



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:11 PM UTC

PDB ID : 1IT8 / pdb_00001it8
Title : Crystal structure of archaeosine tRNA-guanine transglycosylase from *Pyrococcus horikoshii* complexed with archaeosine precursor, preQ0
Authors : Ishitani, R.; Nureki, O.; Fukai, S.; Kijimoto, T.; Nameki, N.; Watanabe, M.; Kondo, H.; Sekine, M.; Okada, N.; Nishimura, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-01-11
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

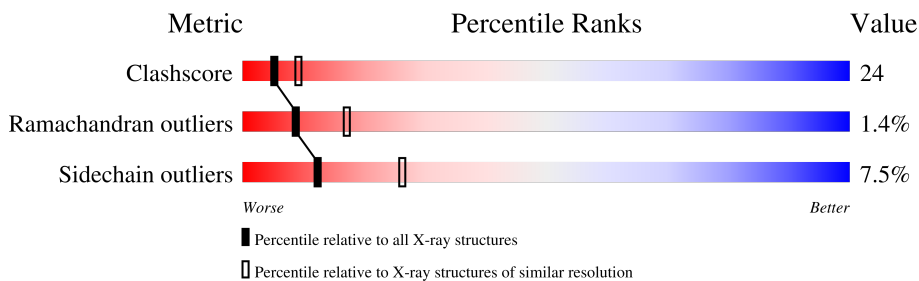
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	
1	B	582	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9463 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 archaeosine tRNA-guanine transglycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4652	2970	815	848	19			
1	B	577	Total	C	N	O	S	0	0	0
			4652	2970	815	848	19			

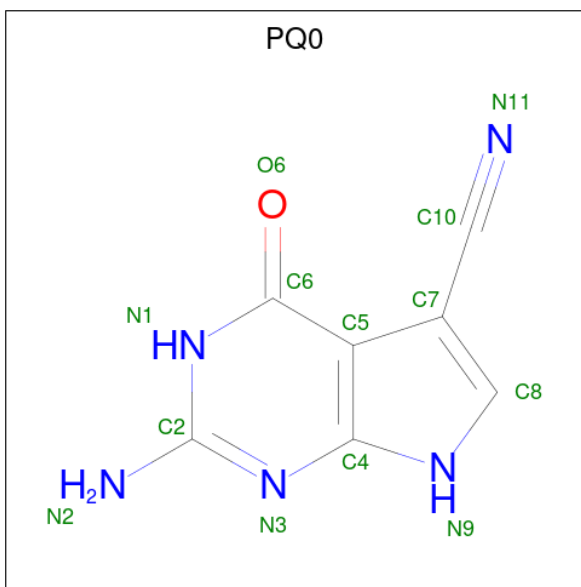
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-AMINO-4-OXO-4,7-DIHYDRO-3H-PYRROLO[2,3-D]PYRIMIDINE-5-CARBONITRILE (CCD ID: PQ0) (formula: C₇H₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	7	5	1		

- Molecule 5 is water.

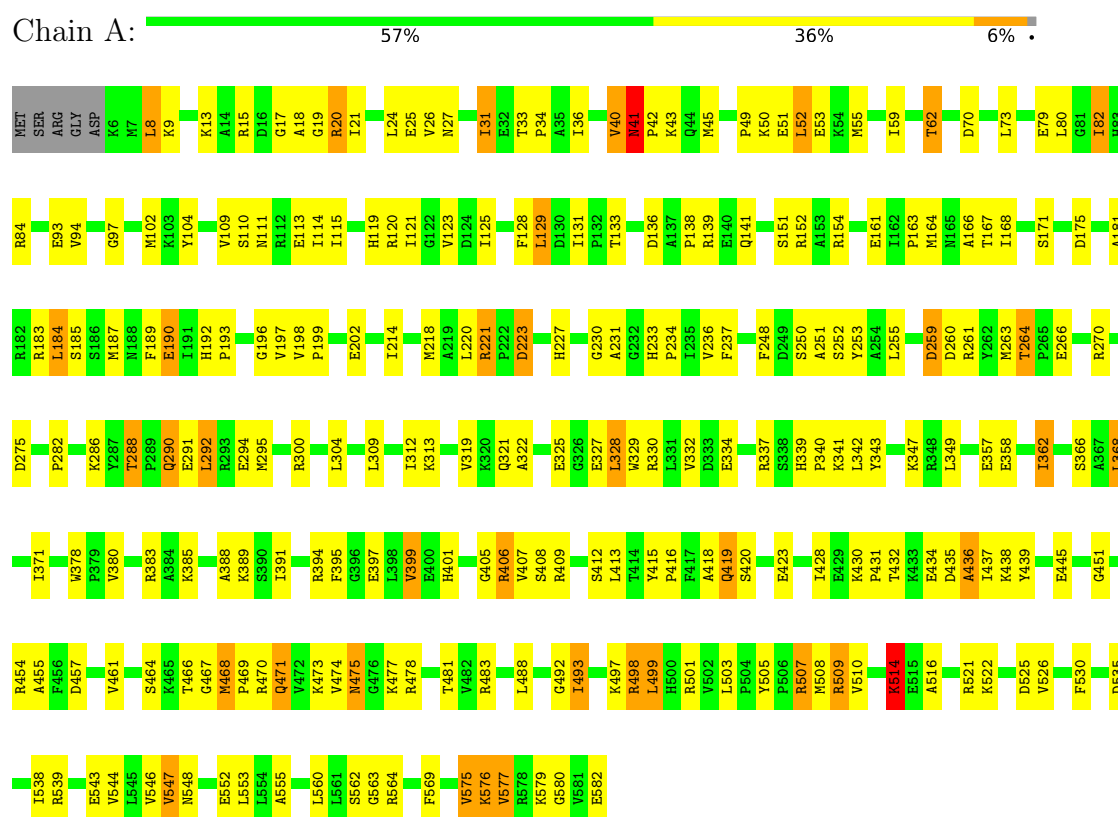
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	B	66	Total	O	0	0
			66	66		

3 Residue-property plots

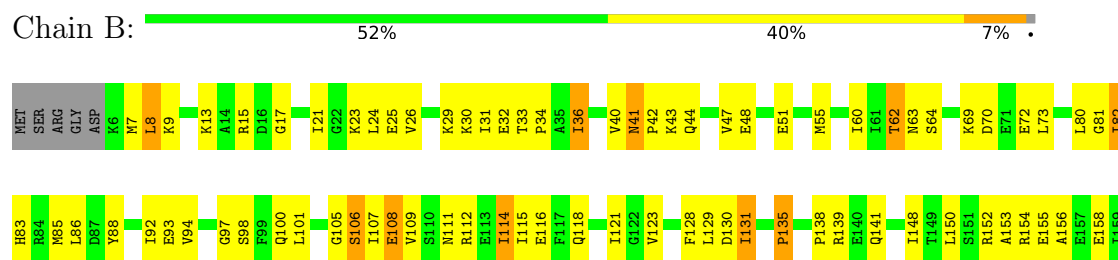
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: archaeosine tRNA-guanine transglycosylase



• Molecule 1: archaeosine tRNA-guanine transglycosylase





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.47 Å 100.47 Å 366.17 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.87 – 2.50	Depositor
% Data completeness (in resolution range)	95.9 (34.87-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9463	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQ0, MG, ZN

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	0.47	0/4745	1.00	21/6391 (0.3%)
1	B	0.44	0/4745	1.01	21/6391 (0.3%)
All	All	0.46	0/9490	1.00	42/12782 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ALA	N-CA-C	-10.26	101.07	114.31
1	A	251	ALA	N-CA-C	-8.41	103.21	113.97
1	A	514	LYS	N-CA-C	-7.94	102.70	111.36
1	B	97	GLY	N-CA-C	-7.12	104.75	115.00
1	A	21	ILE	N-CA-C	-6.84	98.58	108.36
1	B	434	GLU	N-CA-C	-6.82	102.97	112.45
1	A	97	GLY	N-CA-C	-6.46	105.84	114.95
1	A	18	ALA	N-CA-C	-6.38	105.79	112.93
1	A	509	ARG	N-CA-C	6.00	119.86	110.32
1	B	100	GLN	N-CA-C	-6.00	104.86	111.82
1	B	93	GLU	N-CA-C	-5.98	101.15	110.42
1	B	167	THR	N-CA-C	5.98	118.39	109.59
1	A	131	ILE	N-CA-C	5.97	113.47	107.55
1	A	223	ASP	N-CA-C	5.96	120.17	113.02
1	B	169	GLN	N-CA-C	5.83	118.86	109.83
1	B	229	PHE	N-CA-C	5.79	118.88	110.42
1	B	164	MET	N-CA-C	5.74	117.90	109.24
1	B	195	GLY	N-CA-C	5.69	122.54	112.64
1	B	475	ASN	N-CA-C	-5.66	106.76	113.38
1	A	468	MET	N-CA-C	5.61	118.39	109.64
1	A	275	ASP	N-CA-C	-5.57	107.03	113.88
1	B	131	ILE	N-CA-C	5.52	112.58	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	GLU	N-CA-C	-5.42	101.63	110.20
1	A	221	ARG	N-CA-C	-5.41	101.55	109.50
1	B	48	GLU	N-CA-C	5.38	115.78	109.60
1	B	535	ASP	CA-C-N	5.36	125.03	119.56
1	B	535	ASP	C-N-CA	5.36	125.03	119.56
1	A	577	VAL	N-CA-C	5.33	116.26	108.58
1	B	403	ILE	N-CA-C	5.33	116.39	111.81
1	A	52	LEU	N-CA-C	-5.20	105.61	111.28
1	A	41	ASN	CA-C-N	5.15	125.19	119.32
1	A	41	ASN	C-N-CA	5.15	125.19	119.32
1	A	167	THR	N-CA-C	5.14	117.69	110.23
1	B	466	THR	N-CA-C	-5.11	102.81	110.23
1	B	512	VAL	N-CA-C	5.11	117.04	109.17
1	A	164	MET	N-CA-C	5.11	117.14	109.23
1	B	401	HIS	CA-C-N	5.09	125.12	119.32
1	B	401	HIS	C-N-CA	5.09	125.12	119.32
1	A	575	VAL	N-CA-C	5.07	115.57	108.17
1	A	576	LYS	N-CA-C	-5.06	100.91	108.96
1	B	568	VAL	N-CA-C	5.04	117.35	111.05
1	A	505	TYR	N-CA-C	-5.01	102.87	109.84

There are no chirality outliers.

There are no planarity outliers.

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	4652	0	4747	205	0
1	B	4652	0	4747	256	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	5	0	0
5	A	76	0	0	5	0
5	B	66	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9463	0	9499	459	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (459) 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:B:264:THR:HG22	1:B:266:GLU:H	1.12	1.13
1:B:493:ILE:HD11	1:B:579:LYS:HB3	1.24	1.13
1:B:8:LEU:HD23	1:B:190:GLU:HB2	1.48	0.96
1:A:288:THR:HG23	1:A:290:GLN:HG2	1.50	0.91
1:B:8:LEU:HD13	1:B:26:VAL:HG23	1.51	0.91
1:A:111:ASN:HD21	1:A:128:PHE:HB2	1.37	0.89
1:A:436:ALA:HB1	1:A:461:VAL:HB	1.56	0.87
1:B:397:GLU:HB3	1:B:409:ARG:HG2	1.57	0.87
1:A:391:ILE:HD11	1:A:445:GLU:HB3	1.56	0.85
1:A:292:LEU:HA	1:A:295:MET:HE3	1.57	0.85
1:A:514:LYS:H	1:A:514:LYS:HD2	1.39	0.84
1:A:288:THR:HG22	1:A:291:GLU:HG3	1.58	0.84
1:B:221:ARG:HH11	1:B:224:ARG:HE	1.23	0.83
1:B:290:GLN:H	1:B:290:GLN:HE21	1.23	0.83
1:B:156:ALA:O	1:B:160:LYS:HB2	1.79	0.82
1:A:499:LEU:HG	1:A:508:MET:HE1	1.59	0.82
1:B:107:ILE:HD11	1:B:129:LEU:HD21	1.61	0.82
1:A:412:SER:O	1:A:418:ALA:HB2	1.81	0.81
1:A:514:LYS:HD2	1:A:514:LYS:N	1.95	0.81
1:B:264:THR:HG22	1:B:266:GLU:N	1.95	0.80
1:A:264:THR:HG22	1:A:266:GLU:H	1.47	0.80
1:B:459:ALA:HA	1:B:474:VAL:HG22	1.66	0.78
1:B:547:VAL:HG23	1:B:552:GLU:C	2.09	0.78
1:B:162:ILE:HG13	1:B:163:PRO:HD2	1.67	0.77
1:A:288:THR:CG2	1:A:290:GLN:HG2	2.16	0.76
1:B:370:LYS:HE2	1:B:376:LEU:HD21	1.67	0.76
1:A:41:ASN:HD22	1:A:42:PRO:CD	1.99	0.76
1:A:483:ARG:HH12	1:A:488:LEU:HB2	1.50	0.75
1:B:40:VAL:O	1:B:62:THR:HG23	1.86	0.75
1:B:70:ASP:CG	1:B:73:LEU:HD13	2.12	0.74
1:B:295:MET:HE1	1:B:303:LEU:HD12	1.67	0.74
1:B:503:LEU:HD12	1:B:508:MET:HE3	1.69	0.74
1:A:185:SER:HB3	1:A:221:ARG:HG3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD21	1:A:24:LEU:HD21	1.68	0.73
1:B:111:ASN:HD21	1:B:128:PHE:HB2	1.51	0.73
1:A:129:LEU:HB3	1:A:152:ARG:HH11	1.50	0.73
1:A:260:ASP:OD1	1:A:300:ARG:HD2	1.88	0.73
1:A:264:THR:CG2	1:A:266:GLU:H	2.02	0.73
1:A:321:GLN:O	1:A:325:GLU:HG2	1.88	0.72
1:B:521:ARG:HG3	1:B:521:ARG:HH11	1.54	0.72
1:A:84:ARG:NE	1:A:84:ARG:HA	2.04	0.72
1:B:547:VAL:HG23	1:B:552:GLU:O	1.90	0.71
1:A:41:ASN:HD22	1:A:42:PRO:HD2	1.54	0.71
1:A:111:ASN:HD22	1:A:129:LEU:H	1.39	0.71
1:A:391:ILE:CD1	1:A:445:GLU:HB3	2.20	0.71
1:B:498:ARG:O	1:B:502:VAL:HG23	1.91	0.71
1:B:290:GLN:H	1:B:290:GLN:NE2	1.88	0.70
1:B:514:LYS:HD2	1:B:514:LYS:N	2.06	0.70
1:A:432:THR:H	1:A:435:ASP:HB2	1.55	0.69
1:A:114:ILE:HD12	1:A:115:ILE:N	2.06	0.69
1:B:397:GLU:CB	1:B:409:ARG:HG2	2.22	0.69
1:B:41:ASN:C	1:B:41:ASN:HD22	2.01	0.69
1:B:170:GLY:H	1:B:177:ARG:HD3	1.58	0.69
1:A:111:ASN:ND2	1:A:129:LEU:H	1.90	0.68
1:A:525:ASP:HA	1:A:577:VAL:HG23	1.75	0.68
1:B:514:LYS:HD2	1:B:514:LYS:H	1.57	0.68
1:A:41:ASN:O	1:A:45:MET:HG2	1.92	0.68
1:A:109:VAL:HG21	1:A:114:ILE:HG23	1.75	0.68
1:A:282:PRO:O	1:A:286:LYS:HE3	1.92	0.68
1:B:138:PRO:HD2	1:B:141:GLN:HE21	1.59	0.68
1:B:111:ASN:O	1:B:115:ILE:HG13	1.93	0.67
1:A:514:LYS:H	1:A:514:LYS:CD	2.06	0.67
1:B:419:GLN:NE2	1:B:486:ASP:HA	2.08	0.67
1:A:418:ALA:HB1	1:A:428:ILE:HD11	1.76	0.67
1:B:41:ASN:ND2	1:B:43:LYS:H	1.92	0.67
1:A:288:THR:HG22	1:A:291:GLU:CG	2.25	0.67
1:B:162:ILE:HG13	1:B:163:PRO:CD	2.24	0.67
1:A:406:ARG:HD3	1:A:406:ARG:N	2.09	0.67
1:A:55:MET:O	1:A:313:LYS:HE3	1.95	0.67
1:B:503:LEU:HD12	1:B:508:MET:CE	2.24	0.66
1:B:107:ILE:HD11	1:B:129:LEU:HD11	1.77	0.66
1:B:290:GLN:HA	1:B:293:ARG:NH1	2.11	0.66
1:A:548:ASN:ND2	1:A:552:GLU:HB2	2.11	0.66
1:B:82:ILE:HD12	1:B:83:HIS:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HD11	1:A:349:LEU:HD12	1.77	0.65
1:B:330:ARG:NH1	1:B:330:ARG:HB3	2.12	0.65
1:B:480:ALA:HB2	1:B:491:LEU:HD23	1.79	0.65
1:B:41:ASN:HD22	1:B:42:PRO:N	1.94	0.64
1:B:368:LEU:HD11	1:B:381:VAL:HG22	1.79	0.64
1:A:36:ILE:HD13	1:A:312:ILE:HG21	1.80	0.64
1:B:260:ASP:OD1	1:B:300:ARG:HD2	1.98	0.64
1:B:273:GLU:O	1:B:273:GLU:HG2	1.97	0.64
1:A:41:ASN:HD22	1:A:42:PRO:N	1.96	0.64
1:B:474:VAL:C	1:B:476:GLY:H	2.05	0.64
1:B:8:LEU:HD13	1:B:26:VAL:CG2	2.27	0.63
1:A:499:LEU:CG	1:A:508:MET:HE1	2.26	0.63
1:A:560:LEU:HD21	1:A:576:LYS:HE3	1.78	0.63
1:B:41:ASN:C	1:B:41:ASN:ND2	2.56	0.63
1:A:292:LEU:CA	1:A:295:MET:HE3	2.28	0.63
1:B:128:PHE:HB3	1:B:164:MET:HE1	1.80	0.63
1:B:518:PRO:O	1:B:521:ARG:HB2	1.98	0.63
1:B:555:ALA:HB2	1:B:580:GLY:HA2	1.81	0.62
1:A:548:ASN:HD21	1:A:552:GLU:HB2	1.64	0.62
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.65	0.62
1:A:198:VAL:O	1:A:202:GLU:HG3	2.00	0.62
1:B:107:ILE:CD1	1:B:129:LEU:HD21	2.30	0.61
1:B:64:SER:HB3	1:B:94:VAL:CG2	2.30	0.61
1:B:221:ARG:HH11	1:B:224:ARG:NE	1.96	0.61
1:B:290:GLN:HE21	1:B:290:GLN:N	1.97	0.61
1:B:264:THR:CG2	1:B:266:GLU:H	2.02	0.61
1:B:163:PRO:HB3	1:B:190:GLU:HG3	1.82	0.60
1:A:214:ILE:HD11	1:A:349:LEU:CD1	2.31	0.60
1:A:138:PRO:HD2	1:A:141:GLN:HE21	1.66	0.60
1:B:221:ARG:HD2	1:B:224:ARG:CZ	2.31	0.60
1:B:41:ASN:HD22	1:B:42:PRO:CD	2.14	0.60
1:A:327:GLU:O	1:A:327:GLU:HG2	2.01	0.60
1:B:468:MET:HB3	1:B:470:ARG:HH12	1.67	0.60
1:A:184:LEU:HA	1:A:187:MET:HE3	1.82	0.59
1:A:190:GLU:N	1:A:190:GLU:OE1	2.35	0.59
1:A:40:VAL:O	1:A:62:THR:HG23	2.01	0.59
1:A:288:THR:CG2	1:A:291:GLU:HG3	2.30	0.59
1:A:133:THR:CG2	1:A:171:SER:HB2	2.33	0.59
1:A:337:ARG:HB3	1:B:371:ILE:HD12	1.85	0.59
1:A:93:GLU:HG3	1:A:125:ILE:HB	1.83	0.59
1:B:399:VAL:HG21	1:B:429:GLU:OE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:SER:O	1:B:418:ALA:HB2	2.02	0.59
1:A:133:THR:HG22	1:A:171:SER:HB2	1.85	0.58
1:B:519:PHE:HB3	1:B:524:LYS:HB2	1.83	0.58
1:B:60:ILE:HG12	1:B:88:TYR:CE2	2.39	0.58
1:B:112:ARG:NH1	1:B:155:GLU:OE2	2.37	0.58
1:A:183:ARG:HB3	1:A:183:ARG:NH1	2.17	0.58
1:A:264:THR:HG22	1:A:266:GLU:N	2.16	0.58
1:B:297:LYS:O	1:B:297:LYS:HD3	2.02	0.58
1:A:399:VAL:O	1:A:406:ARG:HA	2.04	0.58
1:B:466:THR:O	1:B:468:MET:N	2.32	0.58
1:B:471:GLN:OE1	1:B:473:LYS:HE3	2.03	0.58
1:B:181:ALA:HB3	1:B:219:ALA:HB3	1.85	0.57
1:B:15:ARG:HH21	1:B:359:PHE:HB3	1.68	0.57
1:B:94:VAL:HG11	1:B:118:GLN:HG2	1.86	0.57
1:B:83:HIS:HB2	5:B:612:HOH:O	2.03	0.57
1:A:8:LEU:CD2	1:A:26:VAL:HG22	2.35	0.57
1:B:321:GLN:O	1:B:325:GLU:HG2	2.04	0.57
1:A:330:ARG:NH2	1:A:334:GLU:OE1	2.38	0.57
1:B:555:ALA:CB	1:B:580:GLY:HA2	2.35	0.57
1:A:36:ILE:HD13	1:A:312:ILE:CG2	2.35	0.56
1:B:281:CYS:O	1:B:285:SER:HB2	2.05	0.56
1:B:406:ARG:HD3	1:B:406:ARG:N	2.20	0.56
1:B:461:VAL:HG11	1:B:469:PRO:HB3	1.86	0.56
1:B:474:VAL:C	1:B:476:GLY:N	2.59	0.56
1:A:233:HIS:ND1	1:A:234:PRO:HD2	2.20	0.56
1:B:394:ARG:HD2	1:B:395:PHE:CE1	2.40	0.56
1:A:477:LYS:HG2	1:A:478:ARG:N	2.19	0.56
1:A:477:LYS:HG2	1:A:478:ARG:H	1.71	0.56
1:A:343:TYR:CZ	1:A:347:LYS:HD2	2.41	0.56
1:B:98:SER:HB2	1:B:130:ASP:O	2.06	0.56
1:B:557:GLY:HA2	1:B:578:ARG:HG3	1.87	0.56
1:B:44:GLN:OE1	1:B:258:LYS:HE3	2.06	0.56
1:A:111:ASN:HB2	1:A:152:ARG:HD3	1.88	0.55
1:A:183:ARG:HB3	1:A:183:ARG:HH11	1.70	0.55
1:B:232:GLY:HA3	1:B:250:SER:CB	2.37	0.55
1:A:471:GLN:HG2	1:A:473:LYS:HE3	1.88	0.55
1:B:428:ILE:HD12	1:B:428:ILE:H	1.71	0.55
1:A:406:ARG:HD3	1:A:406:ARG:H	1.71	0.55
1:B:397:GLU:HB3	1:B:409:ARG:CG	2.34	0.55
1:B:428:ILE:HD12	1:B:428:ILE:N	2.22	0.55
1:A:41:ASN:HD22	1:A:41:ASN:C	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:OG	1:A:113:GLU:HG3	2.07	0.55
1:A:368:LEU:HB3	1:A:420:SER:CB	2.37	0.55
1:B:31:ILE:HD12	5:B:648:HOH:O	2.06	0.55
1:B:330:ARG:HB3	1:B:330:ARG:HH11	1.69	0.54
1:A:163:PRO:HB3	1:A:190:GLU:HG3	1.89	0.54
1:B:105:GLY:O	1:B:106:SER:HB3	2.08	0.54
1:B:168:ILE:HD11	1:B:220:LEU:HD21	1.89	0.54
1:A:166:ALA:HB3	1:A:192:HIS:CE1	2.42	0.54
1:A:111:ASN:O	1:A:115:ILE:HG13	2.08	0.54
1:B:70:ASP:OD1	1:B:73:LEU:HD13	2.08	0.54
1:B:8:LEU:HD12	1:B:9:LYS:N	2.23	0.54
1:A:394:ARG:HD2	1:A:395:PHE:CE1	2.43	0.53
1:B:85:MET:O	1:B:85:MET:HG2	2.08	0.53
1:A:483:ARG:NH1	1:A:488:LEU:HB2	2.19	0.53
1:B:232:GLY:HA3	1:B:250:SER:HB2	1.88	0.53
1:A:401:HIS:N	1:A:405:GLY:O	2.35	0.53
1:B:193:PRO:HA	1:B:227:HIS:O	2.08	0.53
1:A:214:ILE:O	1:A:218:MET:HG3	2.08	0.53
1:A:526:VAL:HB	1:A:575:VAL:HB	1.91	0.53
1:B:41:ASN:HD22	1:B:42:PRO:HD2	1.73	0.53
1:A:415:TYR:HB2	1:A:419:GLN:HG3	1.91	0.53
1:B:73:LEU:N	1:B:73:LEU:HD12	2.24	0.53
1:B:163:PRO:HA	1:B:190:GLU:OE1	2.08	0.53
1:B:111:ASN:ND2	1:B:129:LEU:H	2.05	0.53
1:B:290:GLN:HA	1:B:293:ARG:HH11	1.73	0.53
1:B:399:VAL:HG12	1:B:407:VAL:O	2.08	0.53
1:A:41:ASN:C	1:A:41:ASN:ND2	2.66	0.53
1:A:129:LEU:HB3	1:A:152:ARG:NH1	2.20	0.53
1:B:492:GLY:O	1:B:495:GLY:N	2.42	0.53
1:B:330:ARG:NH2	1:B:334:GLU:OE2	2.42	0.52
1:B:339:HIS:ND1	1:B:340:PRO:HD2	2.24	0.52
1:B:328:LEU:O	1:B:332:VAL:HG23	2.09	0.52
1:A:474:VAL:O	1:A:475:ASN:C	2.52	0.52
1:B:471:GLN:NE2	1:B:478:ARG:HG3	2.25	0.52
1:B:107:ILE:HD12	1:B:109:VAL:HG12	1.91	0.52
1:A:477:LYS:CG	1:A:478:ARG:H	2.22	0.52
1:B:98:SER:O	1:B:101:LEU:HB3	2.10	0.52
1:B:221:ARG:HD2	1:B:224:ARG:NE	2.25	0.52
1:B:98:SER:HB3	1:B:129:LEU:HD23	1.92	0.52
1:B:343:TYR:CZ	1:B:347:LYS:HD2	2.44	0.52
1:B:82:ILE:HD12	1:B:83:HIS:H	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:HD22	1:B:129:LEU:H	1.58	0.52
1:B:466:THR:C	1:B:468:MET:H	2.18	0.52
1:B:64:SER:HB3	1:B:94:VAL:HG21	1.90	0.51
1:A:503:LEU:HD12	1:A:508:MET:HE3	1.92	0.51
1:B:112:ARG:O	1:B:116:GLU:HG3	2.11	0.51
1:A:198:VAL:HG22	1:A:230:GLY:HA3	1.93	0.51
1:A:547:VAL:HG23	1:A:552:GLU:C	2.35	0.51
1:B:435:ASP:O	1:B:436:ALA:C	2.53	0.51
1:B:493:ILE:O	1:B:497:LYS:HG3	2.10	0.51
1:B:64:SER:HB3	1:B:94:VAL:HG22	1.91	0.51
1:A:325:GLU:O	1:A:366:SER:HB2	2.10	0.51
1:A:431:PRO:HD2	1:A:467:GLY:O	2.11	0.51
1:A:445:GLU:OE2	1:A:451:GLY:N	2.44	0.51
1:B:7:MET:HG3	1:B:163:PRO:HG3	1.92	0.51
1:A:328:LEU:O	1:A:332:VAL:HG23	2.11	0.51
1:A:510:VAL:HG23	1:A:510:VAL:O	2.10	0.51
1:A:193:PRO:HA	1:A:227:HIS:O	2.10	0.51
1:A:469:PRO:O	1:A:470:ARG:HD3	2.11	0.51
1:B:114:ILE:HD12	1:B:115:ILE:H	1.76	0.51
1:B:62:THR:HG22	1:B:63:ASN:H	1.75	0.50
1:B:82:ILE:HD13	1:B:92:ILE:HD12	1.93	0.50
1:B:473:LYS:HG2	1:B:478:ARG:HA	1.93	0.50
1:A:36:ILE:HD12	1:A:237:PHE:CZ	2.46	0.50
1:A:79:GLU:O	1:A:80:LEU:HD23	2.12	0.50
1:B:70:ASP:OD1	1:B:72:GLU:HB2	2.11	0.50
1:B:448:PHE:HE2	1:B:543:GLU:HB2	1.75	0.50
1:A:31:ILE:HD12	1:A:59:ILE:HB	1.93	0.50
1:B:154:ARG:O	1:B:158:GLU:HG3	2.11	0.50
1:A:36:ILE:HG21	1:A:312:ILE:CG2	2.42	0.50
1:A:111:ASN:HD22	1:A:129:LEU:HB2	1.76	0.50
1:B:190:GLU:CD	1:B:190:GLU:N	2.70	0.50
1:B:437:ILE:HG23	1:B:438:LYS:N	2.25	0.50
1:B:55:MET:HE1	1:B:309:LEU:CD1	2.42	0.50
1:B:69:LYS:NZ	1:B:108:GLU:HB3	2.26	0.50
1:B:232:GLY:CA	1:B:250:SER:HB2	2.42	0.50
1:B:507:ARG:O	1:B:508:MET:HB2	2.12	0.50
1:A:510:VAL:HG23	1:A:546:VAL:HA	1.93	0.50
1:A:197:VAL:HG22	5:A:604:HOH:O	2.11	0.49
1:B:286:LYS:HE3	1:B:287:TYR:CE1	2.47	0.49
1:A:185:SER:HB3	1:A:221:ARG:CG	2.41	0.49
1:B:121:ILE:HG13	1:B:123:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD23	1:A:428:ILE:HG23	1.94	0.49
1:B:148:ILE:O	1:B:152:ARG:HG3	2.11	0.49
1:A:138:PRO:HD2	1:A:141:GLN:NE2	2.26	0.49
1:A:50:LYS:O	1:A:53:GLU:HB3	2.12	0.49
1:A:181:ALA:HB1	1:A:220:LEU:HG	1.94	0.49
1:B:55:MET:HE1	1:B:309:LEU:HD13	1.93	0.49
1:B:107:ILE:HD11	1:B:129:LEU:CD2	2.39	0.49
1:A:121:ILE:HG13	1:A:123:VAL:HG23	1.94	0.49
1:A:436:ALA:O	1:A:439:TYR:HB2	2.13	0.49
1:A:478:ARG:HD2	1:A:481:THR:OG1	2.13	0.49
1:B:431:PRO:HB3	1:B:439:TYR:CE1	2.47	0.49
1:B:436:ALA:HB1	1:B:461:VAL:HB	1.95	0.49
1:A:435:ASP:O	1:A:436:ALA:C	2.55	0.48
1:B:397:GLU:HG3	1:B:410:TYR:CE1	2.47	0.48
1:B:198:VAL:HB	1:B:199:PRO:HD3	1.95	0.48
1:B:492:GLY:O	1:B:494:GLU:N	2.46	0.48
1:A:8:LEU:HG	1:A:190:GLU:HB2	1.96	0.48
1:A:547:VAL:HG22	1:A:552:GLU:N	2.28	0.48
1:B:24:LEU:C	1:B:24:LEU:HD23	2.38	0.48
1:B:578:ARG:HH11	1:B:578:ARG:HG2	1.79	0.48
1:A:260:ASP:HA	1:A:304:LEU:CD1	2.44	0.48
1:A:507:ARG:O	1:A:508:MET:HB2	2.13	0.48
1:B:308:ASN:O	1:B:312:ILE:HG13	2.13	0.48
1:B:521:ARG:HG3	1:B:521:ARG:NH1	2.25	0.48
1:A:430:LYS:NZ	1:A:466:THR:CG2	2.77	0.48
1:B:185:SER:HB3	1:B:221:ARG:HG2	1.95	0.48
1:A:31:ILE:CD1	1:A:59:ILE:HB	2.44	0.48
1:A:477:LYS:CG	1:A:478:ARG:N	2.77	0.48
1:A:24:LEU:HD23	1:A:25:GLU:N	2.29	0.47
1:A:264:THR:HG23	1:A:266:GLU:OE1	2.12	0.47
1:A:104:TYR:CD2	1:A:104:TYR:N	2.78	0.47
1:A:388:ALA:O	1:A:389:LYS:C	2.57	0.47
1:B:510:VAL:HG23	1:B:544:VAL:CG2	2.44	0.47
1:B:292:LEU:HD22	1:B:295:MET:HE2	1.96	0.47
1:B:114:ILE:HD12	1:B:115:ILE:N	2.30	0.47
1:B:206:PHE:O	1:B:210:VAL:HG23	2.15	0.47
1:A:339:HIS:CE1	1:A:341:LYS:HB2	2.50	0.47
1:A:471:GLN:OE1	1:A:478:ARG:HD3	2.14	0.47
1:A:41:ASN:ND2	1:A:42:PRO:HD2	2.25	0.47
1:B:25:GLU:HA	1:B:29:LYS:O	2.15	0.47
1:B:135:PRO:O	1:B:172:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:MET:HB3	1:B:470:ARG:NH1	2.29	0.47
1:B:521:ARG:HH11	1:B:521:ARG:CG	2.26	0.47
1:B:525:ASP:HA	1:B:577:VAL:HG23	1.97	0.47
1:B:391:ILE:N	1:B:391:ILE:HD12	2.30	0.47
1:B:562:SER:O	1:B:563:GLY:C	2.56	0.47
1:B:520:ALA:O	1:B:555:ALA:HB2	2.14	0.47
1:B:31:ILE:HD12	1:B:32:GLU:H	1.80	0.47
1:B:36:ILE:HG21	1:B:312:ILE:HG22	1.97	0.47
1:A:507:ARG:O	1:A:509:ARG:HD2	2.14	0.46
1:A:114:ILE:HD12	1:A:115:ILE:HG13	1.96	0.46
1:B:21:ILE:HA	1:B:33:THR:O	2.15	0.46
1:B:410:TYR:HD2	1:B:439:TYR:CD1	2.33	0.46
1:B:514:LYS:NZ	1:B:549:GLU:HG3	2.29	0.46
1:A:397:GLU:OE1	1:A:409:ARG:HD3	2.16	0.46
1:B:73:LEU:CD1	1:B:73:LEU:H	2.29	0.46
1:A:24:LEU:HD23	1:A:24:LEU:C	2.40	0.46
1:A:120:ARG:HD2	5:A:630:HOH:O	2.15	0.46
1:A:358:GLU:OE2	1:A:564:ARG:NH1	2.46	0.46
1:B:33:THR:HA	1:B:34:PRO:C	2.40	0.46
1:A:385:LYS:O	1:A:388:ALA:HB3	2.16	0.46
1:B:413:LEU:HD23	1:B:428:ILE:CG2	2.45	0.46
1:A:231:ALA:O	1:A:248:PHE:HB3	2.16	0.46
1:B:17:GLY:HA2	1:B:360:GLU:OE1	2.15	0.46
1:B:81:GLY:O	1:B:83:HIS:N	2.49	0.46
1:B:450:GLU:OE2	1:B:451:GLY:N	2.48	0.46
1:B:499:LEU:HD12	1:B:508:MET:HE1	1.97	0.46
1:A:82:ILE:N	1:A:82:ILE:HD12	2.31	0.46
1:A:291:GLU:O	1:A:292:LEU:C	2.59	0.45
1:B:243:MET:HG2	1:B:349:LEU:CD1	2.47	0.45
1:B:478:ARG:HH11	1:B:480:ALA:C	2.23	0.45
1:B:573:ARG:HH12	1:B:576:LYS:NZ	2.14	0.45
1:A:198:VAL:HB	1:A:199:PRO:HD3	1.98	0.45
1:A:198:VAL:CG2	1:A:230:GLY:HA3	2.47	0.45
1:A:252:SER:O	1:A:253:TYR:C	2.60	0.45
1:B:179:TYR:OH	1:B:183:ARG:NH1	2.49	0.45
1:B:292:LEU:HD13	1:B:295:MET:HE2	1.98	0.45
1:A:329:TRP:HB3	1:A:378:TRP:CE2	2.52	0.45
1:A:362:ILE:HD12	1:A:383:ARG:NH1	2.31	0.45
1:A:166:ALA:HB2	1:A:189:PHE:CG	2.52	0.45
1:A:455:ALA:HB1	1:A:498:ARG:HB3	1.99	0.45
1:B:73:LEU:N	1:B:73:LEU:CD1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:HG3	1:B:410:TYR:CZ	2.51	0.45
1:B:462:GLU:OE2	1:B:471:GLN:HB3	2.16	0.45
1:A:454:ARG:HA	1:A:457:ASP:OD2	2.17	0.45
1:B:109:VAL:HG21	1:B:114:ILE:HG23	1.98	0.45
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.30	0.45
1:A:497:LYS:O	1:A:501:ARG:HG2	2.17	0.45
1:B:128:PHE:HD2	1:B:164:MET:CE	2.30	0.45
1:B:496:ALA:HB2	1:B:556:THR:OG1	2.18	0.45
1:B:495:GLY:O	1:B:499:LEU:HD23	2.17	0.44
1:A:466:THR:C	1:A:468:MET:H	2.24	0.44
1:B:252:SER:O	1:B:253:TYR:C	2.60	0.44
1:B:406:ARG:HD3	1:B:406:ARG:H	1.82	0.44
1:A:8:LEU:HD13	1:A:9:LYS:N	2.33	0.44
1:A:371:ILE:C	1:A:371:ILE:HD12	2.42	0.44
1:A:371:ILE:HD13	1:B:337:ARG:HB3	2.00	0.44
1:B:397:GLU:HG3	1:B:410:TYR:OH	2.16	0.44
1:A:151:SER:HA	1:A:154:ARG:NH1	2.32	0.44
1:A:503:LEU:HD12	1:A:508:MET:CE	2.48	0.44
1:B:111:ASN:HD22	1:B:129:LEU:HB2	1.81	0.44
1:B:292:LEU:HD22	1:B:295:MET:CE	2.47	0.44
1:A:368:LEU:HB3	1:A:420:SER:HB3	1.99	0.44
1:A:437:ILE:HG23	1:A:438:LYS:N	2.32	0.44
1:B:42:PRO:HG3	1:B:62:THR:CG2	2.48	0.44
1:B:131:ILE:O	1:B:169:GLN:HG2	2.18	0.44
1:B:339:HIS:CE1	1:B:340:PRO:HD2	2.53	0.44
1:B:493:ILE:HD13	1:B:493:ILE:H	1.82	0.44
1:A:111:ASN:HD22	1:A:129:LEU:N	2.13	0.44
1:A:168:ILE:N	1:A:168:ILE:HD12	2.33	0.44
1:A:339:HIS:CG	1:A:340:PRO:HD2	2.52	0.44
1:B:450:GLU:O	1:B:452:ALA:N	2.51	0.44
1:B:535:ASP:HB3	1:B:538:ILE:HG13	1.99	0.44
1:A:109:VAL:CG2	1:A:114:ILE:HG23	2.45	0.43
1:A:510:VAL:CG2	1:A:546:VAL:HA	2.48	0.43
1:B:42:PRO:HG3	1:B:62:THR:HG22	1.99	0.43
1:A:259:ASP:HB3	1:A:261:ARG:HG3	2.00	0.43
1:B:94:VAL:HG11	1:B:123:VAL:HG21	1.99	0.43
1:B:168:ILE:HD12	1:B:168:ILE:N	2.33	0.43
1:B:394:ARG:HD2	1:B:395:PHE:CD1	2.53	0.43
1:B:330:ARG:HG2	1:B:371:ILE:HD13	2.00	0.43
1:B:437:ILE:CG2	1:B:438:LYS:N	2.81	0.43
1:B:9:LYS:HG2	1:B:571:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:O	1:A:322:ALA:HB3	2.18	0.43
1:A:362:ILE:HD12	1:A:362:ILE:HA	1.83	0.43
1:B:514:LYS:HZ3	1:B:549:GLU:HG3	1.84	0.43
1:B:548:ASN:HD21	1:B:552:GLU:HB2	1.83	0.43
1:A:416:PRO:O	1:A:420:SER:HB3	2.18	0.43
1:B:51:GLU:OE2	1:B:302:ARG:NH1	2.51	0.43
1:B:286:LYS:HE3	1:B:287:TYR:HE1	1.81	0.43
1:B:349:LEU:O	1:B:356:LEU:HD11	2.18	0.43
1:B:135:PRO:HB3	1:B:200:LEU:HD21	2.00	0.43
1:B:138:PRO:HD2	1:B:141:GLN:NE2	2.30	0.43
1:B:286:LYS:HG3	1:B:287:TYR:CD1	2.53	0.43
1:B:448:PHE:HB2	1:B:452:ALA:CB	2.49	0.43
1:B:470:ARG:O	1:B:481:THR:HG23	2.18	0.43
1:B:492:GLY:O	1:B:493:ILE:C	2.59	0.43
1:B:493:ILE:HD13	1:B:493:ILE:N	2.33	0.43
1:A:562:SER:O	1:A:563:GLY:C	2.62	0.43
1:B:201:LEU:O	1:B:202:GLU:C	2.62	0.43
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.91	0.43
1:A:423:GLU:OE2	1:A:423:GLU:N	2.43	0.43
1:B:170:GLY:O	1:B:171:SER:HB3	2.18	0.43
1:A:55:MET:HE1	1:A:309:LEU:CD1	2.49	0.42
1:B:413:LEU:HD22	1:B:468:MET:HE1	2.00	0.42
1:A:139:ARG:NH2	1:A:175:ASP:OD2	2.52	0.42
1:A:223:ASP:HA	1:A:569:PHE:CZ	2.54	0.42
1:A:288:THR:HG23	1:A:290:GLN:N	2.34	0.42
1:A:516:ALA:HB2	1:A:530:PHE:HB3	2.01	0.42
1:A:436:ALA:HB1	1:A:461:VAL:CB	2.37	0.42
1:A:8:LEU:HD13	1:A:8:LEU:C	2.45	0.42
1:A:119:HIS:CD2	1:A:161:GLU:HB2	2.54	0.42
1:A:466:THR:HG22	1:A:467:GLY:N	2.34	0.42
1:B:508:MET:O	1:B:544:VAL:HG22	2.19	0.42
1:A:468:MET:HA	1:A:469:PRO:HD3	1.85	0.42
1:B:23:LYS:HE3	1:B:30:LYS:HD3	2.01	0.42
1:B:179:TYR:O	1:B:182:ARG:HB3	2.20	0.42
1:B:496:ALA:CB	1:B:556:THR:OG1	2.68	0.42
1:A:434:GLU:N	1:A:434:GLU:CD	2.78	0.42
1:A:466:THR:O	1:A:468:MET:N	2.44	0.42
1:A:464:SER:C	1:A:466:THR:N	2.76	0.42
1:B:408:SER:OG	1:B:410:TYR:HD1	2.03	0.42
1:A:20:ARG:HD3	5:A:617:HOH:O	2.19	0.42
1:B:13:LYS:HE3	1:B:23:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LEU:C	1:B:581:VAL:HG23	2.45	0.42
1:A:17:GLY:C	1:A:19:GLY:H	2.27	0.42
1:A:41:ASN:ND2	1:A:43:LYS:H	2.18	0.42
1:A:49:PRO:HA	1:A:52:LEU:HD12	2.01	0.42
1:A:407:VAL:O	1:A:408:SER:C	2.63	0.42
1:B:368:LEU:HD11	1:B:381:VAL:CG2	2.49	0.42
1:B:434:GLU:CD	1:B:434:GLU:H	2.28	0.42
1:B:435:ASP:O	1:B:438:LYS:N	2.52	0.42
1:A:492:GLY:O	1:A:493:ILE:C	2.62	0.41
1:B:521:ARG:NH1	1:B:521:ARG:CG	2.83	0.41
1:A:227:HIS:HD2	5:A:605:HOH:O	2.04	0.41
1:A:252:SER:HB2	1:A:263:MET:HE1	2.01	0.41
1:A:368:LEU:HB3	1:A:420:SER:HB2	2.02	0.41
1:A:535:ASP:HB3	1:A:538:ILE:HG13	2.01	0.41
1:B:41:ASN:HD21	1:B:43:LYS:H	1.65	0.41
1:B:135:PRO:HG2	1:B:199:PRO:HB2	2.02	0.41
1:B:221:ARG:CD	1:B:224:ARG:NE	2.82	0.41
1:B:394:ARG:NH2	1:B:445:GLU:OE2	2.53	0.41
1:A:357:GLU:O	1:A:383:ARG:NH2	2.54	0.41
1:A:471:GLN:CA	1:A:471:GLN:HE21	2.33	0.41
1:B:224:ARG:HA	1:B:225:PRO:HD3	1.95	0.41
1:A:111:ASN:ND2	1:A:128:PHE:HB2	2.18	0.41
1:B:8:LEU:HD12	1:B:8:LEU:C	2.46	0.41
1:B:335:ARG:O	1:B:342:LEU:HD13	2.20	0.41
1:A:406:ARG:O	1:A:406:ARG:HG2	2.19	0.41
1:B:461:VAL:CG1	1:B:469:PRO:HB3	2.48	0.41
1:B:465:LYS:H	1:B:465:LYS:HG2	1.61	0.41
1:B:304:LEU:HD23	1:B:304:LEU:HA	1.89	0.41
1:B:510:VAL:HG23	1:B:544:VAL:HG22	2.02	0.41
1:A:70:ASP:HB3	1:A:73:LEU:HB2	2.02	0.41
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.84	0.41
1:A:236:VAL:O	1:A:237:PHE:C	2.62	0.41
1:B:23:LYS:NZ	1:B:30:LYS:NZ	2.69	0.41
1:B:40:VAL:O	1:B:62:THR:CG2	2.65	0.41
1:B:107:ILE:HD12	1:B:109:VAL:CG1	2.51	0.41
1:B:150:LEU:O	1:B:153:ALA:HB3	2.20	0.41
1:B:289:PRO:O	1:B:293:ARG:HG3	2.21	0.41
1:B:548:ASN:ND2	1:B:552:GLU:HB2	2.36	0.41
1:B:578:ARG:HG2	1:B:578:ARG:NH1	2.36	0.41
1:A:26:VAL:O	1:A:27:ASN:C	2.64	0.41
1:A:380:VAL:O	1:A:380:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ALA:CB	1:A:580:GLY:HA2	2.51	0.41
1:B:36:ILE:HG12	1:B:312:ILE:HG21	2.04	0.41
1:B:237:PHE:O	1:B:238:ALA:C	2.64	0.41
1:B:271:LEU:C	1:B:273:GLU:H	2.28	0.41
1:A:362:ILE:HD13	1:A:539:ARG:CB	2.51	0.40
1:B:233:HIS:ND1	1:B:234:PRO:HD2	2.36	0.40
1:A:102:MET:HE1	1:A:196:GLY:HA2	2.03	0.40
1:B:60:ILE:HG23	1:B:88:TYR:CZ	2.56	0.40
1:B:419:GLN:HE22	1:B:486:ASP:HA	1.81	0.40
1:B:503:LEU:HA	1:B:504:PRO:HD3	1.80	0.40
1:A:185:SER:CB	1:A:221:ARG:HG3	2.45	0.40
1:A:288:THR:HG22	1:A:291:GLU:H	1.85	0.40
1:B:547:VAL:CG2	1:B:552:GLU:N	2.84	0.40
1:A:33:THR:HB	1:A:34:PRO:HA	2.02	0.40
1:A:250:SER:HA	5:A:607:HOH:O	2.20	0.40
1:A:521:ARG:HB3	1:A:582:GLU:HG3	2.03	0.40

There are no symmetry-related clashes.

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	575/582 (99%)	534 (93%)	38 (7%)	3 (0%)	24	43
1	B	575/582 (99%)	514 (89%)	48 (8%)	13 (2%)	5	8
All	All	1150/1164 (99%)	1048 (91%)	86 (8%)	16 (1%)	9	17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	ALA
1	A	475	ASN

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Mol	Chain	Res	Type
1	B	493	ILE
1	B	82	ILE
1	B	436	ALA
1	B	450	GLU
1	B	451	GLY
1	B	106	SER
1	B	432	THR
1	B	467	GLY
1	B	486	ASP
1	B	523	GLY
1	A	136	ASP
1	B	135	PRO
1	B	412	SER
1	B	458	ASP

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	499/503 (99%)	460 (92%)	39 (8%)	11	24
1	B	499/503 (99%)	463 (93%)	36 (7%)	13	28
All	All	998/1006 (99%)	923 (92%)	75 (8%)	12	26

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	13	LYS
1	A	15	ARG
1	A	20	ARG
1	A	31	ILE
1	A	40	VAL
1	A	41	ASN
1	A	51	GLU
1	A	62	THR

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Mol	Chain	Res	Type
1	A	82	ILE
1	A	94	VAL
1	A	129	LEU
1	A	184	LEU
1	A	190	GLU
1	A	259	ASP
1	A	264	THR
1	A	270	ARG
1	A	288	THR
1	A	290	GLN
1	A	292	LEU
1	A	294	GLU
1	A	328	LEU
1	A	342	LEU
1	A	362	ILE
1	A	368	LEU
1	A	399	VAL
1	A	406	ARG
1	A	419	GLN
1	A	471	GLN
1	A	493	ILE
1	A	498	ARG
1	A	499	LEU
1	A	507	ARG
1	A	514	LYS
1	A	522	LYS
1	A	544	VAL
1	A	547	VAL
1	A	553	LEU
1	A	579	LYS
1	B	8	LEU
1	B	36	ILE
1	B	41	ASN
1	B	47	VAL
1	B	62	THR
1	B	80	LEU
1	B	86	LEU
1	B	108	GLU
1	B	114	ILE
1	B	184	LEU
1	B	190	GLU
1	B	221	ARG

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Mol	Chain	Res	Type
1	B	229	PHE
1	B	264	THR
1	B	273	GLU
1	B	290	GLN
1	B	292	LEU
1	B	294	GLU
1	B	302	ARG
1	B	324	LYS
1	B	328	LEU
1	B	330	ARG
1	B	342	LEU
1	B	358	GLU
1	B	365	LYS
1	B	368	LEU
1	B	373	ASN
1	B	406	ARG
1	B	416	PRO
1	B	429	GLU
1	B	465	LYS
1	B	507	ARG
1	B	514	LYS
1	B	522	LYS
1	B	542	ASP
1	B	544	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	111	ASN
1	A	141	GLN
1	A	165	ASN
1	A	188	ASN
1	A	290	GLN
1	A	373	ASN
1	A	419	GLN
1	A	471	GLN
1	B	27	ASN
1	B	41	ASN
1	B	63	ASN
1	B	83	HIS
1	B	111	ASN

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	165	ASN
1	B	188	ASN
1	B	290	GLN

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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PQ0	A	602	-	14,14,14	3.31	7 (50%)	14,20,20	2.08	5 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PQ0	A	602	-	-	0/0/2/2	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	PQ0	C4-N3	7.97	1.48	1.36
4	A	602	PQ0	C8-C7	-5.50	1.32	1.38
4	A	602	PQ0	C5-C4	-4.48	1.35	1.45
4	A	602	PQ0	C4-N9	-3.27	1.29	1.36
4	A	602	PQ0	C8-N9	-3.14	1.29	1.36
4	A	602	PQ0	C5-C6	2.32	1.49	1.44
4	A	602	PQ0	C2-N2	-2.13	1.29	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	PQ0	C2-N3-C4	4.34	121.03	113.36
4	A	602	PQ0	N9-C4-N3	3.05	129.70	125.99
4	A	602	PQ0	O6-C6-C5	-2.50	118.20	125.69
4	A	602	PQ0	C7-C5-C4	-2.14	103.49	105.51
4	A	602	PQ0	C7-C8-N9	2.08	109.76	107.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.