



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID : 1IT8  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

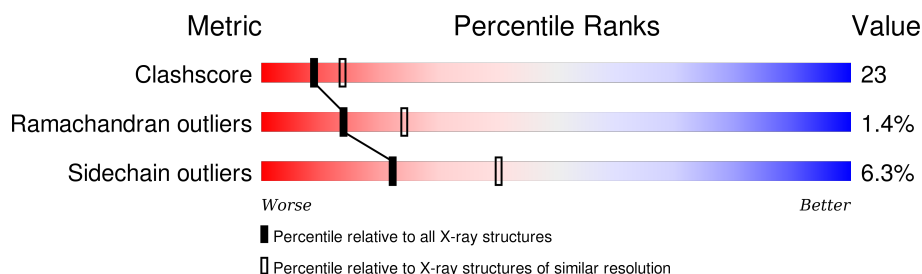
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	 61% 33% 5%
1	B	582	 57% 37% 5%

## 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			

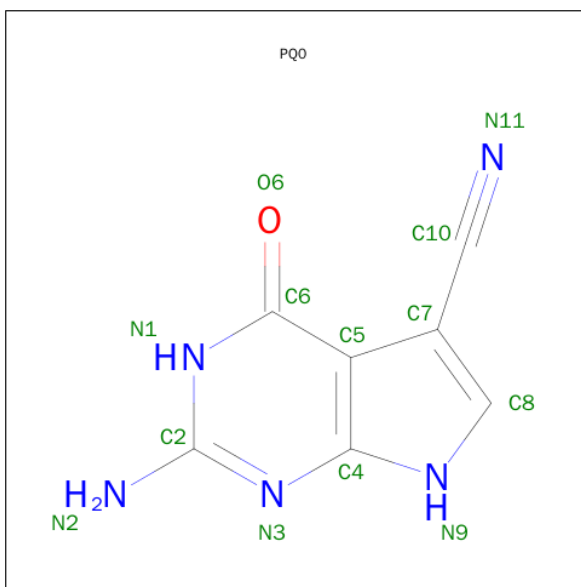
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	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 (three-letter code: PQ0) (formula: C<sub>7</sub>H<sub>5</sub>N<sub>5</sub>O).



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

- Molecule 5 is water.

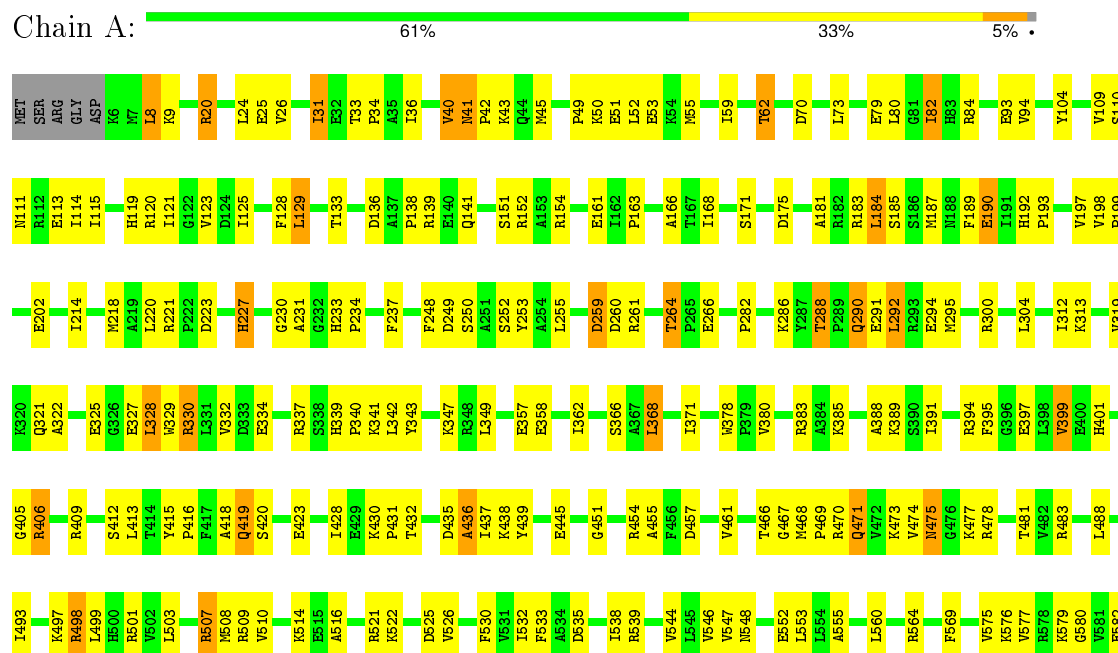
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	B	66	Total	O	0	0
			66	66		

### 3 Residue-property plots

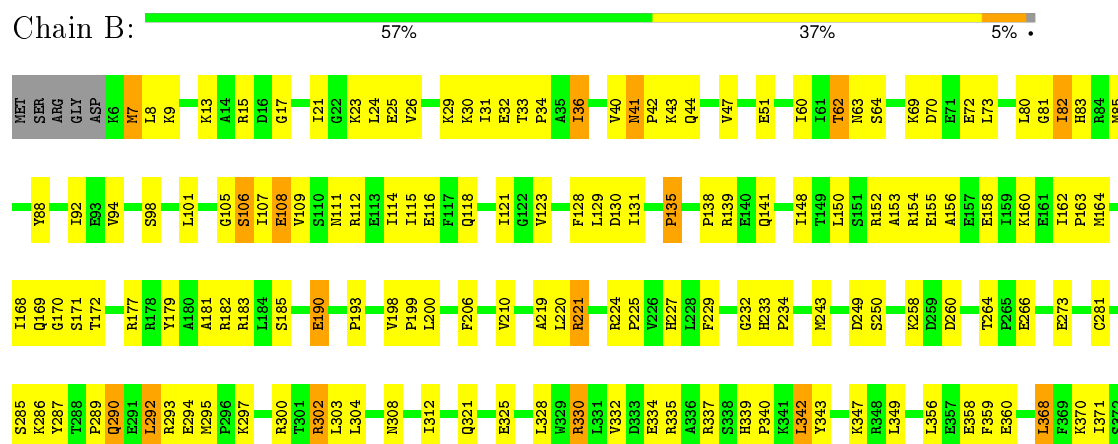
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

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 will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.47Å 100.47Å 366.17Å 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 <sup>2</sup> )	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, 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	0.40	0/4745	0.65	0/6391
1	B	0.38	0/4745	0.64	0/6391
All	All	0.39	0/9490	0.64	0/12782

There are no bond length outliers.

There are no bond angle outliers.

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	193	0
1	B	4652	0	4747	247	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
All	All	9463	0	9499	438	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 23.

All (438) 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: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:B:107:ILE:HD11	1:B:129:LEU:HD21	1.61	0.82
1:A:514:LYS:N	1:A:514:LYS:HD2	1.95	0.81
1:A:412:SER:O	1:A:418:ALA:HB2	1.81	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: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:A:185:SER:HB3	1:A:221:ARG:HG3	1.70	0.74
1:B:111:ASN:HD21	1:B:128:PHE:HB2	1.51	0.73
1:A:8:LEU:HD21	1:A:24:LEU:HD21	1.68	0.73
1:A:129:LEU:HB3	1:A:152:ARG:HH11	1.50	0.73
1:B:547:VAL:HG23	1:B:552:GLU:C	2.09	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:HA	1:A:84:ARG:NE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:514:LYS:HD2	2.06	0.70
1:B:70:ASP:CG	1:B:73:LEU:HD13	2.12	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: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:H	1:B:514:LYS:HD2	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:B:162:ILE:HG13	1:B:163:PRO:CD	2.24	0.67
1:A:288:THR:HG22	1:A:291:GLU:CG	2.25	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:503:LEU:HD12	1:B:508:MET:HE3	1.77	0.65
1:B:82:ILE:HD12	1:B:83:HIS:N	2.11	0.65
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:B:41:ASN:HD22	1:B:41:ASN:C	2.01	0.64
1:A:36:ILE:HD13	1:A:312:ILE:HG21	1.80	0.64
1:B:295:MET:HE1	1:B:303:LEU:HD12	1.79	0.64
1:B:260:ASP:OD1	1:B:300:ARG:HD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:LEU:HD13	1:B:26:VAL:CG2	2.27	0.63
1:A:560:LEU:HD21	1:A:576:LYS:HE3	1.78	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:128:PHE:HB3	1:B:164:MET:HE1	1.81	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:A:327:GLU:HG2	1:A:327:GLU:O	2.01	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:184:LEU:HA	1:A:187:MET:HE3	1.82	0.60
1:B:468:MET:HB3	1:B:470:ARG:HH12	1.67	0.60
1:A:190:GLU:N	1:A:190:GLU:OE1	2.35	0.59
1:B:41:ASN:ND2	1:B:41:ASN:C	2.56	0.59
1:A:40:VAL:O	1:A:62:THR:HG23	2.01	0.59
1:B:292:LEU:HD22	1:B:295:MET:HE1	1.83	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:B:474:VAL:C	1:B:476:GLY:H	2.05	0.59
1:B:399:VAL:HG21	1:B:429:GLU:OE2	2.01	0.59
1:A:93:GLU:HG3	1:A:125:ILE:HB	1.83	0.59
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:264:THR:HG22	1:A:266:GLU:N	2.16	0.58
1:A:183:ARG:NH1	1:A:183:ARG:HB3	2.17	0.58
1:B:297:LYS:HD3	1:B:297:LYS:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:CD1	1:A:508:MET:HE2	2.33	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:499:LEU:HG	1:A:508:MET:HE1	1.85	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:B:555:ALA:CB	1:B:580:GLY:HA2	2.35	0.57
1:A:330:ARG:NH2	1:A:334:GLU:OE1	2.38	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:N	1:B:406:ARG:HD3	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:B:394:ARG:HD2	1:B:395:PHE:CE1	2.40	0.56
1:A:233:HIS:ND1	1:A:234:PRO:HD2	2.20	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: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:A:343:TYR:CZ	1:A:347:LYS:HD2	2.41	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:HH11	1:A:183:ARG:HB3	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:H	1:B:428:ILE:HD12	1.71	0.55
1:B:397:GLU:HB3	1:B:409:ARG:CG	2.34	0.55
1:A:406:ARG:HD3	1:A:406:ARG:H	1.71	0.55
1:B:428:ILE:N	1:B:428:ILE:HD12	2.22	0.55
1:B:31:ILE:HD12	5:B:648:HOH:O	2.06	0.55
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:330:ARG:HH11	1:B:330:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:193:PRO:HA	1:B:227:HIS:O	2.08	0.53
1:A:401:HIS:N	1:A:405:GLY:O	2.35	0.53
1:B:41:ASN:HD22	1:B:42:PRO:HD2	1.73	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:163:PRO:HA	1:B:190:GLU:OE1	2.08	0.53
1:B:73:LEU:HD12	1:B:73:LEU:N	2.24	0.53
1:A:415:TYR:HB2	1:A:419:GLN:HG3	1.91	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:B:492:GLY:O	1:B:495:GLY:N	2.42	0.53
1:A:129:LEU:HB3	1:A:152:ARG:NH1	2.20	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: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:B:221:ARG:HD2	1:B:224:ARG:NE	2.25	0.52
1:B:98:SER:O	1:B:101:LEU:HB3	2.10	0.52
1:A:477:LYS:CG	1:A:478:ARG:H	2.22	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:111:ASN:HD22	1:B:129:LEU:H	1.58	0.52
1:B:82:ILE:HD12	1:B:83:HIS:H	1.72	0.52
1:B:64:SER:HB3	1:B:94:VAL:HG21	1.90	0.51
1:B:112:ARG:O	1:B:116:GLU:HG3	2.11	0.51
1:B:493:ILE:O	1:B:497:LYS:HG3	2.10	0.51
1:A:198:VAL:HG22	1:A:230:GLY:HA3	1.93	0.51
1:B:64:SER:HB3	1:B:94:VAL:HG22	1.91	0.51
1:B:7:MET:HG3	1:B:163:PRO:HG3	1.92	0.51
1:A:445:GLU:OE2	1:A:451:GLY:N	2.44	0.51
1:A:325:GLU:O	1:A:366:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:PRO:HD2	1:A:467:GLY:O	2.11	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:A:41:ASN:HD22	1:A:41:ASN:C	2.12	0.50
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:B:70:ASP:OD1	1:B:72:GLU:HB2	2.11	0.50
1:A:36:ILE:HD12	1:A:237:PHE:CZ	2.46	0.50
1:B:448:PHE:HE2	1:B:543:GLU:HB2	1.75	0.50
1:A:79:GLU:O	1:A:80:LEU:HD23	2.12	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:111:ASN:HD22	1:A:129:LEU:HB2	1.76	0.50
1:A:36:ILE:HG21	1:A:312:ILE:CG2	2.42	0.50
1:B:437:ILE:HG23	1:B:438:LYS:N	2.25	0.50
1:B:69:LYS:NZ	1:B:108:GLU:HB3	2.26	0.50
1:B:507:ARG:O	1:B:508:MET:HB2	2.12	0.50
1:B:232:GLY:CA	1:B:250:SER:HB2	2.42	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
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:292:LEU:HD22	1:A:295:MET:HE3	1.95	0.49
1:A:181:ALA:HB1	1:A:220:LEU:HG	1.94	0.49
1:B:107:ILE:HD11	1:B:129:LEU:CD2	2.39	0.49
1:A:436:ALA:O	1:A:439:TYR:HB2	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:478:ARG:HD2	1:A:481:THR:OG1	2.13	0.49
1:A:121:ILE:HG13	1:A:123:VAL:HG23	1.94	0.49
1:B:397:GLU:HG3	1:B:410:TYR:CE1	2.47	0.48
1:B:492:GLY:O	1:B:494:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HB	1:B:199:PRO:HD3	1.95	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:578:ARG:HG2	1:B:578:ARG:HH11	1.79	0.48
1:A:260:ASP:HA	1:A:304:LEU:CD1	2.44	0.48
1:B:521:ARG:NH1	1:B:521:ARG:HG3	2.25	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:185:SER:HB3	1:B:221:ARG:HG2	1.95	0.48
1:A:430:LYS:NZ	1:A:466:THR:CG2	2.77	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:264:THR:HG23	1:A:266:GLU:OE1	2.12	0.47
1:A:24:LEU:HD23	1:A:25:GLU:N	2.29	0.47
1:B:510:VAL:HG23	1:B:544:VAL:CG2	2.44	0.47
1:A:41:ASN:ND2	1:A:41:ASN:C	2.66	0.47
1:A:104:TYR:CD2	1:A:104:TYR:N	2.78	0.47
1:A:474:VAL:O	1:A:475:ASN:C	2.52	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:471:GLN:OE1	1:A:478:ARG:HD3	2.14	0.47
1:A:339:HIS:CE1	1:A:341:LYS:HB2	2.50	0.47
1:B:503:LEU:CD1	1:B:508:MET:HE2	2.45	0.47
1:A:41:ASN:ND2	1:A:42:PRO:HD2	2.25	0.47
1:B:521:ARG:CG	1:B:521:ARG:HH11	2.26	0.47
1:B:468:MET:HB3	1:B:470:ARG:NH1	2.29	0.47
1:B:135:PRO:O	1:B:172:THR:HG23	2.14	0.47
1:B:25:GLU:HA	1:B:29:LYS:O	2.15	0.47
1:B:525:ASP:HA	1:B:577:VAL:HG23	1.97	0.47
1:B:391:ILE:HD12	1:B:391:ILE:N	2.30	0.47
1:B:499:LEU:HD12	1:B:508:MET:HE1	1.97	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:547:VAL:HG23	1:A:552:GLU:C	2.35	0.46
1:A:503:LEU:HD12	1:A:508:MET:HE2	1.96	0.46
1:A:507:ARG:O	1:A:509:ARG:HD2	2.14	0.46
1:B:435:ASP:O	1:B:436:ALA:C	2.53	0.46
1:A:114:ILE:HD12	1:A:115:ILE:HG13	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HA	1:B:33:THR:O	2.15	0.46
1:A:397:GLU:OE1	1:A:409:ARG:HD3	2.16	0.46
1:B:73:LEU:H	1:B:73:LEU:CD1	2.29	0.46
1:A:358:GLU:OE2	1:A:564:ARG:NH1	2.46	0.46
1:A:120:ARG:HD2	5:A:630:HOH:O	2.15	0.46
1:B:413:LEU:HD23	1:B:428:ILE:CG2	2.45	0.46
1:A:385:LYS:O	1:A:388:ALA:HB3	2.16	0.46
1:B:81:GLY:O	1:B:83:HIS:N	2.49	0.46
1:B:17:GLY:HA2	1:B:360:GLU:OE1	2.15	0.46
1:A:231:ALA:O	1:A:248:PHE:HB3	2.16	0.46
1:B:450:GLU:OE2	1:B:451:GLY:N	2.48	0.46
1:A:82:ILE:HD12	1:A:82:ILE:N	2.31	0.46
1:B:243:MET:HG2	1:B:349:LEU:CD1	2.47	0.45
1:B:190:GLU:N	1:B:190:GLU:CD	2.70	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:B:179:TYR:OH	1:B:183:ARG:NH1	2.49	0.45
1:A:362:ILE:HD12	1:A:383:ARG:NH1	2.31	0.45
1:A:329:TRP:HB3	1:A:378:TRP:CE2	2.52	0.45
1:B:397:GLU:HG3	1:B:410:TYR:CZ	2.51	0.45
1:B:73:LEU:CD1	1:B:73:LEU:N	2.80	0.45
1:B:462:GLU:OE2	1:B:471:GLN:HB3	2.16	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: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:454:ARG:HA	1:A:457:ASP:OD2	2.17	0.45
1:B:128:PHE:HD2	1:B:164:MET:CE	2.30	0.45
1:A:497:LYS:O	1:A:501:ARG:HG2	2.17	0.45
1:B:503:LEU:HD12	1:B:508:MET:HE2	1.98	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:B:406:ARG:HD3	1:B:406:ARG:H	1.82	0.44
1:B:397:GLU:HG3	1:B:410:TYR:OH	2.16	0.44
1:A:8:LEU:HD13	1:A:9:LYS:N	2.33	0.44
1:A:371:ILE:HD13	1:B:337:ARG:HB3	2.00	0.44
1:B:111:ASN:HD22	1:B:129:LEU:HB2	1.81	0.44
1:A:503:LEU:HD12	1:A:508:MET:CE	2.48	0.44
1:A:151:SER:HA	1:A:154:ARG:NH1	2.32	0.44
1:B:42:PRO:HG3	1:B:62:THR:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:493:ILE:HD13	1:B:493:ILE:H	1.82	0.44
1:B:339:HIS:CE1	1:B:340:PRO:HD2	2.53	0.44
1:B:131:ILE:O	1:B:169:GLN:HG2	2.18	0.44
1:A:111:ASN:HD22	1:A:129:LEU:N	2.13	0.44
1:A:435:ASP:O	1:A:436:ALA:C	2.55	0.44
1:B:450:GLU:O	1:B:452:ALA:N	2.51	0.44
1:A:339:HIS:CG	1:A:340:PRO:HD2	2.52	0.44
1:B:535:ASP:HB3	1:B:538:ILE:HG13	1.99	0.44
1:A:168:ILE:N	1:A:168:ILE:HD12	2.33	0.44
1:A:109:VAL:CG2	1:A:114:ILE:HG23	2.45	0.43
1:B:42:PRO:HG3	1:B:62:THR:HG22	1.99	0.43
1:A:510:VAL:CG2	1:A:546:VAL:HA	2.48	0.43
1:B:94:VAL:HG11	1:B:123:VAL:HG21	1.99	0.43
1:B:394:ARG:HD2	1:B:395:PHE:CD1	2.53	0.43
1:B:168:ILE:N	1:B:168:ILE:HD12	2.33	0.43
1:A:259:ASP:HB3	1:A:261:ARG:HG3	2.00	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:24:LEU:C	1:B:24:LEU:HD23	2.38	0.43
1:B:9:LYS:HG2	1:B:571:TYR:CE2	2.54	0.43
1:B:548:ASN:HD21	1:B:552:GLU:HB2	1.83	0.43
1:B:514:LYS:HZ3	1:B:549:GLU:HG3	1.84	0.43
1:A:362:ILE:HD12	1:A:362:ILE:HA	1.83	0.43
1:A:319:VAL:O	1:A:322:ALA:HB3	2.18	0.43
1:A:416:PRO:O	1:A:420:SER:HB3	2.18	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:51:GLU:OE2	1:B:302:ARG:NH1	2.51	0.43
1:B:493:ILE:HD13	1:B:493:ILE:N	2.33	0.43
1:B:138:PRO:HD2	1:B:141:GLN:NE2	2.30	0.43
1:B:470:ARG:O	1:B:481:THR:HG23	2.18	0.43
1:B:448:PHE:HB2	1:B:452:ALA:CB	2.49	0.43
1:B:286:LYS:HG3	1:B:287:TYR:CD1	2.53	0.43
1:B:135:PRO:HB3	1:B:200:LEU:HD21	2.00	0.43
1:A:532:ILE:HG13	1:A:533:PHE:N	2.34	0.43
1:A:388:ALA:O	1:A:389:LYS:C	2.57	0.43
1:B:170:GLY:O	1:B:171:SER:HB3	2.18	0.43
1:A:423:GLU:OE2	1:A:423:GLU:N	2.43	0.43
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HD22	1:B:295:MET:CE	2.47	0.42
1:A:288:THR:HG23	1:A:290:GLN:N	2.34	0.42
1:A:223:ASP:HA	1:A:569:PHE:CZ	2.54	0.42
1:A:139:ARG:NH2	1:A:175:ASP:OD2	2.52	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:B:508:MET:O	1:B:544:VAL:HG22	2.19	0.42
1:A:406:ARG:O	1:A:406:ARG:HG2	2.19	0.42
1:A:466:THR:HG22	1:A:467:GLY:N	2.34	0.42
1:A:119:HIS:CD2	1:A:161:GLU:HB2	2.54	0.42
1:A:468:MET:HA	1:A:469:PRO:HD3	1.85	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:B:23:LYS:HE3	1:B:30:LYS:HD3	2.01	0.42
1:B:562:SER:O	1:B:563:GLY:C	2.56	0.42
1:A:466:THR:O	1:A:468:MET:N	2.44	0.42
1:B:408:SER:OG	1:B:410:TYR:HD1	2.03	0.42
1:B:13:LYS:HE3	1:B:23:LYS:HB2	2.01	0.42
1:A:20:ARG:HD3	5:A:617:HOH:O	2.19	0.42
1:A:41:ASN:ND2	1:A:43:LYS:H	2.18	0.42
1:A:24:LEU:HD23	1:A:24:LEU:C	2.40	0.42
1:B:368:LEU:HD11	1:B:381:VAL:CG2	2.49	0.42
1:B:466:THR:C	1:B:468:MET:H	2.18	0.42
1:B:435:ASP:O	1:B:438:LYS:N	2.52	0.42
1:A:49:PRO:HA	1:A:52:LEU:HD12	2.01	0.42
1:B:521:ARG:NH1	1:B:521:ARG:CG	2.83	0.41
1:B:221:ARG:CD	1:B:224:ARG:NE	2.82	0.41
1:B:41:ASN:HD21	1:B:43:LYS:H	1.65	0.41
1:B:394:ARG:NH2	1:B:445:GLU:OE2	2.53	0.41
1:A:368:LEU:HB3	1:A:420:SER:HB2	2.02	0.41
1:A:227:HIS:HD2	5:A:605:HOH:O	2.04	0.41
1:B:135:PRO:HG2	1:B:199:PRO:HB2	2.02	0.41
1:A:535:ASP:HB3	1:A:538:ILE:HG13	2.01	0.41
1:B:33:THR:HA	1:B:34:PRO:C	2.40	0.41
1:A:357:GLU:O	1:A:383:ARG:NH2	2.54	0.41
1:A:292:LEU:HA	1:A:295:MET:CE	2.51	0.41
1:B:224:ARG:HA	1:B:225:PRO:HD3	1.95	0.41
1:A:471:GLN:HE21	1:A:471:GLN:CA	2.33	0.41
1:A:111:ASN:ND2	1:A:128:PHE:HB2	2.18	0.41
1:B:335:ARG:O	1:B:342:LEU:HD13	2.20	0.41
1:B:461:VAL:CG1	1:B:469:PRO:HB3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:H	1:B:465:LYS:HG2	1.61	0.41
1:B:510:VAL:HG23	1:B:544:VAL:HG22	2.02	0.41
1:B:478:ARG:HH11	1:B:480:ALA:C	2.23	0.41
1:B:304:LEU:HA	1:B:304:LEU:HD23	1.89	0.41
1:A:291:GLU:O	1:A:292:LEU:C	2.59	0.41
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.84	0.41
1:B:289:PRO:O	1:B:293:ARG:HG3	2.21	0.41
1:B:107:ILE:HD12	1:B:109:VAL:CG1	2.51	0.41
1:B:40:VAL:O	1:B:62:THR:CG2	2.65	0.41
1:B:548:ASN:ND2	1:B:552:GLU:HB2	2.36	0.41
1:B:578:ARG:NH1	1:B:578:ARG:HG2	2.36	0.41
1:B:23:LYS:NZ	1:B:30:LYS:NZ	2.69	0.41
1:A:70:ASP:HB3	1:A:73:LEU:HB2	2.02	0.41
1:B:150:LEU:O	1:B:153:ALA:HB3	2.20	0.41
1:B:36:ILE:HG12	1:B:312:ILE:HG21	2.04	0.41
1:A:555:ALA:CB	1:A:580:GLY:HA2	2.51	0.41
1:A:380:VAL:O	1:A:380:VAL:HG22	2.21	0.41
1:B:492:GLY:O	1:B:493:ILE:C	2.59	0.40
1:A:499:LEU:HB3	1:A:508:MET:HE3	2.03	0.40
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:252:SER:O	1:A:253:TYR:C	2.60	0.40
1:B:503:LEU:HA	1:B:504:PRO:HD3	1.80	0.40
1:B:419:GLN:HE22	1:B:486:ASP:HA	1.81	0.40
1:B:60:ILE:HG23	1:B:88:TYR:CZ	2.56	0.40
1:A:288:THR:HG22	1:A:291:GLU:H	1.85	0.40
1:A:185:SER:CB	1:A:221:ARG:HG3	2.45	0.40
1:B:547:VAL:CG2	1:B:552:GLU:N	2.84	0.40
1:A:521:ARG:HB3	1:A:582:GLU:HG3	2.03	0.40
1:A:250:SER:HA	5:A:607:HOH:O	2.20	0.40
1:A:33:THR:HB	1:A:34:PRO:HA	2.02	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%)	534 (93%)	38 (7%)	3 (0%)	34	55
1	B	575/582 (99%)	514 (89%)	48 (8%)	13 (2%)	8	12
All	All	1150/1164 (99%)	1048 (91%)	86 (8%)	16 (1%)	14	24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	ALA
1	A	475	ASN
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%)	464 (93%)	35 (7%)	19	34
1	B	499/503 (99%)	471 (94%)	28 (6%)	26	47
All	All	998/1006 (99%)	935 (94%)	63 (6%)	22	40

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	20	ARG
1	A	31	ILE
1	A	40	VAL
1	A	41	ASN
1	A	51	GLU
1	A	62	THR
1	A	82	ILE
1	A	94	VAL
1	A	129	LEU
1	A	184	LEU
1	A	190	GLU
1	A	227	HIS
1	A	249	ASP
1	A	259	ASP
1	A	264	THR
1	A	288	THR
1	A	290	GLN
1	A	292	LEU
1	A	294	GLU
1	A	328	LEU
1	A	330	ARG
1	A	342	LEU
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	507	ARG
1	A	522	LYS
1	A	544	VAL
1	A	553	LEU
1	A	579	LYS
1	B	7	MET
1	B	36	ILE
1	B	41	ASN
1	B	47	VAL
1	B	62	THR
1	B	80	LEU
1	B	108	GLU
1	B	190	GLU

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Mol	Chain	Res	Type
1	B	221	ARG
1	B	229	PHE
1	B	249	ASP
1	B	290	GLN
1	B	292	LEU
1	B	294	GLU
1	B	302	ARG
1	B	330	ARG
1	B	342	LEU
1	B	358	GLU
1	B	368	LEU
1	B	373	ASN
1	B	406	ARG
1	B	416	PRO
1	B	429	GLU
1	B	445	GLU
1	B	507	ARG
1	B	522	LYS
1	B	542	ASP
1	B	544	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	188	ASN
1	A	290	GLN
1	A	419	GLN
1	A	471	GLN
1	B	41	ASN
1	B	63	ASN
1	B	83	HIS
1	B	111	ASN
1	B	141	GLN
1	B	165	ASN
1	B	290	GLN
1	B	513	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	13,14,14	3.37	9 (69%)	9,20,20	3.64	4 (44%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	PQ0	C8-N9	-3.31	1.29	1.36
4	A	602	PQ0	C5-C4	-2.94	1.35	1.43
4	A	602	PQ0	C4-N9	-2.69	1.29	1.34
4	A	602	PQ0	C2-N2	-2.34	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	PQ0	C2-N1	3.09	1.40	1.35
4	A	602	PQ0	C6-N1	3.72	1.40	1.33
4	A	602	PQ0	C7-C5	4.54	1.47	1.42
4	A	602	PQ0	C6-C5	4.81	1.49	1.41
4	A	602	PQ0	C4-N3	6.58	1.48	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	PQ0	C5-C6-N1	-8.19	117.99	124.19
4	A	602	PQ0	N3-C2-N1	-4.86	120.04	127.44
4	A	602	PQ0	N2-C2-N3	2.03	121.70	117.80
4	A	602	PQ0	C6-N1-C2	4.49	122.17	115.94

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.