



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:13 AM GMT

PDB ID : 2ZZK  
Title : Crystal structure of tRNA wybutosine synthesizing enzyme TYW4  
Authors : Suzuki, Y.; Noma, A.; Suzuki, T.; Ishitani, R.; Nureki, O.  
Deposited on : 2009-02-17  
Resolution : 2.71 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

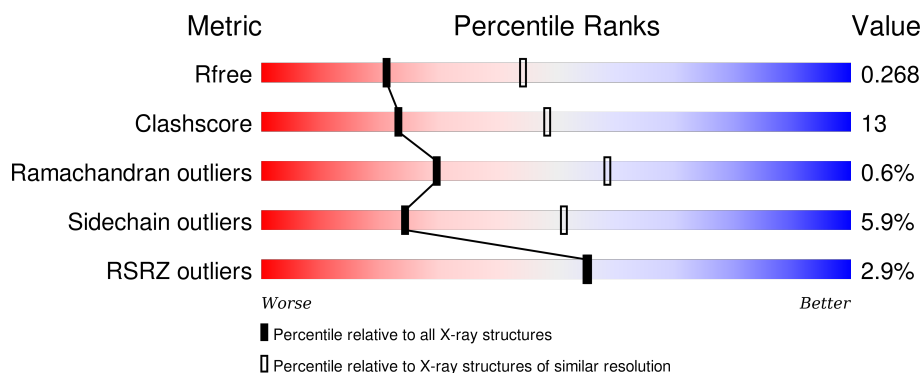
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	695	<div> <div>2%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	B	695	<div> <div>3%</div> <div>66%</div> <div>29%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	802	-	-	-	X
2	CIT	B	802	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10899 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.

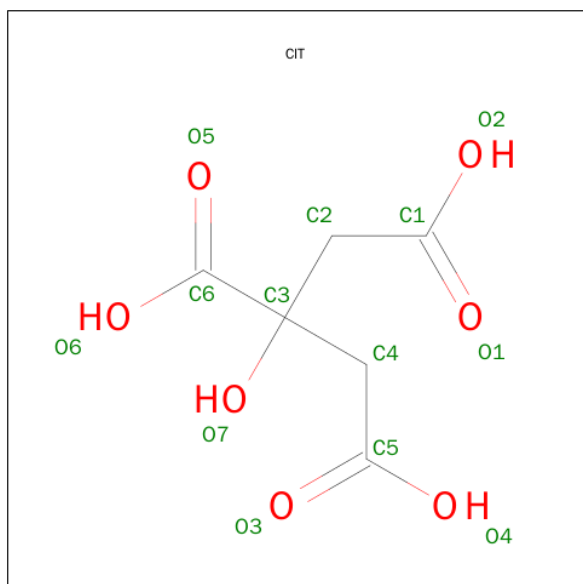
- Molecule 1 is a protein called Leucine carboxyl methyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	0	0
			5411	3465	904	1017	25			
1	B	677	Total	C	N	O	S	0	1	0
			5390	3453	902	1010	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LEU	MET	SEE REMARK 999	UNP Q08282
B	417	LEU	MET	SEE REMARK 999	UNP Q08282

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



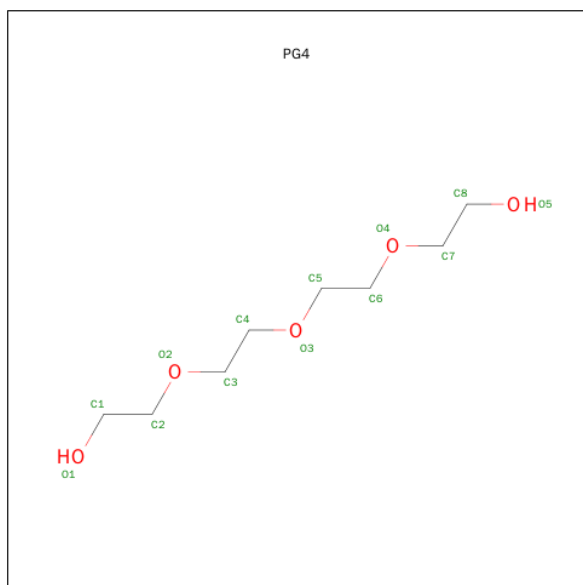
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

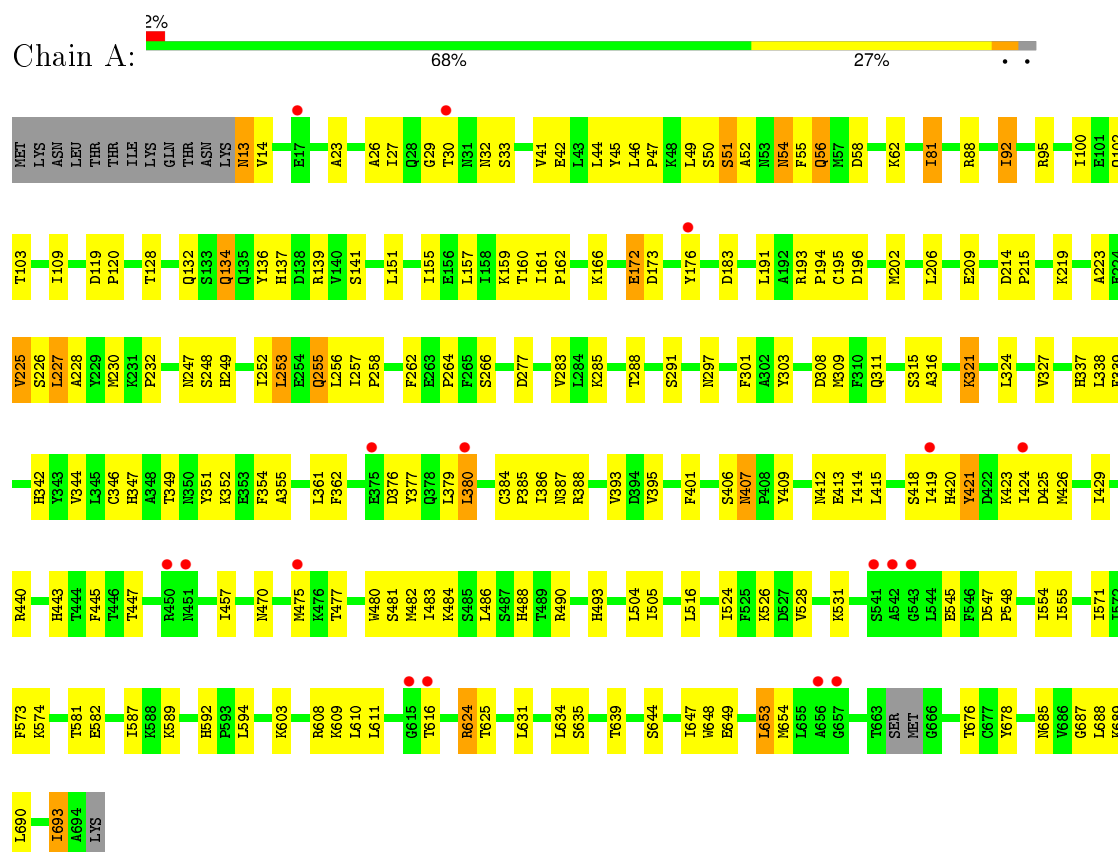
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	13	Total	O	0	0
			13	13		

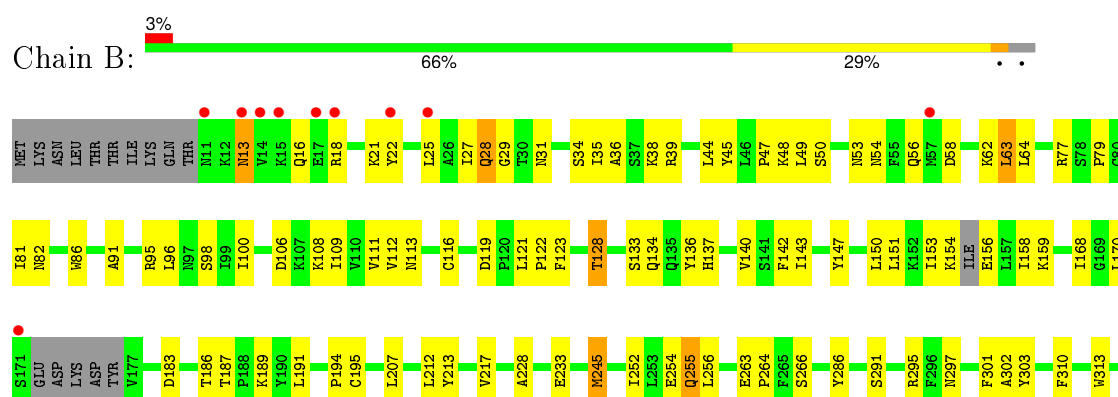
### 3 Residue-property plots

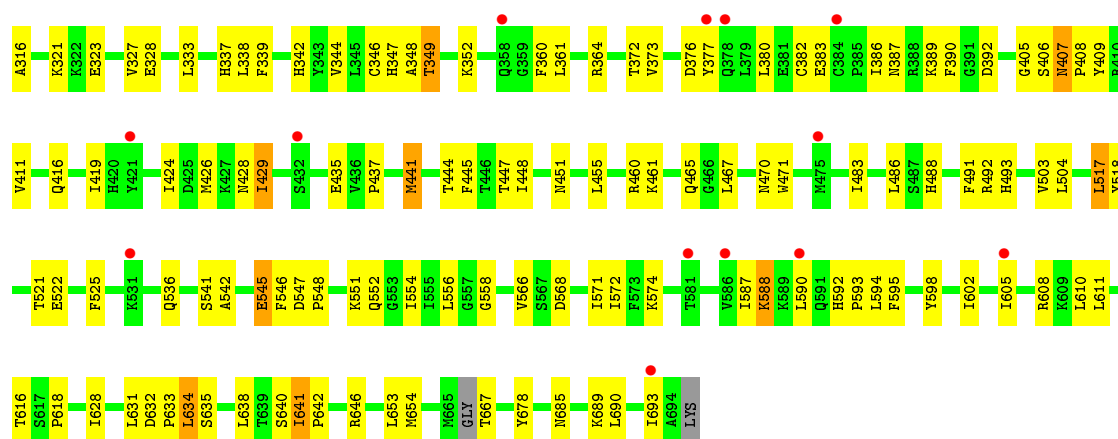
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Leucine carboxyl methyltransferase 2



- Molecule 1: Leucine carboxyl methyltransferase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.83Å 90.14Å 251.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.39 – 2.71 42.39 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.39-2.71) 96.4 (42.39-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.210 , 0.274 0.208 , 0.268	Depositor DCC
$R_{free}$ test set	4820 reflections (11.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	1.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47980 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, CIT

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	0.27	0/5527	0.45	0/7476
1	B	0.27	0/5507	0.46	0/7446
All	All	0.27	0/11034	0.46	0/14922

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	5411	0	5390	137	0
1	B	5390	0	5373	156	0
2	A	26	0	10	3	0
2	B	26	0	10	0	0
3	A	13	0	18	1	0
4	A	20	0	0	0	0
4	B	13	0	0	2	0
All	All	10899	0	10801	291	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 13.

All (291) 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:349:THR:HG22	1:A:351:TYR:H	1.38	0.88
1:A:54:ASN:HD21	1:A:132:GLN:HE21	1.17	0.88
1:B:13:ASN:HD22	1:B:13:ASN:H	1.26	0.83
1:A:102:GLN:HE22	1:A:355:ALA:H	1.28	0.82
1:B:47:PRO:HG3	1:B:63:LEU:HD22	1.59	0.81
1:B:588:LYS:HD2	1:B:590:LEU:HD21	1.62	0.80
1:A:256:LEU:HD11	1:A:344:VAL:HB	1.63	0.80
1:B:134:GLN:HA	1:B:137:HIS:CD2	2.17	0.78
1:A:255:GLN:H	1:A:255:GLN:NE2	1.82	0.77
1:B:654:MET:H	1:B:685:ASN:HD22	1.30	0.76
1:A:589:LYS:O	3:A:803:PG4:H72	1.86	0.76
1:B:113:ASN:HB3	1:B:116:CYS:HB3	1.69	0.74
1:B:303:TYR:OH	1:B:352:LYS:HG3	1.88	0.73
1:B:128:THR:HA	1:B:137:HIS:CE1	2.24	0.73
1:A:252:ILE:HG22	1:A:346:CYS:HB3	1.71	0.73
1:B:338:LEU:O	1:B:342:HIS:HD2	1.73	0.72
1:A:255:GLN:H	1:A:255:GLN:HE21	1.36	0.71
1:A:13:ASN:HD22	1:A:14:VAL:N	1.89	0.71
1:A:100:ILE:HD13	1:A:109:ILE:HD12	1.73	0.71
1:B:256:LEU:HD11	1:B:344:VAL:HB	1.73	0.71
1:B:552:GLN:HE21	1:B:587:ILE:HD12	1.54	0.71
1:B:595:PHE:CZ	1:B:631:LEU:HD22	2.26	0.71
1:B:49:LEU:HD23	1:B:323:GLU:HG2	1.71	0.70
1:B:255:GLN:HE21	1:B:255:GLN:H	1.40	0.70
1:A:554:ILE:HD12	1:A:610:LEU:HD22	1.72	0.70
1:A:338:LEU:O	1:A:342:HIS:HD2	1.73	0.69
1:A:608:ARG:NE	1:A:634:LEU:HD11	2.07	0.69
1:B:310:PHE:CE2	1:B:618:PRO:HB3	2.27	0.69
1:A:134:GLN:HA	1:A:137:HIS:CD2	2.28	0.68
1:B:263:GLU:HG2	1:B:264:PRO:HD2	1.75	0.68
1:B:337:HIS:HD2	1:B:616:THR:OG1	1.77	0.67
1:A:418:SER:HB2	1:A:425:ASP:HB2	1.77	0.67
1:A:608:ARG:HE	1:A:634:LEU:HD11	1.60	0.67
1:A:634:LEU:HD12	1:A:635:SER:N	2.10	0.66
1:B:28:GLN:HA	1:B:29:GLY:C	2.14	0.66
1:A:401:PHE:HE2	1:A:429:ILE:HD11	1.58	0.66
1:A:386:ILE:HG13	1:A:388:ARG:HG2	1.76	0.66
1:A:555:ILE:HB	1:A:571:ILE:HB	1.78	0.66
1:A:592:HIS:CD2	1:A:594:LEU:H	2.13	0.66
1:A:232:PRO:HB3	1:A:285:LYS:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASP:HA	1:B:693:ILE:HD11	1.78	0.65
1:B:18:ARG:O	1:B:21:LYS:HG2	1.96	0.65
1:B:100:ILE:HD13	1:B:109:ILE:HD12	1.78	0.65
1:B:303:TYR:HB2	1:B:349:THR:HG23	1.79	0.64
1:B:252:ILE:CG2	1:B:346:CYS:HB3	2.27	0.64
1:B:58:ASP:HB3	1:B:64:LEU:HD11	1.79	0.63
1:B:133:SER:O	1:B:137:HIS:HD2	1.82	0.63
1:B:634:LEU:HD22	1:B:635:SER:N	2.13	0.63
1:B:123:PHE:HZ	1:B:158:ILE:HD13	1.64	0.62
1:A:88:ARG:NH1	2:A:801:CIT:O6	2.32	0.61
1:B:592:HIS:CD2	1:B:594:LEU:H	2.19	0.61
1:B:382:CYS:HB2	1:B:689:LYS:HG2	1.84	0.60
1:A:166:LYS:HD3	1:A:172:GLU:CD	2.22	0.60
1:B:634:LEU:H	1:B:634:LEU:HD13	1.67	0.59
1:A:644:SER:OG	1:A:647:ILE:HG13	2.01	0.59
1:A:574:LYS:HG3	1:A:587:ILE:HD11	1.85	0.59
1:B:303:TYR:CZ	1:B:352:LYS:HG3	2.37	0.59
1:B:608:ARG:NH2	1:B:634:LEU:HD21	2.18	0.59
1:A:183:ASP:O	1:A:194:PRO:HG3	2.02	0.59
1:B:154:LYS:O	1:B:158:ILE:HG13	2.02	0.59
1:A:406:SER:HA	1:A:409:TYR:O	2.03	0.59
1:B:133:SER:O	1:B:137:HIS:CD2	2.56	0.58
1:A:27:ILE:HA	1:A:30:THR:OG1	2.03	0.58
1:B:592:HIS:HD2	1:B:594:LEU:H	1.52	0.58
1:A:484:LYS:HZ2	1:A:524:ILE:HG22	1.69	0.57
1:A:337:HIS:HD2	1:A:616:THR:OG1	1.86	0.57
1:A:592:HIS:HD2	1:A:594:LEU:H	1.51	0.57
1:A:624:ARG:HD2	1:A:648:TRP:CG	2.40	0.57
1:B:35:ILE:HD11	1:B:119:ASP:HA	1.86	0.57
1:B:255:GLN:NE2	1:B:255:GLN:H	2.02	0.57
1:B:207:LEU:HD23	1:B:212:LEU:HD12	1.87	0.57
1:B:45:TYR:CE1	1:B:82:ASN:HB3	2.39	0.56
1:B:13:ASN:H	1:B:13:ASN:ND2	1.97	0.56
1:A:401:PHE:CE2	1:A:429:ILE:HD11	2.41	0.56
1:B:416:GLN:HB2	1:B:429:ILE:CD1	2.36	0.56
1:A:687:GLY:O	1:A:688:LEU:HD23	2.06	0.56
1:A:26:ALA:O	1:A:30:THR:HG23	2.05	0.56
1:A:470:ASN:HD21	1:A:486:LEU:HG	1.71	0.56
1:B:386:ILE:HA	1:B:426:MET:SD	2.46	0.56
1:B:252:ILE:HG23	1:B:346:CYS:HB3	1.87	0.56
1:A:574:LYS:HE3	1:A:587:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:THR:CG2	1:B:451:ASN:HA	2.36	0.56
1:B:147[B]:TYR:CZ	1:B:150:LEU:HB2	2.41	0.55
1:B:518:TYR:HB2	1:B:525:PHE:CE2	2.41	0.55
1:B:286:TYR:CE2	1:B:295:ARG:HD2	2.42	0.55
1:A:232:PRO:CB	1:A:285:LYS:HD2	2.36	0.55
1:A:611:LEU:HD22	1:A:690:LEU:HD22	1.87	0.55
1:A:440:ARG:HG3	1:A:443:HIS:ND1	2.22	0.55
1:B:153:ILE:O	1:B:156:GLU:HB2	2.07	0.55
1:B:592:HIS:CD2	1:B:593:PRO:HD2	2.42	0.55
1:B:27:ILE:HG22	1:B:28:GLN:N	2.21	0.54
1:A:247:ASN:HA	1:A:351:TYR:CD2	2.43	0.54
1:B:168:ILE:HD12	1:B:187:THR:HG21	1.90	0.54
1:B:100:ILE:HG13	1:B:136:TYR:CZ	2.43	0.54
1:B:419:ILE:HG13	1:B:424:ILE:HD11	1.90	0.53
1:B:266:SER:OG	1:B:342:HIS:HE1	1.91	0.53
1:B:634:LEU:H	1:B:634:LEU:CD1	2.21	0.53
1:B:406:SER:HB2	1:B:408:PRO:O	2.08	0.53
1:B:470:ASN:HD21	1:B:486:LEU:HG	1.73	0.53
1:A:166:LYS:HD3	1:A:172:GLU:OE1	2.08	0.53
1:A:380:LEU:O	1:A:689:LYS:HG2	2.09	0.53
1:B:554:ILE:HG13	1:B:610:LEU:HD22	1.90	0.53
1:A:173:ASP:HB3	1:A:176:TYR:HB3	1.90	0.53
1:A:654:MET:H	1:A:685:ASN:HD22	1.55	0.53
1:B:460:ARG:HA	1:B:467:LEU:HG	1.91	0.52
1:B:159:LYS:HG3	4:B:705:HOH:O	2.07	0.52
1:A:30:THR:O	1:A:33:SER:HB2	2.09	0.52
1:A:415:LEU:HD13	1:A:426:MET:HE3	1.91	0.52
1:A:223:ALA:HB3	1:A:252:ILE:HG13	1.92	0.52
1:B:407:ASN:HD22	1:B:409:TYR:H	1.56	0.52
1:B:602:ILE:HB	1:B:610:LEU:HD11	1.90	0.52
1:B:632:ASP:HB3	1:B:635:SER:HB2	1.92	0.52
1:B:140:VAL:O	1:B:189:LYS:HE2	2.10	0.51
1:B:91:ALA:O	1:B:95:ARG:HG2	2.11	0.51
1:B:389:LYS:HG3	1:B:390:PHE:HD1	1.74	0.51
1:A:482:MET:HG2	1:B:465:GLN:NE2	2.26	0.51
1:B:96:LEU:O	1:B:100:ILE:HG12	2.11	0.51
1:B:108:LYS:HG2	1:B:217:VAL:HG22	1.93	0.51
1:A:393:VAL:HG23	1:A:401:PHE:O	2.11	0.51
1:A:419:ILE:HA	1:A:424:ILE:HG12	1.93	0.51
1:B:81:ILE:HA	1:B:678:TYR:CE1	2.46	0.51
1:A:58:ASP:OD2	1:A:62:LYS:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PRO:HB3	1:B:653:LEU:O	2.11	0.50
1:B:252:ILE:HD11	1:B:254:GLU:OE1	2.11	0.50
1:B:406:SER:HB3	1:B:441:MET:HE3	1.93	0.50
1:B:286:TYR:CZ	1:B:295:ARG:HD2	2.47	0.50
1:A:484:LYS:NZ	1:A:524:ILE:HG22	2.26	0.50
1:A:41:VAL:HG13	1:A:45:TYR:HB2	1.92	0.50
1:B:551:LYS:HB2	1:B:574:LYS:NZ	2.25	0.50
1:B:286:TYR:CD2	1:B:295:ARG:HD2	2.46	0.50
1:B:517:LEU:C	1:B:517:LEU:HD12	2.32	0.50
1:B:542:ALA:HB2	1:B:558:GLY:HA3	1.92	0.50
1:A:100:ILE:HG13	1:A:136:TYR:CE2	2.47	0.49
1:A:384:CYS:SG	1:A:424:ILE:HD12	2.52	0.49
1:B:654:MET:H	1:B:685:ASN:ND2	2.06	0.49
1:B:377:TYR:CE1	1:B:605:ILE:HG21	2.47	0.49
1:B:437:PRO:HG3	1:B:471:TRP:CD2	2.47	0.49
1:A:545:GLU:HG3	1:A:603:LYS:HA	1.94	0.49
1:A:592:HIS:CD2	1:A:594:LEU:HB2	2.48	0.49
1:B:53:ASN:HB3	1:B:86:TRP:HZ2	1.77	0.49
1:A:151:LEU:O	1:A:155:ILE:HG13	2.12	0.49
1:A:155:ILE:CG2	1:A:159:LYS:HE3	2.43	0.49
1:B:372:THR:HG22	1:B:373:VAL:O	2.12	0.48
2:A:802:CIT:O1	2:A:802:CIT:C6	2.60	0.48
1:B:407:ASN:HD22	1:B:407:ASN:C	2.15	0.48
1:A:490:ARG:HG2	1:A:493:HIS:ND1	2.28	0.48
1:A:351:TYR:CE1	1:A:354:PHE:HB2	2.48	0.48
1:A:303:TYR:CZ	1:A:352:LYS:HB3	2.48	0.48
1:B:429:ILE:HG22	1:B:429:ILE:O	2.13	0.48
1:B:646:ARG:O	1:B:646:ARG:HD3	2.14	0.48
1:B:588:LYS:NZ	1:B:588:LYS:HB2	2.28	0.48
1:A:256:LEU:CD1	1:A:344:VAL:HB	2.38	0.48
1:B:552:GLN:HE21	1:B:587:ILE:CD1	2.26	0.47
1:B:444:THR:HG23	1:B:493:HIS:CD2	2.49	0.47
1:A:54:ASN:O	1:A:56:GLN:N	2.46	0.47
1:B:183:ASP:O	1:B:194:PRO:HD3	2.14	0.47
1:B:333:LEU:HB3	1:B:598:TYR:CE2	2.49	0.47
1:B:313:TRP:CZ2	1:B:321:LYS:HG2	2.50	0.47
1:A:160:THR:O	1:A:162:PRO:HD3	2.14	0.47
1:A:379:LEU:HD12	1:A:688:LEU:HB3	1.96	0.47
1:A:421:TYR:N	1:A:421:TYR:CD1	2.78	0.47
1:A:50:SER:O	1:A:51:SER:C	2.53	0.47
1:B:36:ALA:O	1:B:39:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HB2	1:A:248:SER:OG	2.14	0.47
1:A:262:PHE:CG	1:A:649:GLU:HG2	2.50	0.47
1:A:214:ASP:HA	1:A:215:PRO:HD3	1.81	0.47
1:B:266:SER:OG	1:B:342:HIS:CE1	2.69	0.46
1:B:77:ARG:HB2	1:B:82:ASN:OD1	2.15	0.46
1:B:13:ASN:ND2	1:B:13:ASN:N	2.62	0.46
1:B:566:VAL:CG2	1:B:618:PRO:HG3	2.45	0.46
1:B:407:ASN:ND2	1:B:407:ASN:C	2.68	0.46
1:A:92:ILE:HD13	1:A:253:LEU:HD12	1.97	0.46
1:A:88:ARG:NH1	1:A:225:VAL:HG21	2.31	0.46
1:B:186:THR:HG23	1:B:191:LEU:CD2	2.46	0.46
1:A:387:ASN:O	1:A:407:ASN:HB2	2.16	0.46
1:B:405:GLY:O	1:B:411:VAL:HG22	2.15	0.46
1:A:531:LYS:HG3	1:A:582:GLU:OE1	2.15	0.46
1:B:337:HIS:CD2	1:B:616:THR:OG1	2.64	0.46
1:A:155:ILE:HG22	1:A:159:LYS:HE3	1.96	0.46
1:A:376:ASP:O	1:A:693:ILE:HB	2.16	0.46
1:B:631:LEU:HD13	1:B:638:LEU:CD2	2.46	0.46
1:A:414:ILE:HD11	1:A:480:TRP:CZ2	2.51	0.46
1:A:264:PRO:HG3	1:A:653:LEU:HD23	1.98	0.46
1:A:361:LEU:HD23	1:A:362:PHE:N	2.30	0.46
1:B:50:SER:HB3	1:B:323:GLU:OE2	2.16	0.45
1:B:151:LEU:HD12	1:B:194:PRO:HA	1.98	0.45
1:B:301:PHE:HB3	1:B:348:ALA:HB1	1.98	0.45
1:B:628:ILE:HG22	1:B:641:ILE:HG13	1.99	0.45
1:B:158:ILE:HB	4:B:705:HOH:O	2.16	0.45
1:A:206:LEU:HA	1:A:209:GLU:HG3	1.97	0.45
1:B:256:LEU:CD1	1:B:344:VAL:HB	2.46	0.45
1:B:380:LEU:HB2	1:B:689:LYS:HG3	1.97	0.45
1:B:45:TYR:CG	1:B:327:VAL:HG11	2.52	0.45
1:A:256:LEU:C	1:A:258:PRO:HD3	2.37	0.45
1:B:608:ARG:O	1:B:633:PRO:HD2	2.16	0.45
1:B:297:ASN:ND2	1:B:302:ALA:HA	2.32	0.45
1:A:308:ASP:H	1:A:311:GLN:HE21	1.63	0.45
1:A:420:HIS:HB2	1:A:423:LYS:O	2.17	0.45
1:B:392:ASP:HB3	1:B:445:PHE:HB2	1.99	0.45
1:B:554:ILE:HA	1:B:571:ILE:O	2.17	0.45
1:A:352:LYS:HB2	1:A:352:LYS:HE3	1.59	0.45
1:A:23:ALA:O	1:A:27:ILE:HG12	2.17	0.45
1:B:22:TYR:CD2	1:B:25:LEU:HD12	2.52	0.45
1:B:34:SER:O	1:B:38:LYS:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:MET:HA	1:A:309:MET:CE	2.46	0.45
1:A:316:ALA:HB3	1:A:321:LYS:HD2	1.98	0.45
1:A:377:TYR:HD2	1:A:609:LYS:HZ3	1.63	0.45
1:B:111:VAL:HB	1:B:142:PHE:CD2	2.52	0.44
1:A:13:ASN:HD22	1:A:14:VAL:H	1.64	0.44
1:A:103:THR:HG22	1:A:139:ARG:HH12	1.82	0.44
1:B:62:LYS:O	1:B:63:LEU:C	2.55	0.44
1:B:44:LEU:O	1:B:47:PRO:HD2	2.18	0.44
1:B:416:GLN:HB2	1:B:429:ILE:HD11	1.99	0.44
1:B:545:GLU:HG3	1:B:546:PHE:N	2.33	0.44
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.78	0.44
1:A:484:LYS:NZ	2:A:802:CIT:O1	2.31	0.44
1:B:611:LEU:HD22	1:B:690:LEU:HD22	1.98	0.44
1:A:194:PRO:O	1:A:195:CYS:HB2	2.17	0.44
1:A:407:ASN:C	1:A:407:ASN:HD22	2.21	0.44
1:B:448:ILE:HD13	1:B:455:LEU:HB2	1.99	0.44
1:A:81:ILE:HA	1:A:678:TYR:CE1	2.52	0.44
1:A:226:SER:C	1:A:228:ALA:H	2.21	0.44
1:B:595:PHE:HZ	1:B:631:LEU:HD22	1.79	0.44
1:A:608:ARG:HE	1:A:634:LEU:HD21	1.82	0.43
1:A:297:ASN:HA	1:A:301:PHE:O	2.18	0.43
1:B:491:PHE:O	1:B:492:ARG:HB2	2.16	0.43
1:B:228:ALA:HB2	1:B:254:GLU:HB2	2.00	0.43
1:A:488:HIS:CD2	1:B:488:HIS:CD2	3.06	0.43
1:B:79:PRO:HA	1:B:328:GLU:OE1	2.18	0.43
1:A:13:ASN:C	1:A:13:ASN:HD22	2.19	0.43
1:A:42:GLU:HA	1:A:46:LEU:HG	2.00	0.43
1:A:54:ASN:C	1:A:56:GLN:H	2.21	0.43
1:A:505:ILE:HB	1:A:516:LEU:HB2	2.01	0.43
1:A:157:LEU:O	1:A:161:ILE:HG13	2.19	0.43
1:A:308:ASP:H	1:A:311:GLN:NE2	2.16	0.43
1:A:249:HIS:HE1	1:A:354:PHE:CG	2.37	0.43
1:B:316:ALA:HB3	1:B:321:LYS:HE2	1.99	0.43
1:B:338:LEU:O	1:B:342:HIS:CD2	2.63	0.43
1:A:555:ILE:HG13	1:A:573:PHE:HE2	1.84	0.43
1:A:266:SER:OG	1:A:342:HIS:HE1	2.02	0.42
1:B:150:LEU:C	1:B:150:LEU:HD23	2.39	0.42
1:B:339:PHE:CE1	1:B:678:TYR:CZ	3.07	0.42
1:A:92:ILE:CD1	1:A:253:LEU:HD12	2.50	0.42
1:A:377:TYR:HD2	1:A:609:LYS:NZ	2.17	0.42
1:A:547:ASP:HA	1:A:548:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:N	1:A:47:PRO:CD	2.82	0.42
1:A:51:SER:CA	1:A:132:GLN:HE22	2.32	0.42
1:B:552:GLN:HG2	1:B:572:ILE:HG22	2.01	0.42
1:A:634:LEU:HD12	1:A:635:SER:H	1.80	0.42
1:A:196:ASP:H	1:A:202:MET:CE	2.32	0.42
1:B:551:LYS:HB2	1:B:574:LYS:HZ1	1.84	0.42
1:A:227:LEU:HD12	1:A:230:MET:SD	2.58	0.42
1:A:257:ILE:HG13	1:A:257:ILE:O	2.19	0.42
1:A:257:ILE:HG12	1:A:283:VAL:HG22	2.01	0.42
1:B:194:PRO:O	1:B:195:CYS:HB2	2.18	0.42
1:A:526:LYS:O	1:A:528:VAL:HG13	2.20	0.41
1:A:193:ARG:HA	1:A:194:PRO:HD3	1.92	0.41
1:B:551:LYS:O	1:B:574:LYS:HD2	2.20	0.41
1:A:488:HIS:HD2	1:B:488:HIS:CD2	2.38	0.41
1:B:54:ASN:O	1:B:56:GLN:N	2.47	0.41
1:B:213:TYR:HA	1:B:245:MET:HG3	2.02	0.41
1:B:121:LEU:N	1:B:122:PRO:CD	2.83	0.41
1:B:98:SER:HB3	1:B:360:PHE:CE2	2.55	0.41
1:B:592:HIS:ND1	1:B:638:LEU:HD11	2.35	0.41
1:B:207:LEU:CD2	1:B:212:LEU:HD12	2.49	0.41
1:A:457:ILE:HD13	1:A:470:ASN:HB3	2.03	0.41
1:B:286:TYR:CE1	1:B:295:ARG:HD2	2.56	0.41
1:A:324:LEU:HA	1:A:327:VAL:HG23	2.03	0.41
1:B:407:ASN:H	1:B:409:TYR:N	2.18	0.41
1:A:484:LYS:HZ2	1:A:524:ILE:HA	1.85	0.41
1:A:303:TYR:OH	1:A:352:LYS:HB3	2.20	0.41
1:B:297:ASN:HD22	1:B:302:ALA:HA	1.86	0.41
1:B:667:THR:HA	1:B:690:LEU:O	2.20	0.41
1:B:455:LEU:HD23	1:B:503:VAL:HG21	2.03	0.41
1:A:412:ASN:OD1	1:A:412:ASN:C	2.59	0.41
1:B:547:ASP:HA	1:B:548:PRO:HD2	1.86	0.41
1:B:640:SER:O	1:B:642:PRO:HD3	2.21	0.41
1:A:51:SER:HA	1:A:132:GLN:NE2	2.35	0.41
1:A:255:GLN:N	1:A:255:GLN:NE2	2.61	0.41
1:B:568:ASP:O	1:B:595:PHE:HB2	2.20	0.41
1:B:286:TYR:CG	1:B:295:ARG:HD2	2.56	0.40
1:A:119:ASP:HA	1:A:120:PRO:HD3	1.75	0.40
1:A:45:TYR:O	1:A:49:LEU:HG	2.21	0.40
1:A:27:ILE:C	1:A:29:GLY:N	2.75	0.40
1:A:380:LEU:HD22	1:A:380:LEU:HA	1.83	0.40
1:B:382:CYS:O	1:B:383:GLU:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HD13	1:A:379:LEU:HA	1.96	0.40
1:A:258:PRO:HA	1:A:288:THR:HG22	2.02	0.40
1:B:461:LYS:HB2	1:B:465:GLN:OE1	2.20	0.40
1:A:384:CYS:N	1:A:385:PRO:HD3	2.35	0.40
1:B:112:VAL:HG22	1:B:143:ILE:HB	2.04	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	676/695 (97%)	625 (92%)	46 (7%)	5 (1%)	26	55
1	B	670/695 (96%)	619 (92%)	48 (7%)	3 (0%)	39	69
All	All	1346/1390 (97%)	1244 (92%)	94 (7%)	8 (1%)	30	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	483	ILE
1	A	55	PHE
1	B	364	ARG
1	A	52	ALA
1	B	483	ILE
1	B	541	SER
1	A	225	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	607/630 (96%)	566 (93%)	41 (7%)	20	43
1	B	605/630 (96%)	574 (95%)	31 (5%)	29	59
All	All	1212/1260 (96%)	1140 (94%)	72 (6%)	24	51

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	32	ASN
1	A	44	LEU
1	A	54	ASN
1	A	56	GLN
1	A	81	ILE
1	A	92	ILE
1	A	95	ARG
1	A	128	THR
1	A	134	GLN
1	A	141	SER
1	A	172	GLU
1	A	191	LEU
1	A	227	LEU
1	A	253	LEU
1	A	255	GLN
1	A	277	ASP
1	A	291	SER
1	A	315	SER
1	A	321	LYS
1	A	339	PHE
1	A	347	HIS
1	A	380	LEU
1	A	395	VAL
1	A	407	ASN
1	A	413	GLU
1	A	421	TYR

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Mol	Chain	Res	Type
1	A	445	PHE
1	A	447	THR
1	A	475	MET
1	A	477	THR
1	A	481	SER
1	A	504	LEU
1	A	581	THR
1	A	624	ARG
1	A	625	THR
1	A	631	LEU
1	A	639	THR
1	A	653	LEU
1	A	676	THR
1	A	693	ILE
1	B	13	ASN
1	B	16	GLN
1	B	28	GLN
1	B	31	ASN
1	B	63	LEU
1	B	106	ASP
1	B	128	THR
1	B	170	LEU
1	B	233	GLU
1	B	245	MET
1	B	255	GLN
1	B	291	SER
1	B	347	HIS
1	B	349	THR
1	B	361	LEU
1	B	387	ASN
1	B	407	ASN
1	B	428	ASN
1	B	429	ILE
1	B	435	GLU
1	B	441	MET
1	B	504	LEU
1	B	517	LEU
1	B	521	THR
1	B	522	GLU
1	B	536	GLN
1	B	545	GLU
1	B	556	LEU

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Mol	Chain	Res	Type
1	B	588	LYS
1	B	634	LEU
1	B	641	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	54	ASN
1	A	102	GLN
1	A	132	GLN
1	A	134	GLN
1	A	137	HIS
1	A	255	GLN
1	A	272	HIS
1	A	297	ASN
1	A	311	GLN
1	A	337	HIS
1	A	342	HIS
1	A	347	HIS
1	A	407	ASN
1	A	416	GLN
1	A	428	ASN
1	A	488	HIS
1	A	592	HIS
1	A	685	ASN
1	B	13	ASN
1	B	16	GLN
1	B	31	ASN
1	B	137	HIS
1	B	255	GLN
1	B	297	ASN
1	B	337	HIS
1	B	342	HIS
1	B	347	HIS
1	B	358	GLN
1	B	407	ASN
1	B	416	GLN
1	B	470	ASN
1	B	488	HIS
1	B	552	GLN
1	B	592	HIS

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Mol	Chain	Res	Type
1	B	669	HIS
1	B	685	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 ⓘ

5 ligands are modelled in this entry.

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	$\# Z  > 2$
2	CIT	A	801	-	3,12,12	1.21	0	3,17,17	1.49	1 (33%)
2	CIT	A	802	-	3,12,12	1.04	0	3,17,17	1.91	1 (33%)
3	PG4	A	803	-	12,12,12	0.55	0	11,11,11	1.54	0
2	CIT	B	801	-	3,12,12	1.26	0	3,17,17	2.03	2 (66%)
2	CIT	B	802	-	3,12,12	1.13	0	3,17,17	1.54	1 (33%)

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
2	CIT	A	801	-	-	0/6/16/16	0/0/0/0
2	CIT	A	802	-	-	0/6/16/16	0/0/0/0
3	PG4	A	803	-	-	0/10/10/10	0/0/0/0
2	CIT	B	801	-	-	0/6/16/16	0/0/0/0
2	CIT	B	802	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	CIT	C3-C4-C5	-3.16	109.90	114.96
2	B	801	CIT	C3-C4-C5	-2.57	110.85	114.96
2	B	802	CIT	C3-C4-C5	-2.48	110.99	114.96
2	B	801	CIT	C3-C2-C1	-2.36	111.19	114.96
2	A	801	CIT	C3-C4-C5	-2.05	111.69	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CIT	1	0
2	A	802	CIT	2	0
3	A	803	PG4	1	0

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	680/695 (97%)	0.16	17 (2%) 61 61	49, 69, 103, 118	0
1	B	677/695 (97%)	0.11	23 (3%) 49 49	51, 69, 104, 124	0
All	All	1357/1390 (97%)	0.13	40 (2%) 55 55	49, 69, 103, 124	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	LEU	5.9
1	B	22	TYR	5.3
1	B	171	SER	4.5
1	B	421	TYR	4.0
1	A	176	TYR	3.9
1	B	11	ASN	3.7
1	B	18	ARG	3.0
1	A	30	THR	2.9
1	B	15	LYS	2.7
1	B	531	LYS	2.6
1	A	657	GLY	2.6
1	B	57	MET	2.6
1	B	14	VAL	2.6
1	A	542	ALA	2.5
1	A	615	GLY	2.5
1	B	358	GLN	2.5
1	A	375	GLU	2.4
1	B	377	TYR	2.4
1	B	605	ILE	2.4
1	A	17	GLU	2.3
1	A	451	ASN	2.3
1	A	541	SER	2.3
1	B	17	GLU	2.3
1	A	543	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	384	CYS	2.2
1	B	581	THR	2.2
1	B	475	MET	2.2
1	A	450	ARG	2.2
1	B	586	VAL	2.2
1	A	616	THR	2.1
1	B	378	GLN	2.1
1	A	380	LEU	2.1
1	A	419	ILE	2.1
1	B	693	ILE	2.1
1	A	656	ALA	2.1
1	B	590	LEU	2.1
1	B	13	ASN	2.1
1	B	432	SER	2.0
1	A	475	MET	2.0
1	A	424	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CIT	B	802	13/13	0.82	0.32	7.75	74,83,88,89	0
2	CIT	A	802	13/13	0.70	0.40	5.50	92,98,104,105	0
2	CIT	A	801	13/13	0.88	0.18	0.06	65,77,86,88	0
2	CIT	B	801	13/13	0.91	0.18	-0.38	61,69,79,79	0
3	PG4	A	803	13/13	0.81	0.12	-3.95	83,96,105,109	0



## 6.5 Other polymers

There are no such residues in this entry.