Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 12:34 AM EDT

PDB ID	:	1IT7
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 (i) symbol.

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

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

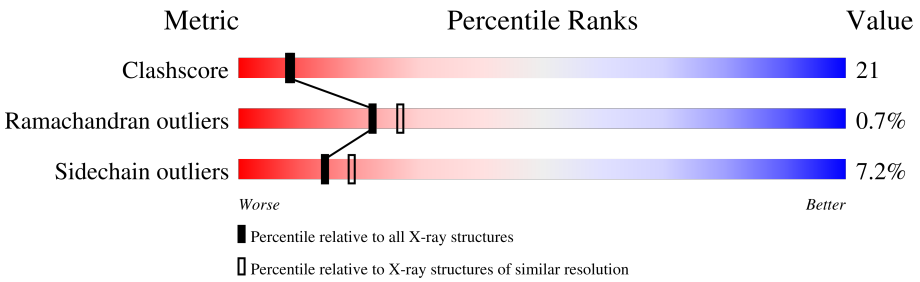
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	61% 33% 5% •
1	B	582	59% 37% • •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	577	4652	2970	815	848	19	0	0	0
1	B	577	4652	2970	815	848	19	0	0	0

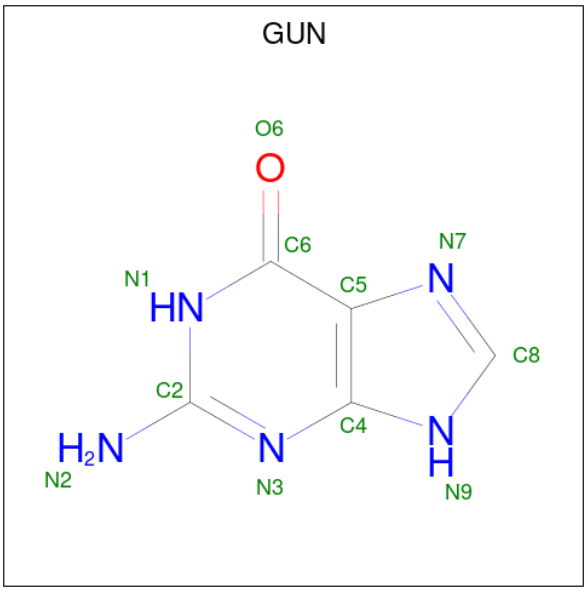
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



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

- Molecule 5 is water.

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

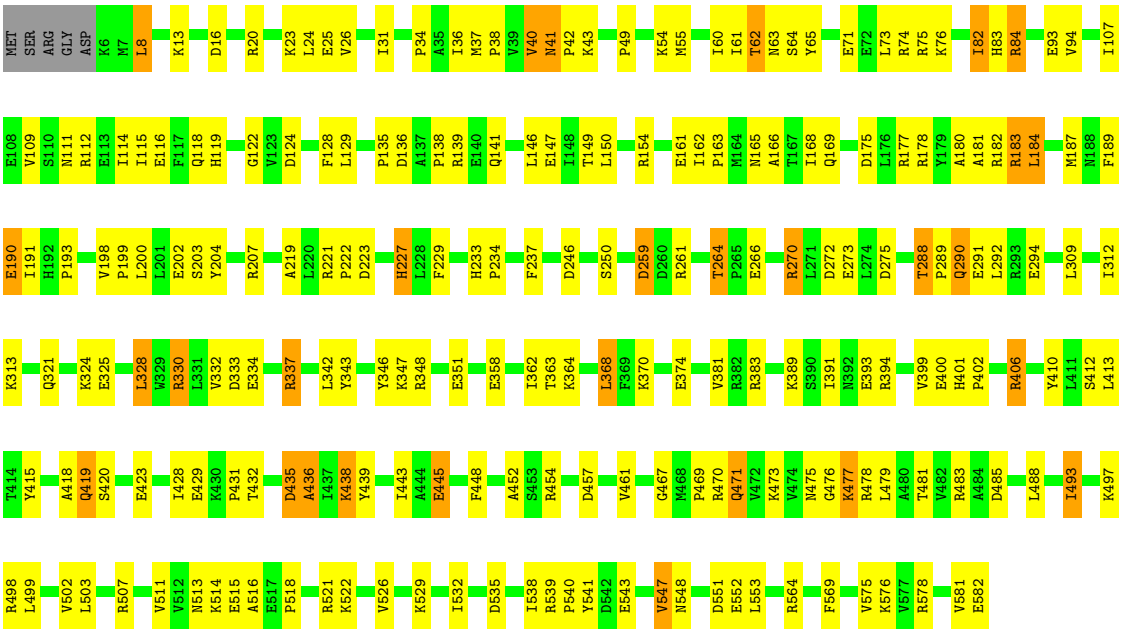
3 Residue-property plots (i)

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

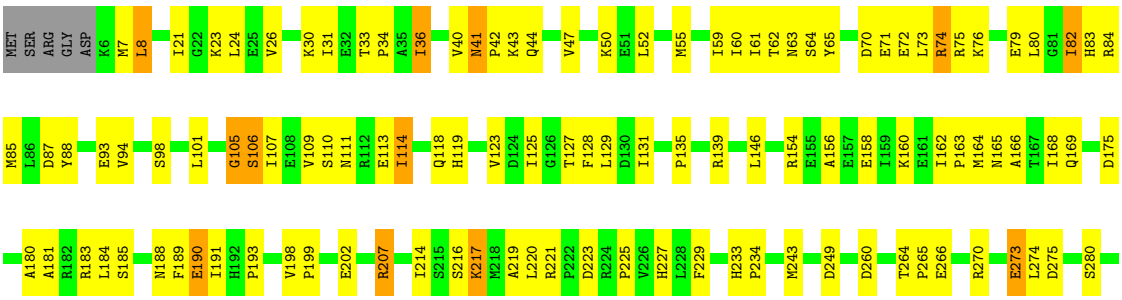
• Molecule 1: Archaeosine tRNA-guanine transglycosylase

Chain A: 61% 33% 5% •



• Molecule 1: Archaeosine tRNA-guanine transglycosylase

Chain B: 59% 37% • •



S285 T288 P289 Q290 E291 L292 R293 E294 M295 P296 K297 R300 T301 R302 L303 I316 Q321 K324 E325 L328 W329 R330 E334 R335 H339 P340 K341 L342 Y343 S344 K347 F355 F359 I362 K365 L368 F369 K370 N373 L376 R377 V381
E386 K389 S390 I391 R394 F395 G396 E397 R406 R409 Y410 L413 T414 Y415 P416 Q419 S420 I428 E429 K430 P431 E434 D435 A436 I437 K438 Y439 I443 F448 A452 A459 K460 V461 T466 G467 M468 P469 R470 K473 V474 N475 G476 K477 R478 R483
A484 D485 L488 I493 A496 K497 R498 L499 H500 R501 V502 L503 P504 R507 M508 R509 V510 V511 K514 F519 A520 R521 K522 G523 K524 D525 V526 K529 F530 V531 I532 D535 I538 Y541 V546 V547 E552 A555 T556 S562 E565 F569 R573
A574 V575 K576 V577 G580 V581 E582

4 Data and refinement statistics (i)

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	100.20Å 100.20Å 364.66Å 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 (i)

5.1 Standard geometry (i)

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	0.38	0/4745	0.63	0/6391
1	B	0.36	0/4745	0.62	0/6391
All	All	0.37	0/9490	0.63	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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4652	0	4747	193	0
1	B	4652	0	4747	208	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	4	0
5	B	79	0	0	3	0
All	All	9503	0	9499	395	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 21.

All (395) 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: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:499:LEU:HB3	1:B:508: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:B:295:MET:HE1	1:B:303:LEU:HD12	1.66	0.78
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:295:MET:CE	1:B:303:LEU:HD12	2.24	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:333:ASP:O	1:A:337:ARG:HD3	2.03	0.59
1:A:111:ASN:HD22	1:A:129:LEU:H	1.51	0.59
1:B:52:LEU:HD23	1:B:55:MET:HE3	1.85	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: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:503:LEU:HD12	1:B:508:MET:CE	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:HB2	1:B:85:MET:HE3	1.87	0.56
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:A:190:GLU:N	1:A:190:GLU:CD	2.59	0.55
1:B:114:ILE:CD1	1:B:129:LEU:HG	2.37	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:A:290:GLN:CD	1:A:290:GLN:H	2.11	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: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:A:107:ILE:HG22	5:A:685:HOH:O	2.08	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: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:198:VAL:O	1:A:202:GLU:HG3	2.09	0.52
1:B:499:LEU:HB3	1:B:508:MET:CE	2.38	0.52
1:A:40:VAL:O	1:A:62:THR:CG2	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ASN:C	1:A:41:ASN:HD22	2.14	0.50
1:A:223:ASP:HA	1:A:569:PHE:CZ	2.46	0.50
1:B:70:ASP:CG	1:B:73:LEU:HD13	2.32	0.50
1:B:127:THR:N	1:B:164:MET:HE2	2.27	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:190:GLU:CD	1:B:190:GLU:N	2.66	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
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:A:82:ILE:HD11	1:A:122:GLY:C	2.33	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:A:576:LYS:HB2	1:A:576:LYS:HZ3	1.76	0.49
1:B:529:LYS:HE3	1:B:530:PHE:CE1	2.47	0.49
1:A:154:ARG:HA	1:A:187:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:190:GLU:CD	1:A:190:GLU:H	2.17	0.48
1:B:503:LEU:HD12	1:B:508:MET:HE1	1.95	0.48
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:B:288:THR:HG22	1:B:291:GLU:CD	2.33	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: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:33:THR:HA	1:B:34:PRO:C	2.34	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:503:LEU:HD12	1:B:508:MET:HE2	1.96	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:B:414:THR:HG22	1:B:415:TYR:N	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:437:ILE:CG2	1:B:438:LYS:N	2.79	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
1:B:496:ALA:HB2	1:B:556:THR:OG1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:24:LEU:HD23	1:A:24:LEU:C	2.36	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: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:415:TYR:CD1	1:B:416:PRO:HA	2.53	0.44
1:B:499:LEU:HD22	1:B:508:MET:HE1	1.99	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
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: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:B:474:VAL:C	1:B:476:GLY:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:292:LEU:HD22	1:B:295:MET:HE1	2.00	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:466:THR:C	1:B:468:MET:H	2.20	0.43
1:A:178:ARG:HB3	1:A:182:ARG:NH2	2.32	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:B:292:LEU:HD13	1:B:295:MET:HE2	2.02	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:B:473:LYS:HG2	1:B:478:ARG:CA	2.43	0.42
1:A:55:MET:HE1	1:A:309:LEU:HD13	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:270:ARG:NH2	1:B:273:GLU:HB2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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:76:LYS:HB2	1:B:85:MET:CE	2.50	0.40
1:A:146:LEU:O	1:A:149:THR:HB	2.22	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 (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%)	553 (96%)	19 (3%)	3 (0%)	29	35
1	B	575/582 (99%)	542 (94%)	28 (5%)	5 (1%)	17	20
All	All	1150/1164 (99%)	1095 (95%)	47 (4%)	8 (1%)	22	26

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/503 (99%)	457 (92%)	42 (8%)	11	13
1	B	499/503 (99%)	469 (94%)	30 (6%)	19	26
All	All	998/1006 (99%)	926 (93%)	72 (7%)	14	18

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

Mol	Chain	Res	Type
1	A	8	LEU
1	A	20	ARG
1	A	40	VAL
1	A	41	ASN
1	A	49	PRO
1	A	62	THR
1	A	74	ARG
1	A	82	ILE

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Mol	Chain	Res	Type
1	A	84	ARG
1	A	136	ASP
1	A	183	ARG
1	A	184	LEU
1	A	190	GLU
1	A	207	ARG
1	A	227	HIS
1	A	229	PHE
1	A	259	ASP
1	A	264	THR
1	A	270	ARG
1	A	288	THR
1	A	290	GLN
1	A	292	LEU
1	A	294	GLU
1	A	328	LEU
1	A	330	ARG
1	A	337	ARG
1	A	342	LEU
1	A	368	LEU
1	A	370	LYS
1	A	394	ARG
1	A	406	ARG
1	A	419	GLN
1	A	429	GLU
1	A	435	ASP
1	A	438	LYS
1	A	445	GLU
1	A	471	GLN
1	A	485	ASP
1	A	493	ILE
1	A	499	LEU
1	A	529	LYS
1	A	547	VAL
1	B	8	LEU
1	B	36	ILE
1	B	41	ASN
1	B	72	GLU
1	B	74	ARG
1	B	114	ILE
1	B	123	VAL
1	B	175	ASP

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Mol	Chain	Res	Type
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	328	LEU
1	B	330	ARG
1	B	342	LEU
1	B	365	LYS
1	B	368	LEU
1	B	406	ARG
1	B	434	GLU
1	B	485	ASP
1	B	501	ARG
1	B	522	LYS
1	B	547	VAL
1	B	582	GLU

Sometimes 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	119	HIS
1	A	141	GLN
1	A	165	ASN
1	A	419	GLN
1	A	513	ASN
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	373	ASN

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Mol	Chain	Res	Type
1	B	475	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	7,12,12	1.37	1 (14%)	8,17,17	0.80	0

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	GUN	C6-N1	2.76	1.42	1.37

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 (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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.