Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:45 PM GMT

PDB ID	:	1QHA
Title	:	HUMAN HEXOKINASE TYPE I COMPLEXED WITH ATP ANALOGUE AMP-PNP
Authors	:	Rosano, C.; Sabini, E.; Deriu, D.; Magnani, M.; Bolognesi, M.
Deposited on	:	1999-05-11
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

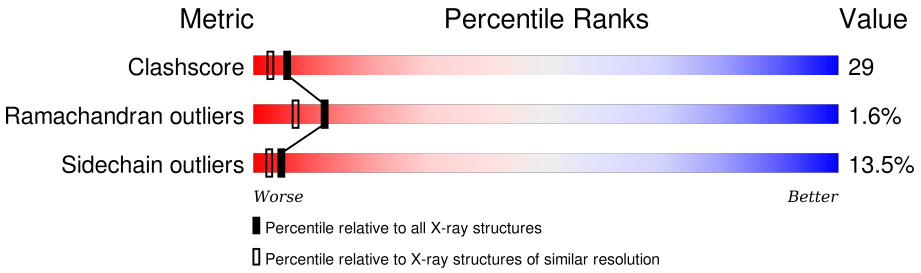
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.25 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	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	917	48% 35% 12%
1	B	917	61% 26% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	A	919	X	-	X	-
3	G6P	A	921	X	-	-	-
3	G6P	B	1916	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	B	1918	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14737 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.

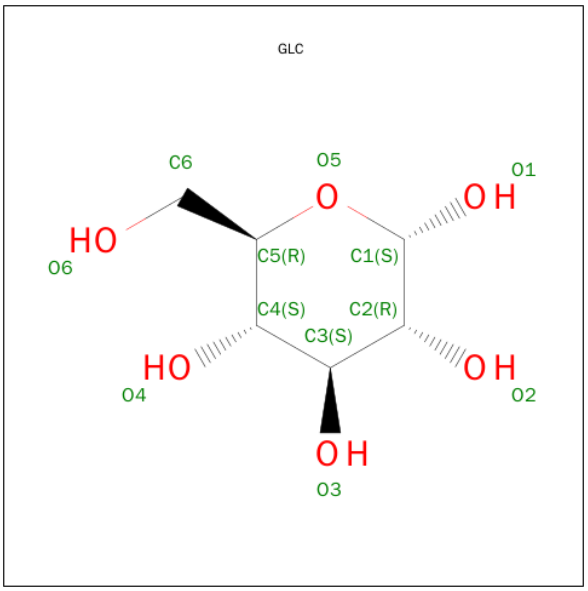
- Molecule 1 is a protein called PROTEIN (HEXOKINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	67	0	0
			7065	4428	1246	1338	53			
1	B	899	Total	C	N	O	S	62	0	0
			7032	4407	1241	1331	53			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	776	LEU	MET	CONFLICT	UNP P19367
B	776	LEU	MET	CONFLICT	UNP P19367

- Molecule 2 is GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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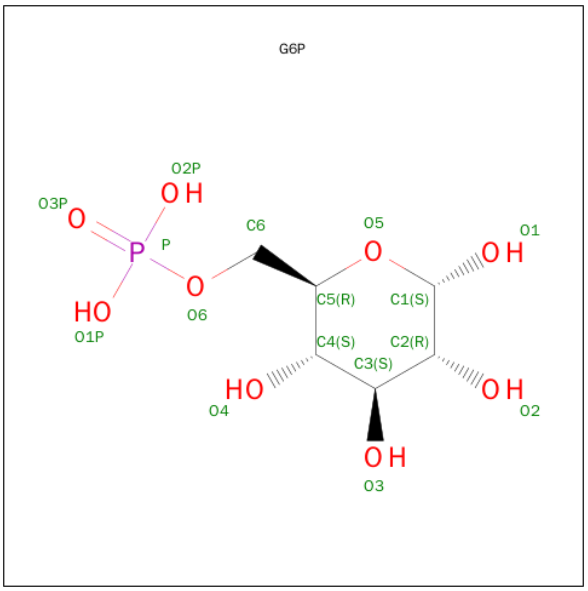
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0

- Molecule 3 is ALPHA-D-GLUCOSE-6-PHOSPHATE (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).

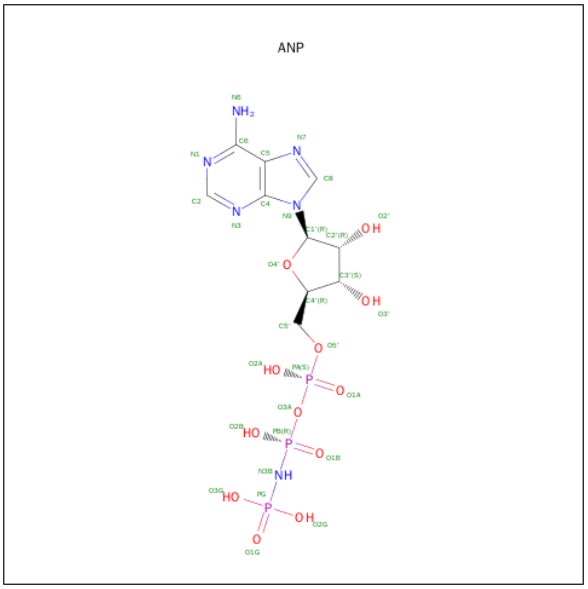


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 16 6 9 1	0	0
3	A	1	Total C O P 16 6 9 1	0	0
3	B	1	Total C O P 16 6 9 1	0	0
3	B	1	Total C O P 16 6 9 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Mg 3 3	0	0
4	A	3	Total Mg 3 3	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	188	Total	O	0	0
			188	188		
6	B	272	Total	O	0	0
			272	272		

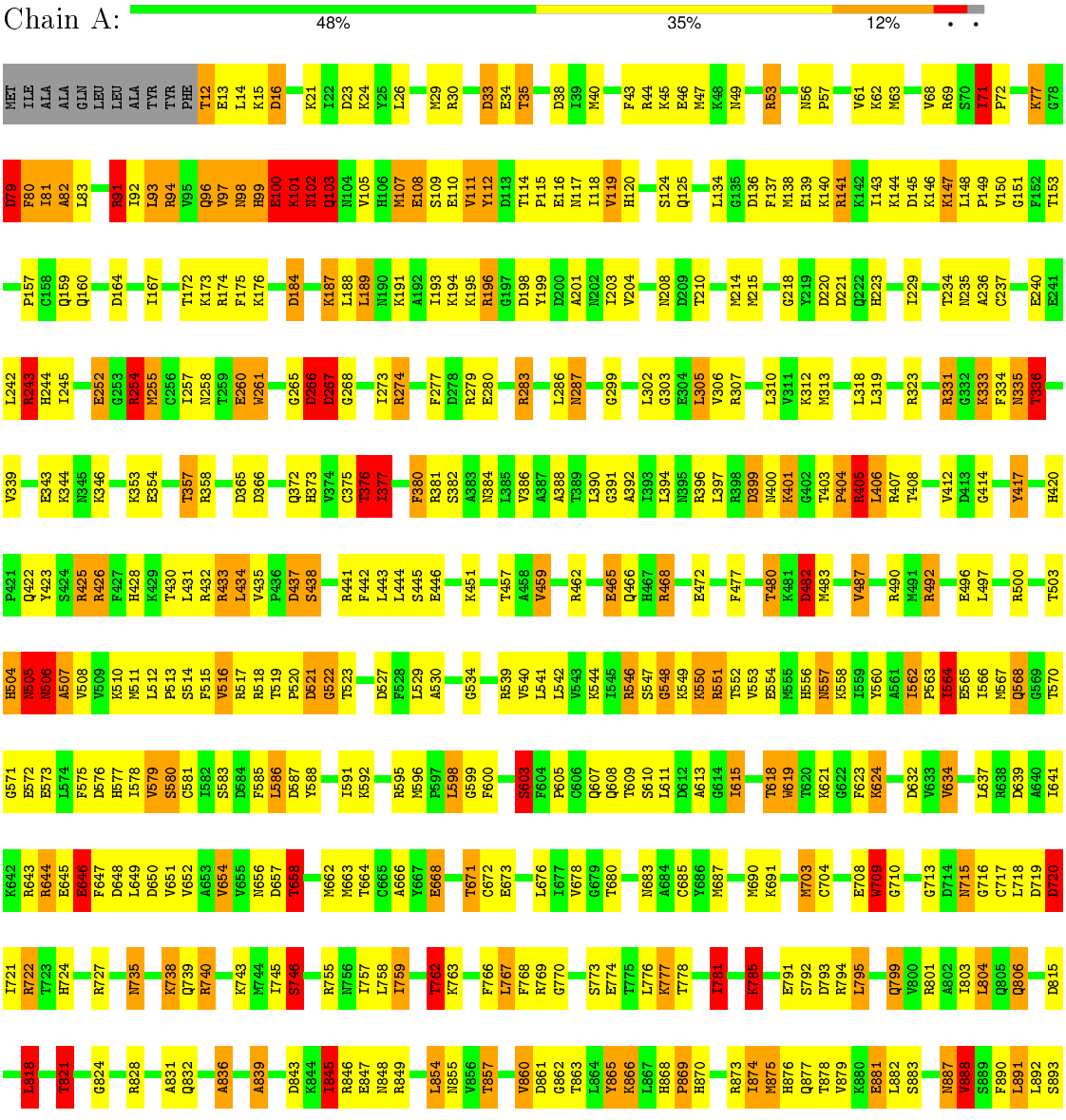
3 Residue-property plots (i)

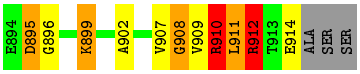
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: PROTEIN (HEXOKINASE)

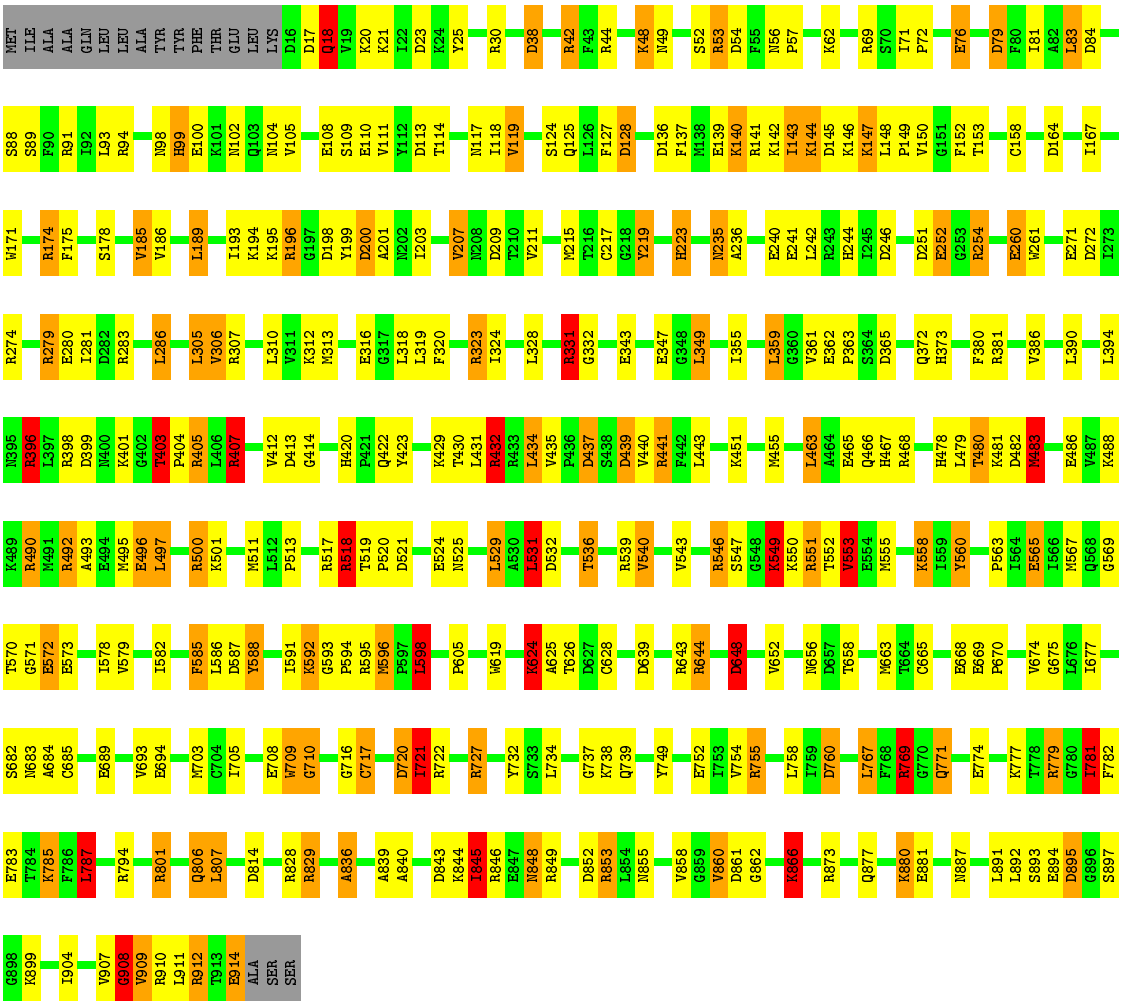
Chain A:





- Molecule 1: PROTEIN (HEXOKINASE)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.59Å 176.17Å 86.76Å 90.00° 90.53° 90.00°	Depositor
Resolution (Å)	12.00 – 2.25	Depositor
% Data completeness (in resolution range)	85.0 (12.00-2.25)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14737	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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, GLC, ANP, G6P

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	0.72	8/7170 (0.1%)	1.75	146/9647 (1.5%)
1	B	0.83	6/7134 (0.1%)	1.89	162/9594 (1.7%)
All	All	0.78	14/14304 (0.1%)	1.82	308/19241 (1.6%)

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	28
1	B	0	16
All	All	0	44

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	914	GLU	CB-CG	-32.64	0.90	1.52
1	A	144	LYS	CG-CD	-17.85	0.91	1.52
1	A	147	LYS	CG-CD	16.68	2.09	1.52
1	B	99	HIS	C-N	14.83	1.68	1.34
1	B	62	LYS	CG-CD	-13.55	1.06	1.52
1	B	18	GLN	CD-OE1	12.41	1.51	1.24
1	A	99	HIS	C-N	-11.80	1.06	1.34
1	B	102	ASN	CA-CB	11.64	1.83	1.53
1	B	99	HIS	CA-CB	9.26	1.74	1.53
1	A	103	GLN	C-N	7.67	1.51	1.34
1	A	912	ARG	CD-NE	6.53	1.57	1.46
1	A	100	GLU	CA-CB	5.29	1.65	1.53
1	A	101	LYS	C-N	-5.13	1.22	1.34
1	A	100	GLU	C-N	-5.07	1.22	1.34

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102	ASN	N-CA-CB	-39.95	38.70	110.60
1	B	829	ARG	NE-CZ-NH2	-27.14	106.73	120.30
1	B	829	ARG	CD-NE-CZ	25.57	159.40	123.60
1	B	100	GLU	CB-CA-C	-25.01	60.37	110.40
1	B	755	ARG	NE-CZ-NH1	-24.72	107.94	120.30
1	B	441	ARG	NE-CZ-NH1	-23.52	108.54	120.30
1	A	283	ARG	NE-CZ-NH2	-23.09	108.76	120.30
1	A	99	HIS	O-C-N	-21.87	87.71	122.70
1	A	144	LYS	CB-CG-CD	21.02	166.24	111.60
1	A	912	ARG	CG-CD-NE	20.66	155.18	111.80
1	B	99	HIS	O-C-N	17.39	150.53	122.70
1	B	279	ARG	NE-CZ-NH2	-16.42	112.09	120.30
1	A	912	ARG	CD-NE-CZ	16.14	146.19	123.60
1	B	727	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	A	53	ARG	NE-CZ-NH2	-14.55	113.03	120.30
1	A	101	LYS	O-C-N	-14.50	99.50	122.70
1	B	99	HIS	CA-C-N	-14.15	86.08	117.20
1	B	42	ARG	CD-NE-CZ	13.57	142.60	123.60
1	B	437	ASP	CB-CG-OD2	-13.56	106.10	118.30
1	B	873	ARG	CD-NE-CZ	13.42	142.38	123.60
1	B	755	ARG	NE-CZ-NH2	13.37	126.99	120.30
1	A	283	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	A	720	ASP	CB-CG-OD1	-13.14	106.47	118.30
1	B	441	ARG	NE-CZ-NH2	13.09	126.85	120.30
1	A	30	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	B	500	ARG	NE-CZ-NH1	-12.89	113.85	120.30
1	B	801	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	B	30	ARG	NE-CZ-NH1	-12.54	114.03	120.30
1	A	801	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	B	18	GLN	CG-CD-OE1	-12.15	97.30	121.60
1	A	260	GLU	OE1-CD-OE2	-11.97	108.94	123.30
1	B	598	LEU	CA-CB-CG	11.86	142.57	115.30
1	B	801	ARG	CD-NE-CZ	11.49	139.69	123.60
1	B	69	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	B	877	GLN	CA-CB-CG	11.41	138.51	113.40
1	B	914	GLU	CA-CB-CG	11.14	137.91	113.40
1	B	829	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	828	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	B	490	ARG	CD-NE-CZ	10.87	138.82	123.60
1	A	102	ASN	N-CA-CB	-10.86	91.06	110.60
1	A	279	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	492	ARG	NE-CZ-NH2	-10.52	115.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	GLN	O-C-N	-10.42	106.02	122.70
1	B	99	HIS	N-CA-CB	-10.36	91.95	110.60
1	A	69	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	B	567	MET	CA-CB-CG	10.28	130.77	113.30
1	A	307	ARG	CD-NE-CZ	10.22	137.91	123.60
1	B	490	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	B	644	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	B	62	LYS	CB-CG-CD	9.95	137.46	111.60
1	B	722	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	B	722	ARG	CD-NE-CZ	9.94	137.51	123.60
1	A	99	HIS	CB-CA-C	-9.90	90.59	110.40
1	B	42	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	B	546	ARG	CD-NE-CZ	9.89	137.45	123.60
1	A	243	ARG	NE-CZ-NH1	-9.75	115.42	120.30
1	A	323	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	A	33	ASP	CB-CG-OD2	9.55	126.90	118.30
1	B	200	ASP	N-CA-CB	9.55	127.78	110.60
1	A	426	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	468	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	B	914	GLU	CB-CG-CD	-9.53	88.47	114.20
1	B	399	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	71	ILE	CA-CB-CG2	9.28	129.45	110.90
1	B	648	ASP	N-CA-CB	9.19	127.14	110.60
1	B	331	ARG	NE-CZ-NH1	-9.17	115.71	120.30
1	B	283	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	A	283	ARG	CD-NE-CZ	9.03	136.25	123.60
1	A	147	LYS	CB-CG-CD	-8.99	88.23	111.60
1	B	365	ASP	CB-CG-OD1	8.98	126.38	118.30
1	B	279	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	B	846	ARG	CD-NE-CZ	8.95	136.13	123.60
1	A	425	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	267	ASP	CB-CG-OD1	8.82	126.24	118.30
1	B	912	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	B	500	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	A	377	ILE	CA-CB-CG2	8.71	128.33	110.90
1	B	492	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	B	44	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	644	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	A	801	ARG	CD-NE-CZ	8.61	135.65	123.60
1	B	53	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	B	94	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	A	100	GLU	CA-C-N	-8.46	98.60	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	407	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	254	ARG	CD-NE-CZ	8.38	135.34	123.60
1	B	785	LYS	CA-CB-CG	8.38	131.83	113.40
1	B	483	MET	CA-CB-CG	8.34	127.48	113.30
1	A	399	ASP	CB-CA-C	8.31	127.02	110.40
1	A	407	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	727	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	323	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	A	396	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	722	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	828	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	B	727	ARG	CD-NE-CZ	-8.15	112.19	123.60
1	A	101	LYS	CA-C-N	8.13	135.08	117.20
1	A	103	GLN	C-N-CA	8.02	141.75	121.70
1	B	546	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	38	ASP	CB-CG-OD1	7.82	125.33	118.30
1	B	895	ASP	CA-CB-CG	7.81	130.57	113.40
1	B	546	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	209	ASP	CB-CG-OD1	-7.77	111.30	118.30
1	A	331	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	A	468	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	912	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	B	551	ARG	CD-NE-CZ	7.65	134.32	123.60
1	A	112	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	B	274	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	866	LYS	CA-CB-CG	7.58	130.06	113.40
1	B	560	TYR	CB-CG-CD1	7.52	125.51	121.00
1	A	720	ASP	CA-CB-CG	-7.47	96.95	113.40
1	A	539	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	A	99	HIS	CA-C-N	7.40	133.48	117.20
1	A	546	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	A	722	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	79	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	433	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	A	794	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	873	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	174	ARG	CD-NE-CZ	-7.29	113.40	123.60
1	B	432	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	B	829	ARG	NH1-CZ-NH2	7.18	127.30	119.40
1	A	69	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	828	ARG	NE-CZ-NH2	-7.14	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	425	ARG	CD-NE-CZ	7.12	133.56	123.60
1	A	709	TRP	CA-CB-CG	7.12	127.22	113.70
1	B	585	PHE	CB-CG-CD1	7.07	125.75	120.80
1	B	518	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	30	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	482	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	815	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	585	PHE	CB-CG-CD2	-6.87	115.99	120.80
1	A	94	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	912	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	A	254	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	894	GLU	OE1-CD-OE2	-6.83	115.11	123.30
1	A	381	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	331	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	818	LEU	CB-CA-C	6.81	123.14	110.20
1	A	99	HIS	C-N-CA	6.80	138.71	121.70
1	B	69	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	B	721	ILE	CA-CB-CG2	6.74	124.38	110.90
1	B	323	ARG	CD-NE-CZ	-6.73	114.18	123.60
1	B	99	HIS	CB-CA-C	6.72	123.85	110.40
1	A	196	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	103	GLN	CA-C-N	6.68	131.90	117.20
1	B	551	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	403	THR	N-CA-CB	-6.63	97.69	110.30
1	B	518	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	B	396	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	644	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	814	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	223	HIS	N-CA-CB	6.50	122.30	110.60
1	A	426	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	91	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	272	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	767	LEU	N-CA-CB	-6.44	97.51	110.40
1	B	398	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	365	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	654	VAL	N-CA-CB	6.36	125.49	111.50
1	B	441	ARG	CD-NE-CZ	-6.36	114.69	123.60
1	B	283	ARG	NH1-CZ-NH2	6.36	126.39	119.40
1	B	511	MET	O-C-N	-6.36	112.53	122.70
1	A	101	LYS	C-N-CA	6.35	137.58	121.70
1	A	323	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	196	ARG	CB-CA-C	6.32	123.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	359	LEU	CA-CB-CG	6.32	129.83	115.30
1	A	767	LEU	CA-CB-CG	6.30	129.78	115.30
1	B	881	GLU	CA-CB-CG	6.28	127.22	113.40
1	A	255	MET	N-CA-CB	6.28	121.90	110.60
1	A	740	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	860	VAL	CB-CA-C	-6.23	99.56	111.40
1	B	551	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	184	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	12	THR	N-CA-CB	-6.22	98.48	110.30
1	B	517	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	267	ASP	N-CA-CB	-6.20	99.44	110.60
1	A	358	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	763	LYS	CA-CB-CG	6.18	127.01	113.40
1	A	405	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	658	THR	CA-CB-CG2	6.17	121.04	112.40
1	B	490	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	558	LYS	N-CA-CB	6.15	121.68	110.60
1	A	426	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	860	VAL	CB-CA-C	-6.12	99.77	111.40
1	B	100	GLU	N-CA-CB	6.12	121.61	110.60
1	A	396	ARG	NH1-CZ-NH2	6.04	126.05	119.40
1	B	279	ARG	CG-CD-NE	-6.04	99.11	111.80
1	A	432	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	B	307	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	560	TYR	CB-CG-CD2	-6.01	117.40	121.00
1	B	648	ASP	CA-CB-CG	-6.00	100.20	113.40
1	B	760	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	79	ASP	CA-CB-CG	5.97	126.54	113.40
1	B	323	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	749	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	B	207	VAL	CA-CB-CG1	5.91	119.77	110.90
1	B	171	TRP	CG-CD2-CE3	-5.91	128.59	133.90
1	A	243	ARG	CD-NE-CZ	-5.88	115.37	123.60
1	B	860	VAL	CA-CB-CG1	5.88	119.72	110.90
1	A	845	ILE	N-CA-CB	5.87	124.31	110.80
1	B	572	GLU	CB-CA-C	5.87	122.15	110.40
1	B	716	GLY	O-C-N	-5.87	113.31	122.70
1	B	260	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	A	12	THR	O-C-N	-5.84	113.36	122.70
1	A	196	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	517	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	769	ARG	NE-CZ-NH2	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	727	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	30	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	785	LYS	CA-CB-CG	5.81	126.19	113.40
1	A	873	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	219	TYR	CB-CG-CD1	5.80	124.48	121.00
1	B	381	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	865	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	A	517	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	306	VAL	CA-CB-CG2	5.68	119.42	110.90
1	B	99	HIS	C-N-CA	-5.68	107.50	121.70
1	B	767	LEU	N-CA-CB	-5.67	99.05	110.40
1	B	749	TYR	CB-CG-CD1	5.66	124.40	121.00
1	A	719	ASP	C-N-CA	5.66	135.84	121.70
1	B	587	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	516	VAL	CA-CB-CG2	5.63	119.34	110.90
1	A	305	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	207	VAL	O-C-N	-5.58	113.76	122.70
1	A	462	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	12	THR	CA-CB-CG2	5.57	120.19	112.40
1	A	746	SER	CB-CA-C	-5.56	99.53	110.10
1	A	839	ALA	N-CA-CB	5.55	117.87	110.10
1	B	128	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	531	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	141	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	727	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	781	ILE	CB-CA-C	5.52	122.64	111.60
1	A	863	THR	CA-CB-CG2	-5.49	104.71	112.40
1	A	274	ARG	CD-NE-CZ	-5.49	115.91	123.60
1	A	153	THR	CA-C-N	-5.48	105.15	117.20
1	B	246	ASP	N-CA-CB	5.44	120.39	110.60
1	B	891	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	100	GLU	C-N-CA	-5.43	108.12	121.70
1	A	35	THR	N-CA-CB	5.42	120.61	110.30
1	A	568	GLN	CA-CB-CG	5.42	125.34	113.40
1	B	785	LYS	N-CA-CB	-5.41	100.86	110.60
1	A	516	VAL	N-CA-CB	5.41	123.39	111.50
1	B	532	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	417	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	38	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	260	GLU	CG-CD-OE1	5.38	129.07	118.30
1	A	174	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	305	LEU	CB-CG-CD1	5.38	120.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	720	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	178	SER	CB-CA-C	-5.37	99.89	110.10
1	B	407	ARG	CD-NE-CZ	5.37	131.12	123.60
1	B	553	VAL	N-CA-CB	5.35	123.26	111.50
1	A	639	ASP	CA-CB-CG	5.34	125.14	113.40
1	A	762	THR	N-CA-CB	5.33	120.44	110.30
1	B	18	GLN	OE1-CD-NE2	-5.33	109.65	121.90
1	A	781	ILE	CA-CB-CG2	5.32	121.54	110.90
1	A	632	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	875	MET	CA-CB-CG	5.31	122.32	113.30
1	B	787	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	220	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	398	ARG	NH1-CZ-NH2	5.28	125.20	119.40
1	B	398	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	B	283	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	254	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	492	ARG	N-CA-CB	5.26	120.07	110.60
1	B	405	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	482	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	580	SER	N-CA-CB	5.24	118.36	110.50
1	B	209	ASP	N-CA-CB	5.23	120.02	110.60
1	A	603	SER	N-CA-CB	-5.22	102.66	110.50
1	B	845	ILE	CA-CB-CG2	5.22	121.33	110.90
1	B	861	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	100	GLU	CB-CA-C	5.21	120.81	110.40
1	A	639	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	643	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	366	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	720	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	376	THR	CA-CB-CG2	5.18	119.65	112.40
1	A	836	ALA	N-CA-CB	5.17	117.33	110.10
1	B	492	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	280	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	517	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	755	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	A	147	LYS	CG-CD-CE	5.14	127.32	111.90
1	B	440	VAL	CB-CA-C	-5.14	101.64	111.40
1	B	588	TYR	CA-CB-CG	5.11	123.12	113.40
1	A	266	ASP	CB-CA-C	5.10	120.61	110.40
1	B	42	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	B	113	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	576	ASP	CB-CG-OD1	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	869	PRO	N-CD-CG	-5.07	95.60	103.20
1	A	821	THR	N-CA-CB	5.06	119.92	110.30
1	A	881	GLU	N-CA-CB	5.06	119.71	110.60
1	A	354	GLU	CA-CB-CG	5.06	124.53	113.40
1	A	396	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	564	ILE	N-CA-CB	5.06	122.43	110.80
1	B	217	CYS	CB-CA-C	5.05	120.50	110.40
1	A	307	ARG	CG-CD-NE	5.05	122.40	111.80
1	A	377	ILE	O-C-N	-5.04	114.64	122.70
1	A	331	ARG	CD-NE-CZ	-5.02	116.57	123.60
1	B	407	ARG	O-C-N	-5.02	114.67	122.70
1	B	125	GLN	CA-CB-CG	5.02	124.44	113.40
1	B	102	ASN	CA-CB-CG	-5.01	102.38	113.40
1	B	500	ARG	CD-NE-CZ	-5.00	116.60	123.60

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	101	LYS	Mainchain,Peptide
1	A	114	THR	Mainchain
1	A	237	CYS	Mainchain
1	A	243	ARG	Mainchain
1	A	258	ASN	Mainchain
1	A	267	ASP	Mainchain
1	A	333	LYS	Mainchain
1	A	336	THR	Mainchain
1	A	346	LYS	Mainchain
1	A	399	ASP	Mainchain
1	A	459	VAL	Mainchain
1	A	505	ASN	Mainchain
1	A	507	ALA	Mainchain
1	A	568	GLN	Mainchain
1	A	618	THR	Mainchain
1	A	634	VAL	Mainchain
1	A	646	GLU	Mainchain
1	A	68	VAL	Mainchain
1	A	738	LYS	Mainchain
1	A	745	ILE	Mainchain
1	A	746	SER	Mainchain
1	A	79	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	854	LEU	Mainchain
1	A	887	ASN	Mainchain
1	A	888	VAL	Mainchain
1	A	99	HIS	Mainchain
1	B	128	ASP	Mainchain
1	B	18	GLN	Sidechain
1	B	286	LEU	Mainchain
1	B	363	PRO	Mainchain
1	B	435	VAL	Mainchain
1	B	466	GLN	Mainchain
1	B	480	THR	Mainchain
1	B	540	VAL	Mainchain
1	B	553	VAL	Mainchain
1	B	710	GLY	Mainchain
1	B	737	GLY	Mainchain
1	B	738	LYS	Mainchain
1	B	807	LEU	Mainchain
1	B	836	ALA	Mainchain
1	B	860	VAL	Mainchain
1	B	908	GLY	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	7065	0	7124	483	0
1	B	7032	0	7087	334	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
3	A	32	0	22	7	0
3	B	32	0	21	8	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	31	0	13	1	0
5	B	31	0	13	1	0
6	A	188	0	0	33	0
6	B	272	0	0	37	0
All	All	14737	0	14328	823	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 29.

All (823) 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:505:ASN:O	1:A:507:ALA:N	1.57	1.31
1:A:521:ASP:HB3	6:A:1169:HOH:O	1.34	1.24
1:A:29:MET:HB2	1:A:377:ILE:HD11	1.27	1.17
1:B:441:ARG:HG3	1:B:441:ARG:HH11	1.13	1.11
1:A:62:LYS:CE	6:A:1057:HOH:O	1.89	1.11
1:A:646:GLU:HG2	1:A:647:PHE:HD1	1.16	1.11
1:A:656:ASN:ND2	1:A:658:THR:HB	1.67	1.09
1:B:71:ILE:HG22	1:B:215:MET:HE1	1.32	1.06
1:A:62:LYS:HE3	6:A:1057:HOH:O	1.44	1.04
1:A:778:THR:HB	1:A:781:ILE:HD13	1.38	1.03
1:A:441:ARG:NH1	1:A:443:LEU:HD22	1.74	1.02
1:B:769:ARG:CD	6:B:2251:HOH:O	2.08	1.01
1:A:303:GLY:N	1:A:336:THR:HG22	1.77	1.00
1:A:189:LEU:HD13	1:A:203:ILE:HD11	1.43	0.98
1:A:71:ILE:HG23	6:A:1102:HOH:O	1.61	0.98
1:A:598:LEU:HD12	1:A:599:GLY:N	1.79	0.98
1:A:71:ILE:HA	1:A:215:MET:HE1	1.46	0.98
1:A:735:ASN:HD22	1:A:735:ASN:H	1.01	0.97
1:B:908:GLY:O	1:B:910:ARG:N	1.98	0.97
1:A:313:MET:HE3	1:A:319:LEU:CD1	1.94	0.97
1:B:480:THR:H	1:B:483:MET:HG3	1.30	0.97
1:B:441:ARG:HG3	1:B:441:ARG:NH1	1.72	0.96
1:B:752:GLU:CD	1:B:755:ARG:HH12	1.67	0.96
1:A:313:MET:HE3	1:A:319:LEU:HD11	1.43	0.96
1:A:313:MET:CE	1:A:319:LEU:HD11	1.93	0.96
1:B:465:GLU:OE1	1:B:468:ARG:NH2	1.97	0.96
1:B:441:ARG:HH11	1:B:441:ARG:CG	1.66	0.95
1:A:110:GLU:O	1:A:111:VAL:HG23	1.67	0.94
1:B:71:ILE:HA	1:B:215:MET:CE	1.98	0.94
1:B:563:PRO:HB2	1:B:565:GLU:HG3	1.49	0.94
1:A:435:VAL:HG12	1:A:438:SER:HB2	1.50	0.94
1:B:752:GLU:OE2	1:B:755:ARG:NH1	2.00	0.93
1:B:72:PRO:HD3	1:B:215:MET:HE2	1.51	0.93
1:B:480:THR:HG22	1:B:483:MET:HG2	1.48	0.93
1:A:832:GLN:HG3	1:A:874:ILE:HD11	1.49	0.93
1:A:644:ARG:HG2	1:A:646:GLU:HB3	1.48	0.93
1:B:578:ILE:HG23	6:B:2246:HOH:O	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HG22	1:B:215:MET:CE	1.98	0.92
1:B:578:ILE:CG2	6:B:2246:HOH:O	2.16	0.92
1:A:658:THR:HG23	1:A:685:CYS:HB3	1.50	0.92
1:B:769:ARG:HD2	6:B:2251:HOH:O	1.69	0.92
1:A:646:GLU:HG2	1:A:647:PHE:CD1	2.05	0.92
1:B:907:VAL:O	1:B:908:GLY:O	1.88	0.92
1:B:513:PRO:HB3	1:B:703:MET:HE1	1.49	0.91
1:A:671:THR:HB	1:A:857:THR:HG23	1.49	0.91
3:B:1918:G6P:H62	6:B:2227:HOH:O	1.70	0.91
1:B:493:ALA:O	1:B:497:LEU:HD23	1.70	0.91
1:B:595:ARG:NH1	1:B:648:ASP:HB3	1.83	0.91
1:A:62:LYS:HE2	6:A:1173:HOH:O	1.71	0.91
1:A:562:ILE:HD11	6:A:1152:HOH:O	1.70	0.91
1:A:81:ILE:HG22	1:A:82:ALA:H	1.35	0.91
1:B:480:THR:HG22	1:B:483:MET:CG	2.01	0.90
1:A:895:ASP:O	1:A:895:ASP:CG	2.09	0.90
1:A:303:GLY:H	1:A:336:THR:HG22	1.31	0.89
3:B:1916:G6P:H62	6:B:2027:HOH:O	1.69	0.89
1:A:792:SER:OG	1:A:795:LEU:HD23	1.72	0.89
1:A:245:ILE:HD13	1:A:257:ILE:HD11	1.54	0.89
1:A:634:VAL:HG23	1:A:654:VAL:CG2	2.02	0.89
3:A:919:G6P:H61	6:A:1033:HOH:O	1.72	0.89
1:B:72:PRO:HB3	1:B:455:MET:CE	2.03	0.89
1:A:656:ASN:HD22	1:A:658:THR:CG2	1.85	0.88
1:A:656:ASN:HD22	1:A:658:THR:HB	1.28	0.88
1:B:420:HIS:HD2	1:B:422:GLN:H	1.20	0.88
1:B:769:ARG:NH2	6:B:2165:HOH:O	2.07	0.87
1:B:496:GLU:OE2	1:B:844:LYS:HE2	1.74	0.87
1:A:895:ASP:OD1	6:A:1161:HOH:O	1.93	0.87
1:B:71:ILE:CG2	1:B:215:MET:HE1	2.03	0.86
1:B:480:THR:HG23	1:B:483:MET:H	1.41	0.86
1:B:189:LEU:HD13	1:B:203:ILE:HD11	1.56	0.86
1:A:335:ASN:C	1:A:335:ASN:HD22	1.72	0.86
1:B:513:PRO:CB	1:B:703:MET:HE1	2.06	0.85
1:A:527:ASP:OD1	1:A:544:LYS:HG2	1.75	0.85
1:B:845:ILE:HD12	1:B:849:ARG:CZ	2.06	0.85
1:B:110:GLU:OE1	1:B:141:ARG:NH2	2.08	0.85
1:A:71:ILE:CD1	1:A:218:GLY:HA3	2.07	0.85
1:A:81:ILE:O	1:A:82:ALA:HB2	1.74	0.85
1:B:479:LEU:HA	1:B:483:MET:HE2	1.58	0.85
1:B:76:GLU:HG3	1:B:455:MET:CE	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ILE:HD11	1:A:776:LEU:HG	1.56	0.85
1:A:353:LYS:O	1:A:357:THR:HG23	1.75	0.84
1:B:111:VAL:HG12	6:B:2155:HOH:O	1.77	0.84
1:A:287:ASN:HD22	1:A:287:ASN:H	1.21	0.84
1:A:33:ASP:OD2	1:A:433:ARG:NE	2.09	0.84
1:A:505:ASN:C	1:A:507:ALA:N	2.27	0.84
1:A:646:GLU:HG2	1:A:647:PHE:H	1.42	0.84
1:B:585:PHE:O	6:B:2249:HOH:O	1.96	0.84
1:B:401:LYS:NZ	1:B:403:THR:HG21	1.91	0.84
1:A:762:THR:HG22	1:A:767:LEU:HD12	1.59	0.84
1:B:492:ARG:HA	1:B:495:MET:HE2	1.58	0.84
1:A:735:ASN:N	1:A:735:ASN:HD22	1.73	0.83
1:A:562:ILE:H	1:A:562:ILE:HD13	1.43	0.83
1:B:313:MET:CE	1:B:319:LEU:HD11	2.08	0.83
1:A:97:VAL:HG13	1:A:105:VAL:HA	1.61	0.83
1:B:200:ASP:OD1	1:B:201:ALA:N	2.12	0.83
1:B:540:VAL:HG12	1:B:585:PHE:CD2	2.13	0.82
1:A:634:VAL:CG2	1:A:654:VAL:CG2	2.58	0.82
1:A:71:ILE:HG12	1:A:215:MET:CE	2.10	0.82
1:B:23:ASP:OD1	1:B:373:HIS:HE1	1.62	0.82
1:A:910:ARG:O	1:A:912:ARG:N	2.13	0.81
1:B:624:LYS:HD3	6:B:2229:HOH:O	1.80	0.81
1:A:845:ILE:HD13	1:A:854:LEU:HD22	1.60	0.81
1:A:143:ILE:HG22	1:A:146:LYS:HD2	1.60	0.81
1:B:215:MET:CE	1:B:215:MET:HA	2.11	0.81
1:A:522:GLY:HA2	1:A:551:ARG:HH21	1.46	0.80
1:A:26:LEU:HD22	1:A:29:MET:HE3	1.62	0.80
3:B:1918:G6P:C6	6:B:2227:HOH:O	2.27	0.80
1:B:252:GLU:HG3	6:B:2028:HOH:O	1.79	0.80
1:A:874:ILE:O	1:A:874:ILE:HD12	1.82	0.80
1:B:143:ILE:HG22	1:B:146:LYS:HE3	1.64	0.79
1:B:17:ASP:OD1	1:B:20:LYS:N	2.15	0.79
1:A:608:GLN:HG2	1:A:613:ALA:O	1.82	0.79
1:A:468:ARG:NH1	1:A:472:GLU:OE2	2.14	0.79
1:A:656:ASN:HD22	1:A:658:THR:CB	1.95	0.79
1:B:451:LYS:O	1:B:455:MET:HG2	1.83	0.78
1:A:544:LYS:HD2	1:A:554:GLU:OE1	1.84	0.78
1:A:513:PRO:HB3	1:A:703:MET:HE3	1.65	0.78
1:B:855:ASN:HD22	1:B:887:ASN:HB3	1.49	0.78
1:A:71:ILE:HD12	1:A:218:GLY:HA3	1.65	0.77
1:B:513:PRO:HB3	1:B:703:MET:CE	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:PRO:HB3	1:B:455:MET:HE2	1.66	0.77
1:B:866:LYS:HD3	1:B:892:LEU:HD11	1.67	0.77
1:A:79:ASP:HB2	1:A:96:GLN:HG2	1.67	0.77
3:A:921:G6P:H61	6:A:1145:HOH:O	1.85	0.76
1:A:713:GLY:HA3	1:A:718:LEU:HD12	1.68	0.76
1:A:558:LYS:HG2	1:A:560:TYR:CE1	2.19	0.76
1:A:735:ASN:ND2	1:A:735:ASN:H	1.82	0.76
1:B:492:ARG:HA	1:B:495:MET:CE	2.15	0.76
1:A:563:PRO:HG2	1:A:566:ILE:HD12	1.65	0.76
1:A:656:ASN:HD22	1:A:658:THR:HG22	1.50	0.76
1:B:420:HIS:CD2	1:B:422:GLN:H	2.03	0.76
1:B:624:LYS:HE2	1:B:734:LEU:HD22	1.68	0.76
1:A:866:LYS:NZ	1:A:892:LEU:HD11	2.01	0.76
1:A:96:GLN:O	1:A:105:VAL:HA	1.86	0.75
1:B:403:THR:CG2	1:B:405:ARG:O	2.34	0.75
1:A:343:GLU:OE2	1:A:420:HIS:HE1	1.69	0.75
1:B:71:ILE:HA	1:B:215:MET:HE1	1.65	0.75
1:A:405:ARG:NH2	1:A:437:ASP:HA	2.02	0.75
1:A:441:ARG:HH12	1:A:443:LEU:HD22	1.49	0.75
1:B:531:LEU:HG	6:B:2246:HOH:O	1.87	0.74
1:A:595:ARG:NH1	1:A:650:ASP:HB2	2.02	0.74
1:A:671:THR:HB	1:A:857:THR:CG2	2.17	0.74
1:A:513:PRO:HB3	1:A:703:MET:CE	2.17	0.74
1:A:97:VAL:HG13	1:A:105:VAL:CA	2.18	0.74
1:B:518:ARG:HH12	1:B:521:ASP:H	1.34	0.74
1:A:283:ARG:NE	6:A:1172:HOH:O	2.19	0.74
1:B:513:PRO:CB	1:B:703:MET:CE	2.65	0.73
1:A:562:ILE:O	1:A:562:ILE:HG12	1.88	0.73
1:A:547:SER:O	1:A:548:GLY:O	2.06	0.73
1:B:774:GLU:OE2	1:B:777:LYS:NZ	2.21	0.73
1:B:480:THR:CG2	1:B:483:MET:HG2	2.18	0.73
1:A:607:GLN:O	1:A:615:ILE:HG12	1.88	0.73
1:A:343:GLU:OE2	1:A:420:HIS:CE1	2.41	0.73
1:A:534:GLY:O	1:A:621:LYS:HE3	1.89	0.72
1:A:527:ASP:OD1	1:A:546:ARG:NH2	2.22	0.72
1:A:607:GLN:HB3	1:A:615:ILE:HG13	1.71	0.72
1:A:896:GLY:O	6:A:1112:HOH:O	2.07	0.72
1:B:401:LYS:HZ2	1:B:403:THR:HG21	1.53	0.72
1:A:634:VAL:CG2	1:A:654:VAL:HG23	2.18	0.72
1:A:759:ILE:CD1	1:A:776:LEU:HG	2.18	0.72
1:B:323:ARG:NH2	1:B:362:GLU:HB2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:ALA:HB3	1:A:874:ILE:HG13	1.71	0.71
1:A:715:ASN:ND2	1:A:715:ASN:H	1.88	0.71
1:A:492:ARG:NH1	1:A:847:GLU:OE1	2.22	0.71
1:B:323:ARG:NH2	1:B:361:VAL:O	2.21	0.71
1:A:570:THR:HB	1:A:573:GLU:OE1	1.88	0.71
1:A:799:GLN:O	1:A:799:GLN:HG3	1.89	0.71
1:A:414:GLY:HA2	3:A:919:G6P:H62	1.72	0.71
1:B:844:LYS:O	1:B:848:ASN:ND2	2.23	0.71
1:A:646:GLU:CG	1:A:647:PHE:H	2.03	0.71
1:B:313:MET:HE3	1:B:319:LEU:CD1	2.21	0.71
1:A:564:ILE:HG22	1:A:567:MET:HG3	1.73	0.71
1:B:137:PHE:O	1:B:141:ARG:NH1	2.23	0.71
1:A:62:LYS:CE	6:A:1173:HOH:O	2.35	0.70
1:A:658:THR:CG2	1:A:685:CYS:HB3	2.21	0.70
1:A:23:ASP:OD1	1:A:373:HIS:HE1	1.75	0.70
1:A:339:VAL:HG13	1:A:375:CYS:HB3	1.74	0.70
1:A:72:PRO:HD2	6:A:1102:HOH:O	1.90	0.70
1:A:514:SER:OG	1:A:704:CYS:HB3	1.92	0.70
1:A:505:ASN:O	1:A:507:ALA:CA	2.39	0.70
1:B:531:LEU:HD22	1:B:598:LEU:HD11	1.74	0.70
1:B:497:LEU:CD1	6:B:2226:HOH:O	2.40	0.70
1:A:891:LEU:N	1:A:891:LEU:HD22	2.06	0.70
1:A:722:ARG:CZ	1:A:740:ARG:HD3	2.22	0.70
1:A:480:THR:HG22	1:A:483:MET:H	1.57	0.70
1:A:857:THR:OG1	1:A:891:LEU:HD21	1.91	0.69
1:A:134:LEU:O	1:A:138:MET:HG3	1.92	0.69
1:B:518:ARG:NH1	1:B:521:ASP:H	1.90	0.69
1:A:832:GLN:HG3	1:A:874:ILE:CD1	2.22	0.69
1:A:845:ILE:CD1	1:A:854:LEU:CD2	2.70	0.69
1:A:534:GLY:HA3	1:A:603:SER:HB2	1.75	0.69
1:B:465:GLU:CD	1:B:468:ARG:HH21	1.96	0.69
1:B:769:ARG:O	1:B:771:GLN:NE2	2.26	0.69
1:A:71:ILE:HA	1:A:215:MET:CE	2.20	0.69
1:A:845:ILE:HD12	1:A:854:LEU:HD21	1.75	0.69
1:A:81:ILE:HG22	1:A:82:ALA:N	2.08	0.69
1:B:390:LEU:HD13	1:B:390:LEU:C	2.13	0.69
1:A:56:ASN:N	1:A:57:PRO:CD	2.55	0.69
1:A:646:GLU:CG	1:A:647:PHE:N	2.56	0.68
1:A:715:ASN:H	1:A:715:ASN:HD22	1.38	0.68
1:B:656:ASN:ND2	1:B:658:THR:OG1	2.25	0.68
1:B:549:LYS:HG2	1:B:550:LYS:H	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:PHE:O	1:A:770:GLY:N	2.27	0.68
1:B:727:ARG:NE	6:B:2180:HOH:O	2.16	0.68
1:B:540:VAL:CG1	1:B:585:PHE:CD2	2.76	0.68
1:B:492:ARG:HD2	1:B:495:MET:HE1	1.75	0.68
1:B:174:ARG:HG2	1:B:174:ARG:HH11	1.58	0.68
1:A:519:THR:OG1	1:A:520:PRO:CD	2.42	0.68
1:A:71:ILE:HG12	1:A:215:MET:HE3	1.75	0.68
1:A:623:PHE:O	1:A:624:LYS:HG3	1.94	0.68
1:B:235:ASN:HD21	1:B:260:GLU:H	1.41	0.68
1:A:245:ILE:CD1	1:A:257:ILE:HD11	2.24	0.68
1:A:673:GLU:OE1	1:A:849:ARG:NH1	2.27	0.68
1:B:586:LEU:HD22	1:B:596:MET:HE1	1.76	0.67
1:A:79:ASP:OD2	1:A:148:LEU:HD22	1.93	0.67
1:A:91:ARG:HG2	1:A:93:LEU:CD2	2.24	0.67
1:B:76:GLU:HG3	1:B:455:MET:HE1	1.74	0.67
1:A:214:MET:HE3	1:A:215:MET:HE2	1.76	0.67
1:A:521:ASP:O	1:A:523:THR:N	2.27	0.67
1:A:562:ILE:HD13	1:A:562:ILE:N	2.10	0.67
1:B:313:MET:HE3	1:B:319:LEU:HD11	1.75	0.67
3:A:919:G6P:C6	6:A:1033:HOH:O	2.38	0.67
1:B:588:TYR:N	6:B:2249:HOH:O	2.28	0.67
1:A:283:ARG:CZ	6:A:1172:HOH:O	2.43	0.67
1:B:479:LEU:HD23	1:B:483:MET:CE	2.25	0.66
1:B:83:LEU:HD12	1:B:152:PHE:CD1	2.30	0.66
1:A:500:ARG:HB2	1:A:503:THR:OG1	1.96	0.66
1:A:845:ILE:CD1	1:A:854:LEU:HD22	2.26	0.66
1:B:215:MET:HE3	1:B:215:MET:HA	1.77	0.66
1:A:687:MET:HE2	1:A:704:CYS:HA	1.77	0.66
3:B:1918:G6P:H61	6:B:2196:HOH:O	1.96	0.66
1:B:525:ASN:HD22	1:B:547:SER:H	1.41	0.66
1:A:400:ASN:OD1	6:A:1147:HOH:O	2.14	0.66
1:B:794:ARG:HD2	6:B:2247:HOH:O	1.95	0.66
1:A:874:ILE:C	1:A:874:ILE:HD12	2.16	0.66
1:A:773:SER:O	1:A:777:LYS:HG2	1.96	0.66
1:B:480:THR:OG1	1:B:481:LYS:N	2.27	0.66
1:A:242:LEU:HD23	1:A:252:GLU:O	1.96	0.66
1:A:303:GLY:H	1:A:336:THR:CG2	2.08	0.65
1:A:56:ASN:N	1:A:57:PRO:HD3	2.12	0.65
1:A:189:LEU:CD1	1:A:203:ILE:HD11	2.22	0.65
1:A:405:ARG:CZ	1:A:437:ASP:HA	2.26	0.65
1:A:575:PHE:O	1:A:579:VAL:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ALA:HA	6:A:1186:HOH:O	1.97	0.65
1:A:145:ASP:OD1	6:A:1008:HOH:O	2.15	0.65
1:A:492:ARG:HD3	6:A:1081:HOH:O	1.95	0.64
1:A:497:LEU:HD13	1:A:506:ASN:OD1	1.97	0.64
1:B:76:GLU:HG3	1:B:455:MET:SD	2.37	0.64
1:A:81:ILE:O	1:A:82:ALA:CB	2.46	0.64
1:B:908:GLY:O	1:B:909:VAL:C	2.35	0.64
1:A:62:LYS:NZ	6:A:1057:HOH:O	1.77	0.64
1:A:515:PHE:HE2	1:A:608:GLN:O	1.81	0.64
1:A:778:THR:HB	1:A:781:ILE:CD1	2.22	0.63
1:A:562:ILE:HD12	6:A:1140:HOH:O	1.98	0.63
1:A:735:ASN:N	1:A:735:ASN:ND2	2.41	0.63
1:B:244:HIS:CD2	1:B:396:ARG:HH21	2.16	0.63
1:B:114:THR:CG2	1:B:118:ILE:HG21	2.27	0.63
1:B:483:MET:HB3	6:B:2176:HOH:O	1.98	0.63
1:A:658:THR:HG23	1:A:685:CYS:CB	2.27	0.63
1:B:727:ARG:NH2	6:B:2180:HOH:O	2.21	0.63
1:A:80:PHE:HB3	1:A:149:PRO:O	1.99	0.63
1:A:26:LEU:HD22	1:A:29:MET:CE	2.27	0.63
1:A:71:ILE:HD13	1:A:218:GLY:HA3	1.81	0.63
1:B:313:MET:CE	1:B:319:LEU:CD1	2.77	0.63
1:B:200:ASP:CG	1:B:201:ALA:H	2.00	0.63
1:A:23:ASP:OD1	1:A:373:HIS:CE1	2.52	0.63
3:B:1916:G6P:C6	6:B:2027:HOH:O	2.38	0.62
1:A:795:LEU:CD1	1:A:799:GLN:HG2	2.29	0.62
1:B:734:LEU:HD13	6:B:2229:HOH:O	1.98	0.62
1:A:710:GLY:O	1:A:739:GLN:HA	1.98	0.62
1:B:845:ILE:CD1	1:B:849:ARG:CZ	2.77	0.62
1:B:114:THR:HG22	1:B:118:ILE:HB	1.81	0.62
1:B:72:PRO:HB3	1:B:455:MET:HE3	1.79	0.62
1:A:518:ARG:NH1	1:A:521:ASP:HB2	2.15	0.62
1:A:313:MET:HG2	1:A:318:LEU:HD12	1.80	0.62
1:B:480:THR:HG22	1:B:483:MET:HG3	1.80	0.62
1:B:549:LYS:CG	1:B:550:LYS:H	2.12	0.62
1:A:16:ASP:CB	6:A:1055:HOH:O	2.48	0.62
1:A:287:ASN:N	1:A:287:ASN:HD22	1.90	0.62
1:A:595:ARG:HG3	1:A:648:ASP:OD2	1.99	0.61
1:A:724:HIS:HE1	6:A:1115:HOH:O	1.82	0.61
1:B:25:TYR:OH	1:B:312:LYS:HG2	1.99	0.61
1:A:16:ASP:CG	6:A:1055:HOH:O	2.38	0.61
1:B:907:VAL:C	1:B:908:GLY:O	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:C	1:A:143:ILE:HD12	2.21	0.61
1:B:215:MET:HE2	1:B:215:MET:HA	1.82	0.61
1:A:634:VAL:HG23	1:A:654:VAL:HG21	1.81	0.61
1:A:715:ASN:N	1:A:715:ASN:HD22	1.97	0.61
1:B:480:THR:N	1:B:483:MET:HG3	2.10	0.61
1:B:200:ASP:CG	1:B:201:ALA:N	2.51	0.61
1:B:463:LEU:HD23	1:B:467:HIS:NE2	2.16	0.61
1:A:437:ASP:N	1:A:437:ASP:OD1	2.33	0.60
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.16	0.60
1:A:306:VAL:HG11	1:A:334:PHE:CE1	2.36	0.60
1:A:29:MET:CB	1:A:377:ILE:HD11	2.16	0.60
1:B:513:PRO:HA	1:B:703:MET:HE3	1.82	0.60
1:B:518:ARG:NH1	1:B:521:ASP:N	2.49	0.60
1:A:671:THR:CB	1:A:857:THR:HG23	2.27	0.60
1:A:16:ASP:HB3	6:A:1055:HOH:O	2.00	0.60
1:B:84:ASP:HA	1:B:153:THR:HB	1.83	0.60
1:B:76:GLU:CG	1:B:455:MET:HE1	2.32	0.60
1:B:595:ARG:HH12	1:B:648:ASP:HB3	1.67	0.60
1:B:492:ARG:HG2	1:B:840:ALA:HB1	1.83	0.60
1:B:479:LEU:HD23	1:B:483:MET:HE2	1.84	0.60
1:A:857:THR:OG1	1:A:891:LEU:CD2	2.50	0.60
1:B:806:GLN:HG3	1:B:806:GLN:O	2.01	0.60
1:A:899:LYS:O	1:A:902:ALA:HB3	2.02	0.60
1:B:570:THR:HG22	1:B:573:GLU:H	1.67	0.60
1:A:115:PRO:HD2	1:A:118:ILE:HG13	1.83	0.59
1:B:323:ARG:HH21	1:B:362:GLU:HB2	1.64	0.59
1:B:586:LEU:C	6:B:2249:HOH:O	2.40	0.59
1:A:335:ASN:C	1:A:335:ASN:ND2	2.51	0.59
1:A:598:LEU:HD12	1:A:598:LEU:C	2.23	0.59
1:B:143:ILE:HG22	1:B:146:LYS:CE	2.32	0.59
1:B:862:GLY:O	1:B:866:LYS:HG2	2.03	0.59
1:B:76:GLU:CG	1:B:455:MET:CE	2.79	0.59
1:A:792:SER:HG	1:A:795:LEU:HD23	1.67	0.59
1:A:550:LYS:O	1:A:552:THR:HG23	2.02	0.59
1:A:687:MET:CE	1:A:704:CYS:SG	2.91	0.59
1:A:541:LEU:HG	1:A:557:ASN:HB3	1.85	0.59
1:B:76:GLU:H	1:B:76:GLU:CD	2.05	0.59
1:B:480:THR:HG23	1:B:483:MET:N	2.16	0.59
1:A:832:GLN:CG	1:A:874:ILE:HD11	2.26	0.59
1:A:722:ARG:NH1	1:A:740:ARG:HD3	2.17	0.59
1:A:570:THR:HG22	1:A:571:GLY:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASP:OD1	6:B:2145:HOH:O	2.17	0.59
1:A:634:VAL:HG21	1:A:654:VAL:HG23	1.85	0.58
1:B:496:GLU:CD	1:B:844:LYS:HE2	2.22	0.58
1:A:420:HIS:HD2	1:A:423:TYR:H	1.50	0.58
1:B:390:LEU:HD13	1:B:390:LEU:O	2.02	0.58
1:B:586:LEU:HD22	1:B:596:MET:CE	2.34	0.58
1:B:136:ASP:OD1	1:B:140:LYS:NZ	2.34	0.58
1:A:907:VAL:O	1:A:908:GLY:O	2.21	0.58
1:B:71:ILE:CA	1:B:215:MET:HE1	2.32	0.58
1:A:138:MET:HB3	1:A:143:ILE:CD1	2.34	0.58
1:B:401:LYS:HZ3	1:B:403:THR:HG21	1.66	0.58
1:A:767:LEU:HD13	1:A:768:PHE:CD2	2.39	0.58
1:B:323:ARG:NH2	1:B:362:GLU:O	2.36	0.58
1:B:429:LYS:NZ	5:B:1999:ANP:O1B	2.36	0.58
1:A:845:ILE:CD1	1:A:854:LEU:HD21	2.32	0.58
1:B:72:PRO:CB	1:B:455:MET:HE2	2.33	0.58
1:B:721:ILE:HD11	6:B:2176:HOH:O	2.04	0.58
1:A:768:PHE:C	1:A:770:GLY:H	2.06	0.58
1:A:588:TYR:CE1	1:B:331:ARG:HB2	2.38	0.58
1:A:503:THR:O	1:A:505:ASN:N	2.37	0.58
1:A:77:LYS:HD3	1:A:98:ASN:OD1	2.03	0.58
1:B:518:ARG:HD2	1:B:519:THR:O	2.03	0.58
1:A:243:ARG:HB3	1:A:243:ARG:NH1	2.18	0.58
1:B:479:LEU:HD22	1:B:721:ILE:HD11	1.85	0.57
1:A:866:LYS:HZ3	1:A:892:LEU:HD11	1.68	0.57
1:B:570:THR:HG22	1:B:572:GLU:H	1.68	0.57
1:A:176:LYS:HD2	1:A:286:LEU:HD22	1.85	0.57
1:A:91:ARG:HG2	1:A:93:LEU:HD21	1.85	0.57
1:B:845:ILE:HD11	1:B:849:ARG:NH1	2.20	0.57
1:A:116:GLU:HG3	1:A:120:HIS:ND1	2.20	0.57
1:A:875:MET:O	1:A:879:VAL:HG23	2.04	0.57
1:A:619:TRP:CD1	1:A:624:LYS:HA	2.40	0.57
1:A:306:VAL:O	1:A:310:LEU:HG	2.04	0.57
1:B:910:ARG:HG2	1:B:911:LEU:HD23	1.86	0.57
1:B:836:ALA:O	1:B:839:ALA:HB3	2.05	0.57
1:A:414:GLY:CA	3:A:919:G6P:H62	2.35	0.56
1:B:481:LYS:HA	6:B:2224:HOH:O	2.06	0.56
1:B:578:ILE:HG21	6:B:2246:HOH:O	1.92	0.56
1:A:299:GLY:O	1:A:336:THR:HG21	2.06	0.56
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.86	0.56
1:A:313:MET:CE	1:A:319:LEU:CD1	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:THR:HB	1:B:573:GLU:HG3	1.88	0.56
1:B:98:ASN:OD1	1:B:104:ASN:ND2	2.39	0.56
1:B:550:LYS:HG2	1:B:552:THR:HG23	1.88	0.56
1:A:431:LEU:HD22	1:A:442:PHE:HZ	1.70	0.56
1:A:888:VAL:HG22	1:A:890:PHE:CE1	2.41	0.56
1:B:72:PRO:HD3	1:B:215:MET:CE	2.32	0.56
1:B:480:THR:O	1:B:483:MET:N	2.36	0.56
1:A:911:LEU:N	1:A:911:LEU:HD23	2.20	0.56
1:A:157:PRO:HB3	1:A:260:GLU:CD	2.26	0.56
1:B:88:SER:OG	3:B:1916:G6P:O2P	2.20	0.56
1:A:77:LYS:HB2	1:A:98:ASN:HA	1.87	0.56
1:A:662:MET:SD	1:A:687:MET:HE3	2.46	0.56
1:B:563:PRO:HB2	1:B:565:GLU:CG	2.30	0.55
1:B:136:ASP:OD1	1:B:140:LYS:CE	2.54	0.55
1:A:652:VAL:CG1	1:A:908:GLY:HA3	2.35	0.55
1:B:911:LEU:HD12	6:B:2253:HOH:O	2.05	0.55
1:B:782:PHE:O	1:B:787:LEU:HD22	2.06	0.55
1:B:769:ARG:HD3	6:B:2251:HOH:O	1.90	0.55
1:A:875:MET:CE	1:A:876:HIS:CD2	2.89	0.55
1:A:71:ILE:HG12	1:A:215:MET:HE1	1.88	0.55
1:B:219:TYR:HD2	1:B:455:MET:HE2	1.70	0.55
1:B:143:ILE:CG2	1:B:146:LYS:HE3	2.33	0.55
1:B:644:ARG:HH11	1:B:644:ARG:HG3	1.72	0.55
1:A:507:ALA:O	1:A:510:LYS:NZ	2.37	0.55
1:A:93:LEU:HD13	1:A:109:SER:HB3	1.89	0.55
1:B:579:VAL:O	1:B:582:ILE:HB	2.06	0.55
1:A:138:MET:HB3	1:A:143:ILE:HD12	1.88	0.55
1:B:136:ASP:O	1:B:140:LYS:HE2	2.07	0.55
1:A:846:ARG:HH11	1:A:846:ARG:HG2	1.72	0.55
1:A:91:ARG:HG2	1:A:93:LEU:HD22	1.87	0.55
1:B:403:THR:HG23	1:B:405:ARG:O	2.06	0.55
1:A:40:MET:HG3	1:A:388:ALA:O	2.07	0.55
1:A:430:THR:HG22	1:A:434:LEU:HD22	1.89	0.55
1:B:668:GLU:OE1	1:B:668:GLU:N	2.35	0.55
1:A:519:THR:OG1	1:A:520:PRO:HD3	2.07	0.54
1:A:93:LEU:N	1:A:93:LEU:CD2	2.70	0.54
1:B:734:LEU:HB3	6:B:2229:HOH:O	2.07	0.54
1:B:862:GLY:HA2	3:B:1918:G6P:H62	1.89	0.54
1:A:690:MET:HE3	1:A:703:MET:HB2	1.89	0.54
1:B:240:GLU:HG3	1:B:241:GLU:N	2.22	0.54
1:A:265:GLY:O	1:A:267:ASP:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:HG3	1:B:54:ASP:N	2.22	0.54
1:A:62:LYS:HZ3	1:A:157:PRO:HB2	1.73	0.54
1:A:687:MET:HE2	1:A:704:CYS:CA	2.37	0.54
1:A:490:ARG:NH1	1:A:717:CYS:O	2.40	0.54
1:B:732:TYR:O	1:B:779:ARG:NH2	2.41	0.54
1:A:521:ASP:CB	6:A:1169:HOH:O	2.14	0.54
1:A:235:ASN:ND2	1:A:236:ALA:H	2.05	0.54
1:A:405:ARG:NH2	6:A:1077:HOH:O	2.40	0.54
1:A:299:GLY:O	1:A:336:THR:CG2	2.56	0.54
1:A:562:ILE:HG13	1:A:567:MET:SD	2.48	0.54
1:A:857:THR:CB	1:A:891:LEU:HD21	2.38	0.54
1:A:570:THR:CG2	1:A:571:GLY:N	2.71	0.54
1:B:235:ASN:HD21	1:B:260:GLU:N	2.06	0.54
1:B:570:THR:CG2	1:B:572:GLU:H	2.20	0.54
1:A:676:LEU:O	1:A:860:VAL:HA	2.09	0.54
1:A:690:MET:CE	1:A:703:MET:HB2	2.38	0.53
1:B:563:PRO:CB	1:B:565:GLU:HG3	2.31	0.53
1:A:583:SER:OG	1:A:592:LYS:NZ	2.41	0.53
1:A:422:GLN:O	1:A:426:ARG:HG3	2.08	0.53
1:A:110:GLU:O	1:A:111:VAL:CG2	2.51	0.53
1:A:265:GLY:O	1:A:266:ASP:O	2.27	0.53
1:A:61:VAL:O	1:A:63:MET:HG2	2.08	0.53
1:B:639:ASP:O	1:B:643:ARG:HG3	2.08	0.53
1:B:595:ARG:HH11	1:B:648:ASP:HB3	1.67	0.53
1:A:83:LEU:HD21	1:A:134:LEU:HD13	1.90	0.53
1:A:767:LEU:HD23	1:A:818:LEU:HD12	1.89	0.53
1:B:553:VAL:HG21	1:B:899:LYS:HG3	1.90	0.53
1:A:550:LYS:O	1:A:551:ARG:C	2.47	0.53
1:A:522:GLY:CA	1:A:551:ARG:HH21	2.18	0.53
1:B:114:THR:HG23	1:B:118:ILE:HG21	1.90	0.53
1:B:652:VAL:HG13	1:B:908:GLY:HA3	1.90	0.53
1:A:895:ASP:OD1	1:A:895:ASP:O	2.26	0.53
1:A:56:ASN:H	1:A:57:PRO:HD3	1.72	0.53
1:B:644:ARG:HG3	1:B:644:ARG:NH1	2.24	0.53
1:B:605:PRO:HB3	1:B:708:GLU:HG3	1.91	0.53
1:B:193:ILE:HD13	1:B:201:ALA:HB3	1.91	0.53
1:A:562:ILE:O	1:A:562:ILE:CG1	2.56	0.52
1:A:641:ILE:CD1	1:A:649:LEU:HD11	2.39	0.52
1:B:478:HIS:O	1:B:483:MET:HE1	2.09	0.52
1:A:647:PHE:HD1	1:A:647:PHE:H	1.58	0.52
1:A:759:ILE:CD1	1:A:776:LEU:CD2	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ASN:HD21	1:A:658:THR:HB	1.68	0.52
1:B:492:ARG:HD2	1:B:495:MET:CE	2.39	0.52
1:A:480:THR:HG23	1:A:482:ASP:H	1.73	0.52
1:A:71:ILE:CG1	1:A:215:MET:HE1	2.39	0.52
1:A:397:LEU:O	1:A:401:LYS:HG2	2.09	0.52
1:B:665:CYS:SG	1:B:893:SER:HB3	2.49	0.52
1:B:324:ILE:HG23	1:B:328:LEU:HD23	1.91	0.52
1:A:656:ASN:ND2	1:A:658:THR:CG2	2.64	0.52
1:B:513:PRO:CA	1:B:703:MET:HE3	2.40	0.52
1:B:114:THR:CG2	1:B:118:ILE:CG2	2.87	0.52
1:B:79:ASP:OD1	1:B:148:LEU:HD13	2.09	0.52
1:B:529:LEU:HB3	1:B:598:LEU:HB2	1.92	0.52
1:A:603:SER:OG	1:A:657:ASP:CG	2.49	0.52
1:A:189:LEU:HD13	1:A:203:ILE:CD1	2.29	0.51
1:B:480:THR:CG2	1:B:483:MET:CG	2.82	0.51
1:A:83:LEU:HD23	1:A:92:ILE:HG12	1.92	0.51
1:A:138:MET:HE1	1:A:143:ILE:HD13	1.92	0.51
1:A:403:THR:OG1	1:A:405:ARG:O	2.22	0.51
1:A:198:ASP:HB3	1:A:199:TYR:HD1	1.75	0.51
1:A:208:ASN:ND2	1:A:210:THR:H	2.08	0.51
1:A:444:LEU:O	1:A:446:GLU:N	2.43	0.51
1:A:510:LYS:O	1:A:511:MET:C	2.49	0.51
1:B:570:THR:HG22	1:B:572:GLU:N	2.24	0.51
1:A:875:MET:HE3	1:A:876:HIS:CD2	2.46	0.51
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.23	0.51
1:A:119:VAL:HG13	1:A:175:PHE:HA	1.93	0.51
1:A:240:GLU:O	1:A:254:ARG:HB3	2.11	0.51
1:A:690:MET:HE2	1:A:703:MET:CB	2.41	0.51
1:A:673:GLU:OE1	1:A:849:ARG:NH2	2.43	0.51
1:A:406:LEU:HD23	1:A:438:SER:OG	2.11	0.51
1:A:83:LEU:N	1:A:151:GLY:O	2.37	0.51
1:A:414:GLY:HA2	3:A:919:G6P:C6	2.39	0.51
1:B:193:ILE:O	1:B:196:ARG:O	2.29	0.51
1:B:56:ASN:N	1:B:57:PRO:CD	2.74	0.51
1:A:138:MET:CE	1:A:143:ILE:HD13	2.41	0.51
1:A:287:ASN:ND2	1:A:287:ASN:H	2.01	0.51
1:A:514:SER:HG	1:A:704:CYS:HB3	1.75	0.51
1:A:138:MET:CE	1:A:143:ILE:CD1	2.89	0.50
1:A:758:LEU:O	1:A:762:THR:CG2	2.59	0.50
1:B:312:LYS:HG3	1:B:316:GLU:OE2	2.12	0.50
1:B:306:VAL:O	1:B:310:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ASP:OD1	1:A:870:HIS:NE2	2.36	0.50
1:A:831:ALA:CB	1:A:874:ILE:HG13	2.41	0.50
1:B:591:ILE:HD12	1:B:596:MET:HE1	1.93	0.50
1:B:136:ASP:OD1	1:B:140:LYS:HE2	2.11	0.50
1:A:553:VAL:HG11	1:A:899:LYS:HG3	1.94	0.50
1:A:34:GLU:CD	1:A:34:GLU:H	2.14	0.50
1:B:845:ILE:CD1	1:B:849:ARG:NH1	2.74	0.50
1:A:77:LYS:HD3	1:A:98:ASN:CG	2.32	0.50
1:A:855:ASN:OD1	1:A:887:ASN:HB3	2.11	0.50
1:B:93:LEU:HG	1:B:109:SER:CB	2.41	0.50
1:A:145:ASP:C	1:A:146:LYS:O	2.48	0.50
1:B:235:ASN:ND2	1:B:236:ALA:H	2.10	0.50
1:A:265:GLY:O	1:A:266:ASP:C	2.49	0.50
1:A:806:GLN:HA	1:A:806:GLN:NE2	2.27	0.50
1:B:591:ILE:O	1:B:596:MET:CE	2.59	0.50
1:A:71:ILE:CA	1:A:215:MET:HE1	2.32	0.50
1:B:845:ILE:HD12	1:B:849:ARG:NH2	2.27	0.50
1:A:198:ASP:CB	1:A:199:TYR:HD1	2.25	0.50
1:B:531:LEU:HD11	1:B:582:ILE:HD11	1.93	0.50
1:B:343:GLU:OE2	1:B:420:HIS:CE1	2.65	0.50
1:A:466:GLN:HG3	1:A:766:PHE:CD1	2.47	0.49
1:B:596:MET:HE3	6:B:2069:HOH:O	2.11	0.49
1:A:564:ILE:C	1:A:564:ILE:CD1	2.80	0.49
1:A:266:ASP:C	1:A:267:ASP:O	2.47	0.49
1:B:413:ASP:OD1	1:B:414:GLY:N	2.43	0.49
1:B:693:VAL:HG11	1:B:703:MET:HE2	1.94	0.49
1:A:910:ARG:O	1:A:911:LEU:C	2.50	0.49
1:A:875:MET:CE	1:A:876:HIS:HD2	2.25	0.49
1:B:355:ILE:HG23	6:B:2019:HOH:O	2.11	0.49
1:A:507:ALA:O	1:A:510:LYS:HE2	2.12	0.49
1:B:595:ARG:HH12	1:B:648:ASP:CB	2.23	0.49
1:A:896:GLY:N	6:A:1112:HOH:O	2.45	0.49
1:A:713:GLY:CA	1:A:718:LEU:HD12	2.40	0.49
1:B:549:LYS:HG2	1:B:550:LYS:N	2.25	0.49
1:A:40:MET:CE	1:A:391:GLY:HA3	2.43	0.49
1:B:349:LEU:HD13	1:B:372:GLN:NE2	2.28	0.49
1:A:44:ARG:HA	1:A:47:MET:HE2	1.94	0.49
1:A:79:ASP:O	1:A:149:PRO:HD2	2.13	0.49
1:A:687:MET:HE2	1:A:704:CYS:SG	2.51	0.49
1:A:400:ASN:HB2	6:A:1147:HOH:O	2.11	0.49
1:B:543:VAL:HG13	1:B:555:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:THR:OG1	1:A:520:PRO:HD2	2.12	0.49
1:A:644:ARG:O	1:A:645:GLU:C	2.51	0.49
1:A:609:THR:O	1:A:610:SER:HB3	2.13	0.49
1:B:71:ILE:HA	1:B:215:MET:HE2	1.89	0.49
1:A:687:MET:HE1	1:A:704:CYS:HB2	1.94	0.49
1:B:361:VAL:O	1:B:362:GLU:C	2.51	0.49
1:A:380:PHE:CE2	1:A:426:ARG:HD3	2.48	0.49
1:B:127:PHE:CE1	1:B:185:VAL:HG23	2.48	0.49
1:A:618:THR:HG23	1:A:618:THR:O	2.13	0.49
1:A:97:VAL:CG1	1:A:105:VAL:CA	2.90	0.49
1:B:430:THR:HG22	1:B:434:LEU:HD22	1.95	0.49
1:A:394:LEU:HD22	1:A:408:THR:HG21	1.95	0.49
1:B:593:GLY:N	1:B:594:PRO:HD2	2.27	0.49
1:A:530:ALA:HA	1:A:598:LEU:CD1	2.43	0.48
1:B:513:PRO:CB	1:B:703:MET:HE3	2.43	0.48
1:A:767:LEU:CD1	1:A:768:PHE:CD2	2.96	0.48
1:A:420:HIS:HD2	1:A:423:TYR:N	2.11	0.48
1:A:505:ASN:O	1:A:507:ALA:C	2.51	0.48
1:B:769:ARG:CG	1:B:769:ARG:HH11	2.25	0.48
1:A:857:THR:HB	1:A:891:LEU:HD21	1.96	0.48
1:A:506:ASN:ND2	1:A:506:ASN:C	2.63	0.48
1:B:271:GLU:OE1	1:B:279:ARG:NH2	2.33	0.48
1:A:112:TYR:OH	1:A:137:PHE:HB2	2.13	0.48
1:A:792:SER:OG	1:A:795:LEU:CD2	2.53	0.48
1:A:79:ASP:OD2	1:A:148:LEU:CD2	2.61	0.48
1:A:687:MET:HE2	1:A:704:CYS:CB	2.43	0.48
1:A:46:GLU:HA	1:A:49:ASN:HB2	1.96	0.48
1:A:29:MET:HB2	1:A:377:ILE:CD1	2.20	0.48
1:B:683:ASN:HA	1:B:709:TRP:CD1	2.49	0.48
1:A:138:MET:CB	1:A:143:ILE:HD11	2.44	0.48
1:A:492:ARG:O	1:A:492:ARG:HD2	2.13	0.48
1:A:529:LEU:O	1:A:598:LEU:HA	2.14	0.48
1:A:758:LEU:O	1:A:762:THR:HG23	2.13	0.48
1:A:652:VAL:HG11	1:A:908:GLY:HA3	1.96	0.48
1:A:720:ASP:HB3	1:A:721:ILE:HG23	1.95	0.48
1:B:119:VAL:CG2	1:B:175:PHE:CZ	2.97	0.48
1:A:62:LYS:NZ	1:A:260:GLU:HG3	2.29	0.48
1:A:150:VAL:HB	1:A:203:ILE:HA	1.95	0.48
1:B:110:GLU:CD	1:B:141:ARG:HH22	2.08	0.48
1:A:892:LEU:HD13	1:A:893:SER:N	2.29	0.48
1:A:425:ARG:NH1	5:A:999:ANP:O1A	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:THR:HG22	1:A:572:GLU:H	1.79	0.48
1:B:83:LEU:HD12	1:B:152:PHE:HD1	1.75	0.48
1:A:598:LEU:HD12	1:A:599:GLY:H	1.71	0.48
1:A:313:MET:HE1	1:A:319:LEU:HD11	1.87	0.48
1:B:174:ARG:CG	1:B:174:ARG:HH11	2.18	0.48
1:A:267:ASP:O	1:A:267:ASP:OD1	2.31	0.48
1:A:910:ARG:HB3	1:A:911:LEU:H	1.55	0.47
1:B:571:GLY:HA2	1:B:628:CYS:SG	2.54	0.47
1:A:846:ARG:HG2	1:A:846:ARG:NH1	2.29	0.47
1:B:675:GLY:O	1:B:684:ALA:HA	2.14	0.47
1:A:803:ILE:HG22	1:A:804:LEU:N	2.29	0.47
1:A:235:ASN:HD21	1:A:260:GLU:N	2.12	0.47
1:A:313:MET:HE3	1:A:319:LEU:CG	2.44	0.47
1:A:759:ILE:HD13	1:A:776:LEU:CD2	2.44	0.47
1:A:687:MET:CE	1:A:704:CYS:CB	2.92	0.47
1:B:412:VAL:HG12	1:B:413:ASP:N	2.30	0.47
1:A:680:THR:O	1:A:746:SER:HB3	2.12	0.47
1:B:38:ASP:OD1	1:B:42:ARG:HD2	2.14	0.47
1:A:563:PRO:CG	1:A:566:ILE:HD12	2.39	0.47
1:A:570:THR:CB	1:A:573:GLU:OE1	2.58	0.47
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.56	0.47
1:A:414:GLY:N	3:A:919:G6P:H62	2.29	0.47
1:B:571:GLY:N	1:B:626:THR:O	2.39	0.47
1:B:148:LEU:HA	1:B:149:PRO:HD3	1.79	0.47
1:A:287:ASN:ND2	1:A:287:ASN:N	2.57	0.47
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.69	0.47
1:B:525:ASN:ND2	1:B:546:ARG:HA	2.30	0.47
1:A:652:VAL:O	1:A:652:VAL:HG12	2.13	0.47
1:A:875:MET:HE1	1:A:876:HIS:CD2	2.49	0.47
1:B:53:ARG:CG	1:B:54:ASP:N	2.77	0.47
1:A:417:TYR:OH	1:A:428:HIS:NE2	2.40	0.47
1:B:185:VAL:HG23	1:B:185:VAL:O	2.13	0.47
1:A:187:LYS:HB3	1:A:187:LYS:HE2	1.60	0.47
1:A:619:TRP:CE3	1:A:619:TRP:HA	2.50	0.47
1:B:752:GLU:CD	1:B:755:ARG:NH1	2.47	0.47
1:A:907:VAL:O	1:A:908:GLY:C	2.52	0.47
1:B:343:GLU:OE2	1:B:420:HIS:HE1	1.98	0.47
1:B:241:GLU:OE2	1:B:254:ARG:HD2	2.14	0.47
1:B:488:LYS:HD2	1:B:839:ALA:HB1	1.97	0.46
1:A:267:ASP:C	1:A:267:ASP:OD1	2.53	0.46
1:B:158:CYS:HA	1:B:167:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:VAL:HG12	1:A:836:ALA:CB	2.45	0.46
1:A:372:GLN:O	1:A:376:THR:HG23	2.15	0.46
1:B:215:MET:HE3	1:B:215:MET:CA	2.43	0.46
1:A:564:ILE:HD12	1:A:564:ILE:C	2.36	0.46
1:A:603:SER:HG	1:A:657:ASP:CG	2.19	0.46
1:B:136:ASP:O	1:B:139:GLU:HB3	2.16	0.46
1:A:878:THR:O	1:A:882:LEU:HG	2.14	0.46
1:B:196:ARG:HG3	1:B:196:ARG:O	2.15	0.46
1:A:506:ASN:HD22	1:A:506:ASN:N	2.13	0.46
1:A:13:GLU:OE2	1:A:15:LYS:HE3	2.15	0.46
1:A:678:VAL:HB	1:A:865:TYR:HB2	1.98	0.46
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.50	0.46
1:A:861:ASP:OD1	1:A:862:GLY:N	2.44	0.46
1:A:868:HIS:HA	1:A:869:PRO:HD2	1.65	0.46
1:A:193:ILE:HD13	1:A:201:ALA:CB	2.46	0.46
1:A:605:PRO:HB3	1:A:708:GLU:HG3	1.97	0.46
1:A:235:ASN:HD21	1:A:260:GLU:H	1.63	0.46
1:A:93:LEU:HD22	1:A:93:LEU:N	2.31	0.46
1:B:93:LEU:HG	1:B:109:SER:HB3	1.98	0.45
1:B:855:ASN:ND2	1:B:887:ASN:HB3	2.25	0.45
1:B:570:THR:O	1:B:571:GLY:C	2.54	0.45
1:B:93:LEU:N	1:B:93:LEU:HD12	2.31	0.45
1:A:891:LEU:CD2	1:A:891:LEU:N	2.75	0.45
1:A:739:GLN:O	1:A:743:LYS:HG3	2.16	0.45
1:A:266:ASP:O	1:A:267:ASP:O	2.35	0.45
1:B:119:VAL:HG22	1:B:175:PHE:CG	2.51	0.45
1:A:107:MET:HB2	1:A:107:MET:HE3	1.86	0.45
1:B:529:LEU:HD22	1:B:596:MET:SD	2.56	0.45
1:A:82:ALA:HA	1:A:151:GLY:O	2.16	0.45
1:B:189:LEU:HD13	1:B:203:ILE:CD1	2.38	0.45
1:A:791:GLU:OE1	1:A:824:GLY:HA2	2.16	0.45
1:A:507:ALA:O	1:A:510:LYS:CE	2.65	0.45
1:B:203:ILE:O	1:B:203:ILE:HG22	2.16	0.45
1:A:480:THR:CG2	1:A:482:ASP:H	2.28	0.45
1:B:848:ASN:N	1:B:848:ASN:HD22	2.15	0.45
1:B:119:VAL:CG2	1:B:175:PHE:CE1	2.99	0.45
1:B:710:GLY:O	1:B:739:GLN:HA	2.16	0.45
1:B:144:LYS:HE2	1:B:199:TYR:HB3	1.98	0.45
1:A:492:ARG:NH2	1:A:496:GLU:OE2	2.39	0.45
1:A:818:LEU:HA	1:A:821:THR:HG23	1.99	0.45
1:B:114:THR:HG22	1:B:118:ILE:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.51	0.45
1:B:880:LYS:HB2	1:B:880:LYS:HE2	1.48	0.45
1:A:45:LYS:O	1:A:45:LYS:HD2	2.17	0.45
1:B:89:SER:N	6:B:2250:HOH:O	2.27	0.45
1:A:759:ILE:HD13	1:A:776:LEU:HD21	1.98	0.45
1:A:71:ILE:CG1	1:A:215:MET:CE	2.87	0.44
1:A:866:LYS:HZ1	1:A:892:LEU:HD11	1.77	0.44
1:B:652:VAL:CG1	1:B:652:VAL:O	2.66	0.44
1:A:80:PHE:CD1	1:A:80:PHE:N	2.85	0.44
1:B:486:GLU:O	1:B:490:ARG:HG3	2.18	0.44
1:A:519:THR:HA	1:A:663:MET:SD	2.57	0.44
1:B:769:ARG:NH1	1:B:769:ARG:HG3	2.32	0.44
1:B:463:LEU:HD23	1:B:467:HIS:CE1	2.51	0.44
1:B:592:LYS:HB2	1:B:592:LYS:HE3	1.42	0.44
1:B:20:LYS:HD3	1:B:20:LYS:HA	1.75	0.44
1:A:540:VAL:HG12	1:A:585:PHE:CD2	2.52	0.44
1:B:754:VAL:O	1:B:758:LEU:HG	2.17	0.44
1:A:214:MET:HE3	1:A:215:MET:CE	2.44	0.44
1:A:563:PRO:O	1:A:565:GLU:N	2.50	0.44
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.53	0.44
1:A:261:TRP:CD1	1:A:261:TRP:C	2.91	0.44
1:A:72:PRO:CD	6:A:1102:HOH:O	2.58	0.44
1:A:598:LEU:CD1	1:A:599:GLY:N	2.66	0.44
1:B:244:HIS:HD2	1:B:396:ARG:HH21	1.65	0.44
1:A:542:LEU:HB3	1:A:556:HIS:HB2	1.99	0.44
1:A:839:ALA:HB1	1:A:883:SER:OG	2.18	0.44
1:A:229:ILE:O	1:A:234:THR:HA	2.17	0.44
1:A:514:SER:O	1:A:515:PHE:HB2	2.17	0.44
1:B:407:ARG:HG3	1:B:439:ASP:HB3	2.00	0.44
1:B:563:PRO:CB	1:B:565:GLU:CG	2.94	0.44
1:A:562:ILE:CD1	1:A:562:ILE:N	2.79	0.44
1:A:595:ARG:CZ	1:A:650:ASP:HB2	2.46	0.44
1:B:518:ARG:NH1	1:B:524:GLU:OE2	2.50	0.44
1:A:596:MET:O	1:A:649:LEU:HB2	2.17	0.44
1:A:13:GLU:OE2	1:A:15:LYS:CE	2.65	0.44
1:B:539:ARG:NH2	6:B:2193:HOH:O	2.21	0.44
1:A:221:ASP:OD1	1:A:223:HIS:HB2	2.17	0.44
1:B:71:ILE:HA	1:B:215:MET:SD	2.58	0.44
1:B:432:ARG:HD2	1:B:432:ARG:HH11	1.67	0.44
1:A:656:ASN:ND2	1:A:658:THR:CB	2.55	0.43
1:A:80:PHE:HD2	1:A:149:PRO:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLN:HB3	1:A:615:ILE:CG1	2.44	0.43
1:A:204:VAL:CG2	1:A:457:THR:HG23	2.48	0.43
1:B:211:VAL:O	1:B:215:MET:HG2	2.18	0.43
1:B:119:VAL:HG22	1:B:175:PHE:CD1	2.53	0.43
1:B:286:LEU:HG	1:B:286:LEU:O	2.18	0.43
1:B:536:THR:OG1	3:B:1918:G6P:O3P	2.29	0.43
1:A:560:TYR:CD2	1:A:581:CYS:HB3	2.53	0.43
1:B:139:GLU:OE1	1:B:139:GLU:CA	2.66	0.43
1:A:558:LYS:HD3	1:A:560:TYR:OH	2.19	0.43
1:B:390:LEU:HD11	1:B:394:LEU:HD11	1.98	0.43
1:A:587:ASP:OD1	1:A:592:LYS:HE2	2.19	0.43
1:A:157:PRO:HB3	1:A:260:GLU:OE1	2.19	0.43
1:A:62:LYS:HZ3	1:A:157:PRO:CB	2.29	0.43
1:B:529:LEU:O	1:B:598:LEU:HA	2.18	0.43
1:A:895:ASP:C	6:A:1112:HOH:O	2.57	0.43
1:B:140:LYS:HB2	1:B:140:LYS:HE3	1.36	0.43
1:B:251:ASP:OD1	1:B:801:ARG:NH2	2.42	0.43
1:A:160:GLN:NE2	6:A:1108:HOH:O	2.14	0.43
1:B:529:LEU:CD2	1:B:596:MET:SD	3.07	0.43
1:B:549:LYS:CG	1:B:550:LYS:N	2.79	0.43
1:A:577:HIS:O	1:A:578:ILE:C	2.55	0.43
1:B:669:GLU:OE2	1:B:670:PRO:HD2	2.18	0.43
1:A:529:LEU:O	1:A:598:LEU:HD13	2.19	0.43
1:A:759:ILE:CD1	1:A:776:LEU:CG	2.94	0.43
1:B:313:MET:HE3	1:B:319:LEU:CG	2.48	0.43
1:A:774:GLU:OE2	1:A:777:LYS:HE2	2.18	0.43
1:A:715:ASN:HD22	1:A:716:GLY:N	2.17	0.43
1:B:139:GLU:HA	1:B:139:GLU:OE1	2.18	0.43
1:A:412:VAL:HG11	1:A:417:TYR:CE2	2.54	0.43
1:A:195:LYS:HG2	1:A:195:LYS:O	2.19	0.43
1:B:685:CYS:HA	1:B:705:ILE:O	2.19	0.43
1:B:219:TYR:CD2	1:B:455:MET:HE2	2.51	0.43
1:B:313:MET:HE3	1:B:319:LEU:HG	2.00	0.43
1:A:243:ARG:HG3	1:A:244:HIS:CD2	2.54	0.43
1:A:208:ASN:ND2	1:A:210:THR:OG1	2.49	0.43
1:A:663:MET:O	1:A:664:THR:C	2.57	0.42
1:A:795:LEU:HD11	1:A:799:GLN:HG2	2.01	0.42
1:B:569:GLY:O	1:B:625:ALA:HA	2.19	0.42
1:A:167:ILE:HD13	1:A:184:ASP:HB2	2.01	0.42
1:A:672:CYS:HA	1:A:857:THR:O	2.19	0.42
1:B:519:THR:HB	1:B:520:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:HE2	1:A:444:LEU:HD23	1.84	0.42
1:A:194:LYS:HB3	1:A:194:LYS:HE2	1.72	0.42
1:A:29:MET:HE1	1:A:277:PHE:CD2	2.54	0.42
1:B:104:ASN:N	1:B:104:ASN:OD1	2.52	0.42
1:A:266:ASP:O	1:A:267:ASP:C	2.58	0.42
1:B:721:ILE:HD12	1:B:721:ILE:HG21	1.75	0.42
1:A:527:ASP:CG	1:A:544:LYS:HG2	2.38	0.42
1:B:682:SER:O	1:B:683:ASN:HB2	2.19	0.42
1:A:487:VAL:HG12	1:A:836:ALA:HB1	2.01	0.42
1:B:558:LYS:HB3	1:B:560:TYR:CE1	2.55	0.42
1:A:77:LYS:CD	1:A:98:ASN:CG	2.88	0.42
1:A:518:ARG:NH1	1:A:519:THR:O	2.50	0.42
1:B:595:ARG:NH1	1:B:648:ASP:CB	2.66	0.42
1:A:138:MET:HE2	1:A:143:ILE:CD1	2.49	0.42
1:A:77:LYS:HA	1:A:97:VAL:O	2.19	0.42
1:A:94:ARG:N	1:A:108:GLU:O	2.50	0.42
1:B:674:VAL:HG12	1:B:858:VAL:HG13	2.01	0.42
1:B:76:GLU:CD	1:B:455:MET:HE3	2.40	0.42
1:B:81:ILE:HB	1:B:150:VAL:HG22	2.02	0.42
1:B:145:ASP:C	1:B:147:LYS:H	2.23	0.42
1:A:176:LYS:HE2	6:A:1176:HOH:O	2.18	0.42
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.87	0.42
1:A:529:LEU:C	1:A:598:LEU:HD13	2.40	0.42
1:B:513:PRO:HB2	1:B:703:MET:HE1	1.94	0.42
1:A:690:MET:CE	1:A:703:MET:CB	2.98	0.42
1:A:570:THR:HB	1:A:573:GLU:CD	2.39	0.42
1:A:444:LEU:HD13	1:A:444:LEU:C	2.40	0.42
1:B:407:ARG:HG3	1:B:439:ASP:CB	2.50	0.42
1:A:172:THR:O	1:A:173:LYS:HB2	2.20	0.42
1:A:382:SER:O	1:A:386:VAL:HG22	2.20	0.42
1:A:274:ARG:HD3	1:A:274:ARG:HH11	1.61	0.42
1:A:138:MET:HB3	1:A:143:ILE:HD11	2.01	0.41
1:A:515:PHE:HA	1:A:703:MET:SD	2.60	0.41
1:A:847:GLU:O	1:A:848:ASN:C	2.57	0.41
1:A:193:ILE:HD13	1:A:201:ALA:HB3	2.02	0.41
1:B:332:GLY:HA2	6:B:2183:HOH:O	2.19	0.41
1:A:637:LEU:HD23	1:A:651:VAL:HG21	2.01	0.41
1:B:769:ARG:CG	1:B:769:ARG:NH1	2.78	0.41
1:A:465:GLU:OE1	1:A:468:ARG:NH2	2.35	0.41
1:A:715:ASN:HD22	1:A:716:GLY:H	1.68	0.41
1:B:53:ARG:HD2	1:B:53:ARG:HH11	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ILE:O	1:B:682:SER:HA	2.19	0.41
1:B:441:ARG:CG	1:B:441:ARG:NH1	2.38	0.41
1:B:76:GLU:HA	6:B:2200:HOH:O	2.19	0.41
1:A:767:LEU:HD13	1:A:768:PHE:CG	2.55	0.41
1:B:17:ASP:OD1	1:B:20:LYS:HG2	2.20	0.41
1:A:403:THR:HB	1:A:404:PRO:CD	2.50	0.41
1:A:875:MET:HE1	1:A:876:HIS:HD2	1.85	0.41
1:B:663:MET:HG3	1:B:904:ILE:HD11	2.03	0.41
1:A:911:LEU:HD23	1:A:911:LEU:H	1.83	0.41
1:B:777:LYS:HE3	1:B:777:LYS:HB2	1.81	0.41
1:A:43:PHE:HD2	1:A:392:ALA:HB3	1.86	0.41
1:B:386:VAL:CG2	1:B:386:VAL:O	2.68	0.41
1:A:143:ILE:CD1	1:A:143:ILE:C	2.87	0.41
1:B:755:ARG:HD3	1:B:755:ARG:HH11	1.15	0.41
1:A:615:ILE:H	1:A:615:ILE:HG12	1.12	0.41
1:A:521:ASP:O	1:A:523:THR:HG23	2.20	0.41
1:B:480:THR:O	1:B:481:LYS:C	2.58	0.41
1:A:91:ARG:HG3	1:A:92:ILE:N	2.36	0.41
1:A:431:LEU:HD22	1:A:442:PHE:CZ	2.54	0.41
1:A:164:ASP:HB3	1:A:204:VAL:O	2.20	0.41
1:A:280:GLU:OE2	1:B:558:LYS:NZ	2.35	0.41
1:B:781:ILE:CD1	1:B:807:LEU:HD13	2.51	0.41
1:A:785:LYS:HB3	1:A:785:LYS:HE3	1.37	0.41
1:B:717:CYS:O	1:B:717:CYS:SG	2.79	0.41
1:B:783:GLU:HG3	6:B:2164:HOH:O	2.21	0.41
1:A:755:ARG:HD2	1:A:776:LEU:O	2.20	0.41
1:B:774:GLU:HA	1:B:777:LYS:CE	2.51	0.41
1:B:593:GLY:N	1:B:594:PRO:CD	2.84	0.41
1:A:384:ASN:HA	1:A:384:ASN:HD22	1.67	0.41
1:B:313:MET:HE2	1:B:313:MET:HB2	1.88	0.40
1:B:521:ASP:C	1:B:521:ASP:OD1	2.58	0.40
1:B:570:THR:HG23	1:B:572:GLU:OE1	2.20	0.40
1:B:853:ARG:O	1:B:853:ARG:HG2	2.20	0.40
1:B:49:ASN:HA	1:B:49:ASN:HD22	1.54	0.40
1:B:420:HIS:CD2	1:B:423:TYR:H	2.40	0.40
1:B:403:THR:HA	1:B:404:PRO:HD3	1.87	0.40
1:A:139:GLU:O	1:A:140:LYS:C	2.60	0.40
1:A:441:ARG:HH11	1:A:443:LEU:HD22	1.74	0.40
1:A:874:ILE:CD1	1:A:874:ILE:O	2.64	0.40
1:A:138:MET:HE2	1:A:143:ILE:HD11	2.04	0.40
1:A:875:MET:HB3	1:A:875:MET:HE3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:MET:HE3	1:A:434:LEU:HB3	2.02	0.40
1:B:478:HIS:O	1:B:483:MET:CE	2.69	0.40
1:A:331:ARG:HD3	1:A:331:ARG:HH11	1.52	0.40
1:B:500:ARG:HH11	1:B:500:ARG:HD3	1.57	0.40
1:B:195:LYS:CG	1:B:195:LYS:O	2.68	0.40
1:B:501:LYS:HE3	1:B:694:GLU:O	2.22	0.40
1:A:666:ALA:C	1:A:668:GLU:N	2.74	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	899/917 (98%)	825 (92%)	51 (6%)	23 (3%)	7 3
1	B	891/917 (97%)	861 (97%)	24 (3%)	6 (1%)	26 26
All	All	1790/1834 (98%)	1686 (94%)	75 (4%)	29 (2%)	12 7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	100	GLU
1	A	111	VAL
1	A	504	HIS
1	A	506	ASN
1	A	522	GLY
1	A	548	GLY
1	A	769	ARG
1	A	910	ARG
1	A	911	LEU
1	B	909	VAL

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Mol	Chain	Res	Type
1	A	81	ILE
1	A	101	LYS
1	A	103	GLN
1	A	551	ARG
1	A	564	ILE
1	A	908	GLY
1	B	549	LYS
1	B	908	GLY
1	A	98	ASN
1	A	102	ASN
1	A	445	SER
1	A	505	ASN
1	B	624	LYS
1	B	147	LYS
1	A	266	ASP
1	B	105	VAL
1	A	268	GLY
1	A	909	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	778/788 (99%)	657 (84%)	121 (16%)	3 1
1	B	774/788 (98%)	686 (89%)	88 (11%)	7 5
All	All	1552/1576 (98%)	1343 (86%)	209 (14%)	5 3

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	14	LEU
1	A	16	ASP
1	A	21	LYS
1	A	24	LYS

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Mol	Chain	Res	Type
1	A	35	THR
1	A	53	ARG
1	A	71	ILE
1	A	77	LYS
1	A	79	ASP
1	A	80	PHE
1	A	91	ARG
1	A	93	LEU
1	A	96	GLN
1	A	97	VAL
1	A	101	LYS
1	A	102	ASN
1	A	103	GLN
1	A	107	MET
1	A	108	GLU
1	A	117	ASN
1	A	119	VAL
1	A	124	SER
1	A	125	GLN
1	A	136	ASP
1	A	141	ARG
1	A	147	LYS
1	A	159	GLN
1	A	187	LYS
1	A	188	LEU
1	A	189	LEU
1	A	191	LYS
1	A	196	ARG
1	A	243	ARG
1	A	252	GLU
1	A	254	ARG
1	A	255	MET
1	A	261	TRP
1	A	273	ILE
1	A	287	ASN
1	A	302	LEU
1	A	305	LEU
1	A	312	LYS
1	A	333	LYS
1	A	335	ASN
1	A	336	THR
1	A	344	LYS

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Mol	Chain	Res	Type
1	A	357	THR
1	A	376	THR
1	A	377	ILE
1	A	380	PHE
1	A	390	LEU
1	A	401	LYS
1	A	404	PRO
1	A	405	ARG
1	A	406	LEU
1	A	434	LEU
1	A	437	ASP
1	A	438	SER
1	A	451	LYS
1	A	459	VAL
1	A	465	GLU
1	A	480	THR
1	A	482	ASP
1	A	487	VAL
1	A	504	HIS
1	A	506	ASN
1	A	508	VAL
1	A	516	VAL
1	A	521	ASP
1	A	549	LYS
1	A	550	LYS
1	A	557	ASN
1	A	562	ILE
1	A	564	ILE
1	A	579	VAL
1	A	580	SER
1	A	586	LEU
1	A	591	ILE
1	A	598	LEU
1	A	600	PHE
1	A	603	SER
1	A	615	ILE
1	A	619	TRP
1	A	624	LYS
1	A	646	GLU
1	A	658	THR
1	A	668	GLU
1	A	671	THR

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Mol	Chain	Res	Type
1	A	691	LYS
1	A	703	MET
1	A	709	TRP
1	A	715	ASN
1	A	720	ASP
1	A	735	ASN
1	A	738	LYS
1	A	759	ILE
1	A	762	THR
1	A	777	LYS
1	A	781	ILE
1	A	785	LYS
1	A	795	LEU
1	A	799	GLN
1	A	804	LEU
1	A	806	GLN
1	A	818	LEU
1	A	821	THR
1	A	843	ASP
1	A	845	ILE
1	A	857	THR
1	A	866	LYS
1	A	874	ILE
1	A	877	GLN
1	A	881	GLU
1	A	888	VAL
1	A	891	LEU
1	A	895	ASP
1	A	899	LYS
1	A	910	ARG
1	A	912	ARG
1	A	914	GLU
1	B	18	GLN
1	B	21	LYS
1	B	48	LYS
1	B	52	SER
1	B	76	GLU
1	B	83	LEU
1	B	91	ARG
1	B	99	HIS
1	B	108	GLU
1	B	117	ASN

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Mol	Chain	Res	Type
1	B	119	VAL
1	B	124	SER
1	B	140	LYS
1	B	142	LYS
1	B	143	ILE
1	B	144	LYS
1	B	185	VAL
1	B	186	VAL
1	B	189	LEU
1	B	194	LYS
1	B	196	ARG
1	B	198	ASP
1	B	207	VAL
1	B	223	HIS
1	B	235	ASN
1	B	242	LEU
1	B	252	GLU
1	B	261	TRP
1	B	281	ILE
1	B	305	LEU
1	B	318	LEU
1	B	320	PHE
1	B	331	ARG
1	B	347	GLU
1	B	349	LEU
1	B	359	LEU
1	B	380	PHE
1	B	396	ARG
1	B	403	THR
1	B	407	ARG
1	B	431	LEU
1	B	432	ARG
1	B	434	LEU
1	B	437	ASP
1	B	439	ASP
1	B	443	LEU
1	B	463	LEU
1	B	483	MET
1	B	496	GLU
1	B	497	LEU
1	B	518	ARG
1	B	529	LEU

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Mol	Chain	Res	Type
1	B	531	LEU
1	B	536	THR
1	B	549	LYS
1	B	551	ARG
1	B	565	GLU
1	B	592	LYS
1	B	596	MET
1	B	598	LEU
1	B	624	LYS
1	B	648	ASP
1	B	689	GLU
1	B	709	TRP
1	B	717	CYS
1	B	720	ASP
1	B	721	ILE
1	B	760	ASP
1	B	767	LEU
1	B	769	ARG
1	B	771	GLN
1	B	779	ARG
1	B	781	ILE
1	B	785	LYS
1	B	787	LEU
1	B	806	GLN
1	B	829	ARG
1	B	843	ASP
1	B	845	ILE
1	B	848	ASN
1	B	852	ASP
1	B	853	ARG
1	B	866	LYS
1	B	880	LYS
1	B	895	ASP
1	B	897	SER
1	B	912	ARG
1	B	914	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	208	ASN
1	A	222	GLN
1	A	235	ASN
1	A	244	HIS
1	A	287	ASN
1	A	335	ASN
1	A	373	HIS
1	A	384	ASN
1	A	420	HIS
1	A	502	GLN
1	A	556	HIS
1	A	631	HIS
1	A	656	ASN
1	A	702	GLN
1	A	715	ASN
1	A	735	ASN
1	A	771	GLN
1	A	806	GLN
1	A	887	ASN
1	B	49	ASN
1	B	56	ASN
1	B	104	ASN
1	B	235	ASN
1	B	244	HIS
1	B	345	ASN
1	B	351	ASN
1	B	372	GLN
1	B	373	HIS
1	B	384	ASN
1	B	400	ASN
1	B	420	HIS
1	B	505	ASN
1	B	525	ASN
1	B	656	ASN
1	B	771	GLN
1	B	855	ASN
1	B	887	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	A	918	-	12,12,12	0.84	1 (8%)	17,17,17	1.75	4 (23%)
3	G6P	A	919	-	16,16,16	1.31	3 (18%)	23,24,24	2.47	11 (47%)
2	GLC	A	920	-	12,12,12	0.96	1 (8%)	17,17,17	2.06	5 (29%)
3	G6P	A	921	-	16,16,16	1.04	0	23,24,24	2.18	5 (21%)
5	ANP	A	999	-	27,33,33	1.59	8 (29%)	30,52,52	1.50	4 (13%)
2	GLC	B	1915	-	12,12,12	0.53	0	17,17,17	1.48	2 (11%)
3	G6P	B	1916	-	16,16,16	1.00	0	23,24,24	2.18	8 (34%)
2	GLC	B	1917	-	12,12,12	1.14	1 (8%)	17,17,17	2.07	7 (41%)
3	G6P	B	1918	-	16,16,16	1.38	3 (18%)	23,24,24	2.65	10 (43%)
5	ANP	B	1999	4	27,33,33	1.58	7 (25%)	30,52,52	1.37	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	918	-	-	0/2/22/22	0/1/1/1
3	G6P	A	919	-	1/1/6/6	0/6/26/26	0/1/1/1
2	GLC	A	920	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	A	921	-	1/1/6/6	0/6/26/26	0/1/1/1
5	ANP	A	999	-	-	0/12/38/38	0/3/3/3
2	GLC	B	1915	-	-	0/2/22/22	0/1/1/1
3	G6P	B	1916	-	1/1/6/6	0/6/26/26	0/1/1/1
2	GLC	B	1917	-	-	0/2/22/22	0/1/1/1
3	G6P	B	1918	-	1/1/6/6	0/6/26/26	0/1/1/1
5	ANP	B	1999	4	-	0/12/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	ANP	C8-N7	-3.15	1.28	1.34
5	B	1999	ANP	C8-N7	-3.02	1.28	1.34
5	A	999	ANP	PG-O3G	-2.90	1.48	1.56
5	A	999	ANP	PG-O2G	-2.89	1.48	1.56
5	B	1999	ANP	PG-O3G	-2.86	1.48	1.56
5	B	1999	ANP	PG-O2G	-2.85	1.48	1.56
5	B	1999	ANP	PB-O2B	-2.81	1.48	1.56
5	A	999	ANP	PB-O2B	-2.71	1.49	1.56
3	B	1918	G6P	O2-C2	-2.67	1.36	1.43
5	A	999	ANP	C5-N7	-2.44	1.31	1.39
3	A	919	G6P	P-O2P	-2.41	1.46	1.54
3	B	1918	G6P	P-O1P	-2.24	1.46	1.54
5	B	1999	ANP	C5-N7	-2.19	1.32	1.39
2	A	918	GLC	C4-C5	2.01	1.57	1.53
2	B	1917	GLC	C4-C5	2.02	1.57	1.53
5	A	999	ANP	C2-N1	2.08	1.37	1.33
2	A	920	GLC	C4-C3	2.11	1.57	1.52
3	B	1918	G6P	C3-C2	2.15	1.58	1.52
3	A	919	G6P	C3-C2	2.15	1.58	1.52
3	A	919	G6P	O5-C5	2.18	1.49	1.44
5	B	1999	ANP	PB-O1B	2.20	1.48	1.46
5	B	1999	ANP	PG-O1G	2.33	1.48	1.46
5	A	999	ANP	PB-O1B	2.39	1.48	1.46
5	A	999	ANP	PG-O1G	2.67	1.49	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1918	G6P	O5-C5-C6	-6.70	92.91	106.61
3	A	921	G6P	C4-C3-C2	-4.12	103.10	110.79
3	A	919	G6P	C4-C3-C2	-4.04	103.26	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	918	GLC	O5-C5-C4	-4.00	102.18	109.68
2	A	920	GLC	O4-C4-C3	-3.94	101.46	110.34
3	B	1918	G6P	O1-C1-O5	-3.93	99.50	110.25
3	A	919	G6P	O5-C5-C6	-3.90	98.64	106.61
3	B	1918	G6P	C4-C3-C2	-3.82	103.66	110.79
2	A	920	GLC	C3-C4-C5	-3.77	103.63	110.20
3	A	919	G6P	O1P-P-O6	-3.69	95.95	106.56
3	B	1916	G6P	O5-C5-C6	-3.61	99.24	106.61
2	A	920	GLC	O5-C5-C4	-3.53	103.05	109.68
2	B	1917	GLC	C3-C4-C5	-3.37	104.32	110.20
3	A	921	G6P	O1P-P-O6	-3.35	96.93	106.56
2	B	1917	GLC	O5-C5-C4	-3.34	103.41	109.68
3	B	1918	G6P	O2-C2-C3	-3.26	102.99	110.34
3	B	1916	G6P	O4-C4-C3	-3.25	103.02	110.34
2	B	1915	GLC	O5-C5-C4	-3.23	103.63	109.68
2	B	1917	GLC	O1-C1-O5	-3.21	101.46	110.25
3	A	919	G6P	C1-C2-C3	-3.14	105.75	110.43
3	A	919	G6P	O5-C5-C4	-3.12	103.83	109.68
2	B	1915	GLC	O5-C1-C2	-3.05	104.94	109.80
3	A	919	G6P	C1-O5-C5	-3.03	107.86	113.47
2	B	1917	GLC	O4-C4-C3	-3.01	103.55	110.34
2	A	918	GLC	C3-C4-C5	-2.95	105.06	110.20
3	B	1918	G6P	O4-C4-C3	-2.79	104.05	110.34
2	A	918	GLC	O4-C4-C3	-2.72	104.21	110.34
3	B	1916	G6P	C4-C3-C2	-2.66	105.83	110.79
3	B	1918	G6P	O5-C1-C2	-2.62	105.61	109.80
5	B	1999	ANP	O3A-PB-N3B	-2.52	99.50	106.44
3	B	1916	G6P	O2-C2-C3	-2.51	104.69	110.34
3	B	1918	G6P	C3-C4-C5	-2.45	105.92	110.20
3	A	919	G6P	O2-C2-C1	-2.41	104.51	109.82
5	A	999	ANP	O3A-PB-N3B	-2.39	99.86	106.44
2	A	920	GLC	C6-C5-C4	-2.34	107.25	113.02
2	A	920	GLC	C1-C2-C3	-2.33	106.96	110.43
2	B	1917	GLC	C1-C2-C3	-2.21	107.13	110.43
2	B	1917	GLC	C6-C5-C4	-2.14	107.72	113.02
5	A	999	ANP	O3G-PG-O1G	-2.10	107.90	113.49
3	B	1918	G6P	C1-C2-C3	-2.09	107.33	110.43
3	A	919	G6P	O4-C4-C3	-2.08	105.66	110.34
3	A	919	G6P	O1-C1-O5	-2.03	104.68	110.25
5	B	1999	ANP	C4'-O4'-C1'	2.10	112.03	109.72
5	B	1999	ANP	O4'-C1'-N9	2.23	112.76	108.10
3	B	1916	G6P	O3-C3-C2	2.41	115.76	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1999	ANP	C1'-N9-C4	2.42	130.60	126.94
2	A	918	GLC	O2-C2-C3	2.46	115.88	110.34
3	B	1916	G6P	O6-P-O3P	2.46	113.41	107.14
3	A	921	G6P	O2P-P-O1P	2.57	117.16	107.38
2	B	1917	GLC	O5-C5-C6	2.78	113.39	106.36
3	B	1918	G6P	O3-C3-C4	2.87	116.80	110.34
5	B	1999	ANP	C4-C5-N7	3.28	112.50	109.48
3	A	919	G6P	O4-C4-C5	3.33	118.07	109.24
5	A	999	ANP	C4-C5-N7	3.89	113.06	109.48
5	A	999	ANP	C1'-N9-C4	4.05	133.05	126.94
3	B	1916	G6P	O3-C3-C4	4.07	119.50	110.34
3	B	1918	G6P	C6-C5-C4	4.70	122.68	112.03
3	A	921	G6P	O5-C5-C4	4.85	118.79	109.68
3	A	919	G6P	C6-C5-C4	4.98	123.32	112.03
3	B	1916	G6P	O5-C1-C2	5.01	117.78	109.80
3	A	921	G6P	O5-C1-C2	5.72	118.93	109.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1916	G6P	C1
3	B	1918	G6P	C1
3	A	919	G6P	C1
3	A	921	G6P	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	919	G6P	6	0
3	A	921	G6P	1	0
5	A	999	ANP	1	0
3	B	1916	G6P	3	0
3	B	1918	G6P	5	0
5	B	1999	ANP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.