



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:33 AM UTC

PDB ID : 3CR8 / pdb_00003cr8
Title : Hexameric APS kinase from Thiobacillus denitrificans
Authors : Gay, S.C.; Segel, I.H.; Fisher, A.J.
Deposited on : 2008-04-04
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

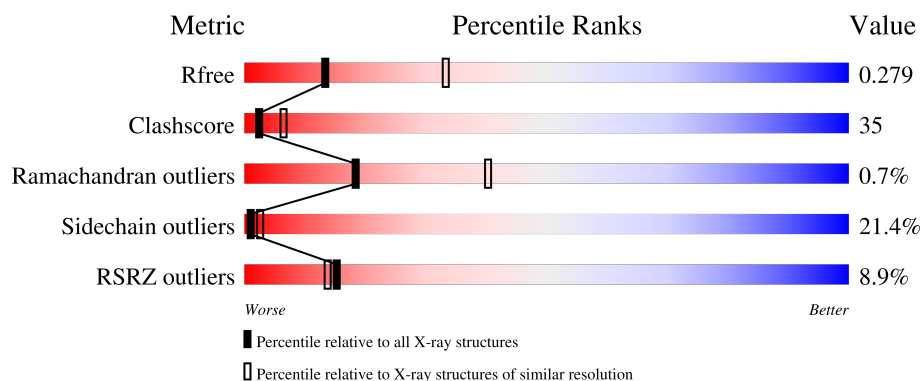
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	9% 46% 31% 11% • 11%
1	B	552	8% 46% 30% 11% • 11%
1	C	552	7% 45% 32% 12% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11339 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 Sulfate adenylyltransferase, adenylylsulfate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3761	2390	676	679	16			
1	B	493	Total	C	N	O	S	0	0	0
			3744	2378	671	679	16			
1	C	493	Total	C	N	O	S	0	0	0
			3748	2380	670	682	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	LEU	-	expression tag	UNP Q3SM86
A	546	GLU	-	expression tag	UNP Q3SM86
A	547	HIS	-	expression tag	UNP Q3SM86
A	548	HIS	-	expression tag	UNP Q3SM86
A	549	HIS	-	expression tag	UNP Q3SM86
A	550	HIS	-	expression tag	UNP Q3SM86
A	551	HIS	-	expression tag	UNP Q3SM86
A	552	HIS	-	expression tag	UNP Q3SM86
B	545	LEU	-	expression tag	UNP Q3SM86
B	546	GLU	-	expression tag	UNP Q3SM86
B	547	HIS	-	expression tag	UNP Q3SM86
B	548	HIS	-	expression tag	UNP Q3SM86
B	549	HIS	-	expression tag	UNP Q3SM86
B	550	HIS	-	expression tag	UNP Q3SM86
B	551	HIS	-	expression tag	UNP Q3SM86
B	552	HIS	-	expression tag	UNP Q3SM86
C	545	LEU	-	expression tag	UNP Q3SM86
C	546	GLU	-	expression tag	UNP Q3SM86
C	547	HIS	-	expression tag	UNP Q3SM86
C	548	HIS	-	expression tag	UNP Q3SM86
C	549	HIS	-	expression tag	UNP Q3SM86
C	550	HIS	-	expression tag	UNP Q3SM86
C	551	HIS	-	expression tag	UNP Q3SM86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	552	HIS	-	expression tag	UNP Q3SM86

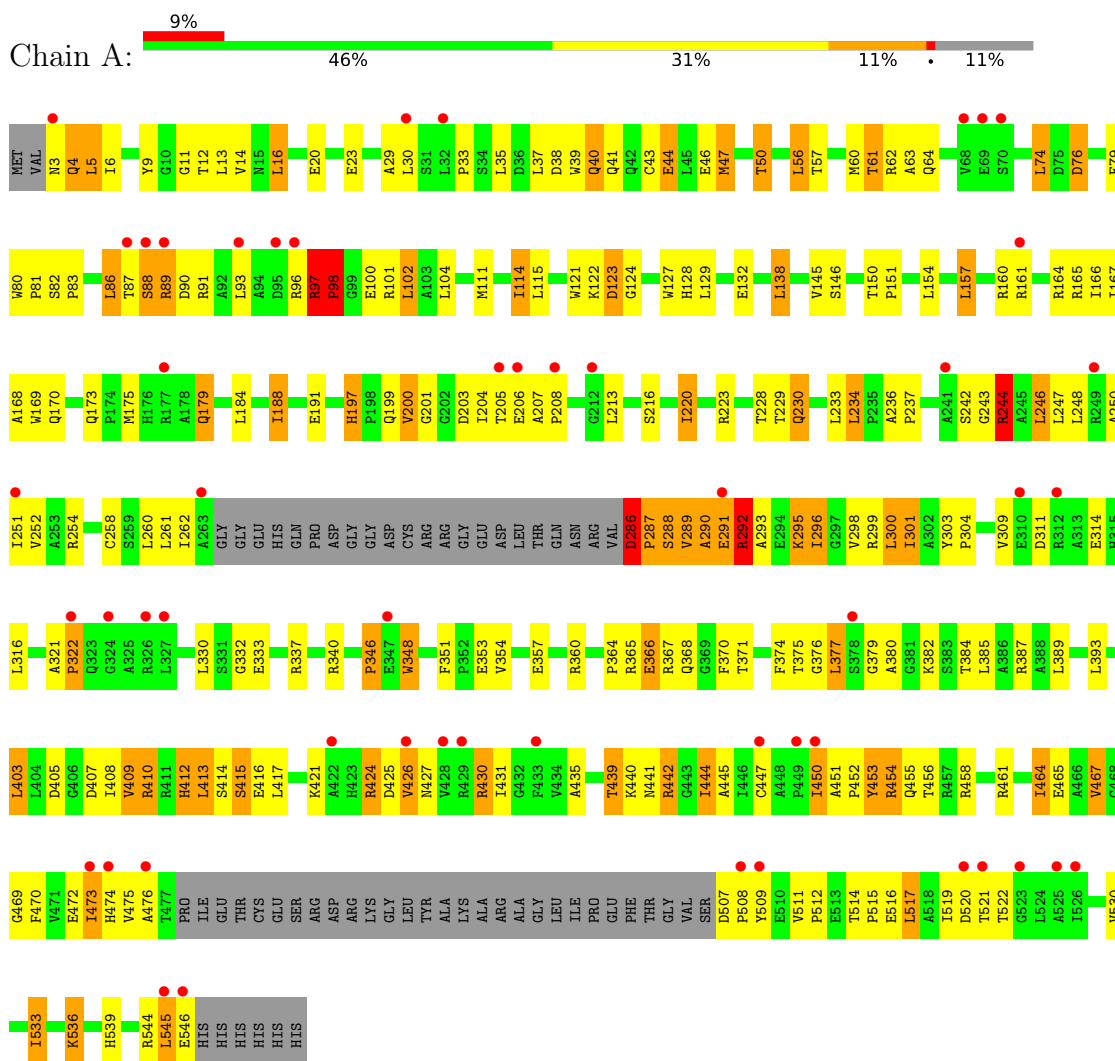
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	O 31	0	0
2	B	22	Total 22	O 22	0	0
2	C	33	Total 33	O 33	0	0

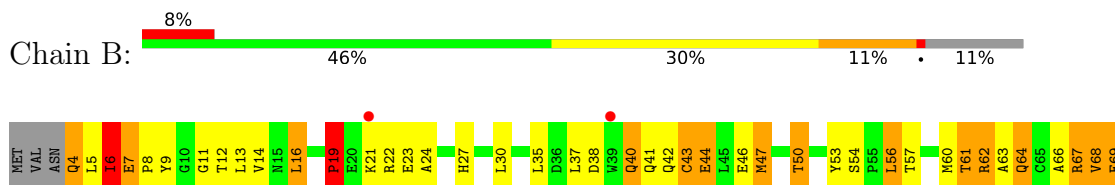
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sulfate adenylyltransferase, adenylylsulfate kinase



- Molecule 1: Sulfate adenylyltransferase, adenylylsulfate kinase



K536	R544
L537	L545
E538	GLU
H539	HIS
	HIS
	HIS
	HIS
	HIS
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	161.07Å 227.21Å 106.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.03 – 2.95 35.03 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.1 (35.03-2.95) 92.1 (35.03-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.282 0.240 , 0.279	Depositor DCC
R_{free} test set	1889 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11339	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.87	1/3843 (0.0%)	1.29	43/5227 (0.8%)
1	B	0.92	4/3825 (0.1%)	1.23	40/5205 (0.8%)
1	C	0.87	3/3829 (0.1%)	1.29	45/5209 (0.9%)
All	All	0.88	8/11497 (0.1%)	1.27	128/15641 (0.8%)

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	1
1	C	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	VAL	CA-CB	-7.10	1.46	1.54
1	C	26	LYS	C-O	6.38	1.31	1.24
1	B	19	PRO	CA-C	6.17	1.61	1.52
1	C	87	THR	C-O	-5.44	1.16	1.23
1	B	333	GLU	N-CA	-5.30	1.39	1.46
1	C	289	VAL	CA-CB	-5.23	1.48	1.54
1	B	296	ILE	CA-CB	-5.14	1.47	1.54
1	B	525	ALA	CA-CB	-5.11	1.45	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLU	N-CA-C	15.54	128.22	111.28
1	B	416	GLU	N-CA-CB	-15.25	93.50	111.79
1	C	522	THR	N-CA-C	14.07	128.99	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	522	THR	N-CA-CB	-13.66	89.85	110.20
1	C	521	THR	CB-CA-C	-13.43	83.03	109.76
1	A	88	SER	CB-CA-C	12.29	131.07	110.43
1	A	410	ARG	N-CA-C	12.19	125.89	111.02
1	B	205	THR	N-CA-C	10.21	127.52	114.56
1	C	205	THR	N-CA-C	10.18	127.49	114.56
1	A	89	ARG	N-CA-C	-10.11	95.69	109.54
1	A	454	ARG	CA-C-N	-10.02	106.85	120.28
1	A	454	ARG	C-N-CA	-10.02	106.85	120.28
1	A	410	ARG	CB-CA-C	-9.83	95.28	110.92
1	A	291	GLU	CB-CA-C	-9.64	94.79	110.79
1	A	244	ARG	N-CA-C	-9.48	100.90	111.14
1	C	286	ASP	CA-C-N	-9.46	109.16	119.19
1	C	286	ASP	C-N-CA	-9.46	109.16	119.19
1	B	294	GLU	N-CA-C	-8.73	101.73	112.38
1	B	237	PRO	N-CA-C	-8.63	100.17	110.70
1	A	88	SER	N-CA-C	-8.48	95.35	108.42
1	C	381	GLY	N-CA-C	-8.45	105.02	114.40
1	A	237	PRO	N-CA-C	-8.34	100.53	110.70
1	A	421	LYS	CA-C-N	-8.28	109.66	122.49
1	A	421	LYS	C-N-CA	-8.28	109.66	122.49
1	C	292	ARG	CB-CA-C	-8.17	98.06	110.88
1	A	289	VAL	N-CA-C	-8.11	104.84	111.81
1	B	380	ALA	N-CA-C	8.02	123.53	113.43
1	A	412	HIS	N-CA-C	8.00	123.72	113.88
1	A	380	ALA	N-CA-C	-7.95	103.37	113.23
1	A	236	ALA	CA-C-N	-7.89	112.26	120.38
1	A	236	ALA	C-N-CA	-7.89	112.26	120.38
1	B	410	ARG	N-CA-C	7.87	120.62	111.02
1	C	27	HIS	N-CA-C	7.83	120.58	111.02
1	B	108	GLU	CA-C-N	-7.79	108.69	122.16
1	B	108	GLU	C-N-CA	-7.79	108.69	122.16
1	C	236	ALA	CA-C-N	-7.60	112.56	120.38
1	C	236	ALA	C-N-CA	-7.60	112.56	120.38
1	B	410	ARG	CA-C-N	7.56	132.16	120.82
1	B	410	ARG	C-N-CA	7.56	132.16	120.82
1	A	295	LYS	N-CA-C	7.56	120.24	111.02
1	C	97	ARG	N-CA-C	7.45	120.30	108.23
1	A	293	ALA	N-CA-C	-7.40	100.23	111.56
1	A	292	ARG	CB-CA-C	-7.40	96.78	109.65
1	C	29	ALA	N-CA-C	7.22	121.35	112.54
1	A	454	ARG	N-CA-C	-7.21	102.46	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	VAL	CA-C-N	-7.21	110.77	120.79
1	B	409	VAL	C-N-CA	-7.21	110.77	120.79
1	C	126	ARG	N-CA-C	7.19	120.67	109.52
1	A	290	ALA	N-CA-C	-7.14	103.67	112.38
1	C	29	ALA	CB-CA-C	-6.81	96.08	110.31
1	A	511	VAL	CB-CA-C	-6.80	98.98	111.36
1	A	340	ARG	CA-C-N	-6.75	111.65	121.98
1	A	340	ARG	C-N-CA	-6.75	111.65	121.98
1	C	447	CYS	CB-CA-C	-6.75	97.49	109.70
1	B	236	ALA	CA-C-N	-6.73	113.45	120.38
1	B	236	ALA	C-N-CA	-6.73	113.45	120.38
1	B	430	ARG	N-CA-C	-6.72	103.95	111.28
1	B	19	PRO	N-CA-C	6.68	126.23	112.47
1	B	447	CYS	CB-CA-C	-6.68	97.61	109.70
1	A	410	ARG	CA-C-N	6.67	130.06	120.79
1	A	410	ARG	C-N-CA	6.67	130.06	120.79
1	C	410	ARG	CA-C-N	6.65	130.80	120.82
1	C	410	ARG	C-N-CA	6.65	130.80	120.82
1	A	97	ARG	N-CA-C	6.54	119.87	108.82
1	A	20	GLU	CA-C-N	-6.43	112.38	122.73
1	A	20	GLU	C-N-CA	-6.43	112.38	122.73
1	B	285	VAL	N-CA-C	6.38	122.61	109.34
1	C	340	ARG	CA-C-N	-6.36	112.63	122.49
1	C	340	ARG	C-N-CA	-6.36	112.63	122.49
1	C	350	SER	CB-CA-C	-6.27	96.69	110.67
1	A	289	VAL	CB-CA-C	-6.14	104.49	111.55
1	A	421	LYS	N-CA-C	-6.10	103.95	111.33
1	C	117	LEU	N-CA-C	6.08	119.02	109.96
1	B	185	LYS	N-CA-C	-6.05	104.01	111.40
1	B	414	SER	CB-CA-C	-6.03	98.75	110.75
1	C	23	GLU	N-CA-C	-6.00	104.81	111.71
1	B	413	LEU	N-CA-C	6.00	121.26	113.88
1	C	426	VAL	CB-CA-C	-5.94	104.03	112.22
1	A	426	VAL	N-CA-C	-5.90	106.74	111.81
1	C	379	GLY	N-CA-C	-5.85	99.33	113.18
1	C	351	PHE	N-CA-C	5.79	118.69	110.24
1	C	448	ALA	N-CA-CB	-5.78	102.64	110.74
1	B	340	ARG	CA-C-N	-5.78	113.07	122.26
1	B	340	ARG	C-N-CA	-5.78	113.07	122.26
1	B	410	ARG	CB-CA-C	-5.66	101.92	110.92
1	C	521	THR	N-CA-C	5.64	118.16	110.55
1	B	447	CYS	N-CA-C	5.59	118.22	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	477	THR	N-CA-C	-5.56	97.52	109.81
1	B	380	ALA	N-CA-CB	-5.53	101.11	110.51
1	C	478	PRO	N-CA-C	-5.52	101.09	112.47
1	A	447	CYS	CB-CA-C	-5.48	98.90	109.37
1	C	523	GLY	N-CA-C	-5.47	100.21	113.18
1	C	325	ALA	CA-C-N	-5.46	113.70	121.50
1	C	325	ALA	C-N-CA	-5.46	113.70	121.50
1	A	288	SER	N-CA-C	-5.45	106.47	113.02
1	A	286	ASP	C-N-CD	-5.45	108.61	120.60
1	B	43	CYS	N-CA-C	-5.43	105.00	111.03
1	A	516	GLU	N-CA-C	-5.43	105.01	111.69
1	C	325	ALA	O-C-N	-5.43	116.46	122.86
1	B	363	PRO	CA-C-N	5.39	125.33	119.78
1	B	363	PRO	C-N-CA	5.39	125.33	119.78
1	C	524	LEU	N-CA-CB	5.35	118.90	110.71
1	B	184	LEU	CB-CA-C	-5.33	102.51	110.88
1	C	447	CYS	N-CA-C	5.31	117.73	108.76
1	A	348	TRP	N-CA-C	-5.29	106.83	113.28
1	C	237	PRO	N-CA-C	-5.27	104.27	110.70
1	B	205	THR	N-CA-CB	-5.24	104.04	111.00
1	C	205	THR	N-CA-CB	-5.23	104.04	111.00
1	B	448	ALA	N-CA-CB	-5.21	103.44	110.74
1	B	288	SER	CA-C-N	-5.21	112.59	121.97
1	B	288	SER	C-N-CA	-5.21	112.59	121.97
1	A	201	GLY	N-CA-C	5.19	119.07	110.97
1	C	43	CYS	N-CA-C	-5.17	105.30	111.03
1	C	80	TRP	CA-C-N	5.14	124.75	119.05
1	C	80	TRP	C-N-CA	5.14	124.75	119.05
1	A	322	PRO	O-C-N	-5.12	116.66	123.01
1	C	289	VAL	CB-CA-C	-5.11	105.43	111.97
1	C	30	LEU	N-CA-CB	-5.11	100.99	110.18
1	B	68	VAL	CB-CA-C	-5.10	105.20	111.94
1	C	27	HIS	CB-CA-C	-5.09	102.82	110.92
1	C	333	GLU	N-CA-C	-5.09	105.86	111.71
1	B	21	LYS	N-CA-C	-5.08	105.86	111.71
1	B	297	GLY	N-CA-C	5.07	125.18	113.18
1	B	333	GLU	N-CA-C	-5.06	105.21	111.33
1	B	381	GLY	N-CA-C	-5.06	107.29	115.08
1	B	97	ARG	N-CA-C	5.06	114.63	108.11
1	A	409	VAL	CA-C-N	-5.04	113.78	120.79
1	A	409	VAL	C-N-CA	-5.04	113.78	120.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ASP	Peptide
1	C	380	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3761	0	3716	266	0
1	B	3744	0	3685	288	1
1	C	3748	0	3684	248	0
2	A	31	0	0	2	0
2	B	22	0	0	0	0
2	C	33	0	0	4	0
All	All	11339	0	11085	783	1

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 35.

All (783) 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:414:SER:HB2	1:A:417:LEU:CD1	1.57	1.35
1:B:4:GLN:NE2	1:B:5:LEU:HB2	1.42	1.34
1:C:288:SER:O	1:C:291:GLU:HB2	1.32	1.28
1:A:244:ARG:HD2	1:A:244:ARG:N	1.40	1.22
1:C:287:PRO:O	1:C:291:GLU:HG2	1.32	1.22
1:C:21:LYS:O	1:C:24:ALA:HB3	1.35	1.22
1:A:286:ASP:CB	1:A:287:PRO:HA	1.69	1.21
1:B:414:SER:CB	1:B:417:LEU:HD12	1.68	1.21
1:B:61:THR:HG22	1:B:64:GLN:CG	1.73	1.18
1:A:244:ARG:H	1:A:244:ARG:CD	1.57	1.16
1:A:545:LEU:HD23	1:A:546:GLU:N	1.59	1.16
1:B:475:VAL:HG13	1:B:519:ILE:HD11	1.24	1.15
1:A:414:SER:CB	1:A:417:LEU:HD12	1.75	1.15
1:B:67:ARG:HH11	1:B:67:ARG:CG	1.59	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:THR:CG2	1:B:64:GLN:HG3	1.79	1.13
1:B:509:TYR:CE2	1:B:510:GLU:O	2.03	1.12
1:B:424:ARG:HE	1:B:450:ILE:HD11	1.01	1.11
1:B:424:ARG:NE	1:B:450:ILE:HD11	1.66	1.11
1:A:539:HIS:CE1	1:C:188:ILE:HA	1.86	1.10
1:B:521:THR:HG21	1:B:524:LEU:HG	1.26	1.10
1:B:507:ASP:CB	1:B:508:PRO:CD	2.30	1.09
1:B:414:SER:CB	1:B:417:LEU:CD1	2.30	1.08
1:A:414:SER:HB2	1:A:417:LEU:HD12	1.10	1.08
1:A:507:ASP:CB	1:A:508:PRO:CD	2.30	1.08
1:A:545:LEU:HD23	1:A:546:GLU:H	0.90	1.07
1:B:507:ASP:CB	1:B:508:PRO:HD3	1.83	1.07
1:A:539:HIS:CD2	1:C:188:ILE:HG22	1.90	1.07
1:C:414:SER:HB2	1:C:417:LEU:HD12	1.09	1.07
1:B:367:ARG:CG	1:B:367:ARG:HH11	1.68	1.06
1:A:414:SER:CB	1:A:417:LEU:CD1	2.30	1.05
1:B:521:THR:CG2	1:B:524:LEU:HG	1.86	1.05
1:B:414:SER:HB2	1:B:417:LEU:HD12	1.30	1.04
1:B:442:ARG:HH11	1:B:442:ARG:HG2	1.22	1.04
1:C:61:THR:HG22	1:C:64:GLN:HG3	1.36	1.04
1:B:367:ARG:HH11	1:B:367:ARG:HG2	1.21	1.03
1:B:285:VAL:HG13	1:B:285:VAL:O	1.57	1.03
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.19	1.03
1:A:286:ASP:CB	1:A:287:PRO:CA	2.30	1.02
1:B:521:THR:HG21	1:B:524:LEU:CG	1.89	1.02
1:C:428:VAL:HG11	1:C:456:THR:CG2	1.90	1.02
1:B:4:GLN:NE2	1:B:5:LEU:H	1.57	1.01
1:B:509:TYR:O	1:B:510:GLU:HG3	1.61	1.00
1:B:424:ARG:HE	1:B:450:ILE:CD1	1.74	0.98
1:C:291:GLU:HA	1:C:291:GLU:OE1	1.63	0.98
1:B:67:ARG:HG3	1:B:67:ARG:NH1	1.63	0.98
1:B:427:ASN:C	1:B:427:ASN:HD22	1.71	0.98
1:B:67:ARG:HH11	1:B:67:ARG:HG3	0.83	0.97
1:A:61:THR:HG22	1:A:64:GLN:HG3	1.44	0.96
1:C:220:ILE:HG22	1:C:354:VAL:HG22	1.47	0.96
1:C:414:SER:CB	1:C:417:LEU:HD12	1.95	0.96
1:A:507:ASP:CB	1:A:508:PRO:HD3	1.91	0.96
1:A:220:ILE:HG22	1:A:354:VAL:HG22	1.47	0.96
1:B:296:ILE:O	1:B:296:ILE:CG1	2.08	0.96
1:B:61:THR:HG22	1:B:64:GLN:HG3	0.98	0.95
1:B:414:SER:HB3	1:B:417:LEU:CD1	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG22	1:B:354:VAL:HG22	1.44	0.94
1:C:289:VAL:HG23	1:C:290:ALA:N	1.81	0.94
1:A:246:LEU:HD22	1:A:246:LEU:O	1.67	0.94
1:B:296:ILE:O	1:B:296:ILE:HG12	1.65	0.94
1:B:509:TYR:CD2	1:B:510:GLU:N	2.34	0.94
1:A:122:LYS:NZ	1:A:127:TRP:CH2	2.35	0.94
1:B:4:GLN:NE2	1:B:5:LEU:CB	2.30	0.93
1:B:4:GLN:HE22	1:B:5:LEU:HB2	0.93	0.93
1:B:521:THR:CB	1:B:524:LEU:HG	1.99	0.93
1:B:161:ARG:HH21	1:B:230:GLN:HG2	1.32	0.92
1:B:89:ARG:H	1:B:89:ARG:HD3	1.35	0.92
1:A:545:LEU:CD2	1:A:546:GLU:H	1.83	0.92
1:B:96:ARG:HG3	1:B:96:ARG:HH11	1.32	0.91
1:B:427:ASN:C	1:B:427:ASN:ND2	2.29	0.90
1:C:96:ARG:HG3	1:C:96:ARG:HH11	1.36	0.90
1:C:415:SER:O	1:C:416:GLU:HG3	1.72	0.89
1:B:464:ILE:HD11	1:B:469:GLY:O	1.72	0.89
1:A:286:ASP:CB	1:A:287:PRO:HG3	2.02	0.89
1:A:414:SER:CA	1:A:417:LEU:HD12	2.01	0.89
1:C:428:VAL:HG11	1:C:456:THR:HG22	1.55	0.89
1:B:424:ARG:HD2	1:B:450:ILE:HD13	1.54	0.89
1:B:475:VAL:CG1	1:B:519:ILE:HD11	2.04	0.88
1:C:292:ARG:O	1:C:295:LYS:CB	2.22	0.88
1:C:161:ARG:HH21	1:C:230:GLN:HG2	1.39	0.87
1:A:290:ALA:HA	1:A:300:LEU:HD21	1.53	0.87
1:A:292:ARG:NH2	1:A:295:LYS:CB	2.38	0.87
1:C:475:VAL:HG13	1:C:519:ILE:HD11	1.55	0.87
1:B:427:ASN:HD22	1:B:428:VAL:N	1.72	0.86
1:C:157:LEU:HD23	1:C:160:ARG:HH21	1.40	0.86
1:A:161:ARG:HH21	1:A:230:GLN:HG2	1.41	0.86
1:A:62:ARG:HG3	1:A:121:TRP:CE2	2.11	0.85
1:A:414:SER:HB2	1:A:417:LEU:HD13	1.57	0.85
1:B:220:ILE:CG2	1:B:354:VAL:HG22	2.05	0.85
1:B:475:VAL:HG13	1:B:519:ILE:CD1	2.06	0.85
1:A:35:LEU:HD11	1:A:88:SER:OG	1.75	0.84
1:B:424:ARG:HD2	1:B:450:ILE:CD1	2.07	0.84
1:B:377:LEU:H	1:B:377:LEU:HD12	1.42	0.83
1:A:475:VAL:HG13	1:A:519:ILE:HD11	1.60	0.83
1:B:4:GLN:CD	1:B:5:LEU:H	1.87	0.83
1:A:377:LEU:HD12	1:A:377:LEU:H	1.44	0.82
1:C:61:THR:CG2	1:C:64:GLN:HG3	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD23	1:A:160:ARG:HH21	1.42	0.82
1:B:414:SER:CA	1:B:417:LEU:CD1	2.58	0.82
1:C:426:VAL:HG12	1:C:427:ASN:N	1.92	0.82
1:B:393:LEU:HD13	1:B:444:ILE:CD1	2.09	0.81
1:A:289:VAL:HG23	1:A:290:ALA:N	1.94	0.81
1:B:414:SER:CA	1:B:417:LEU:HD12	2.10	0.81
1:A:97:ARG:O	1:A:100:GLU:HG3	1.80	0.80
1:C:289:VAL:CG2	1:C:290:ALA:N	2.44	0.80
1:B:424:ARG:NE	1:B:450:ILE:CD1	2.38	0.80
1:B:292:ARG:O	1:B:295:LYS:CB	2.30	0.80
1:C:544:ARG:HG2	1:C:545:LEU:N	1.95	0.80
1:C:19:PRO:O	1:C:22:ARG:CB	2.30	0.80
1:B:157:LEU:HD23	1:B:160:ARG:HH21	1.47	0.80
1:B:367:ARG:HG2	1:B:367:ARG:NH1	1.93	0.80
1:B:393:LEU:HD13	1:B:444:ILE:HD12	1.63	0.80
1:C:384:THR:HG22	2:C:555:HOH:O	1.81	0.80
1:B:4:GLN:NE2	1:B:5:LEU:N	2.30	0.79
1:A:377:LEU:O	1:A:379:GLY:HA3	1.83	0.79
1:C:428:VAL:CG1	1:C:456:THR:CG2	2.61	0.79
1:A:246:LEU:O	1:A:246:LEU:CD2	2.30	0.79
1:A:377:LEU:O	1:A:379:GLY:CA	2.31	0.79
1:B:46:GLU:O	1:B:50:THR:HB	1.83	0.78
1:C:521:THR:O	1:C:521:THR:OG1	1.93	0.78
1:C:21:LYS:C	1:C:24:ALA:HB3	2.08	0.78
1:C:464:ILE:HD11	1:C:469:GLY:O	1.83	0.78
1:A:188:ILE:HG22	1:B:539:HIS:CD2	2.18	0.78
1:A:292:ARG:HH22	1:A:295:LYS:CB	1.97	0.78
1:B:19:PRO:O	1:B:22:ARG:CB	2.32	0.77
1:B:421:LYS:HD3	1:B:421:LYS:H	1.49	0.77
1:A:289:VAL:CG2	1:A:290:ALA:N	2.47	0.77
1:B:284:ARG:O	1:B:285:VAL:HG12	1.83	0.77
1:A:204:ILE:C	1:A:208:PRO:HG3	2.09	0.77
1:B:509:TYR:CG	1:B:510:GLU:N	2.48	0.77
1:A:4:GLN:HE21	1:A:5:LEU:H	1.33	0.76
1:A:220:ILE:CG2	1:A:354:VAL:HG22	2.14	0.76
1:A:517:LEU:CD1	1:A:533:ILE:HG22	2.15	0.76
1:B:424:ARG:CD	1:B:450:ILE:CD1	2.63	0.76
1:B:89:ARG:HD3	1:B:89:ARG:N	2.00	0.76
1:C:220:ILE:CG2	1:C:354:VAL:HG22	2.14	0.76
1:B:414:SER:HA	1:B:417:LEU:HD11	1.67	0.76
1:A:188:ILE:HA	1:B:539:HIS:CE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:TYR:O	1:B:510:GLU:CG	2.33	0.75
1:A:200:VAL:O	1:A:200:VAL:CG1	2.33	0.75
1:B:47:MET:HE2	1:B:47:MET:HA	1.67	0.75
1:C:291:GLU:OE1	1:C:291:GLU:CA	2.30	0.75
1:C:62:ARG:HG3	1:C:121:TRP:CE2	2.22	0.75
1:A:61:THR:CG2	1:A:64:GLN:HG3	2.17	0.74
1:C:461:ARG:O	1:C:465:GLU:HB2	1.87	0.74
1:A:414:SER:CA	1:A:417:LEU:CD1	2.63	0.74
1:A:454:ARG:O	1:A:455:GLN:C	2.27	0.74
1:A:47:MET:HE2	1:A:47:MET:HA	1.69	0.74
1:C:21:LYS:O	1:C:25:LEU:HG	1.87	0.74
1:B:285:VAL:O	1:B:285:VAL:CG1	2.30	0.74
1:A:46:GLU:O	1:A:50:THR:HB	1.88	0.74
1:A:517:LEU:HD13	1:A:533:ILE:HG22	1.70	0.74
1:B:97:ARG:O	1:B:100:GLU:HG3	1.88	0.73
1:A:286:ASP:CB	1:A:287:PRO:CG	2.66	0.73
1:A:203:ASP:O	1:A:208:PRO:HG3	1.88	0.73
1:B:19:PRO:O	1:B:22:ARG:HB3	1.87	0.73
1:A:200:VAL:O	1:A:200:VAL:HG13	1.87	0.73
1:B:138:LEU:HD12	1:B:138:LEU:H	1.53	0.73
1:B:67:ARG:CG	1:B:67:ARG:NH1	2.30	0.73
1:B:519:ILE:HG13	1:B:519:ILE:O	1.88	0.73
1:C:46:GLU:O	1:C:50:THR:HB	1.88	0.73
1:B:106:ASP:C	1:B:106:ASP:OD1	2.29	0.73
1:C:24:ALA:O	1:C:27:HIS:CB	2.37	0.73
1:C:414:SER:HB2	1:C:417:LEU:CD1	2.05	0.72
1:C:89:ARG:HG3	1:C:89:ARG:HH11	1.54	0.72
1:A:122:LYS:HD2	1:A:127:TRP:CZ2	2.25	0.72
1:C:38:ASP:OD1	1:C:41:GLN:HG2	1.90	0.72
1:C:517:LEU:CD1	1:C:533:ILE:HG22	2.20	0.72
1:A:246:LEU:CD2	1:A:246:LEU:C	2.64	0.71
1:B:68:VAL:C	1:B:70:SER:H	1.99	0.71
1:B:517:LEU:CD1	1:B:533:ILE:HG22	2.21	0.71
1:A:458:ARG:HH11	1:A:461:ARG:HD2	1.55	0.71
1:B:424:ARG:CD	1:B:450:ILE:HD13	2.21	0.71
1:C:57:THR:HG23	1:C:132:GLU:OE1	1.90	0.71
1:A:207:ALA:N	1:A:208:PRO:HD3	2.04	0.71
1:B:96:ARG:HG3	1:B:96:ARG:NH1	2.00	0.71
1:A:442:ARG:HH11	1:A:442:ARG:CG	1.99	0.70
1:A:246:LEU:HD22	1:A:246:LEU:C	2.13	0.70
1:C:428:VAL:HG11	1:C:456:THR:HG21	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TRP:CZ3	1:A:262:ILE:HG21	2.25	0.70
1:C:426:VAL:CG1	1:C:427:ASN:N	2.52	0.70
1:A:371:THR:HG23	1:A:464:ILE:HD13	1.74	0.70
1:A:461:ARG:O	1:A:465:GLU:HB2	1.92	0.70
1:B:442:ARG:HH11	1:B:442:ARG:CG	2.03	0.70
1:B:461:ARG:O	1:B:465:GLU:HB2	1.91	0.70
1:B:371:THR:HG23	1:B:464:ILE:HD13	1.73	0.69
1:C:378:SER:C	1:C:380:ALA:H	2.00	0.69
1:A:35:LEU:HD21	1:A:88:SER:CB	2.22	0.69
1:C:20:GLU:C	1:C:22:ARG:H	1.98	0.69
1:C:199:GLN:HG3	1:C:234:LEU:HD13	1.74	0.69
1:B:169:TRP:CZ3	1:B:262:ILE:HG21	2.27	0.69
1:A:371:THR:CG2	1:A:439:THR:HG21	2.23	0.69
1:B:185:LYS:O	1:B:186:SER:C	2.30	0.69
1:C:169:TRP:CZ3	1:C:262:ILE:HG21	2.27	0.69
1:C:138:LEU:HD12	1:C:138:LEU:H	1.57	0.69
1:A:393:LEU:HD13	1:A:444:ILE:CD1	2.22	0.69
1:B:509:TYR:C	1:B:510:GLU:HG3	2.18	0.69
1:A:207:ALA:O	2:A:577:HOH:O	2.11	0.69
1:C:288:SER:OG	1:C:292:ARG:CZ	2.41	0.68
1:C:262:ILE:HG12	1:C:301:ILE:HD11	1.75	0.68
1:C:413:LEU:HG	1:C:430:ARG:HG2	1.76	0.68
1:A:57:THR:HG23	1:A:132:GLU:OE1	1.94	0.68
1:A:61:THR:HG21	2:A:572:HOH:O	1.93	0.68
1:C:47:MET:HA	1:C:47:MET:HE2	1.73	0.68
1:C:371:THR:HG23	1:C:464:ILE:HD13	1.74	0.68
1:B:199:GLN:HG3	1:B:234:LEU:HD13	1.76	0.67
1:C:415:SER:O	1:C:416:GLU:CG	2.42	0.67
1:C:96:ARG:HG3	1:C:96:ARG:NH1	2.04	0.67
1:C:294:GLU:HG3	1:C:294:GLU:O	1.93	0.67
1:C:289:VAL:CG2	1:C:290:ALA:H	2.07	0.67
1:B:414:SER:CA	1:B:417:LEU:HD11	2.23	0.67
1:B:409:VAL:HG11	1:B:431:ILE:HD11	1.75	0.67
1:A:376:GLY:CA	1:A:509:TYR:OH	2.43	0.67
1:B:296:ILE:O	1:B:296:ILE:HG13	1.95	0.67
1:C:287:PRO:O	1:C:291:GLU:CG	2.27	0.67
1:A:393:LEU:HD13	1:A:444:ILE:HD12	1.76	0.67
1:C:374:PHE:CE2	1:C:473:ILE:HD11	2.30	0.67
1:C:475:VAL:HA	1:C:519:ILE:HG12	1.77	0.67
1:C:517:LEU:HD13	1:C:533:ILE:HG22	1.75	0.67
1:B:57:THR:HG23	1:B:132:GLU:OE1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:SER:O	1:C:291:GLU:CB	2.27	0.66
1:C:454:ARG:HG3	1:C:510:GLU:OE1	1.95	0.66
1:A:371:THR:HG23	1:A:439:THR:HG21	1.77	0.66
1:B:517:LEU:HD13	1:B:533:ILE:HG22	1.76	0.66
1:A:464:ILE:HD11	1:A:469:GLY:O	1.96	0.66
1:B:374:PHE:CE2	1:B:473:ILE:HD11	2.29	0.66
1:A:138:LEU:HD12	1:A:138:LEU:H	1.60	0.66
1:B:367:ARG:CG	1:B:367:ARG:NH1	2.39	0.66
1:B:509:TYR:CE2	1:B:510:GLU:C	2.74	0.66
1:A:365:ARG:HA	1:A:368:GLN:HG2	1.76	0.66
1:B:7:GLU:CB	1:B:8:PRO:CD	2.74	0.66
1:B:106:ASP:OD1	1:B:108:GLU:N	2.28	0.66
1:C:378:SER:C	1:C:380:ALA:N	2.53	0.65
1:A:4:GLN:NE2	1:A:5:LEU:H	1.94	0.65
1:A:545:LEU:CD2	1:A:546:GLU:N	2.50	0.65
1:A:122:LYS:HD2	1:A:127:TRP:CE2	2.31	0.65
1:A:507:ASP:CB	1:A:508:PRO:HD2	2.26	0.65
1:B:367:ARG:HH11	1:B:367:ARG:HG3	1.60	0.65
1:A:50:THR:HG23	1:A:151:PRO:HD2	1.77	0.65
1:A:288:SER:O	1:A:291:GLU:CB	2.45	0.65
1:C:289:VAL:HG23	1:C:290:ALA:H	1.62	0.65
1:B:286:ASP:O	1:B:289:VAL:HG22	1.97	0.64
1:B:19:PRO:O	1:B:22:ARG:N	2.29	0.64
1:C:138:LEU:HD12	1:C:138:LEU:N	2.12	0.64
1:A:242:SER:OG	1:A:243:GLY:N	2.30	0.64
1:C:89:ARG:HH11	1:C:89:ARG:CG	2.10	0.64
1:C:288:SER:OG	1:C:292:ARG:NH2	2.30	0.64
1:A:123:ASP:O	1:A:124:GLY:C	2.38	0.64
1:A:114:ILE:C	1:A:114:ILE:HD12	2.23	0.64
1:A:244:ARG:N	1:A:244:ARG:CD	2.29	0.64
1:C:97:ARG:O	1:C:100:GLU:HG3	1.99	0.63
1:A:376:GLY:N	1:A:509:TYR:OH	2.32	0.63
1:B:371:THR:CG2	1:B:439:THR:HG21	2.28	0.63
1:C:19:PRO:O	1:C:22:ARG:N	2.30	0.63
1:C:413:LEU:HG	1:C:430:ARG:CG	2.28	0.63
1:B:38:ASP:OD1	1:B:41:GLN:HG2	1.98	0.63
1:B:50:THR:HG23	1:B:151:PRO:HD2	1.81	0.63
1:B:368:GLN:HA	1:B:442:ARG:HD2	1.80	0.62
1:B:138:LEU:HD12	1:B:138:LEU:N	2.13	0.62
1:C:21:LYS:O	1:C:24:ALA:CB	2.30	0.62
1:A:374:PHE:CE2	1:A:473:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HG2	1:B:121:TRP:CE2	2.34	0.62
1:B:169:TRP:HZ3	1:B:262:ILE:HG21	1.63	0.62
1:B:199:GLN:HG3	1:B:234:LEU:CD1	2.29	0.62
1:C:20:GLU:O	1:C:22:ARG:N	2.32	0.62
1:A:199:GLN:HG3	1:A:234:LEU:HD13	1.81	0.62
1:A:414:SER:HA	1:A:417:LEU:CD1	2.29	0.62
1:C:21:LYS:O	1:C:25:LEU:CD2	2.48	0.62
1:B:521:THR:HG21	1:B:524:LEU:CD1	2.29	0.62
1:A:442:ARG:HG2	1:A:442:ARG:NH1	1.98	0.61
1:C:169:TRP:HZ3	1:C:262:ILE:HG21	1.65	0.61
1:C:371:THR:CG2	1:C:439:THR:HG21	2.30	0.61
1:B:414:SER:HA	1:B:417:LEU:CD1	2.28	0.61
1:B:453:TYR:O	1:B:454:ARG:C	2.43	0.61
1:B:475:VAL:HA	1:B:519:ILE:HG12	1.82	0.61
1:C:114:ILE:C	1:C:114:ILE:HD12	2.25	0.61
1:B:365:ARG:C	1:B:367:ARG:H	2.08	0.61
1:C:300:LEU:H	1:C:300:LEU:CD2	2.14	0.61
1:A:262:ILE:HG12	1:A:301:ILE:HD11	1.82	0.61
1:B:262:ILE:HG12	1:B:301:ILE:HD11	1.81	0.60
1:A:204:ILE:C	1:A:208:PRO:CG	2.74	0.60
1:B:128:HIS:O	1:B:129:LEU:HD23	2.01	0.60
1:B:188:ILE:HG22	1:C:539:HIS:CD2	2.35	0.60
1:B:464:ILE:HG12	1:B:470:PHE:HD1	1.65	0.60
1:B:61:THR:HG22	1:B:64:GLN:H	1.65	0.60
1:B:475:VAL:HA	1:B:519:ILE:CD1	2.31	0.60
1:A:169:TRP:HZ3	1:A:262:ILE:HG21	1.64	0.60
1:B:61:THR:CB	1:B:64:GLN:HG3	2.31	0.60
1:C:393:LEU:HD13	1:C:444:ILE:CD1	2.32	0.60
1:C:409:VAL:HG11	1:C:431:ILE:HD11	1.84	0.60
1:A:366:GLU:HG3	1:A:544:ARG:CB	2.32	0.59
1:B:421:LYS:H	1:B:421:LYS:CD	2.08	0.59
1:A:464:ILE:HG12	1:A:470:PHE:HD1	1.67	0.59
1:A:519:ILE:HG13	1:A:519:ILE:O	2.03	0.59
1:B:114:ILE:HD12	1:B:114:ILE:C	2.27	0.59
1:C:107:GLY:HA2	2:C:574:HOH:O	2.02	0.59
1:B:5:LEU:O	1:B:6:ILE:C	2.46	0.59
1:B:286:ASP:OD1	1:B:287:PRO:HD2	2.02	0.59
1:C:170:GLN:HA	1:C:197:HIS:O	2.02	0.59
1:C:105:ARG:HB3	1:C:110:TYR:O	2.02	0.59
1:C:61:THR:HG22	1:C:64:GLN:CG	2.22	0.59
1:C:50:THR:HG23	1:C:151:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:LEU:HD13	1:C:444:ILE:HD12	1.85	0.59
1:B:170:GLN:HA	1:B:197:HIS:O	2.02	0.59
1:A:114:ILE:HD12	1:A:114:ILE:O	2.03	0.59
1:B:377:LEU:HD12	1:B:377:LEU:N	2.16	0.59
1:C:94:ALA:HB2	1:C:127:TRP:CZ2	2.37	0.59
1:C:453:TYR:O	1:C:454:ARG:C	2.46	0.58
1:A:138:LEU:HD12	1:A:138:LEU:N	2.18	0.58
1:C:427:ASN:O	1:C:430:ARG:N	2.36	0.58
1:A:203:ASP:HB3	1:A:206:GLU:CB	2.33	0.58
1:B:371:THR:HG23	1:B:439:THR:HG21	1.84	0.58
1:C:365:ARG:HA	1:C:368:GLN:HG2	1.85	0.58
1:C:79:PHE:CE2	1:C:81:PRO:HD3	2.39	0.58
1:A:300:LEU:H	1:A:300:LEU:CD2	2.16	0.58
1:C:94:ALA:HB2	1:C:127:TRP:CH2	2.39	0.58
1:A:38:ASP:OD1	1:A:41:GLN:HG2	2.04	0.58
1:B:300:LEU:CD2	1:B:300:LEU:H	2.17	0.58
1:A:188:ILE:HA	1:B:539:HIS:CD2	2.38	0.58
1:B:424:ARG:CD	1:B:450:ILE:HD11	2.28	0.58
1:A:539:HIS:ND1	1:C:188:ILE:HA	2.18	0.58
1:C:89:ARG:HD3	1:C:89:ARG:N	2.19	0.58
1:B:475:VAL:HA	1:B:519:ILE:HD11	1.84	0.57
1:A:300:LEU:H	1:A:300:LEU:HD23	1.69	0.57
1:C:199:GLN:HG3	1:C:234:LEU:CD1	2.34	0.57
1:A:61:THR:HG22	1:A:64:GLN:H	1.69	0.57
1:B:441:ASN:O	1:B:442:ARG:HB2	2.05	0.57
1:C:476:ALA:O	1:C:477:THR:C	2.47	0.57
1:A:375:THR:HG21	1:A:472:GLU:OE2	2.03	0.57
1:C:61:THR:HG22	1:C:64:GLN:H	1.68	0.57
1:A:35:LEU:HD13	1:A:93:LEU:HD21	1.87	0.57
1:B:68:VAL:C	1:B:70:SER:N	2.59	0.57
1:B:521:THR:OG1	1:B:524:LEU:HG	2.04	0.57
1:A:91:ARG:C	1:A:93:LEU:H	2.13	0.57
1:A:461:ARG:HB2	1:A:470:PHE:CE2	2.39	0.57
1:A:403:LEU:HD22	1:A:405:ASP:HB2	1.87	0.56
1:C:544:ARG:CG	1:C:545:LEU:N	2.66	0.56
1:A:204:ILE:O	1:A:208:PRO:HG2	2.05	0.56
1:B:5:LEU:C	1:B:6:ILE:O	2.47	0.56
1:B:429:ARG:NH2	1:B:459:ASP:OD1	2.38	0.56
1:B:475:VAL:HA	1:B:519:ILE:CG1	2.36	0.56
1:A:4:GLN:HE21	1:A:5:LEU:N	1.99	0.56
1:B:97:ARG:HG2	1:B:97:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:PRO:C	1:B:453:TYR:HD1	2.14	0.56
1:C:264:GLY:HA3	1:C:303:TYR:HB3	1.88	0.56
1:C:20:GLU:C	1:C:22:ARG:N	2.51	0.56
1:A:414:SER:HA	1:A:417:LEU:HD11	1.87	0.56
1:B:44:GLU:OE1	1:B:44:GLU:HA	2.04	0.56
1:B:300:LEU:H	1:B:300:LEU:HD23	1.70	0.56
1:B:507:ASP:CB	1:B:508:PRO:HD2	2.29	0.56
1:C:464:ILE:HG12	1:C:470:PHE:HD1	1.69	0.56
1:A:62:ARG:HG3	1:A:121:TRP:NE1	2.21	0.55
1:B:61:THR:CG2	1:B:64:GLN:CG	2.59	0.55
1:C:14:VAL:CG1	1:C:16:LEU:HD13	2.36	0.55
1:C:21:LYS:O	1:C:25:LEU:CG	2.53	0.55
1:A:410:ARG:O	1:A:415:SER:N	2.38	0.55
1:B:89:ARG:N	1:B:89:ARG:CD	2.68	0.55
1:A:188:ILE:HA	1:B:539:HIS:CG	2.42	0.55
1:A:475:VAL:HA	1:A:519:ILE:HG12	1.88	0.55
1:C:377:LEU:C	1:C:379:GLY:H	2.15	0.55
1:A:6:ILE:HD13	1:A:254:ARG:HG3	1.88	0.55
1:C:371:THR:HG23	1:C:439:THR:HG21	1.88	0.55
1:C:521:THR:OG1	1:C:524:LEU:HG	2.07	0.55
1:B:250:ALA:HB1	1:B:298:VAL:HG11	1.88	0.55
1:B:62:ARG:HG2	1:B:121:TRP:CZ2	2.41	0.54
1:A:440:LYS:HB2	1:A:467:VAL:HG21	1.88	0.54
1:B:121:TRP:CH2	1:B:128:HIS:HB3	2.43	0.54
1:A:87:THR:O	1:A:88:SER:HB2	2.07	0.54
1:A:161:ARG:NH2	1:A:229:THR:O	2.41	0.54
1:B:375:THR:HG21	1:B:472:GLU:OE2	2.07	0.54
1:B:86:LEU:HD12	1:B:129:LEU:HD12	1.89	0.54
1:C:6:ILE:HD13	1:C:254:ARG:HG3	1.89	0.54
1:C:86:LEU:HD12	1:C:129:LEU:HD12	1.89	0.54
1:C:519:ILE:O	1:C:519:ILE:HG13	2.08	0.54
1:A:311:ASP:C	1:B:338:ARG:HH21	2.15	0.54
1:A:170:GLN:HA	1:A:197:HIS:O	2.07	0.54
1:A:204:ILE:O	1:A:208:PRO:CG	2.56	0.54
1:B:264:GLY:HA3	1:B:303:TYR:HB3	1.91	0.54
1:A:86:LEU:HD12	1:A:129:LEU:HD12	1.90	0.53
1:B:293:ALA:C	1:B:295:LYS:N	2.58	0.53
1:B:509:TYR:CD2	1:B:510:GLU:C	2.86	0.53
1:B:403:LEU:HD22	1:B:405:ASP:HB2	1.91	0.53
1:C:19:PRO:O	1:C:20:GLU:C	2.50	0.53
1:A:377:LEU:HD12	1:A:377:LEU:N	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD13	1:B:93:LEU:HD21	1.90	0.53
1:B:262:ILE:HG12	1:B:301:ILE:CD1	2.38	0.53
1:C:262:ILE:HG12	1:C:301:ILE:CD1	2.38	0.53
1:B:220:ILE:O	1:B:220:ILE:HG13	2.08	0.53
1:B:393:LEU:CD1	1:B:444:ILE:CD1	2.85	0.53
1:C:428:VAL:CG1	1:C:456:THR:HG21	2.35	0.53
1:A:97:ARG:O	1:A:98:PRO:C	2.50	0.53
1:A:188:ILE:HA	1:B:539:HIS:NE2	2.23	0.53
1:A:452:PRO:C	1:A:453:TYR:HD1	2.17	0.53
1:B:439:THR:HG21	1:B:464:ILE:HD13	1.91	0.53
1:C:476:ALA:C	1:C:477:THR:O	2.48	0.53
1:B:101:ARG:CZ	1:B:114:ILE:HD11	2.39	0.52
1:C:25:LEU:O	1:C:26:LYS:C	2.52	0.52
1:C:29:ALA:C	1:C:31:SER:H	2.17	0.52
1:A:56:LEU:HD11	1:A:60:MET:HE3	1.90	0.52
1:B:67:ARG:O	1:B:67:ARG:HG2	2.09	0.52
1:C:375:THR:HG21	1:C:472:GLU:OE2	2.09	0.52
1:C:439:THR:HG21	1:C:464:ILE:HD13	1.90	0.52
1:B:365:ARG:C	1:B:367:ARG:N	2.68	0.52
1:C:452:PRO:C	1:C:453:TYR:HD1	2.18	0.52
1:A:44:GLU:HA	1:A:44:GLU:OE1	2.09	0.52
1:A:453:TYR:O	1:A:454:ARG:C	2.47	0.52
1:B:440:LYS:HB2	1:B:467:VAL:HG21	1.91	0.52
1:B:68:VAL:O	1:B:70:SER:N	2.43	0.52
1:B:188:ILE:HA	1:C:539:HIS:CE1	2.44	0.52
1:B:374:PHE:CE2	1:B:473:ILE:CD1	2.92	0.52
1:A:104:LEU:HD11	1:A:115:LEU:HB2	1.90	0.52
1:A:262:ILE:HG12	1:A:301:ILE:CD1	2.40	0.52
1:C:453:TYR:HD1	1:C:453:TYR:N	2.08	0.52
1:A:408:ILE:O	1:A:412:HIS:HD2	1.93	0.51
1:B:62:ARG:CG	1:B:121:TRP:CE2	2.93	0.51
1:C:25:LEU:N	1:C:25:LEU:HD23	2.25	0.51
1:C:475:VAL:HG22	1:C:519:ILE:HD11	1.92	0.51
1:A:205:THR:C	1:A:208:PRO:HD3	2.36	0.51
1:B:121:TRP:CE2	1:B:128:HIS:HB2	2.46	0.51
1:C:6:ILE:CD1	1:C:254:ARG:HG3	2.39	0.51
1:A:289:VAL:CG2	1:A:290:ALA:H	2.23	0.51
1:B:220:ILE:CG2	1:B:354:VAL:CG2	2.84	0.51
1:C:374:PHE:CE2	1:C:473:ILE:CD1	2.93	0.51
1:A:414:SER:C	1:A:417:LEU:HD12	2.36	0.51
1:A:199:GLN:HG3	1:A:234:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:CE2	1:B:81:PRO:HD3	2.46	0.51
1:A:9:TYR:C	1:A:11:GLY:H	2.19	0.51
1:A:441:ASN:O	1:A:442:ARG:HB2	2.11	0.51
1:C:128:HIS:O	1:C:129:LEU:HD23	2.10	0.51
1:A:512:PRO:HB2	1:A:515:PRO:HG3	1.92	0.51
1:C:44:GLU:OE1	1:C:44:GLU:HA	2.11	0.51
1:C:220:ILE:O	1:C:220:ILE:HG13	2.12	0.51
1:C:523:GLY:O	1:C:524:LEU:HD23	2.10	0.51
1:B:7:GLU:HB2	1:B:8:PRO:CD	2.39	0.50
1:C:90:ASP:OD1	1:C:91:ARG:N	2.44	0.50
1:C:453:TYR:N	1:C:453:TYR:CD1	2.78	0.50
1:B:365:ARG:O	1:B:367:ARG:N	2.45	0.50
1:C:175:MET:HG3	1:C:179:GLN:CG	2.41	0.50
1:A:220:ILE:O	1:A:220:ILE:HG13	2.11	0.50
1:B:442:ARG:HG2	1:B:442:ARG:NH1	2.01	0.50
1:C:300:LEU:H	1:C:300:LEU:HD23	1.75	0.50
1:C:380:ALA:C	1:C:382:LYS:N	2.67	0.50
1:A:242:SER:OG	1:A:244:ARG:HD3	2.12	0.50
1:A:439:THR:HG21	1:A:464:ILE:HD13	1.93	0.50
1:C:357:GLU:OE1	1:C:360:ARG:NH1	2.43	0.50
1:A:62:ARG:HG3	1:A:121:TRP:CD2	2.47	0.50
1:A:289:VAL:C	1:A:291:GLU:N	2.65	0.49
1:A:251:ILE:HG12	1:A:296:ILE:HD12	1.94	0.49
1:B:390:ALA:O	1:B:394:MET:HG3	2.13	0.49
1:C:455:GLN:HA	1:C:455:GLN:NE2	2.25	0.49
1:C:260:LEU:HA	1:C:299:ARG:O	2.12	0.49
1:C:440:LYS:HB2	1:C:467:VAL:HG21	1.94	0.49
1:B:61:THR:HG23	1:B:63:ALA:H	1.77	0.49
1:B:414:SER:HB3	1:B:417:LEU:HD11	1.90	0.49
1:C:461:ARG:HB2	1:C:470:PHE:CE2	2.47	0.49
1:A:453:TYR:HD1	1:A:453:TYR:N	2.10	0.49
1:B:5:LEU:O	1:B:6:ILE:O	2.30	0.49
1:A:458:ARG:HH11	1:A:461:ARG:CD	2.23	0.49
1:B:440:LYS:HB2	1:B:467:VAL:CG2	2.42	0.49
1:C:250:ALA:HB1	1:C:298:VAL:HG11	1.94	0.49
1:A:539:HIS:NE2	1:C:188:ILE:HA	2.21	0.49
1:B:453:TYR:C	1:B:455:GLN:N	2.71	0.49
1:C:377:LEU:C	1:C:379:GLY:N	2.70	0.49
1:C:475:VAL:HG22	1:C:519:ILE:CD1	2.42	0.49
1:A:157:LEU:HD23	1:A:160:ARG:NH2	2.21	0.49
1:B:364:PRO:O	1:B:365:ARG:C	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:GLN:O	1:B:458:ARG:CB	2.61	0.49
1:A:371:THR:HA	1:A:445:ALA:O	2.13	0.49
1:B:393:LEU:CD1	1:B:444:ILE:HD11	2.43	0.49
1:C:157:LEU:HD23	1:C:160:ARG:NH2	2.19	0.49
1:A:39:TRP:CD1	1:A:206:GLU:CB	2.96	0.49
1:A:414:SER:O	1:A:417:LEU:HD12	2.13	0.49
1:A:440:LYS:HB2	1:A:467:VAL:CG2	2.43	0.49
1:C:312:ARG:O	1:C:314:GLU:HG2	2.13	0.49
1:A:97:ARG:O	1:A:98:PRO:O	2.30	0.48
1:B:377:LEU:C	1:B:379:GLY:H	2.19	0.48
1:C:38:ASP:O	1:C:42:GLN:HG3	2.13	0.48
1:A:453:TYR:N	1:A:453:TYR:CD1	2.80	0.48
1:B:220:ILE:HG22	1:B:354:VAL:CG2	2.29	0.48
1:B:509:TYR:CD2	1:B:510:GLU:O	2.62	0.48
1:C:114:ILE:HD12	1:C:114:ILE:O	2.12	0.48
1:C:427:ASN:O	1:C:428:VAL:C	2.56	0.48
1:B:4:GLN:HE21	1:B:5:LEU:N	2.07	0.48
1:C:20:GLU:O	1:C:21:LYS:C	2.54	0.48
1:B:121:TRP:CZ2	1:B:128:HIS:CB	2.96	0.48
1:C:475:VAL:CG1	1:C:519:ILE:HD11	2.37	0.48
1:A:514:THR:HG23	1:A:514:THR:O	2.14	0.48
1:B:9:TYR:C	1:B:11:GLY:H	2.21	0.48
1:B:47:MET:HA	1:B:47:MET:CE	2.42	0.48
1:B:61:THR:O	1:B:64:GLN:N	2.47	0.48
1:B:114:ILE:HD12	1:B:114:ILE:O	2.14	0.48
1:B:289:VAL:HG23	1:B:290:ALA:N	2.28	0.48
1:C:293:ALA:C	1:C:295:LYS:N	2.69	0.48
1:A:164:ARG:HH21	1:B:532:GLN:HB2	1.78	0.48
1:A:169:TRP:CE3	1:A:262:ILE:HG21	2.48	0.48
1:A:205:THR:HG23	1:A:206:GLU:N	2.28	0.48
1:A:427:ASN:O	1:A:430:ARG:HB3	2.14	0.48
1:A:309:VAL:HG21	1:A:316:LEU:HD12	1.96	0.47
1:B:97:ARG:HG2	1:B:97:ARG:NH1	2.28	0.47
1:C:21:LYS:C	1:C:24:ALA:CB	2.83	0.47
1:C:247:LEU:HD11	1:C:292:ARG:HD2	1.94	0.47
1:A:442:ARG:HA	1:A:442:ARG:HD3	1.62	0.47
1:C:514:THR:N	1:C:515:PRO:HD3	2.29	0.47
1:A:300:LEU:CD2	1:A:300:LEU:N	2.76	0.47
1:C:536:LYS:O	1:C:537:LEU:C	2.55	0.47
1:A:409:VAL:HG11	1:A:431:ILE:HD11	1.96	0.47
1:B:377:LEU:H	1:B:377:LEU:CD1	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:GLY:C	1:C:381:GLY:H	2.20	0.47
1:A:128:HIS:O	1:A:129:LEU:HD23	2.14	0.47
1:C:251:ILE:HG12	1:C:296:ILE:HD12	1.96	0.47
1:C:426:VAL:O	1:C:427:ASN:C	2.56	0.47
1:A:247:LEU:O	1:A:251:ILE:HG13	2.14	0.47
1:A:250:ALA:HB1	1:A:298:VAL:HG11	1.96	0.47
1:B:414:SER:CB	1:B:417:LEU:HD11	2.33	0.47
1:B:461:ARG:HB2	1:B:470:PHE:CE2	2.50	0.47
1:B:157:LEU:HD23	1:B:160:ARG:NH2	2.24	0.47
1:B:300:LEU:CD2	1:B:300:LEU:N	2.77	0.47
1:B:414:SER:C	1:B:417:LEU:HD12	2.39	0.47
1:A:35:LEU:HD21	1:A:88:SER:HB3	1.95	0.47
1:A:314:GLU:CD	1:B:337:ARG:HH22	2.22	0.47
1:B:23:GLU:O	1:B:24:ALA:C	2.58	0.47
1:B:370:PHE:HA	1:B:469:GLY:O	2.15	0.47
1:C:403:LEU:HD22	1:C:405:ASP:HB2	1.97	0.47
1:A:91:ARG:C	1:A:93:LEU:N	2.73	0.46
1:A:539:HIS:CD2	1:C:188:ILE:CG2	2.81	0.46
1:B:14:VAL:CG1	1:B:16:LEU:HD13	2.45	0.46
1:C:530:VAL:O	1:C:533:ILE:HG12	2.15	0.46
1:B:185:LYS:HG3	1:B:186:SER:N	2.30	0.46
1:C:415:SER:OG	1:C:416:GLU:N	2.49	0.46
1:A:14:VAL:CG1	1:A:16:LEU:HD13	2.45	0.46
1:B:56:LEU:HD11	1:B:60:MET:HE3	1.96	0.46
1:B:414:SER:O	1:B:417:LEU:HD12	2.15	0.46
1:C:23:GLU:OE2	1:C:23:GLU:HA	2.15	0.46
1:C:427:ASN:O	1:C:430:ARG:HB3	2.14	0.46
1:B:138:LEU:H	1:B:138:LEU:CD1	2.27	0.46
1:A:371:THR:CG2	1:A:439:THR:CG2	2.92	0.46
1:B:19:PRO:C	1:B:22:ARG:H	2.23	0.46
1:B:514:THR:HG23	1:B:514:THR:O	2.16	0.46
1:C:451:ALA:HA	1:C:452:PRO:HD3	1.72	0.46
1:A:74:LEU:HD13	1:A:80:TRP:CB	2.46	0.46
1:B:451:ALA:HA	1:B:452:PRO:HD3	1.69	0.46
1:C:97:ARG:O	1:C:98:PRO:C	2.58	0.46
1:A:79:PHE:CE2	1:A:81:PRO:HD3	2.50	0.46
1:A:455:GLN:HA	1:A:455:GLN:NE2	2.31	0.46
1:B:61:THR:HG22	1:B:64:GLN:HG2	1.84	0.46
1:B:161:ARG:NH2	1:B:229:THR:O	2.47	0.46
1:A:357:GLU:OE1	1:A:360:ARG:NH1	2.47	0.46
1:A:379:GLY:HA3	1:A:382:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:VAL:O	1:B:410:ARG:C	2.54	0.46
1:C:16:LEU:HD11	1:C:57:THR:OG1	2.16	0.46
1:C:220:ILE:CG2	1:C:354:VAL:CG2	2.92	0.46
1:A:216:SER:O	1:A:220:ILE:HG23	2.16	0.45
1:A:242:SER:OG	1:A:244:ARG:CD	2.64	0.45
1:B:475:VAL:CA	1:B:519:ILE:HD11	2.46	0.45
1:C:509:TYR:CG	1:C:510:GLU:N	2.84	0.45
1:A:292:ARG:HD2	1:A:292:ARG:HA	1.66	0.45
1:B:116:THR:O	1:B:131:GLY:HA3	2.16	0.45
1:C:441:ASN:O	1:C:442:ARG:HB2	2.16	0.45
1:A:530:VAL:O	1:A:533:ILE:HG12	2.15	0.45
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.41	0.45
1:B:247:LEU:O	1:B:251:ILE:HG13	2.15	0.45
1:B:514:THR:N	1:B:515:PRO:HD3	2.31	0.45
1:A:6:ILE:HG23	1:A:6:ILE:O	2.16	0.45
1:A:292:ARG:O	1:A:295:LYS:CB	2.65	0.45
1:A:374:PHE:CE2	1:A:473:ILE:CD1	3.00	0.45
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.79	0.45
1:A:33:PRO:O	1:A:102:LEU:HD23	2.16	0.45
1:A:76:ASP:OD1	1:A:76:ASP:N	2.48	0.45
1:C:29:ALA:O	1:C:30:LEU:C	2.59	0.45
1:C:97:ARG:O	1:C:98:PRO:O	2.35	0.45
1:A:370:PHE:HA	1:A:469:GLY:O	2.16	0.45
1:B:96:ARG:NH1	1:B:96:ARG:CG	2.73	0.45
1:B:260:LEU:HA	1:B:299:ARG:O	2.17	0.45
1:B:371:THR:CG2	1:B:439:THR:CG2	2.95	0.45
1:A:288:SER:C	1:A:291:GLU:CB	2.89	0.45
1:A:450:ILE:HD12	1:A:450:ILE:O	2.16	0.45
1:C:454:ARG:NH1	1:C:511:VAL:O	2.49	0.45
1:A:50:THR:HG23	1:A:151:PRO:CD	2.45	0.45
1:A:168:ALA:HB2	1:A:258:CYS:SG	2.57	0.45
1:C:175:MET:HG3	1:C:179:GLN:HG3	1.99	0.45
1:C:374:PHE:CD2	1:C:473:ILE:HD11	2.52	0.45
1:C:411:ARG:HA	1:C:411:ARG:HD3	1.53	0.45
1:C:440:LYS:HB2	1:C:467:VAL:CG2	2.46	0.45
1:A:188:ILE:HA	1:B:539:HIS:ND1	2.30	0.45
1:A:332:GLY:O	1:A:333:GLU:C	2.55	0.45
1:A:474:HIS:CE1	1:A:476:ALA:HB2	2.52	0.45
1:A:6:ILE:CD1	1:A:254:ARG:HG3	2.47	0.45
1:A:90:ASP:HB3	1:A:93:LEU:HG	1.98	0.45
1:A:101:ARG:CZ	1:A:114:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASP:OD1	1:B:76:ASP:N	2.49	0.45
1:B:96:ARG:HH11	1:B:96:ARG:CG	2.14	0.45
1:B:365:ARG:HA	1:B:368:GLN:HG2	1.97	0.45
1:C:478:PRO:O	1:C:479:ILE:C	2.60	0.45
1:B:40:GLN:O	1:B:43:CYS:HB2	2.17	0.44
1:B:286:ASP:OD1	1:B:287:PRO:CD	2.64	0.44
1:B:474:HIS:CE1	1:B:476:ALA:HB2	2.52	0.44
1:A:254:ARG:NH1	1:A:296:ILE:O	2.49	0.44
1:A:514:THR:N	1:A:515:PRO:HD3	2.31	0.44
1:A:519:ILE:O	1:A:519:ILE:CG1	2.64	0.44
1:C:5:LEU:HD23	1:C:5:LEU:HA	1.64	0.44
1:C:34:SER:HB2	1:C:105:ARG:HD2	1.99	0.44
1:A:314:GLU:OE2	1:B:337:ARG:NH2	2.49	0.44
1:B:450:ILE:HD12	1:B:450:ILE:O	2.17	0.44
1:C:200:VAL:HG21	1:C:233:LEU:HD22	2.00	0.44
1:A:122:LYS:NZ	1:A:127:TRP:CZ3	2.78	0.44
1:A:260:LEU:HA	1:A:299:ARG:O	2.17	0.44
1:B:442:ARG:HA	1:B:442:ARG:HD3	1.65	0.44
1:C:300:LEU:CD2	1:C:300:LEU:N	2.76	0.44
1:C:370:PHE:HA	1:C:469:GLY:O	2.17	0.44
1:B:435:ALA:O	1:B:439:THR:CG2	2.65	0.44
1:B:435:ALA:O	1:B:439:THR:HG22	2.17	0.44
1:C:82:SER:HA	1:C:83:PRO:HD3	1.86	0.44
1:A:220:ILE:CG2	1:A:354:VAL:CG2	2.92	0.44
1:A:451:ALA:HA	1:A:452:PRO:HD3	1.69	0.44
1:A:520:ASP:O	1:A:521:THR:C	2.61	0.44
1:B:27:HIS:O	1:B:30:LEU:HB2	2.17	0.44
1:B:332:GLY:O	1:B:333:GLU:C	2.59	0.44
1:B:509:TYR:OH	1:B:512:PRO:HD3	2.18	0.44
1:C:29:ALA:C	1:C:31:SER:N	2.74	0.44
1:A:371:THR:HG21	1:A:435:ALA:HB1	1.99	0.44
1:C:203:ASP:H	1:C:207:ALA:HB3	1.82	0.44
1:A:414:SER:C	1:A:416:GLU:N	2.73	0.44
1:C:76:ASP:N	1:C:76:ASP:OD1	2.50	0.44
1:C:379:GLY:O	1:C:381:GLY:N	2.47	0.44
1:C:544:ARG:HG2	1:C:545:LEU:H	1.78	0.44
1:A:414:SER:CB	1:A:417:LEU:HD11	2.39	0.44
1:B:19:PRO:HA	1:B:22:ARG:HB2	1.99	0.44
1:C:464:ILE:HD12	1:C:464:ILE:O	2.18	0.44
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.80	0.43
1:C:420:SER:O	1:C:421:LYS:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:HD3	1:A:424:ARG:HA	1.67	0.43
1:B:509:TYR:CZ	1:B:510:GLU:O	2.66	0.43
1:B:38:ASP:O	1:B:42:GLN:HG3	2.18	0.43
1:B:377:LEU:C	1:B:379:GLY:N	2.76	0.43
1:C:22:ARG:C	1:C:24:ALA:N	2.71	0.43
1:C:101:ARG:CZ	1:C:114:ILE:HD11	2.49	0.43
1:C:390:ALA:O	1:C:394:MET:HG3	2.18	0.43
1:A:9:TYR:HD1	1:A:254:ARG:NH1	2.16	0.43
1:B:4:GLN:NE2	1:B:5:LEU:CA	2.81	0.43
1:C:220:ILE:HG22	1:C:354:VAL:CG2	2.33	0.43
1:C:371:THR:HA	1:C:445:ALA:O	2.19	0.43
1:C:385:LEU:HD23	1:C:385:LEU:HA	1.76	0.43
1:C:417:LEU:HD21	1:C:426:VAL:HG11	1.98	0.43
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.72	0.43
1:B:4:GLN:HA	1:B:164:ARG:HD2	2.00	0.43
1:B:216:SER:O	1:B:220:ILE:HG23	2.17	0.43
1:C:56:LEU:HD11	1:C:60:MET:HE3	1.99	0.43
1:C:80:TRP:NE1	1:C:82:SER:O	2.48	0.43
1:C:409:VAL:O	1:C:410:ARG:C	2.59	0.43
1:A:97:ARG:C	1:A:98:PRO:O	2.60	0.43
1:A:364:PRO:O	1:A:365:ARG:C	2.61	0.43
1:A:435:ALA:O	1:A:439:THR:CG2	2.67	0.43
1:B:185:LYS:HA	1:B:188:ILE:CD1	2.48	0.43
1:B:203:ASP:H	1:B:207:ALA:HB3	1.82	0.43
1:B:246:LEU:O	1:B:246:LEU:HD22	2.19	0.43
1:C:96:ARG:HG3	1:C:100:GLU:OE2	2.18	0.43
1:C:169:TRP:CE3	1:C:262:ILE:HG21	2.54	0.43
1:A:200:VAL:HG21	1:A:233:LEU:HD22	2.00	0.43
1:C:47:MET:HA	1:C:47:MET:CE	2.46	0.43
1:A:414:SER:CA	1:A:417:LEU:HD11	2.44	0.43
1:C:40:GLN:O	1:C:43:CYS:HB2	2.19	0.43
1:A:311:ASP:C	1:B:338:ARG:NH2	2.76	0.43
1:B:9:TYR:HD1	1:B:254:ARG:NH1	2.16	0.43
1:B:96:ARG:C	1:B:97:ARG:HG3	2.42	0.43
1:B:228:THR:O	1:B:228:THR:CG2	2.64	0.43
1:C:413:LEU:HG	1:C:430:ARG:HG3	2.01	0.43
1:C:477:THR:CB	1:C:521:THR:O	2.67	0.43
1:A:165:ARG:C	1:A:166:ILE:HG13	2.44	0.42
1:A:175:MET:HG3	1:A:179:GLN:CG	2.49	0.42
1:A:207:ALA:N	1:A:208:PRO:CD	2.81	0.42
1:A:223:ARG:HD2	1:A:351:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:MET:HG3	1:B:179:GLN:CG	2.49	0.42
1:B:234:LEU:HA	1:B:235:PRO:HD3	1.91	0.42
1:B:250:ALA:HB1	1:B:298:VAL:CG1	2.49	0.42
1:B:285:VAL:O	1:B:286:ASP:C	2.62	0.42
1:C:89:ARG:CG	1:C:89:ARG:NH1	2.72	0.42
1:C:512:PRO:HB2	1:C:515:PRO:HG3	2.01	0.42
1:A:289:VAL:HG22	1:A:290:ALA:H	1.84	0.42
1:B:90:ASP:OD1	1:B:91:ARG:N	2.52	0.42
1:B:147:LEU:HB3	1:B:233:LEU:HG	2.00	0.42
1:B:409:VAL:CG1	1:B:431:ILE:HD11	2.48	0.42
1:C:223:ARG:HD2	1:C:351:PHE:CE2	2.54	0.42
1:C:295:LYS:C	1:C:297:GLY:H	2.26	0.42
1:A:169:TRP:CZ3	1:A:262:ILE:CG2	2.99	0.42
1:A:368:GLN:HA	1:A:442:ARG:HD2	2.01	0.42
1:A:413:LEU:O	1:A:430:ARG:NH2	2.48	0.42
1:A:414:SER:O	1:A:415:SER:C	2.63	0.42
1:B:53:TYR:O	1:B:54:SER:C	2.61	0.42
1:B:228:THR:O	1:B:228:THR:HG23	2.19	0.42
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.62	0.42
1:A:82:SER:HA	1:A:83:PRO:HD3	1.93	0.42
1:A:414:SER:O	1:A:416:GLU:N	2.52	0.42
1:C:147:LEU:HD11	1:C:218:LEU:HD21	2.00	0.42
1:A:191:GLU:HA	1:B:539:HIS:CE1	2.53	0.42
1:C:104:LEU:C	1:C:105:ARG:HG2	2.44	0.42
1:A:346:PRO:HB3	1:A:348:TRP:CE2	2.54	0.42
1:A:387:ARG:HG3	1:A:403:LEU:HD11	2.01	0.42
1:A:3:ASN:O	1:A:164:ARG:HD2	2.19	0.42
1:A:425:ASP:O	1:A:425:ASP:OD2	2.36	0.42
1:A:517:LEU:HG	1:A:536:LYS:HG2	2.01	0.42
1:A:29:ALA:O	1:A:30:LEU:C	2.63	0.42
1:A:376:GLY:C	1:A:509:TYR:OH	2.63	0.42
1:C:29:ALA:O	1:C:31:SER:N	2.52	0.42
1:A:167:ILE:HA	1:A:260:LEU:HB2	2.02	0.42
1:B:321:ALA:HA	1:B:322:PRO:HD3	1.95	0.42
1:C:21:LYS:O	1:C:25:LEU:HD21	2.20	0.42
1:A:47:MET:HA	1:A:47:MET:CE	2.47	0.42
1:A:205:THR:HA	1:A:208:PRO:HG2	2.02	0.42
1:A:444:ILE:HD13	1:A:444:ILE:HG21	1.76	0.42
1:B:96:ARG:HG3	1:B:100:GLU:OE2	2.19	0.42
1:B:426:VAL:CG1	1:B:427:ASN:N	2.80	0.42
1:B:453:TYR:O	1:B:455:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:VAL:HG21	1:C:316:LEU:HD12	2.01	0.42
1:C:450:ILE:HD12	1:C:450:ILE:O	2.20	0.42
1:C:138:LEU:N	1:C:138:LEU:CD1	2.83	0.41
1:C:364:PRO:O	1:C:365:ARG:C	2.63	0.41
1:A:74:LEU:HD13	1:A:80:TRP:HB3	2.01	0.41
1:A:536:LYS:HD2	1:A:536:LYS:HA	1.71	0.41
1:B:200:VAL:O	1:B:200:VAL:HG13	2.19	0.41
1:C:94:ALA:CB	1:C:127:TRP:CZ2	3.01	0.41
1:C:435:ALA:O	1:C:439:THR:CG2	2.68	0.41
1:B:332:GLY:O	1:B:336:GLN:HB2	2.21	0.41
1:C:19:PRO:O	1:C:22:ARG:CA	2.69	0.41
1:C:371:THR:HG21	1:C:435:ALA:HB1	2.01	0.41
1:A:184:LEU:HA	1:A:184:LEU:HD23	1.55	0.41
1:B:94:ALA:HB2	1:B:127:TRP:CZ2	2.55	0.41
1:B:139:PRO:HA	1:B:140:PRO:HD3	1.95	0.41
1:C:79:PHE:CD2	1:C:79:PHE:C	2.99	0.41
1:C:168:ALA:HB2	1:C:258:CYS:SG	2.60	0.41
1:C:424:ARG:HA	1:C:424:ARG:HD2	1.25	0.41
1:A:393:LEU:CD1	1:A:444:ILE:HD11	2.50	0.41
1:B:64:GLN:C	1:B:66:ALA:N	2.76	0.41
1:B:307:VAL:O	1:B:315:HIS:HA	2.21	0.41
1:C:176:HIS:H	1:C:179:GLN:HE21	1.68	0.41
1:C:521:THR:H	1:C:521:THR:HG23	1.59	0.41
1:A:371:THR:HG22	1:A:439:THR:CG2	2.50	0.41
1:B:521:THR:HG21	1:B:524:LEU:HD11	2.02	0.41
1:C:107:GLY:CA	2:C:574:HOH:O	2.63	0.41
1:A:35:LEU:HD21	1:A:88:SER:HB2	2.00	0.41
1:B:371:THR:HA	1:B:445:ALA:O	2.19	0.41
1:C:200:VAL:O	1:C:200:VAL:HG13	2.19	0.41
1:C:407:ASP:O	1:C:411:ARG:HG2	2.21	0.41
1:A:5:LEU:HD23	1:A:164:ARG:O	2.21	0.41
1:A:408:ILE:HG22	1:A:409:VAL:N	2.36	0.41
1:B:410:ARG:O	1:B:415:SER:HB3	2.20	0.41
1:B:421:LYS:HD3	1:B:421:LYS:N	2.27	0.41
1:C:9:TYR:HD1	1:C:254:ARG:NH1	2.18	0.41
1:C:247:LEU:O	1:C:251:ILE:HG13	2.20	0.41
1:C:362:THR:HA	1:C:363:PRO:HD3	1.82	0.41
1:A:97:ARG:CB	1:A:98:PRO:CD	2.99	0.41
1:A:150:THR:O	1:A:151:PRO:C	2.61	0.41
1:B:138:LEU:O	1:B:139:PRO:C	2.61	0.41
1:B:286:ASP:OD2	1:B:288:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:CB	1:C:64:GLN:HG3	2.50	0.41
1:C:138:LEU:O	1:C:139:PRO:C	2.64	0.41
1:C:295:LYS:C	1:C:297:GLY:N	2.79	0.41
1:C:384:THR:CG2	2:C:555:HOH:O	2.52	0.41
1:C:408:ILE:HG22	1:C:409:VAL:N	2.35	0.41
1:C:450:ILE:HD12	1:C:450:ILE:H	1.86	0.41
1:A:292:ARG:HH21	1:A:292:ARG:CA	2.33	0.41
1:C:371:THR:CG2	1:C:439:THR:CG2	2.96	0.41
1:A:61:THR:HG23	1:A:63:ALA:H	1.85	0.40
1:A:286:ASP:CB	1:A:287:PRO:CB	2.95	0.40
1:A:301:ILE:O	1:A:301:ILE:HG12	2.20	0.40
1:A:321:ALA:HA	1:A:322:PRO:HD3	1.94	0.40
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.76	0.40
1:B:9:TYR:CE2	1:B:251:ILE:HD13	2.56	0.40
1:B:169:TRP:CZ3	1:B:262:ILE:CG2	3.01	0.40
1:B:169:TRP:CE3	1:B:262:ILE:HG21	2.56	0.40
1:C:105:ARG:CB	1:C:110:TYR:O	2.69	0.40
1:C:161:ARG:NH2	1:C:229:THR:O	2.54	0.40
1:A:40:GLN:O	1:A:43:CYS:HB2	2.21	0.40
1:C:9:TYR:C	1:C:11:GLY:H	2.29	0.40
1:C:32:LEU:HD23	1:C:32:LEU:HA	1.84	0.40
1:A:374:PHE:CE2	1:A:385:LEU:HB3	2.56	0.40
1:B:4:GLN:CG	1:B:5:LEU:H	2.31	0.40
1:C:371:THR:HG22	1:C:439:THR:CG2	2.51	0.40
1:A:303:TYR:HA	1:A:304:PRO:HD3	1.80	0.40
1:A:376:GLY:C	1:A:509:TYR:CZ	2.99	0.40
1:B:248:LEU:O	1:B:252:VAL:HG13	2.21	0.40
1:B:423:HIS:O	1:B:426:VAL:HG12	2.21	0.40
1:C:48:LEU:C	1:C:50:THR:H	2.30	0.40
1:B:408:ILE:HG22	1:B:409:VAL:N	2.36	0.40
1:B:519:ILE:O	1:B:519:ILE:CG1	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ARG:NH2	1:B:430:ARG:NH2[3_455]	1.87	0.33

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/552 (88%)	441 (91%)	44 (9%)	2 (0%)	30	53
1	B	487/552 (88%)	440 (90%)	42 (9%)	5 (1%)	12	32
1	C	487/552 (88%)	438 (90%)	46 (9%)	3 (1%)	21	45
All	All	1461/1656 (88%)	1319 (90%)	132 (9%)	10 (1%)	18	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	GLU
1	C	366	GLU
1	A	98	PRO
1	B	69	GLU
1	B	366	GLU
1	B	6	ILE
1	B	296	ILE
1	C	514	THR
1	C	98	PRO
1	B	519	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/449 (84%)	298 (79%)	78 (21%)	1	3
1	B	373/449 (83%)	287 (77%)	86 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	373/449 (83%)	297 (80%)	76 (20%)	1	3
All	All	1122/1347 (83%)	882 (79%)	240 (21%)	1	2

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	LEU
1	A	12	THR
1	A	13	LEU
1	A	16	LEU
1	A	23	GLU
1	A	37	LEU
1	A	40	GLN
1	A	44	GLU
1	A	47	MET
1	A	50	THR
1	A	56	LEU
1	A	61	THR
1	A	74	LEU
1	A	76	ASP
1	A	86	LEU
1	A	89	ARG
1	A	96	ARG
1	A	97	ARG
1	A	98	PRO
1	A	102	LEU
1	A	111	MET
1	A	114	ILE
1	A	123	ASP
1	A	138	LEU
1	A	145	VAL
1	A	146	SER
1	A	154	LEU
1	A	157	LEU
1	A	173	GLN
1	A	179	GLN
1	A	188	ILE
1	A	197	HIS
1	A	200	VAL
1	A	213	LEU
1	A	220	ILE

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Mol	Chain	Res	Type
1	A	228	THR
1	A	230	GLN
1	A	234	LEU
1	A	244	ARG
1	A	246	LEU
1	A	248	LEU
1	A	252	VAL
1	A	261	LEU
1	A	287	PRO
1	A	292	ARG
1	A	296	ILE
1	A	300	LEU
1	A	301	ILE
1	A	330	LEU
1	A	337	ARG
1	A	346	PRO
1	A	353	GLU
1	A	367	ARG
1	A	377	LEU
1	A	384	THR
1	A	389	LEU
1	A	403	LEU
1	A	407	ASP
1	A	413	LEU
1	A	415	SER
1	A	424	ARG
1	A	426	VAL
1	A	430	ARG
1	A	439	THR
1	A	442	ARG
1	A	444	ILE
1	A	450	ILE
1	A	453	TYR
1	A	456	THR
1	A	464	ILE
1	A	467	VAL
1	A	473	ILE
1	A	517	LEU
1	A	522	THR
1	A	533	ILE
1	A	536	LYS
1	A	545	LEU

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Mol	Chain	Res	Type
1	B	4	GLN
1	B	6	ILE
1	B	7	GLU
1	B	12	THR
1	B	13	LEU
1	B	16	LEU
1	B	19	PRO
1	B	37	LEU
1	B	40	GLN
1	B	44	GLU
1	B	47	MET
1	B	50	THR
1	B	56	LEU
1	B	61	THR
1	B	62	ARG
1	B	64	GLN
1	B	67	ARG
1	B	69	GLU
1	B	74	LEU
1	B	76	ASP
1	B	89	ARG
1	B	96	ARG
1	B	97	ARG
1	B	102	LEU
1	B	105	ARG
1	B	111	MET
1	B	114	ILE
1	B	127	TRP
1	B	138	LEU
1	B	145	VAL
1	B	146	SER
1	B	154	LEU
1	B	157	LEU
1	B	179	GLN
1	B	184	LEU
1	B	185	LYS
1	B	188	ILE
1	B	197	HIS
1	B	200	VAL
1	B	204	ILE
1	B	205	THR
1	B	206	GLU

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Mol	Chain	Res	Type
1	B	213	LEU
1	B	220	ILE
1	B	228	THR
1	B	230	GLN
1	B	234	LEU
1	B	242	SER
1	B	244	ARG
1	B	246	LEU
1	B	248	LEU
1	B	252	VAL
1	B	261	LEU
1	B	285	VAL
1	B	296	ILE
1	B	300	LEU
1	B	301	ILE
1	B	323	GLN
1	B	326	ARG
1	B	330	LEU
1	B	336	GLN
1	B	337	ARG
1	B	367	ARG
1	B	371	THR
1	B	377	LEU
1	B	384	THR
1	B	389	LEU
1	B	403	LEU
1	B	407	ASP
1	B	414	SER
1	B	420	SER
1	B	421	LYS
1	B	426	VAL
1	B	427	ASN
1	B	430	ARG
1	B	439	THR
1	B	442	ARG
1	B	444	ILE
1	B	450	ILE
1	B	464	ILE
1	B	467	VAL
1	B	473	ILE
1	B	512	PRO
1	B	517	LEU

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Mol	Chain	Res	Type
1	B	524	LEU
1	B	533	ILE
1	C	5	LEU
1	C	7	GLU
1	C	12	THR
1	C	13	LEU
1	C	16	LEU
1	C	25	LEU
1	C	37	LEU
1	C	40	GLN
1	C	44	GLU
1	C	47	MET
1	C	50	THR
1	C	61	THR
1	C	74	LEU
1	C	76	ASP
1	C	89	ARG
1	C	96	ARG
1	C	102	LEU
1	C	105	ARG
1	C	111	MET
1	C	114	ILE
1	C	138	LEU
1	C	145	VAL
1	C	146	SER
1	C	154	LEU
1	C	157	LEU
1	C	179	GLN
1	C	188	ILE
1	C	197	HIS
1	C	200	VAL
1	C	204	ILE
1	C	205	THR
1	C	206	GLU
1	C	213	LEU
1	C	220	ILE
1	C	228	THR
1	C	230	GLN
1	C	232	SER
1	C	234	LEU
1	C	242	SER
1	C	246	LEU

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Mol	Chain	Res	Type
1	C	248	LEU
1	C	252	VAL
1	C	261	LEU
1	C	287	PRO
1	C	296	ILE
1	C	300	LEU
1	C	301	ILE
1	C	330	LEU
1	C	336	GLN
1	C	353	GLU
1	C	367	ARG
1	C	371	THR
1	C	384	THR
1	C	389	LEU
1	C	403	LEU
1	C	407	ASP
1	C	408	ILE
1	C	416	GLU
1	C	420	SER
1	C	423	HIS
1	C	424	ARG
1	C	426	VAL
1	C	428	VAL
1	C	439	THR
1	C	444	ILE
1	C	450	ILE
1	C	453	TYR
1	C	456	THR
1	C	464	ILE
1	C	467	VAL
1	C	473	ILE
1	C	517	LEU
1	C	521	THR
1	C	524	LEU
1	C	533	ILE
1	C	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	173	GLN

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Mol	Chain	Res	Type
1	A	197	HIS
1	A	359	HIS
1	A	368	GLN
1	A	412	HIS
1	A	427	ASN
1	A	455	GLN
1	A	474	HIS
1	A	539	HIS
1	B	4	GLN
1	B	27	HIS
1	B	173	GLN
1	B	193	ASN
1	B	336	GLN
1	B	359	HIS
1	B	368	GLN
1	B	427	ASN
1	B	474	HIS
1	B	539	HIS
1	C	197	HIS
1	C	230	GLN
1	C	323	GLN
1	C	368	GLN
1	C	455	GLN
1	C	539	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	493/552 (89%)	0.83	51 (10%)	12 11	22, 55, 94, 118	11 (2%)
1	B	493/552 (89%)	0.65	42 (8%)	16 15	26, 56, 93, 129	6 (1%)
1	C	493/552 (89%)	0.69	39 (7%)	18 16	22, 56, 94, 114	7 (1%)
All	All	1479/1656 (89%)	0.72	132 (8%)	15 14	22, 56, 94, 129	24 (1%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	458	ARG	9.7
1	A	96	ARG	9.4
1	B	453	TYR	8.7
1	B	424	ARG	7.3
1	C	177	ARG	7.2
1	A	326	ARG	7.1
1	C	312	ARG	6.7
1	A	206	GLU	6.6
1	A	177	ARG	6.2
1	A	312	ARG	6.2
1	B	477	THR	6.1
1	A	161	ARG	5.9
1	C	123	ASP	5.6
1	A	378	SER	5.0
1	B	249	ARG	5.0
1	B	423	HIS	5.0
1	C	310	GLU	4.8
1	A	429	ARG	4.8
1	B	418	GLY	4.7
1	A	249	ARG	4.6
1	B	206	GLU	4.6
1	B	320	GLU	4.3
1	B	201	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	520	ASP	4.3
1	A	3	ASN	4.2
1	C	93	LEU	4.1
1	A	525	ALA	4.1
1	A	88	SER	3.9
1	C	124	GLY	3.8
1	A	476	ALA	3.8
1	C	172	ARG	3.7
1	C	92	ALA	3.7
1	C	105	ARG	3.7
1	A	89	ARG	3.6
1	A	347	GLU	3.6
1	B	202	GLY	3.5
1	A	447	CYS	3.4
1	B	414	SER	3.4
1	A	322	PRO	3.4
1	B	422	ALA	3.4
1	A	327	LEU	3.3
1	C	297	GLY	3.3
1	C	286	ASP	3.3
1	C	205	THR	3.2
1	B	438	ILE	3.1
1	A	426	VAL	3.0
1	A	95	ASP	3.0
1	C	398	GLY	2.9
1	B	509	TYR	2.9
1	A	263	ALA	2.9
1	C	418	GLY	2.8
1	B	89	ARG	2.8
1	B	78	SER	2.8
1	B	377	LEU	2.8
1	B	521	THR	2.8
1	A	32	LEU	2.7
1	B	508	PRO	2.7
1	B	204	ILE	2.7
1	A	205	THR	2.7
1	A	324	GLY	2.7
1	B	91	ARG	2.7
1	B	264	GLY	2.7
1	C	207	ALA	2.7
1	C	106	ASP	2.7
1	A	545	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	509	TYR	2.6
1	A	69	GLU	2.6
1	C	27	HIS	2.6
1	A	508	PRO	2.6
1	A	93	LEU	2.6
1	B	420	SER	2.6
1	A	68	VAL	2.6
1	B	378	SER	2.5
1	C	127	TRP	2.5
1	B	381	GLY	2.5
1	C	210	TYR	2.5
1	A	310	GLU	2.5
1	B	71	ALA	2.5
1	C	376	GLY	2.5
1	B	114	ILE	2.4
1	A	251	ILE	2.4
1	B	539	HIS	2.4
1	A	433	PHE	2.4
1	A	422	ALA	2.4
1	A	87	THR	2.4
1	C	512	PRO	2.4
1	B	292	ARG	2.3
1	C	200	VAL	2.3
1	A	523	GLY	2.3
1	C	397	GLY	2.3
1	A	449	PRO	2.3
1	A	212	GLY	2.3
1	A	450	ILE	2.3
1	C	94	ALA	2.3
1	A	509	TYR	2.3
1	A	208	PRO	2.3
1	C	107	GLY	2.3
1	A	291	GLU	2.3
1	C	67	ARG	2.3
1	A	428	VAL	2.3
1	C	59	PHE	2.2
1	A	241	ALA	2.2
1	B	93	LEU	2.2
1	B	527	ASP	2.2
1	A	474	HIS	2.2
1	B	39	TRP	2.2
1	C	39	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	241	ALA	2.2
1	C	412	HIS	2.2
1	A	546	GLU	2.2
1	B	329	THR	2.2
1	C	91	ARG	2.1
1	A	521	THR	2.1
1	A	30	LEU	2.1
1	A	473	ILE	2.1
1	B	21	LYS	2.1
1	B	77	GLY	2.1
1	A	70	SER	2.1
1	C	298	VAL	2.1
1	A	526	ILE	2.1
1	B	110	TYR	2.1
1	C	114	ILE	2.1
1	C	173	GLN	2.1
1	C	122	LYS	2.1
1	B	456	THR	2.1
1	B	520	ASP	2.1
1	B	380	ALA	2.1
1	B	415	SER	2.0
1	B	471	VAL	2.0
1	C	447	CYS	2.0
1	C	26	LYS	2.0
1	C	69	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.