Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:22 PM EDT

PDB ID	:	3PVA
Title	:	PENICILLIN V ACYLASE FROM B. SPHAERICUS
Authors	:	Suresh, C.G.; Pundle, A.V.; Rao, K.N.; Sivaraman, H.; Brannigan, J.A.; Mcvey, C.E.; Verma, C.S.; Dauter, Z.; Dodson, E.J.; Dodson, G.G.
Deposited on	:	1998-11-13
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

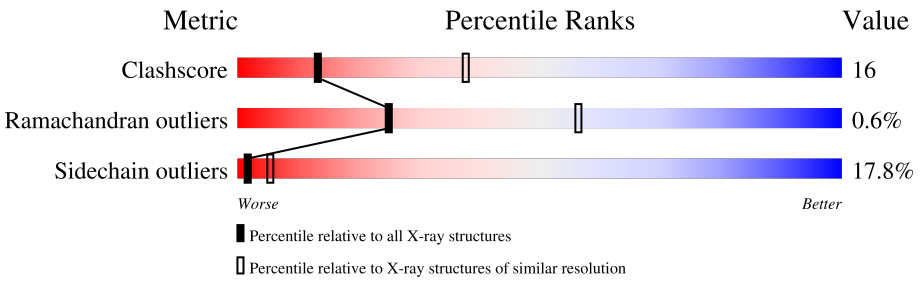
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	64% 25% 9% •
1	B	335	63% 26% 10% •
1	C	335	61% 29% 8% •
1	D	335	63% 27% 8% •
1	E	335	60% 29% 9% •
1	F	335	58% 31% 10% •
1	G	335	61% 28% 9% •
1	H	335	59% 32% 8% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23640 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 PROTEIN (PENICILLIN V ACYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2605	1658	425	508	14	0	0	0
1	B	334	2605	1658	425	508	14	0	0	0
1	C	334	2605	1658	425	508	14	0	0	0
1	D	334	2605	1658	425	508	14	0	0	0
1	E	334	2605	1658	425	508	14	0	0	0
1	F	334	2605	1658	425	508	14	0	0	0
1	G	334	2605	1658	425	508	14	0	0	0
1	H	334	2605	1658	425	508	14	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	346	346	346	0	0
2	B	348	348	348	0	0
2	C	350	350	350	0	0
2	D	356	356	356	0	0
2	E	353	353	353	0	0
2	F	350	350	350	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	G	351	351	351	0	0
			Total	O		
2	H	346	346	346	0	0

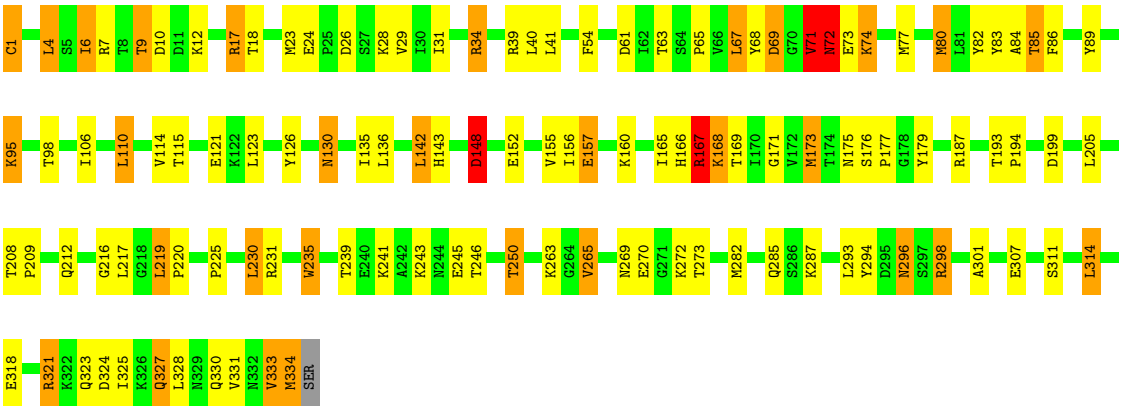
3 Residue-property plots (i)

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.

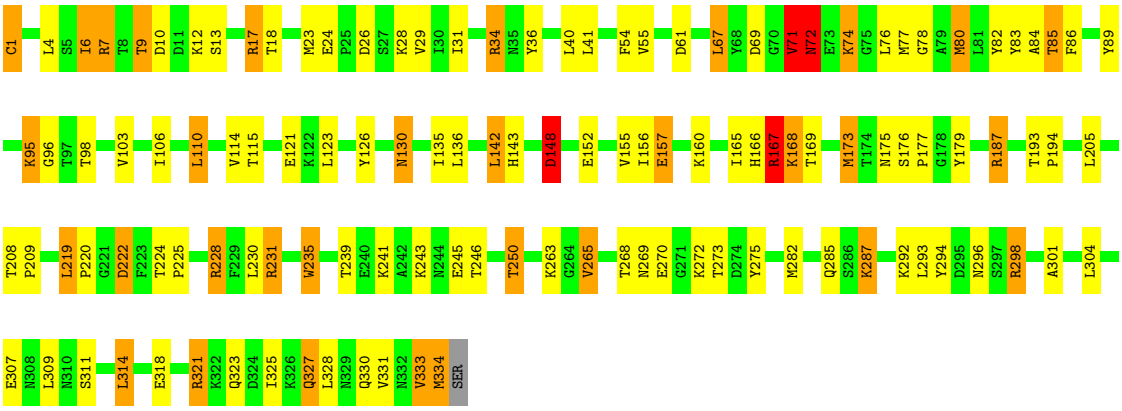
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain A: 64% 25% 9%



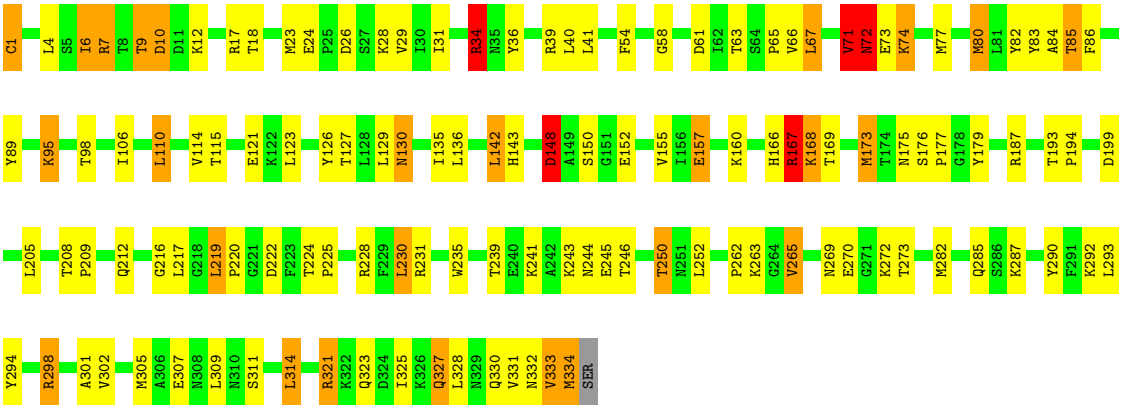
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain B: 63% 26% 10%



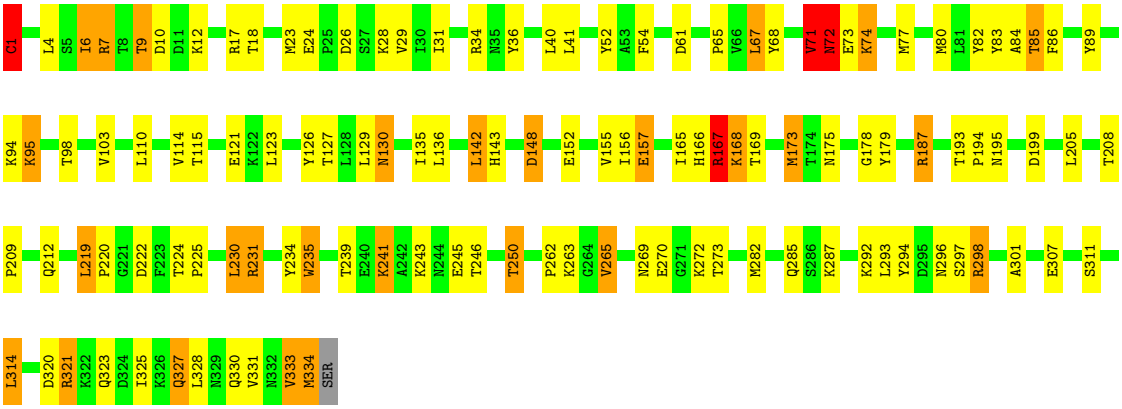
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain C: 61% 29% 8%



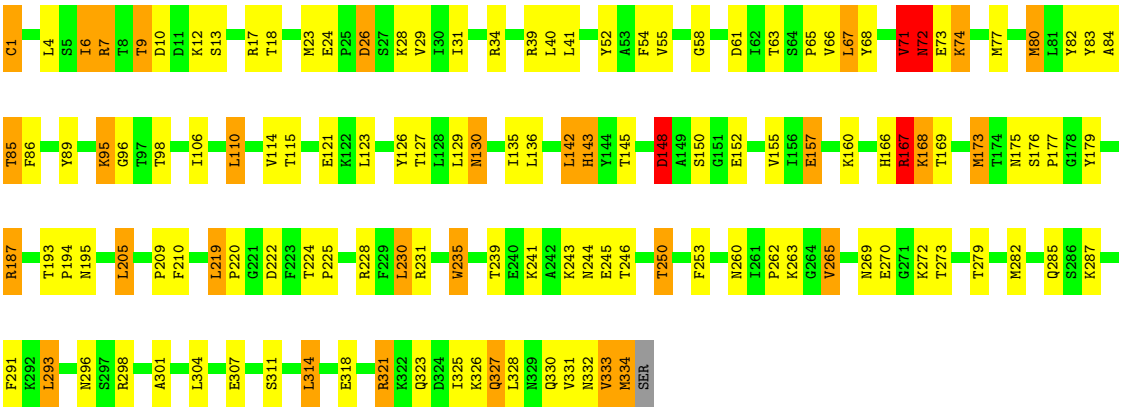
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain D:



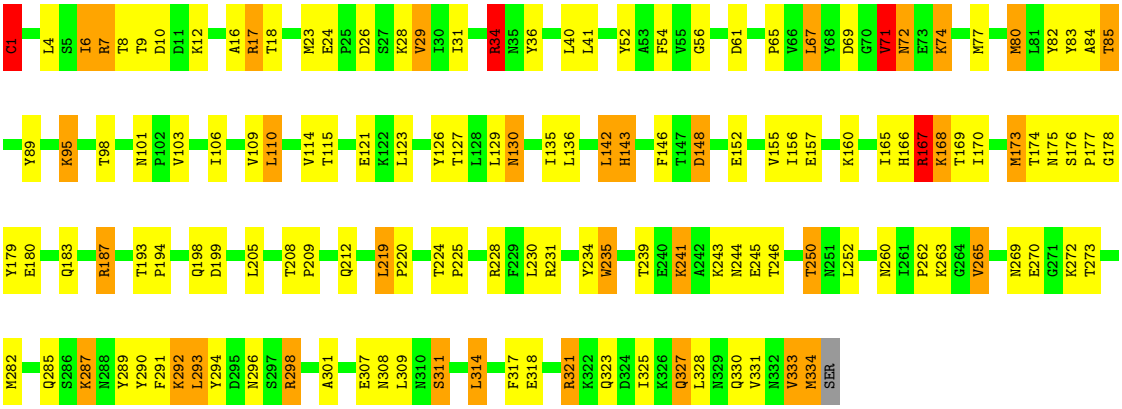
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain E:



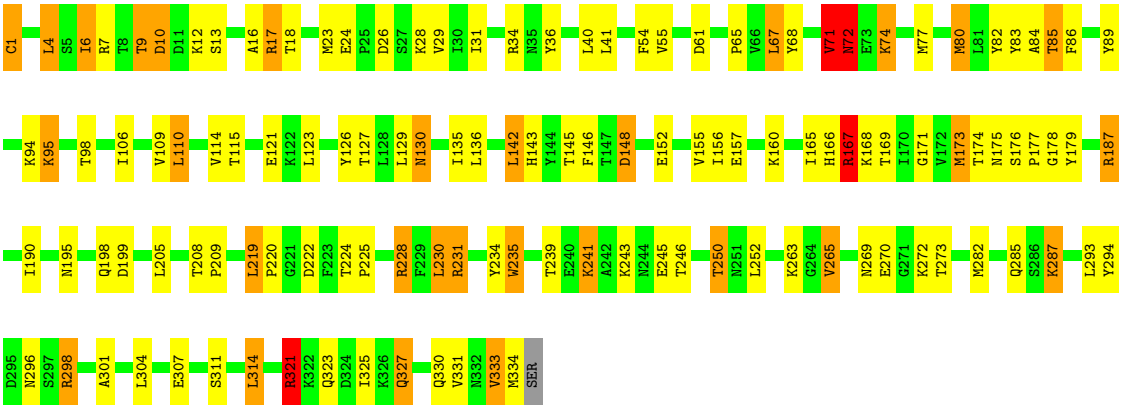
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain F:



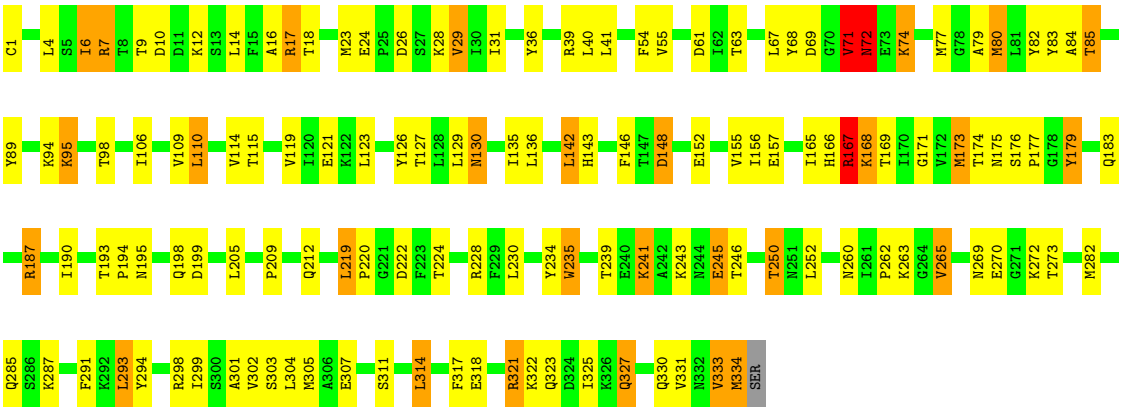
- Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain G:



- Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.40Å 129.60Å 156.70Å 88.30° 83.40° 84.60°	Depositor
Resolution (Å)	14.00 – 2.80	Depositor
% Data completeness (in resolution range)	85.0 (14.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23640	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	0/2660	1.27	20/3617 (0.6%)
1	B	0.51	0/2660	1.30	21/3617 (0.6%)
1	C	0.50	0/2660	1.26	21/3617 (0.6%)
1	D	0.50	0/2660	1.29	24/3617 (0.7%)
1	E	0.48	0/2660	1.26	17/3617 (0.5%)
1	F	0.48	0/2660	1.29	19/3617 (0.5%)
1	G	0.49	0/2660	1.29	25/3617 (0.7%)
1	H	0.48	0/2660	1.26	16/3617 (0.4%)
All	All	0.49	0/21280	1.28	163/28936 (0.6%)

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	A	0	2
1	B	0	2
1	C	0	2
1	E	0	3
1	G	0	1
1	H	0	1
All	All	0	11

There are no bond length outliers.

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	231	ARG	NE-CZ-NH2	10.57	125.58	120.30
1	F	187	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	B	231	ARG	NE-CZ-NH2	10.39	125.49	120.30
1	D	7	ARG	NE-CZ-NH1	10.27	125.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	231	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	B	157	GLU	OE1-CD-OE2	-9.46	111.95	123.30
1	H	7	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	D	231	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	E	80	MET	CA-CB-CG	8.77	128.21	113.30
1	A	167	ARG	CD-NE-CZ	8.77	135.88	123.60
1	G	187	ARG	NE-CZ-NH1	-8.59	116.01	120.30
1	F	167	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	E	167	ARG	CD-NE-CZ	8.40	135.36	123.60
1	A	298	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	D	157	GLU	OE1-CD-OE2	-8.29	113.35	123.30
1	C	167	ARG	CD-NE-CZ	8.29	135.20	123.60
1	B	167	ARG	CD-NE-CZ	8.27	135.18	123.60
1	D	72	ASN	CB-CA-C	-8.21	93.99	110.40
1	G	167	ARG	CD-NE-CZ	8.13	134.99	123.60
1	C	298	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	H	167	ARG	CD-NE-CZ	8.09	134.92	123.60
1	D	167	ARG	CD-NE-CZ	8.06	134.88	123.60
1	F	167	ARG	CD-NE-CZ	7.99	134.78	123.60
1	C	80	MET	CA-CB-CG	7.85	126.65	113.30
1	A	231	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	F	199	ASP	CB-CG-OD1	7.72	125.25	118.30
1	H	72	ASN	CB-CA-C	-7.69	95.02	110.40
1	C	148	ASP	CB-CG-OD2	7.55	125.10	118.30
1	G	72	ASN	CB-CA-C	-7.52	95.35	110.40
1	G	228	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	D	298	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	F	80	MET	CA-CB-CG	7.37	125.82	113.30
1	C	72	ASN	CB-CA-C	-7.32	95.76	110.40
1	A	80	MET	CA-CB-CG	7.27	125.67	113.30
1	B	72	ASN	CB-CA-C	-7.26	95.89	110.40
1	D	7	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	G	71	VAL	CB-CA-C	-7.25	97.63	111.40
1	G	80	MET	CA-CB-CG	7.22	125.58	113.30
1	B	80	MET	CA-CB-CG	7.17	125.49	113.30
1	A	72	ASN	CB-CA-C	-7.15	96.10	110.40
1	C	71	VAL	CB-CA-C	-7.08	97.94	111.40
1	B	9	THR	C-N-CA	7.06	139.36	121.70
1	F	228	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	G	228	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	F	1	CYS	CA-CB-SG	6.97	126.54	114.00
1	D	80	MET	CA-CB-CG	6.94	125.10	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	72	ASN	CB-CA-C	-6.93	96.55	110.40
1	C	228	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	G	298	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	F	298	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	C	142	LEU	CA-CB-CG	6.82	131.00	115.30
1	H	79	ALA	N-CA-CB	-6.79	100.59	110.10
1	H	148	ASP	CB-CA-C	-6.77	96.86	110.40
1	D	142	LEU	CA-CB-CG	6.75	130.83	115.30
1	H	228	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	B	187	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	C	148	ASP	CB-CA-C	-6.74	96.92	110.40
1	G	17	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	G	17	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	G	231	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	B	148	ASP	CB-CG-OD2	6.66	124.29	118.30
1	D	320	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	148	ASP	CB-CA-C	-6.56	97.27	110.40
1	A	231	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	F	199	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	G	142	LEU	CA-CB-CG	6.51	130.27	115.30
1	B	298	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	G	167	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	G	199	ASP	CB-CG-OD1	6.41	124.07	118.30
1	F	148	ASP	CB-CA-C	-6.39	97.61	110.40
1	D	71	VAL	CB-CA-C	-6.39	99.27	111.40
1	F	34	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	148	ASP	CB-CA-C	-6.36	97.68	110.40
1	A	157	GLU	OE1-CD-OE2	-6.34	115.69	123.30
1	G	199	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	298	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	E	142	LEU	CA-CB-CG	6.32	129.84	115.30
1	E	231	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	H	142	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	167	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	231	ARG	NE-CZ-NH2	6.25	123.43	120.30
1	D	9	THR	C-N-CA	6.19	137.17	121.70
1	A	71	VAL	CB-CA-C	-6.18	99.66	111.40
1	F	142	LEU	CA-CB-CG	6.17	129.49	115.30
1	D	148	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	199	ASP	CB-CG-OD1	6.14	123.83	118.30
1	D	157	GLU	CG-CD-OE1	6.14	130.57	118.30
1	B	157	GLU	CG-CD-OE1	6.11	130.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	187	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	199	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	148	ASP	CB-CA-C	-6.09	98.22	110.40
1	B	167	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	157	GLU	CG-CD-OE1	6.07	130.44	118.30
1	B	71	VAL	CB-CA-C	-6.07	99.86	111.40
1	E	71	VAL	CB-CA-C	-6.05	99.90	111.40
1	G	298	ARG	NH1-CZ-NH2	5.99	125.99	119.40
1	C	157	GLU	OE1-CD-OE2	-5.97	116.13	123.30
1	A	68	TYR	CB-CG-CD1	5.90	124.54	121.00
1	E	148	ASP	CB-CA-C	-5.88	98.65	110.40
1	C	9	THR	C-N-CA	5.86	136.35	121.70
1	G	68	TYR	CB-CG-CD1	5.82	124.49	121.00
1	A	69	ASP	CB-CG-OD1	5.82	123.53	118.30
1	E	167	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	H	7	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	H	148	ASP	CB-CG-OD2	5.76	123.48	118.30
1	E	157	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	E	230	LEU	CA-CB-CG	5.74	128.50	115.30
1	G	321	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	G	9	THR	C-N-CA	5.71	135.97	121.70
1	D	1	CYS	CA-CB-SG	5.70	124.27	114.00
1	C	199	ASP	CB-CG-OD1	5.69	123.42	118.30
1	E	9	THR	C-N-CA	5.68	135.90	121.70
1	G	148	ASP	CB-CA-C	-5.68	99.04	110.40
1	C	199	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	E	231	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	H	245	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	E	7	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	9	THR	C-N-CA	5.57	135.63	121.70
1	F	298	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	A	199	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	230	LEU	CA-CB-CG	5.51	127.97	115.30
1	D	292	LYS	N-CA-CB	5.51	120.51	110.60
1	A	148	ASP	CB-CG-OD2	5.51	123.25	118.30
1	B	142	LEU	CA-CB-CG	5.50	127.94	115.30
1	E	187	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	C	292	LYS	N-CA-CB	5.49	120.47	110.60
1	B	222	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	H	80	MET	CA-CB-CG	5.46	122.59	113.30
1	B	292	LYS	N-CA-CB	5.42	120.36	110.60
1	A	142	LEU	CA-CB-CG	5.42	127.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	298	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	228	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	7	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	F	234	TYR	CA-CB-CG	-5.36	103.22	113.40
1	B	228	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	34	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	F	7	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	230	LEU	CA-CB-CG	5.31	127.52	115.30
1	F	292	LYS	N-CA-CB	5.27	120.08	110.60
1	H	234	TYR	CA-CB-CG	-5.26	103.40	113.40
1	H	187	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	34	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	187	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	C	148	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	G	10	ASP	N-CA-CB	-5.21	101.23	110.60
1	H	179	TYR	CB-CG-CD1	5.20	124.12	121.00
1	C	231	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	B	298	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	D	234	TYR	CA-CB-CG	-5.14	103.63	113.40
1	H	199	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	F	71	VAL	CB-CA-C	-5.14	101.64	111.40
1	E	80	MET	CB-CA-C	-5.13	100.14	110.40
1	C	231	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	H	71	VAL	CB-CA-C	-5.10	101.72	111.40
1	D	297	SER	CA-CB-OG	5.07	124.89	111.20
1	G	230	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	7	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	230	LEU	CA-CB-CG	5.05	126.91	115.30
1	G	234	TYR	CA-CB-CG	-5.05	103.81	113.40
1	E	26	ASP	N-CA-CB	5.04	119.67	110.60
1	D	231	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	D	68	TYR	CB-CG-CD1	5.02	124.01	121.00
1	G	80	MET	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ASP	Mainchain
1	A	72	ASN	Mainchain
1	B	148	ASP	Mainchain
1	B	96	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	C	148	ASP	Mainchain
1	C	72	ASN	Mainchain
1	E	148	ASP	Mainchain
1	E	72	ASN	Mainchain
1	E	96	GLY	Mainchain
1	G	72	ASN	Mainchain
1	H	72	ASN	Mainchain

5.2 Too-close contacts (i)

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	2605	0	2582	88	0
1	B	2605	0	2582	89	0
1	C	2605	0	2582	92	0
1	D	2605	0	2582	81	0
1	E	2605	0	2582	97	0
1	F	2605	0	2582	103	0
1	G	2605	0	2582	88	0
1	H	2605	0	2582	107	0
2	A	346	0	0	13	0
2	B	348	0	0	10	0
2	C	350	0	0	10	0
2	D	356	0	0	12	0
2	E	353	0	0	13	0
2	F	350	0	0	15	0
2	G	351	0	0	15	0
2	H	346	0	0	17	0
All	All	23640	0	20656	671	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 16.

All (671) 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:85:THR:HG21	1:C:187:ARG:HH22	1.17	1.08
1:E:187:ARG:HH22	1:G:85:THR:HG21	1.15	1.04
1:E:85:THR:HG21	1:G:187:ARG:HH22	1.19	1.03
1:B:187:ARG:HH22	1:D:85:THR:HG21	1.24	1.00
1:A:187:ARG:HH22	1:C:85:THR:HG21	1.23	1.00
1:B:85:THR:HG21	1:D:187:ARG:HH22	1.23	1.00
1:F:187:ARG:HH22	1:H:85:THR:HG21	1.29	0.98
1:F:85:THR:HG21	1:H:187:ARG:HH22	1.29	0.98
1:H:71:VAL:HG22	1:H:282:MET:HG2	1.53	0.89
1:C:235:TRP:O	1:C:239:THR:HG23	1.78	0.84
1:D:235:TRP:O	1:D:239:THR:HG23	1.78	0.83
1:H:95:LYS:H	1:H:95:LYS:HD2	1.44	0.83
1:B:71:VAL:HG22	1:B:282:MET:HG2	1.61	0.82
1:F:95:LYS:H	1:F:95:LYS:HD2	1.44	0.82
1:B:95:LYS:H	1:B:95:LYS:HD2	1.43	0.81
1:D:95:LYS:H	1:D:95:LYS:HD2	1.46	0.81
1:A:71:VAL:HG22	1:A:282:MET:HG2	1.63	0.80
1:A:235:TRP:O	1:A:239:THR:HG23	1.82	0.80
1:D:71:VAL:HG22	1:D:282:MET:HG2	1.64	0.79
1:E:235:TRP:O	1:E:239:THR:HG23	1.81	0.79
1:G:235:TRP:O	1:G:239:THR:HG23	1.82	0.79
1:G:71:VAL:HG22	1:G:282:MET:HG2	1.63	0.79
1:C:40:LEU:HD21	1:C:126:TYR:HE1	1.46	0.78
1:B:71:VAL:HG13	1:B:77:MET:HG2	1.65	0.78
1:G:95:LYS:H	1:G:95:LYS:HD2	1.47	0.78
1:A:95:LYS:H	1:A:95:LYS:HD2	1.49	0.78
1:D:71:VAL:HG13	1:D:77:MET:HG2	1.66	0.78
1:E:95:LYS:HD2	1:E:95:LYS:H	1.49	0.77
1:F:54:PHE:HE1	1:F:67:LEU:HD13	1.47	0.77
1:H:235:TRP:O	1:H:239:THR:HG23	1.84	0.77
1:E:71:VAL:HG22	1:E:282:MET:HG2	1.65	0.76
1:C:95:LYS:H	1:C:95:LYS:HD2	1.48	0.76
1:B:84:ALA:O	1:B:85:THR:HB	1.86	0.75
1:C:84:ALA:O	1:C:85:THR:HB	1.85	0.75
1:H:68:TYR:HA	1:H:80:MET:HE2	1.68	0.74
1:C:71:VAL:HG22	1:C:282:MET:HG2	1.68	0.74
1:E:54:PHE:HE1	1:E:67:LEU:HD13	1.52	0.73
1:H:40:LEU:HD21	1:H:126:TYR:HE1	1.53	0.73
1:B:235:TRP:O	1:B:239:THR:HG23	1.89	0.73
1:D:84:ALA:O	1:D:85:THR:HB	1.88	0.73
1:F:71:VAL:HG22	1:F:282:MET:HG2	1.70	0.73
1:D:54:PHE:HE1	1:D:67:LEU:HD13	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LEU:HD21	1:E:126:TYR:HE1	1.54	0.72
1:B:54:PHE:HE1	1:B:67:LEU:HD13	1.55	0.72
1:A:84:ALA:O	1:A:85:THR:HB	1.90	0.72
1:B:89:TYR:HB2	1:B:130:ASN:HD22	1.54	0.71
1:E:84:ALA:O	1:E:85:THR:HB	1.89	0.71
1:C:71:VAL:HG13	1:C:77:MET:HG2	1.71	0.71
1:A:89:TYR:HB2	1:A:130:ASN:HD22	1.54	0.71
1:G:40:LEU:HD21	1:G:126:TYR:HE1	1.55	0.71
1:C:54:PHE:HE1	1:C:67:LEU:HD13	1.56	0.71
1:E:155:VAL:HG13	1:E:173:MET:CE	2.21	0.71
1:D:40:LEU:HD21	1:D:126:TYR:HE1	1.55	0.70
1:H:84:ALA:O	1:H:85:THR:HB	1.90	0.70
1:H:71:VAL:HG13	1:H:77:MET:HG2	1.73	0.70
1:H:89:TYR:HB2	1:H:130:ASN:HD22	1.56	0.69
1:D:89:TYR:HB2	1:D:130:ASN:HD22	1.56	0.69
1:A:327:GLN:HB3	1:A:331:VAL:HG23	1.75	0.69
1:F:89:TYR:HB2	1:F:130:ASN:HD22	1.58	0.69
1:A:54:PHE:HE1	1:A:67:LEU:HD13	1.57	0.68
1:G:84:ALA:O	1:G:85:THR:HB	1.93	0.68
1:B:40:LEU:HD21	1:B:126:TYR:HE1	1.58	0.68
1:E:89:TYR:HB2	1:E:130:ASN:HD22	1.58	0.68
1:D:155:VAL:HG13	1:D:173:MET:CE	2.23	0.68
1:F:219:LEU:HD23	1:F:220:PRO:HD2	1.76	0.68
1:B:155:VAL:HG13	1:B:173:MET:CE	2.25	0.67
1:C:89:TYR:HB2	1:C:130:ASN:HD22	1.59	0.67
1:F:235:TRP:O	1:F:239:THR:HG23	1.95	0.67
1:A:40:LEU:HD21	1:A:126:TYR:HE1	1.60	0.66
1:F:40:LEU:HD21	1:F:126:TYR:HE1	1.59	0.66
1:G:54:PHE:HE2	1:G:67:LEU:HD13	1.61	0.66
1:A:71:VAL:HG13	1:A:77:MET:HG2	1.76	0.66
1:E:72:ASN:HB3	1:E:74:LYS:H	1.61	0.65
1:E:71:VAL:HG13	1:E:77:MET:HG2	1.77	0.65
1:H:72:ASN:HB3	1:H:74:LYS:H	1.61	0.65
1:A:85:THR:HG21	1:C:187:ARG:NH2	2.02	0.65
1:E:209:PRO:HG2	2:E:2665:HOH:O	1.96	0.65
1:C:155:VAL:HG13	1:C:173:MET:CE	2.27	0.64
1:F:85:THR:HG21	1:H:187:ARG:NH2	2.08	0.64
1:F:1:CYS:HB3	1:F:18:THR:O	1.97	0.64
1:F:243:LYS:HE3	2:F:1949:HOH:O	1.98	0.64
1:E:298:ARG:HG3	1:H:298:ARG:HG3	1.79	0.64
1:H:31:ILE:HD12	1:H:307:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:VAL:HG13	1:H:173:MET:HE3	1.79	0.64
1:A:74:LYS:HG3	1:A:114:VAL:HG22	1.79	0.64
1:B:72:ASN:HB3	1:B:74:LYS:H	1.63	0.64
1:E:219:LEU:HD23	1:E:220:PRO:HD2	1.78	0.64
1:E:187:ARG:NH2	1:G:85:THR:HG21	2.00	0.63
1:E:323:GLN:HE21	1:H:250:THR:CG2	2.10	0.63
1:F:71:VAL:HG13	1:F:77:MET:HG2	1.80	0.63
1:H:327:GLN:HB3	1:H:331:VAL:HG23	1.79	0.63
1:A:187:ARG:NH2	1:C:85:THR:HG21	2.05	0.63
1:D:12:LYS:HD3	1:D:245:GLU:HB2	1.80	0.63
1:F:187:ARG:NH2	1:H:85:THR:HG21	2.08	0.63
1:G:89:TYR:HB2	1:G:130:ASN:HD22	1.62	0.63
1:F:7:ARG:HB2	2:F:1976:HOH:O	1.98	0.63
1:G:72:ASN:HB3	1:G:74:LYS:H	1.64	0.63
1:C:327:GLN:HB3	1:C:331:VAL:HG23	1.81	0.62
1:A:250:THR:CG2	1:D:323:GLN:HE21	2.12	0.62
1:B:74:LYS:HG3	1:B:114:VAL:HG22	1.82	0.62
1:E:334:MET:O	1:H:245:GLU:HB3	1.99	0.62
1:F:115:THR:HA	1:F:148:ASP:OD1	1.98	0.62
1:G:7:ARG:HB2	2:G:2326:HOH:O	2.00	0.62
1:B:7:ARG:HB2	2:B:535:HOH:O	1.99	0.62
1:C:243:LYS:HE3	2:C:555:HOH:O	2.00	0.62
1:F:84:ALA:O	1:F:85:THR:HB	2.00	0.62
1:A:74:LYS:CG	1:A:114:VAL:HG22	2.30	0.61
1:B:323:GLN:HE21	1:C:250:THR:CG2	2.13	0.61
1:C:72:ASN:HB3	1:C:74:LYS:H	1.65	0.61
1:A:31:ILE:HD12	1:A:307:GLU:HG3	1.80	0.61
1:A:72:ASN:HB3	1:A:74:LYS:H	1.65	0.61
1:B:327:GLN:HB3	1:B:331:VAL:HG23	1.81	0.61
1:E:327:GLN:HB3	1:E:331:VAL:HG23	1.82	0.61
1:C:7:ARG:HB2	2:C:577:HOH:O	2.00	0.61
1:G:71:VAL:HG13	1:G:77:MET:HG2	1.83	0.61
1:F:12:LYS:HD3	1:F:245:GLU:HB2	1.82	0.61
1:G:209:PRO:HG2	2:G:1965:HOH:O	2.01	0.61
1:H:219:LEU:HD23	1:H:220:PRO:HD2	1.82	0.60
1:F:327:GLN:HB3	1:F:331:VAL:HG23	1.82	0.60
1:F:328:LEU:HG	2:G:2408:HOH:O	2.01	0.60
1:G:219:LEU:HD23	1:G:220:PRO:HD2	1.83	0.60
1:A:298:ARG:HG3	1:D:298:ARG:HG3	1.83	0.60
1:C:74:LYS:CG	1:C:114:VAL:HG22	2.32	0.60
1:E:250:THR:CG2	1:H:323:GLN:HE21	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:GLN:HB3	1:D:331:VAL:HG23	1.84	0.60
1:F:167:ARG:HD2	2:F:1984:HOH:O	2.01	0.60
1:E:7:ARG:HB2	2:E:1626:HOH:O	2.01	0.59
1:B:250:THR:CG2	1:C:323:GLN:HE21	2.15	0.59
2:B:598:HOH:O	1:C:328:LEU:HG	2.02	0.59
1:B:74:LYS:CG	1:B:114:VAL:HG22	2.33	0.59
1:A:219:LEU:HD23	1:A:220:PRO:HD2	1.85	0.59
1:B:250:THR:HG21	1:C:323:GLN:HE21	1.67	0.59
1:C:31:ILE:HD12	1:C:307:GLU:HG3	1.84	0.59
1:G:327:GLN:HB3	1:G:331:VAL:HG23	1.84	0.59
1:H:61:ASP:HB3	1:H:135:ILE:HD11	1.84	0.59
1:A:155:VAL:HG13	1:A:173:MET:CE	2.32	0.59
1:E:85:THR:HG21	1:G:187:ARG:NH2	2.04	0.59
1:F:333:VAL:HA	2:G:2200:HOH:O	2.03	0.59
1:G:61:ASP:HB3	1:G:135:ILE:HD11	1.85	0.59
1:B:1:CYS:HB3	1:B:18:THR:O	2.02	0.59
1:F:265:VAL:CG1	1:G:239:THR:HG22	2.33	0.58
1:B:323:GLN:HE21	1:C:250:THR:HG21	1.68	0.58
1:H:9:THR:OG1	1:H:243:LYS:HA	2.03	0.58
1:A:1:CYS:HB3	1:A:18:THR:O	2.02	0.58
1:A:12:LYS:HD3	1:A:245:GLU:HB2	1.84	0.58
1:C:74:LYS:HG3	1:C:114:VAL:HG22	1.84	0.58
1:G:155:VAL:HG13	1:G:173:MET:CE	2.33	0.58
1:H:1:CYS:HB3	1:H:18:THR:O	2.04	0.58
1:H:74:LYS:HG3	1:H:114:VAL:HG22	1.84	0.58
1:B:12:LYS:HD3	1:B:245:GLU:HB2	1.84	0.58
1:E:243:LYS:HE3	2:E:1599:HOH:O	2.03	0.58
1:F:9:THR:OG1	1:F:243:LYS:HA	2.04	0.58
1:E:74:LYS:HG3	1:E:114:VAL:HG22	1.85	0.58
1:A:250:THR:HG21	1:D:323:GLN:HE21	1.69	0.58
1:F:209:PRO:HG2	2:G:2315:HOH:O	2.04	0.58
1:B:209:PRO:HG2	2:C:570:HOH:O	2.04	0.57
1:H:243:LYS:HE3	2:H:576:HOH:O	2.03	0.57
1:D:95:LYS:H	1:D:95:LYS:CD	2.15	0.57
1:E:74:LYS:CG	1:E:114:VAL:HG22	2.35	0.57
1:E:265:VAL:CG1	1:H:239:THR:HG22	2.34	0.57
1:B:31:ILE:HD12	1:B:307:GLU:HG3	1.86	0.57
1:B:95:LYS:H	1:B:95:LYS:CD	2.14	0.57
1:H:54:PHE:HE1	1:H:67:LEU:HD13	1.68	0.57
1:A:323:GLN:HE21	1:D:250:THR:CG2	2.18	0.57
1:D:31:ILE:HD12	1:D:307:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:LYS:CG	1:F:114:VAL:HG22	2.34	0.57
1:B:85:THR:HG21	1:D:187:ARG:NH2	2.07	0.57
1:A:7:ARG:HB2	2:A:513:HOH:O	2.04	0.57
1:D:61:ASP:HB3	1:D:135:ILE:HD11	1.86	0.57
1:E:83:TYR:CE2	1:E:157:GLU:HG2	2.40	0.57
1:B:239:THR:HG22	1:C:265:VAL:CG1	2.35	0.56
1:C:219:LEU:HD23	1:C:220:PRO:HD2	1.87	0.56
1:D:74:LYS:CG	1:D:114:VAL:HG22	2.35	0.56
2:B:527:HOH:O	1:C:209:PRO:HG2	2.05	0.56
1:C:167:ARG:HD2	2:C:584:HOH:O	2.04	0.56
1:G:31:ILE:HD12	1:G:307:GLU:HG3	1.86	0.56
1:A:265:VAL:CG1	1:D:239:THR:HG22	2.35	0.56
1:E:95:LYS:H	1:E:95:LYS:CD	2.18	0.56
1:E:12:LYS:HD3	1:E:245:GLU:HB2	1.86	0.56
1:F:175:ASN:HB2	1:F:225:PRO:HB3	1.88	0.56
2:B:443:HOH:O	1:C:250:THR:HG21	2.05	0.56
1:A:250:THR:HG21	2:D:508:HOH:O	2.05	0.56
1:F:72:ASN:HB3	1:F:74:LYS:H	1.71	0.56
1:G:74:LYS:HG3	1:G:114:VAL:HG22	1.88	0.56
1:G:9:THR:OG1	1:G:243:LYS:HA	2.05	0.56
1:A:209:PRO:HG2	2:D:596:HOH:O	2.05	0.55
1:A:333:VAL:HA	2:D:502:HOH:O	2.06	0.55
1:A:95:LYS:H	1:A:95:LYS:CD	2.19	0.55
1:D:243:LYS:HE3	2:D:582:HOH:O	2.05	0.55
1:C:40:LEU:HD21	1:C:126:TYR:CE1	2.34	0.55
1:F:83:TYR:CZ	1:F:157:GLU:HG2	2.41	0.55
1:H:6:ILE:HD12	1:H:252:LEU:HG	1.89	0.55
1:F:219:LEU:CD2	1:F:220:PRO:HD2	2.36	0.55
1:H:115:THR:HA	1:H:148:ASP:OD1	2.07	0.55
1:E:239:THR:HG22	1:H:265:VAL:CG1	2.37	0.55
1:D:263:LYS:HD2	1:D:294:TYR:CE2	2.42	0.55
1:F:6:ILE:HB	2:F:1809:HOH:O	2.07	0.55
1:F:333:VAL:HG11	2:F:1967:HOH:O	2.07	0.55
1:C:167:ARG:HH11	1:C:167:ARG:HG2	1.72	0.54
1:H:155:VAL:HG13	1:H:173:MET:CE	2.37	0.54
1:C:193:THR:HB	1:C:194:PRO:CD	2.36	0.54
1:E:222:ASP:OD1	1:E:224:THR:HG23	2.08	0.54
1:F:155:VAL:HG13	1:F:173:MET:CE	2.37	0.54
1:A:245:GLU:HB3	1:D:334:MET:O	2.08	0.54
1:C:1:CYS:HB3	1:C:18:THR:O	2.06	0.54
1:E:250:THR:HG21	1:H:323:GLN:HE21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:ILE:HD12	1:H:198:GLN:O	2.08	0.54
1:H:12:LYS:HD3	1:H:245:GLU:HB2	1.89	0.54
1:C:155:VAL:HG13	1:C:173:MET:HE3	1.90	0.54
1:E:6:ILE:HB	2:E:1459:HOH:O	2.07	0.54
1:G:246:THR:O	1:G:250:THR:HG23	2.08	0.54
1:C:95:LYS:H	1:C:95:LYS:CD	2.18	0.54
1:F:61:ASP:HB3	1:F:135:ILE:HD11	1.90	0.54
1:E:83:TYR:CZ	1:E:157:GLU:HG2	2.42	0.54
1:H:169:THR:HB	1:H:179:TYR:CZ	2.43	0.54
1:B:61:ASP:HB3	1:B:135:ILE:HD11	1.90	0.54
1:B:187:ARG:NH2	1:D:85:THR:HG21	2.09	0.54
1:H:167:ARG:HH11	1:H:167:ARG:HG2	1.70	0.54
1:C:24:GLU:OE1	1:C:321:ARG:NH1	2.41	0.54
2:A:413:HOH:O	1:D:333:VAL:HA	2.08	0.54
1:D:167:ARG:HG2	1:D:167:ARG:HH11	1.73	0.54
1:D:219:LEU:HD23	1:D:220:PRO:HD2	1.88	0.54
1:E:323:GLN:HG3	1:E:325:ILE:CD1	2.37	0.54
1:F:167:ARG:HG2	1:F:167:ARG:HH11	1.72	0.54
2:A:419:HOH:O	1:D:250:THR:HG21	2.08	0.54
2:F:1850:HOH:O	1:G:333:VAL:HA	2.08	0.54
2:F:1862:HOH:O	1:G:250:THR:HG21	2.07	0.53
1:D:1:CYS:HB3	1:D:18:THR:O	2.08	0.53
1:E:115:THR:HA	1:E:148:ASP:OD1	2.08	0.53
1:F:72:ASN:ND2	1:F:110:LEU:O	2.30	0.53
1:D:127:THR:HG22	1:D:129:LEU:HD23	1.91	0.53
1:G:224:THR:O	1:G:228:ARG:HG3	2.09	0.53
1:H:6:ILE:HB	2:H:472:HOH:O	2.08	0.53
1:C:323:GLN:HG3	1:C:325:ILE:CD1	2.39	0.53
1:E:1:CYS:HB3	1:E:18:THR:O	2.08	0.53
1:F:74:LYS:HG3	1:F:114:VAL:HG22	1.90	0.53
1:A:323:GLN:HG3	1:A:325:ILE:CD1	2.39	0.53
1:E:31:ILE:HD12	1:E:307:GLU:HG3	1.89	0.53
1:E:323:GLN:HG3	1:E:325:ILE:HD11	1.89	0.53
1:B:9:THR:OG1	1:B:243:LYS:HA	2.08	0.53
1:C:12:LYS:HD3	1:C:245:GLU:HB2	1.91	0.53
1:C:323:GLN:HG3	1:C:325:ILE:HD11	1.90	0.53
1:E:250:THR:HG21	2:H:506:HOH:O	2.09	0.53
1:E:61:ASP:HB3	1:E:135:ILE:HD11	1.90	0.53
1:E:176:SER:HB3	1:E:177:PRO:HA	1.91	0.53
1:H:323:GLN:HG3	1:H:325:ILE:CD1	2.39	0.53
1:F:193:THR:HB	1:F:194:PRO:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:HG22	1:D:265:VAL:CG1	2.39	0.52
1:F:331:VAL:HG21	1:G:301:ALA:HB3	1.91	0.52
1:B:219:LEU:HD23	1:B:220:PRO:HD2	1.90	0.52
1:B:323:GLN:HG3	1:B:325:ILE:CD1	2.38	0.52
1:B:167:ARG:HG2	1:B:167:ARG:HH11	1.74	0.52
1:C:83:TYR:CZ	1:C:157:GLU:HG2	2.44	0.52
1:F:95:LYS:H	1:F:95:LYS:CD	2.16	0.52
1:H:7:ARG:HB2	2:H:596:HOH:O	2.09	0.52
1:A:61:ASP:HB3	1:A:135:ILE:HD11	1.90	0.52
1:A:327:GLN:OE1	1:A:331:VAL:HB	2.09	0.52
1:B:243:LYS:HE3	2:B:513:HOH:O	2.08	0.52
1:D:74:LYS:HG3	1:D:114:VAL:HG22	1.90	0.52
1:C:9:THR:OG1	1:C:243:LYS:HA	2.10	0.52
1:H:241:LYS:HG2	2:H:561:HOH:O	2.09	0.52
1:A:9:THR:OG1	1:A:243:LYS:HA	2.10	0.52
1:A:85:THR:HG22	1:A:86:PHE:CD2	2.45	0.52
1:A:328:LEU:HG	2:D:666:HOH:O	2.09	0.52
1:B:155:VAL:HG13	1:B:173:MET:HE3	1.90	0.52
1:H:95:LYS:H	1:H:95:LYS:CD	2.17	0.52
1:D:72:ASN:HB3	1:D:74:LYS:H	1.74	0.52
1:H:327:GLN:OE1	1:H:331:VAL:HB	2.09	0.52
1:A:6:ILE:HB	2:A:387:HOH:O	2.09	0.51
1:E:219:LEU:CD2	1:E:220:PRO:HD2	2.38	0.51
1:E:333:VAL:HA	2:H:500:HOH:O	2.08	0.51
1:G:74:LYS:CG	1:G:114:VAL:HG22	2.40	0.51
1:C:246:THR:O	1:C:250:THR:HG23	2.10	0.51
1:F:250:THR:HG21	1:G:323:GLN:HE21	1.75	0.51
1:B:7:ARG:HD3	2:B:535:HOH:O	2.10	0.51
1:B:239:THR:HG22	1:C:262:PRO:HB2	1.90	0.51
1:E:127:THR:HG22	1:E:129:LEU:HD23	1.92	0.51
1:H:83:TYR:CE2	1:H:157:GLU:HG2	2.44	0.51
1:D:83:TYR:CZ	1:D:157:GLU:HG2	2.46	0.51
1:F:83:TYR:CE2	1:F:157:GLU:HG2	2.46	0.51
1:A:263:LYS:HD2	1:A:294:TYR:CE2	2.46	0.51
1:E:85:THR:HG22	1:E:86:PHE:CD2	2.45	0.51
1:H:222:ASP:OD1	1:H:224:THR:HG23	2.11	0.51
1:E:106:ILE:O	1:E:110:LEU:HB2	2.11	0.51
1:E:323:GLN:HE21	1:H:250:THR:HG21	1.76	0.51
1:G:243:LYS:HE3	2:G:2299:HOH:O	2.11	0.51
1:H:219:LEU:CD2	1:H:220:PRO:HD2	2.41	0.51
1:A:323:GLN:HE21	1:D:250:THR:HG21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:THR:OG1	1:D:243:LYS:HA	2.10	0.51
1:D:327:GLN:OE1	1:D:331:VAL:HB	2.11	0.51
1:A:24:GLU:OE1	1:A:321:ARG:NH1	2.44	0.51
1:F:323:GLN:HG3	1:F:325:ILE:CD1	2.41	0.51
1:H:74:LYS:CG	1:H:114:VAL:HG22	2.40	0.51
1:C:327:GLN:OE1	1:C:331:VAL:HB	2.10	0.50
1:E:72:ASN:HB3	1:E:74:LYS:N	2.25	0.50
1:F:301:ALA:HB3	1:G:331:VAL:HG21	1.94	0.50
1:G:6:ILE:HB	2:G:2159:HOH:O	2.11	0.50
1:H:94:LYS:HG3	2:H:584:HOH:O	2.11	0.50
1:A:168:LYS:HG3	2:A:615:HOH:O	2.12	0.50
1:B:219:LEU:CD2	1:B:220:PRO:HD2	2.41	0.50
1:B:327:GLN:OE1	1:B:331:VAL:HB	2.10	0.50
1:C:176:SER:HB3	1:C:177:PRO:HA	1.94	0.50
1:D:94:LYS:HG3	2:D:590:HOH:O	2.11	0.50
1:B:24:GLU:OE1	1:B:321:ARG:NH1	2.44	0.50
1:C:115:THR:HA	1:C:148:ASP:OD1	2.11	0.50
1:F:155:VAL:HB	1:F:166:HIS:HB2	1.93	0.50
1:H:16:ALA:HB2	1:H:252:LEU:HD13	1.93	0.50
1:H:83:TYR:CZ	1:H:157:GLU:HG2	2.45	0.50
1:B:9:THR:HG23	1:B:241:LYS:HD2	1.93	0.50
1:A:246:THR:O	1:A:250:THR:HG23	2.11	0.50
1:D:323:GLN:HG3	1:D:325:ILE:CD1	2.41	0.50
1:F:80:MET:HG3	1:F:106:ILE:HG12	1.93	0.50
1:F:327:GLN:OE1	1:F:331:VAL:HB	2.12	0.50
1:H:193:THR:HB	1:H:194:PRO:CD	2.42	0.50
1:H:323:GLN:HG3	1:H:325:ILE:HD11	1.93	0.50
1:E:9:THR:OG1	1:E:243:LYS:HA	2.11	0.50
1:C:84:ALA:O	1:C:85:THR:CB	2.55	0.50
1:E:167:ARG:HH11	1:E:167:ARG:HG2	1.76	0.50
1:G:1:CYS:HB3	1:G:18:THR:O	2.12	0.50
1:A:243:LYS:HE3	2:A:490:HOH:O	2.12	0.50
1:D:167:ARG:HD2	2:D:611:HOH:O	2.10	0.50
1:E:155:VAL:HG13	1:E:173:MET:HE3	1.91	0.50
1:E:327:GLN:OE1	1:E:331:VAL:HB	2.12	0.50
1:H:333:VAL:HG11	2:H:591:HOH:O	2.12	0.50
1:B:7:ARG:NH1	1:B:13:SER:OG	2.40	0.49
1:F:235:TRP:HE3	1:F:235:TRP:HA	1.77	0.49
1:F:250:THR:CG2	1:G:323:GLN:HE21	2.25	0.49
1:B:72:ASN:HB3	1:B:74:LYS:N	2.26	0.49
1:B:323:GLN:HG3	1:B:325:ILE:HD11	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLU:OE1	1:D:321:ARG:NH1	2.46	0.49
1:F:178:GLY:HA3	2:F:2098:HOH:O	2.11	0.49
1:F:239:THR:HG22	1:G:265:VAL:CG1	2.43	0.49
1:C:61:ASP:HB3	1:C:135:ILE:HD11	1.94	0.49
1:E:262:PRO:HB2	1:H:239:THR:CG2	2.42	0.49
1:F:235:TRP:HA	1:F:235:TRP:CE3	2.48	0.49
1:G:24:GLU:OE1	1:G:321:ARG:NH1	2.45	0.49
1:G:83:TYR:CZ	1:G:157:GLU:HG2	2.47	0.49
1:H:72:ASN:HB3	1:H:74:LYS:N	2.28	0.49
1:A:115:THR:HA	1:A:148:ASP:OD1	2.12	0.49
1:C:83:TYR:CE2	1:C:157:GLU:HG2	2.47	0.49
1:G:115:THR:HA	1:G:148:ASP:OD1	2.12	0.49
1:G:327:GLN:OE1	1:G:331:VAL:HB	2.12	0.49
1:H:24:GLU:OE1	1:H:321:ARG:NH1	2.46	0.49
1:B:245:GLU:HB3	1:C:334:MET:O	2.12	0.49
1:C:333:VAL:HG11	2:C:572:HOH:O	2.11	0.49
1:A:167:ARG:HD2	2:A:520:HOH:O	2.12	0.49
1:C:85:THR:HG22	1:C:86:PHE:CD2	2.48	0.49
1:E:205:LEU:HD12	1:F:170:ILE:CG2	2.43	0.49
1:F:24:GLU:OE1	1:F:321:ARG:NH1	2.46	0.48
1:G:12:LYS:HD3	1:G:245:GLU:HB2	1.94	0.48
1:B:263:LYS:HD2	1:B:294:TYR:CE2	2.48	0.48
1:D:222:ASP:OD1	1:D:224:THR:HG23	2.13	0.48
1:D:115:THR:HA	1:D:148:ASP:OD1	2.12	0.48
1:F:7:ARG:HD3	2:F:1976:HOH:O	2.11	0.48
1:G:40:LEU:HD21	1:G:126:TYR:CE1	2.43	0.48
1:B:175:ASN:HB2	1:B:225:PRO:HB3	1.96	0.48
1:E:24:GLU:OE1	1:E:321:ARG:NH1	2.46	0.48
1:E:328:LEU:HD23	1:H:317:PHE:HB3	1.94	0.48
1:D:85:THR:HG22	1:D:86:PHE:CD2	2.49	0.48
1:E:39:ARG:NH1	1:E:63:THR:HG21	2.29	0.48
1:F:9:THR:HG23	1:F:241:LYS:HD2	1.95	0.48
1:F:263:LYS:HD2	1:F:294:TYR:CE2	2.48	0.48
1:H:176:SER:HB3	1:H:177:PRO:HA	1.96	0.48
1:A:72:ASN:HB3	1:A:74:LYS:N	2.28	0.48
1:C:73:GLU:O	1:C:287:LYS:HE2	2.13	0.48
1:C:219:LEU:CD2	1:C:220:PRO:HD2	2.43	0.48
1:E:246:THR:O	1:E:250:THR:HG23	2.14	0.48
1:F:127:THR:HG22	1:F:129:LEU:HD23	1.95	0.48
1:A:39:ARG:NH1	1:A:63:THR:HG21	2.28	0.48
1:G:95:LYS:H	1:G:95:LYS:CD	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:VAL:HA	1:H:303:SER:HB2	1.96	0.48
1:H:235:TRP:HA	1:H:235:TRP:CE3	2.49	0.48
1:B:167:ARG:HD2	2:B:542:HOH:O	2.13	0.48
1:E:167:ARG:HD2	2:E:1634:HOH:O	2.13	0.48
1:H:80:MET:HG3	1:H:106:ILE:HG12	1.96	0.48
1:F:169:THR:HB	1:F:179:TYR:CZ	2.48	0.47
1:G:155:VAL:HB	1:G:166:HIS:HB2	1.96	0.47
1:G:198:GLN:O	1:H:190:ILE:HD12	2.14	0.47
1:D:155:VAL:HG13	1:D:173:MET:HE3	1.96	0.47
1:E:301:ALA:HB3	1:H:331:VAL:HG21	1.96	0.47
1:G:127:THR:HG22	1:G:129:LEU:HD23	1.96	0.47
1:H:55:VAL:CG1	1:H:304:LEU:HB2	2.44	0.47
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.79	0.47
2:A:635:HOH:O	1:D:212:GLN:HG3	2.14	0.47
1:A:67:LEU:O	1:A:80:MET:HE2	2.15	0.47
1:C:127:THR:HG22	1:C:129:LEU:HD23	1.96	0.47
1:D:83:TYR:CE2	1:D:157:GLU:HG2	2.49	0.47
1:A:219:LEU:CD2	1:A:220:PRO:HD2	2.45	0.47
1:B:115:THR:HA	1:B:148:ASP:OD1	2.15	0.47
1:C:72:ASN:HB3	1:C:74:LYS:N	2.28	0.47
1:E:325:ILE:HD12	1:H:299:ILE:CG2	2.44	0.47
1:F:8:THR:OG1	1:F:12:LYS:HB2	2.14	0.47
1:G:4:LEU:HA	1:G:171:GLY:O	2.15	0.47
1:H:40:LEU:HD21	1:H:126:TYR:CE1	2.41	0.47
1:H:135:ILE:HG13	2:H:632:HOH:O	2.14	0.47
1:H:167:ARG:HD2	2:H:603:HOH:O	2.14	0.47
1:D:84:ALA:O	1:D:85:THR:CB	2.61	0.47
1:D:323:GLN:HG3	1:D:325:ILE:HD11	1.96	0.47
2:E:1500:HOH:O	1:H:333:VAL:HA	2.13	0.47
1:F:101:ASN:OD1	1:F:103:VAL:HB	2.15	0.47
1:D:246:THR:O	1:D:250:THR:HG23	2.15	0.47
1:E:169:THR:HB	1:E:179:TYR:CZ	2.50	0.47
1:E:262:PRO:HB2	1:H:239:THR:HG22	1.96	0.47
1:G:167:ARG:HD2	2:G:2334:HOH:O	2.15	0.47
1:A:235:TRP:CE3	1:A:235:TRP:HA	2.50	0.47
1:B:333:VAL:HA	2:C:477:HOH:O	2.14	0.47
1:C:155:VAL:HB	1:C:166:HIS:HB2	1.96	0.47
1:G:72:ASN:HB3	1:G:74:LYS:N	2.28	0.47
1:B:231:ARG:HH11	1:B:231:ARG:HD3	1.51	0.46
1:C:263:LYS:HD2	1:C:294:TYR:CE2	2.51	0.46
1:D:155:VAL:HG13	1:D:173:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:THR:O	1:F:250:THR:HG23	2.15	0.46
1:H:106:ILE:O	1:H:110:LEU:HB2	2.15	0.46
1:G:167:ARG:HG2	1:G:167:ARG:HH11	1.80	0.46
1:H:263:LYS:HD2	1:H:294:TYR:CE2	2.50	0.46
1:B:298:ARG:HG3	1:C:298:ARG:HG3	1.97	0.46
1:B:301:ALA:HB3	1:C:331:VAL:HG21	1.97	0.46
1:G:36:TYR:CE1	1:G:314:LEU:HD13	2.50	0.46
1:B:6:ILE:HB	2:B:410:HOH:O	2.15	0.46
1:H:156:ILE:HG12	1:H:165:ILE:CD1	2.46	0.46
1:H:246:THR:O	1:H:250:THR:HG23	2.14	0.46
1:D:156:ILE:HG12	1:D:165:ILE:CD1	2.46	0.46
1:E:193:THR:HB	1:E:194:PRO:CD	2.46	0.46
1:E:245:GLU:HB3	1:H:334:MET:O	2.16	0.46
1:F:224:THR:HG21	2:H:426:HOH:O	2.15	0.46
1:B:176:SER:HB3	1:B:177:PRO:HA	1.98	0.46
1:B:193:THR:HB	1:B:194:PRO:CD	2.45	0.46
1:B:246:THR:O	1:B:250:THR:HG23	2.16	0.46
1:E:326:LYS:NZ	2:E:1533:HOH:O	2.48	0.46
1:F:115:THR:HB	2:F:1990:HOH:O	2.15	0.46
1:F:176:SER:HB3	1:F:177:PRO:HA	1.97	0.46
1:F:183:GLN:HB3	2:F:1569:HOH:O	2.16	0.46
1:A:323:GLN:HG3	1:A:325:ILE:HD11	1.97	0.46
2:B:437:HOH:O	1:C:333:VAL:HA	2.15	0.46
1:D:175:ASN:HB2	1:D:225:PRO:HB3	1.97	0.46
1:C:6:ILE:HB	2:C:451:HOH:O	2.16	0.46
1:E:7:ARG:NH1	1:E:13:SER:OG	2.41	0.46
1:F:65:PRO:HG3	1:F:314:LEU:HD21	1.98	0.46
1:A:333:VAL:HG11	2:A:506:HOH:O	2.16	0.46
1:C:168:LYS:HG3	2:C:678:HOH:O	2.16	0.46
1:F:31:ILE:HD12	1:F:307:GLU:HG3	1.98	0.46
1:F:56:GLY:HA2	1:F:289:TYR:CE2	2.51	0.46
1:A:72:ASN:HD22	1:A:72:ASN:HA	1.37	0.45
1:A:193:THR:HB	1:A:194:PRO:CD	2.46	0.45
2:A:504:HOH:O	1:D:209:PRO:HG2	2.15	0.45
1:E:263:LYS:HE2	2:H:377:HOH:O	2.16	0.45
1:G:84:ALA:O	1:G:85:THR:CB	2.61	0.45
1:C:36:TYR:CE1	1:C:314:LEU:HD13	2.51	0.45
1:D:7:ARG:HB2	2:D:604:HOH:O	2.16	0.45
1:F:34:ARG:HG3	1:F:309:LEU:O	2.17	0.45
1:G:85:THR:HG22	1:G:86:PHE:CD2	2.51	0.45
1:G:106:ILE:O	1:G:110:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:VAL:HG11	1:H:304:LEU:HB2	1.98	0.45
1:D:9:THR:HG23	1:D:241:LYS:HD2	1.99	0.45
1:D:135:ILE:HG13	2:D:640:HOH:O	2.16	0.45
1:E:55:VAL:HG11	1:E:304:LEU:HB2	1.98	0.45
1:B:239:THR:CG2	1:C:262:PRO:HB2	2.47	0.45
1:B:72:ASN:O	1:B:287:LYS:HG2	2.16	0.45
1:B:265:VAL:CG1	1:C:239:THR:HG22	2.47	0.45
1:E:58:GLY:HA3	1:E:66:VAL:O	2.17	0.45
2:E:2520:HOH:O	1:H:212:GLN:HG3	2.16	0.45
1:G:9:THR:HG23	1:G:241:LYS:HD2	1.99	0.45
1:H:6:ILE:HD13	1:H:14:LEU:HB2	1.99	0.45
1:A:73:GLU:O	1:A:287:LYS:HE2	2.17	0.45
1:B:84:ALA:O	1:B:85:THR:CB	2.61	0.45
1:C:235:TRP:HE3	1:C:235:TRP:HA	1.82	0.45
1:E:244:ASN:HB2	2:E:2770:HOH:O	2.16	0.45
1:F:16:ALA:HB2	1:F:252:LEU:HD13	1.99	0.45
1:F:54:PHE:CE1	1:F:67:LEU:HD13	2.39	0.45
1:G:323:GLN:HG3	1:G:325:ILE:CD1	2.46	0.45
1:E:65:PRO:HG3	1:E:314:LEU:HD21	1.97	0.45
1:F:156:ILE:HG12	1:F:165:ILE:CD1	2.46	0.45
1:H:155:VAL:HB	1:H:166:HIS:HB2	1.99	0.45
1:E:55:VAL:CG1	1:E:304:LEU:HB2	2.47	0.45
1:E:331:VAL:HG21	1:H:301:ALA:HB3	1.99	0.45
1:G:169:THR:HB	1:G:179:TYR:CZ	2.52	0.45
1:A:169:THR:HB	1:A:179:TYR:CZ	2.52	0.45
1:A:301:ALA:HB3	1:D:331:VAL:HG21	1.99	0.45
1:C:222:ASP:OD1	1:C:224:THR:HG23	2.17	0.45
1:F:72:ASN:O	1:F:287:LYS:HG2	2.17	0.45
1:G:36:TYR:CZ	1:G:314:LEU:HD13	2.52	0.45
1:A:80:MET:HG3	1:A:106:ILE:HG12	1.99	0.44
1:B:334:MET:O	1:C:245:GLU:HB3	2.17	0.44
1:C:235:TRP:HA	1:C:235:TRP:CE3	2.52	0.44
1:E:155:VAL:HG13	1:E:173:MET:HE2	1.99	0.44
1:F:323:GLN:HE21	1:G:250:THR:CG2	2.30	0.44
1:B:83:TYR:CE2	1:B:157:GLU:HG2	2.53	0.44
2:E:1512:HOH:O	1:H:250:THR:HG21	2.18	0.44
1:C:106:ILE:O	1:C:110:LEU:HB2	2.16	0.44
1:D:193:THR:HB	1:D:194:PRO:CD	2.48	0.44
1:F:250:THR:HG21	2:G:2212:HOH:O	2.17	0.44
1:G:7:ARG:HD3	2:G:2326:HOH:O	2.17	0.44
1:H:127:THR:HG22	1:H:129:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:THR:OG1	1:H:175:ASN:N	2.49	0.44
1:H:235:TRP:HA	1:H:235:TRP:HE3	1.83	0.44
1:E:168:LYS:HG3	2:E:2053:HOH:O	2.17	0.44
1:F:193:THR:CB	1:F:194:PRO:CD	2.95	0.44
1:G:263:LYS:HD2	1:G:294:TYR:CE2	2.52	0.44
1:H:168:LYS:HG3	2:H:411:HOH:O	2.17	0.44
1:A:235:TRP:HA	1:A:235:TRP:HE3	1.81	0.44
1:A:331:VAL:HG21	1:D:301:ALA:HB3	1.99	0.44
1:B:55:VAL:HG11	1:B:304:LEU:HB2	1.99	0.44
1:E:260:ASN:O	1:E:262:PRO:HD3	2.17	0.44
1:B:156:ILE:HG12	1:B:165:ILE:HD13	1.99	0.44
1:C:175:ASN:HB2	1:C:225:PRO:HB3	2.00	0.44
1:E:40:LEU:HD21	1:E:126:TYR:CE1	2.44	0.44
1:A:65:PRO:HG3	1:A:314:LEU:HD21	1.99	0.44
1:A:176:SER:HB3	1:A:177:PRO:HA	1.99	0.44
1:B:80:MET:HG3	1:B:106:ILE:HG12	2.00	0.44
1:C:39:ARG:NH1	1:C:63:THR:HG21	2.33	0.44
1:C:245:GLU:OE2	1:C:290:TYR:OH	2.30	0.44
1:D:52:TYR:CE1	1:D:74:LYS:HD3	2.53	0.44
1:D:65:PRO:HG3	1:D:314:LEU:HD21	1.99	0.44
1:G:178:GLY:HA3	2:G:2448:HOH:O	2.17	0.44
1:C:67:LEU:O	1:C:80:MET:HE2	2.18	0.44
1:D:52:TYR:CD1	1:D:74:LYS:HD3	2.53	0.44
1:F:244:ASN:HB2	2:G:2420:HOH:O	2.17	0.44
1:F:334:MET:O	1:G:245:GLU:HB3	2.18	0.44
1:G:222:ASP:OD1	1:G:224:THR:HG23	2.18	0.44
1:A:212:GLN:HG3	2:D:340:HOH:O	2.17	0.44
1:C:169:THR:HB	1:C:179:TYR:CZ	2.52	0.44
1:H:4:LEU:HA	1:H:171:GLY:O	2.18	0.44
1:B:55:VAL:CG1	1:B:304:LEU:HB2	2.47	0.43
1:C:148:ASP:HB3	1:C:150:SER:H	1.83	0.43
1:E:84:ALA:O	1:E:85:THR:CB	2.59	0.43
1:E:253:PHE:CE1	1:E:279:THR:HG22	2.53	0.43
1:G:83:TYR:CE2	1:G:157:GLU:HG2	2.52	0.43
1:G:231:ARG:HH11	1:G:231:ARG:HD3	1.58	0.43
1:A:155:VAL:HB	1:A:166:HIS:HB2	2.00	0.43
2:A:575:HOH:O	1:D:328:LEU:HG	2.18	0.43
1:G:333:VAL:HG11	2:G:2317:HOH:O	2.18	0.43
1:B:155:VAL:HB	1:B:166:HIS:HB2	1.99	0.43
1:B:224:THR:O	1:B:228:ARG:HG3	2.18	0.43
1:B:83:TYR:CZ	1:B:157:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ASP:HB3	1:E:150:SER:H	1.83	0.43
1:F:17:ARG:HD2	1:F:69:ASP:OD2	2.18	0.43
1:F:168:LYS:HG3	2:F:1703:HOH:O	2.17	0.43
1:A:17:ARG:HD2	1:A:69:ASP:OD2	2.18	0.43
1:C:6:ILE:HD12	1:C:252:LEU:HG	2.01	0.43
1:C:36:TYR:CZ	1:C:314:LEU:HD13	2.53	0.43
1:G:67:LEU:O	1:G:80:MET:HE2	2.18	0.43
1:H:6:ILE:CD1	1:H:14:LEU:HB2	2.48	0.43
1:H:36:TYR:CZ	1:H:314:LEU:HD13	2.53	0.43
1:F:109:VAL:HG11	1:F:146:PHE:CE1	2.53	0.43
1:F:245:GLU:OE2	1:F:290:TYR:OH	2.31	0.43
1:G:176:SER:HB3	1:G:177:PRO:HA	2.00	0.43
1:F:6:ILE:HD12	1:F:252:LEU:HG	2.00	0.43
1:F:323:GLN:HG3	1:F:325:ILE:HD11	2.00	0.43
1:A:83:TYR:CE2	1:A:157:GLU:HG2	2.54	0.43
1:E:68:TYR:HA	1:E:80:MET:HE3	2.01	0.43
1:A:4:LEU:HA	1:A:171:GLY:O	2.19	0.43
1:B:67:LEU:O	1:B:80:MET:HE2	2.19	0.43
1:C:216:GLY:O	1:C:217:LEU:C	2.54	0.43
1:D:36:TYR:CE1	1:D:314:LEU:HD13	2.53	0.43
1:D:169:THR:HB	1:D:179:TYR:CZ	2.54	0.43
1:D:219:LEU:CD2	1:D:220:PRO:HD2	2.49	0.43
1:E:291:PHE:HE2	1:E:293:LEU:HD21	1.84	0.43
1:F:40:LEU:HD21	1:F:126:TYR:CE1	2.48	0.43
1:G:109:VAL:HG11	1:G:146:PHE:CE1	2.54	0.43
1:F:212:GLN:HG3	2:G:1820:HOH:O	2.18	0.42
1:A:323:GLN:HG3	1:A:325:ILE:HD13	2.01	0.42
1:B:17:ARG:HD2	1:B:69:ASP:OD2	2.19	0.42
1:E:155:VAL:HG22	1:E:173:MET:HE3	2.01	0.42
1:E:210:PHE:CE1	1:F:187:ARG:HB2	2.55	0.42
1:E:333:VAL:HG11	2:E:1617:HOH:O	2.19	0.42
1:H:39:ARG:NH1	1:H:63:THR:HG21	2.35	0.42
1:A:135:ILE:HG13	2:A:548:HOH:O	2.18	0.42
1:B:169:THR:HB	1:B:179:TYR:CZ	2.54	0.42
1:C:58:GLY:HA3	1:C:66:VAL:O	2.20	0.42
1:G:94:LYS:HG3	2:G:2309:HOH:O	2.19	0.42
2:E:1615:HOH:O	1:H:209:PRO:HG2	2.19	0.42
1:F:135:ILE:HG13	2:F:2019:HOH:O	2.19	0.42
1:A:156:ILE:HG12	1:A:165:ILE:CD1	2.50	0.42
1:B:36:TYR:CZ	1:B:314:LEU:HD13	2.55	0.42
1:D:73:GLU:O	1:D:287:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:ASN:HB2	1:G:225:PRO:HB3	2.01	0.42
1:E:83:TYR:CD2	1:E:143:HIS:HB3	2.54	0.42
1:E:332:ASN:HB2	2:H:362:HOH:O	2.20	0.42
1:F:143:HIS:HB2	1:F:157:GLU:HG3	2.01	0.42
1:B:263:LYS:HE3	1:B:275:TYR:CE2	2.54	0.42
1:C:332:ASN:HB2	2:C:556:HOH:O	2.19	0.42
1:D:155:VAL:HB	1:D:166:HIS:HB2	2.02	0.42
1:F:29:VAL:HG13	1:F:317:PHE:HB2	2.02	0.42
1:C:244:ASN:HB2	2:C:391:HOH:O	2.18	0.42
1:G:156:ILE:HG12	1:G:165:ILE:CD1	2.50	0.42
1:H:193:THR:HB	1:H:194:PRO:HD2	2.01	0.42
1:A:9:THR:HG23	1:A:241:LYS:HD2	2.02	0.42
1:A:72:ASN:O	1:A:287:LYS:HG2	2.20	0.42
1:B:193:THR:CB	1:B:194:PRO:CD	2.98	0.42
1:D:167:ARG:O	1:D:168:LYS:C	2.58	0.42
1:H:17:ARG:HH11	1:H:69:ASP:HB3	1.85	0.42
1:F:298:ARG:HG3	1:G:298:ARG:HG3	2.02	0.41
1:F:323:GLN:HG3	1:F:325:ILE:HD13	2.02	0.41
2:F:2413:HOH:O	1:G:263:LYS:HE2	2.19	0.41
1:H:155:VAL:HG11	1:H:179:TYR:HB2	2.02	0.41
1:A:7:ARG:HD3	2:A:513:HOH:O	2.20	0.41
1:A:175:ASN:HB2	1:A:225:PRO:HB3	2.02	0.41
1:B:106:ILE:O	1:B:110:LEU:HB2	2.19	0.41
1:B:222:ASP:OD1	1:B:224:THR:HG23	2.20	0.41
1:E:73:GLU:O	1:E:287:LYS:HE2	2.20	0.41
1:H:29:VAL:HG13	1:H:317:PHE:HB2	2.01	0.41
1:A:216:GLY:O	1:A:217:LEU:C	2.58	0.41
1:B:328:LEU:HD22	1:C:302:VAL:HG23	2.02	0.41
1:D:178:GLY:HA3	2:D:689:HOH:O	2.20	0.41
1:H:166:HIS:CD2	1:H:179:TYR:HB3	2.55	0.41
1:H:291:PHE:HE2	1:H:293:LEU:HD21	1.86	0.41
1:D:235:TRP:HA	1:D:235:TRP:CE3	2.55	0.41
1:F:198:GLN:HB2	2:F:1524:HOH:O	2.20	0.41
1:H:260:ASN:O	1:H:262:PRO:HD3	2.21	0.41
1:E:328:LEU:HD22	1:H:302:VAL:HG23	2.03	0.41
1:G:65:PRO:HG3	1:G:314:LEU:HD21	2.02	0.41
1:G:72:ASN:O	1:G:287:LYS:HG2	2.21	0.41
1:H:7:ARG:HD3	2:H:596:HOH:O	2.19	0.41
1:B:85:THR:HG22	1:B:86:PHE:CD2	2.55	0.41
1:C:65:PRO:HG3	1:C:314:LEU:HD21	2.03	0.41
1:E:52:TYR:CE1	1:E:74:LYS:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:ARG:NH1	1:G:13:SER:OG	2.47	0.41
1:G:55:VAL:CG1	1:G:304:LEU:HB2	2.51	0.41
1:A:83:TYR:CZ	1:A:157:GLU:HG2	2.56	0.41
1:A:84:ALA:O	1:A:85:THR:CB	2.58	0.41
1:A:239:THR:HG22	1:D:262:PRO:HB2	2.02	0.41
1:B:69:ASP:HA	1:B:78:GLY:O	2.21	0.41
1:C:167:ARG:O	1:C:168:LYS:C	2.59	0.41
1:F:52:TYR:CD1	1:F:74:LYS:HD3	2.56	0.41
1:G:219:LEU:CD2	1:G:220:PRO:HD2	2.49	0.41
1:H:29:VAL:HG22	1:H:317:PHE:HD1	1.86	0.41
1:B:34:ARG:HG3	1:B:309:LEU:O	2.20	0.41
1:C:10:ASP:OD2	1:C:12:LYS:HD2	2.21	0.41
1:D:6:ILE:HB	2:D:475:HOH:O	2.20	0.41
1:D:72:ASN:HB3	1:D:74:LYS:N	2.36	0.41
1:F:323:GLN:HE21	1:G:250:THR:HG21	1.85	0.41
1:A:155:VAL:HG13	1:A:173:MET:HE3	2.03	0.41
1:A:219:LEU:HD12	1:A:235:TRP:CZ2	2.55	0.41
1:C:193:THR:HB	1:C:194:PRO:HD2	2.01	0.41
1:D:40:LEU:HD21	1:D:126:TYR:CE1	2.44	0.41
1:E:166:HIS:CD2	1:E:179:TYR:HB3	2.55	0.41
1:E:175:ASN:HB2	1:E:225:PRO:HB3	2.03	0.41
1:F:260:ASN:O	1:F:262:PRO:HD3	2.21	0.41
1:F:291:PHE:HE2	1:F:293:LEU:HD21	1.86	0.41
1:G:110:LEU:HD12	1:G:110:LEU:HA	1.95	0.41
1:H:36:TYR:CE1	1:H:314:LEU:HD13	2.56	0.41
1:A:334:MET:O	1:D:245:GLU:HB3	2.21	0.41
1:E:9:THR:HG23	1:E:241:LYS:HD2	2.03	0.41
1:E:52:TYR:CD1	1:E:74:LYS:HD3	2.56	0.41
1:F:106:ILE:O	1:F:110:LEU:HB2	2.21	0.41
1:G:16:ALA:HB2	1:G:252:LEU:HD13	2.03	0.41
1:B:72:ASN:HB2	1:B:76:LEU:H	1.86	0.40
1:B:235:TRP:HA	1:B:235:TRP:CE3	2.56	0.40
1:F:36:TYR:CZ	1:F:314:LEU:HD13	2.56	0.40
1:G:55:VAL:HG11	1:G:304:LEU:HB2	2.03	0.40
1:H:109:VAL:HG11	1:H:146:PHE:CE1	2.56	0.40
1:H:183:GLN:HB3	2:H:404:HOH:O	2.20	0.40
1:H:322:LYS:HB3	2:H:637:HOH:O	2.20	0.40
1:A:155:VAL:HG22	1:A:173:MET:HE3	2.02	0.40
1:B:167:ARG:O	1:B:168:LYS:C	2.59	0.40
1:F:308:ASN:O	1:F:311:SER:OG	2.38	0.40
1:G:174:THR:OG1	1:G:175:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:TRP:HA	1:G:235:TRP:CE3	2.56	0.40
1:H:109:VAL:HG13	1:H:119:VAL:HG22	2.03	0.40
1:B:331:VAL:HG21	1:C:301:ALA:HB3	2.03	0.40
1:F:174:THR:OG1	1:F:175:ASN:N	2.54	0.40
1:G:235:TRP:HA	1:G:235:TRP:HE3	1.87	0.40
1:H:72:ASN:HD22	1:H:72:ASN:HA	1.35	0.40
1:A:106:ILE:O	1:A:110:LEU:HB2	2.21	0.40
1:B:156:ILE:HG12	1:B:165:ILE:CD1	2.51	0.40
1:B:268:THR:HA	1:C:212:GLN:NE2	2.37	0.40
1:D:231:ARG:HH11	1:D:231:ARG:HD3	1.64	0.40
1:F:166:HIS:CD2	1:F:179:TYR:HB3	2.56	0.40
1:A:296:ASN:ND2	1:A:324:ASP:H	2.19	0.40
1:B:135:ILE:HG13	2:B:571:HOH:O	2.21	0.40
1:C:34:ARG:HG3	1:C:309:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	25	56
1	B	332/335 (99%)	318 (96%)	12 (4%)	2 (1%)	25	56
1	C	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	25	56
1	D	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	25	56
1	E	332/335 (99%)	316 (95%)	14 (4%)	2 (1%)	25	56
1	F	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	25	56
1	G	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	25	56
1	H	332/335 (99%)	314 (95%)	16 (5%)	2 (1%)	25	56
All	All	2656/2680 (99%)	2533 (95%)	107 (4%)	16 (1%)	25	56

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	B	168	LYS
1	C	168	LYS
1	D	168	LYS
1	E	333	VAL
1	G	333	VAL
1	H	168	LYS
1	C	333	VAL
1	D	333	VAL
1	E	168	LYS
1	F	168	LYS
1	F	333	VAL
1	G	168	LYS
1	A	168	LYS
1	B	333	VAL
1	H	333	VAL

5.3.2 Protein sidechains (i)

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	291/292 (100%)	240 (82%)	51 (18%)	2	6
1	B	291/292 (100%)	238 (82%)	53 (18%)	1	5
1	C	291/292 (100%)	241 (83%)	50 (17%)	2	6
1	D	291/292 (100%)	239 (82%)	52 (18%)	2	5
1	E	291/292 (100%)	239 (82%)	52 (18%)	2	5
1	F	291/292 (100%)	236 (81%)	55 (19%)	1	5
1	G	291/292 (100%)	237 (81%)	54 (19%)	1	5
1	H	291/292 (100%)	243 (84%)	48 (16%)	2	7
All	All	2328/2336 (100%)	1913 (82%)	415 (18%)	2	5

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	4	LEU
1	A	6	ILE
1	A	10	ASP
1	A	17	ARG
1	A	23	MET
1	A	26	ASP
1	A	28	LYS
1	A	29	VAL
1	A	34	ARG
1	A	41	LEU
1	A	67	LEU
1	A	71	VAL
1	A	72	ASN
1	A	74	LYS
1	A	82	TYR
1	A	85	THR
1	A	95	LYS
1	A	98	THR
1	A	110	LEU
1	A	121	GLU
1	A	123	LEU
1	A	130	ASN
1	A	136	LEU
1	A	142	LEU
1	A	143	HIS
1	A	152	GLU
1	A	160	LYS
1	A	167	ARG
1	A	173	MET
1	A	205	LEU
1	A	208	THR
1	A	219	LEU
1	A	230	LEU
1	A	235	TRP
1	A	250	THR
1	A	265	VAL
1	A	269	ASN
1	A	270	GLU
1	A	272	LYS
1	A	273	THR
1	A	285	GLN
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	296	ASN
1	A	311	SER
1	A	314	LEU
1	A	318	GLU
1	A	321	ARG
1	A	327	GLN
1	A	330	GLN
1	A	334	MET
1	B	1	CYS
1	B	4	LEU
1	B	6	ILE
1	B	10	ASP
1	B	17	ARG
1	B	23	MET
1	B	26	ASP
1	B	28	LYS
1	B	29	VAL
1	B	34	ARG
1	B	41	LEU
1	B	67	LEU
1	B	71	VAL
1	B	72	ASN
1	B	74	LYS
1	B	82	TYR
1	B	85	THR
1	B	95	LYS
1	B	98	THR
1	B	103	VAL
1	B	110	LEU
1	B	121	GLU
1	B	123	LEU
1	B	130	ASN
1	B	136	LEU
1	B	142	LEU
1	B	143	HIS
1	B	152	GLU
1	B	160	LYS
1	B	167	ARG
1	B	173	MET
1	B	205	LEU
1	B	208	THR
1	B	219	LEU

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Mol	Chain	Res	Type
1	B	230	LEU
1	B	235	TRP
1	B	250	THR
1	B	265	VAL
1	B	269	ASN
1	B	270	GLU
1	B	272	LYS
1	B	273	THR
1	B	285	GLN
1	B	287	LYS
1	B	293	LEU
1	B	296	ASN
1	B	311	SER
1	B	314	LEU
1	B	318	GLU
1	B	321	ARG
1	B	327	GLN
1	B	330	GLN
1	B	334	MET
1	C	1	CYS
1	C	4	LEU
1	C	6	ILE
1	C	10	ASP
1	C	17	ARG
1	C	23	MET
1	C	26	ASP
1	C	28	LYS
1	C	29	VAL
1	C	34	ARG
1	C	41	LEU
1	C	67	LEU
1	C	71	VAL
1	C	72	ASN
1	C	74	LYS
1	C	82	TYR
1	C	85	THR
1	C	95	LYS
1	C	98	THR
1	C	110	LEU
1	C	121	GLU
1	C	123	LEU
1	C	130	ASN

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	142	LEU
1	C	143	HIS
1	C	152	GLU
1	C	160	LYS
1	C	167	ARG
1	C	173	MET
1	C	205	LEU
1	C	208	THR
1	C	219	LEU
1	C	230	LEU
1	C	241	LYS
1	C	250	THR
1	C	265	VAL
1	C	269	ASN
1	C	270	GLU
1	C	272	LYS
1	C	273	THR
1	C	285	GLN
1	C	293	LEU
1	C	305	MET
1	C	311	SER
1	C	314	LEU
1	C	321	ARG
1	C	327	GLN
1	C	330	GLN
1	C	334	MET
1	D	1	CYS
1	D	4	LEU
1	D	6	ILE
1	D	10	ASP
1	D	17	ARG
1	D	23	MET
1	D	26	ASP
1	D	28	LYS
1	D	29	VAL
1	D	34	ARG
1	D	41	LEU
1	D	67	LEU
1	D	71	VAL
1	D	72	ASN
1	D	74	LYS

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Mol	Chain	Res	Type
1	D	82	TYR
1	D	85	THR
1	D	95	LYS
1	D	98	THR
1	D	103	VAL
1	D	110	LEU
1	D	121	GLU
1	D	123	LEU
1	D	130	ASN
1	D	136	LEU
1	D	142	LEU
1	D	143	HIS
1	D	152	GLU
1	D	167	ARG
1	D	173	MET
1	D	195	ASN
1	D	205	LEU
1	D	208	THR
1	D	219	LEU
1	D	230	LEU
1	D	235	TRP
1	D	241	LYS
1	D	250	THR
1	D	265	VAL
1	D	269	ASN
1	D	270	GLU
1	D	272	LYS
1	D	273	THR
1	D	285	GLN
1	D	293	LEU
1	D	296	ASN
1	D	311	SER
1	D	314	LEU
1	D	321	ARG
1	D	327	GLN
1	D	330	GLN
1	D	334	MET
1	E	1	CYS
1	E	4	LEU
1	E	6	ILE
1	E	10	ASP
1	E	17	ARG

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Mol	Chain	Res	Type
1	E	23	MET
1	E	26	ASP
1	E	28	LYS
1	E	29	VAL
1	E	34	ARG
1	E	41	LEU
1	E	67	LEU
1	E	71	VAL
1	E	72	ASN
1	E	74	LYS
1	E	82	TYR
1	E	85	THR
1	E	95	LYS
1	E	98	THR
1	E	110	LEU
1	E	121	GLU
1	E	123	LEU
1	E	130	ASN
1	E	136	LEU
1	E	142	LEU
1	E	143	HIS
1	E	145	THR
1	E	152	GLU
1	E	160	LYS
1	E	167	ARG
1	E	173	MET
1	E	195	ASN
1	E	205	LEU
1	E	219	LEU
1	E	230	LEU
1	E	235	TRP
1	E	250	THR
1	E	265	VAL
1	E	269	ASN
1	E	270	GLU
1	E	272	LYS
1	E	273	THR
1	E	285	GLN
1	E	293	LEU
1	E	296	ASN
1	E	311	SER
1	E	314	LEU

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Mol	Chain	Res	Type
1	E	318	GLU
1	E	321	ARG
1	E	327	GLN
1	E	330	GLN
1	E	334	MET
1	F	1	CYS
1	F	4	LEU
1	F	6	ILE
1	F	10	ASP
1	F	17	ARG
1	F	23	MET
1	F	26	ASP
1	F	28	LYS
1	F	29	VAL
1	F	34	ARG
1	F	41	LEU
1	F	67	LEU
1	F	71	VAL
1	F	72	ASN
1	F	74	LYS
1	F	82	TYR
1	F	85	THR
1	F	95	LYS
1	F	98	THR
1	F	110	LEU
1	F	121	GLU
1	F	123	LEU
1	F	130	ASN
1	F	136	LEU
1	F	142	LEU
1	F	143	HIS
1	F	152	GLU
1	F	160	LYS
1	F	167	ARG
1	F	173	MET
1	F	180	GLU
1	F	205	LEU
1	F	208	THR
1	F	219	LEU
1	F	230	LEU
1	F	235	TRP
1	F	241	LYS

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Mol	Chain	Res	Type
1	F	250	THR
1	F	265	VAL
1	F	269	ASN
1	F	270	GLU
1	F	272	LYS
1	F	273	THR
1	F	285	GLN
1	F	287	LYS
1	F	292	LYS
1	F	293	LEU
1	F	296	ASN
1	F	311	SER
1	F	314	LEU
1	F	318	GLU
1	F	321	ARG
1	F	327	GLN
1	F	330	GLN
1	F	334	MET
1	G	1	CYS
1	G	4	LEU
1	G	6	ILE
1	G	10	ASP
1	G	17	ARG
1	G	23	MET
1	G	26	ASP
1	G	28	LYS
1	G	29	VAL
1	G	34	ARG
1	G	41	LEU
1	G	67	LEU
1	G	71	VAL
1	G	72	ASN
1	G	74	LYS
1	G	82	TYR
1	G	85	THR
1	G	95	LYS
1	G	98	THR
1	G	110	LEU
1	G	121	GLU
1	G	123	LEU
1	G	130	ASN
1	G	136	LEU

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Mol	Chain	Res	Type
1	G	142	LEU
1	G	143	HIS
1	G	145	THR
1	G	152	GLU
1	G	160	LYS
1	G	167	ARG
1	G	173	MET
1	G	195	ASN
1	G	205	LEU
1	G	208	THR
1	G	219	LEU
1	G	230	LEU
1	G	235	TRP
1	G	241	LYS
1	G	250	THR
1	G	265	VAL
1	G	269	ASN
1	G	270	GLU
1	G	272	LYS
1	G	273	THR
1	G	285	GLN
1	G	287	LYS
1	G	293	LEU
1	G	296	ASN
1	G	311	SER
1	G	314	LEU
1	G	321	ARG
1	G	327	GLN
1	G	330	GLN
1	G	334	MET
1	H	6	ILE
1	H	10	ASP
1	H	17	ARG
1	H	23	MET
1	H	26	ASP
1	H	28	LYS
1	H	29	VAL
1	H	41	LEU
1	H	71	VAL
1	H	72	ASN
1	H	74	LYS
1	H	82	TYR

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Mol	Chain	Res	Type
1	H	85	THR
1	H	95	LYS
1	H	98	THR
1	H	110	LEU
1	H	121	GLU
1	H	123	LEU
1	H	130	ASN
1	H	136	LEU
1	H	142	LEU
1	H	143	HIS
1	H	152	GLU
1	H	167	ARG
1	H	173	MET
1	H	195	ASN
1	H	205	LEU
1	H	219	LEU
1	H	230	LEU
1	H	235	TRP
1	H	241	LYS
1	H	250	THR
1	H	265	VAL
1	H	269	ASN
1	H	270	GLU
1	H	272	LYS
1	H	273	THR
1	H	285	GLN
1	H	287	LYS
1	H	293	LEU
1	H	305	MET
1	H	311	SER
1	H	314	LEU
1	H	318	GLU
1	H	321	ARG
1	H	327	GLN
1	H	330	GLN
1	H	334	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	72	ASN
1	A	130	ASN
1	A	133	ASN
1	A	185	ASN
1	A	212	GLN
1	A	251	ASN
1	A	269	ASN
1	A	288	ASN
1	A	296	ASN
1	B	35	ASN
1	B	49	ASN
1	B	72	ASN
1	B	130	ASN
1	B	133	ASN
1	B	185	ASN
1	B	251	ASN
1	B	269	ASN
1	B	288	ASN
1	B	296	ASN
1	C	72	ASN
1	C	130	ASN
1	C	133	ASN
1	C	185	ASN
1	C	212	GLN
1	C	251	ASN
1	C	269	ASN
1	C	288	ASN
1	C	296	ASN
1	D	72	ASN
1	D	130	ASN
1	D	133	ASN
1	D	185	ASN
1	D	251	ASN
1	D	269	ASN
1	D	288	ASN
1	D	296	ASN
1	E	35	ASN
1	E	49	ASN
1	E	72	ASN
1	E	130	ASN
1	E	133	ASN
1	E	185	ASN

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Mol	Chain	Res	Type
1	E	212	GLN
1	E	251	ASN
1	E	269	ASN
1	E	288	ASN
1	E	296	ASN
1	F	130	ASN
1	F	133	ASN
1	F	166	HIS
1	F	185	ASN
1	F	212	GLN
1	F	251	ASN
1	F	269	ASN
1	F	288	ASN
1	F	296	ASN
1	G	72	ASN
1	G	130	ASN
1	G	133	ASN
1	G	185	ASN
1	G	251	ASN
1	G	269	ASN
1	G	288	ASN
1	G	296	ASN
1	H	72	ASN
1	H	130	ASN
1	H	133	ASN
1	H	185	ASN
1	H	251	ASN
1	H	269	ASN
1	H	288	ASN
1	H	296	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.