



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 1DBR / pdb_00001dbr
Title : HYPOXANTHINE GUANINE XANTHINE
Authors : Schumacher, M.A.; Carter, D.; Roos, D.; Ullman, B.; Brennan, R.G.
Deposited on : 1996-02-13
Resolution : 2.40 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

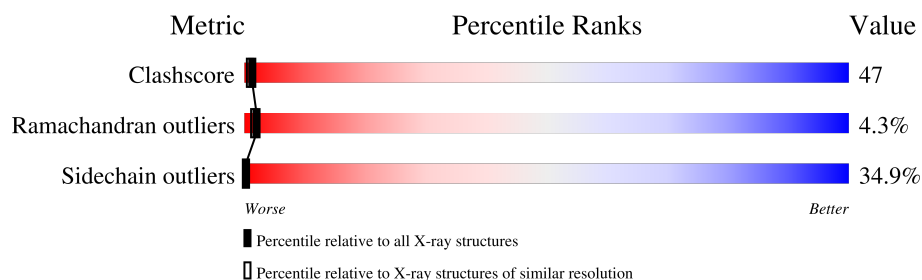
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7494 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 HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1834	1180	306	341	7			
1	B	219	Total	C	N	O	S	0	0	0
			1775	1149	294	325	7			
1	C	215	Total	C	N	O	S	0	0	0
			1746	1130	289	320	7			
1	D	215	Total	C	N	O	S	0	0	0
			1748	1132	289	320	7			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

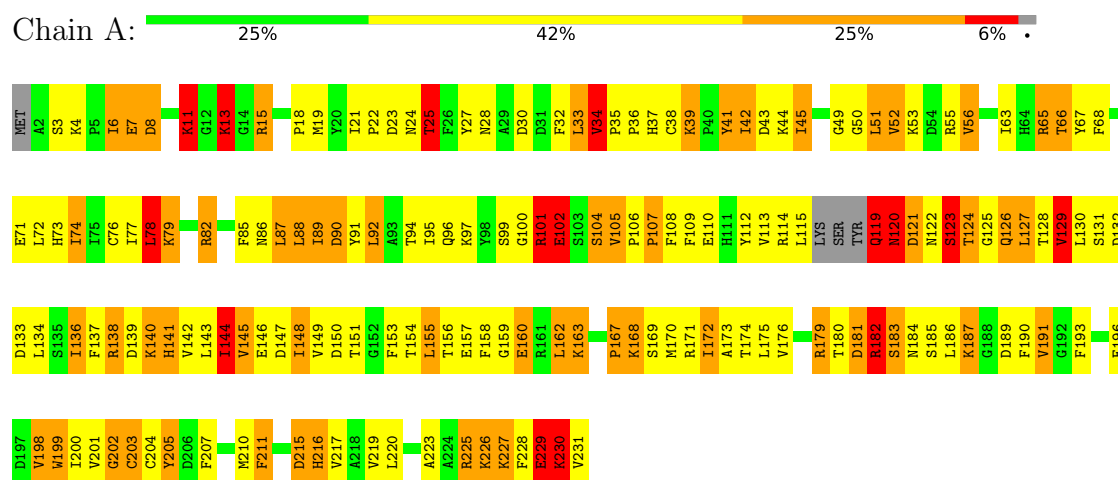
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	97	Total	O	0	0
			97	97		
3	C	95	Total	O	0	0
			95	95		
3	D	88	Total	O	0	0
			88	88		

3 Residue-property plots [i](#)

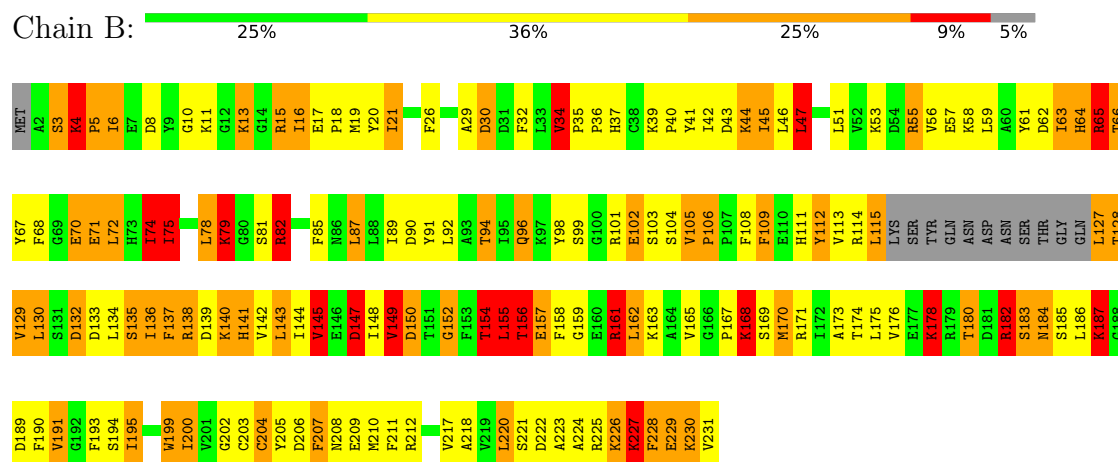
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

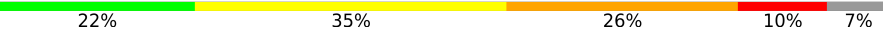
• Molecule 1: HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE

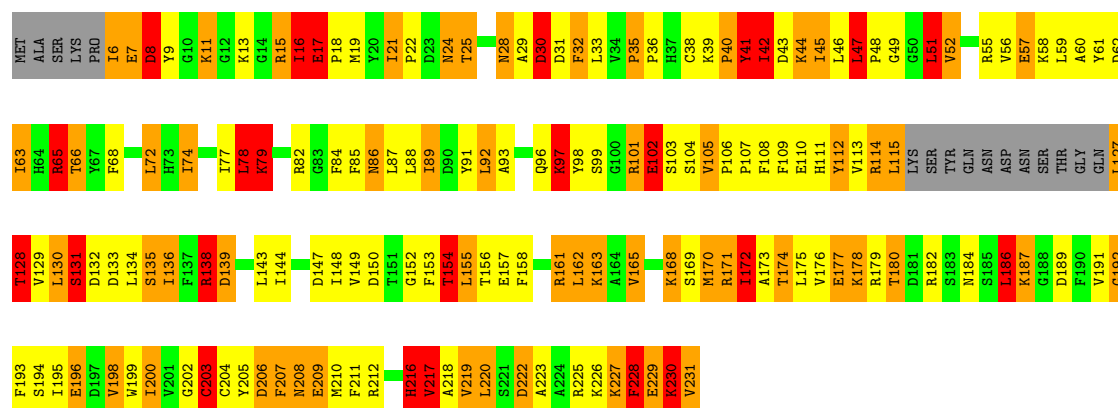


• Molecule 1: HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE

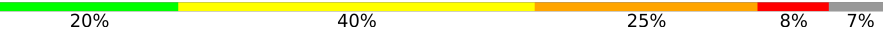


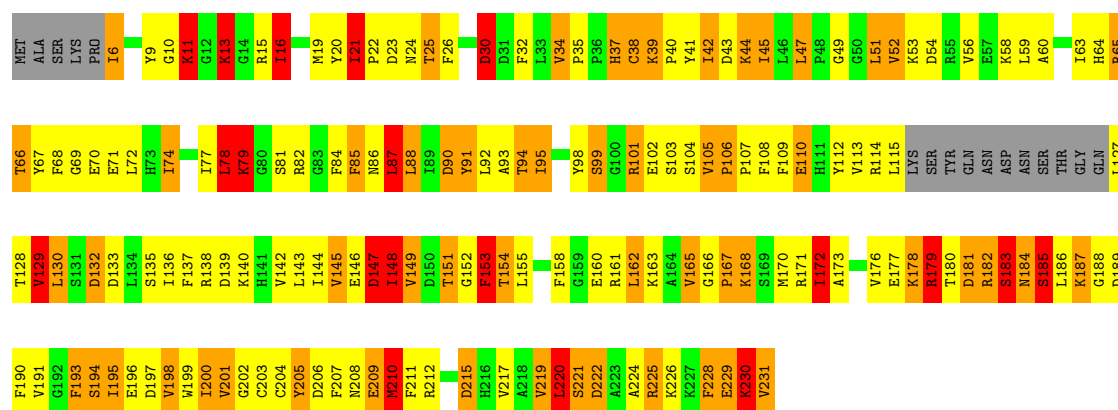
• Molecule 1: HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE

Chain C: 



• Molecule 1: HYPOXANTHINE GUANINE XANTHINE PHOSPHORIBOSYLTRANSFERASE

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.15Å 109.22Å 79.74Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	90.0 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.57	16/1876 (0.9%)	1.90	69/2530 (2.7%)
1	B	1.44	16/1817 (0.9%)	2.04	75/2450 (3.1%)
1	C	1.20	7/1787 (0.4%)	1.89	51/2409 (2.1%)
1	D	1.37	6/1789 (0.3%)	1.97	65/2412 (2.7%)
All	All	1.40	45/7269 (0.6%)	1.95	260/9801 (2.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	1
1	D	0	1
All	All	2	2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	ASN	N-CA	25.21	1.78	1.46
1	A	203	CYS	CA-CB	18.11	1.81	1.53
1	B	204	CYS	CA-CB	-10.97	1.39	1.54
1	A	203	CYS	CB-SG	10.66	2.16	1.81
1	A	144	ILE	CA-CB	7.65	1.62	1.53
1	B	156	THR	C-O	7.06	1.32	1.24
1	A	18	PRO	CA-C	-7.05	1.46	1.53
1	C	111	HIS	CA-C	6.98	1.61	1.52
1	B	175	LEU	CA-C	-6.94	1.44	1.52
1	A	86	ASN	CA-C	-6.72	1.44	1.52
1	B	4	LYS	N-CA	6.48	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ALA	CA-C	6.47	1.60	1.52
1	D	21	ILE	N-CA	-6.42	1.41	1.46
1	D	34	VAL	CA-C	6.32	1.58	1.52
1	C	172	ILE	CA-C	-5.86	1.45	1.52
1	A	78	LEU	CA-C	-5.74	1.45	1.52
1	C	60	ALA	CA-C	-5.69	1.45	1.52
1	B	112	TYR	CA-C	-5.67	1.45	1.52
1	B	3	SER	C-N	5.61	1.45	1.33
1	D	21	ILE	CA-CB	-5.61	1.48	1.53
1	C	203	CYS	CB-SG	5.58	1.99	1.81
1	B	75	ILE	CA-CB	5.54	1.60	1.53
1	B	194	SER	C-O	5.53	1.30	1.24
1	B	144	ILE	C-N	5.47	1.40	1.33
1	B	91	TYR	CA-CB	-5.44	1.44	1.53
1	B	199	TRP	NE1-CE2	-5.35	1.31	1.37
1	A	217	VAL	CA-CB	-5.33	1.47	1.54
1	B	143	LEU	CA-C	5.32	1.59	1.52
1	A	187	LYS	CA-C	-5.32	1.46	1.52
1	C	21	ILE	CA-CB	5.30	1.59	1.53
1	A	147	ASP	C-O	-5.27	1.17	1.24
1	A	230	LYS	CA-C	5.26	1.59	1.52
1	D	94	THR	CA-C	-5.22	1.45	1.52
1	B	56	VAL	CA-CB	-5.21	1.47	1.54
1	B	64	HIS	C-N	-5.21	1.27	1.33
1	A	216	HIS	CA-CB	5.19	1.63	1.54
1	C	229	GLU	N-CA	5.12	1.52	1.46
1	D	16	ILE	CA-CB	-5.12	1.48	1.54
1	B	144	ILE	N-CA	5.05	1.52	1.46
1	B	106	PRO	CA-C	-5.03	1.47	1.52
1	A	33	LEU	CA-C	5.02	1.59	1.52
1	A	95	ILE	CA-CB	5.02	1.60	1.54
1	D	95	ILE	CA-CB	-5.02	1.48	1.54
1	C	31	ASP	N-CA	-5.01	1.40	1.46
1	A	231	VAL	N-CA	5.01	1.55	1.46

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	TYR	N-CA-C	14.68	129.75	111.69
1	B	78	LEU	N-CA-C	14.43	131.48	110.42
1	D	153	PHE	N-CA-C	-11.37	97.71	111.69
1	A	105	VAL	N-CA-C	-10.79	100.34	109.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	VAL	CB-CA-C	10.73	119.84	109.33
1	B	184	ASN	N-CA-C	-10.44	88.56	110.80
1	C	180	THR	N-CA-C	10.41	124.97	109.24
1	C	219	VAL	N-CA-C	-10.41	93.05	108.87
1	C	135	SER	N-CA-C	-10.38	101.12	113.88
1	D	228	PHE	CA-CB-CG	-10.27	103.53	113.80
1	B	147	ASP	N-CA-C	-10.23	99.95	111.82
1	A	120	ASN	N-CA-CB	10.10	127.56	110.49
1	C	222	ASP	N-CA-C	-9.94	100.45	111.28
1	D	16	ILE	N-CA-C	-9.80	94.35	108.36
1	C	97	LYS	N-CA-C	9.78	122.02	111.36
1	B	104	SER	N-CA-C	-9.60	100.87	112.59
1	D	38	CYS	N-CA-C	-9.43	101.46	113.72
1	C	228	PHE	N-CA-C	9.18	130.35	110.80
1	B	187	LYS	N-CA-C	-9.06	95.19	109.50
1	A	78	LEU	N-CA-C	9.05	123.00	110.24
1	D	195	ILE	N-CA-C	8.98	123.00	108.99
1	B	185	SER	N-CA-C	8.95	121.09	108.74
1	B	94	THR	N-CA-C	8.94	120.63	111.07
1	D	101	ARG	N-CA-C	-8.91	94.71	109.24
1	B	137	PHE	N-CA-C	8.91	124.15	113.28
1	C	31	ASP	CB-CA-C	8.84	125.36	111.13
1	A	144	ILE	N-CA-CB	8.80	122.42	111.41
1	B	154	THR	CB-CA-C	8.56	124.51	110.81
1	C	30	ASP	CA-C-N	-8.52	109.83	122.86
1	C	30	ASP	C-N-CA	-8.52	109.83	122.86
1	D	66	THR	N-CA-C	8.52	120.34	111.14
1	B	228	PHE	CA-CB-CG	-8.39	105.41	113.80
1	C	55	ARG	CG-CD-NE	-8.35	93.63	112.00
1	B	103	SER	N-CA-C	-8.30	96.74	109.85
1	B	78	LEU	CA-C-N	8.26	137.31	121.54
1	B	78	LEU	C-N-CA	8.26	137.31	121.54
1	B	167	PRO	N-CA-C	-8.26	98.83	111.13
1	B	145	VAL	N-CA-C	8.21	119.61	108.11
1	A	66	THR	N-CA-C	8.18	121.31	111.82
1	D	193	PHE	N-CA-C	8.17	122.40	109.50
1	B	5	PRO	O-C-N	8.16	133.66	122.64
1	B	99	SER	N-CA-C	8.13	121.25	111.82
1	B	183	SER	N-CA-C	8.12	128.09	110.80
1	C	7	GLU	N-CA-C	-8.09	103.57	113.19
1	A	82	ARG	N-CA-C	8.03	120.81	111.02
1	B	74	ILE	CB-CA-C	7.98	122.28	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	SER	N-CA-C	7.98	122.60	113.02
1	C	78	LEU	N-CA-C	7.97	127.78	110.80
1	D	222	ASP	N-CA-C	-7.92	102.63	111.82
1	A	228	PHE	N-CA-C	7.90	123.01	111.87
1	D	205	TYR	N-CA-C	-7.85	98.86	110.48
1	A	144	ILE	CA-CB-CG2	7.71	123.61	110.50
1	C	186	LEU	N-CA-C	7.71	120.26	110.24
1	A	11	LYS	N-CA-C	-7.66	99.17	111.04
1	D	16	ILE	CB-CA-C	-7.66	100.42	110.84
1	C	57	GLU	N-CA-C	-7.64	102.95	111.28
1	B	144	ILE	CA-C-N	-7.63	113.14	123.14
1	B	144	ILE	C-N-CA	-7.63	113.14	123.14
1	A	78	LEU	O-C-N	7.47	132.09	122.97
1	C	15	ARG	N-CA-C	7.38	126.52	110.80
1	C	35	PRO	C-N-CD	-7.37	94.78	125.00
1	B	44	LYS	N-CA-C	7.36	121.54	109.24
1	D	42	ILE	CB-CA-C	7.36	121.61	111.31
1	A	156	THR	N-CA-C	-7.34	103.22	111.07
1	C	172	ILE	CB-CA-C	-7.21	99.15	110.69
1	D	147	ASP	N-CA-C	-7.18	103.18	112.23
1	D	21	ILE	CB-CA-C	7.14	119.39	111.18
1	B	204	CYS	CA-CB-SG	-7.13	98.01	114.40
1	A	88	LEU	N-CA-C	7.08	119.00	111.28
1	B	87	LEU	N-CA-C	-7.06	103.33	112.23
1	D	198	VAL	N-CA-CB	-7.06	104.54	112.45
1	B	3	SER	N-CA-C	7.05	120.60	110.24
1	B	82	ARG	CB-CA-C	7.04	122.12	110.92
1	A	127	LEU	N-CA-C	-7.01	99.05	109.15
1	D	220	LEU	N-CA-C	7.01	119.89	109.59
1	A	78	LEU	CA-C-N	7.00	134.92	121.54
1	A	78	LEU	C-N-CA	7.00	134.92	121.54
1	A	141	HIS	CA-C-N	-7.00	112.17	122.68
1	A	141	HIS	C-N-CA	-7.00	112.17	122.68
1	C	38	CYS	N-CA-C	-6.96	103.31	114.09
1	D	87	LEU	N-CA-C	-6.95	103.39	110.97
1	B	78	LEU	O-C-N	6.93	130.87	123.11
1	C	32	PHE	CA-C-N	-6.93	113.27	123.11
1	C	32	PHE	C-N-CA	-6.93	113.27	123.11
1	B	3	SER	O-C-N	6.89	131.33	123.06
1	B	71	GLU	N-CA-C	6.86	120.33	110.24
1	C	109	PHE	N-CA-C	-6.86	97.17	108.76
1	C	227	LYS	N-CA-C	6.83	119.59	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	ASN	N-CA-C	6.82	119.58	111.33
1	D	30	ASP	N-CA-C	-6.82	103.87	111.71
1	A	15	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	B	149	VAL	N-CA-CB	6.80	118.65	112.06
1	D	129	VAL	N-CA-CB	6.77	119.90	110.56
1	B	178	LYS	N-CA-C	6.75	121.30	109.96
1	B	74	ILE	N-CA-C	6.75	117.35	107.37
1	A	123	SER	N-CA-C	6.69	125.05	110.80
1	B	34	VAL	CA-C-N	6.67	124.53	119.66
1	B	34	VAL	C-N-CA	6.67	124.53	119.66
1	D	172	ILE	CB-CA-C	6.62	120.00	110.33
1	D	196	GLU	N-CA-C	-6.59	100.67	110.23
1	A	97	LYS	N-CA-C	6.55	119.24	111.71
1	D	208	ASN	N-CA-C	-6.53	97.71	108.49
1	B	102	GLU	N-CA-C	6.52	120.50	110.20
1	B	132	ASP	N-CA-C	-6.52	98.72	109.80
1	A	7	GLU	N-CA-C	6.50	124.64	110.80
1	A	18	PRO	CB-CA-C	-6.48	100.73	110.20
1	A	167	PRO	N-CA-C	-6.48	101.72	111.57
1	C	206	ASP	N-CA-C	6.47	119.97	110.59
1	D	13	LYS	N-CA-C	6.46	124.57	110.80
1	B	182	ARG	N-CA-C	6.46	124.56	110.80
1	B	111	HIS	CA-C-N	-6.45	112.68	122.81
1	B	111	HIS	C-N-CA	-6.45	112.68	122.81
1	D	10	GLY	N-CA-C	-6.44	106.84	115.21
1	D	106	PRO	CB-CA-C	-6.41	105.36	111.39
1	D	92	LEU	CB-CA-C	-6.40	100.16	110.79
1	A	183	SER	N-CA-C	-6.36	99.32	108.60
1	A	24	ASN	CB-CA-C	-6.34	101.70	111.66
1	C	25	THR	CB-CA-C	6.34	120.59	110.19
1	C	47	LEU	CB-CA-C	-6.34	101.64	110.13
1	B	140	LYS	N-CA-C	6.30	119.85	110.52
1	B	82	ARG	N-CA-C	6.27	118.67	111.02
1	A	27	TYR	N-CA-C	-6.27	100.92	110.14
1	C	216	HIS	N-CA-C	6.24	118.95	110.35
1	D	98	TYR	N-CA-C	-6.23	105.50	113.23
1	C	217	VAL	CB-CA-C	6.21	120.02	110.96
1	C	47	LEU	N-CA-C	6.20	120.50	108.85
1	B	195	ILE	N-CA-C	6.15	119.10	108.95
1	A	187	LYS	N-CA-C	-6.12	99.02	109.24
1	D	11	LYS	N-CA-C	6.10	121.00	113.50
1	B	90	ASP	N-CA-C	-6.07	103.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	THR	N-CA-C	6.07	119.12	108.75
1	B	30	ASP	CB-CA-C	-6.06	98.36	110.42
1	C	24	ASN	CA-C-N	-6.05	114.57	123.05
1	C	24	ASN	C-N-CA	-6.05	114.57	123.05
1	A	25	THR	N-CA-C	-6.05	99.38	109.24
1	D	185	SER	N-CA-C	6.05	119.70	111.17
1	D	194	SER	CA-CB-OG	-6.04	99.02	111.10
1	B	109	PHE	N-CA-C	-6.02	98.03	108.69
1	C	131	SER	N-CA-C	6.01	123.61	110.80
1	D	99	SER	N-CA-C	5.99	123.56	110.80
1	D	103	SER	CA-C-N	-5.97	112.92	122.66
1	D	103	SER	C-N-CA	-5.97	112.92	122.66
1	D	230	LYS	N-CA-C	5.97	123.51	110.80
1	B	152	GLY	N-CA-C	5.96	122.81	113.86
1	C	40	PRO	N-CA-C	-5.96	105.76	113.57
1	D	60	ALA	N-CA-C	-5.95	104.71	111.14
1	A	34	VAL	N-CA-CB	5.94	117.97	111.61
1	B	227	LYS	CA-C-N	-5.93	113.79	122.86
1	B	227	LYS	C-N-CA	-5.93	113.79	122.86
1	B	157	GLU	CB-CA-C	5.93	120.19	110.88
1	D	184	ASN	N-CA-C	-5.90	104.58	113.89
1	A	182	ARG	O-C-N	5.89	130.43	122.59
1	A	228	PHE	CA-C-N	-5.89	114.68	122.99
1	A	228	PHE	C-N-CA	-5.89	114.68	122.99
1	D	142	VAL	N-CA-C	5.89	116.09	107.37
1	B	207	PHE	CA-CB-CG	-5.86	107.94	113.80
1	D	129	VAL	O-C-N	5.86	129.63	122.83
1	B	141	HIS	CA-C-N	-5.83	115.35	123.10
1	B	141	HIS	C-N-CA	-5.83	115.35	123.10
1	A	15	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	B	85	PHE	CA-C-O	-5.79	114.70	121.07
1	A	160	GLU	N-CA-C	-5.78	104.67	110.97
1	A	184	ASN	N-CA-C	-5.78	104.15	110.91
1	C	200	ILE	N-CA-C	5.77	116.89	108.53
1	A	169	SER	N-CA-C	-5.74	99.70	108.76
1	A	179	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	A	90	ASP	N-CA-C	-5.73	104.73	110.97
1	C	102	GLU	N-CA-C	5.72	118.13	110.35
1	C	128	THR	N-CA-C	5.71	122.96	110.80
1	C	51	LEU	N-CA-C	-5.70	105.15	111.36
1	C	17	GLU	CA-C-N	5.68	125.63	119.78
1	C	17	GLU	C-N-CA	5.68	125.63	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CB-CA-C	-5.67	101.33	110.74
1	B	16	ILE	N-CA-C	-5.67	98.27	107.28
1	D	85	PHE	CA-C-N	5.65	128.12	120.44
1	D	85	PHE	C-N-CA	5.65	128.12	120.44
1	D	37	HIS	CA-C-N	-5.64	113.30	122.26
1	D	37	HIS	C-N-CA	-5.64	113.30	122.26
1	A	202	GLY	O-C-N	5.61	129.15	122.64
1	C	60	ALA	N-CA-C	-5.61	105.07	111.07
1	B	157	GLU	N-CA-C	-5.58	105.10	111.07
1	C	8	ASP	N-CA-C	5.57	120.06	113.16
1	A	8	ASP	N-CA-C	-5.56	101.47	110.32
1	A	121	ASP	N-CA-C	5.56	122.65	110.80
1	B	45	ILE	N-CA-C	5.56	115.96	108.17
1	B	29	ALA	N-CA-C	-5.56	105.12	111.07
1	A	34	VAL	CB-CA-C	5.54	116.30	110.37
1	C	42	ILE	CB-CA-C	5.53	119.11	111.38
1	C	86	ASN	CA-C-N	5.49	128.65	120.31
1	C	86	ASN	C-N-CA	5.49	128.65	120.31
1	C	16	ILE	N-CA-C	-5.48	100.55	108.87
1	B	168	LYS	N-CA-C	-5.44	106.14	112.89
1	B	194	SER	N-CA-C	-5.44	99.65	108.52
1	B	75	ILE	CB-CA-C	5.44	118.16	111.25
1	D	42	ILE	N-CA-C	5.43	115.61	107.51
1	D	66	THR	CB-CA-C	-5.42	102.33	110.90
1	D	52	VAL	CB-CA-C	-5.41	104.78	111.70
1	A	205	TYR	N-CA-C	-5.41	100.88	109.96
1	B	203	CYS	CB-CA-C	-5.41	103.84	111.95
1	D	91	TYR	N-CA-C	5.40	117.59	111.11
1	A	162	LEU	CA-CB-CG	5.40	135.19	116.30
1	D	78	LEU	CA-C-N	5.39	131.84	121.54
1	D	78	LEU	C-N-CA	5.39	131.84	121.54
1	A	126	GLN	N-CA-C	-5.38	103.88	110.61
1	D	167	PRO	CA-C-N	5.38	127.92	120.29
1	D	167	PRO	C-N-CA	5.38	127.92	120.29
1	D	65	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	182	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	B	47	LEU	CA-C-N	5.34	125.64	119.93
1	B	47	LEU	C-N-CA	5.34	125.64	119.93
1	D	200	ILE	N-CA-C	5.33	116.16	108.48
1	C	65	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	129	VAL	CB-CA-C	-5.32	103.39	111.69
1	A	41	TYR	CA-C-N	-5.32	116.03	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	TYR	C-N-CA	-5.32	116.03	123.10
1	D	79	LYS	CA-C-N	5.29	125.82	120.00
1	D	79	LYS	C-N-CA	5.29	125.82	120.00
1	D	179	ARG	CB-CA-C	-5.28	102.43	110.88
1	B	75	ILE	N-CA-CB	5.27	117.80	111.31
1	A	41	TYR	N-CA-C	5.26	120.35	113.30
1	D	210	MET	N-CA-C	5.25	118.62	110.17
1	B	65	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	3	SER	N-CA-C	-5.23	102.03	110.14
1	A	120	ASN	N-CA-C	-5.23	99.67	110.80
1	B	71	GLU	N-CA-CB	5.21	117.56	109.48
1	B	10	GLY	N-CA-C	-5.21	108.13	115.32
1	D	44	LYS	N-CA-C	5.20	117.38	108.90
1	A	119	GLN	CA-C-N	5.18	131.44	121.54
1	A	119	GLN	C-N-CA	5.18	131.44	121.54
1	A	203	CYS	CA-CB-SG	5.17	126.28	114.40
1	A	211	PHE	N-CA-C	5.16	121.79	110.80
1	A	120	ASN	CA-C-N	5.16	131.39	121.54
1	A	120	ASN	C-N-CA	5.16	131.39	121.54
1	A	229	GLU	O-C-N	5.15	129.43	123.30
1	D	206	ASP	N-CA-C	5.15	116.90	109.07
1	D	162	LEU	N-CA-C	-5.14	105.76	111.36
1	A	101	ARG	CA-C-N	5.14	131.36	121.54
1	A	101	ARG	C-N-CA	5.14	131.36	121.54
1	C	16	ILE	N-CA-CB	5.12	117.62	110.56
1	D	178	LYS	CA-C-N	-5.11	113.38	122.07
1	D	178	LYS	C-N-CA	-5.11	113.38	122.07
1	C	138	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	13	LYS	N-CA-C	5.11	121.67	110.80
1	C	42	ILE	N-CA-C	5.09	117.01	109.17
1	D	54	ASP	CB-CA-C	-5.08	102.36	110.79
1	B	161	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	B	85	PHE	N-CA-C	-5.07	104.83	111.02
1	D	93	ALA	N-CA-C	-5.06	105.45	110.97
1	B	228	PHE	N-CA-C	5.06	118.94	112.26
1	A	102	GLU	N-CA-C	5.04	121.54	110.80
1	A	138	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	55	ARG	CG-CD-NE	-5.03	100.93	112.00
1	D	94	THR	N-CA-C	5.03	117.66	111.82
1	A	74	ILE	CB-CA-C	-5.03	104.00	110.84
1	A	50	GLY	O-C-N	5.03	127.07	122.19
1	B	155	LEU	N-CA-C	5.03	116.45	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	PHE	CB-CA-C	-5.03	104.88	111.82
1	B	39	LYS	N-CA-C	5.02	120.90	109.81
1	B	5	PRO	N-CA-C	5.01	122.78	112.47
1	C	112	TYR	N-CA-C	5.01	117.06	108.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	78	LEU	CA
1	C	228	PHE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	LYS	Peptide
1	D	179	ARG	Sidechain

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	1834	0	1813	156	0
1	B	1775	0	1766	154	0
1	C	1746	0	1729	207	0
1	D	1748	0	1736	168	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	107	0	0	10	0
3	B	97	0	0	13	0
3	C	95	0	0	5	0
3	D	88	0	0	6	0
All	All	7494	0	7044	659	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 47.

All (659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:CYS:CB	1:A:203:CYS:CA	1.82	1.57
1:A:120:ASN:N	1:A:120:ASN:CA	1.78	1.44
1:A:203:CYS:CB	1:A:203:CYS:SG	2.16	1.34
1:C:115:LEU:HD13	1:C:130:LEU:HB2	1.32	1.08
1:C:78:LEU:HD22	1:C:79:LYS:H	1.17	1.04
1:C:28:ASN:N	1:C:28:ASN:HD22	1.56	1.01
1:D:151:THR:HG22	1:D:153:PHE:H	1.22	1.01
1:B:105:VAL:HG23	1:B:106:PRO:HD2	1.42	1.01
1:C:203:CYS:HB2	1:C:217:VAL:HG12	1.43	1.00
1:D:129:VAL:HG13	1:D:158:PHE:HB2	1.41	1.00
1:D:180:THR:HG22	1:D:181:ASP:H	1.27	1.00
1:D:11:LYS:HD2	1:D:13:LYS:HA	1.45	0.98
1:C:96:GLN:HG3	1:C:107:PRO:HB3	1.45	0.97
1:C:28:ASN:HD22	1:C:28:ASN:H	1.10	0.93
1:C:42:ILE:HD11	1:C:45:ILE:HD11	1.51	0.93
1:D:11:LYS:NZ	1:D:13:LYS:HD2	1.84	0.92
1:A:114:ARG:NE	1:A:130:LEU:HD11	1.83	0.92
1:A:49:GLY:H	1:A:216:HIS:HD2	1.12	0.91
1:D:172:ILE:HG12	1:D:188:GLY:HA2	1.52	0.91
1:D:229:GLU:OE1	1:D:229:GLU:HA	1.71	0.91
1:D:19:MET:HE3	1:D:21:ILE:HD11	1.53	0.90
1:C:115:LEU:CD1	1:C:130:LEU:HB2	2.01	0.89
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.36	0.89
1:C:128:THR:HA	1:C:154:THR:HG22	1.55	0.89
1:C:222:ASP:HB3	1:C:226:LYS:HZ2	1.38	0.88
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.38	0.88
1:A:144:ILE:HD11	1:A:155:LEU:HD11	1.55	0.88
1:C:42:ILE:HD13	1:C:218:ALA:CB	2.03	0.88
1:C:143:LEU:HD11	1:C:173:ALA:HB2	1.55	0.88
1:A:6:ILE:HD12	1:A:170:MET:HG2	1.57	0.87
1:D:105:VAL:HG22	1:D:106:PRO:HD2	1.56	0.86
1:D:178:LYS:HD2	1:D:197:ASP:HA	1.55	0.86
1:C:156:THR:CG2	1:C:186:LEU:HD21	2.05	0.86
1:B:152:GLY:O	1:B:156:THR:HG23	1.77	0.85
1:A:34:VAL:HG22	1:A:39:LYS:HG2	1.56	0.85
1:C:155:LEU:HB3	1:C:186:LEU:CD1	2.06	0.85
1:A:73:HIS:CD2	1:A:140:LYS:HG2	2.12	0.85
1:B:147:ASP:HB2	1:B:205:TYR:CE1	2.12	0.83
1:D:11:LYS:HD2	1:D:13:LYS:CA	2.08	0.83
1:C:42:ILE:HD13	1:C:218:ALA:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:MET:CE	1:D:21:ILE:HD11	2.09	0.82
1:A:78:LEU:HD21	1:B:78:LEU:HD11	1.62	0.82
1:C:28:ASN:H	1:C:28:ASN:ND2	1.71	0.82
1:A:52:VAL:O	1:A:56:VAL:HG13	1.79	0.81
1:C:19:MET:HE1	1:C:51:LEU:HD11	1.61	0.81
1:C:136:ILE:HD13	1:C:136:ILE:O	1.80	0.81
1:D:39:LYS:HB3	1:D:40:PRO:HD3	1.62	0.81
1:A:225:ARG:HH11	1:A:225:ARG:HG2	1.46	0.81
1:B:63:ILE:HD11	1:B:72:LEU:HD11	1.62	0.80
1:A:225:ARG:HD2	3:A:309:HOH:O	1.81	0.80
1:B:18:PRO:HB3	1:B:191:VAL:HG22	1.64	0.80
1:C:89:ILE:HG22	1:C:108:PHE:CD2	2.15	0.80
1:B:15:ARG:NH2	1:B:187:LYS:HD2	1.96	0.80
1:B:159:GLY:O	1:B:163:LYS:HG3	1.81	0.80
1:A:49:GLY:H	1:A:216:HIS:CD2	1.99	0.80
1:A:113:VAL:HG12	1:A:131:SER:HB3	1.65	0.78
1:A:41:TYR:HE2	1:A:227:LYS:HG3	1.48	0.78
1:D:107:PRO:HB2	1:D:108:PHE:HD1	1.47	0.78
1:A:226:LYS:HD3	1:A:227:LYS:N	1.99	0.78
1:A:119:GLN:CD	1:A:120:ASN:H	1.92	0.78
1:C:163:LYS:NZ	1:C:163:LYS:HB2	1.96	0.78
1:B:6:ILE:HG13	1:B:6:ILE:O	1.83	0.77
1:D:105:VAL:CG2	1:D:106:PRO:HD2	2.14	0.77
1:D:207:PHE:CE2	1:D:225:ARG:HA	2.20	0.77
1:C:29:ALA:HA	1:C:45:ILE:HD13	1.66	0.77
1:B:41:TYR:HB3	1:B:224:ALA:HB2	1.66	0.77
1:C:28:ASN:N	1:C:28:ASN:ND2	2.29	0.77
1:A:41:TYR:CE2	1:A:227:LYS:HG3	2.20	0.77
1:B:149:VAL:HG21	1:B:186:LEU:HB2	1.66	0.77
1:B:180:THR:CG2	1:B:182:ARG:HD3	2.15	0.77
1:C:155:LEU:HB3	1:C:186:LEU:HD12	1.66	0.76
1:B:142:VAL:HG12	1:B:169:SER:O	1.85	0.76
1:B:174:THR:O	1:B:191:VAL:HA	1.86	0.76
1:D:127:LEU:O	1:D:154:THR:HB	1.86	0.76
1:A:133:ASP:O	1:A:136:ILE:HG22	1.86	0.75
1:C:42:ILE:HD11	1:C:45:ILE:CD1	2.16	0.75
1:D:133:ASP:OD2	1:D:135:SER:HB2	1.86	0.75
1:C:128:THR:HG23	1:C:157:GLU:OE2	1.87	0.75
1:B:11:LYS:HB3	3:B:311:HOH:O	1.87	0.74
1:C:222:ASP:HA	1:C:225:ARG:HD3	1.69	0.74
1:A:34:VAL:HG22	1:A:39:LYS:CG	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:PRO:HB2	1:D:108:PHE:CD1	2.23	0.74
1:B:62:ASP:O	1:B:66:THR:HG22	1.88	0.73
1:D:11:LYS:HD2	1:D:13:LYS:N	2.03	0.73
1:C:207:PHE:CZ	1:C:225:ARG:HA	2.23	0.73
1:D:78:LEU:HD23	1:D:79:LYS:H	1.53	0.73
1:A:90:ASP:O	1:A:94:THR:HG22	1.89	0.72
1:A:110:GLU:OE1	1:B:82:ARG:HD2	1.88	0.72
1:B:47:LEU:HD12	1:B:217:VAL:HG21	1.70	0.72
1:A:11:LYS:HD3	3:A:281:HOH:O	1.89	0.72
1:B:63:ILE:CD1	1:B:72:LEU:HD11	2.20	0.72
1:D:22:PRO:O	1:D:25:THR:HG23	1.90	0.72
1:D:130:LEU:HD13	1:D:130:LEU:C	2.14	0.72
1:C:210:MET:HB3	1:C:211:PHE:CD2	2.25	0.72
1:D:47:LEU:HB2	1:D:217:VAL:HB	1.70	0.72
1:D:91:TYR:O	1:D:95:ILE:HG13	1.90	0.72
1:C:19:MET:HE1	1:C:51:LEU:HD21	1.71	0.71
1:A:44:LYS:HE2	3:A:264:HOH:O	1.89	0.71
1:C:210:MET:HB3	1:C:211:PHE:CE2	2.25	0.71
1:A:181:ASP:O	1:A:182:ARG:HB2	1.89	0.71
1:D:149:VAL:HG22	1:D:149:VAL:O	1.89	0.71
1:D:78:LEU:HD23	1:D:79:LYS:N	2.04	0.71
1:D:19:MET:HE2	1:D:193:PHE:CD1	2.26	0.71
1:A:49:GLY:N	1:A:216:HIS:HD2	1.86	0.71
1:C:203:CYS:CB	1:C:217:VAL:HG12	2.20	0.71
1:C:207:PHE:O	1:C:210:MET:HB2	1.91	0.71
1:B:75:ILE:HD13	1:B:75:ILE:O	1.90	0.71
1:B:158:PHE:HD1	1:B:161:ARG:NH1	1.88	0.71
1:D:19:MET:HE2	1:D:193:PHE:HD1	1.56	0.71
1:A:129:VAL:HG11	1:A:158:PHE:HB2	1.73	0.70
1:B:15:ARG:HD3	1:B:17:GLU:OE2	1.90	0.70
1:B:105:VAL:CG2	1:B:106:PRO:HD2	2.21	0.70
1:C:158:PHE:CE2	1:C:162:LEU:HD21	2.27	0.69
1:D:230:LYS:CD	1:D:231:VAL:H	2.05	0.69
1:B:199:TRP:CD1	1:B:220:LEU:HB2	2.28	0.69
1:C:230:LYS:O	1:C:231:VAL:HB	1.91	0.69
1:D:180:THR:CG2	1:D:182:ARG:HG3	2.22	0.69
1:B:43:ASP:HA	3:B:254:HOH:O	1.91	0.69
3:B:247:HOH:O	1:D:19:MET:HG3	1.93	0.68
1:D:101:ARG:HG3	3:D:252:HOH:O	1.91	0.68
1:A:71:GLU:HG2	1:A:109:PHE:HE2	1.58	0.68
1:B:68:PHE:CE2	1:B:101:ARG:HG2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:THR:HG21	1:B:182:ARG:HD3	1.75	0.68
1:A:225:ARG:HG2	1:A:225:ARG:NH1	2.08	0.68
1:A:136:ILE:HG13	1:A:136:ILE:O	1.93	0.67
1:C:136:ILE:HD13	1:C:136:ILE:C	2.19	0.67
1:D:151:THR:HG22	1:D:153:PHE:N	2.02	0.67
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.59	0.67
1:D:16:ILE:HG12	3:D:234:HOH:O	1.95	0.67
1:C:148:ILE:HD11	1:C:178:LYS:HD2	1.76	0.67
1:C:178:LYS:HA	1:C:195:ILE:O	1.95	0.67
1:D:209:GLU:HA	1:D:209:GLU:OE1	1.93	0.67
1:C:174:THR:HG22	1:C:191:VAL:HG23	1.75	0.66
1:C:8:ASP:N	1:C:8:ASP:OD1	2.28	0.66
1:A:15:ARG:NH1	1:A:191:VAL:HG11	2.08	0.66
1:C:56:VAL:HG22	1:C:84:PHE:HE1	1.60	0.66
1:C:171:ARG:HG3	1:C:171:ARG:NH1	2.10	0.66
1:D:129:VAL:CG1	1:D:158:PHE:HB2	2.22	0.66
1:B:142:VAL:HG13	1:B:170:MET:HA	1.77	0.66
1:C:222:ASP:O	1:C:226:LYS:HD2	1.95	0.66
1:A:37:HIS:CE1	1:B:96:GLN:HE22	2.14	0.66
1:C:89:ILE:HD12	1:C:89:ILE:H	1.59	0.66
1:C:153:PHE:O	1:C:154:THR:HG23	1.95	0.66
1:B:63:ILE:HD11	1:B:72:LEU:CD1	2.26	0.66
1:C:42:ILE:HD13	1:C:218:ALA:HB1	1.76	0.66
1:D:11:LYS:CE	1:D:13:LYS:HD2	2.26	0.66
1:B:147:ASP:OD1	1:B:147:ASP:N	2.29	0.65
1:B:210:MET:HB3	1:B:211:PHE:CD2	2.31	0.65
1:C:78:LEU:HD22	1:C:79:LYS:N	2.02	0.65
1:C:131:SER:HB3	1:C:161:ARG:NH2	2.11	0.65
1:C:207:PHE:HZ	1:C:225:ARG:HA	1.62	0.65
1:C:6:ILE:HG23	1:C:7:GLU:CD	2.20	0.65
1:C:202:GLY:HA2	1:C:211:PHE:O	1.97	0.65
1:D:180:THR:HG22	1:D:182:ARG:HG3	1.77	0.65
1:A:113:VAL:CG1	1:A:131:SER:HB3	2.26	0.65
1:D:220:LEU:HD22	1:D:225:ARG:HG2	1.77	0.65
1:D:220:LEU:HD23	1:D:224:ALA:HB3	1.77	0.65
1:B:15:ARG:HG2	1:B:16:ILE:N	2.12	0.65
1:B:161:ARG:HH11	1:B:161:ARG:CG	2.08	0.65
1:D:71:GLU:CG	1:D:109:PHE:HE2	2.09	0.65
1:A:114:ARG:HE	1:A:130:LEU:HD11	1.62	0.65
1:A:77:ILE:HD12	1:A:146:GLU:HG2	1.78	0.64
1:A:215:ASP:N	1:A:215:ASP:OD1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASP:HB2	1:B:205:TYR:HE1	1.58	0.64
1:C:35:PRO:HB2	1:C:36:PRO:HD2	1.79	0.64
1:C:89:ILE:HG22	1:C:108:PHE:CE2	2.32	0.64
1:D:149:VAL:O	1:D:149:VAL:CG2	2.45	0.64
1:B:26:PHE:HB2	3:B:257:HOH:O	1.95	0.64
1:B:180:THR:HG23	1:B:182:ARG:HD3	1.80	0.64
1:C:68:PHE:CZ	1:C:101:ARG:HG2	2.32	0.64
1:C:155:LEU:HB3	1:C:186:LEU:HD11	1.79	0.64
1:B:162:LEU:O	1:B:165:VAL:HG22	1.98	0.64
1:D:11:LYS:HZ2	1:D:13:LYS:HD2	1.62	0.64
1:C:48:PRO:HA	1:C:216:HIS:HD2	1.63	0.64
1:B:40:PRO:HG2	1:B:41:TYR:CE2	2.33	0.64
1:D:138:ARG:HA	1:D:165:VAL:HG23	1.80	0.63
3:A:329:HOH:O	1:B:114:ARG:HD3	1.98	0.63
1:A:110:GLU:OE2	1:B:82:ARG:NH1	2.30	0.63
1:C:28:ASN:HB2	1:C:30:ASP:OD1	1.99	0.63
1:D:107:PRO:HG2	1:D:108:PHE:CE1	2.32	0.63
1:C:79:LYS:HZ2	1:D:112:TYR:HD1	1.47	0.63
1:D:178:LYS:HD3	1:D:195:ILE:HG13	1.81	0.62
1:C:131:SER:HB3	1:C:161:ARG:HH22	1.64	0.62
1:C:158:PHE:HD1	1:C:161:ARG:NH1	1.98	0.62
1:C:105:VAL:HG13	1:C:106:PRO:O	1.99	0.62
1:A:19:MET:CE	1:A:21:ILE:HD11	2.29	0.62
1:B:32:PHE:C	1:D:58:LYS:HD3	2.24	0.61
1:C:82:ARG:HD2	1:C:86:ASN:HD22	1.65	0.61
1:C:105:VAL:HG22	1:C:106:PRO:HD2	1.81	0.61
1:D:163:LYS:HD3	3:D:313:HOH:O	2.00	0.61
1:D:105:VAL:HG22	1:D:106:PRO:CD	2.29	0.61
1:C:209:GLU:OE1	1:C:212:ARG:HD2	2.00	0.61
1:C:86:ASN:HA	1:C:89:ILE:HD11	1.83	0.61
1:A:207:PHE:O	1:A:210:MET:HB2	2.00	0.61
1:C:158:PHE:O	1:C:162:LEU:HD22	2.01	0.61
1:C:29:ALA:HA	1:C:45:ILE:CD1	2.30	0.61
1:C:207:PHE:O	1:C:208:ASN:HB3	2.01	0.60
1:A:226:LYS:HD3	1:A:227:LYS:H	1.67	0.60
1:C:89:ILE:HD12	1:C:89:ILE:N	2.16	0.60
1:A:120:ASN:N	1:A:120:ASN:C	2.57	0.60
1:C:129:VAL:HG11	1:C:158:PHE:HB2	1.84	0.60
1:C:156:THR:HG22	1:C:186:LEU:HD21	1.80	0.60
1:D:201:VAL:HG13	1:D:220:LEU:HD12	1.83	0.60
1:A:142:VAL:HB	3:A:296:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:HG3	3:C:272:HOH:O	2.01	0.59
1:C:163:LYS:HB2	1:C:163:LYS:HZ2	1.67	0.59
1:C:198:VAL:HG13	1:C:199:TRP:N	2.17	0.59
1:B:161:ARG:HG3	1:B:161:ARG:NH1	2.10	0.59
1:B:199:TRP:HD1	1:B:220:LEU:HB2	1.66	0.59
1:C:115:LEU:HB3	1:C:128:THR:O	2.03	0.59
1:D:35:PRO:HB2	1:D:37:HIS:CE1	2.38	0.59
1:C:222:ASP:HB3	1:C:226:LYS:NZ	2.14	0.59
1:A:49:GLY:O	1:A:53:LYS:HG3	2.02	0.58
1:A:151:THR:C	1:A:153:PHE:H	2.10	0.58
1:C:19:MET:CE	1:C:51:LEU:HD11	2.33	0.58
1:D:82:ARG:HD2	1:D:82:ARG:O	2.03	0.58
1:A:151:THR:HG22	1:A:153:PHE:H	1.67	0.58
1:A:181:ASP:O	1:A:181:ASP:CG	2.45	0.58
1:C:143:LEU:HD11	1:C:173:ALA:CB	2.33	0.58
1:A:203:CYS:CB	1:A:203:CYS:C	2.74	0.58
1:C:18:PRO:HB3	1:C:191:VAL:HG13	1.85	0.58
1:C:78:LEU:HD11	1:D:112:TYR:CD2	2.39	0.58
1:C:39:LYS:N	1:C:40:PRO:HD2	2.18	0.58
1:D:11:LYS:HE3	1:D:13:LYS:CD	2.34	0.57
1:B:142:VAL:CG1	1:B:170:MET:HA	2.34	0.57
1:B:19:MET:HE2	1:B:21:ILE:HD11	1.86	0.57
1:C:19:MET:HE2	1:C:21:ILE:HD11	1.85	0.57
1:D:32:PHE:CD1	1:D:45:ILE:HD13	2.40	0.57
1:D:74:ILE:HG22	1:D:85:PHE:HE1	1.68	0.57
1:D:147:ASP:O	1:D:148:ILE:HB	2.05	0.57
1:A:28:ASN:OD1	1:A:30:ASP:HB2	2.04	0.57
1:B:129:VAL:HG13	1:B:158:PHE:HB2	1.86	0.57
1:A:182:ARG:HB2	1:A:182:ARG:CZ	2.34	0.57
1:C:115:LEU:HB2	1:C:130:LEU:H	1.69	0.57
1:C:22:PRO:O	1:C:25:THR:HG23	2.04	0.57
1:C:78:LEU:CD2	1:C:79:LYS:H	2.05	0.57
1:D:172:ILE:CG1	1:D:188:GLY:HA2	2.31	0.57
1:B:222:ASP:HB2	3:B:316:HOH:O	2.05	0.56
1:C:6:ILE:HG23	1:C:7:GLU:N	2.19	0.56
1:C:11:LYS:HZ1	1:C:13:LYS:HD3	1.69	0.56
1:D:180:THR:HG22	1:D:181:ASP:N	2.09	0.56
1:A:119:GLN:HB3	1:A:125:GLY:N	2.20	0.56
1:C:127:LEU:O	1:C:154:THR:HG21	2.06	0.56
1:D:11:LYS:HZ1	1:D:13:LYS:HD2	1.70	0.56
1:A:74:ILE:HG22	1:A:145:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HG3	1:A:155:LEU:HD21	1.88	0.56
1:B:156:THR:HG22	1:B:186:LEU:HD11	1.86	0.56
1:C:9:TYR:CD1	1:C:170:MET:HE2	2.41	0.56
1:D:11:LYS:HE3	1:D:13:LYS:HD2	1.86	0.56
1:D:71:GLU:HG2	1:D:109:PHE:HE2	1.71	0.56
1:D:78:LEU:HD12	1:D:112:TYR:HD2	1.71	0.56
1:B:75:ILE:HG12	1:B:113:VAL:HG22	1.87	0.56
1:D:6:ILE:HG21	1:D:163:LYS:HD2	1.88	0.56
1:A:171:ARG:HG2	1:A:189:ASP:CG	2.30	0.56
1:C:180:THR:HG23	1:C:182:ARG:H	1.69	0.56
1:C:89:ILE:H	1:C:89:ILE:CD1	2.16	0.56
1:C:186:LEU:N	1:C:186:LEU:HD23	2.21	0.56
1:A:114:ARG:HE	1:A:130:LEU:HD21	1.70	0.56
1:B:15:ARG:HH22	1:B:187:LYS:HD2	1.69	0.56
1:C:162:LEU:O	1:C:165:VAL:HG22	2.06	0.56
1:A:225:ARG:O	1:A:229:GLU:HB3	2.06	0.56
1:C:115:LEU:HD13	1:C:130:LEU:CB	2.22	0.56
1:B:41:TYR:OH	1:B:227:LYS:HE3	2.06	0.55
1:C:49:GLY:HA2	1:C:52:VAL:HG13	1.87	0.55
1:C:82:ARG:HD2	1:C:86:ASN:ND2	2.19	0.55
1:A:175:LEU:HG	1:A:175:LEU:O	2.07	0.55
1:B:74:ILE:HG13	1:B:145:VAL:CG1	2.36	0.55
1:B:223:ALA:O	1:B:227:LYS:HB3	2.06	0.55
1:D:230:LYS:HD2	1:D:231:VAL:O	2.06	0.55
1:A:126:GLN:HA	1:A:153:PHE:CE2	2.41	0.55
1:C:19:MET:HE1	1:C:51:LEU:CD1	2.35	0.55
1:A:105:VAL:CG2	1:A:106:PRO:HD2	2.37	0.55
1:B:47:LEU:HD12	1:B:217:VAL:CG2	2.36	0.55
1:C:153:PHE:O	1:C:153:PHE:CG	2.60	0.55
1:B:63:ILE:HD12	1:B:67:TYR:CD2	2.41	0.55
1:C:61:TYR:HE2	1:C:65:ARG:HH11	1.55	0.55
1:D:229:GLU:O	1:D:230:LYS:HB2	2.07	0.55
1:A:199:TRP:CE3	1:A:220:LEU:HD22	2.42	0.55
1:B:134:LEU:HD23	1:B:137:PHE:HE2	1.72	0.55
1:D:81:SER:OG	1:D:146:GLU:HA	2.06	0.55
1:B:65:ARG:HG2	1:B:65:ARG:NH1	2.22	0.55
1:C:128:THR:HA	1:C:154:THR:CG2	2.33	0.55
1:C:199:TRP:HB3	1:C:220:LEU:HD21	1.89	0.55
1:A:74:ILE:HG22	1:A:145:VAL:CG1	2.38	0.54
1:A:88:LEU:O	1:A:92:LEU:HB2	2.06	0.54
1:A:151:THR:HG22	1:A:153:PHE:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:CG	1:C:18:PRO:HD2	2.37	0.54
1:D:138:ARG:CA	1:D:165:VAL:HG23	2.37	0.54
1:C:99:SER:C	1:C:101:ARG:H	2.16	0.54
1:C:199:TRP:HB3	1:C:220:LEU:CD2	2.37	0.54
1:D:186:LEU:O	3:D:243:HOH:O	2.18	0.54
1:A:105:VAL:HG23	1:A:106:PRO:HD2	1.90	0.54
1:A:196:GLU:HG2	3:A:272:HOH:O	2.07	0.54
1:B:129:VAL:HG13	3:B:293:HOH:O	2.07	0.54
1:B:17:GLU:HG2	3:B:295:HOH:O	2.08	0.54
1:C:19:MET:CE	1:C:21:ILE:HD11	2.38	0.54
1:D:138:ARG:HA	1:D:165:VAL:O	2.08	0.54
1:C:102:GLU:HB3	3:C:258:HOH:O	2.08	0.54
1:B:75:ILE:CG1	1:B:113:VAL:HG22	2.38	0.54
1:C:222:ASP:O	1:C:225:ARG:HB2	2.08	0.54
1:A:6:ILE:HG22	1:A:6:ILE:O	2.07	0.54
1:D:6:ILE:CG2	1:D:163:LYS:HD2	2.38	0.54
1:A:63:ILE:HD11	1:A:190:PHE:CG	2.42	0.53
1:D:20:TYR:CE2	1:D:179:ARG:NH2	2.76	0.53
1:D:11:LYS:HG3	1:D:13:LYS:H	1.73	0.53
1:B:63:ILE:HD13	1:B:143:LEU:HD22	1.90	0.53
1:B:71:GLU:O	1:B:141:HIS:HB2	2.08	0.53
1:B:134:LEU:CD2	1:B:137:PHE:HE2	2.21	0.53
1:C:175:LEU:O	1:C:175:LEU:HD12	2.08	0.53
1:D:67:TYR:OH	1:D:171:ARG:HD2	2.08	0.53
1:D:71:GLU:HG2	1:D:109:PHE:CE2	2.43	0.53
1:D:130:LEU:HD13	1:D:130:LEU:O	2.09	0.53
1:D:178:LYS:HE2	1:D:198:VAL:H	1.74	0.53
1:A:138:ARG:HG2	1:A:139:ASP:OD2	2.09	0.53
1:C:48:PRO:HA	1:C:216:HIS:CD2	2.44	0.53
1:B:178:LYS:HG3	1:B:195:ILE:HG13	1.91	0.53
1:C:139:ASP:O	1:C:168:LYS:HB2	2.09	0.53
1:C:79:LYS:NZ	1:D:112:TYR:HD1	2.05	0.53
1:B:98:TYR:OH	1:C:57:GLU:OE2	2.26	0.53
1:A:114:ARG:CD	1:A:130:LEU:HD11	2.38	0.52
1:A:19:MET:HE3	1:A:21:ILE:HD11	1.90	0.52
1:A:19:MET:HE2	1:A:193:PHE:HD2	1.75	0.52
1:A:159:GLY:O	1:A:163:LYS:HG3	2.09	0.52
1:C:158:PHE:CD1	1:C:161:ARG:NH1	2.78	0.52
1:D:85:PHE:HB2	1:D:145:VAL:HG21	1.92	0.52
1:A:141:HIS:CE1	1:A:168:LYS:HD3	2.44	0.52
1:A:144:ILE:HD11	1:A:155:LEU:CD1	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASP:O	1:B:11:LYS:HG3	2.09	0.52
1:B:133:ASP:OD1	1:B:135:SER:HB3	2.10	0.52
1:D:34:VAL:CG1	1:D:39:LYS:HA	2.39	0.52
1:B:173:ALA:HA	1:B:190:PHE:O	2.10	0.52
1:A:198:VAL:CG2	1:A:219:VAL:HG13	2.39	0.52
1:B:32:PHE:O	1:D:58:LYS:HD3	2.09	0.51
1:C:82:ARG:NH1	1:D:110:GLU:OE1	2.43	0.51
1:B:129:VAL:CG1	1:B:158:PHE:HB2	2.39	0.51
1:A:76:CYS:HB2	1:A:85:PHE:CD1	2.45	0.51
1:B:155:LEU:HB3	1:B:186:LEU:CD1	2.41	0.51
1:C:207:PHE:HD2	1:C:211:PHE:HE2	1.59	0.51
1:A:100:GLY:HA3	1:D:65:ARG:NH2	2.26	0.51
1:C:130:LEU:C	1:C:130:LEU:HD13	2.34	0.51
1:A:34:VAL:CG2	1:A:39:LYS:HG2	2.34	0.51
1:C:8:ASP:O	1:C:11:LYS:HB2	2.11	0.51
1:A:19:MET:HE2	1:A:193:PHE:CD2	2.45	0.51
1:B:162:LEU:CB	1:B:170:MET:HE3	2.41	0.51
1:A:182:ARG:HD2	1:A:185:SER:HB2	1.93	0.51
1:B:162:LEU:HB3	1:B:170:MET:HE3	1.92	0.51
1:D:87:LEU:O	1:D:90:ASP:HB3	2.11	0.51
1:A:67:TYR:OH	1:A:171:ARG:HD2	2.10	0.51
1:D:49:GLY:O	1:D:52:VAL:HB	2.11	0.51
1:D:130:LEU:C	1:D:130:LEU:CD1	2.84	0.51
1:A:38:CYS:HB3	1:A:42:ILE:HD12	1.93	0.50
1:B:115:LEU:HD12	1:B:129:VAL:HA	1.94	0.50
1:B:57:GLU:OE2	1:C:98:TYR:OH	2.21	0.50
1:C:77:ILE:HD13	1:C:113:VAL:HG22	1.93	0.50
1:A:114:ARG:O	1:A:115:LEU:HB2	2.10	0.50
1:B:89:ILE:HB	1:B:108:PHE:CZ	2.46	0.50
1:B:128:THR:HG22	1:B:129:VAL:O	2.12	0.50
1:D:11:LYS:HE3	1:D:13:LYS:HB2	1.93	0.50
1:B:68:PHE:CD2	1:B:101:ARG:NH1	2.79	0.50
1:C:114:ARG:O	1:C:115:LEU:HB2	2.10	0.50
1:D:129:VAL:HG13	1:D:158:PHE:CB	2.28	0.50
1:D:202:GLY:HA2	1:D:211:PHE:O	2.12	0.50
1:C:17:GLU:HG3	1:C:18:PRO:HD2	1.94	0.50
1:B:42:ILE:HD12	1:B:218:ALA:CB	2.42	0.49
1:B:206:ASP:HB3	1:B:212:ARG:HG2	1.94	0.49
1:C:147:ASP:O	1:C:175:LEU:HB3	2.12	0.49
1:C:174:THR:CG2	1:C:191:VAL:HG23	2.41	0.49
1:C:177:GLU:OE1	3:C:321:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:TYR:CE2	1:D:170:MET:HE2	2.47	0.49
1:D:13:LYS:O	1:D:13:LYS:HG3	2.10	0.49
1:D:19:MET:HE3	1:D:21:ILE:CD1	2.34	0.49
1:B:71:GLU:HA	3:B:287:HOH:O	2.11	0.49
1:B:174:THR:HG23	1:B:191:VAL:HB	1.94	0.49
1:D:129:VAL:HG22	1:D:158:PHE:CD1	2.46	0.49
1:B:158:PHE:HD1	1:B:161:ARG:HH12	1.61	0.49
1:C:220:LEU:HD23	1:C:220:LEU:N	2.27	0.49
1:B:142:VAL:HG13	1:B:142:VAL:O	2.13	0.49
1:A:137:PHE:O	1:A:167:PRO:HA	2.13	0.49
1:B:199:TRP:CD1	1:B:220:LEU:CB	2.96	0.49
1:D:165:VAL:HG23	1:D:165:VAL:O	2.11	0.49
1:C:128:THR:CG2	1:C:129:VAL:N	2.76	0.49
1:C:129:VAL:HG11	1:C:158:PHE:CD1	2.48	0.49
1:C:19:MET:HE1	1:C:51:LEU:CD2	2.42	0.49
1:C:62:ASP:O	1:C:66:THR:HG23	2.13	0.49
1:A:82:ARG:HD3	1:B:112:TYR:OH	2.12	0.49
1:B:15:ARG:CG	1:B:16:ILE:N	2.75	0.49
1:C:168:LYS:HG2	1:C:168:LYS:O	2.13	0.49
1:D:230:LYS:HD2	1:D:231:VAL:H	1.75	0.49
3:A:329:HOH:O	1:B:130:LEU:HD12	2.12	0.48
1:B:13:LYS:HG2	3:B:311:HOH:O	2.13	0.48
1:A:151:THR:HG22	1:A:153:PHE:HB3	1.94	0.48
1:B:26:PHE:HD2	3:B:257:HOH:O	1.95	0.48
1:B:176:VAL:HG13	1:B:195:ILE:HG12	1.95	0.48
1:D:207:PHE:CD2	1:D:228:PHE:HB2	2.48	0.48
1:B:75:ILE:HD13	1:B:75:ILE:C	2.38	0.48
1:C:41:TYR:CE2	1:C:228:PHE:CZ	3.01	0.48
1:C:29:ALA:O	1:C:32:PHE:HB2	2.14	0.48
1:C:96:GLN:HB2	3:C:253:HOH:O	2.13	0.48
1:C:202:GLY:O	1:C:205:TYR:HB2	2.14	0.48
1:A:23:ASP:OD1	1:A:196:GLU:HB3	2.13	0.48
1:C:93:ALA:O	1:C:96:GLN:HB2	2.14	0.48
1:C:114:ARG:CG	1:C:115:LEU:N	2.77	0.48
1:D:172:ILE:HG12	1:D:188:GLY:CA	2.35	0.48
1:D:210:MET:HE3	1:D:228:PHE:CD1	2.48	0.48
1:A:68:PHE:HZ	1:A:102:GLU:O	1.97	0.48
1:A:142:VAL:HG12	3:A:296:HOH:O	2.13	0.48
1:A:151:THR:C	1:A:153:PHE:N	2.70	0.48
1:A:172:ILE:O	1:A:189:ASP:N	2.39	0.48
1:B:112:TYR:N	1:B:112:TYR:CD1	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LYS:NZ	1:C:13:LYS:HD3	2.28	0.48
1:A:182:ARG:HG2	1:A:183:SER:N	2.29	0.48
1:B:59:LEU:O	1:B:63:ILE:HG23	2.14	0.48
1:D:24:ASN:HA	1:D:26:PHE:CE1	2.47	0.48
1:A:74:ILE:HG23	1:A:143:LEU:HD23	1.96	0.48
1:C:6:ILE:C	1:C:6:ILE:HD13	2.38	0.48
1:D:225:ARG:O	1:D:229:GLU:HB2	2.13	0.48
1:A:33:LEU:N	1:C:58:LYS:HG2	2.29	0.47
1:A:37:HIS:CD2	1:B:106:PRO:HA	2.48	0.47
1:B:70:GLU:O	3:B:287:HOH:O	2.20	0.47
1:C:114:ARG:HH22	1:D:114:ARG:HE	1.60	0.47
1:A:78:LEU:CD2	1:B:78:LEU:HD11	2.40	0.47
1:B:127:LEU:O	1:B:154:THR:HB	2.14	0.47
1:C:187:LYS:HG2	3:C:263:HOH:O	2.12	0.47
1:D:129:VAL:CG2	1:D:158:PHE:CD1	2.97	0.47
1:B:155:LEU:HB3	1:B:186:LEU:HD13	1.96	0.47
1:C:89:ILE:HA	1:C:92:LEU:HB2	1.96	0.47
1:D:230:LYS:HA	1:D:230:LYS:HD3	1.73	0.47
1:A:33:LEU:C	1:A:33:LEU:HD23	2.39	0.47
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.51	0.47
1:A:173:ALA:HA	1:A:190:PHE:O	2.13	0.47
1:C:85:PHE:HE2	1:C:112:TYR:OH	1.97	0.47
1:A:114:ARG:HG3	1:A:130:LEU:HG	1.96	0.47
1:C:115:LEU:CB	1:C:130:LEU:H	2.26	0.47
1:C:150:ASP:OD1	1:C:150:ASP:N	2.48	0.47
1:C:155:LEU:CB	1:C:186:LEU:HD12	2.40	0.47
1:D:41:TYR:O	1:D:221:SER:HB2	2.14	0.47
1:D:136:ILE:HG23	1:D:137:PHE:CD1	2.50	0.47
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.51	0.47
1:A:126:GLN:HA	1:A:153:PHE:HE2	1.79	0.47
1:C:97:LYS:NZ	1:D:215:ASP:OD2	2.48	0.47
1:A:119:GLN:HB3	1:A:124:THR:C	2.40	0.47
1:D:52:VAL:O	1:D:56:VAL:HG23	2.15	0.47
1:B:222:ASP:O	1:B:226:LYS:HB2	2.15	0.46
1:C:57:GLU:HB2	1:C:91:TYR:CZ	2.50	0.46
1:D:19:MET:CE	1:D:193:PHE:CE1	2.98	0.46
1:D:144:ILE:HD13	1:D:158:PHE:HE2	1.79	0.46
1:B:40:PRO:HG2	1:B:41:TYR:CD2	2.49	0.46
1:B:207:PHE:CE2	1:B:228:PHE:HB2	2.49	0.46
1:B:229:GLU:CG	1:B:230:LYS:N	2.75	0.46
1:A:49:GLY:HA2	1:A:52:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.62	0.46
1:B:34:VAL:HA	1:B:35:PRO:HD3	1.69	0.46
1:A:126:GLN:O	1:A:126:GLN:HG3	2.15	0.46
1:A:142:VAL:CG1	3:A:296:HOH:O	2.64	0.46
1:A:104:SER:O	1:A:104:SER:OG	2.30	0.46
1:C:41:TYR:CE2	1:C:228:PHE:CE2	3.03	0.46
1:A:140:LYS:O	1:A:168:LYS:N	2.48	0.46
1:C:158:PHE:CE2	1:C:162:LEU:CD2	2.96	0.46
1:C:187:LYS:HD2	1:C:187:LYS:HA	1.74	0.46
1:D:39:LYS:CB	1:D:40:PRO:HD3	2.32	0.46
1:D:63:ILE:O	1:D:66:THR:HB	2.15	0.46
1:C:158:PHE:HD1	1:C:161:ARG:HH12	1.64	0.46
1:D:136:ILE:HG23	1:D:137:PHE:CE1	2.51	0.46
1:C:89:ILE:CG2	1:C:108:PHE:CE2	2.99	0.46
1:B:202:GLY:HA2	1:B:211:PHE:O	2.16	0.46
1:C:198:VAL:CG1	1:C:199:TRP:N	2.79	0.46
1:C:206:ASP:OD1	1:C:209:GLU:HA	2.16	0.46
1:D:69:GLY:O	1:D:70:GLU:HG2	2.16	0.46
1:D:108:PHE:CD1	1:D:108:PHE:N	2.83	0.46
1:A:196:GLU:O	1:A:198:VAL:HG12	2.16	0.45
1:D:176:VAL:CG1	1:D:177:GLU:N	2.79	0.45
1:C:61:TYR:CE2	1:C:65:ARG:HD2	2.52	0.45
1:C:136:ILE:C	1:C:136:ILE:CD1	2.88	0.45
1:C:200:ILE:O	1:C:200:ILE:HG13	2.16	0.45
1:D:6:ILE:CG2	1:D:163:LYS:CD	2.93	0.45
1:A:144:ILE:CD1	1:A:155:LEU:HD11	2.37	0.45
1:B:220:LEU:HD22	1:B:221:SER:N	2.32	0.45
1:D:43:ASP:HA	3:D:280:HOH:O	2.15	0.45
1:A:77:ILE:HD11	1:A:144:ILE:HD11	1.98	0.45
1:C:59:LEU:O	1:C:63:ILE:HD12	2.15	0.45
1:C:79:LYS:HZ2	1:C:79:LYS:HG2	1.68	0.45
1:C:131:SER:HB2	1:C:132:ASP:H	1.43	0.45
1:C:148:ILE:CG1	1:C:149:VAL:N	2.78	0.45
1:C:171:ARG:HA	1:C:189:ASP:OD2	2.17	0.45
1:A:52:VAL:HA	1:A:193:PHE:HZ	1.82	0.45
1:A:96:GLN:CG	1:A:107:PRO:HG3	2.47	0.45
1:A:129:VAL:O	1:A:129:VAL:HG22	2.12	0.45
1:D:39:LYS:N	1:D:40:PRO:CD	2.79	0.45
1:D:77:ILE:HG13	1:D:146:GLU:HG2	1.98	0.45
1:B:134:LEU:CD2	1:B:137:PHE:CE2	2.99	0.45
1:B:141:HIS:CD2	1:B:168:LYS:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ILE:HD13	1:B:148:ILE:HG21	1.67	0.45
1:B:230:LYS:O	1:B:230:LYS:HG3	2.16	0.45
1:C:202:GLY:O	1:C:205:TYR:HD2	1.99	0.45
1:D:34:VAL:HG12	1:D:39:LYS:HA	1.99	0.45
1:A:142:VAL:CB	3:A:296:HOH:O	2.61	0.45
1:B:4:LYS:HA	1:B:4:LYS:HD2	1.39	0.45
1:B:207:PHE:O	1:B:210:MET:HB2	2.17	0.45
1:C:170:MET:O	1:C:171:ARG:HG2	2.17	0.45
1:C:179:ARG:HH21	1:C:196:GLU:HB2	1.82	0.45
1:A:22:PRO:HG2	1:A:25:THR:OG1	2.17	0.45
1:D:22:PRO:HB2	1:D:25:THR:HG21	1.98	0.45
1:D:78:LEU:HD12	1:D:112:TYR:CD2	2.50	0.45
1:D:224:ALA:O	1:D:228:PHE:HB2	2.17	0.45
1:B:134:LEU:HD13	1:B:162:LEU:HD13	1.99	0.45
1:B:200:ILE:HA	1:B:218:ALA:O	2.17	0.45
1:D:39:LYS:HB3	1:D:40:PRO:CD	2.42	0.45
1:D:51:LEU:C	1:D:51:LEU:HD22	2.41	0.45
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.69	0.45
1:C:39:LYS:N	1:C:40:PRO:CD	2.80	0.45
1:A:108:PHE:CD1	1:A:108:PHE:N	2.85	0.44
1:B:208:ASN:O	1:B:209:GLU:HB2	2.17	0.44
1:C:139:ASP:O	1:C:139:ASP:OD1	2.36	0.44
1:D:74:ILE:HG22	1:D:85:PHE:CE1	2.50	0.44
1:C:138:ARG:O	1:C:139:ASP:HB2	2.15	0.44
1:A:6:ILE:HG21	1:A:170:MET:CG	2.47	0.44
1:B:55:ARG:HD2	1:B:55:ARG:HA	1.70	0.44
1:C:216:HIS:ND1	1:C:216:HIS:N	2.49	0.44
1:D:129:VAL:O	1:D:161:ARG:NH2	2.50	0.44
1:C:138:ARG:CG	1:C:138:ARG:HH11	2.30	0.44
1:D:51:LEU:HD23	1:D:51:LEU:HA	1.67	0.44
1:A:63:ILE:CD1	1:A:190:PHE:CG	3.00	0.44
1:A:100:GLY:CA	1:D:65:ARG:HH21	2.30	0.44
1:B:106:PRO:HG2	1:B:109:PHE:CZ	2.53	0.44
1:C:72:LEU:HD13	1:C:74:ILE:HG12	1.98	0.44
1:C:77:ILE:HD13	1:C:113:VAL:CG2	2.47	0.44
1:C:207:PHE:CE2	1:C:225:ARG:HA	2.51	0.44
1:D:79:LYS:HE2	1:D:212:ARG:NH2	2.33	0.44
1:B:227:LYS:CD	1:B:227:LYS:O	2.65	0.44
1:B:61:TYR:O	1:B:64:HIS:HB3	2.17	0.44
1:B:66:THR:HG21	1:B:190:PHE:HZ	1.83	0.44
1:B:136:ILE:O	1:B:140:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PRO:CB	1:C:191:VAL:HG13	2.47	0.44
1:D:23:ASP:O	1:D:25:THR:HG23	2.18	0.44
1:B:155:LEU:HB2	3:B:315:HOH:O	2.18	0.43
1:A:15:ARG:HH12	1:A:191:VAL:HG11	1.78	0.43
1:C:35:PRO:CB	1:C:36:PRO:HD2	2.45	0.43
1:C:148:ILE:HG22	1:C:205:TYR:HE1	1.84	0.43
1:D:207:PHE:HE2	1:D:225:ARG:HA	1.78	0.43
1:B:134:LEU:HD23	1:B:137:PHE:CE2	2.51	0.43
1:C:220:LEU:HD23	1:C:220:LEU:H	1.82	0.43
1:D:19:MET:HE1	1:D:193:PHE:HE1	1.82	0.43
1:A:51:LEU:HD22	1:A:51:LEU:O	2.18	0.43
1:C:56:VAL:HG22	1:C:84:PHE:CE1	2.48	0.43
1:C:79:LYS:NZ	1:D:112:TYR:CD1	2.86	0.43
1:C:175:LEU:O	1:C:192:GLY:HA3	2.18	0.43
1:D:151:THR:HG22	1:D:152:GLY:N	2.33	0.43
1:A:148:ILE:HD12	1:A:176:VAL:HG23	2.00	0.43
1:A:182:ARG:HB2	1:A:182:ARG:NH1	2.33	0.43
1:B:20:TYR:CD1	1:B:20:TYR:C	2.97	0.43
1:B:79:LYS:HE3	3:B:261:HOH:O	2.18	0.43
1:B:133:ASP:CG	1:B:135:SER:HB3	2.44	0.43
1:C:47:LEU:O	1:C:216:HIS:HB3	2.18	0.43
1:C:208:ASN:C	1:C:210:MET:N	2.77	0.43
1:A:35:PRO:HA	1:A:36:PRO:HD3	1.78	0.43
1:C:16:ILE:HG13	1:C:17:GLU:N	2.32	0.43
1:D:202:GLY:O	1:D:205:TYR:HD2	2.01	0.43
1:A:89:ILE:HB	1:A:108:PHE:CZ	2.54	0.43
1:D:143:LEU:HD11	1:D:173:ALA:HB2	2.01	0.43
1:B:130:LEU:HA	1:B:130:LEU:HD23	1.47	0.43
1:B:142:VAL:CG1	1:B:170:MET:HG3	2.49	0.43
1:B:220:LEU:HD11	1:B:225:ARG:HB2	2.00	0.43
1:C:29:ALA:CA	1:C:45:ILE:CD1	2.97	0.43
1:C:29:ALA:HB2	1:C:45:ILE:CD1	2.48	0.43
1:C:148:ILE:HG12	1:C:149:VAL:N	2.34	0.43
1:D:114:ARG:O	1:D:130:LEU:HB3	2.18	0.43
1:D:151:THR:CG2	1:D:153:PHE:HB3	2.48	0.43
1:D:180:THR:CG2	1:D:181:ASP:N	2.77	0.43
1:A:19:MET:HE2	1:A:21:ILE:HD11	1.99	0.43
1:A:99:SER:C	1:A:101:ARG:N	2.76	0.43
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.50	0.42
1:B:42:ILE:CD1	1:B:218:ALA:CB	2.97	0.42
1:D:15:ARG:NH1	1:D:191:VAL:HG21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LYS:N	1:D:168:LYS:H	2.17	0.42
1:A:56:VAL:HG23	1:A:91:TYR:CD2	2.54	0.42
1:B:137:PHE:O	1:B:140:LYS:HB2	2.19	0.42
1:C:68:PHE:CZ	1:C:101:ARG:CG	3.02	0.42
1:D:230:LYS:HD3	1:D:231:VAL:H	1.78	0.42
1:A:32:PHE:C	1:C:58:LYS:HG2	2.44	0.42
1:A:210:MET:O	1:A:211:PHE:HB2	2.19	0.42
1:B:227:LYS:HG3	1:B:228:PHE:CD2	2.55	0.42
1:C:48:PRO:O	1:C:52:VAL:HG13	2.19	0.42
1:C:99:SER:C	1:C:101:ARG:N	2.75	0.42
1:B:129:VAL:HG21	1:B:158:PHE:CE1	2.55	0.42
1:C:21:ILE:HD12	1:C:21:ILE:HG23	1.71	0.42
1:B:187:LYS:HA	1:B:187:LYS:HD3	1.08	0.42
1:D:64:HIS:O	1:D:68:PHE:HB2	2.20	0.42
1:D:129:VAL:CG1	1:D:158:PHE:CB	2.93	0.42
1:D:210:MET:HE2	1:D:210:MET:HB2	1.94	0.42
1:A:182:ARG:CZ	1:A:182:ARG:CB	2.98	0.42
1:B:155:LEU:CB	1:B:186:LEU:CD1	2.98	0.42
1:D:189:ASP:HB3	3:D:294:HOH:O	2.18	0.42
1:A:63:ILE:CD1	1:A:190:PHE:CD2	3.03	0.42
1:A:182:ARG:HG2	1:A:183:SER:O	2.19	0.42
1:D:56:VAL:HG11	1:D:87:LEU:HB3	2.00	0.42
1:D:82:ARG:HD2	1:D:82:ARG:C	2.45	0.42
1:D:172:ILE:HD12	1:D:172:ILE:HG21	1.86	0.42
1:A:110:GLU:CD	1:B:82:ARG:HH11	2.27	0.42
1:A:113:VAL:HG12	1:A:131:SER:CB	2.42	0.42
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.87	0.42
1:C:127:LEU:C	1:C:154:THR:CG2	2.93	0.42
1:D:178:LYS:HD3	1:D:195:ILE:CG1	2.49	0.42
1:D:183:SER:HB3	1:D:185:SER:H	1.85	0.42
1:D:207:PHE:CD2	1:D:228:PHE:CB	3.03	0.42
1:A:143:LEU:HD11	1:A:173:ALA:HB2	2.01	0.41
1:A:202:GLY:O	1:A:205:TYR:HB2	2.20	0.41
1:B:58:LYS:NZ	1:D:30:ASP:O	2.53	0.41
1:C:9:TYR:C	1:C:11:LYS:N	2.77	0.41
1:A:78:LEU:HD13	1:A:112:TYR:HD1	1.85	0.41
1:A:123:SER:HB2	1:A:124:THR:H	1.57	0.41
1:B:59:LEU:O	1:B:63:ILE:CG2	2.69	0.41
1:B:171:ARG:HG2	1:B:189:ASP:CG	2.45	0.41
1:C:9:TYR:C	1:C:11:LYS:H	2.27	0.41
1:C:130:LEU:HD22	1:C:130:LEU:HA	1.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HG23	1:B:106:PRO:CD	2.31	0.41
1:A:151:THR:CG2	1:A:153:PHE:HB3	2.50	0.41
1:C:82:ARG:CD	1:C:86:ASN:ND2	2.83	0.41
1:A:174:THR:O	1:A:191:VAL:HA	2.21	0.41
1:A:202:GLY:HA2	1:A:211:PHE:O	2.20	0.41
1:D:187:LYS:HE3	1:D:187:LYS:HB3	1.74	0.41
1:A:56:VAL:HG21	1:A:87:LEU:HB3	2.03	0.41
1:B:155:LEU:HB2	1:B:186:LEU:HD12	2.03	0.41
1:C:174:THR:O	1:C:191:VAL:HA	2.20	0.41
1:D:79:LYS:HD2	1:D:79:LYS:HA	1.22	0.41
1:A:100:GLY:HA3	1:D:65:ARG:HH21	1.85	0.41
1:B:138:ARG:O	1:B:139:ASP:HB2	2.21	0.41
1:C:44:LYS:HG3	1:C:219:VAL:CB	2.51	0.41
1:C:114:ARG:HG2	1:C:115:LEU:N	2.33	0.41
1:A:6:ILE:HG21	1:A:170:MET:HG3	2.03	0.41
1:A:45:ILE:HD13	1:A:216:HIS:HB2	2.03	0.41
1:A:114:ARG:CG	1:A:130:LEU:HD11	2.51	0.41
1:C:6:ILE:HG23	1:C:7:GLU:OE2	2.21	0.41
1:A:100:GLY:CA	1:D:65:ARG:NH2	2.83	0.41
1:A:198:VAL:HG22	1:A:199:TRP:N	2.35	0.41
1:B:58:LYS:O	1:B:58:LYS:HG3	2.21	0.41
1:B:206:ASP:HA	1:B:210:MET:O	2.20	0.41
1:B:220:LEU:CD1	1:B:225:ARG:HB2	2.51	0.41
1:C:77:ILE:CD1	1:C:113:VAL:CG2	2.98	0.41
1:D:82:ARG:HD2	1:D:86:ASN:HD22	1.85	0.41
1:D:84:PHE:O	1:D:88:LEU:HB2	2.21	0.41
1:B:193:PHE:CD1	1:B:193:PHE:N	2.89	0.41
1:C:17:GLU:CD	1:C:18:PRO:HD2	2.46	0.41
1:C:155:LEU:HA	1:C:155:LEU:HD12	1.11	0.41
1:D:210:MET:HE3	1:D:228:PHE:CE1	2.55	0.41
1:A:107:PRO:HB2	1:A:108:PHE:CD1	2.56	0.40
1:B:36:PRO:HG2	1:B:37:HIS:H	1.86	0.40
1:C:82:ARG:O	1:C:86:ASN:HB2	2.21	0.40
1:A:78:LEU:HA	1:A:78:LEU:HD12	1.61	0.40
1:B:156:THR:CG2	1:B:186:LEU:HD11	2.51	0.40
1:C:85:PHE:HE2	1:C:112:TYR:HH	1.68	0.40
1:C:172:ILE:HG22	1:C:173:ALA:N	2.35	0.40
1:D:44:LYS:HE2	1:D:219:VAL:HG11	2.03	0.40
1:D:178:LYS:CD	1:D:197:ASP:HA	2.38	0.40
1:A:6:ILE:HD12	1:A:170:MET:CG	2.38	0.40
1:B:105:VAL:CG2	1:B:106:PRO:CD	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:HE2	1:B:228:PHE:HB2	1.86	0.40
1:D:107:PRO:CB	1:D:108:PHE:CD1	3.01	0.40
1:D:207:PHE:HD2	1:D:228:PHE:HB2	1.87	0.40
1:D:166:GLY:N	1:D:167:PRO:HD3	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/231 (96%)	184 (82%)	28 (13%)	11 (5%)	1	1
1	B	215/231 (93%)	189 (88%)	18 (8%)	8 (4%)	2	2
1	C	211/231 (91%)	171 (81%)	27 (13%)	13 (6%)	1	0
1	D	211/231 (91%)	186 (88%)	20 (10%)	5 (2%)	4	5
All	All	860/924 (93%)	730 (85%)	93 (11%)	37 (4%)	2	1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	79	LYS
1	A	121	ASP
1	A	230	LYS
1	B	182	ARG
1	B	183	SER
1	B	229	GLU
1	B	230	LYS
1	C	15	ARG
1	C	131	SER
1	C	139	ASP

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Mol	Chain	Res	Type
1	C	154	THR
1	D	79	LYS
1	A	122	ASN
1	A	182	ARG
1	C	128	THR
1	C	207	PHE
1	C	208	ASN
1	D	13	LYS
1	D	132	ASP
1	D	183	SER
1	A	102	GLU
1	A	120	ASN
1	A	132	ASP
1	B	5	PRO
1	C	79	LYS
1	C	228	PHE
1	A	13	LYS
1	B	79	LYS
1	C	152	GLY
1	C	223	ALA
1	C	184	ASN
1	D	148	ILE
1	A	148	ILE
1	B	136	ILE
1	C	192	GLY
1	B	4	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/206 (98%)	139 (69%)	63 (31%)	0	0
1	B	195/206 (95%)	133 (68%)	62 (32%)	0	0
1	C	191/206 (93%)	115 (60%)	76 (40%)	0	0
1	D	192/206 (93%)	121 (63%)	71 (37%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	780/824 (95%)	508 (65%)	272 (35%)	0 0

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	ILE
1	A	8	ASP
1	A	11	LYS
1	A	13	LYS
1	A	25	THR
1	A	34	VAL
1	A	39	LYS
1	A	42	ILE
1	A	43	ASP
1	A	45	ILE
1	A	51	LEU
1	A	52	VAL
1	A	56	VAL
1	A	65	ARG
1	A	66	THR
1	A	72	LEU
1	A	78	LEU
1	A	79	LYS
1	A	87	LEU
1	A	89	ILE
1	A	92	LEU
1	A	101	ARG
1	A	104	SER
1	A	107	PRO
1	A	119	GLN
1	A	120	ASN
1	A	123	SER
1	A	127	LEU
1	A	128	THR
1	A	129	VAL
1	A	136	ILE
1	A	140	LYS
1	A	144	ILE
1	A	145	VAL
1	A	149	VAL
1	A	150	ASP

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Mol	Chain	Res	Type
1	A	154	THR
1	A	155	LEU
1	A	157	GLU
1	A	160	GLU
1	A	162	LEU
1	A	163	LYS
1	A	168	LYS
1	A	172	ILE
1	A	179	ARG
1	A	180	THR
1	A	181	ASP
1	A	182	ARG
1	A	186	LEU
1	A	187	LYS
1	A	191	VAL
1	A	198	VAL
1	A	199	TRP
1	A	200	ILE
1	A	201	VAL
1	A	204	CYS
1	A	215	ASP
1	A	225	ARG
1	A	226	LYS
1	A	227	LYS
1	A	229	GLU
1	A	230	LYS
1	B	3	SER
1	B	4	LYS
1	B	6	ILE
1	B	13	LYS
1	B	15	ARG
1	B	21	ILE
1	B	30	ASP
1	B	34	VAL
1	B	44	LYS
1	B	45	ILE
1	B	46	LEU
1	B	47	LEU
1	B	51	LEU
1	B	53	LYS
1	B	55	ARG
1	B	63	ILE

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Mol	Chain	Res	Type
1	B	65	ARG
1	B	66	THR
1	B	70	GLU
1	B	72	LEU
1	B	74	ILE
1	B	75	ILE
1	B	79	LYS
1	B	82	ARG
1	B	87	LEU
1	B	92	LEU
1	B	94	THR
1	B	96	GLN
1	B	102	GLU
1	B	105	VAL
1	B	115	LEU
1	B	127	LEU
1	B	128	THR
1	B	129	VAL
1	B	130	LEU
1	B	132	ASP
1	B	135	SER
1	B	138	ARG
1	B	145	VAL
1	B	147	ASP
1	B	149	VAL
1	B	150	ASP
1	B	154	THR
1	B	155	LEU
1	B	156	THR
1	B	157	GLU
1	B	161	ARG
1	B	162	LEU
1	B	168	LYS
1	B	170	MET
1	B	178	LYS
1	B	180	THR
1	B	182	ARG
1	B	184	ASN
1	B	187	LYS
1	B	191	VAL
1	B	200	ILE
1	B	204	CYS

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Mol	Chain	Res	Type
1	B	220	LEU
1	B	226	LYS
1	B	227	LYS
1	B	231	VAL
1	C	6	ILE
1	C	8	ASP
1	C	11	LYS
1	C	16	ILE
1	C	17	GLU
1	C	24	ASN
1	C	28	ASN
1	C	30	ASP
1	C	33	LEU
1	C	41	TYR
1	C	42	ILE
1	C	43	ASP
1	C	44	LYS
1	C	45	ILE
1	C	46	LEU
1	C	47	LEU
1	C	51	LEU
1	C	52	VAL
1	C	63	ILE
1	C	65	ARG
1	C	66	THR
1	C	72	LEU
1	C	74	ILE
1	C	78	LEU
1	C	79	LYS
1	C	87	LEU
1	C	88	LEU
1	C	89	ILE
1	C	92	LEU
1	C	97	LYS
1	C	101	ARG
1	C	102	GLU
1	C	103	SER
1	C	104	SER
1	C	105	VAL
1	C	114	ARG
1	C	115	LEU
1	C	127	LEU

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Mol	Chain	Res	Type
1	C	130	LEU
1	C	133	ASP
1	C	134	LEU
1	C	135	SER
1	C	136	ILE
1	C	138	ARG
1	C	144	ILE
1	C	154	THR
1	C	155	LEU
1	C	161	ARG
1	C	162	LEU
1	C	163	LYS
1	C	165	VAL
1	C	168	LYS
1	C	169	SER
1	C	170	MET
1	C	171	ARG
1	C	172	ILE
1	C	174	THR
1	C	176	VAL
1	C	177	GLU
1	C	178	LYS
1	C	186	LEU
1	C	187	LYS
1	C	193	PHE
1	C	194	SER
1	C	196	GLU
1	C	198	VAL
1	C	203	CYS
1	C	204	CYS
1	C	209	GLU
1	C	216	HIS
1	C	217	VAL
1	C	220	LEU
1	C	227	LYS
1	C	229	GLU
1	C	230	LYS
1	C	231	VAL
1	D	6	ILE
1	D	11	LYS
1	D	16	ILE
1	D	21	ILE

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Mol	Chain	Res	Type
1	D	25	THR
1	D	30	ASP
1	D	38	CYS
1	D	39	LYS
1	D	42	ILE
1	D	45	ILE
1	D	47	LEU
1	D	51	LEU
1	D	53	LYS
1	D	59	LEU
1	D	72	LEU
1	D	74	ILE
1	D	78	LEU
1	D	79	LYS
1	D	87	LEU
1	D	88	LEU
1	D	90	ASP
1	D	94	THR
1	D	99	SER
1	D	102	GLU
1	D	104	SER
1	D	105	VAL
1	D	110	GLU
1	D	113	VAL
1	D	115	LEU
1	D	128	THR
1	D	129	VAL
1	D	130	LEU
1	D	132	ASP
1	D	139	ASP
1	D	145	VAL
1	D	147	ASP
1	D	148	ILE
1	D	149	VAL
1	D	151	THR
1	D	153	PHE
1	D	154	THR
1	D	155	LEU
1	D	160	GLU
1	D	162	LEU
1	D	165	VAL
1	D	168	LYS

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Mol	Chain	Res	Type
1	D	172	ILE
1	D	181	ASP
1	D	182	ARG
1	D	183	SER
1	D	184	ASN
1	D	185	SER
1	D	187	LYS
1	D	194	SER
1	D	199	TRP
1	D	200	ILE
1	D	201	VAL
1	D	203	CYS
1	D	204	CYS
1	D	209	GLU
1	D	210	MET
1	D	215	ASP
1	D	219	VAL
1	D	220	LEU
1	D	221	SER
1	D	222	ASP
1	D	225	ARG
1	D	226	LYS
1	D	229	GLU
1	D	230	LYS
1	D	231	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	216	HIS
1	B	96	GLN
1	B	184	ASN
1	C	28	ASN
1	C	86	ASN
1	D	24	ASN
1	D	64	HIS
1	D	86	ASN
1	D	96	GLN
1	D	184	ASN
1	D	208	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.