



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:05 AM UTC

PDB ID : 3CDJ / pdb\_00003cdj  
Title : Crystal structure of the E. coli KH/S1 domain truncated PNPase  
Authors : Shi, Z.; Yang, W.Z.; Lin-Chao, S.; Chak, K.F.; Yuan, H.S.  
Deposited on : 2008-02-27  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

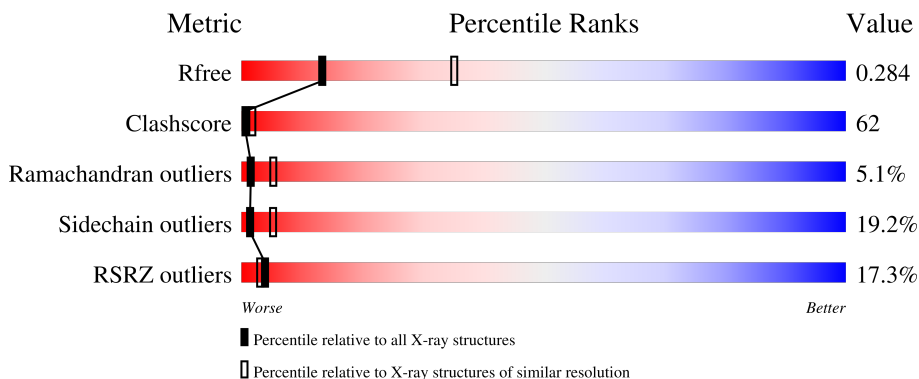
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	559	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3418 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 Polynucleotide phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3382	2132	585	647	18	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.09Å 160.09Å 153.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.80) 95.1 (50.00-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.30 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.270 , 0.294 0.280 , 0.284	Depositor DCC
$R_{free}$ test set	1817 reflections (9.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtrriage
Anisotropy	0.998	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 94.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.54	48/3432 (1.4%)	1.88	118/4648 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	THR	CA-C	-12.92	1.34	1.52
1	A	91	TYR	CA-CB	12.14	1.74	1.53
1	A	90	THR	CA-C	11.97	1.68	1.52
1	A	91	TYR	CG-CD2	11.93	1.64	1.39
1	A	92	ALA	C-O	8.69	1.34	1.24
1	A	91	TYR	CE1-CZ	8.21	1.57	1.38
1	A	398	THR	CA-CB	-8.12	1.39	1.53
1	A	450	VAL	N-CA	-8.10	1.36	1.46
1	A	151	ILE	CA-CB	8.07	1.64	1.54
1	A	256	TRP	N-CA	-8.02	1.35	1.46
1	A	89	ARG	CA-CB	7.91	1.65	1.53
1	A	395	ARG	N-CA	-7.88	1.36	1.46
1	A	91	TYR	N-CA	7.70	1.56	1.46
1	A	441	MET	SD-CE	-7.66	1.60	1.79
1	A	258	PRO	CA-CB	-7.61	1.43	1.53
1	A	397	ASP	N-CA	-7.55	1.36	1.46
1	A	397	ASP	CA-C	-7.48	1.43	1.52
1	A	399	PHE	C-O	-7.11	1.16	1.24
1	A	449	ARG	C-N	7.02	1.43	1.33
1	A	256	TRP	CA-C	-6.60	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	VAL	CA-CB	6.30	1.61	1.53
1	A	65	VAL	CA-CB	-6.30	1.46	1.54
1	A	90	THR	C-O	6.15	1.31	1.24
1	A	448	VAL	N-CA	-6.06	1.39	1.46
1	A	176	ARG	N-CA	-6.05	1.38	1.46
1	A	175	ALA	CA-C	6.04	1.60	1.52
1	A	140	VAL	CA-C	-5.61	1.46	1.52
1	A	62	ALA	C-O	-5.59	1.17	1.24
1	A	174	ALA	CA-CB	5.57	1.62	1.53
1	A	451	VAL	CA-C	-5.51	1.45	1.52
1	A	84	VAL	C-O	-5.50	1.18	1.24
1	A	448	VAL	C-O	5.44	1.30	1.24
1	A	230	PHE	C-O	5.39	1.30	1.24
1	A	164	SER	CA-C	-5.38	1.46	1.52
1	A	70	GLN	N-CA	5.36	1.53	1.46
1	A	397	ASP	CA-CB	-5.36	1.44	1.53
1	A	399	PHE	N-CA	-5.32	1.40	1.46
1	A	213	GLU	C-O	-5.31	1.18	1.24
1	A	468	GLY	C-N	5.29	1.40	1.33
1	A	90	THR	CA-CB	5.29	1.61	1.53
1	A	449	ARG	CA-C	5.25	1.58	1.52
1	A	143	VAL	CA-CB	5.24	1.62	1.54
1	A	450	VAL	C-N	5.20	1.40	1.33
1	A	403	TYR	C-O	-5.19	1.17	1.24
1	A	185	VAL	C-O	5.15	1.29	1.24
1	A	472	ALA	C-O	5.12	1.30	1.24
1	A	257	GLN	N-CA	-5.09	1.41	1.45
1	A	141	VAL	C-N	-5.06	1.27	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	N-CA-C	21.72	157.07	110.80
1	A	461	SER	N-CA-C	20.07	135.47	108.38
1	A	257	GLN	CA-C-N	19.13	143.75	119.84
1	A	257	GLN	C-N-CA	19.13	143.75	119.84
1	A	164	SER	N-CA-C	-18.01	84.12	110.23
1	A	257	GLN	N-CA-C	-16.57	82.70	108.55
1	A	406	PRO	CA-C-N	16.38	140.31	119.84
1	A	406	PRO	C-N-CA	16.38	140.31	119.84
1	A	428	ARG	N-CA-C	-14.59	95.50	113.01
1	A	325	LYS	N-CA-C	13.70	125.73	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ARG	N-CA-C	13.62	139.81	110.80
1	A	544	VAL	N-CA-C	-13.35	97.87	110.82
1	A	256	TRP	N-CA-C	-12.76	83.62	110.80
1	A	25	LEU	N-CA-C	12.68	127.26	110.53
1	A	335	GLY	N-CA-C	-12.61	92.73	111.14
1	A	442	ASP	N-CA-C	-12.53	98.09	113.50
1	A	23	THR	N-CA-C	12.21	128.08	111.24
1	A	331	ARG	N-CA-C	-12.12	98.49	113.28
1	A	463	MET	N-CA-C	-12.05	85.12	110.80
1	A	339	ILE	N-CA-C	-11.59	92.59	108.12
1	A	342	ARG	N-CA-C	-11.53	93.21	110.28
1	A	357	LEU	CA-C-N	11.25	130.67	118.97
1	A	357	LEU	C-N-CA	11.25	130.67	118.97
1	A	395	ARG	N-CA-CB	-11.24	91.50	110.49
1	A	457	SER	N-CA-C	10.46	133.08	110.80
1	A	337	PRO	CA-C-N	10.43	141.47	121.54
1	A	337	PRO	C-N-CA	10.43	141.47	121.54
1	A	132	ASN	N-CA-C	-10.16	92.60	109.46
1	A	192	GLU	N-CA-C	-10.11	100.36	112.89
1	A	396	THR	CA-C-N	-9.47	107.54	120.90
1	A	396	THR	C-N-CA	-9.47	107.54	120.90
1	A	182	ASP	N-CA-C	9.04	123.60	112.58
1	A	446	TYR	N-CA-C	8.97	124.38	110.20
1	A	456	GLU	N-CA-C	8.71	122.67	108.55
1	A	510	HIS	N-CA-C	-8.62	102.35	112.86
1	A	215	GLU	N-CA-C	-8.57	94.49	109.06
1	A	339	ILE	CB-CA-C	8.28	120.37	111.35
1	A	407	PRO	N-CA-C	8.27	129.51	112.47
1	A	115	ALA	N-CA-C	-8.19	102.55	112.54
1	A	328	VAL	N-CA-C	-7.97	101.11	112.35
1	A	61	THR	N-CA-C	-7.96	93.85	108.02
1	A	199	ASP	N-CA-C	-7.84	93.96	107.61
1	A	458	ASN	N-CA-C	7.62	122.02	112.87
1	A	358	PRO	N-CA-C	7.54	124.25	113.47
1	A	256	TRP	CB-CA-C	-7.50	95.50	110.42
1	A	466	VAL	N-CA-C	-7.42	103.56	110.53
1	A	111	GLU	N-CA-C	-7.35	103.78	112.89
1	A	74	LYS	CA-C-N	-7.30	111.94	119.83
1	A	74	LYS	C-N-CA	-7.30	111.94	119.83
1	A	24	LEU	N-CA-C	-7.30	103.63	112.54
1	A	226	GLY	N-CA-C	-7.26	106.68	114.67
1	A	345	ASP	N-CA-C	-7.22	101.78	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	SER	CB-CA-C	-7.20	97.77	109.72
1	A	255	ASP	N-CA-C	-7.02	98.86	110.17
1	A	75	PRO	N-CA-C	-6.92	100.37	111.03
1	A	144	ASN	N-CA-C	-6.78	96.11	108.85
1	A	91	TYR	O-C-N	6.76	131.48	122.43
1	A	70	GLN	CA-CB-CG	-6.67	100.76	114.10
1	A	396	THR	CB-CA-C	-6.52	98.07	109.02
1	A	257	GLN	N-CA-CB	6.47	122.83	111.18
1	A	465	SER	N-CA-C	-6.45	104.90	112.89
1	A	460	SER	CA-C-N	-6.39	111.50	122.10
1	A	460	SER	C-N-CA	-6.39	111.50	122.10
1	A	445	PRO	N-CA-C	6.35	122.29	114.35
1	A	460	SER	N-CA-C	6.30	124.21	110.80
1	A	79	PHE	N-CA-C	-6.23	99.50	108.60
1	A	90	THR	CA-C-N	-6.17	110.41	120.72
1	A	90	THR	C-N-CA	-6.17	110.41	120.72
1	A	90	THR	O-C-N	6.12	128.60	122.12
1	A	165	GLY	N-CA-C	-6.08	105.22	115.62
1	A	170	GLY	C-N-CD	-6.03	100.28	125.00
1	A	444	PHE	N-CA-C	-6.00	95.41	108.74
1	A	70	GLN	N-CA-C	6.00	123.57	110.80
1	A	542	MET	N-CA-C	-5.92	98.05	108.23
1	A	396	THR	N-CA-C	5.86	121.86	114.31
1	A	258	PRO	N-CA-C	5.86	124.53	112.47
1	A	398	THR	N-CA-C	-5.84	105.81	113.17
1	A	341	GLY	N-CA-C	-5.84	99.34	113.18
1	A	26	ASN	N-CA-C	5.80	122.62	109.81
1	A	539	LYS	N-CA-C	5.79	123.13	110.80
1	A	336	GLU	CA-C-N	5.74	127.01	119.84
1	A	336	GLU	C-N-CA	5.74	127.01	119.84
1	A	29	VAL	N-CA-C	5.64	115.72	107.37
1	A	164	SER	O-C-N	5.63	129.79	122.87
1	A	397	ASP	CA-C-N	-5.62	113.28	122.54
1	A	397	ASP	C-N-CA	-5.62	113.28	122.54
1	A	110	GLY	N-CA-C	-5.60	99.92	113.18
1	A	337	PRO	N-CA-C	5.58	123.97	112.47
1	A	327	VAL	CB-CA-C	-5.54	104.66	112.14
1	A	197	LYS	N-CA-C	-5.53	106.21	113.17
1	A	548	GLN	N-CA-C	-5.52	104.90	111.69
1	A	407	PRO	CA-N-CD	-5.48	104.33	112.00
1	A	524	GLY	N-CA-C	5.47	119.53	110.55
1	A	92	ALA	O-C-N	5.47	127.92	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	GLN	CA-C-O	5.46	125.52	120.50
1	A	150	ASP	N-CA-C	5.44	116.89	111.07
1	A	394	GLU	CA-CB-CG	-5.44	103.22	114.10
1	A	535	GLU	N-CA-C	5.37	120.51	112.94
1	A	258	PRO	N-CA-CB	-5.35	97.63	103.25
1	A	179	TYR	N-CA-C	-5.30	99.45	108.26
1	A	337	PRO	O-C-N	5.27	129.76	122.64
1	A	462	SER	N-CA-C	-5.24	99.65	110.80
1	A	406	PRO	N-CA-C	5.21	117.05	110.70
1	A	62	ALA	N-CA-C	5.20	117.38	108.90
1	A	337	PRO	CA-N-CD	-5.20	104.72	112.00
1	A	445	PRO	CA-C-N	5.17	128.82	121.42
1	A	445	PRO	C-N-CA	5.17	128.82	121.42
1	A	71	LYS	O-C-N	5.16	129.46	122.59
1	A	24	LEU	CA-CB-CG	5.13	134.26	116.30
1	A	79	PHE	CB-CA-C	5.10	121.17	111.17
1	A	461	SER	CA-C-N	5.10	131.28	121.54
1	A	461	SER	C-N-CA	5.10	131.28	121.54
1	A	71	LYS	CA-C-N	5.10	130.91	121.94
1	A	71	LYS	C-N-CA	5.10	130.91	121.94
1	A	483	ALA	N-CA-C	-5.10	103.67	110.55
1	A	60	ASP	N-CA-C	5.06	118.37	111.39
1	A	258	PRO	CA-CB-CG	-5.06	94.89	104.50
1	A	90	THR	CB-CA-C	-5.02	102.45	110.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	GLU	Mainchain,Peptide

## 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	3382	0	3415	418	2
2	A	36	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3418	0	3415	418	2

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 62.

All (418) 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:91:TYR:CB	1:A:91:TYR:CA	1.74	1.58
1:A:325:LYS:O	1:A:327:VAL:N	1.76	1.18
1:A:69:GLY:C	1:A:70:GLN:HG3	1.55	1.14
1:A:70:GLN:CD	1:A:71:LYS:N	2.07	1.12
1:A:394:GLU:OE2	2:A:599:HOH:O	1.63	1.12
1:A:395:ARG:HG2	1:A:396:THR:CB	1.79	1.12
1:A:534:ILE:HG13	1:A:537:ILE:HD11	1.12	1.12
1:A:487:ILE:HG12	1:A:489:MET:HE2	1.32	1.11
1:A:395:ARG:NE	1:A:396:THR:HB	1.64	1.10
1:A:131:VAL:HG12	1:A:131:VAL:O	1.52	1.09
1:A:257:GLN:HB3	1:A:258:PRO:HD2	1.27	1.09
1:A:325:LYS:HE3	1:A:326:ASN:H	1.15	1.08
1:A:395:ARG:HG2	1:A:396:THR:N	1.40	1.07
1:A:116:ARG:HH11	1:A:116:ARG:HB3	1.21	1.04
1:A:335:GLY:C	1:A:337:PRO:HD2	1.84	1.02
1:A:338:ARG:HH11	1:A:338:ARG:HB2	1.21	1.02
1:A:395:ARG:HG2	1:A:396:THR:HB	1.40	1.02
1:A:25:LEU:HD23	1:A:45:MET:HG3	1.41	1.01
1:A:325:LYS:C	1:A:327:VAL:H	1.65	1.00
1:A:395:ARG:HG2	1:A:396:THR:CA	1.90	1.00
1:A:342:ARG:NH2	1:A:346:MET:O	1.95	0.99
1:A:325:LYS:CE	1:A:326:ASN:H	1.75	0.99
1:A:395:ARG:CG	1:A:396:THR:N	2.20	0.99
1:A:257:GLN:HB3	1:A:258:PRO:CD	1.93	0.98
1:A:323:ILE:HD12	2:A:582:HOH:O	1.63	0.98
1:A:332:VAL:HG13	1:A:333:LEU:HD22	1.44	0.98
1:A:327:VAL:O	1:A:331:ARG:HG2	1.65	0.96
1:A:351:ASP:HB3	1:A:367:THR:HG23	1.46	0.96
1:A:344:LYS:O	1:A:344:LYS:HG2	1.62	0.96
1:A:395:ARG:CG	1:A:396:THR:CB	2.44	0.96
1:A:336:GLU:N	1:A:337:PRO:HD2	1.82	0.94
1:A:441:MET:HE3	1:A:445:PRO:HA	1.50	0.93
1:A:325:LYS:HB2	1:A:328:VAL:HG23	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:CG1	1:A:537:ILE:HD11	1.98	0.92
1:A:340:ASP:O	1:A:342:ARG:N	2.03	0.91
1:A:70:GLN:NE2	1:A:70:GLN:C	2.29	0.90
1:A:69:GLY:O	1:A:70:GLN:NE2	2.05	0.90
1:A:342:ARG:HH21	1:A:346:MET:C	1.80	0.89
1:A:343:GLU:N	1:A:346:MET:HG3	1.88	0.89
1:A:395:ARG:CG	1:A:396:THR:HB	2.02	0.89
1:A:372:GLN:HB3	1:A:456:GLU:HG2	1.54	0.88
1:A:232:HIS:HA	1:A:235:GLN:HE21	1.37	0.88
1:A:462:SER:OG	1:A:465:SER:HB2	1.74	0.87
1:A:69:GLY:O	1:A:70:GLN:HG3	1.72	0.87
1:A:395:ARG:HG2	1:A:396:THR:H	1.39	0.86
1:A:69:GLY:C	1:A:70:GLN:CG	2.44	0.85
1:A:225:LEU:HD21	1:A:542:MET:HE3	1.59	0.85
1:A:332:VAL:CG1	1:A:333:LEU:HD22	2.06	0.85
1:A:395:ARG:NE	1:A:396:THR:CB	2.39	0.83
1:A:331:ARG:CB	1:A:331:ARG:HH11	1.90	0.83
1:A:441:MET:O	1:A:441:MET:HG3	1.76	0.83
1:A:259:GLU:HB3	1:A:260:PRO:HD2	1.61	0.82
1:A:395:ARG:CD	1:A:396:THR:HB	2.09	0.82
1:A:513:ASP:HA	1:A:534:ILE:HG23	1.60	0.82
1:A:327:VAL:HG22	1:A:331:ARG:HD3	1.62	0.82
1:A:441:MET:HE1	1:A:445:PRO:O	1.80	0.81
1:A:70:GLN:CD	1:A:70:GLN:C	2.49	0.81
1:A:225:LEU:HD21	1:A:542:MET:CE	2.11	0.81
1:A:425:GLY:C	1:A:427:GLY:H	1.89	0.81
1:A:70:GLN:HE22	1:A:71:LYS:HA	1.45	0.80
1:A:441:MET:CE	1:A:445:PRO:O	2.29	0.80
1:A:91:TYR:CA	1:A:91:TYR:CG	2.62	0.80
1:A:498:TYR:CE2	1:A:541:ILE:HD12	2.16	0.80
1:A:338:ARG:HH12	1:A:339:ILE:HD12	1.45	0.80
1:A:539:LYS:O	1:A:542:MET:O	2.00	0.79
1:A:540:GLU:O	1:A:544:VAL:HG23	1.81	0.79
1:A:116:ARG:HB3	1:A:116:ARG:NH1	1.96	0.79
1:A:116:ARG:HH21	1:A:426:HIS:HB3	1.48	0.79
1:A:323:ILE:HD13	1:A:324:GLU:H	1.47	0.79
1:A:70:GLN:NE2	1:A:71:LYS:HA	1.97	0.78
1:A:340:ASP:O	1:A:342:ARG:HG2	1.82	0.78
1:A:534:ILE:HG13	1:A:537:ILE:CD1	2.06	0.77
1:A:325:LYS:HE3	1:A:326:ASN:N	1.98	0.77
1:A:329:ARG:O	1:A:329:ARG:HD3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:HE1	1:A:62:ALA:HB1	1.67	0.77
1:A:371:THR:HA	1:A:457:SER:HB2	1.67	0.76
1:A:344:LYS:O	1:A:344:LYS:CG	2.34	0.76
1:A:148:ASN:HD22	1:A:149:PRO:N	1.84	0.76
1:A:259:GLU:HB3	1:A:260:PRO:CD	2.15	0.76
1:A:456:GLU:O	1:A:457:SER:HB2	1.86	0.76
1:A:396:THR:O	1:A:397:ASP:C	2.21	0.76
1:A:331:ARG:HH11	1:A:331:ARG:HB3	1.49	0.76
1:A:70:GLN:NE2	1:A:71:LYS:N	2.34	0.75
1:A:537:ILE:H	1:A:537:ILE:HD12	1.49	0.75
1:A:70:GLN:CD	1:A:71:LYS:CA	2.60	0.74
1:A:117:LEU:O	1:A:154:MET:HE3	1.86	0.74
1:A:242:ILE:O	1:A:246:VAL:HG23	1.88	0.74
1:A:325:LYS:HG2	1:A:326:ASN:N	2.01	0.74
1:A:131:VAL:O	1:A:131:VAL:CG1	2.27	0.73
1:A:257:GLN:CB	1:A:258:PRO:CD	2.49	0.73
1:A:70:GLN:NE2	1:A:71:LYS:CA	2.51	0.73
1:A:396:THR:O	1:A:396:THR:HG23	1.86	0.73
1:A:498:TYR:HE2	1:A:541:ILE:HD12	1.53	0.73
1:A:327:VAL:O	1:A:331:ARG:CG	2.36	0.73
1:A:428:ARG:O	1:A:432:ARG:HG3	1.88	0.73
1:A:67:VAL:HG23	1:A:160:ALA:HB1	1.70	0.73
1:A:441:MET:HA	1:A:444:PHE:O	1.90	0.71
1:A:326:ASN:O	1:A:330:SER:N	2.24	0.71
1:A:23:THR:O	1:A:23:THR:OG1	2.04	0.71
1:A:336:GLU:OE1	1:A:341:GLY:HA3	1.90	0.71
1:A:259:GLU:CB	1:A:260:PRO:CD	2.68	0.71
1:A:396:THR:O	1:A:396:THR:CG2	2.33	0.71
1:A:113:LEU:HD11	1:A:425:GLY:HA3	1.71	0.71
1:A:70:GLN:O	1:A:71:LYS:HD3	1.91	0.70
1:A:425:GLY:C	1:A:427:GLY:N	2.44	0.70
1:A:259:GLU:CB	1:A:260:PRO:HD2	2.22	0.70
1:A:74:LYS:HB2	1:A:75:PRO:CD	2.23	0.69
1:A:325:LYS:N	1:A:325:LYS:HE2	2.08	0.69
1:A:375:VAL:HG11	1:A:469:ALA:HA	1.72	0.69
1:A:395:ARG:CG	1:A:396:THR:OG1	2.41	0.69
1:A:538:THR:HG23	1:A:539:LYS:N	2.08	0.69
1:A:173:GLY:HA3	1:A:235:GLN:HB3	1.72	0.68
1:A:368:ARG:HG2	1:A:368:ARG:HH11	1.58	0.68
1:A:522:ARG:HG3	1:A:554:LEU:HD22	1.74	0.68
1:A:437:VAL:HG21	1:A:484:VAL:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:O	1:A:503:ASP:OD1	2.12	0.68
1:A:69:GLY:O	1:A:70:GLN:CG	2.41	0.68
1:A:437:VAL:HG12	1:A:480:ILE:HB	1.75	0.68
1:A:148:ASN:HD22	1:A:149:PRO:CD	2.07	0.67
1:A:323:ILE:CD1	1:A:324:GLU:H	2.07	0.67
1:A:343:GLU:H	1:A:346:MET:HG3	1.55	0.67
1:A:245:LEU:HD23	1:A:245:LEU:O	1.94	0.67
1:A:427:GLY:C	1:A:429:LEU:N	2.49	0.67
1:A:113:LEU:O	1:A:116:ARG:HB2	1.95	0.67
1:A:92:ALA:HB1	1:A:143:VAL:HG23	1.77	0.67
1:A:338:ARG:HH11	1:A:339:ILE:H	1.42	0.67
1:A:325:LYS:O	1:A:327:VAL:HG12	1.95	0.66
1:A:31:LYS:HG2	1:A:40:THR:HB	1.77	0.66
1:A:91:TYR:CB	1:A:91:TYR:C	2.66	0.66
1:A:221:GLU:HG3	1:A:546:LEU:HD12	1.77	0.66
1:A:489:MET:HE3	1:A:549:ALA:HA	1.76	0.66
1:A:504:ILE:O	1:A:504:ILE:HG13	1.95	0.66
1:A:395:ARG:CD	1:A:396:THR:CB	2.71	0.66
1:A:125:LEU:HD11	1:A:172:ILE:CG2	2.25	0.65
1:A:116:ARG:HH21	1:A:426:HIS:CB	2.09	0.65
1:A:325:LYS:CB	1:A:328:VAL:HG23	2.26	0.65
1:A:543:GLN:O	1:A:547:ASN:HB2	1.97	0.65
1:A:209:VAL:C	1:A:210:LEU:HD23	2.22	0.65
1:A:30:ARG:HG3	1:A:30:ARG:HH11	1.62	0.65
1:A:70:GLN:O	1:A:71:LYS:CD	2.45	0.65
1:A:328:VAL:O	1:A:332:VAL:HB	1.96	0.64
1:A:351:ASP:OD1	1:A:353:ARG:NH1	2.30	0.64
1:A:70:GLN:OE1	1:A:71:LYS:C	2.41	0.64
1:A:491:LEU:HD11	1:A:498:TYR:HB2	1.80	0.64
1:A:342:ARG:O	1:A:343:GLU:O	2.16	0.64
1:A:70:GLN:OE1	1:A:71:LYS:CA	2.46	0.64
1:A:542:MET:O	1:A:543:GLN:HB2	1.97	0.64
1:A:258:PRO:O	1:A:258:PRO:HG2	1.97	0.64
1:A:480:ILE:HD13	1:A:480:ILE:H	1.63	0.63
1:A:148:ASN:HD22	1:A:148:ASN:C	2.05	0.63
1:A:350:LEU:HD21	1:A:368:ARG:HD3	1.80	0.63
1:A:426:HIS:O	1:A:429:LEU:HB3	1.98	0.63
1:A:454:ILE:HD12	1:A:454:ILE:H	1.63	0.63
1:A:342:ARG:HB3	1:A:346:MET:HB2	1.81	0.63
1:A:491:LEU:HD12	1:A:492:VAL:N	2.13	0.63
1:A:518:VAL:CG1	1:A:525:ILE:HD12	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:HB2	1:A:338:ARG:NH1	2.04	0.63
1:A:179:TYR:O	1:A:196:SER:HA	1.98	0.62
1:A:437:VAL:CG1	1:A:482:ALA:H	2.12	0.62
1:A:82:LEU:HD11	1:A:122:ILE:HD11	1.79	0.62
1:A:498:TYR:OH	1:A:544:VAL:HG21	1.99	0.62
1:A:406:PRO:CB	1:A:407:PRO:HD2	2.27	0.62
1:A:125:LEU:HD21	1:A:210:LEU:HD11	1.81	0.62
1:A:331:ARG:CB	1:A:331:ARG:NH1	2.63	0.61
1:A:70:GLN:OE1	1:A:71:LYS:N	2.32	0.61
1:A:74:LYS:HB2	1:A:75:PRO:HD2	1.82	0.61
1:A:441:MET:CE	1:A:445:PRO:C	2.73	0.61
1:A:257:GLN:CB	1:A:258:PRO:HD2	2.10	0.61
1:A:79:PHE:O	1:A:131:VAL:HG22	2.00	0.61
1:A:487:ILE:CG1	1:A:489:MET:HE2	2.21	0.61
1:A:326:ASN:HA	1:A:329:ARG:HB3	1.82	0.61
1:A:395:ARG:CZ	1:A:396:THR:HB	2.29	0.61
1:A:161:LEU:HA	1:A:164:SER:OG	2.00	0.61
1:A:161:LEU:O	1:A:164:SER:O	2.19	0.60
1:A:206:GLU:HG3	1:A:207:ALA:N	2.15	0.60
1:A:500:VAL:HG21	1:A:545:ALA:HA	1.83	0.60
1:A:343:GLU:H	1:A:346:MET:CG	2.13	0.60
1:A:340:ASP:C	1:A:342:ARG:N	2.58	0.60
1:A:55:MET:HG2	1:A:64:PHE:HD1	1.66	0.60
1:A:356:VAL:HG21	1:A:365:LEU:HB2	1.83	0.60
1:A:127:PRO:HG3	1:A:167:PRO:HB3	1.84	0.59
1:A:441:MET:HE3	1:A:445:PRO:C	2.26	0.59
1:A:327:VAL:O	1:A:331:ARG:CD	2.50	0.59
1:A:437:VAL:HG11	1:A:482:ALA:O	2.02	0.59
1:A:56:VAL:HG21	1:A:156:GLY:CA	2.32	0.59
1:A:159:ALA:HB2	1:A:242:ILE:HD12	1.85	0.59
1:A:539:LYS:O	1:A:540:GLU:C	2.44	0.59
1:A:231:GLY:O	1:A:235:GLN:HG3	2.03	0.59
1:A:148:ASN:ND2	1:A:150:ASP:H	1.99	0.58
1:A:427:GLY:C	1:A:429:LEU:H	2.08	0.58
1:A:221:GLU:HG2	1:A:546:LEU:O	2.03	0.58
1:A:491:LEU:HD12	1:A:492:VAL:H	1.69	0.58
1:A:25:LEU:HD12	1:A:25:LEU:N	2.18	0.58
1:A:325:LYS:CG	1:A:326:ASN:N	2.66	0.58
1:A:426:HIS:O	1:A:429:LEU:CB	2.52	0.58
1:A:403:TYR:OH	1:A:462:SER:CB	2.52	0.57
1:A:72:LYS:HB2	1:A:72:LYS:NZ	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:HG12	1:A:489:MET:CE	2.22	0.57
1:A:69:GLY:O	1:A:70:GLN:CD	2.47	0.57
1:A:209:VAL:O	1:A:210:LEU:HD23	2.04	0.57
1:A:375:VAL:HG11	1:A:469:ALA:CA	2.34	0.57
1:A:229:VAL:O	1:A:233:GLU:HG3	2.04	0.57
1:A:327:VAL:HG13	1:A:328:VAL:N	2.18	0.57
1:A:329:ARG:CZ	1:A:492:VAL:HG23	2.34	0.57
1:A:27:PRO:HB3	1:A:45:MET:HB2	1.87	0.57
1:A:258:PRO:O	1:A:259:GLU:O	2.23	0.57
1:A:338:ARG:HH12	1:A:339:ILE:CD1	2.15	0.57
1:A:525:ILE:HD11	1:A:553:ARG:NH1	2.19	0.57
1:A:148:ASN:HD22	1:A:149:PRO:HD2	1.68	0.57
1:A:159:ALA:HB2	1:A:242:ILE:CD1	2.36	0.56
1:A:340:ASP:HB3	1:A:342:ARG:HG2	1.86	0.56
1:A:323:ILE:O	1:A:324:GLU:O	2.23	0.56
1:A:508:GLU:O	1:A:511:LEU:HD22	2.06	0.56
1:A:344:LYS:O	1:A:345:ASP:OD2	2.24	0.56
1:A:79:PHE:O	1:A:131:VAL:HG13	2.06	0.55
1:A:437:VAL:HG12	1:A:437:VAL:O	2.06	0.55
1:A:325:LYS:C	1:A:327:VAL:N	2.33	0.55
1:A:441:MET:HE3	1:A:445:PRO:CA	2.29	0.55
1:A:343:GLU:N	1:A:346:MET:CG	2.66	0.55
1:A:395:ARG:HG3	1:A:396:THR:OG1	2.06	0.55
1:A:40:THR:HG23	1:A:57:SER:HB3	1.89	0.55
1:A:59:ASP:HB2	1:A:147:VAL:HG21	1.88	0.55
1:A:323:ILE:CG1	1:A:324:GLU:N	2.70	0.55
1:A:347:ILE:HG13	1:A:555:HIS:HD2	1.72	0.54
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.20	0.54
1:A:245:LEU:HD23	1:A:245:LEU:C	2.33	0.54
1:A:395:ARG:CD	1:A:396:THR:OG1	2.56	0.54
1:A:396:THR:O	1:A:398:THR:HG23	2.07	0.54
1:A:538:THR:CG2	1:A:539:LYS:N	2.70	0.54
1:A:438:MET:HE1	1:A:473:LEU:HD22	1.90	0.54
1:A:34:TYR:CE2	1:A:186:LEU:HD11	2.43	0.54
1:A:130:PHE:HE1	1:A:167:PRO:HG2	1.73	0.54
1:A:371:THR:HA	1:A:457:SER:CB	2.38	0.53
1:A:539:LYS:HD2	1:A:539:LYS:C	2.34	0.53
1:A:350:LEU:CD2	1:A:368:ARG:HD3	2.38	0.53
1:A:336:GLU:N	1:A:337:PRO:CD	2.66	0.53
1:A:30:ARG:NE	1:A:244:GLU:OE2	2.42	0.53
1:A:74:LYS:O	1:A:75:PRO:C	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:HG13	1:A:333:LEU:CD2	2.30	0.53
1:A:85:ASN:HD22	1:A:137:ILE:HG12	1.74	0.53
1:A:25:LEU:CD2	1:A:45:MET:HG3	2.29	0.53
1:A:163:LEU:HD21	1:A:245:LEU:CD2	2.39	0.53
1:A:39:VAL:HG12	1:A:40:THR:N	2.23	0.53
1:A:70:GLN:C	1:A:71:LYS:CG	2.82	0.53
1:A:323:ILE:HG12	1:A:324:GLU:N	2.23	0.53
1:A:327:VAL:HG22	1:A:331:ARG:CD	2.38	0.53
1:A:70:GLN:HG2	1:A:132:ASN:HB3	1.91	0.53
1:A:251:LYS:HB3	1:A:252:PRO:CD	2.39	0.52
1:A:70:GLN:O	1:A:71:LYS:CG	2.57	0.52
1:A:116:ARG:O	1:A:120:ARG:HG3	2.09	0.52
1:A:246:VAL:O	1:A:250:GLY:N	2.42	0.52
1:A:204:GLY:HA2	1:A:210:LEU:HG	1.91	0.52
1:A:331:ARG:NH1	1:A:331:ARG:HB2	2.25	0.52
1:A:395:ARG:CG	1:A:396:THR:CA	2.76	0.52
1:A:539:LYS:O	1:A:542:MET:N	2.42	0.52
1:A:200:LEU:HD21	1:A:202:VAL:CG2	2.40	0.52
1:A:437:VAL:HG13	1:A:481:LYS:HB2	1.92	0.52
1:A:505:LEU:CD1	1:A:508:GLU:HG3	2.40	0.52
1:A:489:MET:CE	1:A:549:ALA:HA	2.40	0.52
1:A:162:SER:C	1:A:164:SER:O	2.53	0.52
1:A:70:GLN:O	1:A:71:LYS:CB	2.58	0.51
1:A:404:ASN:O	1:A:454:ILE:HD12	2.10	0.51
1:A:25:LEU:N	1:A:25:LEU:CD1	2.73	0.51
1:A:538:THR:HG23	1:A:539:LYS:H	1.74	0.51
1:A:542:MET:O	1:A:543:GLN:CB	2.59	0.51
1:A:70:GLN:C	1:A:71:LYS:HG2	2.33	0.51
1:A:329:ARG:NH2	1:A:513:ASP:OD1	2.42	0.51
1:A:489:MET:HG3	1:A:549:ALA:HB2	1.93	0.51
1:A:56:VAL:HG21	1:A:156:GLY:HA2	1.91	0.51
1:A:258:PRO:O	1:A:258:PRO:CG	2.59	0.51
1:A:82:LEU:HD11	1:A:122:ILE:CD1	2.41	0.51
1:A:325:LYS:C	1:A:327:VAL:HG12	2.36	0.51
1:A:90:THR:HG22	1:A:95:ARG:O	2.12	0.50
1:A:395:ARG:HE	1:A:396:THR:CB	2.24	0.50
1:A:89:ARG:O	1:A:92:ALA:HB3	2.12	0.50
1:A:125:LEU:HD11	1:A:172:ILE:HG23	1.93	0.50
1:A:325:LYS:HB2	1:A:327:VAL:HG12	1.94	0.49
1:A:123:ARG:N	1:A:124:PRO:HD2	2.27	0.49
1:A:329:ARG:O	1:A:329:ARG:CD	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ALA:N	1:A:132:ASN:OD1	2.46	0.49
1:A:150:ASP:OD1	1:A:151:ILE:N	2.45	0.49
1:A:462:SER:HA	1:A:465:SER:H	1.78	0.49
1:A:148:ASN:C	1:A:148:ASN:ND2	2.70	0.49
1:A:211:MET:HA	1:A:530:MET:O	2.12	0.49
1:A:33:GLN:HA	1:A:33:GLN:NE2	2.28	0.49
1:A:325:LYS:CE	1:A:326:ASN:N	2.59	0.49
1:A:347:ILE:HD13	1:A:347:ILE:H	1.78	0.49
1:A:120:ARG:HB2	1:A:121:PRO:HD3	1.95	0.49
1:A:257:GLN:CB	1:A:258:PRO:HD3	2.27	0.49
1:A:327:VAL:O	1:A:331:ARG:HD3	2.12	0.49
1:A:159:ALA:CB	1:A:242:ILE:HD12	2.42	0.48
1:A:480:ILE:HD13	1:A:480:ILE:N	2.28	0.48
1:A:67:VAL:HG11	1:A:161:LEU:HD23	1.95	0.48
1:A:437:VAL:HG11	1:A:482:ALA:H	1.75	0.48
1:A:480:ILE:H	1:A:480:ILE:CD1	2.25	0.48
1:A:55:MET:HG2	1:A:64:PHE:CD1	2.46	0.48
1:A:86:TYR:C	1:A:87:GLN:HG3	2.37	0.48
1:A:372:GLN:CB	1:A:456:GLU:HG2	2.34	0.48
1:A:347:ILE:O	1:A:348:ARG:HB2	2.13	0.48
1:A:350:LEU:HD23	1:A:368:ARG:HB2	1.94	0.48
1:A:343:GLU:HB3	1:A:346:MET:HG2	1.96	0.48
1:A:493:LYS:HG3	1:A:498:TYR:HB3	1.96	0.48
1:A:518:VAL:HG12	1:A:525:ILE:HD12	1.95	0.48
1:A:509:ASP:C	1:A:511:LEU:N	2.68	0.48
1:A:191:ASP:HA	1:A:194:LYS:HG3	1.96	0.48
1:A:338:ARG:HH11	1:A:338:ARG:CB	2.08	0.47
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.78	0.47
1:A:33:GLN:NE2	1:A:38:THR:HB	2.29	0.47
1:A:522:ARG:HG3	1:A:554:LEU:CD2	2.42	0.47
1:A:325:LYS:CA	1:A:327:VAL:HG12	2.45	0.47
1:A:523:ASP:N	1:A:523:ASP:OD1	2.47	0.47
1:A:538:THR:CG2	1:A:539:LYS:H	2.28	0.47
1:A:125:LEU:HD11	1:A:172:ILE:HG21	1.96	0.47
1:A:347:ILE:O	1:A:348:ARG:CB	2.63	0.47
1:A:148:ASN:ND2	1:A:149:PRO:HD2	2.30	0.46
1:A:110:GLY:O	1:A:114:ILE:HD12	2.16	0.46
1:A:171:PRO:HB2	1:A:239:ILE:HG23	1.97	0.46
1:A:505:LEU:O	1:A:506:GLY:C	2.59	0.46
1:A:440:ASP:OD2	1:A:440:ASP:N	2.48	0.46
1:A:323:ILE:CG1	1:A:324:GLU:H	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:HG13	1:A:555:HIS:CD2	2.50	0.46
1:A:90:THR:HG21	1:A:97:PRO:HD3	1.97	0.46
1:A:362:GLY:HA3	1:A:476:ALA:HB2	1.98	0.46
1:A:206:GLU:HG3	1:A:207:ALA:H	1.81	0.45
1:A:379:LEU:HD23	1:A:379:LEU:N	2.30	0.45
1:A:33:GLN:HE22	1:A:38:THR:HB	1.81	0.45
1:A:122:ILE:C	1:A:122:ILE:HD12	2.41	0.45
1:A:500:VAL:CG1	1:A:548:GLN:CD	2.89	0.45
1:A:127:PRO:O	1:A:128:GLU:C	2.59	0.45
1:A:539:LYS:O	1:A:542:MET:C	2.59	0.45
1:A:350:LEU:CD2	1:A:368:ARG:HB2	2.46	0.45
1:A:454:ILE:HD12	1:A:454:ILE:N	2.30	0.45
1:A:154:MET:HE1	1:A:211:MET:HE2	1.99	0.45
1:A:28:ILE:N	1:A:28:ILE:HD12	2.32	0.45
1:A:375:VAL:HG21	1:A:468:GLY:HA3	1.98	0.45
1:A:403:TYR:HD1	1:A:454:ILE:HD11	1.82	0.45
1:A:537:ILE:HD12	1:A:537:ILE:N	2.25	0.45
1:A:177:VAL:HA	1:A:185:VAL:O	2.17	0.45
1:A:401:PHE:HA	1:A:450:VAL:O	2.16	0.45
1:A:209:VAL:HG23	1:A:232:HIS:ND1	2.31	0.45
1:A:36:GLN:H	1:A:36:GLN:HG3	1.54	0.44
1:A:332:VAL:CG2	1:A:492:VAL:HG11	2.46	0.44
1:A:424:ILE:HG23	1:A:426:HIS:CD2	2.52	0.44
1:A:522:ARG:HH12	1:A:557:LEU:HB2	1.81	0.44
1:A:460:SER:O	1:A:461:SER:HB3	2.17	0.44
1:A:41:LEU:HD13	1:A:242:ILE:HD13	2.00	0.44
1:A:30:ARG:HG3	1:A:30:ARG:NH1	2.30	0.44
1:A:22:ILE:C	1:A:23:THR:HG23	2.43	0.44
1:A:108:SER:O	1:A:111:GLU:HB2	2.18	0.44
1:A:151:ILE:HD13	1:A:151:ILE:H	1.83	0.44
1:A:489:MET:HE3	1:A:549:ALA:CA	2.45	0.44
1:A:323:ILE:HD13	1:A:323:ILE:H	1.82	0.43
1:A:338:ARG:HH12	1:A:339:ILE:CG1	2.32	0.43
1:A:403:TYR:OH	1:A:462:SER:HB3	2.18	0.43
1:A:461:SER:HB2	1:A:462:SER:H	1.51	0.43
1:A:328:VAL:HG13	1:A:338:ARG:HG2	2.00	0.43
1:A:333:LEU:HD22	1:A:333:LEU:N	2.33	0.43
1:A:123:ARG:N	1:A:124:PRO:CD	2.81	0.43
1:A:230:PHE:O	1:A:234:GLN:HG2	2.17	0.43
1:A:237:VAL:O	1:A:241:ASN:ND2	2.48	0.43
1:A:171:PRO:HG2	1:A:243:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:HB3	1:A:246:VAL:HG21	2.01	0.43
1:A:352:VAL:HG13	1:A:471:LEU:CD1	2.49	0.43
1:A:368:ARG:HG2	1:A:368:ARG:NH1	2.28	0.43
1:A:329:ARG:O	1:A:332:VAL:HG11	2.19	0.43
1:A:512:GLY:O	1:A:513:ASP:HB2	2.19	0.43
1:A:127:PRO:HG3	1:A:167:PRO:CB	2.49	0.43
1:A:326:ASN:O	1:A:330:SER:CB	2.67	0.43
1:A:327:VAL:CG1	1:A:328:VAL:N	2.82	0.43
1:A:493:LYS:HE2	1:A:495:GLY:O	2.18	0.43
1:A:232:HIS:HA	1:A:235:GLN:NE2	2.18	0.42
1:A:333:LEU:O	1:A:334:ALA:C	2.60	0.42
1:A:543:GLN:O	1:A:547:ASN:CB	2.63	0.42
1:A:30:ARG:HB3	1:A:245:LEU:HD12	2.00	0.42
1:A:41:LEU:CD1	1:A:242:ILE:HD13	2.49	0.42
1:A:337:PRO:O	1:A:341:GLY:HA2	2.19	0.42
1:A:214:SER:OG	1:A:528:LEU:HB3	2.19	0.42
1:A:353:ARG:HG3	1:A:353:ARG:HH11	1.85	0.42
1:A:489:MET:SD	1:A:502:SER:HA	2.60	0.42
1:A:176:ARG:HA	1:A:200:LEU:O	2.19	0.42
1:A:437:VAL:CG1	1:A:480:ILE:HB	2.48	0.42
1:A:535:GLU:HA	2:A:579:HOH:O	2.20	0.42
1:A:72:LYS:HG2	1:A:73:ALA:O	2.19	0.42
1:A:82:LEU:C	1:A:82:LEU:HD22	2.44	0.42
1:A:332:VAL:HG22	1:A:492:VAL:HG11	2.02	0.42
1:A:332:VAL:HG12	1:A:333:LEU:HD22	1.98	0.42
1:A:22:ILE:C	1:A:23:THR:CG2	2.92	0.42
1:A:462:SER:HB2	1:A:465:SER:OG	2.20	0.42
1:A:525:ILE:CD1	1:A:553:ARG:NH1	2.83	0.42
1:A:534:ILE:CD1	1:A:537:ILE:HD11	2.48	0.42
1:A:225:LEU:C	1:A:227:ALA:N	2.78	0.42
1:A:403:TYR:CE2	1:A:427:GLY:HA3	2.54	0.42
1:A:438:MET:HA	1:A:438:MET:HE2	2.01	0.42
1:A:340:ASP:O	1:A:342:ARG:CG	2.61	0.41
1:A:329:ARG:NH2	1:A:513:ASP:CG	2.78	0.41
1:A:72:LYS:HB2	1:A:72:LYS:HZ1	1.86	0.41
1:A:323:ILE:O	1:A:324:GLU:C	2.63	0.41
1:A:342:ARG:NH2	1:A:347:ILE:HA	2.35	0.41
1:A:439:PRO:HG3	1:A:479:PRO:O	2.21	0.41
1:A:361:HIS:O	1:A:476:ALA:HA	2.20	0.41
1:A:438:MET:CE	1:A:473:LEU:HD13	2.51	0.41
1:A:326:ASN:O	1:A:329:ARG:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:HB2	1:A:453:GLU:HG2	2.02	0.41
1:A:539:LYS:C	1:A:541:ILE:N	2.79	0.41
1:A:396:THR:C	1:A:397:ASP:O	2.57	0.41
1:A:130:PHE:CE1	1:A:167:PRO:HD2	2.56	0.41
1:A:338:ARG:NH1	1:A:339:ILE:H	2.15	0.41
1:A:435:LEU:CD2	1:A:435:LEU:O	2.69	0.41
1:A:496:ASP:OD1	1:A:496:ASP:N	2.53	0.41
1:A:26:ASN:O	1:A:27:PRO:C	2.64	0.41
1:A:179:TYR:CE2	1:A:182:ASP:HA	2.56	0.40
1:A:230:PHE:CD1	1:A:230:PHE:C	2.98	0.40
1:A:162:SER:O	1:A:164:SER:O	2.40	0.40
1:A:426:HIS:O	1:A:429:LEU:HB2	2.21	0.40
1:A:440:ASP:O	1:A:441:MET:HB3	2.21	0.40
1:A:77:GLN:O	1:A:78:ASP:HB3	2.21	0.40
1:A:462:SER:CB	1:A:465:SER:HB2	2.50	0.40
1:A:94:GLY:HA2	2:A:584:HOH:O	2.20	0.40

All (2) 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:A:30:ARG:NH1	1:A:30:ARG:NH1[18_444]	2.09	0.11
1:A:30:ARG:NH2	1:A:30:ARG:NH2[18_444]	2.15	0.05

## 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	433/559 (78%)	381 (88%)	30 (7%)	22 (5%)	<b>1</b> <b>5</b>

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	PRO
1	A	256	TRP
1	A	324	GLU
1	A	326	ASN
1	A	337	PRO
1	A	343	GLU
1	A	407	PRO
1	A	457	SER
1	A	460	SER
1	A	71	LYS
1	A	259	GLU
1	A	338	ARG
1	A	341	GLY
1	A	506	GLY
1	A	543	GLN
1	A	74	LYS
1	A	344	LYS
1	A	167	PRO
1	A	463	MET
1	A	78	ASP
1	A	26	ASN
1	A	76	GLY

### 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	364/456 (80%)	294 (81%)	70 (19%)	<b>1</b> <b>5</b>

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	23	THR
1	A	33	GLN
1	A	36	GLN
1	A	38	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	40	THR
1	A	66	THR
1	A	68	VAL
1	A	70	GLN
1	A	71	LYS
1	A	72	LYS
1	A	74	LYS
1	A	82	LEU
1	A	83	THR
1	A	87	GLN
1	A	89	ARG
1	A	109	GLU
1	A	113	LEU
1	A	116	ARG
1	A	139	THR
1	A	151	ILE
1	A	164	SER
1	A	183	GLN
1	A	186	LEU
1	A	198	LEU
1	A	200	LEU
1	A	206	GLU
1	A	211	MET
1	A	214	SER
1	A	217	GLN
1	A	222	ASP
1	A	225	LEU
1	A	253	ARG
1	A	258	PRO
1	A	259	GLU
1	A	323	ILE
1	A	324	GLU
1	A	325	LYS
1	A	331	ARG
1	A	337	PRO
1	A	338	ARG
1	A	340	ASP
1	A	342	ARG
1	A	344	LYS
1	A	346	MET
1	A	347	ILE
1	A	354	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	365	LEU
1	A	367	THR
1	A	374	LEU
1	A	378	THR
1	A	394	GLU
1	A	395	ARG
1	A	396	THR
1	A	428	ARG
1	A	435	LEU
1	A	440	ASP
1	A	457	SER
1	A	458	ASN
1	A	463	MET
1	A	474	MET
1	A	480	ILE
1	A	496	ASP
1	A	500	VAL
1	A	528	LEU
1	A	533	LYS
1	A	537	ILE
1	A	540	GLU
1	A	546	LEU
1	A	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	33	GLN
1	A	70	GLN
1	A	85	ASN
1	A	148	ASN
1	A	181	ASN
1	A	183	GLN
1	A	217	GLN
1	A	372	GLN
1	A	426	HIS
1	A	548	GLN
1	A	555	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	445/559 (79%)	1.02	77 (17%) <b>4</b> <b>3</b>	19, 84, 151, 166	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	457	SER	5.6
1	A	563	ALA	5.3
1	A	424	ILE	5.2
1	A	536	GLY	4.7
1	A	461	SER	4.6
1	A	538	THR	4.5
1	A	339	ILE	4.4
1	A	462	SER	4.3
1	A	110	GLY	4.2
1	A	333	LEU	4.1
1	A	340	ASP	4.0
1	A	426	HIS	3.9
1	A	334	ALA	3.8
1	A	425	GLY	3.8
1	A	108	SER	3.7
1	A	541	ILE	3.6
1	A	459	GLY	3.5
1	A	21	ASP	3.3
1	A	338	ARG	3.3
1	A	427	GLY	3.3
1	A	502	SER	3.2
1	A	258	PRO	3.2
1	A	407	PRO	3.2
1	A	539	LYS	3.1
1	A	22	ILE	3.1
1	A	131	VAL	3.0
1	A	335	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	130	PHE	3.0
1	A	322	ALA	3.0
1	A	501	LEU	3.0
1	A	458	ASN	2.9
1	A	336	GLU	2.9
1	A	25	LEU	2.9
1	A	164	SER	2.8
1	A	254	TRP	2.8
1	A	79	PHE	2.8
1	A	78	ASP	2.8
1	A	537	ILE	2.8
1	A	443	LYS	2.7
1	A	332	VAL	2.7
1	A	24	LEU	2.7
1	A	337	PRO	2.7
1	A	511	LEU	2.7
1	A	165	GLY	2.7
1	A	499	VAL	2.6
1	A	460	SER	2.6
1	A	80	PHE	2.5
1	A	397	ASP	2.4
1	A	513	ASP	2.4
1	A	166	ILE	2.4
1	A	23	THR	2.3
1	A	253	ARG	2.3
1	A	38	THR	2.3
1	A	260	PRO	2.3
1	A	170	GLY	2.3
1	A	463	MET	2.2
1	A	125	LEU	2.2
1	A	408	TYR	2.2
1	A	423	GLU	2.2
1	A	242	ILE	2.2
1	A	442	ASP	2.2
1	A	252	PRO	2.2
1	A	330	SER	2.2
1	A	445	PRO	2.2
1	A	495	GLY	2.2
1	A	546	LEU	2.2
1	A	70	GLN	2.2
1	A	498	TYR	2.2
1	A	207	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	500	VAL	2.1
1	A	35	GLY	2.1
1	A	256	TRP	2.1
1	A	36	GLN	2.1
1	A	328	VAL	2.1
1	A	440	ASP	2.0
1	A	163	LEU	2.0
1	A	551	GLY	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.