



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:14 PM UTC

PDB ID : 1IT7 / pdb_00001it7
Title : Crystal structure of archaeosine tRNA-guanine transglycosylase complexed with guanine
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 : 2.30 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

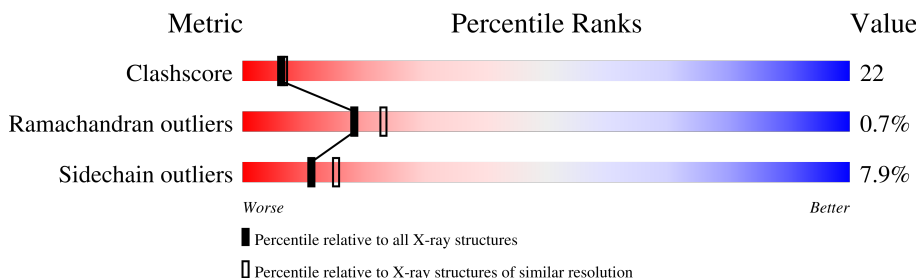
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 9503 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			

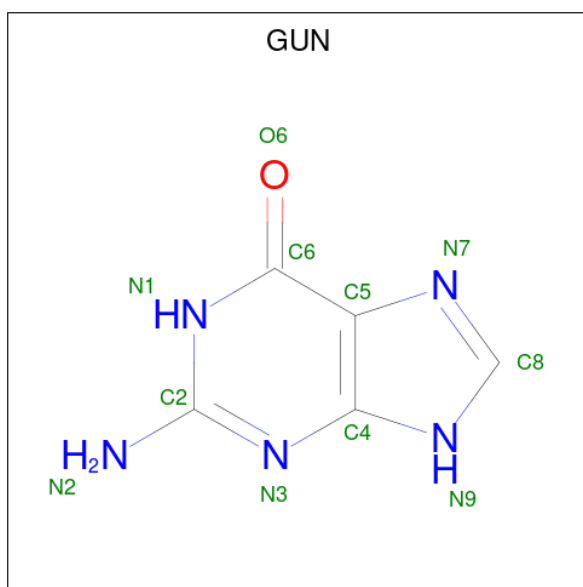
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 5 is water.

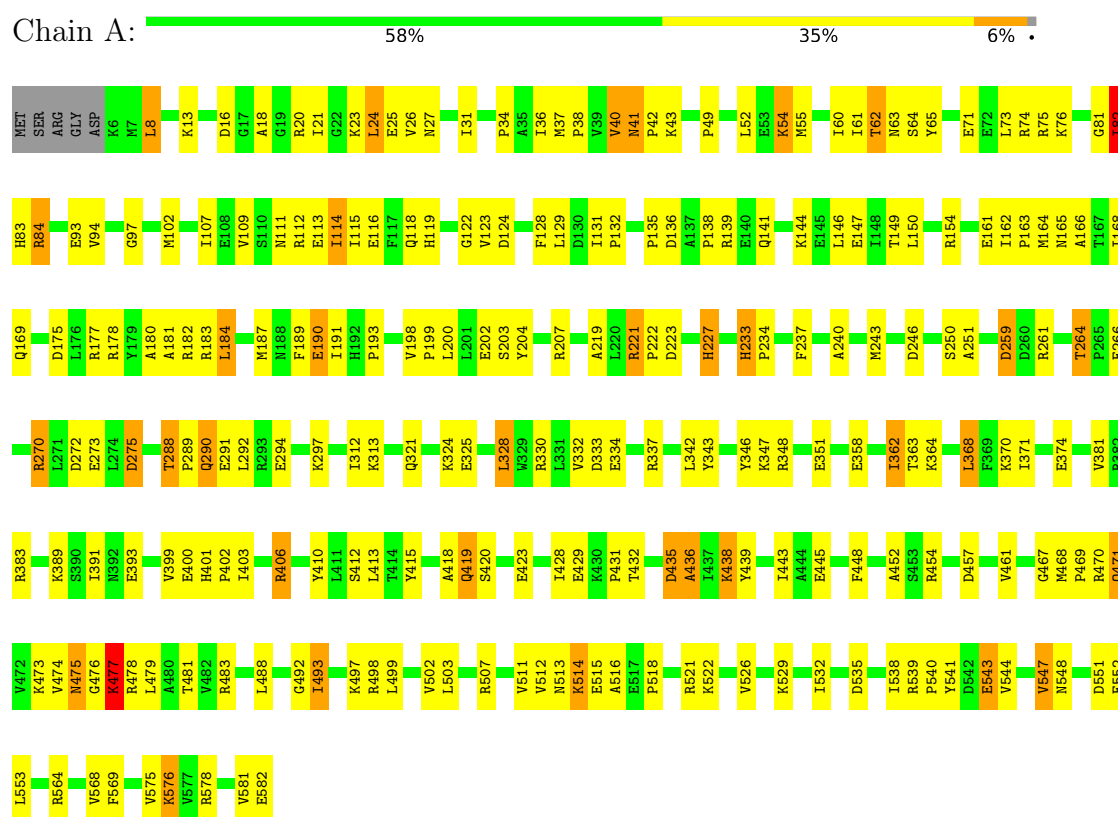
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	79	Total	O	0	0
			79	79		

3 Residue-property plots

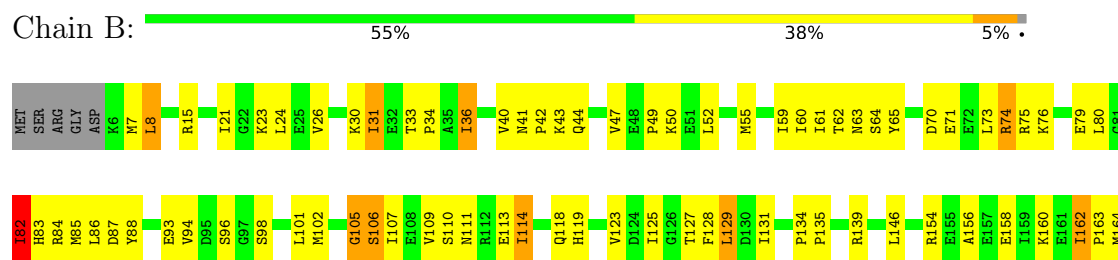
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



A452	I362	R270	N165
A459	K365	L271	A166
K460	L368	D272	T167
V461	F369	E273	I168
T466	K370	L274	Q169
G467		D275	
M468	N373	S280	A180
P469	E374		A181
R470	S375	S285	R182
	L376		R183
K473	R377	T288	L184
V474	V381		S185
N475		P289	N188
G476	E386	Q290	F189
K477		E291	E190
R478	K389	L292	I191
	S390	R293	H192
R483	S390	M294	P193
A484	I391	P296	V198
D485		K297	P199
	R394		
L488	F395	R300	E202
L489	G396	T301	
T490	E397	R302	E207
K491		L303	
G492	I403	L309	I214
I493			S215
	R406	I316	S216
A496	R409		K217
K497	Y410	Q321	M218
R498			A219
L499			L220
	L413	K324	R221
V502	T414	E325	P222
L503	Y415		D223
P504	P416	L328	R224
Y505	F417	W329	P225
P506	A418	R330	R226
R507	Q419		H227
M508	S420		V227
R509		D333	L228
V510	I428	E334	F229
V511	E429	R335	
	K430	A336	H233
K514	P431	S338	P234
	T432	H339	
F519	K433	P340	M243
A520	E434		
R521	D435	K341	D249
	A436	L342	S250
K524	I437	Y343	A251
D525	K438	S344	S252
V526	Y439		Y253
		K347	
	I443	F355	D260
K529			
F530	F448	F359	T264
V531			P265
I532			E266

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	100.20 Å 100.20 Å 364.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	98.3 (50.00-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9503	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: MG, GUN, 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	0.44	0/4745	0.97	20/6391 (0.3%)
1	B	0.42	0/4745	0.97	19/6391 (0.3%)
All	All	0.43	0/9490	0.97	39/12782 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ALA	N-CA-C	-7.63	104.20	113.97
1	A	221	ARG	CA-C-N	7.24	127.57	119.32
1	A	221	ARG	C-N-CA	7.24	127.57	119.32
1	A	514	LYS	N-CA-C	-7.22	103.49	111.36
1	A	251	ALA	N-CA-C	-6.93	105.37	114.31
1	A	543	GLU	N-CA-C	-6.67	100.61	110.48
1	B	167	THR	N-CA-C	6.54	119.20	109.59
1	B	514	LYS	N-CA-C	-6.41	104.16	112.23
1	A	568	VAL	N-CA-C	6.35	116.52	110.42
1	A	492	GLY	N-CA-C	-6.28	101.78	112.51
1	B	134	PRO	CA-C-N	6.17	127.55	119.84
1	B	134	PRO	C-N-CA	6.17	127.55	119.84
1	A	82	ILE	CB-CA-C	-6.15	103.84	112.14
1	B	418	ALA	N-CA-C	6.09	118.45	111.02
1	A	113	GLU	N-CA-C	6.08	117.58	111.07
1	A	512	VAL	N-CA-C	6.08	118.63	109.20
1	A	18	ALA	N-CA-C	-6.03	105.50	112.92
1	B	510	VAL	N-CA-C	-5.97	98.93	107.77
1	A	21	ILE	N-CA-C	-5.96	99.29	107.99
1	A	131	ILE	N-CA-C	5.95	114.43	107.77
1	B	485	ASP	N-CA-C	5.74	117.34	111.14
1	B	15	ARG	N-CA-C	5.71	116.93	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	GLN	N-CA-C	5.63	119.93	109.56
1	A	81	GLY	N-CA-C	-5.63	105.67	112.48
1	B	417	PHE	N-CA-C	5.55	117.01	111.07
1	A	233	HIS	CA-C-N	5.55	126.78	119.84
1	A	233	HIS	C-N-CA	5.55	126.78	119.84
1	A	97	GLY	N-CA-C	-5.54	107.38	115.63
1	A	275	ASP	N-CA-C	-5.51	106.73	113.50
1	A	81	GLY	CA-C-O	-5.38	117.56	122.24
1	B	505	TYR	N-CA-C	-5.22	102.59	109.84
1	B	503	LEU	CA-C-N	5.18	124.94	119.76
1	B	503	LEU	C-N-CA	5.18	124.94	119.76
1	B	568	VAL	N-CA-C	5.09	115.86	110.72
1	B	129	LEU	N-CA-C	5.08	117.47	109.39
1	B	432	THR	N-CA-C	-5.08	101.88	109.95
1	B	403	ILE	N-CA-C	5.04	116.14	111.81
1	A	403	ILE	N-CA-C	5.03	116.44	111.67
1	B	96	SER	N-CA-C	5.02	116.83	111.36

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	204	0
1	B	4652	0	4747	217	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	11	0	5	0	0
5	A	105	0	0	5	0
5	B	79	0	0	3	0
All	All	9503	0	9499	415	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 22.

All (415) 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:84:ARG:HA	1:A:84:ARG:HH11	1.16	1.04
1:B:264:THR:HG22	1:B:266:GLU:H	1.24	1.03
1:B:295:MET:HE1	1:B:303:LEU:HD12	1.36	1.03
1:B:503:LEU:HD12	1:B:508:MET:HE2	1.40	1.02
1:B:514:LYS:H	1:B:514:LYS:HD2	1.24	0.99
1:A:471:GLN:HG2	1:A:473:LYS:HE3	1.47	0.96
1:A:503:LEU:HD22	1:A:507:ARG:HH21	1.26	0.95
1:B:290:GLN:H	1:B:290:GLN:HE21	1.10	0.95
1:A:477:LYS:HD3	1:A:478:ARG:H	1.34	0.91
1:B:290:GLN:H	1:B:290:GLN:NE2	1.71	0.89
1:A:514:LYS:H	1:A:514:LYS:HD2	1.34	0.89
1:B:111:ASN:HD21	1:B:128:PHE:HB2	1.40	0.86
1:B:82:ILE:HD12	1:B:83:HIS:H	1.41	0.86
1:B:8:LEU:HD22	1:B:26:VAL:HG22	1.56	0.84
1:A:84:ARG:HA	1:A:84:ARG:NH1	1.93	0.83
1:A:111:ASN:HD21	1:A:128:PHE:HB2	1.42	0.83
1:A:119:HIS:HE1	1:A:161:GLU:H	1.26	0.82
1:B:84:ARG:HE	1:B:84:ARG:HA	1.45	0.82
1:B:76:LYS:HB2	1:B:85:MET:HE3	1.63	0.81
1:A:264:THR:HG22	1:A:266:GLU:H	1.45	0.81
1:B:514:LYS:HD2	1:B:514:LYS:N	1.96	0.79
1:B:290:GLN:HE21	1:B:290:GLN:N	1.80	0.79
1:A:36:ILE:HD13	1:A:312:ILE:HG21	1.65	0.77
1:A:431:PRO:HG2	1:A:469:PRO:HG3	1.65	0.77
1:A:119:HIS:CE1	1:A:161:GLU:H	2.01	0.77
1:A:183:ARG:HB3	1:A:183:ARG:NH1	2.01	0.75
1:A:518:PRO:O	1:A:522:LYS:HD3	1.87	0.75
1:A:503:LEU:CD2	1:A:507:ARG:HH21	2.00	0.74
1:A:264:THR:CG2	1:A:266:GLU:H	2.01	0.73
1:B:470:ARG:HH12	1:B:484:ALA:HA	1.54	0.73
1:A:275:ASP:OD1	1:B:324:LYS:HG2	1.89	0.72
1:A:288:THR:HG22	1:A:291:GLU:H	1.55	0.72
1:A:362:ILE:HD13	1:A:539:ARG:HB2	1.71	0.71
1:A:413:LEU:HD22	1:A:468:MET:HE1	1.72	0.71
1:A:514:LYS:HD2	1:A:514:LYS:N	2.04	0.71
1:A:521:ARG:HB3	1:A:582:GLU:HG2	1.71	0.71
1:B:473:LYS:HG2	1:B:478:ARG:HA	1.70	0.71
1:B:82:ILE:HD12	1:B:83:HIS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:THR:OG1	1:A:435:ASP:HB2	1.90	0.70
1:A:40:VAL:HG23	1:A:62:THR:HG23	1.73	0.70
1:A:477:LYS:HD3	1:A:478:ARG:N	2.06	0.70
1:B:110:SER:OG	1:B:113:GLU:HG3	1.91	0.70
1:B:114:ILE:HD11	1:B:129:LEU:HG	1.72	0.70
1:B:535:ASP:HB3	1:B:538:ILE:HG13	1.74	0.70
1:B:114:ILE:O	1:B:118:GLN:HG3	1.91	0.70
1:B:499:LEU:HB3	1:B:508:MET:HE1	1.73	0.70
1:A:514:LYS:H	1:A:514:LYS:CD	2.05	0.69
1:B:406:ARG:HD3	1:B:406:ARG:N	2.05	0.69
1:B:84:ARG:HA	1:B:84:ARG:NE	2.07	0.69
1:A:288:THR:CG2	1:A:290:GLN:HG2	2.23	0.68
1:A:471:GLN:OE1	1:A:478:ARG:HD3	1.93	0.68
1:A:183:ARG:HB3	1:A:183:ARG:HH11	1.57	0.68
1:A:348:ARG:HD3	5:A:683:HOH:O	1.92	0.68
1:A:576:LYS:HB2	1:A:576:LYS:NZ	2.09	0.68
1:B:321:GLN:O	1:B:325:GLU:HG3	1.94	0.67
1:B:105:GLY:O	1:B:106:SER:HB3	1.94	0.67
1:A:270:ARG:O	1:A:273:GLU:HG2	1.94	0.67
1:B:207:ARG:HH11	1:B:207:ARG:HB3	1.60	0.67
1:A:71:GLU:HG2	1:A:75:ARG:HH12	1.59	0.67
1:A:406:ARG:HD3	1:A:406:ARG:N	2.08	0.66
1:B:406:ARG:HD3	1:B:406:ARG:H	1.60	0.66
1:B:156:ALA:O	1:B:160:LYS:HB2	1.96	0.65
1:B:514:LYS:H	1:B:514:LYS:CD	2.03	0.65
1:A:362:ILE:HD12	1:A:383:ARG:NH1	2.12	0.64
1:B:41:ASN:HB3	1:B:44:GLN:O	1.97	0.64
1:B:288:THR:HG23	1:B:291:GLU:H	1.62	0.64
1:B:503:LEU:CD1	1:B:508:MET:HE2	2.21	0.64
1:A:330:ARG:NH2	1:A:334:GLU:OE2	2.30	0.64
1:B:469:PRO:O	1:B:470:ARG:HD3	1.98	0.64
1:A:410:TYR:CE2	1:A:438:LYS:HB3	2.34	0.63
1:B:470:ARG:NH1	1:B:484:ALA:HA	2.13	0.63
1:A:415:TYR:HA	1:A:419:GLN:HG2	1.80	0.63
1:A:8:LEU:HG	1:A:190:GLU:HB2	1.81	0.63
1:A:109:VAL:HG21	1:A:114:ILE:HG23	1.80	0.62
1:A:112:ARG:O	1:A:116:GLU:HG3	1.99	0.62
1:B:217:LYS:HD3	1:B:243:MET:O	1.98	0.62
1:B:23:LYS:CE	1:B:30:LYS:HD3	2.29	0.62
1:A:264:THR:HG22	1:A:266:GLU:N	2.13	0.62
1:B:273:GLU:O	1:B:273:GLU:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ASP:HA	1:B:577:VAL:HG23	1.81	0.62
1:B:40:VAL:O	1:B:62:THR:HG23	1.99	0.62
1:B:339:HIS:ND1	1:B:340:PRO:HD2	2.13	0.62
1:B:131:ILE:O	1:B:169:GLN:HG2	2.00	0.62
1:B:64:SER:HB3	1:B:94:VAL:CG2	2.29	0.61
1:A:40:VAL:O	1:A:62:THR:HG23	2.01	0.61
1:A:436:ALA:HB1	1:A:461:VAL:HB	1.81	0.61
1:A:187:MET:HE2	1:A:189:PHE:HE1	1.66	0.61
1:B:510:VAL:HG13	1:B:546:VAL:HA	1.83	0.61
1:A:321:GLN:O	1:A:325:GLU:HG2	1.99	0.61
1:B:70:ASP:OD1	1:B:73:LEU:HD13	2.01	0.61
1:B:394:ARG:HD2	1:B:395:PHE:CE1	2.36	0.61
1:B:413:LEU:HD22	1:B:468:MET:HE1	1.83	0.60
1:A:111:ASN:ND2	1:A:129:LEU:H	1.97	0.60
1:A:412:SER:O	1:A:418:ALA:HB2	2.01	0.60
1:B:473:LYS:HE2	1:B:478:ARG:HB2	1.83	0.60
1:B:42:PRO:HG3	1:B:62:THR:HG21	1.83	0.60
1:B:260:ASP:OD1	1:B:300:ARG:HD2	2.01	0.60
1:A:190:GLU:N	1:A:190:GLU:CD	2.59	0.59
1:B:413:LEU:HD23	1:B:428:ILE:HG21	1.83	0.59
1:B:288:THR:HG22	1:B:291:GLU:CG	2.32	0.59
1:A:36:ILE:HD13	1:A:312:ILE:CG2	2.32	0.59
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.68	0.59
1:A:290:GLN:CD	1:A:290:GLN:H	2.11	0.59
1:A:333:ASP:O	1:A:337:ARG:HD3	2.03	0.59
1:A:576:LYS:HB2	1:A:576:LYS:HZ3	1.66	0.59
1:A:111:ASN:HD22	1:A:129:LEU:H	1.51	0.59
1:B:111:ASN:ND2	1:B:129:LEU:H	1.99	0.59
1:A:41:ASN:ND2	1:A:43:LYS:H	2.01	0.58
1:B:8:LEU:CD2	1:B:26:VAL:HG22	2.33	0.58
1:B:295:MET:CE	1:B:303:LEU:HD12	2.24	0.58
1:B:483:ARG:NH1	1:B:488:LEU:HB2	2.17	0.58
1:B:573:ARG:HH12	1:B:576:LYS:HE2	1.67	0.58
1:B:274:LEU:O	1:B:293:ARG:NH2	2.36	0.58
1:A:368:LEU:HD11	1:A:381:VAL:HG22	1.85	0.58
1:B:98:SER:O	1:B:101:LEU:HB2	2.04	0.58
1:A:8:LEU:HD22	1:A:26:VAL:HG22	1.84	0.58
1:A:163:PRO:HB3	1:A:190:GLU:HG3	1.85	0.57
1:A:548:ASN:HD21	1:A:552:GLU:HB2	1.69	0.57
1:B:101:LEU:HD12	1:B:107:ILE:HG23	1.87	0.57
1:B:185:SER:HB3	1:B:221:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ARG:O	1:B:502:VAL:HG23	2.04	0.57
1:A:13:LYS:HD2	1:A:23:LYS:HB2	1.86	0.57
1:A:61:ILE:HA	1:A:93:GLU:O	2.04	0.57
1:B:70:ASP:O	1:B:74:ARG:HB2	2.04	0.57
1:B:93:GLU:HG3	1:B:125:ILE:HB	1.85	0.57
1:A:42:PRO:HG3	1:A:62:THR:CG2	2.35	0.57
1:B:193:PRO:HA	1:B:227:HIS:O	2.05	0.57
1:A:139:ARG:NH2	1:A:175:ASP:OD2	2.38	0.56
1:A:36:ILE:HD11	1:A:250:SER:HB2	1.88	0.56
1:A:83:HIS:HD2	5:A:640:HOH:O	1.88	0.56
1:B:227:HIS:HE1	1:B:249:ASP:OD2	1.89	0.56
1:A:183:ARG:HH11	1:A:183:ARG:CB	2.18	0.55
1:A:431:PRO:HG2	1:A:469:PRO:CG	2.34	0.55
1:B:105:GLY:O	1:B:106:SER:CB	2.54	0.55
1:B:419:GLN:HB2	5:B:669:HOH:O	2.05	0.55
1:B:41:ASN:HD22	1:B:42:PRO:CD	2.19	0.55
1:B:264:THR:HG22	1:B:266:GLU:N	2.07	0.55
1:B:114:ILE:CD1	1:B:129:LEU:HG	2.37	0.55
1:B:292:LEU:HD13	1:B:295:MET:HE2	1.88	0.55
1:A:114:ILE:HD12	1:A:115:ILE:N	2.20	0.55
1:A:288:THR:HG22	1:A:291:GLU:N	2.22	0.55
1:A:521:ARG:HB3	1:A:582:GLU:CG	2.36	0.55
1:B:41:ASN:HD22	1:B:42:PRO:HD2	1.72	0.55
1:B:70:ASP:CG	1:B:73:LEU:HD13	2.32	0.55
1:A:41:ASN:C	1:A:41:ASN:HD22	2.14	0.54
1:B:190:GLU:CD	1:B:190:GLU:N	2.66	0.54
1:A:82:ILE:HD11	1:A:122:GLY:C	2.33	0.54
1:B:119:HIS:HD2	1:B:162:ILE:HD12	1.72	0.54
1:A:178:ARG:HB3	1:A:182:ARG:HH21	1.73	0.54
1:A:330:ARG:NH2	1:B:266:GLU:HG2	2.23	0.54
1:B:76:LYS:CB	1:B:85:MET:HE3	2.35	0.54
1:A:548:ASN:ND2	1:A:552:GLU:HB2	2.23	0.54
1:A:270:ARG:HB3	1:A:272:ASP:OD1	2.07	0.54
1:A:513:ASN:HD22	1:A:515:GLU:H	1.55	0.54
1:A:288:THR:HG23	1:A:290:GLN:HG2	1.89	0.54
1:A:288:THR:HG21	1:A:290:GLN:HG2	1.89	0.53
1:A:42:PRO:HG3	1:A:62:THR:HG21	1.90	0.53
1:B:42:PRO:HG3	1:B:62:THR:CG2	2.38	0.53
1:A:553:LEU:O	1:A:581:VAL:HG21	2.07	0.53
1:B:288:THR:HG22	1:B:291:GLU:CD	2.33	0.53
1:A:107:ILE:HG22	5:A:685:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:HB3	1:B:508:MET:CE	2.38	0.53
1:B:23:LYS:HE3	1:B:30:LYS:HD3	1.91	0.53
1:A:493:ILE:HG23	1:A:497:LYS:HE3	1.91	0.53
1:B:64:SER:HB3	1:B:94:VAL:HG21	1.89	0.53
1:A:337:ARG:HD2	1:A:337:ARG:N	2.22	0.53
1:B:33:THR:HA	1:B:34:PRO:C	2.34	0.52
1:B:165:ASN:HB3	1:B:193:PRO:HG2	1.90	0.52
1:B:339:HIS:CE1	1:B:340:PRO:HD2	2.44	0.52
1:B:507:ARG:O	1:B:509:ARG:HD2	2.10	0.52
1:A:415:TYR:HB2	1:A:419:GLN:HG3	1.91	0.52
1:A:190:GLU:CD	1:A:190:GLU:H	2.17	0.52
1:A:198:VAL:O	1:A:202:GLU:HG3	2.09	0.52
1:A:102:MET:HE3	1:A:132:PRO:O	2.10	0.52
1:B:52:LEU:HD23	1:B:55:MET:HE3	1.92	0.52
1:A:40:VAL:O	1:A:62:THR:CG2	2.57	0.51
1:B:65:TYR:CZ	1:B:107:ILE:HB	2.45	0.51
1:B:207:ARG:HB3	1:B:207:ARG:NH1	2.26	0.51
1:A:8:LEU:CD2	1:A:26:VAL:HG22	2.40	0.51
1:B:386:GLU:HA	1:B:389:LYS:NZ	2.24	0.51
1:B:8:LEU:HG	1:B:190:GLU:HB2	1.92	0.51
1:A:503:LEU:HD22	1:A:507:ARG:NH2	2.09	0.51
1:B:74:ARG:HG3	1:B:74:ARG:NH1	2.25	0.51
1:B:109:VAL:HG21	1:B:114:ILE:HG23	1.93	0.51
1:B:119:HIS:HA	1:B:162:ILE:HD12	1.91	0.51
1:A:111:ASN:HD22	1:A:129:LEU:HB2	1.76	0.50
1:A:193:PRO:HA	1:A:227:HIS:O	2.11	0.50
1:A:526:VAL:HB	1:A:575:VAL:HB	1.93	0.50
1:A:337:ARG:N	1:A:337:ARG:CD	2.74	0.50
1:B:343:TYR:CZ	1:B:347:LYS:HD2	2.46	0.50
1:B:391:ILE:N	1:B:391:ILE:HD12	2.27	0.50
1:A:454:ARG:HA	1:A:457:ASP:OD2	2.10	0.50
1:B:461:VAL:HG11	1:B:469:PRO:HB3	1.93	0.50
1:A:540:PRO:O	1:A:541:TYR:HB2	2.11	0.50
1:B:162:ILE:HG22	1:B:163:PRO:O	2.12	0.50
1:B:474:VAL:O	1:B:477:LYS:HG2	2.12	0.50
1:A:24:LEU:C	1:A:24:LEU:HD23	2.36	0.50
1:A:223:ASP:HA	1:A:569:PHE:CZ	2.46	0.50
1:B:397:GLU:CB	1:B:409:ARG:HG2	2.41	0.50
1:B:73:LEU:N	1:B:73:LEU:HD12	2.27	0.50
1:B:368:LEU:HD11	1:B:381:VAL:HG22	1.93	0.50
1:B:466:THR:O	1:B:468:MET:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HG12	1:A:532:ILE:HD11	1.94	0.49
1:B:190:GLU:O	1:B:225:PRO:HD2	2.12	0.49
1:B:437:ILE:HG23	1:B:438:LYS:N	2.25	0.49
1:A:16:ASP:OD1	1:A:364:LYS:HE2	2.12	0.49
1:B:431:PRO:HD2	1:B:467:GLY:O	2.10	0.49
1:A:24:LEU:HD23	1:A:25:GLU:N	2.28	0.49
1:B:529:LYS:HE3	1:B:530:PHE:CE1	2.47	0.49
1:B:330:ARG:NH2	1:B:334:GLU:OE2	2.45	0.49
1:B:483:ARG:HH12	1:B:488:LEU:HB2	1.76	0.49
1:B:74:ARG:HG3	1:B:74:ARG:HH11	1.76	0.49
1:B:131:ILE:O	1:B:169:GLN:CG	2.61	0.49
1:B:288:THR:HG22	1:B:291:GLU:HB2	1.94	0.49
1:A:324:LYS:HG2	1:B:275:ASP:OD1	2.13	0.49
1:B:163:PRO:HB3	1:B:190:GLU:HG3	1.95	0.49
1:A:270:ARG:HB2	1:A:270:ARG:HH11	1.78	0.49
1:B:373:ASN:HD22	1:B:377:ARG:HH12	1.61	0.49
1:B:62:THR:HG22	1:B:63:ASN:H	1.78	0.48
1:A:259:ASP:HB3	1:A:261:ARG:HG3	1.95	0.48
1:B:135:PRO:HG2	1:B:199:PRO:HB2	1.94	0.48
1:A:165:ASN:HD22	1:A:191:ILE:HB	1.78	0.48
1:A:535:ASP:HB3	1:A:538:ILE:HG13	1.96	0.48
1:A:348:ARG:NH1	1:A:351:GLU:OE1	2.46	0.48
1:B:165:ASN:HD22	1:B:191:ILE:HB	1.78	0.48
1:B:474:VAL:C	1:B:476:GLY:H	2.22	0.48
1:B:562:SER:OG	1:B:565:GLU:HG3	2.14	0.48
1:A:432:THR:H	1:A:435:ASP:CB	2.26	0.48
1:B:526:VAL:HB	1:B:575:VAL:HB	1.95	0.48
1:A:82:ILE:HD11	1:A:122:GLY:O	2.14	0.48
1:B:511:VAL:HG12	1:B:532:ILE:HD11	1.95	0.48
1:A:270:ARG:HH11	1:A:270:ARG:CB	2.27	0.47
1:B:280:SER:O	1:B:285:SER:HB3	2.14	0.47
1:B:431:PRO:HG3	1:B:439:TYR:CE2	2.49	0.47
1:B:119:HIS:HB3	5:B:634:HOH:O	2.14	0.47
1:A:55:MET:O	1:A:313:LYS:HE3	2.14	0.47
1:A:198:VAL:HB	1:A:199:PRO:HD3	1.97	0.47
1:B:466:THR:C	1:B:468:MET:H	2.20	0.47
1:B:547:VAL:HG22	1:B:552:GLU:N	2.29	0.47
1:A:64:SER:HB3	1:A:94:VAL:HG21	1.96	0.47
1:A:343:TYR:CZ	1:A:347:LYS:HD2	2.49	0.47
1:B:146:LEU:HD21	1:B:180:ALA:HB2	1.96	0.47
1:B:519:PHE:HB3	1:B:524:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:ALA:HB2	1:B:580:GLY:HA2	1.97	0.47
1:A:168:ILE:HG23	1:A:180:ALA:HB3	1.96	0.47
1:A:135:PRO:HB3	1:A:200:LEU:HD21	1.97	0.47
1:A:471:GLN:HG2	1:A:473:LYS:CE	2.33	0.47
1:B:343:TYR:CE1	1:B:347:LYS:HD2	2.50	0.47
1:B:555:ALA:CB	1:B:580:GLY:HA2	2.44	0.47
1:A:169:GLN:O	1:A:177:ARG:HD3	2.15	0.47
1:B:524:LYS:O	1:B:577:VAL:HG21	2.14	0.47
1:A:64:SER:HB3	1:A:94:VAL:CG2	2.45	0.47
1:B:216:SER:O	1:B:220:LEU:HG	2.14	0.47
1:B:160:LYS:HE2	1:B:188:ASN:O	2.15	0.46
1:B:290:GLN:HA	1:B:293:ARG:NH1	2.31	0.46
1:A:362:ILE:HD13	1:A:539:ARG:CB	2.43	0.46
1:A:547:VAL:HG21	1:A:551:ASP:OD2	2.13	0.46
1:B:24:LEU:HB3	1:B:31:ILE:HG22	1.98	0.46
1:A:138:PRO:HD2	1:A:141:GLN:HE21	1.81	0.46
1:A:547:VAL:HG13	1:A:548:ASN:O	2.15	0.46
1:B:21:ILE:HA	1:B:33:THR:O	2.15	0.46
1:B:73:LEU:CD1	1:B:73:LEU:H	2.29	0.46
1:A:478:ARG:HD2	1:A:481:THR:OG1	2.16	0.46
1:B:190:GLU:N	1:B:190:GLU:OE1	2.48	0.46
1:B:198:VAL:O	1:B:202:GLU:HG3	2.15	0.46
1:B:264:THR:HG23	1:B:265:PRO:HD2	1.97	0.46
1:B:333:ASP:CG	1:B:337:ARG:HH21	2.23	0.46
1:B:437:ILE:CG2	1:B:438:LYS:N	2.79	0.46
1:B:414:THR:HG22	1:B:415:TYR:N	2.30	0.46
1:B:355:PHE:CE1	1:B:359:PHE:HE1	2.34	0.46
1:A:389:LYS:O	1:A:393:GLU:HG3	2.16	0.46
1:A:391:ILE:HD12	1:A:445:GLU:HB3	1.98	0.46
1:A:431:PRO:HG3	1:A:439:TYR:CE2	2.50	0.46
1:B:79:GLU:HG3	1:B:80:LEU:HG	1.97	0.46
1:B:154:ARG:O	1:B:158:GLU:HG3	2.16	0.46
1:B:61:ILE:HA	1:B:93:GLU:O	2.16	0.45
1:B:459:ALA:HA	1:B:474:VAL:HG22	1.98	0.45
1:A:346:TYR:CE2	1:A:374:GLU:HG2	2.51	0.45
1:A:423:GLU:OE2	1:A:423:GLU:N	2.47	0.45
1:B:198:VAL:HB	1:B:199:PRO:HD3	1.97	0.45
1:A:368:LEU:HB3	1:A:420:SER:HB3	1.98	0.45
1:A:391:ILE:CD1	1:A:445:GLU:HB3	2.46	0.45
1:B:335:ARG:HD2	5:B:651:HOH:O	2.15	0.45
1:B:397:GLU:HB2	1:B:409:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ALA:HB2	1:B:556:THR:OG1	2.16	0.45
1:A:128:PHE:HB3	1:A:164:MET:HE1	1.99	0.45
1:A:165:ASN:ND2	1:A:191:ILE:HB	2.31	0.45
1:A:181:ALA:HB3	1:A:219:ALA:HB3	1.98	0.45
1:B:31:ILE:CD1	1:B:59:ILE:HB	2.47	0.45
1:B:162:ILE:HG23	1:B:163:PRO:HD2	1.98	0.45
1:A:289:PRO:HD2	1:A:290:GLN:OE1	2.16	0.45
1:B:474:VAL:HG12	1:B:475:ASN:ND2	2.31	0.45
1:A:297:LYS:NZ	5:A:639:HOH:O	2.48	0.45
1:B:413:LEU:HD23	1:B:428:ILE:CG2	2.46	0.45
1:B:436:ALA:HB1	1:B:461:VAL:HB	1.98	0.45
1:B:503:LEU:HA	1:B:504:PRO:HD3	1.80	0.45
1:B:566:MET:HE2	1:B:574:ALA:O	2.17	0.45
1:A:476:GLY:O	1:A:477:LYS:O	2.35	0.45
1:B:439:TYR:O	1:B:443:ILE:HG13	2.17	0.45
1:A:483:ARG:NH2	1:A:543:GLU:OE2	2.50	0.45
1:A:513:ASN:HB3	1:A:516:ALA:H	1.82	0.45
1:A:270:ARG:HB2	1:A:273:GLU:HG2	1.99	0.45
1:B:288:THR:HG22	1:B:291:GLU:CB	2.47	0.45
1:A:41:ASN:ND2	1:A:41:ASN:C	2.75	0.44
1:A:180:ALA:O	1:A:184:LEU:HD22	2.17	0.44
1:A:578:ARG:HG2	1:A:578:ARG:HH11	1.81	0.44
1:B:41:ASN:ND2	1:B:43:LYS:H	2.15	0.44
1:B:50:LYS:HD3	1:B:87:ASP:OD2	2.18	0.44
1:B:181:ALA:HB3	1:B:219:ALA:HB3	1.98	0.44
1:B:223:ASP:HA	1:B:569:PHE:CZ	2.52	0.44
1:A:343:TYR:CE1	1:A:347:LYS:HD2	2.52	0.44
1:B:374:GLU:H	1:B:374:GLU:CD	2.25	0.44
1:B:415:TYR:CD1	1:B:416:PRO:HA	2.53	0.44
1:A:187:MET:HE2	1:A:189:PHE:CE1	2.49	0.44
1:A:432:THR:H	1:A:435:ASP:HB2	1.81	0.44
1:A:448:PHE:HB2	1:A:452:ALA:CB	2.48	0.44
1:B:47:VAL:HG21	1:B:52:LEU:HD21	1.99	0.44
1:A:41:ASN:HD22	1:A:42:PRO:N	2.16	0.44
1:A:419:GLN:CA	1:A:419:GLN:HE21	2.31	0.44
1:A:399:VAL:HG22	1:A:400:GLU:N	2.33	0.44
1:A:166:ALA:HB2	1:A:189:PHE:CG	2.53	0.43
1:A:368:LEU:HB3	1:A:420:SER:CB	2.48	0.43
1:B:7:MET:CB	1:B:163:PRO:HG3	2.48	0.43
1:B:154:ARG:HH11	1:B:183:ARG:HH22	1.65	0.43
1:A:233:HIS:HA	1:A:234:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HD22	1:A:332:VAL:HG23	1.99	0.43
1:B:529:LYS:HE3	1:B:530:PHE:CZ	2.54	0.43
1:B:64:SER:HB3	1:B:94:VAL:HG22	1.99	0.43
1:B:272:ASP:OD1	1:B:272:ASP:C	2.61	0.43
1:B:410:TYR:HD2	1:B:439:TYR:CD1	2.36	0.43
1:A:413:LEU:CD2	1:A:428:ILE:HD12	2.48	0.43
1:A:34:PRO:HA	1:A:246:ASP:O	2.19	0.43
1:B:431:PRO:HG3	1:B:439:TYR:CZ	2.53	0.43
1:B:448:PHE:HB2	1:B:452:ALA:CB	2.48	0.43
1:A:42:PRO:HG3	1:A:62:THR:HG22	2.01	0.43
1:A:406:ARG:N	1:A:406:ARG:CD	2.80	0.43
1:B:362:ILE:HG22	1:B:541:TYR:HB2	2.01	0.43
1:A:362:ILE:HG22	1:A:363:THR:HG22	2.00	0.43
1:B:55:MET:HE1	1:B:309:LEU:HD13	2.00	0.43
1:B:60:ILE:HG12	1:B:88:TYR:CE2	2.53	0.43
1:A:83:HIS:CE1	1:A:124:ASP:OD2	2.72	0.43
1:A:150:LEU:O	1:A:154:ARG:HG3	2.18	0.43
1:B:41:ASN:HD22	1:B:42:PRO:N	2.17	0.43
1:B:73:LEU:N	1:B:73:LEU:CD1	2.82	0.43
1:B:288:THR:HG23	1:B:290:GLN:HG2	1.99	0.43
1:A:24:LEU:HB3	1:A:31:ILE:HG22	2.01	0.43
1:A:38:PRO:HD2	1:A:60:ILE:HG22	2.01	0.43
1:B:492:GLY:O	1:B:493:ILE:C	2.62	0.42
1:A:178:ARG:HB3	1:A:182:ARG:NH2	2.32	0.42
1:B:41:ASN:HD22	1:B:41:ASN:C	2.26	0.42
1:A:42:PRO:HB2	1:A:73:LEU:HD13	2.01	0.42
1:A:266:GLU:HG2	1:B:330:ARG:HH22	1.84	0.42
1:A:401:HIS:HA	1:A:402:PRO:HD3	1.88	0.42
1:A:423:GLU:HG3	1:B:344:SER:HB2	2.02	0.42
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.34	0.42
1:A:578:ARG:HD2	5:A:646:HOH:O	2.19	0.42
1:A:83:HIS:HE1	1:A:124:ASP:OD2	2.03	0.42
1:A:147:GLU:OE2	1:A:147:GLU:HA	2.19	0.42
1:A:221:ARG:HA	1:A:222:PRO:HD3	1.79	0.42
1:A:348:ARG:HD2	1:A:351:GLU:OE1	2.20	0.42
1:B:168:ILE:HD12	1:B:168:ILE:N	2.34	0.42
1:B:370:LYS:HD3	1:B:376:LEU:HD21	2.02	0.42
1:A:507:ARG:HA	1:A:535:ASP:OD2	2.20	0.42
1:A:240:ALA:HA	1:A:243:MET:HE3	2.02	0.42
1:B:292:LEU:HD22	1:B:295:MET:HE2	2.02	0.42
1:B:473:LYS:HG2	1:B:478:ARG:CA	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD23	1:A:55:MET:HE3	2.02	0.41
1:A:63:ASN:OD1	1:A:65:TYR:HB3	2.20	0.41
1:A:266:GLU:HG2	1:B:330:ARG:NH2	2.35	0.41
1:A:358:GLU:OE2	1:A:564:ARG:HD3	2.20	0.41
1:A:483:ARG:NH1	1:A:488:LEU:HB2	2.35	0.41
1:B:127:THR:N	1:B:164:MET:HE2	2.35	0.41
1:B:270:ARG:NH2	1:B:273:GLU:HB2	2.35	0.41
1:A:371:ILE:C	1:A:371:ILE:HD12	2.45	0.41
1:A:493:ILE:O	1:A:497:LYS:HG3	2.21	0.41
1:B:71:GLU:O	1:B:75:ARG:HG3	2.20	0.41
1:B:292:LEU:CD1	1:B:300:ARG:HG3	2.50	0.41
1:A:37:MET:HB2	1:A:60:ILE:HA	2.02	0.41
1:B:82:ILE:HA	1:B:85:MET:HB3	2.01	0.41
1:B:119:HIS:CD2	1:B:162:ILE:HB	2.56	0.41
1:B:166:ALA:HB2	1:B:189:PHE:CG	2.56	0.41
1:B:430:LYS:HA	1:B:431:PRO:HD3	1.83	0.41
1:B:521:ARG:HB3	1:B:582:GLU:HB3	2.01	0.41
1:A:54:LYS:NZ	1:A:54:LYS:HB2	2.35	0.41
1:A:362:ILE:HD12	1:A:362:ILE:HA	1.90	0.41
1:A:76:LYS:HE3	1:A:76:LYS:HB2	1.85	0.41
1:A:410:TYR:HE2	1:A:435:ASP:OD1	2.04	0.41
1:B:36:ILE:HG22	1:B:316:ILE:HG13	2.02	0.41
1:A:24:LEU:C	1:A:24:LEU:CD2	2.94	0.41
1:A:36:ILE:HD12	1:A:237:PHE:CZ	2.56	0.41
1:A:36:ILE:HG21	1:A:312:ILE:CG2	2.51	0.41
1:A:399:VAL:O	1:A:406:ARG:HA	2.20	0.41
1:A:436:ALA:O	1:A:439:TYR:HB2	2.21	0.41
1:B:214:ILE:HD12	1:B:355:PHE:CD2	2.56	0.41
1:B:395:PHE:HB3	1:B:410:TYR:CD1	2.56	0.41
1:A:26:VAL:O	1:A:27:ASN:C	2.64	0.41
1:A:114:ILE:O	1:A:118:GLN:HG3	2.20	0.41
1:A:203:SER:O	1:A:204:TYR:HB2	2.20	0.41
1:B:7:MET:HB3	1:B:163:PRO:HG3	2.02	0.41
1:B:252:SER:O	1:B:253:TYR:C	2.64	0.41
1:A:454:ARG:NH1	1:A:502:VAL:HG13	2.36	0.40
1:A:469:PRO:O	1:A:470:ARG:NH1	2.50	0.40
1:B:62:THR:HG22	1:B:63:ASN:N	2.37	0.40
1:B:102:MET:HE1	1:B:198:VAL:HB	2.02	0.40
1:A:431:PRO:HD2	1:A:467:GLY:O	2.21	0.40
1:A:119:HIS:CE1	1:A:162:ILE:HG23	2.56	0.40
1:B:217:LYS:HE2	1:B:217:LYS:HB3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:HIS:HA	1:B:234:PRO:HD3	1.96	0.40
1:A:439:TYR:O	1:A:443:ILE:HG13	2.22	0.40
1:A:479:LEU:HD22	1:A:498:ARG:HD2	2.03	0.40
1:B:499:LEU:HD22	1:B:508:MET:HE1	2.03	0.40
1:A:146:LEU:O	1:A:149:THR:HB	2.22	0.40
1:A:474:VAL:O	1:A:475:ASN:C	2.64	0.40
1:B:493:ILE:O	1:B:497:LYS:HG3	2.21	0.40
1:B:519:PHE:H	1:B:519:PHE:HD1	1.69	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%)	553 (96%)	19 (3%)	3 (0%)	24	31
1	B	575/582 (99%)	542 (94%)	28 (5%)	5 (1%)	14	17
All	All	1150/1164 (99%)	1095 (95%)	47 (4%)	8 (1%)	18	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	ASN
1	A	477	LYS
1	B	82	ILE
1	B	106	SER
1	A	436	ALA
1	B	420	SER
1	B	105	GLY
1	B	467	GLY

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%)	455 (91%)	44 (9%)	9	12
1	B	499/503 (99%)	464 (93%)	35 (7%)	14	19
All	All	998/1006 (99%)	919 (92%)	79 (8%)	11	15

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	20	ARG
1	A	24	LEU
1	A	40	VAL
1	A	41	ASN
1	A	49	PRO
1	A	54	LYS
1	A	62	THR
1	A	74	ARG
1	A	82	ILE
1	A	84	ARG
1	A	114	ILE
1	A	123	VAL
1	A	136	ASP
1	A	144	LYS
1	A	184	LEU
1	A	190	GLU
1	A	207	ARG
1	A	227	HIS
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

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	362	ILE
1	A	368	LEU
1	A	370	LYS
1	A	406	ARG
1	A	419	GLN
1	A	429	GLU
1	A	435	ASP
1	A	438	LYS
1	A	471	GLN
1	A	477	LYS
1	A	493	ILE
1	A	499	LEU
1	A	529	LYS
1	A	544	VAL
1	A	547	VAL
1	A	576	LYS
1	B	8	LEU
1	B	31	ILE
1	B	36	ILE
1	B	49	PRO
1	B	74	ARG
1	B	82	ILE
1	B	86	LEU
1	B	114	ILE
1	B	123	VAL
1	B	162	ILE
1	B	184	LEU
1	B	190	GLU
1	B	207	ARG
1	B	217	LYS
1	B	229	PHE
1	B	273	GLU
1	B	290	GLN
1	B	292	LEU
1	B	297	LYS
1	B	302	ARG
1	B	324	LYS
1	B	328	LEU
1	B	330	ARG
1	B	342	LEU
1	B	365	LYS

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Mol	Chain	Res	Type
1	B	368	LEU
1	B	406	ARG
1	B	434	GLU
1	B	485	ASP
1	B	490	THR
1	B	493	ILE
1	B	507	ARG
1	B	510	VAL
1	B	547	VAL
1	B	582	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	44	GLN
1	A	83	HIS
1	A	111	ASN
1	A	119	HIS
1	A	141	GLN
1	A	165	ASN
1	A	419	GLN
1	A	513	ASN
1	B	41	ASN
1	B	111	ASN
1	B	119	HIS
1	B	141	GLN
1	B	165	ASN
1	B	227	HIS
1	B	290	GLN
1	B	373	ASN
1	B	471	GLN
1	B	475	ASN

5.3.3 RNA ⓘ

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	GUN	A	602	-	12,12,12	1.51	3 (25%)	15,17,17	0.91	2 (13%)

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	GUN	A	602	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	GUN	C4-N3	2.85	1.40	1.36
4	A	602	GUN	C8-N9	2.52	1.39	1.35
4	A	602	GUN	C4-N9	2.51	1.41	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	GUN	C8-N9-C4	-2.21	103.79	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	GUN	N9-C8-N7	2.01	115.31	112.98

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.