Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 08:37 AM EDT

PDB ID	:	3CDJ
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

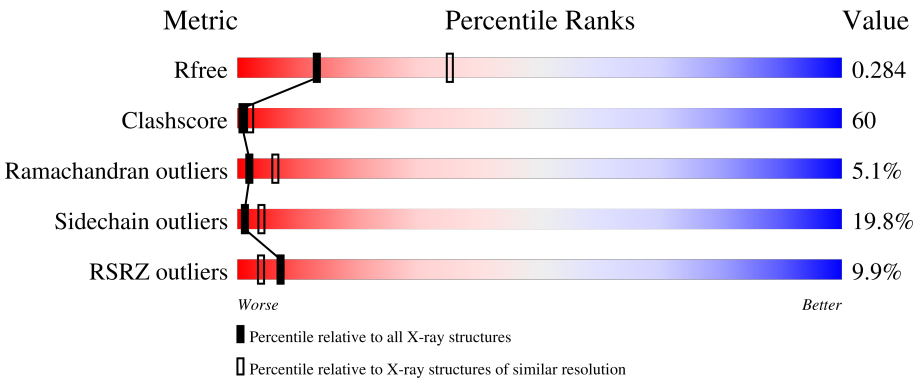
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	8%; 30%, 34%, 11%, •, 20%

2 Entry composition (i)

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.

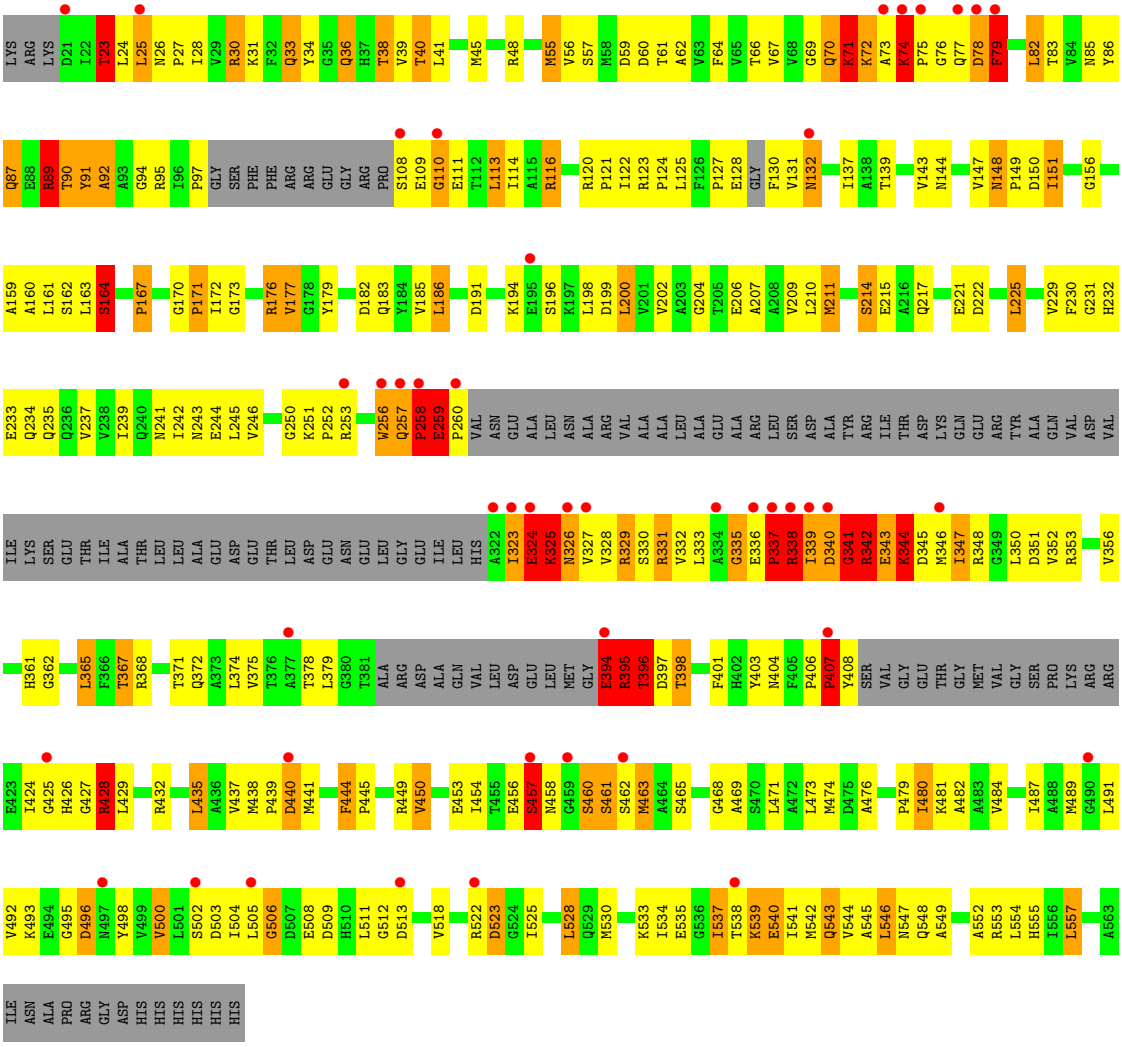
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	36	36	36	0	0

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: Polynucleotide phosphorylase

Chain A: 8% 30% 34% 11% • 20%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	160.09Å 160.09Å 153.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.80) 95.2 (49.58-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.30 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.270 , 0.294 0.280 , 0.284	Depositor DCC
R_{free} test set	1817 reflections (10.22%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 82.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3418	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.18	17/3432 (0.5%)	1.29	49/4648 (1.1%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TYR	CG-CD2	19.43	1.64	1.39
1	A	91	TYR	CE1-CZ	14.92	1.57	1.38
1	A	91	TYR	CA-CB	9.33	1.74	1.53
1	A	91	TYR	CE2-CZ	7.95	1.48	1.38
1	A	396	THR	CA-C	-7.09	1.34	1.52
1	A	90	THR	CA-C	5.92	1.68	1.52
1	A	92	ALA	C-O	5.75	1.34	1.23
1	A	91	TYR	CB-CG	-5.49	1.43	1.51
1	A	398	THR	CA-CB	-5.32	1.39	1.53
1	A	258	PRO	CA-CB	-5.29	1.43	1.53
1	A	256	TRP	N-CA	-5.25	1.35	1.46
1	A	395	ARG	N-CA	-5.16	1.36	1.46
1	A	450	VAL	N-CA	-5.15	1.36	1.46
1	A	257	GLN	C-N	-5.10	1.24	1.34
1	A	177	VAL	CB-CG2	5.09	1.63	1.52
1	A	89	ARG	CA-CB	5.08	1.65	1.53
1	A	91	TYR	N-CA	5.04	1.56	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	395	ARG	N-CA-C	17.06	157.07	111.00
1	A	91	TYR	CB-CG-CD1	11.83	128.10	121.00
1	A	91	TYR	CB-CG-CD2	-11.70	113.98	121.00
1	A	338	ARG	N-CA-C	10.67	139.81	111.00
1	A	395	ARG	N-CA-CB	-10.61	91.50	110.60
1	A	257	GLN	N-CA-C	-10.48	82.70	111.00
1	A	256	TRP	N-CA-C	-10.14	83.62	111.00
1	A	164	SER	N-CA-C	-9.96	84.12	111.00
1	A	463	MET	N-CA-C	-9.58	85.12	111.00
1	A	170	GLY	C-N-CD	-9.24	100.28	120.60
1	A	461	SER	N-CA-C	9.06	135.47	111.00
1	A	24	LEU	CA-CB-CG	8.24	134.26	115.30
1	A	457	SER	N-CA-C	8.18	133.08	111.00
1	A	335	GLY	N-CA-C	-8.15	92.73	113.10
1	A	337	PRO	C-N-CA	7.91	141.47	121.70
1	A	256	TRP	CB-CA-C	-7.45	95.50	110.40
1	A	339	ILE	N-CA-C	-6.82	92.59	111.00
1	A	132	ASN	N-CA-C	-6.82	92.60	111.00
1	A	257	GLN	N-CA-CB	6.79	122.83	110.60
1	A	407	PRO	N-CA-C	6.70	129.51	112.10
1	A	342	ARG	N-CA-C	-6.59	93.21	111.00
1	A	257	GLN	C-N-CD	-6.54	106.22	120.60
1	A	164	SER	CB-CA-C	-6.49	97.77	110.10
1	A	61	THR	N-CA-C	-6.35	93.85	111.00
1	A	394	GLU	CA-C-N	-6.34	103.25	117.20
1	A	23	THR	N-CA-C	6.33	128.08	111.00
1	A	199	ASP	N-CA-C	-6.31	93.96	111.00
1	A	89	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	91	TYR	CG-CD1-CE1	6.23	126.28	121.30
1	A	215	GLU	N-CA-C	-6.11	94.49	111.00
1	A	25	LEU	N-CA-C	6.02	127.26	111.00
1	A	337	PRO	CA-C-N	-5.95	104.12	117.20
1	A	444	PHE	N-CA-C	-5.77	95.41	111.00
1	A	70	GLN	CA-CB-CG	-5.75	100.76	113.40
1	A	428	ARG	N-CA-C	-5.74	95.50	111.00
1	A	396	THR	C-N-CA	-5.66	107.54	121.70
1	A	144	ASN	N-CA-C	-5.51	96.11	111.00
1	A	341	GLY	N-CA-C	-5.50	99.34	113.10
1	A	91	TYR	O-C-N	5.49	131.48	122.70
1	A	325	LYS	N-CA-C	5.46	125.73	111.00
1	A	79	PHE	CB-CA-C	5.38	121.17	110.40
1	A	461	SER	CA-C-N	-5.31	105.52	117.20
1	A	395	ARG	CA-C-N	-5.29	105.56	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	GLY	N-CA-C	-5.27	99.92	113.10
1	A	176	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	257	GLN	C-N-CA	5.18	143.75	122.00
1	A	407	PRO	CA-N-CD	-5.12	104.33	111.50
1	A	449	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	396	THR	CB-CA-C	-5.01	98.07	111.60

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	405	2
2	A	36	0	0	4	0
All	All	3418	0	3415	405	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 60.

All (405) 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:395:ARG:HG2	1:A:396:THR:N	1.40	1.19
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: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:395:ARG:NE	1:A:396:THR:HB	1.64	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:GLN:CD	1:A:71:LYS:N	2.07	1.07
1:A:116:ARG:HH11	1:A:116:ARG:HB3	1.21	1.04
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: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:335:GLY:C	1:A:337:PRO:HD2	1.84	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:325:LYS:C	1:A:327:VAL:H	1.65	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:325:LYS:HB2	1:A:328:VAL:HG23	1.52	0.92
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:69:GLY:O	1:A:70:GLN:NE2	2.05	0.90
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:70:GLN:NE2	1:A:70:GLN:C	2.29	0.86
1:A:395:ARG:HG2	1:A:396:THR:H	1.39	0.86
1:A:332:VAL:CG1	1:A:333:LEU:HD22	2.06	0.85
1:A:225:LEU:HD21	1:A:542:MET:HE3	1.57	0.84
1:A:342:ARG:HH21	1:A:346:MET:C	1.80	0.84
1:A:69:GLY:C	1:A:70:GLN:CG	2.44	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:A:445:PRO:C	2.01	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:225:LEU:HD21	1:A:542:MET:CE	2.11	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
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:425:GLY:C	1:A:427:GLY:H	1.89	0.76
1:A:456:GLU:O	1:A:457:SER:HB2	1.86	0.76
1:A:441:MET:HE3	1:A:445:PRO:O	1.86	0.76
1:A:487:ILE:HG12	1:A:489:MET:HE2	1.65	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:325:LYS:HG2	1:A:326:ASN:N	2.01	0.74
1:A:242:ILE:O	1:A:246:VAL:HG23	1.88	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:HG23	1:A:396:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:396:THR:O	1:A:397:ASP:C	2.21	0.71
1:A:23:THR:O	1:A:23:THR:OG1	2.04	0.71
1:A:70:GLN:CD	1:A:70:GLN:C	2.49	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:259:GLU:CB	1:A:260:PRO:HD2	2.22	0.70
1:A:70:GLN:CD	1:A:71:LYS:CA	2.60	0.70
1:A:74:LYS:HB2	1:A:75:PRO:CD	2.23	0.69
1:A:487:ILE:HG12	1:A:489:MET:CE	2.22	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
1:A:347:ILE:O	1:A:503:ASP:OD1	2.12	0.68
1:A:425:GLY:C	1:A:427:GLY:N	2.44	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: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:221:GLU:HG3	1:A:546:LEU:HD12	1.77	0.66
1:A:504:ILE:O	1:A:504:ILE:HG13	1.95	0.66
1:A:462:SER:HG	1:A:465:SER:HB2	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:427:GLY:C	1:A:429:LEU:N	2.49	0.64
1:A:351:ASP:OD1	1:A:353:ARG:NH1	2.30	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: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
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: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: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:209:VAL:C	1:A:210:LEU:HD23	2.22	0.60
1:A:343:GLU:H	1:A:346:MET:CG	2.13	0.60
1:A:55:MET:HG2	1:A:64:PHE:HD1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:327:VAL:O	1:A:331:ARG:CD	2.50	0.59
1:A:438:MET:HE3	1:A:473:LEU:HD13	1.84	0.59
1:A:70:GLN:OE1	1:A:71:LYS:C	2.41	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:231:GLY:O	1:A:235:GLN:HG3	2.03	0.59
1:A:327:VAL:HG13	1:A:328:VAL:N	2.18	0.59
1:A:148:ASN:HD22	1:A:148:ASN:C	2.05	0.58
1:A:148:ASN:ND2	1:A:150:ASP:H	1.99	0.58
1:A:91:TYR:CB	1:A:91:TYR:C	2.66	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
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: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:489:MET:HE1	1:A:549:ALA:HA	1.88	0.56
1:A:340:ASP:C	1:A:342:ARG:N	2.58	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:539:LYS:O	1:A:540:GLU:C	2.44	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: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: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: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:69:GLY:O	1:A:70:GLN:CD	2.47	0.52
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: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:329:ARG:NH2	1:A:513:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:441:MET:CE	1:A:445:PRO:C	2.73	0.50
1:A:90:THR:HG22	1:A:95:ARG:O	2.12	0.50
1:A:325:LYS:C	1:A:327:VAL:N	2.33	0.50
1:A:441:MET:CE	1:A:445:PRO:HA	2.41	0.50
1:A:441:MET:HE2	1:A:445:PRO:HA	1.92	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:245:LEU:HD23	1:A:245:LEU:C	2.33	0.49
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
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: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:487:ILE:CG1	1:A:489:MET:HE2	2.40	0.49
1:A:539:LYS:HD2	1:A:539:LYS:C	2.34	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:74:LYS:O	1:A:75:PRO:C	2.48	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:427:GLY:C	1:A:429:LEU:H	2.08	0.48
1:A:493:LYS:HG3	1:A:498:TYR:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:HG12	1:A:525:ILE:HD12	1.95	0.48
1:A:438:MET:HE3	1:A:473:LEU:CD1	2.44	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:162:SER:C	1:A:164:SER:O	2.53	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:70:GLN:C	1:A:71:LYS:HG2	2.33	0.46
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:509:ASP:C	1:A:511:LEU:N	2.68	0.46
1:A:440:ASP:OD2	1:A:440:ASP:N	2.48	0.46
1:A:325:LYS:C	1:A:327:VAL:HG12	2.36	0.46
1:A:323:ILE:CG1	1:A:324:GLU:H	2.27	0.46
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:441:MET:HE1	1:A:445:PRO:O	2.15	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: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: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:148:ASN:C	1:A:148:ASN:ND2	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:GLN:C	1:A:71:LYS:CG	2.82	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: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:86:TYR:C	1:A:87:GLN:HG3	2.37	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
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:489:MET:HE1	1:A:552:ALA:HB3	1.99	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: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:332:VAL:HG22	1:A:492:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:HG12	1:A:333:LEU:HD22	1.98	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:403:TYR:CE2	1:A:427:GLY:HA3	2.54	0.42
1:A:340:ASP:O	1:A:342:ARG:CG	2.61	0.41
1:A:505:LEU:O	1:A:506:GLY:C	2.59	0.41
1:A:72:LYS:HB2	1:A:72:LYS:HZ1	1.86	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:122:ILE:C	1:A:122:ILE:HD12	2.41	0.41
1:A:55:MET:HE1	1:A:62:ALA:HB1	2.02	0.41
1:A:404:ASN:HB2	1:A:453:GLU:HG2	2.02	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:127:PRO:O	1:A:128:GLU:C	2.59	0.41
1:A:500:VAL:CG1	1:A:548:GLN:CD	2.89	0.40
1:A:539:LYS:O	1:A:542:MET:C	2.59	0.40
1:A:179:TYR:CE2	1:A:182:ASP:HA	2.56	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%)	2 6

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%)	292 (80%)	72 (20%)	1 4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	30	ARG
1	A	33	GLN
1	A	36	GLN
1	A	38	THR
1	A	40	THR
1	A	48	ARG
1	A	55	MET
1	A	60	ASP
1	A	66	THR
1	A	71	LYS
1	A	72	LYS
1	A	74	LYS
1	A	79	PHE
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	148	ASN
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	211	MET
1	A	214	SER
1	A	217	GLN
1	A	222	ASP
1	A	225	LEU
1	A	253	ARG

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Mol	Chain	Res	Type
1	A	258	PRO
1	A	259	GLU
1	A	323	ILE
1	A	324	GLU
1	A	325	LYS
1	A	329	ARG
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	347	ILE
1	A	365	LEU
1	A	367	THR
1	A	374	LEU
1	A	378	THR
1	A	395	ARG
1	A	396	THR
1	A	408	TYR
1	A	428	ARG
1	A	435	LEU
1	A	440	ASP
1	A	457	SER
1	A	458	ASN
1	A	474	MET
1	A	480	ILE
1	A	496	ASP
1	A	500	VAL
1	A	523	ASP
1	A	528	LEU
1	A	533	LYS
1	A	537	ILE
1	A	539	LYS
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	70	GLN
1	A	85	ASN
1	A	148	ASN
1	A	181	ASN
1	A	183	GLN
1	A	372	GLN
1	A	497	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	445/559 (79%)	0.72	44 (9%) 7 4	19, 84, 151, 166	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	5.2
1	A	336	GLU	4.4
1	A	78	ASP	4.3
1	A	260	PRO	4.2
1	A	257	GLN	4.1
1	A	339	ILE	4.1
1	A	338	ARG	3.9
1	A	457	SER	3.6
1	A	132	ASN	3.4
1	A	538	THR	3.4
1	A	327	VAL	3.3
1	A	322	ALA	3.2
1	A	258	PRO	3.2
1	A	79	PHE	3.2
1	A	75	PRO	3.1
1	A	77	GLN	3.1
1	A	394	GLU	3.0
1	A	25	LEU	3.0
1	A	108	SER	3.0
1	A	505	LEU	2.9
1	A	110	GLY	2.7
1	A	497	ASN	2.7
1	A	462	SER	2.6
1	A	253	ARG	2.6
1	A	323	ILE	2.6
1	A	502	SER	2.5
1	A	425	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	440	ASP	2.5
1	A	21	ASP	2.4
1	A	256	TRP	2.4
1	A	337	PRO	2.3
1	A	346	MET	2.3
1	A	74	LYS	2.2
1	A	195	GLU	2.2
1	A	326	ASN	2.2
1	A	407	PRO	2.2
1	A	340	ASP	2.2
1	A	324	GLU	2.1
1	A	513	ASP	2.1
1	A	459	GLY	2.1
1	A	377	ALA	2.1
1	A	522	ARG	2.1
1	A	490	GLY	2.0
1	A	73	ALA	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 monosaccharides 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.