



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:55 PM UTC

PDB ID : 1XHZ / pdb_00001xhz
Title : Phi29 DNA polymerase, orthorhombic crystal form, ssDNA complex
Authors : Kamtekar, S.; Berman, A.J.; Wang, J.; Lazaro, J.M.; de Vega, M.; Blanco, L.; Salas, M.; Steitz, T.A.
Deposited on : 2004-09-21
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:

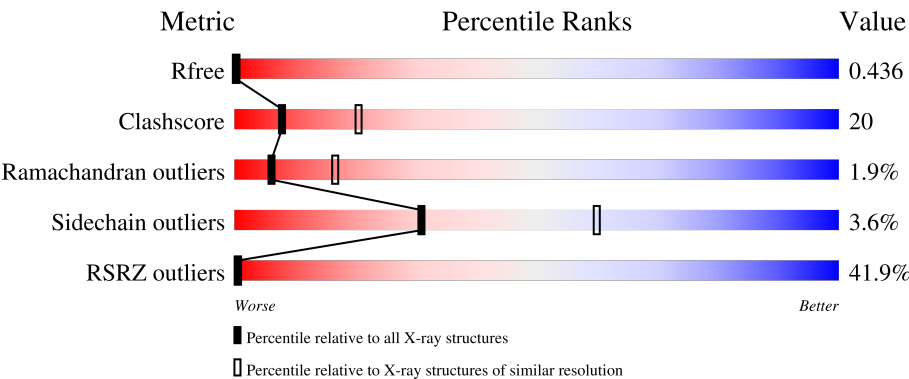
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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	E	5	100% 100%
1	F	5	40% 20% 20% 60%
1	G	5	100% 100%
1	H	5	100% 80% 20%
2	A	575	45% 57% 38% ...

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Mol	Chain	Length	Quality of chain
2	B	575	46% 59% 37% ..
2	C	575	36% 62% 32% ..
2	D	575	38% 64% 33% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19512 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 DNA chain called 5'-D(*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			
1	F	2	Total	C	N	O	P	0	0	0
			37	20	4	12	1			
1	G	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			
1	H	5	Total	C	N	O	P	0	0	0
			97	50	10	33	4			

- Molecule 2 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
2	B	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
2	C	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
2	D	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	ASP	engineered mutation	UNP P03680
A	66	ALA	ASP	engineered mutation	UNP P03680
B	12	ALA	ASP	engineered mutation	UNP P03680
B	66	ALA	ASP	engineered mutation	UNP P03680
C	12	ALA	ASP	engineered mutation	UNP P03680
C	66	ALA	ASP	engineered mutation	UNP P03680
D	12	ALA	ASP	engineered mutation	UNP P03680
D	66	ALA	ASP	engineered mutation	UNP P03680

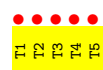
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	O 1	0	0
3	H	2	Total 2	O 2	0	0
3	A	124	Total 124	O 124	0	0
3	B	129	Total 129	O 129	0	0
3	C	140	Total 140	O 140	0	0
3	D	116	Total 116	O 116	0	0

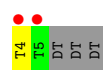
3 Residue-property plots

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.

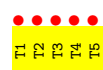
- Molecule 1: 5'-D(*TP*TP*TP*TP*T)-3'



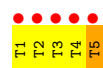
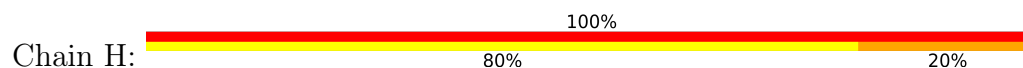
- Molecule 1: 5'-D(*TP*TP*TP*TP*T)-3'



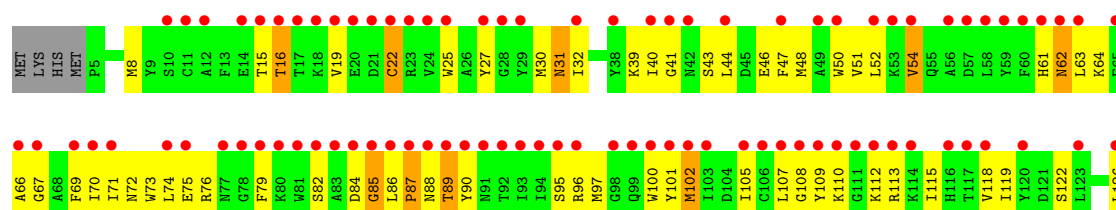
- Molecule 1: 5'-D(*TP*TP*TP*TP*T)-3'

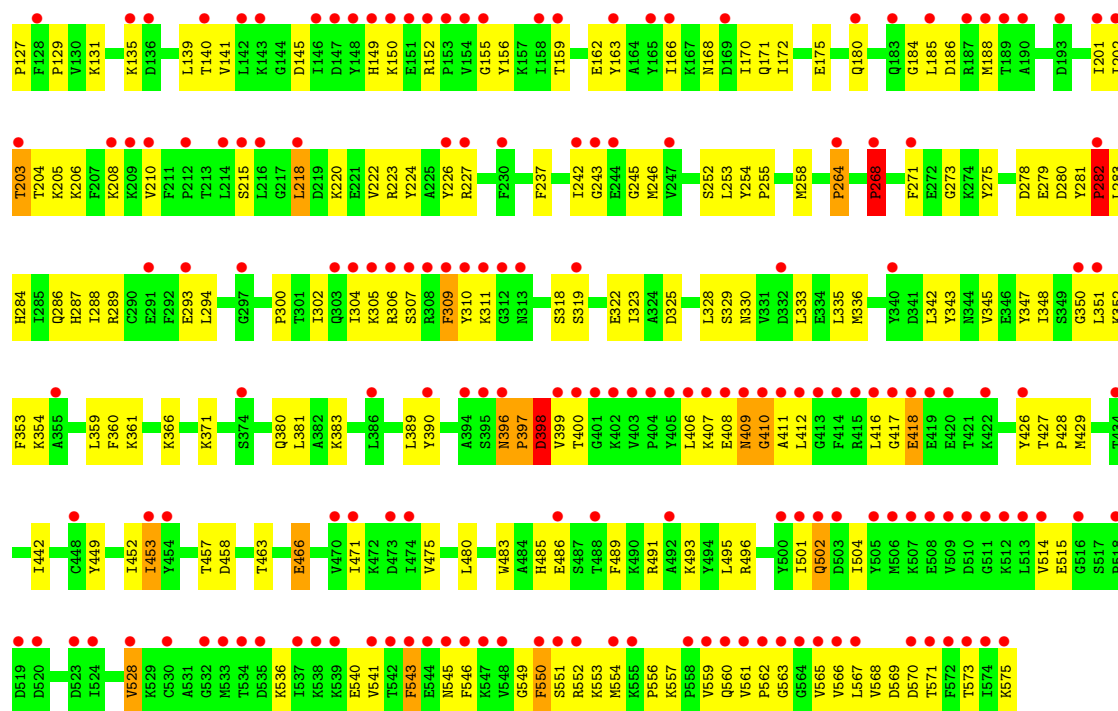


- Molecule 1: 5'-D(*TP*TP*TP*TP*T)-3'

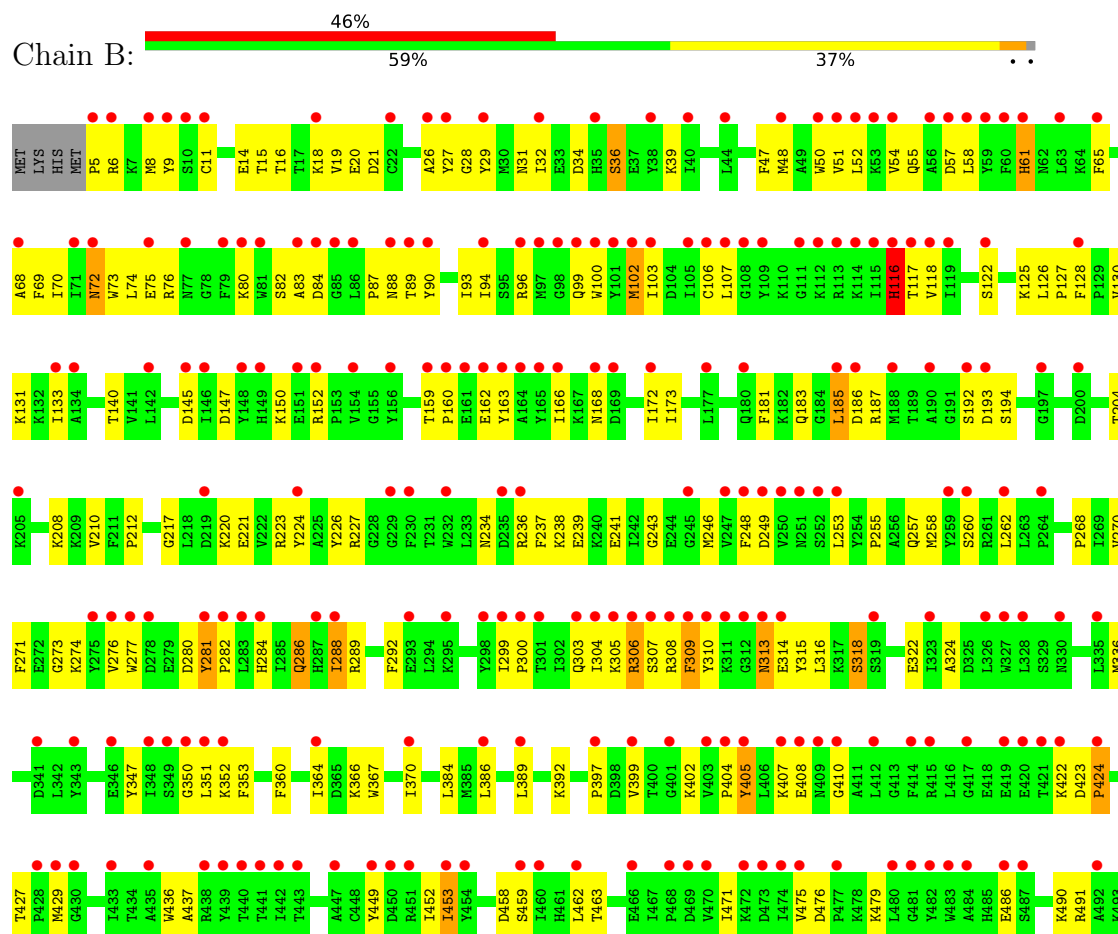


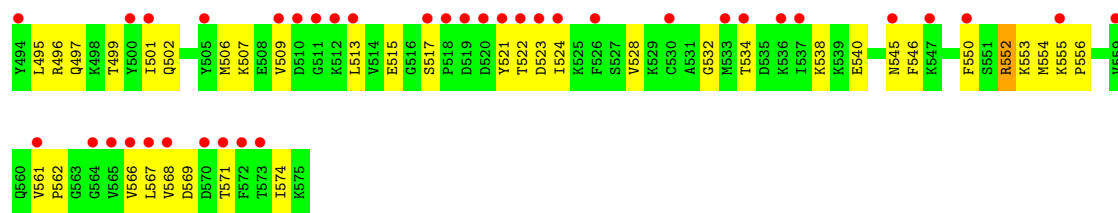
- Molecule 2: DNA polymerase



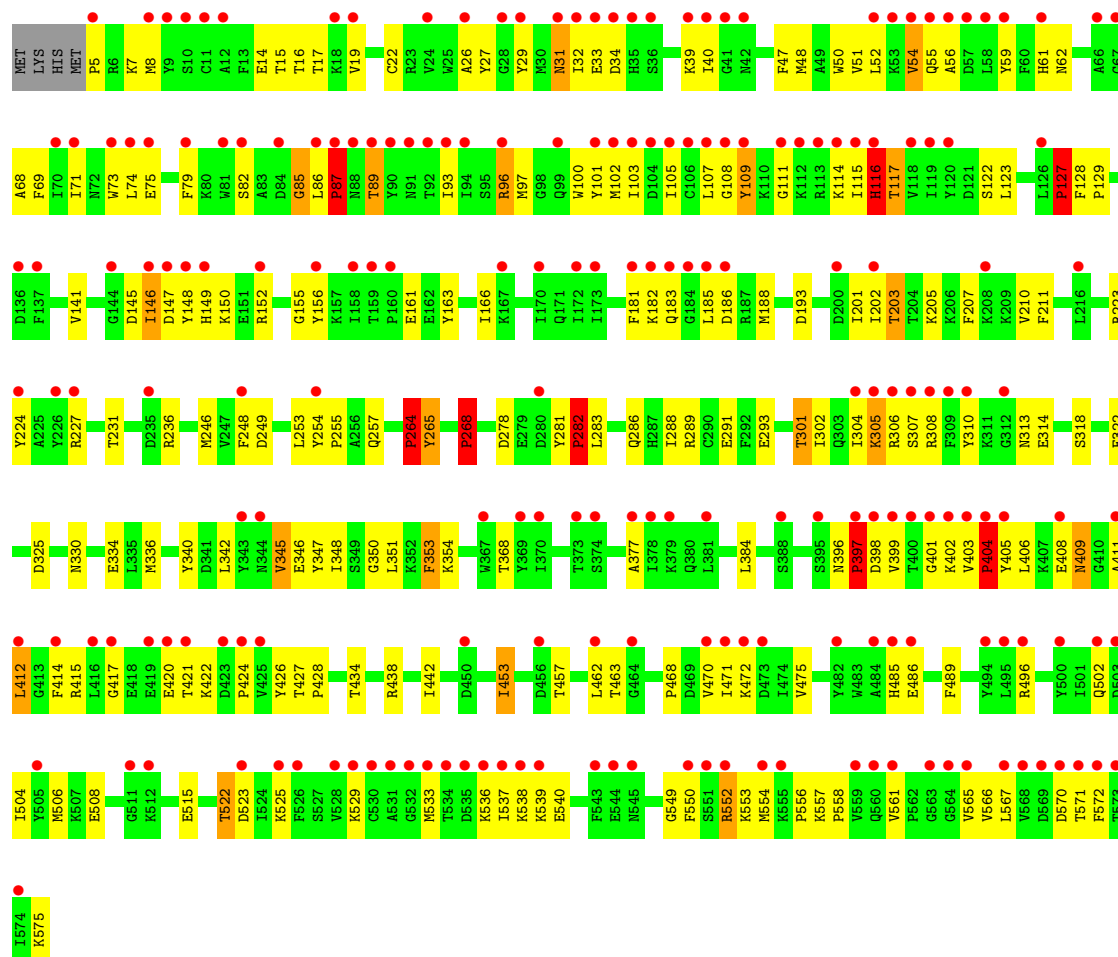


- Molecule 2: DNA polymerase

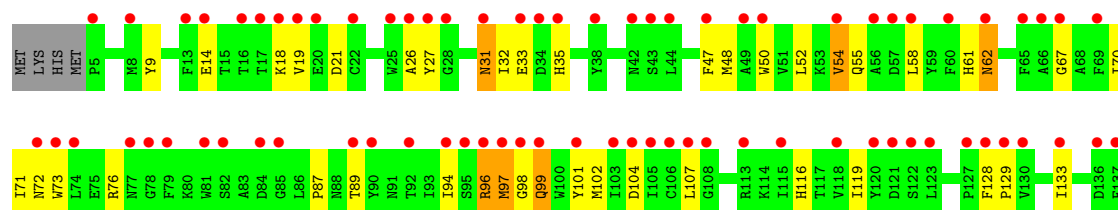
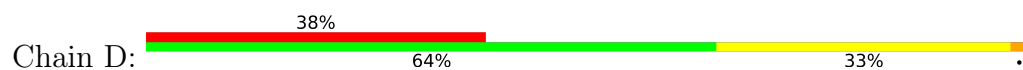


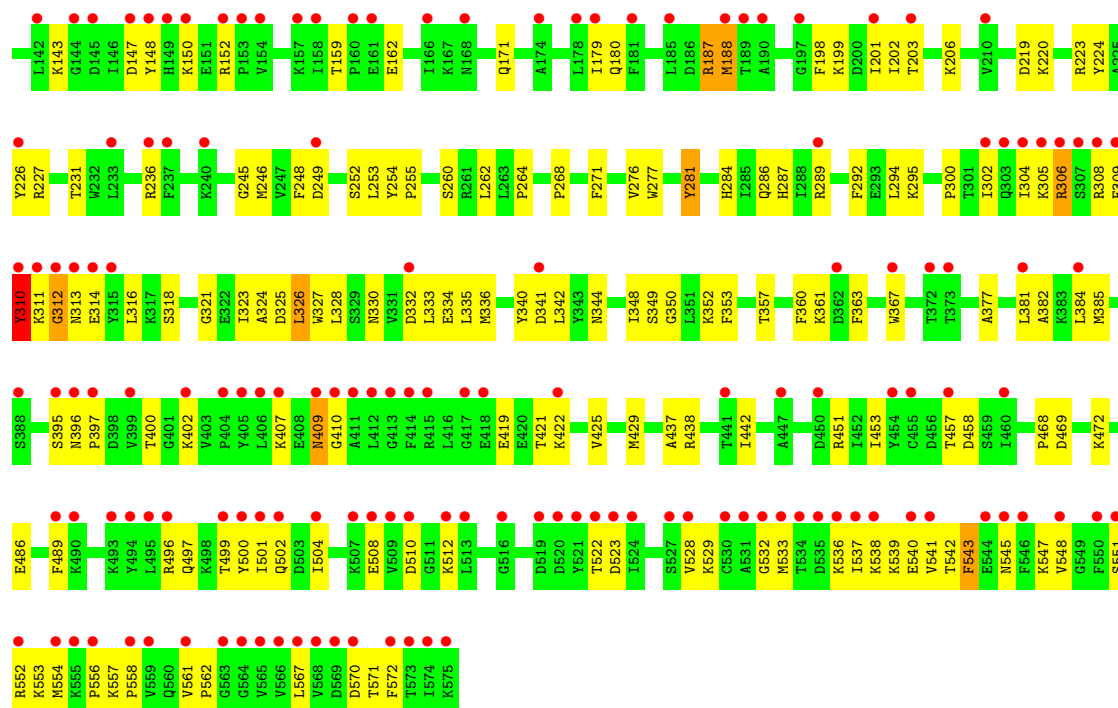


• Molecule 2: DNA polymerase



• Molecule 2: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.66Å 150.40Å 198.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.99-2.70) 99.7 (19.99-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.34Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.268 0.299 , 0.436	Depositor DCC
R_{free} test set	41700 reflections (34.77%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	19512	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	E	0.30	0/106	0.99	0/162
1	F	0.29	0/40	1.08	0/60
1	G	0.48	0/106	1.15	0/162
1	H	0.37	0/106	1.05	1/162 (0.6%)
2	A	0.47	0/4788	1.01	22/6459 (0.3%)
2	B	0.46	0/4788	0.98	18/6459 (0.3%)
2	C	0.53	0/4788	1.09	25/6459 (0.4%)
2	D	0.47	0/4788	0.98	20/6459 (0.3%)
All	All	0.48	0/19510	1.02	86/26382 (0.3%)

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	268	PRO	CA-N-CD	-16.77	88.52	112.00
2	C	264	PRO	CA-N-CD	-14.24	92.07	112.00
2	C	404	PRO	CA-N-CD	-13.91	92.53	112.00
2	A	397	PRO	CA-N-CD	-12.04	95.15	112.00
2	C	127	PRO	CA-N-CD	-11.78	95.51	112.00
2	B	502	GLN	OE1-CD-NE2	-10.46	112.14	122.60
2	C	397	PRO	CA-N-CD	-10.43	97.40	112.00
2	B	453	ILE	CB-CA-C	-10.30	102.95	111.71
2	A	502	GLN	OE1-CD-NE2	-10.23	112.37	122.60
2	C	286	GLN	OE1-CD-NE2	-10.04	112.56	122.60
2	B	286	GLN	OE1-CD-NE2	-9.97	112.63	122.60
2	D	99	GLN	OE1-CD-NE2	-9.93	112.67	122.60
2	C	282	PRO	CA-N-CD	-9.89	98.15	112.00
2	C	453	ILE	CB-CA-C	-9.87	102.06	111.44
2	A	286	GLN	OE1-CD-NE2	-9.75	112.85	122.60
2	D	286	GLN	OE1-CD-NE2	-9.68	112.92	122.60
2	C	502	GLN	OE1-CD-NE2	-9.41	113.19	122.60
2	A	282	PRO	CA-N-CD	-9.30	98.98	112.00
2	D	55	GLN	OE1-CD-NE2	-9.06	113.54	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	264	PRO	CA-N-CD	-8.62	99.92	112.00
2	C	111	GLY	N-CA-C	-8.42	103.93	111.67
2	A	268	PRO	CA-N-CD	-7.89	100.96	112.00
2	A	453	ILE	CB-CA-C	-7.77	104.14	111.05
2	A	54	VAL	N-CA-C	7.76	118.54	110.62
2	D	281	TYR	CA-C-N	7.67	127.31	119.56
2	D	281	TYR	C-N-CA	7.67	127.31	119.56
2	D	314	GLU	N-CA-C	7.66	120.89	110.55
2	C	87	PRO	CA-N-CD	-7.57	101.40	112.00
2	C	54	VAL	N-CA-C	7.30	118.07	110.62
2	C	286	GLN	CG-CD-NE2	7.20	127.20	116.40
2	B	423	ASP	CA-C-N	7.20	128.84	119.84
2	B	423	ASP	C-N-CA	7.20	128.84	119.84
2	B	286	GLN	CG-CD-NE2	7.19	127.19	116.40
2	B	502	GLN	CG-CD-NE2	7.11	127.06	116.40
2	D	99	GLN	CG-CD-NE2	7.10	127.05	116.40
2	B	61	HIS	CA-CB-CG	-7.07	106.73	113.80
2	D	453	ILE	CB-CA-C	-6.92	104.87	111.44
2	B	116	HIS	N-CA-C	6.83	117.29	108.34
2	D	286	GLN	CG-CD-NE2	6.75	126.53	116.40
2	A	126	LEU	CA-C-N	6.75	128.28	119.84
2	A	126	LEU	C-N-CA	6.75	128.28	119.84
2	A	502	GLN	CG-CD-NE2	6.67	126.40	116.40
2	C	502	GLN	CG-CD-NE2	6.63	126.34	116.40
2	A	286	GLN	CG-CD-NE2	6.34	125.91	116.40
2	A	543	PHE	N-CA-C	6.32	118.17	111.28
2	A	307	SER	N-CA-C	6.30	120.05	111.17
2	C	201	ILE	N-CA-C	6.09	116.73	110.82
2	A	410	GLY	N-CA-C	-6.08	106.69	115.27
2	C	396	ASN	CA-C-N	6.03	127.37	119.84
2	C	396	ASN	C-N-CA	6.03	127.37	119.84
2	D	55	GLN	CG-CD-NE2	6.01	125.42	116.40
2	B	102	MET	N-CA-C	6.01	118.25	108.76
2	A	398	ASP	CA-CB-CG	6.00	118.60	112.60
2	D	361	LYS	N-CA-C	6.00	118.31	111.11
2	B	309	PHE	N-CA-C	-5.94	104.47	113.51
2	C	268	PRO	CB-CA-C	-5.93	103.32	111.21
2	D	334	GLU	N-CA-C	-5.90	104.85	111.28
2	B	36	SER	N-CA-C	-5.84	106.31	113.50
2	D	382	ALA	N-CA-C	-5.83	105.00	111.36
2	D	396	ASN	CA-C-N	5.78	125.48	119.82
2	D	396	ASN	C-N-CA	5.78	125.48	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	326	LEU	N-CA-C	5.73	118.80	109.06
2	C	442	ILE	N-CA-C	5.71	116.44	110.62
2	C	116	HIS	N-CA-C	5.64	118.08	109.95
2	C	345	VAL	N-CA-C	5.64	116.89	108.54
2	B	126	LEU	CA-C-N	5.59	126.83	119.84
2	B	126	LEU	C-N-CA	5.59	126.83	119.84
1	H	5	DT	C2'-C3'-O3'	-5.54	103.18	111.50
2	C	302	ILE	N-CA-C	5.51	116.70	108.54
2	D	264	PRO	N-CA-C	5.41	119.53	111.41
2	B	281	TYR	CA-C-N	5.38	125.20	119.28
2	B	281	TYR	C-N-CA	5.38	125.20	119.28
2	B	299	ILE	CA-C-N	5.37	125.53	119.90
2	B	299	ILE	C-N-CA	5.37	125.53	119.90
2	A	329	SER	N-CA-C	-5.30	103.53	110.53
2	D	102	MET	N-CA-C	5.30	117.14	108.55
2	A	354	LYS	N-CA-C	-5.26	102.69	110.48
2	C	368	THR	N-CA-C	-5.25	105.64	111.36
2	C	377	ALA	N-CA-C	5.18	117.32	111.11
2	A	396	ASN	CA-C-N	5.16	124.61	119.24
2	A	396	ASN	C-N-CA	5.16	124.61	119.24
2	D	96	ARG	N-CA-C	-5.12	105.61	111.14
2	D	543	PHE	N-CA-C	-5.04	103.83	110.43
2	A	361	LYS	N-CA-C	5.04	116.46	111.07
2	A	442	ILE	N-CA-C	5.01	115.62	110.36
2	C	354	LYS	N-CA-C	-5.01	103.44	110.50

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	E	97	0	62	10	0
1	F	37	0	26	1	0
1	G	97	0	62	13	0
1	H	97	0	62	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4668	0	4676	206	0
2	B	4668	0	4676	167	0
2	C	4668	0	4676	206	0
2	D	4668	0	4676	165	0
3	A	124	0	0	4	0
3	B	129	0	0	6	0
3	C	140	0	0	2	0
3	D	116	0	0	5	0
3	G	1	0	0	0	0
3	H	2	0	0	0	0
All	All	19512	0	18916	751	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 20.

All (751) 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)
2:A:264:PRO:HD3	2:A:283:LEU:CD1	1.41	1.47
2:A:264:PRO:CD	2:A:283:LEU:HD12	1.60	1.28
2:A:264:PRO:CD	2:A:283:LEU:CD1	2.18	1.18
1:G:3:DT:H5'	2:C:129:PRO:HG3	1.24	1.13
2:B:453:ILE:HD11	2:B:463:THR:HG23	1.20	1.12
1:H:3:DT:H5'	2:D:129:PRO:HG3	1.28	1.10
1:E:3:DT:H5'	2:A:129:PRO:HG3	1.27	1.10
2:C:434:THR:HG22	2:C:438:ARG:NH1	1.68	1.09
2:C:404:PRO:HD3	2:C:414:PHE:HD2	1.19	1.03
1:H:1:DT:H3'	1:H:2:DT:H5'	1.39	1.02
2:A:86:LEU:O	2:A:89:THR:HB	1.62	0.98
2:C:87:PRO:HG3	2:C:108:GLY:HA2	1.44	0.98
2:A:52:LEU:HD22	2:A:107:LEU:HD21	1.42	0.97
2:C:278:ASP:O	2:C:282:PRO:HD3	1.64	0.96
2:A:82:SER:HB3	2:A:89:THR:HG23	1.46	0.95
2:A:323:ILE:HD12	2:B:307:SER:HB3	1.48	0.95
1:H:4:DT:H4'	1:H:4:DT:OP1	1.67	0.93
2:C:96:ARG:HH11	2:C:96:ARG:HB2	1.34	0.92
2:D:306:ARG:H	2:D:311:LYS:HD3	1.33	0.92
2:C:404:PRO:HD3	2:C:414:PHE:CD2	2.05	0.92
2:C:55:GLN:HE21	2:C:115:ILE:HG23	1.35	0.92
2:C:97:MET:HE1	2:C:308:ARG:HB3	1.50	0.91
2:D:311:LYS:HG3	2:D:312:GLY:H	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:ARG:HH11	2:C:96:ARG:CB	1.82	0.91
2:C:288:ILE:HD11	2:C:345:VAL:HG13	1.54	0.90
2:C:96:ARG:HB2	2:C:96:ARG:NH1	1.87	0.89
2:C:289:ARG:HG3	2:C:348:ILE:HD11	1.52	0.89
2:D:304:ILE:HB	2:D:309:PHE:HE1	1.38	0.89
2:C:522:THR:HG22	2:C:523:ASP:OD2	1.72	0.88
2:C:223:ARG:NH2	2:C:397:PRO:HG2	1.87	0.88
1:G:1:DT:H3'	1:G:2:DT:H5'	1.54	0.87
2:D:333:LEU:HD12	2:D:336:MET:HE2	1.58	0.86
2:C:404:PRO:HG3	2:C:414:PHE:CE2	2.11	0.86
2:A:398:ASP:OD1	2:A:398:ASP:O	1.94	0.85
2:A:268:PRO:HG3	2:A:353:PHE:CE2	2.12	0.84
2:A:15:THR:HG22	2:A:16:THR:N	1.93	0.83
2:C:85:GLY:HA3	2:C:114:LYS:HZ3	1.44	0.83
2:D:19:VAL:O	2:D:561:VAL:HG11	1.79	0.83
2:D:306:ARG:N	2:D:311:LYS:HD3	1.93	0.82
2:B:553:LYS:HA	2:B:571:THR:HA	1.62	0.82
2:A:220:LYS:HE2	2:A:224:TYR:OH	1.81	0.80
2:A:86:LEU:HB2	2:A:89:THR:OG1	1.79	0.80
2:D:305:LYS:HA	2:D:311:LYS:CB	2.13	0.79
2:B:471:ILE:O	2:B:475:VAL:HG23	1.82	0.79
2:C:264:PRO:HD3	2:C:283:LEU:HD12	1.64	0.79
2:A:30:MET:HB2	2:A:170:ILE:HD12	1.63	0.79
2:B:55:GLN:HA	2:B:116:HIS:O	1.83	0.79
2:A:264:PRO:HD3	2:A:283:LEU:HD12	0.79	0.78
2:A:82:SER:HB3	2:A:89:THR:CG2	2.14	0.78
2:C:264:PRO:HD3	2:C:283:LEU:CD1	2.14	0.78
2:A:278:ASP:O	2:A:282:PRO:HD3	1.82	0.78
2:A:493:LYS:HE2	2:A:495:LEU:HD21	1.65	0.78
2:C:434:THR:HG22	2:C:438:ARG:HH12	1.49	0.77
1:E:1:DT:H3'	1:E:2:DT:H5'	1.67	0.77
1:G:4:DT:H4'	1:G:4:DT:OP1	1.85	0.77
2:C:146:ILE:HD12	2:C:146:ILE:H	1.50	0.77
2:B:162:GLU:O	2:B:166:ILE:HG12	1.85	0.77
1:H:1:DT:H3'	1:H:2:DT:C5'	2.16	0.76
2:D:305:LYS:HA	2:D:311:LYS:HB2	1.67	0.76
2:B:183:GLN:HB2	2:B:185:LEU:HD22	1.67	0.76
2:A:101:TYR:HB3	2:A:188:MET:HE3	1.68	0.75
2:B:159:THR:OG1	2:B:162:GLU:HG3	1.87	0.75
2:D:96:ARG:O	2:D:402:LYS:HE3	1.87	0.75
2:A:345:VAL:HB	2:B:322:GLU:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:HIS:O	2:C:123:LEU:HB2	1.86	0.75
2:B:168:ASN:O	2:B:172:ILE:HG12	1.87	0.75
1:G:3:DT:H2''	1:G:4:DT:O5'	1.86	0.74
2:C:289:ARG:HE	2:C:348:ILE:HD11	1.51	0.74
2:C:350:GLY:O	2:C:351:LEU:HD23	1.88	0.74
2:D:409:ASN:N	2:D:409:ASN:HD22	1.83	0.74
2:A:264:PRO:HD3	2:A:283:LEU:HD11	1.65	0.74
2:D:536:LYS:HG2	2:D:554:MET:HE2	1.69	0.74
2:B:31:ASN:HD22	2:B:32:ILE:N	1.86	0.74
2:C:308:ARG:H	2:C:308:ARG:HD2	1.52	0.74
2:D:336:MET:HE3	2:D:342:LEU:HD11	1.70	0.73
2:B:226:TYR:HD2	2:B:306:ARG:HH21	1.36	0.73
2:B:183:GLN:HB2	2:B:185:LEU:CD2	2.18	0.73
2:B:506:MET:HE3	2:B:513:LEU:HB3	1.69	0.73
2:D:48:MET:O	2:D:52:LEU:HG	1.88	0.73
2:A:74:LEU:O	2:A:79:PHE:HB2	1.89	0.73
1:H:1:DT:C3'	1:H:2:DT:H5'	2.18	0.72
2:A:496:ARG:HG3	2:A:496:ARG:HH11	1.55	0.72
2:A:202:ILE:O	2:A:203:THR:HB	1.87	0.72
2:A:204:THR:HG22	2:A:208:LYS:HE2	1.71	0.72
2:B:5:PRO:HG2	2:C:5:PRO:HG3	1.72	0.72
1:H:4:DT:OP1	1:H:4:DT:C4'	2.37	0.71
2:A:264:PRO:CG	2:A:283:LEU:HD12	2.20	0.71
2:B:366:LYS:O	2:B:370:ILE:HG12	1.91	0.71
2:B:304:ILE:HD12	2:B:314:GLU:OE1	1.91	0.71
2:C:301:THR:HB	2:C:340:TYR:HE1	1.56	0.71
2:C:293:GLU:OE2	2:C:318:SER:HB2	1.90	0.71
2:C:85:GLY:HA3	2:C:114:LYS:NZ	2.04	0.70
2:C:223:ARG:HH12	2:C:227:ARG:HH22	1.39	0.70
1:G:1:DT:H3'	1:G:2:DT:C5'	2.20	0.70
2:A:560:GLN:HG2	2:A:565:VAL:HG22	1.73	0.70
2:B:47:PHE:O	2:B:51:VAL:HG23	1.91	0.70
2:C:306:ARG:HD3	2:C:310:TYR:HB3	1.74	0.70
2:A:293:GLU:OE2	2:A:318:SER:HB2	1.91	0.70
2:C:408:GLU:CD	2:C:408:GLU:H	2.00	0.70
2:D:304:ILE:HB	2:D:309:PHE:CE1	2.24	0.70
2:A:15:THR:HG22	2:A:16:THR:H	1.57	0.70
2:D:67:GLY:O	2:D:71:ILE:HG12	1.92	0.69
2:B:14:GLU:HB2	2:B:26:ALA:HB3	1.73	0.69
2:C:202:ILE:O	2:C:203:THR:HB	1.89	0.69
2:D:542:THR:H	2:D:545:ASN:HD22	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:TYR:CZ	2:C:39:LYS:HB3	2.27	0.69
2:D:302:ILE:HD11	2:D:336:MET:SD	2.33	0.69
2:A:87:PRO:HG3	2:A:108:GLY:HA2	1.74	0.69
2:C:453:ILE:HD11	2:C:463:THR:HG23	1.73	0.69
2:D:304:ILE:HD11	2:D:326:LEU:HD21	1.73	0.69
2:A:264:PRO:CD	2:A:283:LEU:HD13	2.21	0.68
2:A:273:GLY:HA2	2:A:347:TYR:O	1.93	0.68
2:C:97:MET:HE1	2:C:308:ARG:CB	2.23	0.68
2:C:71:ILE:HB	2:C:412:LEU:HD11	1.75	0.68
2:A:501:ILE:HG22	2:A:528:VAL:HG13	1.75	0.68
2:B:286:GLN:HG3	2:B:288:ILE:CG2	2.23	0.68
2:B:210:VAL:O	2:B:212:PRO:HD3	1.93	0.68
2:C:399:VAL:HG12	2:C:399:VAL:O	1.91	0.68
1:E:3:DT:H2''	1:E:4:DT:O5'	1.94	0.67
2:D:220:LYS:HE2	2:D:224:TYR:OH	1.94	0.67
2:D:496:ARG:HH11	2:D:496:ARG:HG3	1.58	0.67
2:A:15:THR:HG21	2:A:69:PHE:CZ	2.29	0.67
2:D:289:ARG:HG3	2:D:348:ILE:HD11	1.76	0.67
2:D:143:LYS:HE3	3:D:601:HOH:O	1.95	0.67
2:A:15:THR:CG2	2:A:16:THR:H	2.07	0.67
2:A:15:THR:CG2	2:A:16:THR:N	2.57	0.67
2:C:289:ARG:HG2	2:C:325:ASP:OD1	1.95	0.67
2:A:281:TYR:N	2:A:282:PRO:CD	2.58	0.67
2:A:67:GLY:O	2:A:71:ILE:HG12	1.95	0.66
2:B:130:VAL:HG22	2:B:173:ILE:HD11	1.77	0.66
2:B:289:ARG:HA	2:B:324:ALA:O	1.95	0.66
2:D:311:LYS:CG	2:D:312:GLY:H	2.01	0.66
2:A:61:HIS:HA	2:A:122:SER:OG	1.95	0.66
2:C:52:LEU:HD22	2:C:107:LEU:HD21	1.77	0.66
2:D:561:VAL:CG1	2:D:562:PRO:HD2	2.26	0.66
2:B:220:LYS:HE2	2:B:224:TYR:OH	1.96	0.66
2:A:215:SER:OG	2:A:218:LEU:HB2	1.96	0.65
2:B:50:TRP:CE2	2:B:54:VAL:HG11	2.32	0.65
2:C:434:THR:CG2	2:C:438:ARG:NH1	2.53	0.65
2:B:226:TYR:CD2	2:B:306:ARG:NH2	2.63	0.65
2:C:50:TRP:CE2	2:C:54:VAL:HG11	2.32	0.65
2:A:302:ILE:HD11	2:A:336:MET:SD	2.37	0.65
2:D:31:ASN:C	2:D:31:ASN:HD22	2.05	0.65
2:A:226:TYR:O	2:A:227:ARG:HG3	1.97	0.64
2:B:253:LEU:HD21	2:B:437:ALA:HB1	1.79	0.64
2:C:55:GLN:NE2	2:C:115:ILE:HG23	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:403:VAL:HG23	2:C:417:GLY:HA3	1.78	0.64
2:C:146:ILE:HD12	2:C:146:ILE:N	2.11	0.64
2:A:323:ILE:HD11	2:B:305:LYS:HB2	1.78	0.64
2:A:19:VAL:HG13	2:A:561:VAL:HG11	1.80	0.64
2:B:522:THR:HG22	2:B:523:ASP:OD2	1.96	0.64
2:B:545:ASN:HD21	2:B:550:PHE:HD1	1.45	0.64
2:A:75:GLU:HB3	2:A:406:LEU:HD11	1.78	0.63
2:D:180:GLN:HE21	2:D:381:LEU:HD13	1.62	0.63
2:C:87:PRO:HG3	2:C:108:GLY:CA	2.24	0.63
2:C:264:PRO:O	2:C:265:TYR:HB3	1.98	0.63
2:C:434:THR:HG22	2:C:438:ARG:HH11	1.63	0.63
2:A:203:THR:HG22	2:A:205:LYS:H	1.63	0.63
1:E:4:DT:H4'	1:E:4:DT:OP1	1.99	0.63
2:A:206:LYS:O	2:A:210:VAL:HG23	1.99	0.63
2:D:333:LEU:CD1	2:D:336:MET:HE2	2.27	0.63
2:C:61:HIS:HA	2:C:122:SER:OG	1.99	0.63
2:C:289:ARG:NE	2:C:348:ILE:HD11	2.13	0.62
2:D:542:THR:N	2:D:545:ASN:HD22	1.97	0.62
2:A:252:SER:HA	3:A:690:HOH:O	1.99	0.62
1:H:2:DT:OP1	2:D:532:GLY:N	2.31	0.62
2:A:224:TYR:HA	2:A:305:LYS:NZ	2.14	0.62
2:B:286:GLN:HG3	2:B:288:ILE:HG22	1.81	0.62
2:B:399:VAL:HG21	2:B:422:LYS:HG3	1.80	0.62
2:B:453:ILE:HD11	2:B:463:THR:CG2	2.12	0.62
2:C:55:GLN:HA	2:C:116:HIS:O	1.99	0.62
2:C:404:PRO:HG3	2:C:414:PHE:HE2	1.60	0.62
2:A:131:LYS:O	2:A:135:LYS:HG3	2.00	0.62
2:C:506:MET:HG3	2:C:525:LYS:HB2	1.81	0.62
2:A:150:LYS:O	2:A:152:ARG:HG3	1.99	0.61
2:B:52:LEU:HD22	2:B:107:LEU:HD21	1.81	0.61
2:B:360:PHE:CZ	2:B:429:MET:HE3	2.35	0.61
1:G:4:DT:H5''	1:G:4:DT:H6	1.64	0.61
2:C:31:ASN:C	2:C:31:ASN:HD22	2.08	0.61
2:C:96:ARG:O	2:C:402:LYS:HE3	2.00	0.61
2:C:289:ARG:HE	2:C:348:ILE:CD1	2.13	0.61
2:D:561:VAL:HG12	2:D:562:PRO:HD2	1.81	0.61
2:C:288:ILE:HD11	2:C:345:VAL:CG1	2.30	0.61
2:A:184:GLY:O	2:A:186:ASP:N	2.34	0.61
2:D:249:ASP:CG	2:D:486:GLU:HG3	2.24	0.61
2:B:308:ARG:O	2:B:309:PHE:HB2	2.01	0.61
2:C:31:ASN:ND2	2:C:33:GLU:H	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:LYS:HG3	2:D:312:GLY:N	2.13	0.61
1:H:4:DT:H5''	1:H:4:DT:H6	1.66	0.60
2:A:268:PRO:HG3	2:A:353:PHE:CD2	2.37	0.60
2:A:453:ILE:HD11	2:A:463:THR:CG2	2.31	0.60
2:C:93:ILE:HG12	2:C:102:MET:HE2	1.82	0.60
2:A:15:THR:HG21	2:A:69:PHE:CE2	2.36	0.60
2:D:504:ILE:N	2:D:504:ILE:HD12	2.15	0.60
2:C:31:ASN:HD22	2:C:34:ASP:H	1.48	0.60
2:C:223:ARG:NH1	2:C:227:ARG:HH22	1.99	0.60
2:B:192:SER:HA	2:B:392:LYS:HE3	1.84	0.60
2:B:210:VAL:C	2:B:212:PRO:HD3	2.27	0.60
2:D:19:VAL:HG13	2:D:561:VAL:HG21	1.84	0.60
2:D:543:PHE:C	2:D:545:ASN:H	2.10	0.60
2:B:310:TYR:OH	2:B:314:GLU:HB3	2.01	0.59
2:C:223:ARG:NH2	2:C:424:PRO:HG3	2.17	0.59
2:B:399:VAL:HG12	2:B:399:VAL:O	2.02	0.59
2:D:538:LYS:C	2:D:540:GLU:H	2.09	0.59
2:B:52:LEU:O	2:B:107:LEU:HD11	2.02	0.59
2:C:96:ARG:NH1	2:C:398:ASP:OD1	2.35	0.59
2:A:553:LYS:HA	2:A:571:THR:HA	1.84	0.59
2:C:210:VAL:HG13	2:C:265:TYR:HB2	1.83	0.59
2:C:82:SER:HB3	2:C:89:THR:CG2	2.33	0.59
2:D:50:TRP:CE2	2:D:54:VAL:HG11	2.38	0.59
1:E:1:DT:H3'	1:E:2:DT:C5'	2.31	0.59
2:A:453:ILE:HD11	2:A:463:THR:HG22	1.84	0.59
2:D:305:LYS:O	2:D:306:ARG:HB2	2.03	0.59
2:D:409:ASN:H	2:D:409:ASN:ND2	1.99	0.59
2:A:171:GLN:O	2:A:175:GLU:HG3	2.03	0.59
2:B:495:LEU:HG	2:B:546:PHE:CE2	2.38	0.59
2:D:325:ASP:O	2:D:326:LEU:HD23	2.02	0.59
2:A:284:HIS:CE1	2:A:330:ASN:HB3	2.38	0.59
2:C:48:MET:HE2	2:C:51:VAL:HG21	1.84	0.59
2:A:281:TYR:N	2:A:282:PRO:HD2	2.18	0.58
2:D:409:ASN:N	2:D:409:ASN:ND2	2.49	0.58
2:B:540:GLU:OE2	2:B:552:ARG:HD3	2.04	0.58
2:C:409:ASN:N	2:C:409:ASN:HD22	1.99	0.58
2:D:9:TYR:HB2	2:D:58:LEU:HD22	1.86	0.58
2:D:31:ASN:ND2	2:D:33:GLU:H	2.01	0.58
2:C:305:LYS:HB3	2:D:344:ASN:CG	2.27	0.58
2:D:305:LYS:HA	2:D:311:LYS:HB3	1.86	0.58
2:D:327:TRP:O	2:D:328:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:PRO:HG3	2:C:353:PHE:CE2	2.39	0.58
2:D:504:ILE:HD12	2:D:504:ILE:H	1.68	0.58
2:B:496:ARG:HH11	2:B:496:ARG:HG2	1.68	0.57
2:C:19:VAL:HG13	2:C:561:VAL:HG11	1.86	0.57
2:A:271:PHE:CZ	2:A:275:TYR:HB2	2.39	0.57
2:A:328:LEU:HD12	2:A:333:LEU:HD13	1.86	0.57
2:D:310:TYR:CE1	2:D:316:LEU:HD23	2.39	0.57
2:B:87:PRO:O	2:B:89:THR:HG23	2.04	0.57
2:A:224:TYR:HA	2:A:305:LYS:HZ2	1.68	0.57
1:E:5:DT:C2	2:A:567:LEU:HD12	2.39	0.57
2:A:466:GLU:CD	2:A:466:GLU:H	2.12	0.57
2:B:258:MET:HE1	2:B:389:LEU:HG	1.87	0.57
2:D:147:ASP:O	2:D:152:ARG:NH2	2.37	0.57
2:C:540:GLU:OE1	2:C:552:ARG:HD3	2.05	0.57
2:A:302:ILE:HD11	2:A:336:MET:HG3	1.86	0.57
2:B:5:PRO:HG2	2:C:5:PRO:CG	2.35	0.57
2:B:227:ARG:HD2	2:B:303:GLN:HE21	1.68	0.57
2:A:31:ASN:C	2:A:31:ASN:HD22	2.13	0.56
2:A:536:LYS:HE2	2:A:554:MET:HE2	1.87	0.56
2:D:541:VAL:HA	2:D:545:ASN:ND2	2.20	0.56
2:B:367:TRP:HB2	2:B:386:LEU:HD21	1.87	0.56
2:C:289:ARG:HG3	2:C:348:ILE:CD1	2.29	0.56
2:D:253:LEU:HD21	2:D:437:ALA:HB1	1.86	0.56
2:D:262:LEU:HA	2:D:357:THR:HG22	1.88	0.56
2:C:291:GLU:HG2	2:C:322:GLU:O	2.05	0.56
2:A:416:LEU:HD12	2:A:417:GLY:H	1.70	0.56
2:B:68:ALA:O	2:B:72:ASN:HB2	2.05	0.56
2:D:50:TRP:O	2:D:54:VAL:HG22	2.05	0.56
2:C:306:ARG:HD3	2:C:310:TYR:CB	2.36	0.56
2:C:14:GLU:HB2	2:C:26:ALA:HB3	1.88	0.56
2:B:75:GLU:OE2	2:B:80:LYS:HA	2.06	0.56
2:B:102:MET:HG2	2:B:103:ILE:N	2.20	0.56
2:A:168:ASN:O	2:A:172:ILE:HG13	2.05	0.56
2:C:427:THR:OG1	2:C:428:PRO:HD3	2.05	0.56
2:C:554:MET:O	2:C:556:PRO:HD3	2.05	0.56
2:A:336:MET:HE3	2:A:342:LEU:CD2	2.37	0.55
1:E:1:DT:C3'	1:E:2:DT:H5'	2.36	0.55
2:A:202:ILE:O	2:A:203:THR:CB	2.55	0.55
2:A:258:MET:HE2	2:A:360:PHE:CD2	2.41	0.55
2:C:96:ARG:CB	2:C:96:ARG:NH1	2.55	0.55
2:D:180:GLN:NE2	2:D:381:LEU:HD13	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:294:LEU:HD22	2:A:300:PRO:HG3	1.89	0.55
2:D:407:LYS:HB2	2:D:409:ASN:HD21	1.70	0.55
1:H:5:DT:C2	2:D:567:LEU:HD12	2.42	0.55
2:A:162:GLU:O	2:A:166:ILE:HG13	2.07	0.55
2:A:258:MET:HE2	2:A:360:PHE:CE2	2.42	0.55
2:A:495:LEU:O	2:A:496:ARG:HG3	2.06	0.55
2:C:31:ASN:ND2	2:C:33:GLU:N	2.55	0.55
2:A:159:THR:OG1	2:A:162:GLU:HG3	2.07	0.55
2:D:159:THR:OG1	2:D:162:GLU:HG3	2.07	0.55
2:D:302:ILE:HD11	2:D:336:MET:HG3	1.89	0.55
2:A:253:LEU:HD22	2:A:458:ASP:HB3	1.88	0.55
2:C:31:ASN:ND2	2:C:34:ASP:H	2.04	0.55
2:C:453:ILE:HD11	2:C:463:THR:CG2	2.37	0.55
2:A:287:HIS:HE1	2:A:325:ASP:OD1	1.90	0.55
2:D:409:ASN:HD22	2:D:409:ASN:H	1.49	0.55
2:C:51:VAL:O	2:C:117:THR:HG21	2.07	0.55
2:C:150:LYS:HD3	2:C:152:ARG:NH1	2.22	0.54
2:C:223:ARG:NH2	2:C:424:PRO:CG	2.70	0.54
2:D:31:ASN:HD22	2:D:33:GLU:H	1.56	0.54
2:B:217:GLY:O	2:B:221:GLU:HG3	2.07	0.54
2:C:223:ARG:HH21	2:C:424:PRO:CG	2.20	0.54
2:D:496:ARG:HG3	2:D:496:ARG:NH1	2.23	0.54
2:D:501:ILE:HG22	2:D:528:VAL:HG13	1.89	0.54
2:A:47:PHE:CD2	2:A:48:MET:HE2	2.42	0.54
2:A:410:GLY:O	2:A:562:PRO:HA	2.08	0.54
2:A:350:GLY:O	2:A:351:LEU:HD23	2.08	0.54
2:C:223:ARG:NH2	2:C:397:PRO:CG	2.67	0.54
2:C:289:ARG:CG	2:C:348:ILE:HD11	2.32	0.54
2:A:27:TYR:CE2	2:A:41:GLY:HA3	2.43	0.54
2:B:545:ASN:ND2	2:B:550:PHE:HD1	2.04	0.54
2:C:231:THR:HB	2:C:313:ASN:HD22	1.73	0.54
2:A:471:ILE:HG22	2:A:475:VAL:CG2	2.38	0.54
2:C:420:GLU:O	2:C:421:THR:OG1	2.23	0.54
2:C:489:PHE:HB3	2:C:504:ILE:HD13	1.90	0.54
2:D:14:GLU:HB2	2:D:26:ALA:HB3	1.89	0.54
2:D:397:PRO:HA	2:D:422:LYS:HG2	1.89	0.54
2:B:5:PRO:HG2	2:C:5:PRO:CB	2.37	0.54
2:C:31:ASN:HD22	2:C:33:GLU:N	2.05	0.54
2:A:549:GLY:O	2:A:550:PHE:C	2.50	0.53
2:B:93:ILE:HG13	2:B:102:MET:HE2	1.90	0.53
2:D:253:LEU:HD22	2:D:458:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:246:MET:HE2	2:C:248:PHE:CZ	2.44	0.53
2:D:202:ILE:O	2:D:206:LYS:HB3	2.08	0.53
2:D:554:MET:O	2:D:556:PRO:HD3	2.09	0.53
2:C:101:TYR:HD2	2:C:188:MET:HE3	1.74	0.53
2:C:281:TYR:N	2:C:282:PRO:CD	2.71	0.53
2:C:506:MET:HE2	2:C:525:LYS:HD2	1.91	0.53
2:D:284:HIS:CE1	2:D:330:ASN:HB3	2.44	0.53
2:B:424:PRO:HB3	2:B:427:THR:HG23	1.91	0.53
2:A:501:ILE:HG23	2:A:546:PHE:CE2	2.44	0.53
2:B:501:ILE:HG22	2:B:528:VAL:HG22	1.90	0.53
2:C:538:LYS:C	2:C:540:GLU:H	2.17	0.53
2:D:500:TYR:CZ	2:D:529:LYS:HG3	2.44	0.53
2:A:97:MET:HA	2:A:97:MET:HE2	1.91	0.52
2:A:203:THR:HG22	2:A:205:LYS:N	2.23	0.52
2:A:289:ARG:NH2	2:B:309:PHE:HB3	2.25	0.52
2:B:253:LEU:O	2:B:257:GLN:HG2	2.10	0.52
2:D:202:ILE:HB	2:D:206:LYS:HD3	1.92	0.52
2:B:160:PRO:O	2:B:163:TYR:HB3	2.10	0.52
2:B:550:PHE:HB3	2:B:574:ILE:HD12	1.91	0.52
2:D:295:LYS:HE3	2:D:340:TYR:O	2.09	0.52
2:C:421:THR:HG22	2:C:422:LYS:N	2.24	0.52
2:B:31:ASN:HD22	2:B:31:ASN:C	2.13	0.52
2:A:407:LYS:O	2:A:409:ASN:N	2.42	0.52
2:B:140:THR:O	2:B:172:ILE:HD11	2.09	0.52
2:C:31:ASN:HD21	2:C:33:GLU:HB2	1.74	0.52
2:D:101:TYR:HB3	2:D:188:MET:HE3	1.92	0.52
2:D:179:ILE:HD12	2:D:377:ALA:HB1	1.92	0.52
2:C:185:LEU:HD22	2:C:193:ASP:HB3	1.91	0.52
2:D:311:LYS:O	2:D:313:ASN:N	2.43	0.52
2:B:236:ARG:NH1	3:B:601:HOH:O	2.42	0.52
2:C:50:TRP:CZ2	2:C:54:VAL:HG11	2.44	0.52
2:C:434:THR:CG2	2:C:438:ARG:HH12	2.20	0.52
2:A:31:ASN:HD22	2:A:32:ILE:N	2.08	0.52
2:A:549:GLY:O	2:A:573:THR:HG23	2.10	0.52
2:A:62:ASN:O	2:A:63:LEU:C	2.53	0.51
2:B:271:PHE:CZ	2:B:350:GLY:HA3	2.45	0.51
2:B:281:TYR:HB3	2:B:352:LYS:HB3	1.93	0.51
2:C:399:VAL:O	2:C:399:VAL:CG1	2.58	0.51
2:D:451:ARG:NH1	2:D:468:PRO:HG3	2.25	0.51
2:A:86:LEU:C	2:A:89:THR:HB	2.33	0.51
2:C:405:TYR:CE2	2:C:415:ARG:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:PHE:O	2:D:201:ILE:HG22	2.11	0.51
2:A:180:GLN:HE21	2:A:381:LEU:HD22	1.75	0.51
2:A:502:GLN:HB2	2:A:504:ILE:HD11	1.93	0.51
2:B:51:VAL:HG13	2:B:117:THR:HG21	1.93	0.51
2:B:515:GLU:H	2:B:515:GLU:CD	2.19	0.51
2:A:223:ARG:HG2	2:A:427:THR:HG21	1.92	0.51
2:C:305:LYS:HD3	2:D:344:ASN:ND2	2.25	0.51
2:A:222:VAL:HG11	2:A:428:PRO:HG3	1.91	0.51
2:A:79:PHE:CE2	2:A:88:ASN:HA	2.45	0.51
2:A:71:ILE:HG23	2:A:90:TYR:OH	2.11	0.51
2:B:257:GLN:OE1	2:B:436:TRP:HB3	2.11	0.51
2:D:281:TYR:HB3	2:D:352:LYS:HB3	1.91	0.51
2:D:469:ASP:HA	2:D:472:LYS:HG3	1.92	0.51
2:D:538:LYS:O	2:D:540:GLU:N	2.44	0.51
2:A:25:TRP:CD2	2:A:152:ARG:HD3	2.46	0.51
2:A:541:VAL:HG22	2:A:550:PHE:CZ	2.45	0.51
2:C:350:GLY:C	2:C:351:LEU:HD23	2.35	0.51
2:C:468:PRO:O	2:C:472:LYS:HG3	2.10	0.51
2:A:201:ILE:HD11	2:A:366:LYS:HD3	1.93	0.51
2:B:9:TYR:HB2	2:B:58:LEU:HD22	1.93	0.51
2:B:360:PHE:O	2:B:364:ILE:HG12	2.11	0.51
2:C:223:ARG:NH1	2:C:227:ARG:NH2	2.59	0.51
2:C:540:GLU:OE2	2:C:554:MET:SD	2.68	0.51
2:D:48:MET:HG3	2:D:73:TRP:CD2	2.46	0.51
2:A:74:LEU:HD21	2:A:105:ILE:HD13	1.93	0.50
2:A:264:PRO:HD2	2:A:283:LEU:CD1	2.32	0.50
2:B:226:TYR:HD2	2:B:306:ARG:NH2	2.02	0.50
2:C:146:ILE:HG22	2:C:147:ASP:N	2.26	0.50
2:D:50:TRP:CZ2	2:D:54:VAL:HG11	2.45	0.50
2:C:47:PHE:O	2:C:51:VAL:HG23	2.11	0.50
2:C:249:ASP:HB2	2:C:486:GLU:HG2	1.92	0.50
2:A:8:MET:HB3	2:A:32:ILE:HD12	1.94	0.50
2:A:471:ILE:HG22	2:A:475:VAL:HG23	1.91	0.50
2:A:96:ARG:HB2	2:A:400:THR:O	2.10	0.50
2:D:52:LEU:O	2:D:107:LEU:CD1	2.60	0.50
2:D:70:ILE:HD13	2:D:119:ILE:HD13	1.93	0.50
2:D:499:THR:HA	2:D:529:LYS:O	2.11	0.50
2:B:274:LYS:HE2	3:B:631:HOH:O	2.12	0.50
2:C:31:ASN:C	2:C:31:ASN:ND2	2.69	0.50
2:C:161:GLU:HB2	3:C:603:HOH:O	2.11	0.50
2:C:506:MET:CG	2:C:525:LYS:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:86:LEU:HB2	2:A:89:THR:CB	2.40	0.50
2:C:75:GLU:OE1	2:C:75:GLU:HA	2.11	0.50
2:C:146:ILE:H	2:C:146:ILE:CD1	2.22	0.50
2:C:353:PHE:CD1	2:C:353:PHE:N	2.80	0.50
2:B:234:ASN:OD1	2:B:236:ARG:HG2	2.12	0.50
2:C:304:ILE:O	2:C:306:ARG:N	2.45	0.49
2:D:542:THR:OG1	2:D:545:ASN:HB3	2.12	0.49
1:G:5:DT:H5'	2:C:14:GLU:OE1	2.12	0.49
2:C:97:MET:CE	2:C:308:ARG:HB3	2.32	0.49
2:C:202:ILE:O	2:C:203:THR:CB	2.59	0.49
2:B:147:ASP:OD2	2:B:150:LYS:HE3	2.11	0.49
2:C:404:PRO:CD	2:C:414:PHE:CD2	2.88	0.49
2:A:281:TYR:HB3	2:A:352:LYS:HB3	1.94	0.49
2:C:508:GLU:HB2	2:C:522:THR:HG21	1.94	0.49
2:D:150:LYS:HD3	2:D:152:ARG:HH12	1.76	0.49
2:A:279:GLU:O	2:A:282:PRO:CD	2.61	0.49
2:B:6:ARG:HH22	2:B:118:VAL:HG23	1.78	0.49
2:C:86:LEU:O	2:C:89:THR:HG22	2.12	0.49
2:C:203:THR:HG22	2:C:205:LYS:N	2.28	0.49
2:B:273:GLY:HA2	2:B:347:TYR:O	2.13	0.49
2:B:476:ASP:OD2	2:B:479:LYS:HE3	2.12	0.49
1:G:1:DT:C3'	1:G:2:DT:H5'	2.35	0.49
2:A:496:ARG:HG3	2:A:496:ARG:NH1	2.22	0.49
2:C:336:MET:HE2	2:C:342:LEU:HD21	1.93	0.49
2:D:31:ASN:HD22	2:D:32:ILE:N	2.10	0.49
2:D:245:GLY:HA3	2:D:489:PHE:CZ	2.48	0.49
2:D:553:LYS:C	2:D:554:MET:HG3	2.38	0.49
2:B:227:ARG:HG2	2:B:227:ARG:HH11	1.78	0.49
2:C:336:MET:HE2	2:C:342:LEU:CD2	2.43	0.49
2:A:8:MET:CB	2:A:32:ILE:HD12	2.43	0.48
2:C:68:ALA:CB	2:C:565:VAL:HG23	2.42	0.48
2:D:268:PRO:HG3	2:D:353:PHE:CE2	2.48	0.48
2:D:538:LYS:C	2:D:540:GLU:N	2.71	0.48
2:D:561:VAL:HG12	2:D:562:PRO:CD	2.43	0.48
2:A:245:GLY:HA3	2:A:489:PHE:CZ	2.48	0.48
2:C:74:LEU:HD11	2:C:105:ILE:CD1	2.43	0.48
2:C:570:ASP:OD1	2:C:571:THR:N	2.46	0.48
2:A:557:LYS:O	2:A:559:VAL:HG23	2.13	0.48
2:B:246:MET:HE2	2:B:248:PHE:CZ	2.49	0.48
2:C:281:TYR:N	2:C:282:PRO:HD2	2.29	0.48
2:C:409:ASN:N	2:C:409:ASN:ND2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:410:GLY:O	2:D:562:PRO:HA	2.13	0.48
2:D:502:GLN:HB2	2:D:504:ILE:HD11	1.95	0.48
2:A:100:TRP:N	2:A:100:TRP:CD1	2.81	0.48
2:A:400:THR:HG23	2:A:418:GLU:O	2.13	0.48
2:B:532:GLY:O	2:B:555:LYS:HE2	2.13	0.48
2:C:307:SER:HG	2:C:310:TYR:HD1	1.59	0.48
2:D:304:ILE:O	2:D:311:LYS:HB3	2.14	0.48
2:B:522:THR:HG22	2:B:523:ASP:CG	2.37	0.48
2:C:181:PHE:C	2:C:183:GLN:H	2.22	0.48
2:A:96:ARG:O	2:A:97:MET:HE2	2.14	0.48
2:B:18:LYS:HB2	2:B:21:ASP:HB3	1.96	0.48
2:D:367:TRP:CE2	2:D:385:MET:HE2	2.48	0.48
1:G:4:DT:H1'	2:C:62:ASN:HD22	1.79	0.48
2:C:7:LYS:O	2:C:56:ALA:HB1	2.14	0.48
2:C:82:SER:HB3	2:C:89:THR:HG23	1.94	0.48
2:A:252:SER:HB2	2:A:480:LEU:HD12	1.95	0.48
2:A:360:PHE:CZ	2:A:429:MET:HE3	2.48	0.48
2:D:252:SER:HA	3:D:629:HOH:O	2.14	0.48
2:A:39:LYS:HG3	2:A:40:ILE:N	2.27	0.48
2:A:40:ILE:HD12	2:A:163:TYR:CE1	2.47	0.48
2:A:258:MET:HE1	2:A:389:LEU:HG	1.96	0.48
2:A:380:GLN:HE22	2:A:383:LYS:NZ	2.12	0.48
2:B:255:PRO:HD3	3:B:612:HOH:O	2.13	0.48
2:C:22:CYS:SG	2:C:566:VAL:HG23	2.54	0.48
2:A:304:ILE:O	2:A:305:LYS:C	2.57	0.47
2:A:399:VAL:HG12	2:A:399:VAL:O	2.14	0.47
2:C:203:THR:HG22	2:C:205:LYS:H	1.79	0.47
2:C:330:ASN:O	2:C:334:GLU:HG2	2.13	0.47
2:C:406:LEU:HD12	2:C:411:ALA:O	2.14	0.47
2:C:453:ILE:HD11	2:C:463:THR:N	2.29	0.47
2:D:150:LYS:HD3	2:D:152:ARG:NH1	2.29	0.47
2:D:302:ILE:HD11	2:D:336:MET:CG	2.44	0.47
2:D:561:VAL:CG1	2:D:562:PRO:CD	2.92	0.47
2:B:300:PRO:HB2	2:B:315:TYR:HB2	1.97	0.47
2:C:470:VAL:HG23	2:C:471:ILE:HG23	1.95	0.47
2:A:61:HIS:O	2:A:62:ASN:CB	2.62	0.47
2:D:540:GLU:OE2	2:D:554:MET:HE1	2.13	0.47
2:B:11:CYS:HA	2:B:28:GLY:O	2.14	0.47
2:B:268:PRO:HG3	2:B:353:PHE:CE2	2.49	0.47
2:C:207:PHE:CE1	2:C:211:PHE:HD1	2.33	0.47
1:G:4:DT:C1'	2:C:62:ASN:HD22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:302:ILE:HD11	2:A:336:MET:CG	2.45	0.47
2:D:561:VAL:HG13	2:D:562:PRO:HD2	1.95	0.47
2:B:94:ILE:HG23	2:B:100:TRP:CD1	2.50	0.47
2:B:303:GLN:NE2	3:B:639:HOH:O	2.47	0.47
2:C:48:MET:CE	2:C:51:VAL:HG21	2.45	0.47
2:C:223:ARG:HH21	2:C:424:PRO:HG2	1.80	0.47
2:D:27:TYR:C	2:D:27:TYR:CD1	2.92	0.47
2:A:50:TRP:CE2	2:A:54:VAL:HG11	2.50	0.47
2:A:319:SER:HB2	2:A:322:GLU:O	2.14	0.47
2:C:155:GLY:O	2:C:156:TYR:C	2.58	0.47
2:C:403:VAL:CG2	2:C:417:GLY:HA3	2.42	0.47
2:D:551:SER:O	2:D:552:ARG:CG	2.63	0.47
2:B:61:HIS:HA	2:B:122:SER:OG	2.14	0.47
2:A:514:VAL:HG12	2:A:515:GLU:N	2.30	0.46
2:B:5:PRO:HG2	2:C:5:PRO:HB3	1.97	0.46
2:B:73:TRP:CE3	2:B:74:LEU:HD23	2.50	0.46
2:B:73:TRP:HE3	2:B:74:LEU:HD23	1.80	0.46
2:C:288:ILE:HD13	2:C:347:TYR:CE2	2.49	0.46
2:A:466:GLU:CD	2:A:466:GLU:N	2.72	0.46
2:D:254:TYR:HB2	2:D:255:PRO:HD3	1.97	0.46
2:A:66:ALA:O	2:A:70:ILE:HG13	2.15	0.46
2:B:9:TYR:HB2	2:B:58:LEU:CD2	2.45	0.46
2:B:106:CYS:HA	2:B:116:HIS:HB3	1.97	0.46
2:B:238:LYS:HG2	2:B:239:GLU:HG3	1.97	0.46
2:A:52:LEU:CD2	2:A:107:LEU:HD21	2.30	0.46
2:A:75:GLU:HB3	2:A:406:LEU:CD1	2.45	0.46
2:A:246:MET:HE3	2:A:485:HIS:CE1	2.50	0.46
2:D:287:HIS:HE1	2:D:325:ASP:OD1	1.98	0.46
2:A:570:ASP:OD1	2:A:571:THR:N	2.38	0.46
2:B:561:VAL:HG13	2:B:562:PRO:HD2	1.96	0.46
2:B:568:VAL:HG12	2:B:569:ASP:N	2.31	0.46
2:C:86:LEU:O	2:C:87:PRO:C	2.59	0.46
2:D:52:LEU:O	2:D:107:LEU:HD11	2.16	0.46
2:D:76:ARG:NH2	2:D:410:GLY:O	2.49	0.46
2:D:305:LYS:O	2:D:306:ARG:CB	2.63	0.46
2:A:102:MET:HG3	2:A:118:VAL:CG1	2.46	0.46
2:A:281:TYR:HA	2:A:353:PHE:O	2.15	0.46
2:A:336:MET:HE3	2:A:342:LEU:HD21	1.98	0.46
2:B:125:LYS:NZ	2:B:193:ASP:OD2	2.46	0.46
2:B:405:TYR:CE1	2:B:407:LYS:HA	2.50	0.46
2:B:534:THR:O	2:B:538:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:TYR:N	2:C:109:TYR:CD1	2.83	0.46
2:B:187:ARG:HB3	2:B:192:SER:HB2	1.98	0.46
2:D:246:MET:HE2	2:D:248:PHE:CZ	2.51	0.46
2:A:310:TYR:O	2:A:311:LYS:C	2.58	0.46
2:A:556:PRO:HA	2:A:568:VAL:O	2.16	0.46
2:D:333:LEU:CD1	2:D:336:MET:CE	2.93	0.46
2:A:110:LYS:HG3	2:A:115:ILE:HD11	1.98	0.45
2:C:17:THR:HG21	2:C:149:HIS:CE1	2.51	0.45
2:C:254:TYR:HB2	2:C:255:PRO:HD3	1.97	0.45
2:D:570:ASP:OD1	2:D:571:THR:N	2.41	0.45
2:A:43:SER:O	2:A:46:GLU:HB3	2.15	0.45
2:A:101:TYR:O	2:A:102:MET:HB2	2.16	0.45
2:A:280:ASP:C	2:A:282:PRO:HD2	2.41	0.45
2:A:540:GLU:O	2:A:545:ASN:ND2	2.48	0.45
2:A:565:VAL:HG12	2:A:566:VAL:N	2.30	0.45
2:C:268:PRO:HG3	2:C:353:PHE:HE2	1.79	0.45
2:D:397:PRO:O	2:D:421:THR:HA	2.16	0.45
2:D:551:SER:C	2:D:552:ARG:HG3	2.40	0.45
2:A:64:LYS:HA	2:A:100:TRP:CD1	2.51	0.45
2:A:553:LYS:HA	2:A:570:ASP:O	2.16	0.45
1:E:3:DT:H5'	2:A:129:PRO:CG	2.20	0.45
2:A:309:PHE:O	2:A:309:PHE:CD2	2.69	0.45
2:B:55:GLN:CA	2:B:116:HIS:O	2.61	0.45
2:B:237:PHE:CE1	2:B:453:ILE:HD12	2.51	0.45
2:B:486:GLU:O	2:B:515:GLU:HG2	2.16	0.45
2:C:8:MET:HB3	2:C:32:ILE:HD12	1.97	0.45
2:D:226:TYR:O	2:D:227:ARG:HG3	2.16	0.45
2:C:27:TYR:CD2	2:C:47:PHE:HB2	2.51	0.45
2:A:48:MET:HE2	2:A:51:VAL:HG21	1.98	0.45
2:A:252:SER:HB2	2:A:480:LEU:CD1	2.47	0.45
2:C:150:LYS:O	2:C:152:ARG:HG3	2.17	0.45
2:A:76:ARG:NH2	2:A:410:GLY:O	2.50	0.45
2:D:533:MET:HG2	2:D:537:ILE:HB	1.98	0.45
2:A:22:CYS:O	2:A:22:CYS:SG	2.75	0.45
2:C:86:LEU:O	2:C:89:THR:CG2	2.65	0.45
2:B:288:ILE:HD11	2:B:336:MET:HE1	1.99	0.44
2:C:40:ILE:HD12	2:C:166:ILE:CG2	2.47	0.44
2:C:253:LEU:O	2:C:257:GLN:HG2	2.17	0.44
2:C:408:GLU:CD	2:C:408:GLU:N	2.71	0.44
2:A:63:LEU:O	2:A:64:LYS:C	2.60	0.44
2:A:271:PHE:CZ	2:A:350:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:412:LEU:HD23	2:A:560:GLN:NE2	2.32	0.44
2:A:575:LYS:OXT	2:A:575:LYS:HG3	2.17	0.44
2:B:384:LEU:HD23	2:B:384:LEU:HA	1.81	0.44
2:C:496:ARG:NH1	2:C:575:LYS:OXT	2.49	0.44
2:B:48:MET:CE	2:B:70:ILE:HG12	2.47	0.44
2:B:561:VAL:O	2:B:562:PRO:C	2.59	0.44
2:C:109:TYR:CZ	2:C:114:LYS:HG2	2.52	0.44
2:C:289:ARG:HB2	2:C:346:GLU:HB2	2.00	0.44
2:B:150:LYS:O	2:B:152:ARG:HG3	2.17	0.44
2:B:308:ARG:O	2:B:309:PHE:CB	2.65	0.44
2:C:150:LYS:HD3	2:C:152:ARG:HH12	1.82	0.44
2:D:231:THR:HG22	2:D:497:GLN:HB3	1.99	0.44
2:A:264:PRO:CG	2:A:283:LEU:CD1	2.89	0.44
2:A:293:GLU:CD	2:A:318:SER:HB2	2.41	0.44
2:B:292:PHE:CE1	2:B:318:SER:C	2.96	0.44
2:C:307:SER:HA	2:D:323:ILE:HD12	1.99	0.44
2:B:243:GLY:O	2:B:491:ARG:HA	2.18	0.44
2:D:400:THR:OG1	2:D:419:GLU:HA	2.18	0.44
2:A:243:GLY:O	2:A:491:ARG:HA	2.16	0.44
2:B:241:GLU:HG2	3:B:607:HOH:O	2.17	0.44
2:D:96:ARG:C	2:D:98:GLY:H	2.26	0.44
2:D:541:VAL:HA	2:D:545:ASN:HD21	1.80	0.44
2:A:86:LEU:O	2:A:87:PRO:C	2.57	0.44
2:B:96:ARG:O	2:B:402:LYS:HE3	2.18	0.44
2:B:303:GLN:OE1	2:B:313:ASN:ND2	2.51	0.44
2:B:313:ASN:HB2	2:B:497:GLN:OE1	2.18	0.44
2:B:360:PHE:HZ	2:B:429:MET:HE3	1.81	0.44
2:C:289:ARG:NH2	2:D:341:ASP:OD1	2.50	0.44
2:A:288:ILE:HG12	2:A:289:ARG:N	2.32	0.43
2:C:305:LYS:HB3	2:D:344:ASN:OD1	2.18	0.43
2:D:236:ARG:NH1	3:D:619:HOH:O	2.51	0.43
2:A:72:ASN:CG	2:A:563:GLY:C	2.85	0.43
2:C:223:ARG:O	2:C:224:TYR:C	2.60	0.43
2:A:139:LEU:O	2:A:140:THR:C	2.61	0.43
2:B:262:LEU:HB2	3:B:618:HOH:O	2.18	0.43
2:A:245:GLY:HA3	2:A:489:PHE:CE1	2.53	0.43
2:A:551:SER:O	2:A:552:ARG:CD	2.66	0.43
2:C:264:PRO:O	2:C:265:TYR:CB	2.64	0.43
2:B:280:ASP:C	2:B:282:PRO:HD3	2.44	0.43
2:B:8:MET:HA	2:B:57:ASP:O	2.19	0.43
2:C:141:VAL:O	2:C:141:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:510:ASP:C	2:D:512:LYS:H	2.27	0.43
2:D:543:PHE:C	2:D:545:ASN:N	2.76	0.43
2:A:48:MET:HG3	2:A:73:TRP:CD2	2.54	0.43
2:A:70:ILE:HD13	2:A:119:ILE:CD1	2.49	0.43
2:B:48:MET:HE3	2:B:70:ILE:HG12	2.00	0.43
2:C:529:LYS:HD3	2:C:529:LYS:HA	1.74	0.43
1:G:4:DT:OP1	1:G:4:DT:C4'	2.60	0.43
2:A:64:LYS:HG3	2:A:100:TRP:NE1	2.34	0.43
2:A:84:ASP:O	2:A:85:GLY:O	2.36	0.43
2:A:279:GLU:C	2:A:282:PRO:HD3	2.44	0.43
2:C:403:VAL:HG23	2:C:417:GLY:CA	2.48	0.43
2:C:453:ILE:CD1	2:C:462:LEU:C	2.92	0.43
2:C:549:GLY:O	2:C:550:PHE:C	2.62	0.43
2:D:308:ARG:HD2	2:D:308:ARG:HA	1.62	0.43
2:A:475:VAL:HA	2:A:483:TRP:O	2.19	0.43
2:A:545:ASN:OD1	2:A:545:ASN:C	2.61	0.43
2:B:76:ARG:NH2	2:B:410:GLY:O	2.49	0.43
2:B:556:PRO:HA	2:B:568:VAL:O	2.19	0.43
2:C:486:GLU:O	2:C:515:GLU:HG2	2.18	0.43
2:D:226:TYR:C	2:D:227:ARG:HG3	2.44	0.43
2:A:19:VAL:HG23	3:A:579:HOH:O	2.19	0.43
2:C:536:LYS:HE2	2:C:554:MET:CE	2.49	0.43
2:D:128:PHE:HB2	2:D:133:ILE:HG13	2.01	0.43
2:A:19:VAL:CG1	2:A:561:VAL:HG11	2.49	0.42
2:C:100:TRP:CZ3	2:C:103:ILE:HD11	2.54	0.42
2:A:201:ILE:HD11	2:A:366:LYS:CD	2.49	0.42
2:B:82:SER:O	2:B:83:ALA:C	2.61	0.42
2:D:87:PRO:O	2:D:89:THR:HG23	2.19	0.42
2:D:276:VAL:O	2:D:277:TRP:C	2.62	0.42
2:A:310:TYR:OH	2:A:322:GLU:HB2	2.19	0.42
2:A:411:ALA:HA	2:A:562:PRO:HA	2.01	0.42
2:A:566:VAL:HG12	2:A:567:LEU:N	2.35	0.42
2:B:15:THR:HG21	2:B:69:PHE:CZ	2.54	0.42
2:B:31:ASN:HB3	2:B:34:ASP:O	2.19	0.42
2:B:397:PRO:O	2:B:399:VAL:HG23	2.18	0.42
2:C:471:ILE:O	2:C:475:VAL:HG23	2.19	0.42
2:D:508:GLU:HG3	2:D:512:LYS:O	2.19	0.42
2:A:48:MET:CE	2:A:51:VAL:HG21	2.49	0.42
2:B:181:PHE:CE2	2:B:186:ASP:HA	2.54	0.42
2:B:284:HIS:HA	2:B:351:LEU:O	2.18	0.42
2:C:310:TYR:HE1	2:D:289:ARG:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:LYS:HB2	2:D:21:ASP:HB3	2.01	0.42
2:D:219:ASP:O	2:D:223:ARG:HB2	2.20	0.42
1:G:5:DT:H2'	2:C:148:TYR:CD1	2.54	0.42
2:A:254:TYR:HB2	2:A:255:PRO:HD3	2.02	0.42
2:B:507:LYS:HG3	2:B:509:VAL:HG23	1.99	0.42
2:C:59:TYR:HB3	2:C:122:SER:HB3	2.01	0.42
2:D:201:ILE:HD13	2:D:363:PHE:HA	2.02	0.42
2:D:294:LEU:HD22	2:D:300:PRO:HG3	2.01	0.42
2:B:304:ILE:HG12	2:B:316:LEU:HG	2.02	0.42
2:B:517:SER:O	2:B:521:TYR:HB3	2.20	0.42
2:B:566:VAL:HG12	2:B:567:LEU:N	2.34	0.42
2:C:31:ASN:ND2	2:C:34:ASP:N	2.67	0.42
2:D:171:GLN:NE2	3:D:606:HOH:O	2.53	0.42
2:D:289:ARG:HA	2:D:324:ALA:O	2.20	0.42
2:A:110:LYS:HD2	2:A:113:ARG:NH2	2.34	0.42
2:C:71:ILE:HG21	2:C:412:LEU:HD21	2.00	0.42
2:C:227:ARG:C	2:C:434:THR:HG21	2.45	0.42
2:D:50:TRP:NE1	2:D:54:VAL:CG1	2.82	0.42
2:D:547:LYS:HB2	3:D:622:HOH:O	2.19	0.42
2:A:52:LEU:O	2:A:107:LEU:HD11	2.20	0.42
2:B:27:TYR:CD1	2:B:27:TYR:C	2.98	0.42
2:B:50:TRP:NE1	2:B:54:VAL:HG11	2.34	0.42
2:B:248:PHE:O	2:B:459:SER:HA	2.20	0.42
2:B:424:PRO:CB	2:B:427:THR:HG23	2.50	0.42
2:C:453:ILE:CD1	2:C:463:THR:N	2.83	0.42
2:D:187:ARG:HD2	2:D:187:ARG:HA	1.80	0.42
1:E:2:DT:H5''	1:E:2:DT:H6	1.84	0.42
1:H:1:DT:C3'	1:H:2:DT:C5'	2.90	0.42
2:B:281:TYR:HB2	2:B:352:LYS:HD2	2.02	0.42
2:C:40:ILE:HB	2:C:163:TYR:CE1	2.55	0.42
2:B:404:PRO:O	2:B:405:TYR:HB3	2.19	0.42
2:C:100:TRP:HZ3	2:C:103:ILE:HD11	1.85	0.42
1:E:3:DT:C2'	1:E:4:DT:O5'	2.60	0.41
2:B:29:TYR:C	2:B:29:TYR:CD1	2.98	0.41
2:C:236:ARG:NH2	3:C:618:HOH:O	2.52	0.41
2:A:50:TRP:O	2:A:54:VAL:HG22	2.20	0.41
2:A:237:PHE:HD2	2:A:242:ILE:HG21	1.85	0.41
2:D:72:ASN:O	2:D:76:ARG:HG3	2.19	0.41
2:D:94:ILE:HA	2:D:99:GLN:O	2.20	0.41
2:A:289:ARG:CD	2:A:348:ILE:HD11	2.50	0.41
2:C:48:MET:HG3	2:C:73:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:LEU:O	2:C:79:PHE:HB2	2.20	0.41
2:B:204:THR:O	2:B:208:LYS:HG3	2.20	0.41
2:B:286:GLN:CG	2:B:288:ILE:CG2	2.96	0.41
2:D:547:LYS:O	2:D:548:VAL:C	2.63	0.41
1:H:5:DT:H2'	2:D:148:TYR:CD2	2.55	0.41
2:A:108:GLY:C	2:A:109:TYR:CD1	2.98	0.41
2:B:276:VAL:O	2:B:277:TRP:C	2.62	0.41
2:C:15:THR:HG21	2:C:69:PHE:CZ	2.56	0.41
2:D:271:PHE:CZ	2:D:350:GLY:HA3	2.56	0.41
2:D:287:HIS:HB3	2:D:349:SER:O	2.21	0.41
2:A:155:GLY:O	2:A:156:TYR:C	2.63	0.41
2:A:491:ARG:HG3	2:A:543:PHE:CZ	2.55	0.41
2:B:270:VAL:HG12	2:B:271:PHE:N	2.35	0.41
2:B:306:ARG:HB2	2:B:307:SER:H	1.71	0.41
2:B:501:ILE:HG22	2:B:528:VAL:HG13	2.02	0.41
2:D:360:PHE:CZ	2:D:429:MET:HE3	2.54	0.41
2:D:551:SER:HA	2:D:572:PHE:O	2.20	0.41
2:A:95:SER:C	2:A:97:MET:N	2.78	0.41
2:A:226:TYR:C	2:A:227:ARG:HG3	2.45	0.41
2:A:371:LYS:HE3	3:A:637:HOH:O	2.19	0.41
2:B:94:ILE:HA	2:B:99:GLN:O	2.21	0.41
2:B:227:ARG:HD2	2:B:303:GLN:NE2	2.34	0.41
2:B:253:LEU:HD22	2:B:458:ASP:HB3	2.01	0.41
2:B:553:LYS:C	2:B:554:MET:HG3	2.45	0.41
1:H:2:DT:H6	1:H:2:DT:H5''	1.85	0.41
2:B:187:ARG:HB3	2:B:192:SER:CB	2.50	0.41
2:C:223:ARG:NH1	2:C:397:PRO:HD2	2.36	0.41
2:D:35:HIS:N	2:D:35:HIS:CD2	2.88	0.41
2:D:199:LYS:C	2:D:201:ILE:N	2.79	0.41
2:D:304:ILE:HD12	2:D:309:PHE:CE1	2.55	0.41
2:A:44:LEU:CD1	2:A:48:MET:HG2	2.51	0.41
2:A:218:LEU:O	2:A:222:VAL:HG23	2.21	0.41
2:A:449:TYR:O	2:A:452:ILE:HG22	2.20	0.41
2:B:11:CYS:SG	2:B:58:LEU:HB3	2.61	0.41
2:C:533:MET:HE3	2:C:533:MET:HB2	1.72	0.41
2:C:553:LYS:O	2:C:554:MET:HG3	2.21	0.41
2:D:304:ILE:CD1	2:D:326:LEU:HD21	2.45	0.41
1:G:5:DT:C2	2:C:567:LEU:HD12	2.56	0.41
2:A:453:ILE:HD11	2:A:463:THR:HG23	2.02	0.41
2:B:226:TYR:CD2	2:B:226:TYR:C	2.99	0.41
2:B:490:LYS:HD2	2:B:524:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:ASP:CG	2:D:438:ARG:HH21	2.29	0.41
2:A:95:SER:C	2:A:97:MET:H	2.28	0.40
2:B:28:GLY:HA2	2:B:39:LYS:O	2.21	0.40
2:B:34:ASP:CG	2:B:36:SER:HG	2.28	0.40
2:B:496:ARG:NH1	2:B:499:THR:OG1	2.54	0.40
2:B:554:MET:O	2:B:556:PRO:HD3	2.21	0.40
2:D:61:HIS:O	2:D:62:ASN:HB3	2.21	0.40
2:A:486:GLU:O	2:A:515:GLU:HG2	2.20	0.40
2:C:52:LEU:HB3	2:C:107:LEU:HD11	2.02	0.40
2:C:223:ARG:HH21	2:C:424:PRO:HG3	1.81	0.40
2:C:537:ILE:HG21	2:C:572:PHE:CE2	2.56	0.40
2:D:292:PHE:O	2:D:318:SER:HA	2.22	0.40
2:B:90:TYR:CD1	2:B:90:TYR:C	2.99	0.40
2:B:449:TYR:O	2:B:452:ILE:HG22	2.21	0.40
2:C:557:LYS:HA	2:C:558:PRO:HD3	1.92	0.40
2:D:47:PHE:O	2:D:50:TRP:HB3	2.21	0.40
2:D:104:ASP:OD2	2:D:116:HIS:HD2	2.04	0.40
2:D:551:SER:C	2:D:552:ARG:CG	2.94	0.40
2:A:89:THR:CG2	2:A:90:TYR:N	2.83	0.40
2:A:359:LEU:HB2	3:A:688:HOH:O	2.21	0.40
2:B:452:ILE:HA	2:B:462:LEU:HD23	2.01	0.40
2:D:335:LEU:HD21	2:D:442:ILE:HD12	2.03	0.40
2:D:522:THR:C	2:D:523:ASP:OD2	2.64	0.40
1:F:4:DT:O2	2:B:65:PHE:HB2	2.22	0.40
2:A:343:TYR:CE2	2:B:289:ARG:HD3	2.57	0.40
2:A:540:GLU:HB3	2:A:552:ARG:HH12	1.85	0.40
2:B:128:PHE:HB2	2:B:133:ILE:HG13	2.03	0.40
2:B:308:ARG:C	2:B:310:TYR:H	2.29	0.40
2:C:288:ILE:HD12	2:C:346:GLU:O	2.22	0.40
2:C:334:GLU:HA	2:C:334:GLU:OE1	2.20	0.40
2:D:557:LYS:HA	2:D:558:PRO:HD3	1.88	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	
2	A	569/575 (99%)	506 (89%)	47 (8%)	16 (3%)	4	9
2	B	569/575 (99%)	513 (90%)	51 (9%)	5 (1%)	14	35
2	C	569/575 (99%)	518 (91%)	39 (7%)	12 (2%)	5	15
2	D	569/575 (99%)	519 (91%)	39 (7%)	11 (2%)	6	17
All	All	2276/2300 (99%)	2056 (90%)	176 (8%)	44 (2%)	6	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	62	ASN
2	A	85	GLY
2	A	309	PHE
2	A	408	GLU
2	A	185	LEU
2	A	306	ARG
2	A	409	ASN
2	A	418	GLU
2	B	306	ARG
2	B	408	GLU
2	C	85	GLY
2	C	182	LYS
2	D	312	GLY
2	D	395	SER
2	D	539	LYS
2	A	426	TYR
2	A	569	ASP
2	C	117	THR
2	C	305	LYS
2	C	397	PRO
2	D	62	ASN
2	D	97	MET
2	D	310	TYR
2	A	550	PHE
2	C	203	THR
2	C	401	GLY
2	C	426	TYR
2	C	457	THR
2	D	203	THR
2	D	306	ARG

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Mol	Chain	Res	Type
2	D	457	THR
2	A	127	PRO
2	A	457	THR
2	B	127	PRO
2	B	405	TYR
2	C	539	LYS
2	A	102	MET
2	A	112	LYS
2	A	203	THR
2	C	127	PRO
2	D	425	VAL
2	D	321	GLY
2	C	87	PRO
2	B	424	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	502/506 (99%)	484 (96%)	18 (4%)	31	60
2	B	502/506 (99%)	484 (96%)	18 (4%)	31	60
2	C	502/506 (99%)	475 (95%)	27 (5%)	20	45
2	D	502/506 (99%)	493 (98%)	9 (2%)	51	78
All	All	2008/2024 (99%)	1936 (96%)	72 (4%)	31	60

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	16	THR
2	A	22	CYS
2	A	31	ASN
2	A	87	PRO
2	A	89	THR
2	A	141	VAL
2	A	145	ASP

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Mol	Chain	Res	Type
2	A	149	HIS
2	A	218	LEU
2	A	268	PRO
2	A	282	PRO
2	A	335	LEU
2	A	390	TYR
2	A	396	ASN
2	A	397	PRO
2	A	398	ASP
2	A	466	GLU
2	A	528	VAL
2	B	16	THR
2	B	19	VAL
2	B	20	GLU
2	B	72	ASN
2	B	84	ASP
2	B	88	ASN
2	B	116	HIS
2	B	131	LYS
2	B	145	ASP
2	B	185	LEU
2	B	194	SER
2	B	223	ARG
2	B	249	ASP
2	B	260	SER
2	B	288	ILE
2	B	313	ASN
2	B	318	SER
2	B	552	ARG
2	C	16	THR
2	C	31	ASN
2	C	87	PRO
2	C	89	THR
2	C	96	ARG
2	C	109	TYR
2	C	116	HIS
2	C	127	PRO
2	C	128	PHE
2	C	145	ASP
2	C	146	ILE
2	C	186	ASP
2	C	264	PRO

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Mol	Chain	Res	Type
2	C	265	TYR
2	C	268	PRO
2	C	282	PRO
2	C	301	THR
2	C	314	GLU
2	C	353	PHE
2	C	384	LEU
2	C	397	PRO
2	C	404	PRO
2	C	409	ASN
2	C	412	LEU
2	C	485	HIS
2	C	522	THR
2	C	552	ARG
2	D	31	ASN
2	D	54	VAL
2	D	97	MET
2	D	187	ARG
2	D	188	MET
2	D	260	SER
2	D	310	TYR
2	D	384	LEU
2	D	409	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	ASN
2	A	55	GLN
2	A	171	GLN
2	A	180	GLN
2	A	287	HIS
2	A	303	GLN
2	A	380	GLN
2	A	485	HIS
2	B	31	ASN
2	B	99	GLN
2	B	171	GLN
2	B	287	HIS
2	B	303	GLN
2	B	313	ASN
2	B	396	ASN

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Mol	Chain	Res	Type
2	B	545	ASN
2	C	31	ASN
2	C	35	HIS
2	C	55	GLN
2	C	62	ASN
2	C	72	ASN
2	C	116	HIS
2	C	171	GLN
2	C	183	GLN
2	C	313	ASN
2	C	339	HIS
2	C	409	ASN
2	C	502	GLN
2	D	31	ASN
2	D	55	GLN
2	D	171	GLN
2	D	180	GLN
2	D	287	HIS
2	D	396	ASN
2	D	409	ASN
2	D	545	ASN
2	D	560	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	E	5/5 (100%)	5.15	5 (100%) 0 0	98, 113, 125, 129	0
1	F	2/5 (40%)	4.55	2 (100%) 0 0	128, 128, 128, 130	0
1	G	5/5 (100%)	4.35	5 (100%) 0 0	72, 77, 81, 98	0
1	H	5/5 (100%)	4.53	5 (100%) 0 0	65, 76, 100, 112	0
2	A	571/575 (99%)	2.07	259 (45%) 0 0	31, 65, 116, 130	0
2	B	571/575 (99%)	2.00	263 (46%) 0 0	29, 56, 96, 130	0
2	C	571/575 (99%)	1.77	205 (35%) 1 0	25, 54, 110, 130	0
2	D	571/575 (99%)	1.83	221 (38%) 1 0	28, 51, 86, 130	0
All	All	2301/2320 (99%)	1.94	965 (41%) 0 0	25, 56, 111, 130	0

All (965) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	533	MET	7.7
1	E	5	DT	7.4
2	C	572	PHE	6.9
2	C	148	TYR	6.7
2	A	572	PHE	6.6
2	D	19	VAL	6.6
2	D	413	GLY	6.3
2	A	154	VAL	6.3
1	E	4	DT	6.2
2	A	541	VAL	6.2
2	A	533	MET	6.0
2	C	535	ASP	6.0
2	D	572	PHE	6.0
2	D	533	MET	5.9
2	B	106	CYS	5.9
2	A	532	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
2	C	304	ILE	5.6
2	D	534	THR	5.5
2	D	564	GLY	5.5
2	A	396	ASN	5.5
2	B	310	TYR	5.4
2	A	564	GLY	5.4
1	H	1	DT	5.4
2	C	532	GLY	5.3
2	A	85	GLY	5.3
2	D	412	LEU	5.3
1	G	5	DT	5.3
2	A	113	ARG	5.2
2	C	421	THR	5.1
2	A	574	ILE	5.1
2	A	562	PRO	5.0
2	C	184	GLY	5.0
2	D	532	GLY	5.0
2	D	314	GLU	4.9
2	B	148	TYR	4.9
2	D	574	ILE	4.9
2	A	149	HIS	4.9
2	A	70	ILE	4.9
2	A	567	LEU	4.8
2	D	565	VAL	4.8
2	D	566	VAL	4.8
2	A	555	LYS	4.8
2	B	306	ARG	4.8
2	C	57	ASP	4.8
2	A	310	TYR	4.8
2	A	146	ILE	4.7
2	A	508	GLU	4.7
2	D	535	ASP	4.7
2	D	554	MET	4.7
1	H	3	DT	4.7
1	F	4	DT	4.7
1	G	4	DT	4.7
1	E	3	DT	4.6
2	D	530	CYS	4.6
2	A	409	ASN	4.6
2	D	310	TYR	4.6
2	A	417	GLY	4.6
2	C	105	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	309	PHE	4.5
2	A	95	SER	4.5
2	D	148	TYR	4.5
2	B	165	TYR	4.5
2	C	149	HIS	4.5
2	D	85	GLY	4.5
2	A	74	LEU	4.5
2	A	412	LEU	4.4
2	D	570	ASP	4.4
1	F	5	DT	4.4
1	G	2	DT	4.4
2	B	117	THR	4.4
2	C	398	ASP	4.4
1	H	5	DT	4.4
2	C	306	ARG	4.4
2	C	310	TYR	4.3
2	A	56	ALA	4.3
2	C	107	LEU	4.3
2	A	410	GLY	4.3
2	A	14	GLU	4.3
2	B	405	TYR	4.3
1	H	4	DT	4.3
2	A	112	LYS	4.2
2	A	395	SER	4.2
2	A	16	THR	4.2
2	B	307	SER	4.2
2	C	377	ALA	4.2
2	A	311	LYS	4.2
2	A	399	VAL	4.2
2	C	568	VAL	4.2
2	C	87	PRO	4.1
2	A	534	THR	4.1
2	B	568	VAL	4.1
2	C	534	THR	4.1
2	A	563	GLY	4.1
2	A	546	PHE	4.1
2	D	531	ALA	4.1
2	A	473	ASP	4.1
2	D	541	VAL	4.1
2	A	571	THR	4.1
2	D	536	LYS	4.1
2	A	309	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	A	15	THR	4.1
2	C	26	ALA	4.0
2	A	543	PHE	4.0
2	B	421	THR	4.0
2	A	148	TYR	4.0
2	B	10	SER	4.0
2	C	539	LYS	4.0
2	A	405	TYR	4.0
2	C	369	TYR	4.0
2	C	104	ASP	4.0
2	A	150	LYS	4.0
2	A	565	VAL	4.0
2	B	295	LYS	4.0
2	C	118	VAL	4.0
2	D	399	VAL	4.0
2	D	97	MET	4.0
2	A	83	ALA	4.0
2	D	567	LEU	4.0
2	A	505	TYR	4.0
2	D	303	GLN	3.9
2	B	107	LEU	3.9
2	D	414	PHE	3.9
2	D	54	VAL	3.9
1	H	2	DT	3.9
2	A	560	GLN	3.9
2	B	346	GLU	3.9
2	D	312	GLY	3.9
2	B	190	ALA	3.9
2	B	50	TRP	3.9
2	B	276	VAL	3.9
2	C	34	ASP	3.9
2	C	75	GLU	3.9
2	D	304	ILE	3.9
2	A	535	ASP	3.9
2	A	404	PRO	3.8
2	A	180	GLN	3.8
2	C	395	SER	3.8
1	E	1	DT	3.8
2	A	32	ILE	3.8
2	A	561	VAL	3.8
2	A	406	LEU	3.8
1	G	3	DT	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	397	PRO	3.8
2	C	400	THR	3.8
2	D	313	ASN	3.8
2	A	24	VAL	3.8
2	A	566	VAL	3.7
1	E	2	DT	3.7
2	A	189	THR	3.7
2	A	510	ASP	3.7
2	B	35	HIS	3.7
2	D	573	THR	3.7
2	B	304	ILE	3.7
2	D	79	PHE	3.7
2	B	518	PRO	3.7
2	B	115	ILE	3.7
2	D	523	ASP	3.7
2	A	27	TYR	3.7
2	B	319	SER	3.7
2	D	89	THR	3.6
2	C	114	LYS	3.6
2	A	106	CYS	3.6
2	D	190	ALA	3.6
2	A	488	THR	3.6
1	G	1	DT	3.6
2	C	424	PRO	3.6
2	D	309	PHE	3.6
2	A	416	LEU	3.6
2	C	116	HIS	3.6
2	A	516	GLY	3.6
2	B	410	GLY	3.6
2	B	312	GLY	3.6
2	C	404	PRO	3.6
2	B	248	PHE	3.6
2	D	22	CYS	3.6
2	C	115	ILE	3.5
2	D	501	ILE	3.5
2	B	275	TYR	3.5
2	A	408	GLU	3.5
2	D	402	LYS	3.5
2	D	521	TYR	3.5
2	B	146	ILE	3.5
2	D	537	ILE	3.5
2	A	17	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	A	84	ASP	3.5
2	B	108	GLY	3.5
2	D	508	GLU	3.5
2	B	58	LEU	3.5
2	B	128	PHE	3.5
2	B	567	LEU	3.5
2	D	513	LEU	3.5
2	A	101	TYR	3.5
2	A	537	ILE	3.5
2	A	573	THR	3.5
2	C	42	ASN	3.5
2	A	411	ALA	3.5
2	A	264	PRO	3.5
2	C	419	GLU	3.5
2	A	216	LEU	3.5
2	D	13	PHE	3.5
2	D	509	VAL	3.5
2	B	348	ILE	3.4
2	B	370	ILE	3.4
2	D	103	ILE	3.4
2	D	405	TYR	3.4
2	C	89	THR	3.4
2	A	402	LYS	3.4
2	B	164	ALA	3.4
2	B	180	GLN	3.4
2	C	35	HIS	3.4
2	A	509	VAL	3.4
2	A	40	ILE	3.4
2	C	530	CYS	3.4
2	A	87	PRO	3.4
2	D	121	ASP	3.4
2	D	411	ALA	3.4
2	A	86	LEU	3.4
2	B	412	LEU	3.4
2	C	24	VAL	3.4
2	C	370	ILE	3.4
2	D	157	LYS	3.4
2	C	399	VAL	3.4
2	D	522	THR	3.4
2	B	44	LEU	3.4
2	B	415	ARG	3.4
2	C	503	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	168	ASN	3.4
2	A	414	PHE	3.4
2	B	509	VAL	3.4
2	A	306	ARG	3.3
2	C	185	LEU	3.3
2	C	545	ASN	3.3
2	D	43	SER	3.3
2	A	63	LEU	3.3
2	A	123	LEU	3.3
2	B	513	LEU	3.3
2	A	492	ALA	3.3
2	D	502	GLN	3.3
2	D	409	ASN	3.3
2	D	561	VAL	3.3
2	D	73	TRP	3.3
2	A	82	SER	3.3
2	B	264	PRO	3.3
2	C	59	TYR	3.3
2	D	404	PRO	3.3
2	B	97	MET	3.3
2	B	407	LYS	3.3
2	B	571	THR	3.3
2	A	188	MET	3.3
2	D	149	HIS	3.3
2	C	417	GLY	3.3
2	B	118	VAL	3.3
2	C	54	VAL	3.3
2	C	147	ASP	3.3
2	A	75	GLU	3.2
2	B	522	THR	3.2
2	B	521	TYR	3.2
2	D	108	GLY	3.2
2	B	57	ASP	3.2
2	B	520	ASP	3.2
2	B	419	GLU	3.2
2	C	538	LYS	3.2
2	D	58	LEU	3.2
2	B	517	SER	3.2
2	B	26	ALA	3.2
2	A	403	VAL	3.2
2	C	88	ASN	3.2
2	B	523	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	114	LYS	3.2
2	B	422	LYS	3.2
2	C	472	LYS	3.2
2	A	151	GLU	3.2
2	B	283	LEU	3.2
2	A	511	GLY	3.2
2	C	511	GLY	3.2
2	A	90	TYR	3.2
2	A	163	TYR	3.2
2	D	237	PHE	3.2
2	B	570	ASP	3.2
2	C	186	ASP	3.2
2	C	544	GLU	3.2
2	D	35	HIS	3.2
2	B	90	TYR	3.2
2	B	109	TYR	3.2
2	C	181	PHE	3.2
2	C	420	GLU	3.1
2	A	203	THR	3.1
2	A	400	THR	3.1
2	B	68	ALA	3.1
2	D	56	ALA	3.1
2	B	163	TYR	3.1
2	B	298	TYR	3.1
2	D	538	LYS	3.1
2	C	86	LEU	3.1
2	A	413	GLY	3.1
2	B	430	GLY	3.1
2	D	516	GLY	3.1
2	A	81	TRP	3.1
2	B	435	ALA	3.1
2	C	496	ARG	3.1
2	A	554	MET	3.1
2	C	74	LEU	3.1
2	D	104	ASP	3.1
2	B	282	PRO	3.1
2	B	417	GLY	3.1
2	C	56	ALA	3.1
2	C	309	PHE	3.1
2	C	536	LYS	3.1
2	D	507	LYS	3.1
2	D	555	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	520	ASP	3.1
2	A	153	PRO	3.1
2	C	160	PRO	3.1
2	D	94	ILE	3.1
2	B	308	ARG	3.1
2	B	250	VAL	3.1
2	B	168	ASN	3.0
2	A	21	ASP	3.0
2	C	560	GLN	3.0
2	A	110	LYS	3.0
2	A	422	LYS	3.0
2	A	242	ILE	3.0
2	D	417	GLY	3.0
2	B	572	PHE	3.0
2	A	120	TYR	3.0
2	B	149	HIS	3.0
2	B	494	TYR	3.0
2	C	33	GLU	3.0
2	B	313	ASN	3.0
2	A	512	LYS	3.0
2	A	67	GLY	3.0
2	A	152	ARG	3.0
2	B	229	GLY	3.0
2	A	49	ALA	3.0
2	D	130	VAL	3.0
2	A	107	LEU	3.0
2	D	495	LEU	3.0
2	B	151	GLU	3.0
2	A	518	PRO	3.0
2	B	343	TYR	3.0
2	B	249	ASP	3.0
2	C	112	LYS	3.0
2	C	554	MET	3.0
2	D	203	THR	3.0
2	A	528	VAL	3.0
2	D	528	VAL	3.0
2	D	129	PRO	3.0
2	A	545	ASN	3.0
2	C	109	TYR	3.0
2	C	423	ASP	3.0
2	B	433	ILE	3.0
2	C	378	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	302	ILE	3.0
2	C	564	GLY	3.0
2	B	86	LEU	2.9
2	A	303	GLN	2.9
2	B	113	ARG	2.9
2	B	288	ILE	2.9
2	B	474	ILE	2.9
2	C	574	ILE	2.9
2	B	511	GLY	2.9
2	C	41	GLY	2.9
2	D	66	ALA	2.9
2	B	79	PHE	2.9
2	B	561	VAL	2.9
2	B	480	LEU	2.9
2	A	544	GLU	2.9
2	D	544	GLU	2.9
2	A	558	PRO	2.9
2	D	496	ARG	2.9
2	A	193	ASP	2.9
2	B	101	TYR	2.9
2	C	120	TYR	2.9
2	D	34	ASP	2.9
2	A	111	GLY	2.9
2	C	108	GLY	2.9
2	D	457	THR	2.9
2	A	12	ALA	2.9
2	B	134	ALA	2.9
2	D	65	PHE	2.9
2	B	450	ASP	2.9
2	D	120	TYR	2.9
2	C	28	GLY	2.9
2	C	19	VAL	2.9
2	A	407	LYS	2.9
2	D	550	PHE	2.9
2	C	61	HIS	2.9
2	B	160	PRO	2.9
2	D	556	PRO	2.9
2	A	25	TRP	2.9
2	B	103	ILE	2.9
2	B	501	ILE	2.9
2	D	144	GLY	2.9
2	B	83	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	205	LYS	2.9
2	C	555	LYS	2.9
2	D	493	LYS	2.9
2	B	408	GLU	2.8
2	B	486	GLU	2.8
2	A	105	ILE	2.8
2	A	524	ILE	2.8
2	C	32	ILE	2.8
2	D	545	ASN	2.8
2	B	278	ASP	2.8
2	A	22	CYS	2.8
2	A	109	TYR	2.8
2	B	112	LYS	2.8
2	B	564	GLY	2.8
2	D	315	TYR	2.8
2	C	425	VAL	2.8
2	B	466	GLU	2.8
2	B	100	TRP	2.8
2	D	25	TRP	2.8
2	D	105	ILE	2.8
2	A	538	LYS	2.8
2	B	18	LYS	2.8
2	D	78	GLY	2.8
2	D	84	ASP	2.8
2	A	226	TYR	2.8
2	A	542	THR	2.8
2	B	449	TYR	2.8
2	B	484	ALA	2.8
2	B	500	TYR	2.8
2	C	90	TYR	2.8
2	C	567	LEU	2.8
2	D	101	TYR	2.8
2	D	123	LEU	2.8
2	C	411	ALA	2.8
2	D	546	PHE	2.8
2	B	420	GLU	2.8
2	C	8	MET	2.8
2	B	468	PRO	2.8
2	D	415	ARG	2.8
2	A	71	ILE	2.8
2	C	81	TRP	2.8
2	C	537	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	252	SER	2.8
2	A	570	ASP	2.8
2	B	186	ASP	2.8
2	D	74	LEU	2.8
2	B	443	THR	2.8
2	D	17	THR	2.8
2	B	281	TYR	2.8
2	C	403	VAL	2.8
2	D	5	PRO	2.8
2	A	502	GLN	2.8
2	A	208	LYS	2.8
2	C	93	ILE	2.8
2	A	126	LEU	2.8
2	B	245	GLY	2.8
2	C	563	GLY	2.8
2	A	169	ASP	2.8
2	D	60	PHE	2.8
2	C	482	TYR	2.8
2	C	55	GLN	2.7
2	A	80	LYS	2.7
2	D	18	LYS	2.7
2	D	524	ILE	2.7
2	A	185	LEU	2.7
2	B	386	LEU	2.7
2	B	469	ASP	2.7
2	C	565	VAL	2.7
2	D	418	GLU	2.7
2	D	510	ASP	2.7
2	D	137	PHE	2.7
2	A	165	TYR	2.7
2	A	114	LYS	2.7
2	B	555	LYS	2.7
2	D	311	LYS	2.7
2	B	460	ILE	2.7
2	B	262	LEU	2.7
2	D	44	LEU	2.7
2	A	88	ASN	2.7
2	A	100	TRP	2.7
2	A	307	SER	2.7
2	A	313	ASN	2.7
2	B	192	SER	2.7
2	D	395	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	54	VAL	2.7
2	A	60	PHE	2.7
2	A	514	VAL	2.7
2	A	559	VAL	2.7
2	B	54	VAL	2.7
2	B	470	VAL	2.7
2	B	492	ALA	2.7
2	C	552	ARG	2.7
2	D	441	THR	2.7
2	D	226	TYR	2.7
2	D	166	ILE	2.7
2	A	187	ARG	2.7
2	A	244	GLU	2.7
2	B	60	PHE	2.7
2	B	89	THR	2.7
2	C	137	PHE	2.7
2	C	200	ASP	2.7
2	D	147	ASP	2.7
2	A	268	PRO	2.7
2	A	575	LYS	2.7
2	B	537	ILE	2.7
2	D	201	ILE	2.7
2	B	462	LEU	2.7
2	C	58	LEU	2.7
2	C	216	LEU	2.7
2	D	552	ARG	2.7
2	A	374	SER	2.7
2	D	95	SER	2.7
2	B	230	PHE	2.7
2	B	512	LYS	2.7
2	C	543	PHE	2.7
2	D	26	ALA	2.7
2	A	519	ASP	2.7
2	B	510	ASP	2.7
2	B	482	TYR	2.6
2	A	166	ILE	2.6
2	B	105	ILE	2.6
2	B	453	ILE	2.6
2	D	306	ARG	2.6
2	A	20	GLU	2.6
2	B	88	ASN	2.6
2	B	547	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	374	SER	2.6
2	C	528	VAL	2.6
2	D	447	ALA	2.6
2	B	473	ASP	2.6
2	B	519	ASP	2.6
2	D	332	ASP	2.6
2	D	450	ASP	2.6
2	C	102	MET	2.6
2	A	11	CYS	2.6
2	A	419	GLU	2.6
2	B	481	GLY	2.6
2	A	62	ASN	2.6
2	A	10	SER	2.6
2	D	307	SER	2.6
2	A	501	ILE	2.6
2	C	103	ILE	2.6
2	C	500	TYR	2.6
2	D	27	TYR	2.6
2	A	227	ARG	2.6
2	A	305	LYS	2.6
2	A	293	GLU	2.6
2	A	78	GLY	2.6
2	B	72	ASN	2.6
2	B	397	PRO	2.6
2	C	484	ALA	2.6
2	C	561	VAL	2.6
2	D	128	PHE	2.6
2	B	232	TRP	2.6
2	C	92	THR	2.6
2	C	84	ASP	2.6
2	C	202	ILE	2.6
2	D	133	ILE	2.6
2	A	218	LEU	2.6
2	A	308	ARG	2.6
2	C	525	LYS	2.6
2	D	512	LYS	2.6
2	A	212	PRO	2.6
2	A	65	PHE	2.6
2	A	66	ALA	2.6
2	D	568	VAL	2.6
2	A	99	GLN	2.6
2	A	551	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	81	TRP	2.5
2	D	57	ASP	2.5
2	A	453	ILE	2.5
2	B	40	ILE	2.5
2	D	142	LEU	2.5
2	C	308	ARG	2.5
2	D	236	ARG	2.5
2	B	38	TYR	2.5
2	C	9	TYR	2.5
2	C	29	TYR	2.5
2	A	28	GLY	2.5
2	A	98	GLY	2.5
2	D	98	GLY	2.5
2	A	19	VAL	2.5
2	A	247	VAL	2.5
2	C	414	PHE	2.5
2	C	526	PHE	2.5
2	B	251	ASN	2.5
2	B	440	THR	2.5
2	D	42	ASN	2.5
2	D	77	ASN	2.5
2	C	551	SER	2.5
2	B	327	TRP	2.5
2	B	219	ASP	2.5
2	A	158	ILE	2.5
2	B	52	LEU	2.5
2	D	96	ARG	2.5
2	B	27	TYR	2.5
2	B	259	TYR	2.5
2	D	47	PHE	2.5
2	B	48	MET	2.5
2	D	188	MET	2.5
2	C	373	THR	2.5
2	D	16	THR	2.5
2	D	62	ASN	2.5
2	C	10	SER	2.5
2	A	507	LYS	2.5
2	A	547	LYS	2.5
2	A	552	ARG	2.5
2	B	166	ILE	2.5
2	C	18	LYS	2.5
2	C	416	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	462	LEU	2.5
2	A	418	GLU	2.5
2	A	59	TYR	2.5
2	A	390	TYR	2.5
2	D	28	GLY	2.5
2	D	67	GLY	2.5
2	B	5	PRO	2.5
2	B	99	GLN	2.5
2	B	154	VAL	2.5
2	A	128	PHE	2.5
2	A	18	LYS	2.5
2	B	349	SER	2.5
2	C	70	ILE	2.5
2	C	71	ILE	2.5
2	D	115	ILE	2.5
2	D	152	ARG	2.5
2	A	420	GLU	2.5
2	B	428	PRO	2.5
2	D	397	PRO	2.5
2	A	79	PHE	2.5
2	B	56	ALA	2.5
2	B	65	PHE	2.5
2	B	305	LYS	2.4
2	C	53	LYS	2.4
2	A	415	ARG	2.4
2	C	31	ASN	2.4
2	D	72	ASN	2.4
2	B	172	ILE	2.4
2	B	326	LEU	2.4
2	C	172	ILE	2.4
2	B	84	ASP	2.4
2	B	235	ASP	2.4
2	A	41	GLY	2.4
2	B	8	MET	2.4
2	B	533	MET	2.4
2	C	401	GLY	2.4
2	C	101	TYR	2.4
2	A	539	LYS	2.4
2	B	80	LYS	2.4
2	B	303	GLN	2.4
2	A	271	PHE	2.4
2	B	352	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	502	GLN	2.4
2	D	240	LYS	2.4
2	B	6	ARG	2.4
2	C	227	ARG	2.4
2	D	373	THR	2.4
2	A	77	ASN	2.4
2	B	32	ILE	2.4
2	B	94	ILE	2.4
2	B	389	LEU	2.4
2	C	126	LEU	2.4
2	D	31	ASN	2.4
2	A	523	ASP	2.4
2	B	200	ASP	2.4
2	B	277	TRP	2.4
2	C	473	ASP	2.4
2	B	75	GLU	2.4
2	B	162	GLU	2.4
2	D	161	GLU	2.4
2	C	5	PRO	2.4
2	A	183	GLN	2.4
2	A	355	ALA	2.4
2	B	335	LEU	2.4
2	C	173	ILE	2.4
2	C	571	THR	2.4
2	D	179	ILE	2.4
2	A	50	TRP	2.4
2	B	81	TRP	2.4
2	B	314	GLU	2.4
2	C	456	ASP	2.4
2	D	455	CYS	2.4
2	A	108	GLY	2.4
2	A	243	GLY	2.4
2	D	197	GLY	2.4
2	D	410	GLY	2.4
2	C	183	GLN	2.4
2	A	92	THR	2.4
2	A	304	ILE	2.4
2	A	351	LEU	2.4
2	A	474	ILE	2.4
2	C	94	ILE	2.4
2	C	158	ILE	2.4
2	C	36	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	249	ASP	2.4
2	A	506	MET	2.4
2	C	73	TRP	2.4
2	C	367	TRP	2.4
2	C	305	LYS	2.4
2	D	407	LYS	2.4
2	A	401	GLY	2.4
2	C	111	GLY	2.4
2	B	152	ARG	2.4
2	B	247	VAL	2.4
2	B	559	VAL	2.4
2	B	550	PHE	2.4
2	D	181	PHE	2.4
2	A	386	LEU	2.3
2	D	381	LEU	2.3
2	B	524	ILE	2.3
2	C	146	ILE	2.3
2	B	284	HIS	2.3
2	B	341	ASP	2.3
2	A	282	PRO	2.3
2	C	106	CYS	2.3
2	D	153	PRO	2.3
2	D	558	PRO	2.3
2	A	155	GLY	2.3
2	C	113	ARG	2.3
2	D	99	GLN	2.3
2	D	113	ARG	2.3
2	D	49	ALA	2.3
2	D	178	LEU	2.3
2	A	93	ILE	2.3
2	A	94	ILE	2.3
2	B	442	ILE	2.3
2	A	29	TYR	2.3
2	A	500	TYR	2.3
2	D	500	TYR	2.3
2	B	534	THR	2.3
2	D	189	THR	2.3
2	D	33	GLU	2.3
2	A	136	ASP	2.3
2	A	147	ASP	2.3
2	B	169	ASP	2.3
2	C	136	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	145	ASP	2.3
2	A	96	ARG	2.3
2	A	350	GLY	2.3
2	B	236	ARG	2.3
2	B	530	CYS	2.3
2	D	106	CYS	2.3
2	D	118	VAL	2.3
2	A	550	PHE	2.3
2	B	253	LEU	2.3
2	C	495	LEU	2.3
2	C	550	PHE	2.3
2	D	174	ALA	2.3
2	C	471	ILE	2.3
2	C	485	HIS	2.3
2	B	59	TYR	2.3
2	A	102	MET	2.3
2	A	135	LYS	2.3
2	D	575	LYS	2.3
2	D	396	ASN	2.3
2	B	122	SER	2.3
2	B	459	SER	2.3
2	B	477	PRO	2.3
2	C	96	ARG	2.3
2	D	289	ARG	2.3
2	B	85	GLY	2.3
2	A	52	LEU	2.3
2	A	448	CYS	2.3
2	C	79	PHE	2.3
2	A	190	ALA	2.3
2	A	201	ILE	2.3
2	A	116	HIS	2.3
2	A	53	LYS	2.3
2	A	159	THR	2.3
2	B	311	LYS	2.3
2	C	208	LYS	2.3
2	D	92	THR	2.3
2	C	156	TYR	2.3
2	D	90	TYR	2.3
2	A	91	ASN	2.3
2	B	409	ASN	2.3
2	A	23	ARG	2.3
2	C	235	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	401	GLY	2.3
2	A	210	VAL	2.3
2	A	470	VAL	2.3
2	D	154	VAL	2.3
2	D	559	VAL	2.3
2	B	447	ALA	2.2
2	C	11	CYS	2.2
2	C	119	ILE	2.2
2	C	531	ALA	2.2
2	B	472	LYS	2.2
2	B	293	GLU	2.2
2	D	14	GLU	2.2
2	B	505	TYR	2.2
2	C	343	TYR	2.2
2	A	57	ASP	2.2
2	B	145	ASP	2.2
2	A	58	LEU	2.2
2	A	548	VAL	2.2
2	B	403	VAL	2.2
2	C	381	LEU	2.2
2	A	143	LYS	2.2
2	B	526	PHE	2.2
2	B	536	LYS	2.2
2	C	39	LYS	2.2
2	D	158	ILE	2.2
2	D	305	LYS	2.2
2	D	422	LYS	2.2
2	D	460	ILE	2.2
2	B	102	MET	2.2
2	A	117	THR	2.2
2	B	573	THR	2.2
2	C	159	THR	2.2
2	C	573	THR	2.2
2	D	20	GLU	2.2
2	C	226	TYR	2.2
2	B	404	PRO	2.2
2	B	260	SER	2.2
2	B	487	SER	2.2
2	C	523	ASP	2.2
2	D	527	SER	2.2
2	B	63	LEU	2.2
2	B	565	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	167	LYS	2.2
2	C	559	VAL	2.2
2	D	490	LYS	2.2
2	B	71	ILE	2.2
2	B	133	ILE	2.2
2	B	299	ILE	2.2
2	B	429	MET	2.2
2	C	40	ILE	2.2
2	C	405	TYR	2.2
2	B	111	GLY	2.2
2	B	193	ASP	2.2
2	B	350	GLY	2.2
2	C	450	ASP	2.2
2	C	464	GLY	2.2
2	D	136	ASP	2.2
2	D	341	ASP	2.2
2	D	384	LEU	2.2
2	D	563	GLY	2.2
2	B	566	VAL	2.2
2	D	548	VAL	2.2
2	B	116	HIS	2.2
2	B	364	ILE	2.2
2	A	291	GLU	2.2
2	D	540	GLU	2.2
2	D	372	THR	2.2
2	A	38	TYR	2.2
2	A	426	TYR	2.2
2	B	424	PRO	2.2
2	C	344	ASN	2.2
2	B	142	LEU	2.2
2	B	177	LEU	2.2
2	B	185	LEU	2.2
2	C	312	GLY	2.2
2	D	519	ASP	2.2
2	A	118	VAL	2.2
2	C	307	SER	2.2
2	D	122	SER	2.2
2	D	210	VAL	2.2
2	D	367	TRP	2.1
2	C	486	GLU	2.1
2	B	441	THR	2.1
2	B	300	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	160	PRO	2.1
2	B	330	ASN	2.1
2	C	91	ASN	2.1
2	A	340	TYR	2.1
2	C	402	LYS	2.1
2	C	505	TYR	2.1
2	B	328	LEU	2.1
2	C	52	LEU	2.1
2	C	412	LEU	2.1
2	D	8	MET	2.1
2	D	107	LEU	2.1
2	A	103	ILE	2.1
2	A	332	ASP	2.1
2	B	475	VAL	2.1
2	C	170	ILE	2.1
2	C	470	VAL	2.1
2	C	570	ASP	2.1
2	A	69	PHE	2.1
2	D	489	PHE	2.1
2	C	12	ALA	2.1
2	A	486	GLU	2.1
2	B	483	TRP	2.1
2	C	408	GLU	2.1
2	B	438	ARG	2.1
2	D	308	ARG	2.1
2	A	89	THR	2.1
2	B	301	THR	2.1
2	A	209	LYS	2.1
2	D	127	PRO	2.1
2	A	142	LEU	2.1
2	A	513	LEU	2.1
2	B	77	ASN	2.1
2	B	224	TYR	2.1
2	C	494	TYR	2.1
2	D	38	TYR	2.1
2	D	406	LEU	2.1
2	B	197	GLY	2.1
2	A	202	ILE	2.1
2	A	319	SER	2.1
2	D	388	SER	2.1
2	A	394	ALA	2.1
2	B	53	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	379	LYS	2.1
2	A	214	LEU	2.1
2	B	351	LEU	2.1
2	B	11	CYS	2.1
2	A	61	HIS	2.1
2	A	312	GLY	2.1
2	B	9	TYR	2.1
2	B	156	TYR	2.1
2	C	67	GLY	2.1
2	C	569	ASP	2.1
2	D	69	PHE	2.1
2	D	569	ASP	2.1
2	A	215	SER	2.1
2	C	66	ALA	2.1
2	C	82	SER	2.1
2	D	82	SER	2.1
2	D	551	SER	2.1
2	B	451	ARG	2.1
2	C	182	LYS	2.1
2	A	140	THR	2.1
2	B	159	THR	2.1
2	A	44	LEU	2.1
2	D	233	LEU	2.1
2	A	530	CYS	2.1
2	B	287	HIS	2.1
2	A	454	TYR	2.1
2	A	471	ILE	2.1
2	B	29	TYR	2.1
2	B	119	ILE	2.1
2	C	224	TYR	2.1
2	D	494	TYR	2.1
2	D	504	ILE	2.1
2	A	520	ASP	2.0
2	C	248	PHE	2.1
2	C	152	ARG	2.0
2	C	280	ASP	2.0
2	B	161	GLU	2.0
2	C	512	LYS	2.0
2	D	50	TRP	2.0
2	A	434	THR	2.0
2	B	188	MET	2.0
2	C	99	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	22	CYS	2.0
2	B	454	TYR	2.0
2	C	254	TYR	2.0
2	D	454	TYR	2.0
2	A	47	PHE	2.0
2	A	230	PHE	2.0
2	B	414	PHE	2.0
2	A	503	ASP	2.0
2	D	362	ASP	2.0
2	C	529	LYS	2.0
2	D	150	LYS	2.0
2	C	388	SER	2.0
2	D	499	THR	2.0
2	D	185	LEU	2.0
2	B	61	HIS	2.0
2	A	42	ASN	2.0
2	A	297	GLY	2.0
2	B	98	GLY	2.0
2	B	323	ILE	2.0
2	B	545	ASN	2.0
2	C	144	GLY	2.0
2	B	51	VAL	2.0
2	B	96	ARG	2.0
2	B	399	VAL	2.0
2	B	439	TYR	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.