O	3:D:482:ALA:N	2.53	0.41
3:D:740:ASN:O	3:D:741:PRO:C	2.63	0.41
1:A:34:VAL:O	1:A:36:LEU:N	2.54	0.41
1:A:121:GLU:C	1:A:123:MET:N	2.77	0.41
1:B:128:HIS:O	1:B:130:ALA:N	2.53	0.41
1:B:215:VAL:O	1:B:219:LYS:N	2.41	0.41
2:C:583:LEU:O	2:C:585:GLU:N	2.53	0.41
2:C:957:LYS:O	2:C:958:SER:O	2.39	0.41
2:C:438:ILE:O	2:C:439:CYS:C	2.62	0.41
2:C:730:SER:O	2:C:732:ALA:N	2.53	0.41
2:C:891:GLY:C	2:C:893:ALA:N	2.75	0.41
3:D:465:GLN:O	3:D:466:ALA:C	2.63	0.41
3:D:661:ASP:C	3:D:663:ALA:N	2.77	0.41
3:D:820:ASP:C	3:D:822:GLY:H	2.29	0.41
3:D:916:TYR:O	3:D:917:ASP:C	2.64	0.41
3:D:1436:SER:O	3:D:1437:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:SER:C	2:C:391:LEU:H	2.29	0.41
2:C:889:HIS:C	2:C:891:GLY:N	2.75	0.41
2:C:963:LEU:O	2:C:966:LEU:N	2.54	0.41
3:D:382:ALA:O	3:D:383:ARG:C	2.64	0.41
3:D:1391:GLU:C	3:D:1392:GLY:O	2.63	0.41
1:B:222:LEU:C	1:B:224:TYR:H	2.28	0.41
2:C:871:LEU:O	2:C:872:ASN:C	2.63	0.41
2:C:1047:HIS:C	2:C:1049:LEU:H	2.27	0.41
3:D:219:GLU:O	3:D:220:TRP:C	2.63	0.41
3:D:347:LYS:O	3:D:348:LEU:O	2.38	0.41
3:D:527:ARG:C	3:D:529:GLU:N	2.79	0.41
3:D:659:GLY:O	3:D:662:ASP:N	2.41	0.41
3:D:1347:TYR:O	3:D:1348:LEU:O	2.38	0.41
1:A:223:ASN:C	1:A:225:PHE:N	2.79	0.41
1:B:104:GLU:O	1:B:136:GLY:O	2.39	0.41
2:C:34:VAL:O	2:C:35:PRO:C	2.63	0.41
3:D:864:ALA:C	3:D:866:GLY:H	2.29	0.41
1:A:233:LEU:O	1:A:234:PRO:C	2.63	0.41
3:D:85:VAL:C	3:D:87:ARG:N	2.79	0.41
3:D:561:ALA:C	3:D:563:ALA:N	2.79	0.41
3:D:933:VAL:O	3:D:934:ALA:O	2.39	0.41
1:A:38:ASN:O	1:A:39:PRO:C	2.63	0.41
1:A:84:GLU:O	1:A:85:LEU:C	2.64	0.41
3:D:463:PHE:O	3:D:464:ALA:C	2.64	0.41
3:D:745:ARG:C	3:D:747:LEU:N	2.79	0.41
3:D:804:THR:O	3:D:805:ARG:O	2.39	0.41
3:D:847:SER:O	3:D:850:GLU:N	2.54	0.41
3:D:1349:VAL:O	3:D:1352:ILE:N	2.54	0.41
2:C:553:ASP:C	2:C:554:ASP:O	2.61	0.41
2:C:883:GLY:O	2:C:886:LEU:N	2.53	0.41
3:D:493:ASP:O	3:D:496:LEU:N	2.55	0.41
3:D:777:LEU:C	3:D:779:TYR:N	2.76	0.41
3:D:1350:ASP:O	3:D:1353:GLN:N	2.54	0.41
3:D:1353:GLN:O	3:D:1354:LYS:C	2.64	0.41
2:C:1021:LEU:O	2:C:1022:GLY:C	2.62	0.40
3:D:373:LYS:O	3:D:374:ALA:C	2.64	0.40
3:D:387:GLU:C	3:D:389:GLN:H	2.29	0.40
3:D:559:LEU:O	3:D:562:VAL:N	2.54	0.40
3:D:607:GLU:O	3:D:608:LEU:C	2.62	0.40
2:C:560:MET:O	2:C:563:ASN:O	2.40	0.40
2:C:1082:PRO:O	2:C:1083:GLU:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:390:ARG:O	3:D:391:ASP:C	2.63	0.40
1:A:171:PHE:O	1:A:173:PRO:N	2.55	0.40
2:C:15:LEU:O	2:C:16:PRO:O	2.39	0.40
3:D:645:TYR:O	3:D:647:GLY:N	2.54	0.40
3:D:731:VAL:O	3:D:732:MET:C	2.64	0.40
1:B:219:LYS:O	1:B:222:LEU:N	2.50	0.40
2:C:292:ARG:O	2:C:293:PHE:C	2.63	0.40
2:C:504:GLU:O	2:C:505:GLY:C	2.62	0.40
2:C:559:LEU:O	2:C:560:MET:C	2.65	0.40
2:C:573:ARG:O	2:C:574:ALA:O	2.39	0.40
2:C:654:LEU:C	2:C:656:ALA:H	2.29	0.40
3:D:177:LEU:O	3:D:178:ASP:C	2.63	0.40
3:D:200:LYS:O	3:D:201:ALA:C	2.63	0.40
3:D:263:LEU:C	3:D:265:LYS:H	2.28	0.40
3:D:497:GLY:O	3:D:499:TYR:N	2.54	0.40
3:D:743:GLN:C	3:D:745:ARG:N	2.78	0.40
3:D:845:LYS:O	3:D:846:ARG:O	2.38	0.40
1:B:36:LEU:O	1:B:37:GLY:C	2.65	0.40
2:C:536:PRO:C	2:C:538:GLN:N	2.78	0.40
3:D:911:GLN:C	3:D:913:CYS:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/314 (73%)	138 (60%)	48 (21%)	42 (18%)	0	2
1	B	223/314 (71%)	133 (60%)	58 (26%)	32 (14%)	0	3
2	C	1112/1119 (99%)	640 (58%)	275 (25%)	197 (18%)	0	2
3	D	1192/1233 (97%)	536 (45%)	339 (28%)	317 (27%)	0	0
All	All	2755/2980 (92%)	1447 (52%)	720 (26%)	588 (21%)	0	1

All (588) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	45	LEU
1	A	59	GLU
1	A	74	ASP
1	A	75	VAL
1	A	90	LEU
1	A	94	MET
1	A	111	ALA
1	A	118	ALA
1	A	138	LEU
1	A	188	GLN
1	A	191	ASP
1	A	198	ARG
1	A	203	GLY
1	A	226	ALA
1	A	230	ALA
1	B	36	LEU
1	B	38	ASN
1	B	63	HIS
1	B	113	ASP
1	B	116	PRO
1	B	117	SER
1	B	133	GLU
1	B	173	PRO
1	B	226	ALA
2	C	19	THR
2	C	42	VAL
2	C	55	GLU
2	C	61	LYS
2	C	63	GLY
2	C	111	ASP
2	C	124	ASP
2	C	132	ALA
2	C	183	THR
2	C	230	ARG
2	C	258	PHE
2	C	260	LEU
2	C	261	LEU
2	C	264	PRO
2	C	266	ARG
2	C	283	VAL
2	C	293	PHE

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Mol	Chain	Res	Type
2	C	300	ASP
2	C	309	TYR
2	C	315	ALA
2	C	316	GLY
2	C	394	PHE
2	C	395	LYS
2	C	422	ARG
2	C	434	HIS
2	C	449	ILE
2	C	510	THR
2	C	574	ALA
2	C	615	TYR
2	C	619	ARG
2	C	635	THR
2	C	636	ALA
2	C	656	ALA
2	C	680	ASP
2	C	686	ASP
2	C	731	GLU
2	C	735	ARG
2	C	767	PRO
2	C	768	SER
2	C	770	GLU
2	C	775	ARG
2	C	780	GLU
2	C	788	THR
2	C	790	LEU
2	C	796	GLU
2	C	800	VAL
2	C	801	VAL
2	C	816	LYS
2	C	832	LYS
2	C	972	VAL
2	C	1001	VAL
2	C	1045	ALA
2	C	1046	ALA
2	C	1055	ILE
2	C	1059	ASP
2	C	1069	ALA
2	C	1076	VAL
2	C	1077	PRO
2	C	1078	GLU

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Mol	Chain	Res	Type
2	C	1083	GLU
2	C	1084	SER
2	C	1095	LEU
2	C	1113	GLU
3	D	23	TYR
3	D	25	GLU
3	D	29	PRO
3	D	32	ILE
3	D	34	TYR
3	D	40	GLU
3	D	41	ARG
3	D	57	GLU
3	D	82	ARG
3	D	85	VAL
3	D	102	ILE
3	D	103	TRP
3	D	120	ALA
3	D	130	ASN
3	D	137	PRO
3	D	146	PRO
3	D	147	VAL
3	D	149	LYS
3	D	158	TYR
3	D	164	ARG
3	D	208	VAL
3	D	212	LEU
3	D	219	GLU
3	D	232	ASP
3	D	239	VAL
3	D	254	ARG
3	D	295	ARG
3	D	310	ARG
3	D	322	ARG
3	D	325	GLN
3	D	348	LEU
3	D	349	HIS
3	D	356	ARG
3	D	358	ALA
3	D	364	PRO
3	D	365	PHE
3	D	367	LEU
3	D	374	ALA

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Mol	Chain	Res	Type
3	D	379	VAL
3	D	395	GLU
3	D	396	VAL
3	D	421	GLY
3	D	426	GLN
3	D	431	GLU
3	D	439	PRO
3	D	440	LEU
3	D	442	CYS
3	D	444	ALA
3	D	468	ALA
3	D	492	ARG
3	D	493	ASP
3	D	495	ILE
3	D	496	LEU
3	D	504	VAL
3	D	514	ALA
3	D	532	LEU
3	D	533	ASN
3	D	536	ILE
3	D	584	THR
3	D	606	GLN
3	D	611	MET
3	D	613	VAL
3	D	617	LYS
3	D	619	SER
3	D	624	VAL
3	D	641	ASP
3	D	645	TYR
3	D	648	PHE
3	D	651	SER
3	D	655	GLY
3	D	660	ILE
3	D	713	THR
3	D	730	TYR
3	D	731	VAL
3	D	737	ALA
3	D	742	GLN
3	D	743	GLN
3	D	799	ASP
3	D	800	SER
3	D	802	TYR

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Mol	Chain	Res	Type
3	D	805	ARG
3	D	808	VAL
3	D	846	ARG
3	D	861	GLU
3	D	865	LEU
3	D	890	GLY
3	D	901	LEU
3	D	903	CYS
3	D	917	ASP
3	D	933	VAL
3	D	936	GLU
3	D	943	THR
3	D	1255	GLY
3	D	1262	LEU
3	D	1271	LYS
3	D	1296	SER
3	D	1313	VAL
3	D	1314	LYS
3	D	1317	ASP
3	D	1327	ARG
3	D	1335	LEU
3	D	1336	LEU
3	D	1339	LYS
3	D	1348	LEU
3	D	1349	VAL
3	D	1377	LYS
3	D	1424	VAL
3	D	1425	THR
3	D	1427	SER
3	D	1428	ALA
3	D	1438	ALA
3	D	1439	SER
3	D	1441	GLN
3	D	1448	THR
3	D	1450	ALA
3	D	1452	ILE
3	D	1472	ILE
1	A	73	GLU
1	A	105	GLY
1	A	122	ILE
1	A	128	HIS
1	A	152	PRO

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Mol	Chain	Res	Type
1	A	157	GLY
1	A	166	PRO
1	A	199	ILE
1	A	232	LEU
1	B	30	ARG
1	B	37	GLY
1	B	42	ARG
1	B	60	ASP
1	B	105	GLY
1	B	119	ASP
1	B	129	ILE
1	B	204	SER
2	C	7	GLY
2	C	11	GLU
2	C	14	PRO
2	C	18	LEU
2	C	38	LYS
2	C	41	ASN
2	C	66	LEU
2	C	83	CYS
2	C	90	TYR
2	C	148	PHE
2	C	288	ARG
2	C	290	LEU
2	C	336	VAL
2	C	337	GLY
2	C	350	ARG
2	C	390	GLN
2	C	409	ARG
2	C	432	ARG
2	C	433	THR
2	C	435	TYR
2	C	445	GLU
2	C	457	ALA
2	C	465	GLY
2	C	505	GLY
2	C	541	SER
2	C	557	ARG
2	C	572	ILE
2	C	573	ARG
2	C	583	LEU
2	C	584	GLU

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Mol	Chain	Res	Type
2	C	602	GLU
2	C	616	GLU
2	C	654	LEU
2	C	659	PRO
2	C	684	PHE
2	C	685	GLU
2	C	722	ILE
2	C	771	GLU
2	C	774	LEU
2	C	808	ARG
2	C	821	GLU
2	C	867	VAL
2	C	874	LEU
2	C	877	PRO
2	C	883	GLY
2	C	909	ALA
2	C	936	VAL
2	C	977	GLY
2	C	1016	ILE
2	C	1022	GLY
2	C	1048	THR
2	C	1057	SER
2	C	1080	SER
3	D	5	VAL
3	D	26	VAL
3	D	33	ASN
3	D	39	PRO
3	D	58	CYS
3	D	68	PHE
3	D	97	THR
3	D	111	LYS
3	D	136	ASP
3	D	148	GLU
3	D	150	ARG
3	D	155	ASP
3	D	195	ARG
3	D	206	GLU
3	D	213	ASP
3	D	218	PRO
3	D	220	TRP
3	D	235	PRO
3	D	260	ASN

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Mol	Chain	Res	Type
3	D	285	GLU
3	D	293	ASN
3	D	294	GLY
3	D	305	SER
3	D	309	LEU
3	D	318	GLY
3	D	338	SER
3	D	352	GLY
3	D	400	LEU
3	D	432	GLY
3	D	441	VAL
3	D	484	GLY
3	D	497	GLY
3	D	512	GLY
3	D	538	VAL
3	D	539	ALA
3	D	547	ARG
3	D	565	GLY
3	D	592	ALA
3	D	596	GLY
3	D	607	GLU
3	D	626	GLN
3	D	637	ALA
3	D	728	PRO
3	D	729	LEU
3	D	735	SER
3	D	744	ILE
3	D	778	GLU
3	D	798	ALA
3	D	807	LEU
3	D	814	ILE
3	D	848	ASP
3	D	849	ILE
3	D	870	GLU
3	D	907	TYR
3	D	915	GLY
3	D	930	VAL
3	D	934	ALA
3	D	935	ALA
3	D	938	ILE
3	D	944	GLN
3	D	1265	ALA

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Mol	Chain	Res	Type
3	D	1322	GLY
3	D	1328	GLY
3	D	1332	PRO
3	D	1337	GLU
3	D	1363	LEU
3	D	1367	HIS
3	D	1370	ILE
3	D	1371	VAL
3	D	1372	VAL
3	D	1391	GLU
3	D	1444	THR
3	D	1446	VAL
3	D	1455	LYS
3	D	1464	GLU
3	D	1465	ASN
3	D	1475	GLY
3	D	1489	GLN
1	A	15	THR
1	A	44	LEU
1	A	204	SER
1	A	209	GLU
1	A	234	PRO
1	B	32	PHE
1	B	61	VAL
1	B	75	VAL
1	B	96	SER
1	B	157	GLY
1	B	193	ASP
2	C	16	PRO
2	C	54	ILE
2	C	58	ASP
2	C	64	LEU
2	C	112	GLU
2	C	144	PRO
2	C	168	ARG
2	C	209	ARG
2	C	271	GLU
2	C	281	LEU
2	C	304	LEU
2	C	370	ALA
2	C	398	THR
2	C	532	MET

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Mol	Chain	Res	Type
2	C	567	GLN
2	C	617	ASP
2	C	683	ASN
2	C	728	HIS
2	C	739	GLU
2	C	781	LYS
2	C	794	PRO
2	C	846	LYS
2	C	857	ASP
2	C	859	PRO
2	C	1058	ASP
2	C	1061	GLU
2	C	1063	ARG
2	C	1087	VAL
2	C	1110	ASP
3	D	6	ARG
3	D	7	LYS
3	D	22	SER
3	D	56	TYR
3	D	72	VAL
3	D	108	VAL
3	D	132	TYR
3	D	152	LEU
3	D	153	LEU
3	D	169	ALA
3	D	172	GLU
3	D	175	LYS
3	D	227	PRO
3	D	273	GLU
3	D	332	VAL
3	D	353	LEU
3	D	377	PRO
3	D	391	ASP
3	D	483	SER
3	D	491	SER
3	D	498	LEU
3	D	509	LYS
3	D	556	ASP
3	D	597	GLU
3	D	602	GLU
3	D	605	ALA
3	D	634	GLU

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Mol	Chain	Res	Type
3	D	638	ARG
3	D	642	ALA
3	D	646	TYR
3	D	732	MET
3	D	746	GLN
3	D	793	THR
3	D	806	LYS
3	D	809	ASP
3	D	847	SER
3	D	1277	ILE
3	D	1287	GLU
3	D	1333	HIS
3	D	1343	ALA
3	D	1366	LYS
3	D	1369	GLU
3	D	1373	ARG
3	D	1406	ARG
3	D	1413	VAL
3	D	1451	ALA
1	A	26	GLU
1	A	126	ASP
1	A	139	TYR
1	A	171	PHE
1	A	223	ASN
1	B	5	LYS
1	B	138	LEU
2	C	39	ARG
2	C	76	PRO
2	C	223	ASP
2	C	224	GLU
2	C	519	GLY
2	C	829	GLN
2	C	878	SER
2	C	891	GLY
2	C	958	SER
2	C	1002	GLU
2	C	1079	PRO
2	C	1099	VAL
3	D	21	TRP
3	D	42	ASP
3	D	69	GLU
3	D	119	SER

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Mol	Chain	Res	Type
3	D	161	ILE
3	D	171	GLN
3	D	193	PRO
3	D	271	ALA
3	D	290	VAL
3	D	296	ARG
3	D	297	GLY
3	D	363	LYS
3	D	372	GLU
3	D	376	ALA
3	D	394	ASP
3	D	580	ARG
3	D	629	LEU
3	D	636	THR
3	D	639	LEU
3	D	644	LYS
3	D	670	GLN
3	D	724	TYR
3	D	745	ARG
3	D	750	MET
3	D	794	ALA
3	D	804	THR
3	D	810	VAL
3	D	852	GLY
3	D	914	TYR
3	D	1267	ARG
3	D	1307	LYS
3	D	1334	GLN
3	D	1395	LEU
3	D	1410	GLU
3	D	1426	LYS
1	A	165	ILE
1	A	172	SER
1	B	6	LEU
1	B	26	GLU
1	B	35	THR
2	C	91	GLN
2	C	93	PRO
2	C	105	THR
2	C	181	VAL
2	C	220	GLY
2	C	418	LEU

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Mol	Chain	Res	Type
2	C	544	THR
2	C	546	LEU
2	C	895	TYR
2	C	904	PRO
2	C	949	LYS
2	C	1005	MET
2	C	1012	PRO
2	C	1035	MET
2	C	1097	LEU
2	C	1100	GLN
2	C	1106	ASP
2	C	1109	VAL
3	D	110	SER
3	D	141	VAL
3	D	176	GLU
3	D	286	ALA
3	D	289	ALA
3	D	303	PRO
3	D	317	SER
3	D	346	LEU
3	D	389	GLN
3	D	445	PHE
3	D	557	GLU
3	D	558	ALA
3	D	578	LEU
3	D	621	LYS
3	D	627	ALA
3	D	690	GLY
3	D	703	GLN
3	D	825	ASN
3	D	931	GLY
3	D	1272	ALA
3	D	1350	ASP
3	D	1386	ASP
3	D	1449	GLU
1	A	16	GLN
1	A	217	ILE
1	B	227	ASN
2	C	65	VAL
2	C	152	PRO
2	C	292	ARG
2	C	631	SER

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Mol	Chain	Res	Type
2	C	761	PHE
2	C	807	ARG
2	C	835	VAL
2	C	935	GLY
2	C	1062	GLY
2	C	1071	ILE
3	D	98	PRO
3	D	118	LEU
3	D	144	GLY
3	D	494	ILE
3	D	932	VAL
3	D	1263	PHE
3	D	1268	PRO
3	D	1345	GLU
1	A	76	VAL
1	B	115	THR
1	B	135	GLY
2	C	9	ILE
2	C	52	PHE
2	C	417	GLY
2	C	535	SER
2	C	548	PRO
3	D	562	VAL
3	D	1415	VAL
1	A	228	PRO
2	C	1029	GLY
3	D	274	ILE
3	D	518	PRO
3	D	776	VAL
3	D	900	PRO
1	A	49	PRO
1	B	215	VAL
2	C	296	GLY
2	C	1023	GLY
3	D	595	VAL
3	D	725	PRO
2	C	125	GLY
2	C	136	ILE
2	C	894	GLY
3	D	594	ILE
2	C	645	VAL
3	D	1259	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1435:LEU	C	1436:SER	N	1.18
1	D	943:THR	C	944:GLN	N	1.11

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	230/314 (73%)	1.16	46 (20%) 3 8	194, 194, 194, 194	0
1	B	225/314 (71%)	1.13	51 (22%) 2 7	194, 194, 194, 194	0
2	C	1114/1119 (99%)	1.28	247 (22%) 2 7	194, 194, 194, 194	0
3	D	1196/1233 (96%)	1.35	285 (23%) 2 6	194, 194, 194, 194	0
All	All	2765/2980 (92%)	1.28	629 (22%) 2 7	194, 194, 194, 194	0

All (629) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1315	ASP	27.7
3	D	241	GLY	17.9
3	D	242	GLY	16.7
3	D	505	ARG	11.7
3	D	74	GLU	11.3
2	C	741	GLY	10.9
2	C	246	ASP	10.5
3	D	1314	LYS	10.1
3	D	1287	GLU	9.8
1	A	50	GLY	9.7
3	D	914	TYR	9.3
2	C	118	LEU	7.8
3	D	377	PRO	7.8
3	D	1307	LYS	7.6
3	D	749	GLY	7.4
2	C	633	GLN	7.4
3	D	70	GLY	7.3
3	D	1496	GLU	7.2
3	D	51	GLY	7.1
3	D	294	GLY	7.1
3	D	910	CYS	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	175	ARG	7.0
3	D	821	CYS	7.0
3	D	520	GLU	6.8
1	B	160	ASP	6.6
3	D	62	LYS	6.4
1	B	134	GLU	6.4
2	C	226	VAL	6.3
3	D	67	ARG	6.3
3	D	240	ASP	6.3
3	D	1489	GLN	6.3
3	D	1308	ASP	6.2
2	C	255	ALA	6.2
3	D	136	ASP	6.1
3	D	69	GLU	5.9
2	C	227	LEU	5.9
3	D	913	CYS	5.9
3	D	855	GLY	5.8
3	D	1500	LYS	5.8
3	D	903	CYS	5.8
1	A	51	THR	5.7
3	D	1497	GLU	5.7
2	C	889	HIS	5.7
3	D	1297	GLU	5.6
1	B	49	PRO	5.6
2	C	212	SER	5.6
1	A	60	ASP	5.6
2	C	152	PRO	5.6
3	D	822	GLY	5.5
3	D	1495	ILE	5.5
3	D	1298	GLY	5.4
2	C	970	GLY	5.4
2	C	178	ALA	5.4
3	D	1286	GLY	5.4
3	D	1488	ASP	5.4
3	D	915	GLY	5.4
2	C	71	TYR	5.3
3	D	75	ARG	5.3
2	C	11	GLU	5.2
1	B	175	ARG	5.2
3	D	196	ALA	5.2
3	D	1380	GLU	5.1
3	D	688	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
3	D	1313	VAL	5.0
1	B	17	GLY	5.0
3	D	63	TYR	4.9
1	A	174	VAL	4.9
2	C	757	GLY	4.9
3	D	165	MET	4.9
3	D	1402	ALA	4.8
3	D	484	GLY	4.8
3	D	504	VAL	4.8
2	C	843	HIS	4.8
2	C	364	PRO	4.8
2	C	12	VAL	4.8
2	C	115	LEU	4.7
3	D	657	THR	4.7
3	D	77	GLY	4.7
2	C	1055	ILE	4.6
3	D	900	PRO	4.6
1	B	64	GLU	4.6
2	C	840	ALA	4.5
2	C	211	LEU	4.5
2	C	396	ASP	4.5
1	B	135	GLY	4.5
2	C	245	GLY	4.5
2	C	51	THR	4.5
3	D	1309	ALA	4.5
3	D	948	ARG	4.4
3	D	549	LYS	4.4
3	D	859	ALA	4.4
2	C	166	PRO	4.4
2	C	739	GLU	4.3
2	C	784	ASP	4.3
2	C	150	PRO	4.3
2	C	369	PRO	4.3
1	B	89	PHE	4.3
2	C	807	ARG	4.3
2	C	842	ARG	4.3
3	D	1401	GLU	4.3
3	D	376	ALA	4.3
1	B	95	ALA	4.3
2	C	367	LEU	4.2
2	C	231	PRO	4.2
3	D	76	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	678	PRO	4.2
2	C	296	GLY	4.2
3	D	194	SER	4.2
3	D	1278	ASP	4.2
3	D	512	GLY	4.1
2	C	167	LYS	4.1
3	D	1490	ARG	4.1
3	D	789	GLY	4.1
3	D	1300	SER	4.1
3	D	1498	ALA	4.1
3	D	611	MET	4.1
2	C	225	ALA	4.0
2	C	320	HIS	4.0
3	D	819	ALA	4.0
2	C	580	MET	4.0
3	D	782	SER	4.0
3	D	73	CYS	4.0
2	C	179	SER	4.0
1	B	96	SER	4.0
3	D	544	SER	4.0
2	C	50	GLU	4.0
1	B	70	GLY	4.0
2	C	442	GLU	3.9
2	C	116	GLY	3.9
3	D	20	SER	3.9
3	D	344	PRO	3.9
1	B	166	PRO	3.9
3	D	911	GLN	3.9
3	D	85	VAL	3.9
3	D	1319	VAL	3.9
2	C	363	SER	3.9
2	C	579	VAL	3.9
2	C	441	VAL	3.9
3	D	506	LYS	3.9
3	D	533	ASN	3.9
3	D	551	VAL	3.9
2	C	1044	GLY	3.8
1	B	161	ARG	3.8
3	D	132	TYR	3.8
2	C	1084	SER	3.8
2	C	188	LYS	3.8
2	C	321	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	872	ASN	3.8
1	A	49	PRO	3.8
3	D	751	ARG	3.8
2	C	365	ASP	3.8
3	D	66	GLN	3.8
2	C	268	ASP	3.8
3	D	1379	VAL	3.7
2	C	371	LYS	3.7
2	C	936	VAL	3.7
3	D	408	VAL	3.7
2	C	119	PRO	3.7
3	D	899	SER	3.7
1	B	76	VAL	3.7
3	D	615	GLN	3.7
3	D	690	GLY	3.7
1	A	134	GLU	3.7
2	C	370	ALA	3.7
3	D	1279	GLY	3.7
1	A	72	LYS	3.6
3	D	1288	ASP	3.6
1	B	162	ILE	3.6
3	D	30	GLU	3.6
3	D	888	GLU	3.6
2	C	1007	ALA	3.6
3	D	773	GLY	3.6
2	C	177	GLU	3.6
3	D	81	THR	3.6
3	D	689	MET	3.6
2	C	117	HIS	3.5
3	D	1484	THR	3.5
3	D	665	ILE	3.5
1	A	20	TYR	3.5
3	D	64	LYS	3.5
2	C	841	ASN	3.5
3	D	1501	GLU	3.5
3	D	759	GLY	3.5
3	D	68	PHE	3.5
3	D	256	LEU	3.5
3	D	470	ILE	3.5
2	C	685	GLU	3.5
3	D	153	LEU	3.5
3	D	1499	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	783	SER	3.5
3	D	610	GLN	3.5
2	C	306	THR	3.5
1	B	111	ALA	3.5
2	C	821	GLU	3.4
2	C	282	GLY	3.4
3	D	53	ILE	3.4
1	A	141	GLU	3.4
3	D	519	GLU	3.4
2	C	971	LYS	3.4
3	D	243	ARG	3.4
3	D	581	ARG	3.4
3	D	1480	PHE	3.4
2	C	755	LEU	3.4
2	C	176	VAL	3.4
2	C	1114	GLY	3.4
3	D	448	ASP	3.4
2	C	161	SER	3.4
3	D	58	CYS	3.4
1	A	21	GLY	3.4
2	C	251	ASP	3.3
2	C	1023	GLY	3.3
2	C	544	THR	3.3
2	C	617	ASP	3.3
3	D	163	ALA	3.3
1	A	195	LEU	3.3
2	C	289	THR	3.3
2	C	302	VAL	3.3
2	C	485	TYR	3.3
3	D	684	GLU	3.3
2	C	132	ALA	3.3
3	D	1491	THR	3.3
1	A	135	GLY	3.3
2	C	190	LYS	3.3
3	D	31	THR	3.3
3	D	417	LEU	3.3
2	C	632	ASN	3.3
2	C	551	GLU	3.3
2	C	812	GLY	3.3
3	D	43	GLY	3.3
3	D	342	VAL	3.3
3	D	1471	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	101	HIS	3.2
3	D	451	GLY	3.2
1	B	75	VAL	3.2
3	D	586	PRO	3.2
2	C	436	GLY	3.2
2	C	724	ARG	3.2
3	D	1255	GLY	3.2
3	D	1320	GLU	3.2
2	C	596	TYR	3.2
1	A	204	SER	3.2
3	D	61	GLY	3.2
3	D	471	GLN	3.2
1	B	159	LYS	3.2
1	B	187	GLY	3.2
3	D	24	GLY	3.2
2	C	186	VAL	3.2
1	A	172	SER	3.2
3	D	100	ALA	3.2
3	D	658	ILE	3.2
1	A	35	THR	3.1
2	C	360	VAL	3.1
3	D	947	MET	3.1
2	C	162	ILE	3.1
2	C	903	SER	3.1
2	C	451	LEU	3.1
2	C	761	PHE	3.1
3	D	334	TYR	3.1
1	A	6	LEU	3.1
1	A	202	ASP	3.1
2	C	281	LEU	3.1
3	D	758	SER	3.1
3	D	666	PRO	3.1
3	D	1483	PHE	3.1
3	D	552	PHE	3.1
2	C	280	LYS	3.1
1	B	34	VAL	3.1
3	D	60	CYS	3.1
2	C	581	THR	3.1
2	C	628	TYR	3.1
2	C	776	SER	3.1
2	C	779	GLY	3.1
3	D	1437	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	144	PRO	3.1
2	C	7	GLY	3.1
2	C	286	SER	3.1
2	C	1017	THR	3.1
3	D	726	PHE	3.0
3	D	388	ARG	3.0
1	A	27	PRO	3.0
3	D	565	GLY	3.0
3	D	553	ALA	3.0
2	C	300	ASP	3.0
3	D	904	GLN	3.0
2	C	142	ARG	3.0
2	C	398	THR	3.0
2	C	711	GLU	3.0
2	C	498	GLN	3.0
3	D	534	ALA	3.0
2	C	283	VAL	3.0
3	D	164	ARG	3.0
3	D	419	ARG	3.0
2	C	657	ASP	3.0
3	D	768	SER	3.0
3	D	439	PRO	3.0
3	D	1306	PRO	3.0
2	C	252	LYS	3.0
2	C	868	ASP	2.9
3	D	1316	GLY	2.9
1	A	137	LYS	2.9
2	C	434	HIS	2.9
2	C	500	ASN	2.9
3	D	215	GLY	2.9
3	D	1328	GLY	2.9
2	C	835	VAL	2.9
1	A	73	GLU	2.9
2	C	278	GLU	2.9
3	D	185	GLU	2.9
2	C	223	ASP	2.9
2	C	209	ARG	2.9
3	D	108	VAL	2.9
3	D	909	VAL	2.9
2	C	224	GLU	2.9
3	D	940	GLU	2.9
2	C	158	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	256	TYR	2.9
2	C	539	VAL	2.9
2	C	808	ARG	2.9
3	D	462	SER	2.9
1	A	159	LYS	2.9
2	C	771	GLU	2.9
2	C	577	PRO	2.9
3	D	141	VAL	2.9
1	B	50	GLY	2.9
3	D	48	ARG	2.8
3	D	438	HIS	2.8
2	C	31	GLN	2.8
2	C	319	GLY	2.8
3	D	82	ARG	2.8
3	D	458	VAL	2.8
3	D	655	GLY	2.8
1	A	176	ARG	2.8
2	C	1058	ASP	2.8
3	D	207	VAL	2.8
2	C	26	TYR	2.8
2	C	93	PRO	2.8
3	D	34	TYR	2.8
2	C	39	ARG	2.8
2	C	182	VAL	2.8
1	B	47	SER	2.8
2	C	541	SER	2.8
2	C	1043	TYR	2.8
3	D	748	CYS	2.8
3	D	260	ASN	2.8
3	D	226	VAL	2.8
2	C	299	LYS	2.7
1	B	133	GLU	2.7
3	D	59	ALA	2.7
3	D	818	GLU	2.7
3	D	1403	LEU	2.7
3	D	1485	GLN	2.7
2	C	429	ASP	2.7
2	C	855	VAL	2.7
3	D	418	HIS	2.7
1	B	228	PRO	2.7
3	D	1359	GLN	2.7
3	D	905	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	323	ASP	2.7
3	D	1277	ILE	2.7
3	D	429	LEU	2.7
2	C	303	PHE	2.7
2	C	570	PRO	2.7
3	D	27	GLU	2.7
2	C	953	VAL	2.7
1	A	23	PHE	2.7
2	C	556	ASN	2.7
2	C	247	PRO	2.7
3	D	52	PRO	2.7
3	D	697	ARG	2.7
3	D	1492	LEU	2.7
3	D	1270	ALA	2.7
1	A	166	PRO	2.7
2	C	748	GLU	2.7
3	D	1334	GLN	2.7
1	B	136	GLY	2.7
2	C	837	ASP	2.6
3	D	46	ASP	2.6
1	B	165	ILE	2.6
3	D	44	LEU	2.6
2	C	102	HIS	2.6
2	C	1053	LEU	2.6
3	D	848	ASP	2.6
3	D	1317	ASP	2.6
1	B	188	GLN	2.6
3	D	389	GLN	2.6
3	D	1486	VAL	2.6
3	D	137	PRO	2.6
1	B	63	HIS	2.6
3	D	1493	LYS	2.6
2	C	606	VAL	2.6
2	C	368	THR	2.6
1	A	55	SER	2.6
2	C	180	GLY	2.6
2	C	187	ASN	2.6
2	C	1025	ALA	2.6
3	D	89	ARG	2.6
1	B	117	SER	2.5
3	D	832	PHE	2.5
3	D	919	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	372	LEU	2.5
3	D	494	ILE	2.5
3	D	890	GLY	2.5
1	B	53	VAL	2.5
2	C	458	TYR	2.5
2	C	725	ASP	2.5
3	D	813	GLU	2.5
2	C	699	PHE	2.5
2	C	1036	GLU	2.5
1	B	173	PRO	2.5
2	C	143	SER	2.5
3	D	96	ALA	2.5
3	D	1494	ALA	2.5
3	D	45	PHE	2.5
3	D	341	VAL	2.5
2	C	677	MET	2.5
2	C	366	THR	2.5
2	C	99	GLN	2.5
3	D	734	GLN	2.5
1	A	181	VAL	2.5
2	C	189	ARG	2.5
2	C	356	ARG	2.5
2	C	978	ARG	2.5
3	D	33	ASN	2.5
1	B	203	GLY	2.5
3	D	304	GLY	2.5
3	D	14	SER	2.5
2	C	834	GLN	2.5
2	C	870	ILE	2.5
3	D	84	ILE	2.5
3	D	1280	VAL	2.5
1	B	227	ASN	2.5
1	B	52	ALA	2.5
2	C	495	THR	2.4
2	C	911	GLU	2.4
1	B	69	PRO	2.4
1	B	74	ASP	2.4
2	C	137	VAL	2.4
2	C	973	VAL	2.4
3	D	191	LYS	2.4
3	D	212	LEU	2.4
2	C	453	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	301	GLU	2.4
3	D	296	ARG	2.4
3	D	1318	TYR	2.4
1	B	204	SER	2.4
2	C	243	ARG	2.4
3	D	728	PRO	2.4
3	D	898	ARG	2.4
1	B	195	LEU	2.4
2	C	909	ALA	2.4
2	C	449	ILE	2.4
2	C	309	TYR	2.4
1	A	88	ARG	2.4
2	C	752	GLY	2.4
1	A	124	ASN	2.4
2	C	901	TYR	2.4
3	D	857	VAL	2.4
1	B	196	THR	2.4
2	C	55	GLU	2.4
2	C	314	THR	2.4
3	D	763	GLU	2.4
2	C	228	ALA	2.4
2	C	136	ILE	2.4
3	D	42	ASP	2.4
2	C	305	PRO	2.4
1	B	98	THR	2.4
2	C	279	GLU	2.4
3	D	774	LEU	2.4
1	B	164	ALA	2.4
2	C	431	HIS	2.4
3	D	29	PRO	2.3
1	A	196	THR	2.3
2	C	1048	THR	2.3
3	D	140	ALA	2.3
2	C	322	VAL	2.3
2	C	791	ARG	2.3
1	A	183	ASP	2.3
3	D	314	ASP	2.3
2	C	1047	HIS	2.3
1	B	141	GLU	2.3
3	D	455	ALA	2.3
3	D	1378	TYR	2.3
2	C	133	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	151	ASP	2.3
2	C	1006	HIS	2.3
2	C	531	PHE	2.3
3	D	193	PRO	2.3
2	C	836	GLY	2.3
3	D	752	GLY	2.3
3	D	1360	GLY	2.3
1	A	230	ALA	2.3
1	B	22	GLU	2.3
2	C	578	VAL	2.3
2	C	235	MET	2.3
3	D	1366	LYS	2.3
2	C	90	TYR	2.3
1	B	202	ASP	2.3
3	D	568	ASP	2.3
2	C	153	ALA	2.3
3	D	447	ALA	2.3
3	D	539	ALA	2.3
3	D	1302	GLU	2.3
3	D	750	MET	2.3
3	D	251	ASP	2.3
2	C	86	LYS	2.3
3	D	80	VAL	2.3
3	D	189	GLU	2.3
3	D	1487	VAL	2.3
2	C	335	THR	2.3
3	D	311	SER	2.3
3	D	491	SER	2.3
2	C	440	PRO	2.3
2	C	216	ASP	2.3
2	C	1024	LYS	2.3
2	C	291	VAL	2.3
3	D	1479	ASP	2.3
3	D	616	GLU	2.3
3	D	907	TYR	2.3
3	D	949	THR	2.3
1	B	27	PRO	2.3
2	C	63	GLY	2.3
3	D	901	LEU	2.3
2	C	1101	THR	2.2
3	D	1283	ILE	2.2
2	C	809	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	177	VAL	2.2
3	D	831	LEU	2.2
2	C	173	ASP	2.2
2	C	968	ASP	2.2
3	D	340	ILE	2.2
2	C	537	LYS	2.2
1	A	37	GLY	2.2
2	C	671	ASN	2.2
3	D	537	VAL	2.2
3	D	545	VAL	2.2
2	C	184	MET	2.2
3	D	19	ARG	2.2
3	D	295	ARG	2.2
3	D	696	GLU	2.2
3	D	1413	VAL	2.2
3	D	725	PRO	2.2
3	D	817	ARG	2.2
2	C	44	ILE	2.2
2	C	781	LYS	2.2
3	D	1398	TRP	2.2
3	D	659	GLY	2.2
2	C	415	PRO	2.2
3	D	97	THR	2.2
3	D	247	SER	2.2
2	C	103	LYS	2.2
3	D	1343	ALA	2.2
1	B	158	ILE	2.2
1	A	197	LEU	2.2
2	C	269	LEU	2.2
1	A	86	VAL	2.2
1	B	102	ARG	2.2
2	C	1034	GLU	2.2
2	C	590	ASP	2.1
3	D	799	ASP	2.1
3	D	10	ILE	2.1
3	D	840	THR	2.1
1	A	231	SER	2.1
2	C	168	ARG	2.1
3	D	667	GLU	2.1
1	B	105	GLY	2.1
2	C	295	ASP	2.1
2	C	738	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	773	LEU	2.1
3	D	1368	ILE	2.1
3	D	1412	LYS	2.1
2	C	359	MET	2.1
3	D	335	SER	2.1
3	D	244	PHE	2.1
1	B	168	ASP	2.1
3	D	662	ASP	2.1
3	D	472	MET	2.1
1	A	133	GLU	2.1
1	A	203	GLY	2.1
2	C	670	GLN	2.1
2	C	338	GLU	2.1
2	C	445	GLU	2.1
2	C	636	ALA	2.1
3	D	13	ALA	2.1
2	C	350	ARG	2.1
3	D	1310	ARG	2.1
1	A	131	THR	2.1
2	C	95	TYR	2.1
2	C	543	ASN	2.1
3	D	812	HIS	2.1
3	D	874	TYR	2.1
3	D	902	THR	2.1
2	C	768	SER	2.1
2	C	194	VAL	2.1
3	D	826	TYR	2.1
1	A	97	THR	2.1
2	C	433	THR	2.1
2	C	48	PHE	2.1
2	C	390	GLN	2.1
2	C	528	GLU	2.1
3	D	305	SER	2.1
3	D	190	MET	2.1
1	B	183	ASP	2.1
2	C	754	ILE	2.1
2	C	923	ASN	2.1
3	D	785	GLY	2.1
2	C	171	TRP	2.1
2	C	192	PRO	2.1
3	D	1323	GLN	2.1
1	A	53	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	174	VAL	2.1
2	C	648	ARG	2.0
2	C	492	ASP	2.0
3	D	612	ASP	2.0
1	A	67	THR	2.0
3	D	825	ASN	2.0
3	D	183	GLU	2.0
1	A	87	VAL	2.0
2	C	64	LEU	2.0
1	A	191	ASP	2.0
2	C	170	PRO	2.0
3	D	518	PRO	2.0
3	D	554	ASN	2.0
3	D	921	ALA	2.0
2	C	548	PRO	2.0
2	C	988	VAL	2.0
3	D	459	PRO	2.0
3	D	716	VAL	2.0
1	A	59	GLU	2.0
2	C	386	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.