



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:36 PM UTC

PDB ID : 1IQ8 / pdb_00001iq8
Title : Crystal Structure of archaeosine tRNA-guanine transglycosylase from *Pyrococcus horikoshii*
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 : 2001-07-09
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

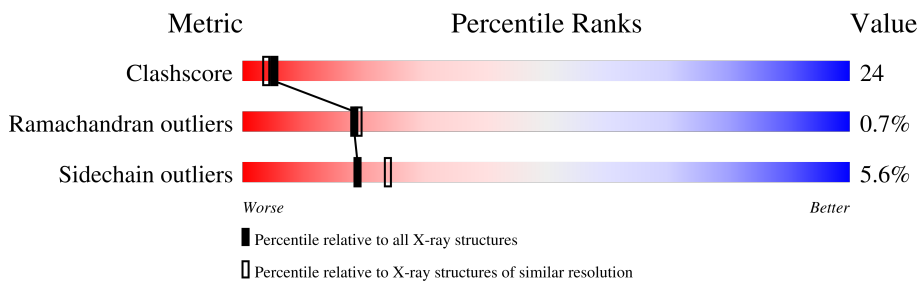
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	 61% 33% 5%
1	B	582	 54% 40% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9599 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 water.

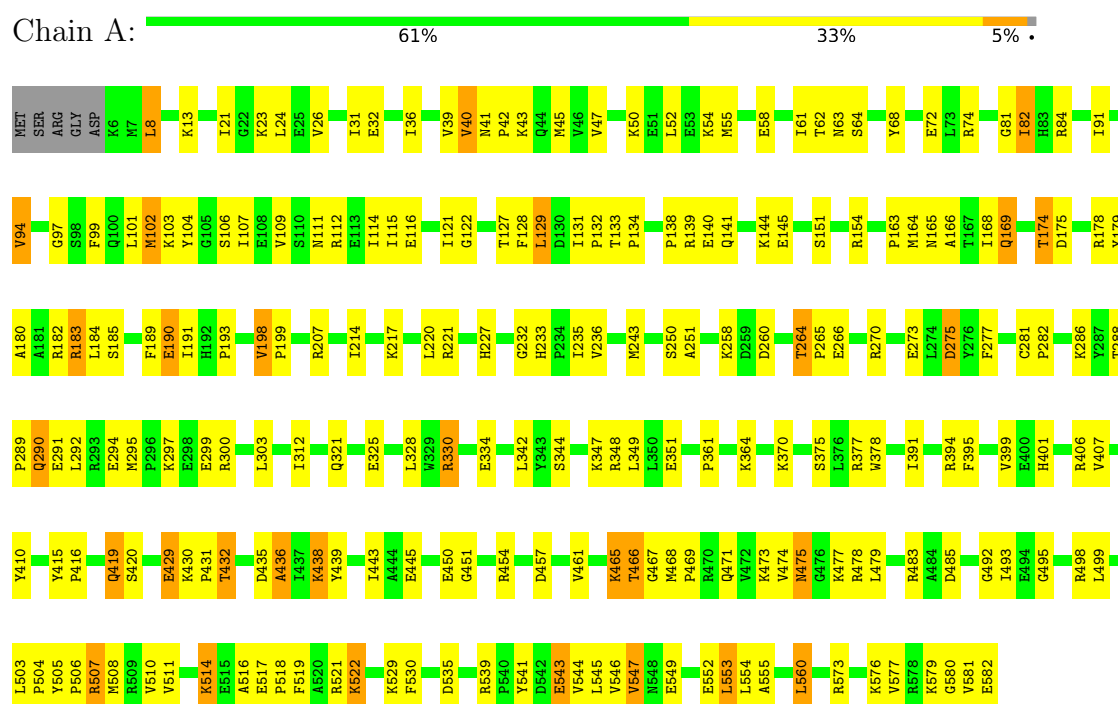
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	175	Total	O	0	0
			175	175		
4	B	116	Total	O	0	0
			116	116		

3 Residue-property plots

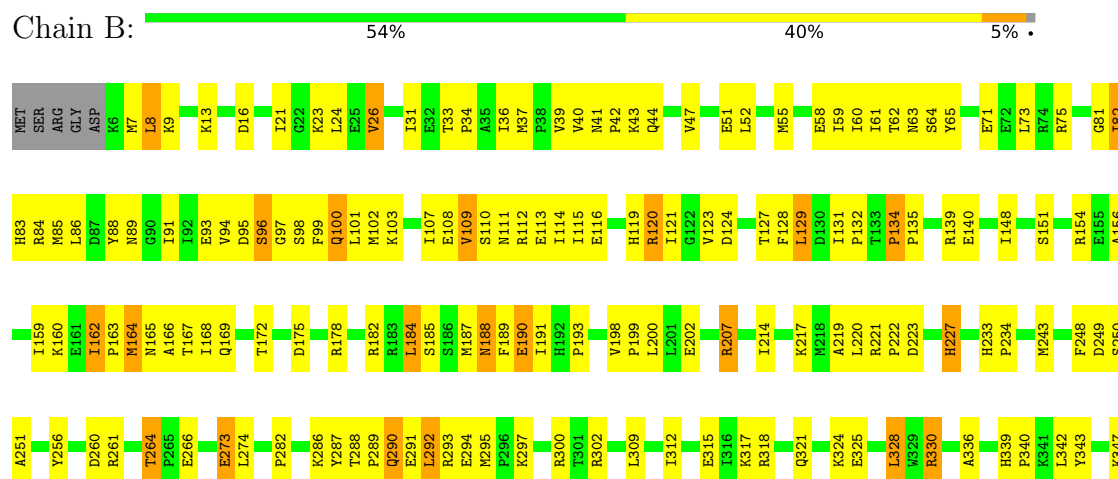
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ARCHAEOSE TRNA-GUANINE TRANSGLYCOSYLASE



• Molecule 1: ARCHAEOSE 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	99.28Å 99.28Å 363.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9599	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: ZN, MG

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	0.42	0/4745	0.97	20/6391 (0.3%)
1	B	0.39	0/4745	0.92	14/6391 (0.2%)
All	All	0.41	0/9490	0.94	34/12782 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ALA	N-CA-C	-8.63	102.92	113.97
1	A	251	ALA	N-CA-C	-8.38	103.25	113.97
1	B	514	LYS	N-CA-C	-7.71	102.52	112.23
1	A	81	GLY	N-CA-C	-7.10	103.89	112.48
1	A	233	HIS	CA-C-N	7.01	127.60	119.47
1	A	233	HIS	C-N-CA	7.01	127.60	119.47
1	A	492	GLY	N-CA-C	-6.73	101.00	112.51
1	B	134	PRO	CA-C-N	6.73	128.25	119.84
1	B	134	PRO	C-N-CA	6.73	128.25	119.84
1	A	432	THR	N-CA-C	-6.43	100.18	110.14
1	A	466	THR	N-CA-C	-6.35	101.12	110.52
1	A	169	GLN	N-CA-C	6.17	118.89	110.06
1	A	514	LYS	N-CA-C	-6.05	104.60	112.23
1	B	167	THR	N-CA-C	6.05	119.03	109.96
1	A	543	GLU	N-CA-C	-5.95	100.81	110.20
1	B	81	GLY	N-CA-C	-5.74	104.49	112.18
1	A	401	HIS	CA-C-N	5.74	126.12	119.47
1	A	401	HIS	C-N-CA	5.74	126.12	119.47
1	A	485	ASP	N-CA-C	5.68	118.41	111.82
1	B	505	TYR	N-CA-C	-5.67	103.08	109.60
1	A	21	ILE	N-CA-C	-5.60	99.81	107.99
1	A	465	LYS	N-CA-C	-5.56	105.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	VAL	N-CA-C	5.54	116.20	108.89
1	A	275	ASP	N-CA-C	-5.46	106.98	113.97
1	B	100	GLN	N-CA-C	-5.43	106.50	113.23
1	B	560	LEU	N-CA-C	-5.42	107.03	113.97
1	B	148	ILE	N-CA-C	-5.42	105.44	110.53
1	B	120	ARG	N-CA-C	5.38	118.06	111.82
1	A	560	LEU	N-CA-C	-5.30	107.19	113.97
1	A	198	VAL	CB-CA-C	-5.28	108.69	113.70
1	B	129	LEU	N-CA-C	5.21	117.68	109.39
1	B	250	SER	N-CA-C	5.20	117.55	108.76
1	A	102	MET	N-CA-C	-5.18	106.64	113.12
1	B	164	MET	N-CA-C	5.18	117.26	109.23

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	213	0
1	B	4652	0	4747	248	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	175	0	0	5	0
4	B	116	0	0	5	0
All	All	9599	0	9494	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:A:477:LYS:HG2	1:A:478:ARG:H	1.03	1.15
1:A:503:LEU:HD12	1:A:508:MET:HE2	1.33	1.07
1:A:295:MET:HE1	1:A:303:LEU:HD12	1.38	1.04
1:B:503:LEU:HD12	1:B:508:MET:HE2	1.41	1.02
1:B:413:LEU:HD22	1:B:468:MET:HE1	1.44	0.99
1:A:499:LEU:HB3	1:A:508:MET:HE1	1.43	0.98
1:A:264:THR:HG22	1:A:266:GLU:H	1.24	0.97
1:A:13:LYS:HE3	1:A:23:LYS:HB2	1.45	0.97
1:A:514:LYS:H	1:A:514:LYS:HD2	1.28	0.96
1:B:514:LYS:HE3	1:B:514:LYS:H	1.33	0.93
1:B:290:GLN:H	1:B:290:GLN:NE2	1.65	0.93
1:B:514:LYS:HE3	1:B:514:LYS:N	1.85	0.91
1:A:477:LYS:HG2	1:A:478:ARG:N	1.86	0.91
1:B:264:THR:HG22	1:B:266:GLU:H	1.33	0.90
1:B:101:LEU:HD21	1:B:131:ILE:HG12	1.53	0.89
1:A:471:GLN:HG2	1:A:473:LYS:HE3	1.52	0.88
1:A:510:VAL:HG23	1:A:546:VAL:HA	1.55	0.86
1:A:344:SER:HB2	1:B:423:GLU:HG3	1.58	0.86
1:B:499:LEU:HG	1:B:508:MET:HE1	1.57	0.85
1:A:477:LYS:CG	1:A:478:ARG:H	1.89	0.84
1:B:510:VAL:HG13	1:B:544:VAL:HG11	1.59	0.83
1:B:84:ARG:HE	1:B:84:ARG:HA	1.43	0.83
1:A:514:LYS:HD2	1:A:514:LYS:N	1.94	0.83
1:A:63:ASN:HD21	1:A:97:GLY:HA2	1.44	0.82
1:B:131:ILE:O	1:B:169:GLN:HG2	1.82	0.80
1:B:168:ILE:HD11	1:B:220:LEU:HD21	1.62	0.80
1:B:290:GLN:H	1:B:290:GLN:HE21	1.29	0.80
1:A:178:ARG:HB3	1:A:182:ARG:HH21	1.44	0.79
1:B:64:SER:HB3	1:B:94:VAL:HG21	1.63	0.79
1:A:131:ILE:O	1:A:169:GLN:HG2	1.82	0.79
1:B:40:VAL:O	1:B:62:THR:HG23	1.82	0.79
1:B:292:LEU:HA	1:B:295:MET:HE2	1.65	0.78
1:B:382:ARG:O	1:B:386:GLU:HG3	1.84	0.77
1:A:138:PRO:HD2	1:A:141:GLN:NE2	2.00	0.76
1:B:510:VAL:CG1	1:B:544:VAL:HG11	2.15	0.76
1:A:270:ARG:O	1:A:273:GLU:HG2	1.85	0.76
1:A:138:PRO:HD2	1:A:141:GLN:HE21	1.50	0.76
1:A:292:LEU:HD13	1:A:295:MET:HE2	1.68	0.76
1:B:525:ASP:HA	1:B:577:VAL:HG23	1.68	0.75
1:B:110:SER:OG	1:B:113:GLU:HG3	1.87	0.74
1:B:406:ARG:HD3	1:B:406:ARG:N	2.01	0.74
1:A:264:THR:HG22	1:A:266:GLU:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:MET:HE1	1:A:303:LEU:CD1	2.17	0.74
1:A:31:ILE:HD12	1:A:91:ILE:HD12	1.70	0.74
1:B:111:ASN:HD21	1:B:128:PHE:HB2	1.52	0.74
1:A:471:GLN:HE21	1:A:478:ARG:HG3	1.53	0.73
1:B:397:GLU:HB3	1:B:409:ARG:HG2	1.70	0.73
1:B:8:LEU:HD22	1:B:26:VAL:HG22	1.71	0.73
1:A:151:SER:HA	1:A:154:ARG:NH1	2.04	0.72
1:B:84:ARG:HH22	1:B:89:ASN:ND2	1.87	0.72
1:A:111:ASN:HD21	1:A:128:PHE:HB2	1.54	0.72
1:B:41:ASN:HD22	1:B:42:PRO:CD	2.04	0.71
1:A:214:ILE:HD11	1:A:349:LEU:CD1	2.21	0.70
1:B:264:THR:HG22	1:B:266:GLU:N	2.06	0.70
1:B:84:ARG:HH22	1:B:89:ASN:HD21	1.39	0.70
1:B:386:GLU:HA	1:B:389:LYS:HZ3	1.57	0.70
1:A:178:ARG:HB3	1:A:182:ARG:NH2	2.07	0.69
1:B:82:ILE:HD12	1:B:83:HIS:N	2.08	0.69
1:A:288:THR:HG22	1:A:291:GLU:CG	2.23	0.69
1:A:8:LEU:HG	1:A:190:GLU:HB2	1.74	0.69
1:A:445:GLU:OE2	1:A:450:GLU:HA	1.93	0.68
1:B:114:ILE:HD12	1:B:115:ILE:N	2.09	0.68
1:B:519:PHE:HA	1:B:522:LYS:HE3	1.75	0.68
1:A:40:VAL:O	1:A:62:THR:HG23	1.93	0.68
1:A:288:THR:HG22	1:A:291:GLU:HG3	1.77	0.67
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.60	0.67
1:B:380:VAL:HG23	4:B:603:HOH:O	1.93	0.67
1:A:168:ILE:HD11	1:A:220:LEU:HD11	1.77	0.67
1:B:82:ILE:HD12	1:B:83:HIS:H	1.60	0.67
1:A:42:PRO:HG3	1:A:62:THR:HG21	1.76	0.67
1:A:36:ILE:HD13	1:A:312:ILE:HG21	1.76	0.67
1:B:207:ARG:HH11	1:B:207:ARG:HB3	1.60	0.67
1:A:474:VAL:HG22	1:A:475:ASN:OD1	1.94	0.66
1:B:214:ILE:HD11	1:B:349:LEU:CD1	2.25	0.66
1:A:514:LYS:H	1:A:514:LYS:CD	2.05	0.66
1:B:330:ARG:HH11	1:B:330:ARG:HB3	1.61	0.66
1:B:290:GLN:HE21	1:B:290:GLN:N	1.94	0.66
1:A:163:PRO:HB3	1:A:190:GLU:HG3	1.79	0.65
1:B:493:ILE:HD12	1:B:497:LYS:HE3	1.78	0.65
1:A:165:ASN:HD22	1:A:191:ILE:HB	1.62	0.64
1:B:31:ILE:HD12	1:B:91:ILE:HD12	1.79	0.64
1:B:85:MET:HE2	1:B:86:LEU:HD11	1.78	0.64
1:A:510:VAL:HG13	1:A:544:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:HG13	1:B:544:VAL:CG1	2.28	0.64
1:A:36:ILE:HD13	1:A:312:ILE:CG2	2.28	0.64
1:B:386:GLU:HA	1:B:389:LYS:NZ	2.12	0.64
1:A:52:LEU:HA	1:A:55:MET:HE3	1.77	0.64
1:A:432:THR:H	1:A:435:ASP:HB2	1.61	0.63
1:A:529:LYS:HE3	1:A:530:PHE:CE1	2.34	0.63
1:B:413:LEU:HD23	1:B:428:ILE:CG2	2.28	0.63
1:A:99:PHE:CE2	1:A:103:LYS:HD2	2.35	0.62
1:A:114:ILE:HD12	1:A:115:ILE:N	2.14	0.62
1:A:198:VAL:HB	1:A:199:PRO:HD3	1.80	0.62
1:B:41:ASN:HD22	1:B:42:PRO:HD2	1.64	0.62
1:B:264:THR:CG2	1:B:266:GLU:H	2.10	0.62
1:A:275:ASP:OD1	1:B:324:LYS:HG2	1.98	0.62
1:B:185:SER:OG	1:B:221:ARG:HG3	1.98	0.62
1:A:102:MET:HE3	1:A:132:PRO:O	1.99	0.62
1:A:510:VAL:CG2	1:A:546:VAL:HA	2.26	0.61
1:B:274:LEU:O	1:B:293:ARG:NH2	2.34	0.61
1:A:270:ARG:H	1:A:273:GLU:CD	2.08	0.61
1:B:330:ARG:HB3	1:B:330:ARG:NH1	2.16	0.61
1:B:41:ASN:HD22	1:B:42:PRO:N	1.98	0.61
1:B:399:VAL:O	1:B:406:ARG:HA	2.01	0.60
1:A:479:LEU:HD22	1:A:498:ARG:HD2	1.84	0.60
1:A:499:LEU:HB3	1:A:508:MET:CE	2.24	0.60
1:A:264:THR:CG2	1:A:266:GLU:H	2.08	0.60
1:B:13:LYS:HD2	1:B:23:LYS:HB2	1.83	0.60
1:B:135:PRO:HB3	1:B:200:LEU:HD21	1.82	0.60
1:B:198:VAL:HB	1:B:199:PRO:HD3	1.82	0.60
1:B:286:LYS:HE2	1:B:287:TYR:CE1	2.36	0.60
1:B:395:PHE:HB3	1:B:410:TYR:CD1	2.37	0.60
1:A:185:SER:HB3	1:A:221:ARG:HG3	1.84	0.60
1:B:7:MET:HB3	1:B:163:PRO:HG3	1.83	0.60
1:B:273:GLU:O	1:B:273:GLU:HG2	2.01	0.60
1:A:499:LEU:CB	1:A:508:MET:HE1	2.25	0.60
1:A:406:ARG:H	1:A:406:ARG:HD3	1.66	0.60
1:A:406:ARG:HD3	1:A:406:ARG:N	2.17	0.59
1:B:286:LYS:HE2	1:B:287:TYR:HE1	1.67	0.59
1:B:493:ILE:O	1:B:493:ILE:HD13	2.02	0.59
1:A:553:LEU:HD22	1:A:581:VAL:CG2	2.32	0.59
1:B:474:VAL:HG11	1:B:498:ARG:HH22	1.67	0.59
1:B:135:PRO:HG2	1:B:199:PRO:HB2	1.84	0.59
1:B:165:ASN:HD22	1:B:191:ILE:HB	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:ND2	1:A:191:ILE:HB	2.17	0.59
1:A:260:ASP:OD1	1:A:300:ARG:HD2	2.03	0.59
1:B:471:GLN:NE2	1:B:478:ARG:HG3	2.17	0.59
1:B:321:GLN:O	1:B:325:GLU:HG2	2.02	0.58
1:A:112:ARG:O	1:A:116:GLU:HG3	2.03	0.58
1:A:431:PRO:HD2	1:A:467:GLY:O	2.03	0.58
1:B:499:LEU:CG	1:B:508:MET:HE1	2.30	0.58
1:B:477:LYS:HE3	1:B:494:GLU:CD	2.28	0.58
1:B:84:ARG:HA	1:B:84:ARG:NE	2.15	0.58
1:B:436:ALA:HB1	1:B:461:VAL:HB	1.85	0.58
1:B:217:LYS:HD3	1:B:243:MET:O	2.04	0.58
1:A:174:THR:HG22	1:A:178:ARG:NH2	2.19	0.58
1:B:222:PRO:HD2	1:B:568:VAL:HG21	1.85	0.58
1:B:413:LEU:HD23	1:B:428:ILE:HG21	1.86	0.58
1:A:64:SER:HB3	1:A:94:VAL:HG11	1.86	0.57
1:B:84:ARG:HE	1:B:84:ARG:CA	2.13	0.57
1:A:290:GLN:CD	1:A:290:GLN:H	2.12	0.57
1:A:183:ARG:CB	1:A:183:ARG:HH11	2.17	0.57
1:B:288:THR:HG23	1:B:291:GLU:H	1.68	0.57
1:A:63:ASN:ND2	1:A:97:GLY:HA2	2.17	0.56
1:A:553:LEU:HD23	1:A:554:LEU:N	2.20	0.56
1:B:119:HIS:HA	1:B:162:ILE:HD12	1.87	0.56
1:B:112:ARG:HD3	1:B:159:ILE:HD13	1.86	0.56
1:A:415:TYR:HA	1:A:419:GLN:HG2	1.88	0.56
1:A:483:ARG:NH2	1:A:543:GLU:OE2	2.38	0.56
1:B:111:ASN:ND2	1:B:129:LEU:H	2.03	0.56
1:B:114:ILE:HD12	1:B:115:ILE:HG13	1.87	0.56
1:B:184:LEU:HA	1:B:187:MET:HE3	1.88	0.56
1:A:560:LEU:HD21	1:A:576:LYS:HE3	1.87	0.56
1:A:151:SER:HA	1:A:154:ARG:HH11	1.71	0.55
1:A:507:ARG:HD2	4:A:761:HOH:O	2.06	0.55
1:B:286:LYS:HG3	1:B:287:TYR:CD1	2.41	0.55
1:A:183:ARG:HH11	1:A:183:ARG:HA	1.72	0.55
1:A:214:ILE:HD11	1:A:349:LEU:HD13	1.88	0.55
1:B:513:ASN:HD22	1:B:530:PHE:HD2	1.55	0.55
1:A:68:TYR:O	1:A:74:ARG:HD2	2.06	0.55
1:A:394:ARG:HD2	1:A:395:PHE:CE1	2.42	0.55
1:B:439:TYR:O	1:B:443:ILE:HG13	2.07	0.55
1:B:524:LYS:O	1:B:577:VAL:HG21	2.07	0.55
1:B:71:GLU:O	1:B:75:ARG:HG3	2.08	0.54
1:B:282:PRO:O	1:B:286:LYS:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:HG3	1:A:62:THR:CG2	2.38	0.54
1:A:84:ARG:NE	1:A:84:ARG:HA	2.23	0.54
1:B:95:ASP:C	1:B:97:GLY:H	2.14	0.54
1:B:214:ILE:HD11	1:B:349:LEU:HD12	1.89	0.54
1:B:395:PHE:HB3	1:B:410:TYR:HD1	1.70	0.54
1:A:31:ILE:HD11	1:A:58:GLU:O	2.08	0.54
1:A:555:ALA:HB2	1:A:580:GLY:HA2	1.89	0.54
1:B:555:ALA:HB2	1:B:580:GLY:HA2	1.90	0.54
1:B:116:GLU:O	1:B:120:ARG:HG3	2.08	0.54
1:A:471:GLN:HG2	1:A:473:LYS:CE	2.31	0.53
1:B:353:TYR:CE1	1:B:382:ARG:HB2	2.43	0.53
1:B:474:VAL:O	1:B:477:LYS:HG2	2.08	0.53
1:B:517:GLU:HG3	1:B:554:LEU:HD11	1.89	0.53
1:A:107:ILE:HG12	1:A:109:VAL:HG12	1.90	0.53
1:B:64:SER:HB3	1:B:94:VAL:CG2	2.33	0.53
1:B:107:ILE:HD11	1:B:129:LEU:HD13	1.89	0.53
1:A:183:ARG:HH11	1:A:183:ARG:HB3	1.74	0.53
1:A:364:LYS:HE3	4:A:728:HOH:O	2.08	0.53
1:B:221:ARG:HB3	1:B:223:ASP:OD1	2.09	0.53
1:A:282:PRO:O	1:A:286:LYS:HG2	2.07	0.53
1:B:188:ASN:CG	1:B:188:ASN:O	2.51	0.53
1:B:24:LEU:C	1:B:24:LEU:HD23	2.34	0.53
1:B:41:ASN:ND2	1:B:43:LYS:H	2.06	0.53
1:B:431:PRO:HG2	1:B:469:PRO:CG	2.39	0.53
1:A:183:ARG:HH11	1:A:183:ARG:CA	2.21	0.53
1:A:217:LYS:HD3	1:A:243:MET:O	2.08	0.53
1:B:227:HIS:HE1	1:B:249:ASP:OD2	1.92	0.53
1:B:508:MET:O	1:B:544:VAL:HG13	2.09	0.53
1:A:517:GLU:OE2	1:A:521:ARG:NH1	2.33	0.53
1:B:31:ILE:HD11	1:B:58:GLU:O	2.09	0.53
1:B:403:ILE:HD12	1:B:420:SER:OG	2.09	0.53
1:B:140:GLU:HG3	4:B:618:HOH:O	2.10	0.52
1:A:64:SER:HB3	1:A:94:VAL:CG1	2.38	0.52
1:A:183:ARG:HB3	1:A:183:ARG:NH1	2.24	0.52
1:B:510:VAL:HG23	1:B:510:VAL:O	2.08	0.52
1:A:439:TYR:O	1:A:443:ILE:HG13	2.09	0.52
1:B:198:VAL:O	1:B:202:GLU:HG3	2.09	0.52
1:A:127:THR:HG22	1:A:128:PHE:H	1.74	0.52
1:B:360:GLU:HB3	1:B:383:ARG:NH2	2.25	0.52
1:A:519:PHE:HA	1:A:522:LYS:HE3	1.92	0.52
1:B:190:GLU:CD	1:B:190:GLU:N	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:NH1	1:B:488:LEU:HB2	2.24	0.52
1:A:8:LEU:CD2	1:A:26:VAL:HG22	2.39	0.52
1:A:82:ILE:HD11	1:A:122:GLY:O	2.09	0.52
1:B:85:MET:HE2	1:B:86:LEU:CD1	2.38	0.52
1:B:98:SER:O	1:B:101:LEU:HB3	2.10	0.52
1:A:140:GLU:HB2	4:A:746:HOH:O	2.10	0.51
1:B:62:THR:HG22	1:B:63:ASN:H	1.75	0.51
1:A:435:ASP:O	1:A:438:LYS:N	2.41	0.51
1:B:52:LEU:HD23	1:B:55:MET:HE3	1.91	0.51
1:A:82:ILE:HG13	1:A:121:ILE:O	2.10	0.51
1:B:55:MET:HE1	1:B:309:LEU:HD13	1.91	0.51
1:A:24:LEU:HD21	1:A:26:VAL:CG2	2.39	0.51
1:A:510:VAL:HG23	1:A:510:VAL:O	2.10	0.51
1:B:7:MET:HE1	1:B:160:LYS:NZ	2.25	0.51
1:B:166:ALA:HB2	1:B:189:PHE:CG	2.46	0.51
1:B:288:THR:HG22	1:B:291:GLU:CG	2.41	0.51
1:A:429:GLU:OE1	1:A:429:GLU:HA	2.11	0.51
1:A:180:ALA:O	1:A:184:LEU:HD23	2.09	0.51
1:A:24:LEU:CD2	1:A:26:VAL:HG23	2.41	0.51
1:A:506:PRO:O	1:A:535:ASP:HB2	2.11	0.51
1:B:493:ILE:CD1	1:B:497:LYS:HE3	2.41	0.51
1:A:474:VAL:O	1:A:475:ASN:C	2.54	0.50
1:B:163:PRO:HB3	1:B:190:GLU:HG3	1.92	0.50
1:B:33:THR:HA	1:B:34:PRO:C	2.36	0.50
1:B:387:ARG:O	1:B:391:ILE:HD13	2.10	0.50
1:B:554:LEU:C	1:B:581:VAL:HG23	2.37	0.50
1:A:40:VAL:HG22	1:A:62:THR:OG1	2.12	0.50
1:A:133:THR:OG1	1:A:145:GLU:OE2	2.25	0.50
1:A:24:LEU:C	1:A:24:LEU:HD23	2.37	0.50
1:A:41:ASN:O	1:A:45:MET:HG3	2.12	0.50
1:A:514:LYS:HE3	1:A:549:GLU:OE1	2.11	0.50
1:B:431:PRO:HG3	1:B:439:TYR:CE2	2.46	0.50
1:B:493:ILE:HD11	1:B:581:VAL:HG22	1.93	0.50
1:A:47:VAL:HG11	1:A:55:MET:HE1	1.94	0.50
1:A:109:VAL:CG2	1:A:114:ILE:HG23	2.42	0.50
1:A:395:PHE:HB3	1:A:410:TYR:CD1	2.47	0.50
1:B:165:ASN:ND2	1:B:191:ILE:HB	2.26	0.50
1:B:292:LEU:HD13	1:B:295:MET:CE	2.42	0.50
1:B:343:TYR:CZ	1:B:347:LYS:HD2	2.47	0.50
1:B:498:ARG:O	1:B:502:VAL:HG23	2.11	0.50
1:B:517:GLU:HB3	1:B:518:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ARG:N	1:A:406:ARG:CD	2.75	0.49
1:B:41:ASN:HB3	1:B:44:GLN:O	2.11	0.49
1:A:435:ASP:O	1:A:438:LYS:HB2	2.11	0.49
1:B:8:LEU:HD13	1:B:9:LYS:N	2.27	0.49
1:B:109:VAL:CG2	1:B:114:ILE:HG23	2.41	0.49
1:A:31:ILE:HG22	1:A:32:GLU:N	2.27	0.49
1:A:510:VAL:HG13	1:A:544:VAL:CG2	2.43	0.49
1:A:529:LYS:HE3	1:A:530:PHE:CZ	2.48	0.49
1:B:41:ASN:HD22	1:B:41:ASN:C	2.20	0.49
1:A:111:ASN:ND2	1:A:129:LEU:H	2.10	0.49
1:A:174:THR:CG2	1:A:178:ARG:HH22	2.26	0.49
1:B:399:VAL:HG22	1:B:400:GLU:N	2.28	0.49
1:B:96:SER:HB2	1:B:129:LEU:HD23	1.95	0.49
1:A:193:PRO:HA	1:A:227:HIS:HB3	1.95	0.49
1:A:174:THR:CG2	1:A:178:ARG:NH2	2.75	0.49
1:A:289:PRO:HD2	1:A:290:GLN:OE1	2.13	0.49
1:A:330:ARG:NH2	1:A:334:GLU:OE2	2.38	0.49
1:A:554:LEU:C	1:A:581:VAL:HG23	2.38	0.49
1:B:555:ALA:CB	1:B:580:GLY:HA2	2.43	0.49
1:A:479:LEU:O	1:A:495:GLY:HA3	2.13	0.48
1:B:451:GLY:HA3	1:B:454:ARG:HH21	1.78	0.48
1:B:465:LYS:HG3	1:B:466:THR:N	2.28	0.48
1:A:214:ILE:HD11	1:A:349:LEU:HD12	1.95	0.48
1:A:227:HIS:HD2	4:A:602:HOH:O	1.96	0.48
1:A:508:MET:HE3	1:A:545:LEU:HD11	1.95	0.48
1:B:547:VAL:HG23	1:B:552:GLU:C	2.38	0.48
1:B:36:ILE:HD12	1:B:248:PHE:C	2.37	0.48
1:B:207:ARG:HB3	1:B:207:ARG:NH1	2.27	0.48
1:B:397:GLU:CB	1:B:409:ARG:HG2	2.43	0.48
1:A:41:ASN:HD22	1:A:42:PRO:CD	2.27	0.48
1:A:410:TYR:CE2	1:A:438:LYS:HB3	2.48	0.48
1:A:471:GLN:NE2	1:A:478:ARG:HG3	2.24	0.48
1:B:156:ALA:O	1:B:160:LYS:HB2	2.13	0.48
1:B:399:VAL:HG21	1:B:429:GLU:OE2	2.14	0.48
1:B:506:PRO:O	1:B:535:ASP:HB2	2.13	0.48
1:A:264:THR:HG23	1:A:265:PRO:HD2	1.96	0.48
1:A:41:ASN:ND2	1:A:43:LYS:H	2.10	0.48
1:A:416:PRO:O	1:A:420:SER:HB3	2.14	0.48
1:B:47:VAL:HG21	1:B:52:LEU:HD21	1.96	0.48
1:B:406:ARG:HD3	1:B:406:ARG:H	1.75	0.48
1:B:162:ILE:HG23	1:B:163:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:HG2	1:B:219:ALA:HB1	1.94	0.48
1:B:525:ASP:HA	1:B:577:VAL:CG2	2.42	0.48
1:A:82:ILE:HD11	1:A:122:GLY:C	2.39	0.47
1:A:42:PRO:O	1:A:45:MET:HE2	2.14	0.47
1:A:465:LYS:HG3	1:A:466:THR:N	2.29	0.47
1:A:573:ARG:NH1	1:A:576:LYS:HE2	2.30	0.47
1:A:521:ARG:HD3	1:A:582:GLU:CD	2.39	0.47
1:A:445:GLU:OE2	1:A:451:GLY:N	2.48	0.47
1:A:466:THR:C	1:A:468:MET:H	2.23	0.47
1:B:8:LEU:CD2	1:B:26:VAL:HG22	2.41	0.47
1:B:47:VAL:HG22	4:B:707:HOH:O	2.15	0.47
1:B:102:MET:HE3	1:B:132:PRO:O	2.15	0.47
1:B:112:ARG:HD3	1:B:159:ILE:CD1	2.44	0.47
1:B:465:LYS:HG3	1:B:466:THR:HG23	1.96	0.47
1:B:493:ILE:O	1:B:497:LYS:HG3	2.14	0.47
1:B:510:VAL:CG2	1:B:546:VAL:HA	2.45	0.47
1:A:436:ALA:HB1	1:A:461:VAL:HB	1.95	0.47
1:B:459:ALA:HA	1:B:474:VAL:HG22	1.95	0.47
1:B:497:LYS:HG2	1:B:553:LEU:HD23	1.97	0.47
1:A:24:LEU:HD21	1:A:26:VAL:HG23	1.96	0.47
1:B:31:ILE:CD1	1:B:91:ILE:HD12	2.43	0.47
1:A:139:ARG:HG2	1:A:139:ARG:NH1	2.27	0.47
1:B:114:ILE:CD1	1:B:115:ILE:HG13	2.45	0.47
1:B:490:THR:HG23	1:B:578:ARG:CZ	2.45	0.47
1:A:573:ARG:HH11	1:A:576:LYS:HE2	1.80	0.46
1:B:65:TYR:HB2	1:B:97:GLY:HA3	1.96	0.46
1:A:190:GLU:N	1:A:190:GLU:CD	2.72	0.46
1:B:343:TYR:CE1	1:B:347:LYS:HD2	2.50	0.46
1:B:491:LEU:HD11	1:B:499:LEU:HD23	1.97	0.46
1:B:282:PRO:O	1:B:286:LYS:NZ	2.45	0.46
1:A:511:VAL:HA	1:A:547:VAL:O	2.16	0.46
1:B:399:VAL:HG12	1:B:407:VAL:O	2.16	0.46
1:B:52:LEU:HD23	1:B:55:MET:CE	2.46	0.46
1:B:162:ILE:HG22	1:B:163:PRO:O	2.16	0.46
1:A:166:ALA:HB2	1:A:189:PHE:CG	2.50	0.46
1:A:41:ASN:HD22	1:A:41:ASN:C	2.24	0.46
1:B:151:SER:HA	1:B:154:ARG:HE	1.81	0.46
1:A:555:ALA:CB	1:A:580:GLY:HA2	2.45	0.46
1:B:31:ILE:CD1	1:B:59:ILE:HB	2.46	0.46
1:B:178:ARG:HD3	1:B:182:ARG:HH22	1.81	0.46
1:A:288:THR:CG2	1:A:291:GLU:HG3	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PRO:HB3	1:A:541:TYR:HD1	1.81	0.45
1:B:95:ASP:O	1:B:97:GLY:N	2.49	0.45
1:B:288:THR:OG1	1:B:289:PRO:HD2	2.16	0.45
1:B:52:LEU:HA	1:B:55:MET:HE3	1.99	0.45
1:A:258:LYS:O	1:A:297:LYS:NZ	2.50	0.45
1:A:299:GLU:OE1	1:A:299:GLU:HA	2.16	0.45
1:B:233:HIS:ND1	1:B:234:PRO:HD2	2.31	0.45
1:A:391:ILE:CD1	1:A:445:GLU:HB3	2.46	0.45
1:B:468:MET:HA	1:B:469:PRO:HD3	1.88	0.45
1:B:557:GLY:HA2	1:B:578:ARG:HG3	1.99	0.45
1:A:31:ILE:CD1	1:A:91:ILE:HD12	2.43	0.45
1:A:127:THR:CA	1:A:164:MET:HE3	2.47	0.45
1:B:41:ASN:ND2	1:B:41:ASN:C	2.74	0.45
1:B:443:ILE:O	1:B:447:GLN:N	2.43	0.45
1:B:95:ASP:C	1:B:97:GLY:N	2.72	0.44
1:B:416:PRO:O	1:B:420:SER:HB2	2.17	0.44
1:A:101:LEU:O	1:A:101:LEU:HD12	2.18	0.44
1:A:347:LYS:HG2	1:A:377:ARG:HH22	1.81	0.44
1:A:431:PRO:HG2	1:A:469:PRO:HG3	1.99	0.44
1:B:474:VAL:HG12	1:B:475:ASN:ND2	2.33	0.44
1:A:399:VAL:HG12	1:A:407:VAL:O	2.17	0.44
1:B:260:ASP:OD1	1:B:300:ARG:HD2	2.17	0.44
1:A:41:ASN:HD22	1:A:42:PRO:HD2	1.83	0.44
1:A:235:ILE:HG23	1:A:236:VAL:HG13	1.98	0.44
1:B:39:VAL:HG22	1:B:61:ILE:CG2	2.48	0.44
1:B:510:VAL:HG23	1:B:546:VAL:HA	2.00	0.44
1:B:234:PRO:HG3	1:B:312:ILE:HG12	2.00	0.44
1:B:291:GLU:O	1:B:295:MET:HG3	2.18	0.44
1:B:519:PHE:HA	1:B:522:LYS:CE	2.44	0.44
1:B:273:GLU:O	1:B:273:GLU:CG	2.66	0.44
1:A:41:ASN:ND2	1:A:41:ASN:C	2.74	0.44
1:A:264:THR:CG2	1:A:266:GLU:OE1	2.66	0.44
1:B:60:ILE:HG12	1:B:88:TYR:CE2	2.53	0.44
1:B:119:HIS:HD2	1:B:162:ILE:HD12	1.83	0.44
1:B:193:PRO:HA	1:B:227:HIS:O	2.18	0.44
1:B:286:LYS:HD3	4:B:699:HOH:O	2.17	0.44
1:B:497:LYS:O	1:B:501:ARG:HG2	2.18	0.44
1:B:84:ARG:NH2	1:B:89:ASN:OD1	2.51	0.43
1:B:461:VAL:HG11	1:B:469:PRO:HB3	2.00	0.43
1:B:166:ALA:HB1	1:B:184:LEU:HG	2.00	0.43
1:B:391:ILE:N	1:B:391:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:CG2	1:A:32:GLU:N	2.81	0.43
1:A:127:THR:C	1:A:164:MET:HE3	2.43	0.43
1:B:214:ILE:HD12	1:B:352:HIS:CD2	2.53	0.43
1:A:516:ALA:HB2	1:A:530:PHE:CG	2.53	0.43
1:B:62:THR:HG22	1:B:63:ASN:N	2.34	0.43
1:B:97:GLY:O	1:B:100:GLN:OE1	2.37	0.43
1:B:499:LEU:HD12	1:B:499:LEU:HA	1.87	0.43
1:A:168:ILE:CD1	1:A:220:LEU:HD11	2.47	0.43
1:A:277:PHE:CD1	1:A:289:PRO:HG3	2.53	0.43
1:A:468:MET:HA	1:A:469:PRO:HD3	1.84	0.43
1:B:109:VAL:HG21	1:B:114:ILE:HG23	2.00	0.43
1:B:435:ASP:O	1:B:439:TYR:HD1	2.01	0.43
1:B:544:VAL:CG1	1:B:545:LEU:N	2.82	0.43
1:A:164:MET:HE2	1:A:164:MET:HB3	1.95	0.43
1:A:553:LEU:O	1:A:581:VAL:HG21	2.19	0.43
1:B:16:ASP:OD1	1:B:364:LYS:HE2	2.19	0.43
1:B:16:ASP:OD2	1:B:328:LEU:HB2	2.19	0.43
1:B:139:ARG:HH22	1:B:175:ASP:CG	2.26	0.43
1:B:339:HIS:ND1	1:B:340:PRO:HD2	2.33	0.43
1:B:544:VAL:HG12	1:B:545:LEU:N	2.33	0.43
1:A:179:TYR:O	1:A:183:ARG:HG2	2.19	0.42
1:A:295:MET:HE3	1:A:299:GLU:HG3	2.01	0.42
1:A:139:ARG:NH2	1:A:175:ASP:OD2	2.52	0.42
1:A:361:PRO:HB3	1:A:541:TYR:CD1	2.55	0.42
1:B:51:GLU:HG2	1:B:55:MET:HE2	2.00	0.42
1:B:99:PHE:O	1:B:103:LYS:HG3	2.19	0.42
1:B:430:LYS:NZ	1:B:466:THR:HB	2.33	0.42
1:A:435:ASP:O	1:A:436:ALA:C	2.62	0.42
1:A:348:ARG:NH1	1:A:351:GLU:OE1	2.52	0.42
1:A:62:THR:HG22	1:A:63:ASN:H	1.83	0.42
1:B:227:HIS:CE1	1:B:249:ASP:OD2	2.70	0.42
1:A:102:MET:HE2	1:A:134:PRO:HG3	2.01	0.42
1:A:517:GLU:HB3	1:A:518:PRO:HD3	2.02	0.42
1:B:82:ILE:HG23	1:B:121:ILE:HD12	2.02	0.42
1:B:135:PRO:O	1:B:172:THR:HG23	2.19	0.42
1:A:50:LYS:O	1:A:54:LYS:HG3	2.18	0.42
1:B:290:GLN:NE2	1:B:290:GLN:N	2.47	0.42
1:A:419:GLN:HG2	1:A:419:GLN:H	1.58	0.42
1:A:454:ARG:HA	1:A:457:ASP:OD2	2.20	0.41
1:A:132:PRO:HA	1:A:169:GLN:CD	2.45	0.41
1:A:375:SER:HA	1:A:378:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:HH22	1:B:89:ASN:CG	2.27	0.41
1:A:8:LEU:HD22	1:A:26:VAL:HG22	2.02	0.41
1:B:227:HIS:HD2	4:B:602:HOH:O	2.04	0.41
1:B:526:VAL:HB	1:B:575:VAL:HB	2.02	0.41
1:A:430:LYS:NZ	1:A:466:THR:HG23	2.36	0.41
1:A:103:LYS:HE2	1:A:103:LYS:HB3	1.87	0.41
1:A:391:ILE:HD12	1:A:445:GLU:HB3	2.00	0.41
1:B:547:VAL:CG2	1:B:551:ASP:C	2.94	0.41
1:A:281:CYS:HB2	1:A:282:PRO:HD2	2.01	0.41
1:B:21:ILE:HA	1:B:33:THR:O	2.21	0.41
1:B:37:MET:HG2	1:B:248:PHE:O	2.21	0.41
1:A:62:THR:HG22	1:A:63:ASN:N	2.36	0.41
1:B:8:LEU:HG	1:B:190:GLU:HB2	2.03	0.41
1:A:576:LYS:HE3	1:A:576:LYS:HB2	1.83	0.41
1:B:134:PRO:HA	1:B:135:PRO:HD3	1.89	0.41
1:B:160:LYS:HD2	1:B:164:MET:HB2	2.01	0.41
1:B:547:VAL:CG2	1:B:551:ASP:HA	2.51	0.41
1:A:321:GLN:O	1:A:325:GLU:HG2	2.20	0.41
1:A:471:GLN:HB2	4:A:720:HOH:O	2.21	0.41
1:A:510:VAL:HG22	1:A:545:LEU:O	2.20	0.41
1:B:40:VAL:O	1:B:40:VAL:HG23	2.21	0.41
1:B:61:ILE:HA	1:B:93:GLU:O	2.21	0.41
1:B:127:THR:HG22	1:B:128:PHE:N	2.36	0.41
1:B:290:GLN:HA	1:B:293:ARG:NH1	2.36	0.41
1:B:434:GLU:N	1:B:434:GLU:CD	2.79	0.41
1:A:39:VAL:HG22	1:A:61:ILE:HG23	2.03	0.41
1:A:82:ILE:HG13	1:A:82:ILE:H	1.53	0.41
1:B:315:GLU:OE2	1:B:318:ARG:NH1	2.50	0.41
1:B:471:GLN:HG3	1:B:478:ARG:HD3	2.02	0.41
1:B:83:HIS:CE1	1:B:124:ASP:OD2	2.74	0.40
1:B:415:TYR:HB2	1:B:419:GLN:HE22	1.85	0.40
1:A:232:GLY:CA	1:A:250:SER:HB2	2.51	0.40
1:A:430:LYS:NZ	1:A:466:THR:CG2	2.84	0.40
1:A:579:LYS:HE3	1:A:579:LYS:HB2	1.75	0.40
1:B:336:ALA:HB1	1:B:343:TYR:HA	2.03	0.40
1:A:399:VAL:O	1:A:406:ARG:HA	2.21	0.40
1:A:504:PRO:O	1:A:505:TYR:C	2.63	0.40
1:B:41:ASN:ND2	1:B:42:PRO:HD2	2.34	0.40
1:B:108:GLU:N	1:B:108:GLU:CD	2.79	0.40
1:B:256:TYR:HB3	1:B:261:ARG:HB2	2.03	0.40
1:B:464:SER:O	1:B:465:LYS:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:C	1:A:106:SER:H	2.29	0.40
1:A:131:ILE:O	1:A:169:GLN:CG	2.60	0.40
1:A:547:VAL:HG23	1:A:552:GLU:C	2.46	0.40
1:A:431:PRO:HG2	1:A:469:PRO:CG	2.51	0.40
1:B:42:PRO:HB2	1:B:73:LEU:HD21	2.04	0.40
1:B:86:LEU:N	1:B:86:LEU:HD12	2.36	0.40
1:B:582:GLU:O	1:B:582:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/582 (99%)	554 (96%)	18 (3%)	3 (0%)	24	27
1	B	575/582 (99%)	540 (94%)	30 (5%)	5 (1%)	14	14
All	All	1150/1164 (99%)	1094 (95%)	48 (4%)	8 (1%)	18	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	ASN
1	A	436	ALA
1	B	96	SER
1	B	418	ALA
1	B	464	SER
1	B	466	THR
1	A	129	LEU
1	B	109	VAL

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%)	473 (95%)	26 (5%)	21	26
1	B	499/503 (99%)	469 (94%)	30 (6%)	17	21
All	All	998/1006 (99%)	942 (94%)	56 (6%)	19	24

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	40	VAL
1	A	72	GLU
1	A	82	ILE
1	A	94	VAL
1	A	144	LYS
1	A	174	THR
1	A	183	ARG
1	A	190	GLU
1	A	207	ARG
1	A	264	THR
1	A	290	GLN
1	A	294	GLU
1	A	328	LEU
1	A	330	ARG
1	A	342	LEU
1	A	370	LYS
1	A	419	GLN
1	A	429	GLU
1	A	438	LYS
1	A	493	ILE
1	A	507	ARG
1	A	522	LYS
1	A	539	ARG
1	A	547	VAL
1	A	553	LEU
1	B	8	LEU

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Mol	Chain	Res	Type
1	B	26	VAL
1	B	82	ILE
1	B	123	VAL
1	B	162	ILE
1	B	184	LEU
1	B	188	ASN
1	B	190	GLU
1	B	207	ARG
1	B	227	HIS
1	B	264	THR
1	B	273	GLU
1	B	290	GLN
1	B	292	LEU
1	B	294	GLU
1	B	297	LYS
1	B	302	ARG
1	B	317	LYS
1	B	328	LEU
1	B	330	ARG
1	B	342	LEU
1	B	368	LEU
1	B	371	ILE
1	B	429	GLU
1	B	477	LYS
1	B	493	ILE
1	B	499	LEU
1	B	506	PRO
1	B	514	LYS
1	B	522	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	83	HIS
1	A	111	ASN
1	A	141	GLN
1	A	165	ASN
1	A	227	HIS
1	A	352	HIS
1	A	419	GLN
1	A	471	GLN

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Mol	Chain	Res	Type
1	B	41	ASN
1	B	83	HIS
1	B	111	ASN
1	B	141	GLN
1	B	165	ASN
1	B	227	HIS
1	B	290	GLN
1	B	471	GLN
1	B	475	ASN
1	B	513	ASN
1	B	570	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.