



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:24 pm GMT

PDB ID : 1P1K  
Title : Crystal structure of the 1L-myo-inositol 1-phosphate synthase complexed with NADH in the presence of EDTA  
Authors : Jin, X.; Geiger, J.H.  
Deposited on : 2003-04-12  
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

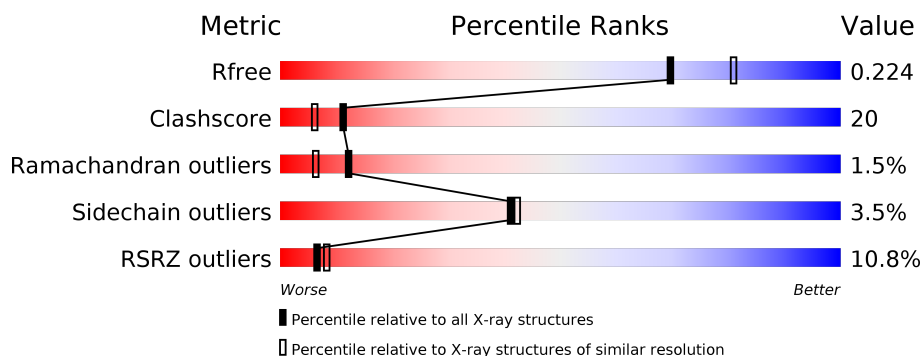
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	533	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>• •</div> </div> </div>
1	B	533	<div> <div>13%</div> <div> <div></div> <div>60%</div> <div>32%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8450 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.

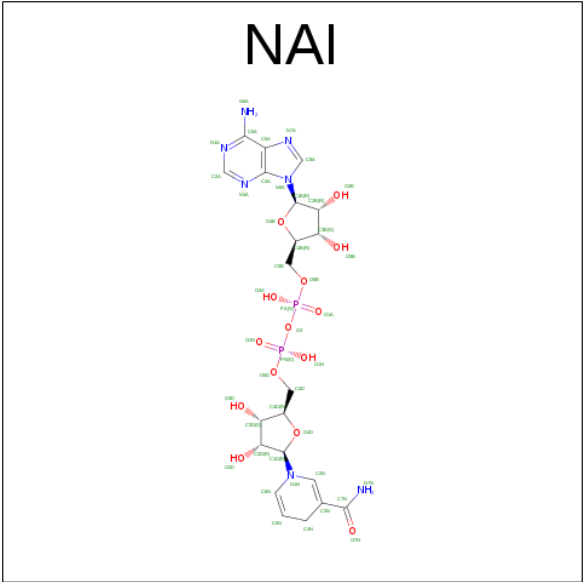
- Molecule 1 is a protein called Inositol-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4138	2632	695	795	16			
1	B	512	Total	C	N	O	S	0	0	0
			4046	2577	680	773	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986
B	14	VAL	LEU	SEE REMARK 999	UNP P11986
B	?	-	PHE	SEE REMARK 999	UNP P11986
B	60	LEU	GLU	SEE REMARK 999	UNP P11986
B	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

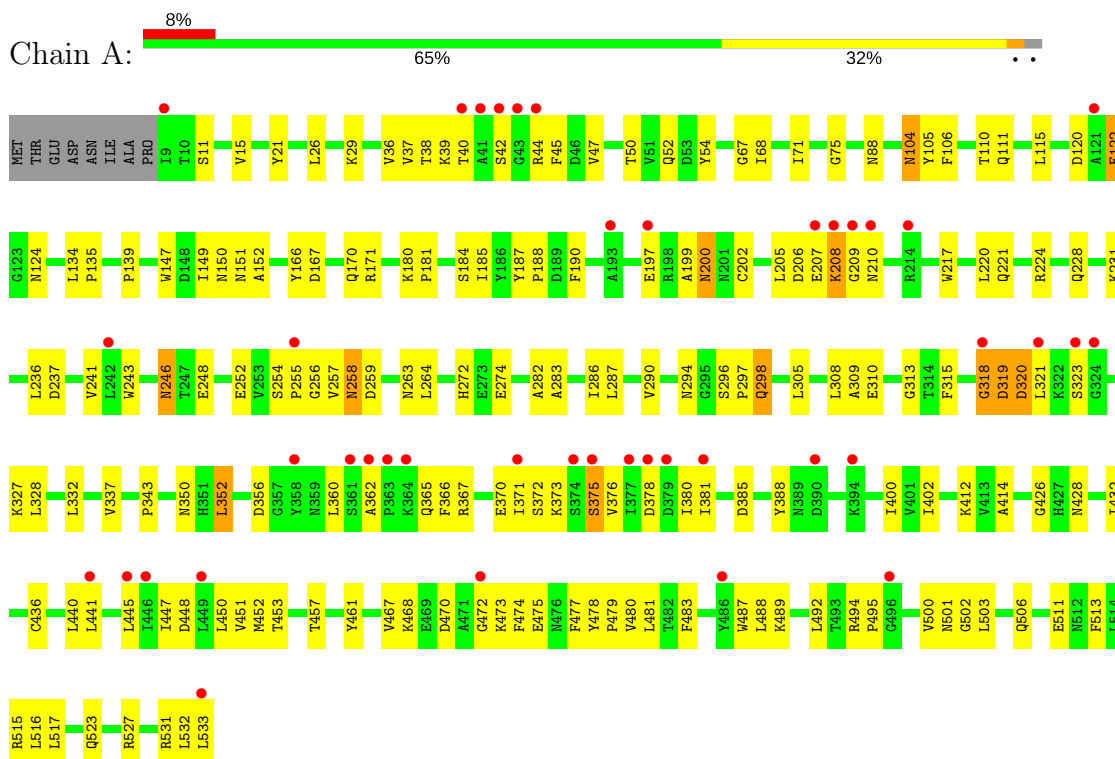
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	79	Total	O	0	0
			79	79		

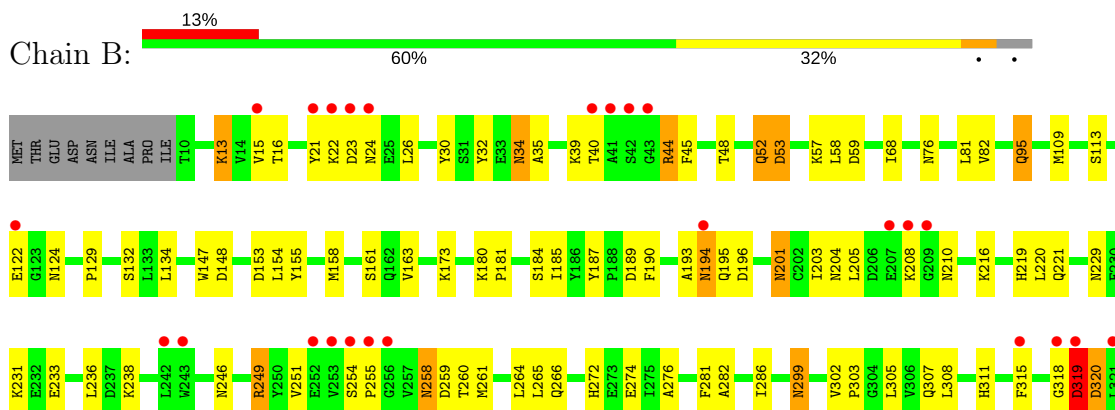
### 3 Residue-property plots [i](#)

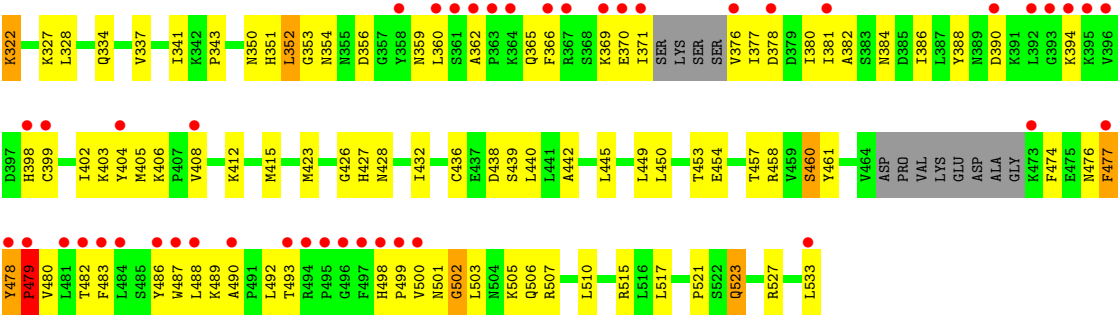
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Inositol-3-phosphate synthase



#### • Molecule 1: Inositol-3-phosphate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.98Å 97.61Å 121.72Å 90.00° 126.15° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 35.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.10) 98.6 (35.93-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.261 0.230 , 0.224	Depositor DCC
$R_{free}$ test set	4132 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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:  
NAI

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	0.37	0/4219	0.62	1/5719 (0.0%)
1	B	0.37	0/4124	0.62	0/5588
All	All	0.37	0/8343	0.62	1/11307 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	GLY	N-CA-C	5.04	125.71	113.10

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	4138	0	4147	164	0
1	B	4046	0	4055	180	0
2	A	44	0	27	1	0
2	B	44	0	27	4	0
3	A	99	0	0	3	0
3	B	79	0	0	5	0
All	All	8450	0	8256	329	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 20.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LEU:HD21	1:B:487:TRP:HB3	1.31	1.12
1:A:332:LEU:HD13	1:A:432:ILE:HD11	1.37	1.06
1:A:115:LEU:HD22	1:A:511:GLU:HG3	1.37	1.04
1:B:445:LEU:CD2	1:B:487:TRP:HB3	2.10	0.82
1:A:110:THR:HG23	1:A:111:GLN:HE21	1.50	0.76
1:A:110:THR:HG22	1:A:448:ASP:OD2	1.85	0.76
1:A:104:ASN:ND2	1:A:106:PHE:H	1.84	0.76
1:B:221:GLN:HG3	3:B:704:HOH:O	1.86	0.75
1:B:493:THR:HG21	1:B:499:PRO:HD3	1.68	0.75
1:A:367:ARG:CZ	1:A:371:ILE:HD11	2.16	0.74
1:A:15:VAL:HG11	1:B:48:THR:HG22	1.72	0.72
1:A:104:ASN:HD22	1:A:106:PHE:H	1.37	0.72
1:B:251:VAL:H	1:B:299:ASN:HD21	1.36	0.71
1:A:515:ARG:CZ	1:A:523:GLN:HE21	2.04	0.71
1:A:318:GLY:HA2	1:A:488:LEU:HD13	1.73	0.70
1:A:533:LEU:HD22	1:B:478:TYR:HB2	1.72	0.70
1:B:15:VAL:O	1:B:15:VAL:HG23	1.89	0.70
1:A:254:SER:H	1:A:258:ASN:HD21	1.40	0.70
1:A:445:LEU:HD21	1:A:487:TRP:HB3	1.73	0.68
1:B:381:ILE:HG13	1:B:388:TYR:CG	2.29	0.68
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.09	0.68
1:A:531:ARG:HG3	1:B:482:THR:HB	1.75	0.68
1:A:321:LEU:HD22	1:A:445:LEU:HD22	1.74	0.67
1:A:318:GLY:HA2	1:A:488:LEU:CD1	2.25	0.67
1:B:13:LYS:HE2	1:B:13:LYS:HA	1.74	0.67
1:B:405:MET:O	1:B:408:VAL:HG22	1.95	0.67
1:A:255:PRO:HA	1:A:259:ASP:OD1	1.96	0.66
1:A:412:LYS:HE3	1:A:414:ALA:HB2	1.75	0.66
1:A:376:VAL:HA	1:A:501:ASN:OD1	1.96	0.66
1:B:258:ASN:HD22	1:B:258:ASN:H	1.42	0.66
1:B:445:LEU:O	1:B:445:LEU:HD23	1.96	0.66
1:A:272:HIS:CD2	1:A:274:GLU:HB2	2.31	0.66
1:A:40:THR:HG22	1:A:42:SER:H	1.60	0.66
1:A:367:ARG:NH2	1:A:371:ILE:HD11	2.11	0.65
1:B:320:ASP:O	1:B:488:LEU:HD23	1.95	0.65
1:A:375:SER:HA	1:A:378:ASP:OD2	1.97	0.64
1:A:150:ASN:ND2	1:A:152:ALA:H	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ALA:HB3	1:A:365:GLN:HE21	1.62	0.64
1:A:318:GLY:CA	1:A:488:LEU:HD13	2.28	0.64
1:A:502:GLY:O	1:A:506:GLN:HG3	1.98	0.64
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.28	0.64
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.34	0.63
1:A:272:HIS:HD2	1:A:274:GLU:HB2	1.63	0.63
1:B:492:LEU:HD13	1:B:493:THR:N	2.14	0.63
1:B:238:LYS:HE2	1:B:454:GLU:OE2	2.00	0.62
1:B:377:ILE:O	1:B:381:ILE:HG22	1.99	0.62
1:B:378:ASP:HA	1:B:381:ILE:CG2	2.30	0.62
1:A:328:LEU:O	1:A:328:LEU:HD23	2.00	0.62
1:B:442:ALA:HB2	2:B:660:NAI:H42N	1.82	0.62
1:B:95:GLN:HA	1:B:95:GLN:HE21	1.65	0.62
1:A:315:PHE:CZ	1:A:477:PHE:HB2	2.36	0.61
1:B:477:PHE:HZ	1:B:483:PHE:CE1	2.18	0.61
1:A:15:VAL:CG1	1:B:48:THR:HG22	2.30	0.61
1:B:315:PHE:CD2	1:B:479:PRO:HA	2.36	0.61
1:B:318:GLY:CA	1:B:488:LEU:HD13	2.31	0.61
1:A:328:LEU:HD21	1:A:432:ILE:HD13	1.82	0.60
1:B:34:ASN:ND2	1:B:35:ALA:H	1.99	0.60
1:B:315:PHE:HD2	1:B:479:PRO:HA	1.66	0.60
1:B:320:ASP:HB3	1:B:489:LYS:HB3	1.82	0.60
1:A:21:TYR:CZ	1:A:26:LEU:HD13	2.37	0.60
1:A:352:LEU:H	1:A:352:LEU:HD23	1.67	0.60
1:B:52:GLN:C	1:B:52:GLN:HE21	2.04	0.60
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.02	0.59
1:B:30:TYR:HE1	1:B:32:TYR:HB2	1.68	0.59
1:B:246:ASN:HD22	1:B:359:ASN:HB2	1.67	0.59
1:B:318:GLY:HA2	1:B:488:LEU:HD13	1.86	0.58
1:B:320:ASP:O	1:B:488:LEU:HA	2.03	0.58
1:B:502:GLY:HA3	1:B:505:LYS:HE2	1.84	0.58
1:B:30:TYR:CE1	1:B:32:TYR:HB2	2.39	0.58
1:A:350:ASN:HD21	1:A:402:ILE:HG12	1.68	0.58
1:A:315:PHE:CD1	1:A:481:LEU:HD11	2.39	0.58
1:B:264:LEU:HD21	1:B:305:LEU:HD13	1.86	0.58
1:A:356:ASP:O	1:A:360:LEU:HG	2.04	0.57
1:A:104:ASN:HD21	1:B:423:MET:HA	1.68	0.57
1:B:299:ASN:HD22	1:B:299:ASN:N	2.03	0.57
1:A:256:GLY:HA2	1:A:263:ASN:OD1	2.04	0.57
1:A:328:LEU:CD2	1:A:432:ILE:HD13	2.34	0.57
1:B:260:THR:HA	1:B:307:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LYS:C	1:B:371:ILE:H	2.09	0.56
1:B:327:LYS:HG2	1:B:503:LEU:HD22	1.86	0.56
1:B:498:HIS:CD2	1:B:498:HIS:N	2.70	0.56
1:A:104:ASN:HD22	1:A:104:ASN:C	2.09	0.56
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.88	0.56
1:A:500:VAL:HG21	1:B:527:ARG:CZ	2.34	0.56
1:B:352:LEU:HD23	1:B:352:LEU:N	2.20	0.56
1:A:217:TRP:O	1:A:221:GLN:HG2	2.06	0.56
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.41	0.55
1:A:373:LYS:HG2	1:A:489:LYS:HD3	1.87	0.55
1:A:320:ASP:HB3	1:A:489:LYS:HB3	1.88	0.55
1:B:376:VAL:HG23	1:B:501:ASN:HB2	1.89	0.55
1:B:334:GLN:NE2	1:B:380:ILE:HG12	2.21	0.55
1:B:377:ILE:HG13	1:B:398:HIS:HD1	1.72	0.55
1:B:95:GLN:HA	1:B:95:GLN:NE2	2.22	0.55
1:B:231:LYS:HG2	1:B:236:LEU:O	2.07	0.55
1:B:122:GLU:HB2	1:B:124:ASN:ND2	2.22	0.54
1:B:95:GLN:CA	1:B:95:GLN:HE21	2.18	0.54
1:A:258:ASN:H	1:A:258:ASN:HD22	1.55	0.54
1:A:318:GLY:O	1:A:319:ASP:HB2	2.07	0.54
1:B:203:ILE:HG13	1:B:204:ASN:N	2.22	0.54
1:B:377:ILE:HG13	1:B:398:HIS:ND1	2.22	0.54
1:A:208:LYS:H	1:A:208:LYS:HD3	1.73	0.54
1:A:68:ILE:HD12	1:A:450:LEU:HD13	1.90	0.54
1:A:258:ASN:ND2	1:A:258:ASN:H	2.05	0.54
1:A:151:ASN:H	1:A:200:ASN:HD21	1.54	0.54
1:B:318:GLY:HA2	1:B:488:LEU:CD1	2.38	0.54
1:B:22:LYS:O	1:B:23:ASP:HB2	2.07	0.53
1:B:318:GLY:O	1:B:319:ASP:HB2	2.07	0.53
1:A:494:ARG:HG3	1:A:495:PRO:HD2	1.90	0.53
1:B:483:PHE:HB3	1:B:510:LEU:CD2	2.39	0.53
1:A:224:ARG:O	1:A:228:GLN:HG3	2.08	0.53
1:B:194:ASN:HD22	1:B:195:GLN:N	2.07	0.53
1:B:258:ASN:HD22	1:B:258:ASN:N	2.02	0.53
1:B:322:LYS:NZ	1:B:506:GLN:HE22	2.06	0.53
1:B:82:VAL:HG21	1:B:154:LEU:CD1	2.39	0.53
1:B:381:ILE:HD11	1:B:394:LYS:O	2.09	0.53
1:B:15:VAL:CG2	1:B:15:VAL:O	2.57	0.53
1:A:477:PHE:HZ	1:A:513:PHE:CZ	2.27	0.52
1:B:57:LYS:HE3	1:B:474:PHE:CE2	2.44	0.52
1:A:461:TYR:O	1:A:474:PHE:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.09	0.52
1:B:352:LEU:HD12	1:B:354:ASN:OD1	2.09	0.52
1:A:29:LYS:HE2	3:A:697:HOH:O	2.09	0.52
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.10	0.52
1:B:190:PHE:CE2	1:B:276:ALA:HB2	2.46	0.52
1:B:299:ASN:HD22	1:B:299:ASN:H	1.57	0.51
1:B:57:LYS:HE3	1:B:474:PHE:CD2	2.45	0.51
1:B:109:MET:HE2	1:B:507:ARG:HE	1.75	0.51
1:A:352:LEU:N	1:A:352:LEU:HD23	2.26	0.51
1:A:373:LYS:CG	1:A:489:LYS:HD3	2.41	0.51
1:B:362:ALA:HB3	1:B:365:GLN:OE1	2.11	0.51
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.23	0.51
1:B:261:MET:CE	1:B:311:HIS:HB2	2.40	0.51
1:B:486:TYR:CE1	1:B:503:LEU:HG	2.45	0.51
1:B:147:TRP:HB3	1:B:184:SER:HB2	1.91	0.51
1:A:184:SER:OG	1:A:185:ILE:N	2.44	0.51
1:B:129:PRO:HB2	1:B:132:SER:HB3	1.92	0.51
1:B:477:PHE:CZ	1:B:483:PHE:CE1	2.99	0.51
1:B:52:GLN:NE2	1:B:53:ASP:N	2.58	0.51
1:A:527:ARG:CZ	1:B:500:VAL:HG21	2.40	0.51
1:B:220:LEU:C	1:B:220:LEU:HD23	2.31	0.51
1:A:272:HIS:HD2	1:A:274:GLU:H	1.59	0.50
1:A:515:ARG:NH1	1:A:523:GLN:HE21	2.07	0.50
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.94	0.50
1:B:445:LEU:HD23	1:B:445:LEU:C	2.31	0.50
1:A:15:VAL:HG13	1:A:15:VAL:O	2.11	0.50
1:A:367:ARG:O	1:A:371:ILE:HG12	2.12	0.50
1:A:500:VAL:HG21	1:B:527:ARG:NH2	2.27	0.50
1:B:258:ASN:ND2	1:B:258:ASN:N	2.59	0.50
1:B:76:ASN:HB3	1:B:439:SER:OG	2.10	0.50
1:A:294:ASN:ND2	1:A:296:SER:H	2.10	0.50
1:A:52:GLN:HG3	1:A:54:TYR:CE1	2.47	0.50
1:A:122:GLU:CD	1:A:122:GLU:N	2.65	0.50
1:A:220:LEU:HD12	1:A:221:GLN:HE21	1.77	0.50
1:A:44:ARG:HG2	1:A:45:PHE:N	2.27	0.50
1:B:58:LEU:HD22	1:B:134:LEU:HD13	1.94	0.49
1:A:272:HIS:CD2	1:A:274:GLU:H	2.30	0.49
1:A:40:THR:HG22	1:A:42:SER:N	2.27	0.49
1:B:205:LEU:HA	1:B:210:ASN:O	2.11	0.49
1:A:531:ARG:CG	1:B:482:THR:HB	2.42	0.49
1:A:315:PHE:HZ	1:A:477:PHE:HB2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:THR:O	1:A:457:THR:HG23	2.13	0.49
1:B:26:LEU:O	1:B:57:LYS:HA	2.12	0.49
1:B:327:LYS:HG3	1:B:503:LEU:HD13	1.94	0.49
1:B:394:LYS:HG2	3:B:709:HOH:O	2.11	0.49
1:A:531:ARG:O	1:A:532:LEU:HD23	2.13	0.49
1:B:258:ASN:H	1:B:258:ASN:ND2	2.09	0.49
1:B:341:ILE:O	1:B:343:PRO:HD3	2.12	0.49
1:B:337:VAL:HG21	1:B:380:ILE:HG22	1.95	0.49
1:A:200:ASN:HD22	1:A:200:ASN:C	2.16	0.48
1:A:205:LEU:HA	1:A:210:ASN:O	2.13	0.48
1:B:39:LYS:HD3	1:B:45:PHE:CE1	2.48	0.48
1:A:323:SER:HA	3:A:710:HOH:O	2.12	0.48
1:B:486:TYR:HB2	1:B:506:GLN:HB3	1.95	0.48
1:B:81:LEU:C	1:B:81:LEU:HD13	2.34	0.48
1:B:328:LEU:HD12	1:B:328:LEU:O	2.12	0.48
1:A:516:LEU:C	1:A:516:LEU:HD12	2.34	0.48
1:B:249:ARG:O	1:B:249:ARG:HG3	2.14	0.48
1:A:447:ILE:O	1:A:451:VAL:HG23	2.13	0.48
1:A:372:SER:O	1:A:489:LYS:HG2	2.14	0.48
1:B:148:ASP:HA	2:B:660:NAI:N3A	2.28	0.48
1:A:134:LEU:HB3	1:A:135:PRO:HD2	1.96	0.47
1:A:206:ASP:O	1:A:209:GLY:N	2.46	0.47
1:B:153:ASP:OD2	1:B:155:TYR:HB3	2.14	0.47
1:A:258:ASN:ND2	1:A:258:ASN:N	2.60	0.47
1:B:493:THR:HG21	1:B:499:PRO:CD	2.42	0.47
1:A:296:SER:HB3	1:A:297:PRO:HD2	1.96	0.47
1:A:350:ASN:HB2	1:A:412:LYS:HD3	1.96	0.47
1:B:460:SER:HB2	1:B:474:PHE:HB3	1.96	0.47
1:A:110:THR:CG2	1:A:111:GLN:HE21	2.25	0.47
1:B:220:LEU:HD23	1:B:220:LEU:O	2.15	0.47
1:A:105:TYR:CE2	1:A:139:PRO:HG2	2.50	0.47
1:A:328:LEU:HD23	1:A:328:LEU:C	2.35	0.47
1:A:531:ARG:HG2	3:B:737:HOH:O	2.15	0.47
1:B:378:ASP:HA	1:B:381:ILE:HG22	1.96	0.47
1:B:259:ASP:HA	1:B:303:PRO:HB2	1.97	0.47
1:A:385:ASP:HA	1:A:388:TYR:O	2.15	0.46
1:A:200:ASN:H	1:A:200:ASN:HD22	1.62	0.46
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.97	0.46
1:A:381:ILE:HG23	1:A:388:TYR:CG	2.50	0.46
1:A:231:LYS:HE3	1:A:237:ASP:O	2.15	0.46
1:A:286:ILE:HG21	1:A:308:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:OD2	1:A:124:ASN:HB2	2.16	0.46
1:A:370:GLU:HG2	1:A:370:GLU:O	2.15	0.46
1:A:428:ASN:HD22	1:B:436:CYS:HB3	1.79	0.46
1:A:36:VAL:HG23	1:A:50:THR:HG21	1.98	0.46
1:B:266:GLN:HA	1:B:266:GLN:NE2	2.31	0.46
1:B:153:ASP:OD2	1:B:155:TYR:N	2.46	0.46
1:A:315:PHE:CZ	1:A:481:LEU:HD21	2.51	0.46
1:B:384:ASN:OD1	1:B:386:ILE:HB	2.15	0.46
1:A:104:ASN:C	1:A:104:ASN:ND2	2.69	0.45
1:A:110:THR:HG23	1:A:111:GLN:NE2	2.25	0.45
1:B:356:ASP:O	1:B:360:LEU:HG	2.16	0.45
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.99	0.45
1:B:155:TYR:CE2	1:B:173:LYS:HE3	2.51	0.45
1:B:453:THR:O	1:B:457:THR:HG23	2.16	0.45
1:B:52:GLN:NE2	1:B:53:ASP:O	2.49	0.45
1:A:149:ILE:O	1:A:199:ALA:HA	2.16	0.45
1:A:254:SER:HB2	1:A:257:VAL:HG21	1.97	0.45
1:A:489:LYS:HB2	1:A:489:LYS:HE3	1.86	0.45
1:B:483:PHE:HB3	1:B:510:LEU:HD23	1.98	0.45
1:A:180:LYS:HA	1:A:181:PRO:HD3	1.81	0.45
1:A:475:GLU:HB3	1:B:533:LEU:HD12	1.98	0.45
1:A:445:LEU:CD2	1:A:487:TRP:HB3	2.44	0.45
1:A:298:GLN:HE21	1:A:298:GLN:HB3	1.62	0.45
1:B:194:ASN:C	1:B:194:ASN:HD22	2.20	0.45
1:A:283:ALA:O	1:A:287:LEU:HG	2.17	0.44
1:B:366:PHE:HE1	1:B:402:ILE:HG12	1.81	0.44
1:A:37:VAL:HG12	1:A:38:THR:N	2.32	0.44
1:B:180:LYS:HA	1:B:181:PRO:HD3	1.87	0.44
1:B:229:ASN:O	1:B:233:GLU:HB3	2.16	0.44
1:A:190:PHE:O	1:A:248:GLU:HA	2.18	0.44
1:A:254:SER:H	1:A:258:ASN:ND2	2.13	0.44
1:A:513:PHE:O	1:A:516:LEU:HG	2.17	0.44
1:B:480:VAL:CG1	1:B:492:LEU:HD12	2.47	0.44
1:B:415:MET:HA	1:B:432:ILE:O	2.17	0.44
1:B:449:LEU:HD21	1:B:487:TRP:HB2	1.98	0.44
1:A:39:LYS:HA	1:A:44:ARG:O	2.17	0.44
1:A:494:ARG:CG	1:A:495:PRO:HD2	2.47	0.44
1:A:252:GLU:N	1:A:274:GLU:OE1	2.50	0.44
1:A:241:VAL:HG23	1:A:290:VAL:HG11	1.98	0.44
1:A:373:LYS:HB3	1:A:400:ILE:HD13	2.00	0.44
1:A:440:LEU:CD1	1:B:426:GLY:HA3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:660:NAI:H2N	2:B:660:NAI:O5D	2.18	0.44
1:A:452:MET:HG3	1:A:487:TRP:CH2	2.53	0.44
1:B:282:ALA:HB3	1:B:305:LEU:HD21	2.00	0.44
1:B:327:LYS:HG3	1:B:503:LEU:CD1	2.48	0.44
1:B:109:MET:HE1	1:B:507:ARG:HD2	1.99	0.44
1:A:533:LEU:N	1:B:461:TYR:OH	2.51	0.43
1:A:263:ASN:HD22	1:A:263:ASN:N	2.15	0.43
1:B:427:HIS:HE1	3:B:710:HOH:O	2.00	0.43
1:B:480:VAL:HG13	1:B:492:LEU:HD12	2.01	0.43
1:A:75:GLY:HA3	2:A:650:NAI:O5B	2.19	0.43
1:A:110:THR:HG23	1:A:111:GLN:HG2	2.01	0.43
1:A:366:PHE:HE1	1:A:402:ILE:HG13	1.83	0.43
1:A:71:ILE:HG21	1:A:243:TRP:CE3	2.54	0.43
1:B:492:LEU:HD13	1:B:493:THR:H	1.80	0.43
1:B:184:SER:OG	1:B:185:ILE:N	2.51	0.43
1:B:44:ARG:HB3	1:B:44:ARG:HH11	1.82	0.43
1:B:68:ILE:HD12	1:B:450:LEU:HD13	1.99	0.43
1:A:67:GLY:HA3	1:A:236:LEU:HD13	2.00	0.43
1:B:193:ALA:O	1:B:196:ASP:HB2	2.18	0.43
1:B:390:ASP:OD1	1:B:394:LYS:HE2	2.18	0.43
1:B:412:LYS:HA	3:B:715:HOH:O	2.19	0.43
1:B:523:GLN:HA	1:B:523:GLN:HE21	1.83	0.43
1:B:398:HIS:HD2	1:B:399:CYS:H	1.67	0.43
1:B:476:ASN:O	1:B:478:TYR:N	2.51	0.43
1:A:426:GLY:HA3	1:B:440:LEU:CD1	2.48	0.42
1:A:88:ASN:HD21	1:A:104:ASN:HA	1.82	0.42
1:B:21:TYR:CD1	1:B:21:TYR:N	2.86	0.42
1:B:52:GLN:HE21	1:B:53:ASP:N	2.17	0.42
1:A:282:ALA:CB	1:A:305:LEU:HD21	2.49	0.42
1:A:436:CYS:HB3	1:B:428:ASN:ND2	2.34	0.42
1:B:261:MET:HE1	1:B:311:HIS:HB2	2.01	0.42
1:B:354:ASN:O	1:B:404:TYR:HE2	2.01	0.42
1:A:187:TYR:HB2	1:A:190:PHE:HD1	1.85	0.42
1:A:516:LEU:HD12	1:A:517:LEU:N	2.34	0.42
1:B:161:SER:HB3	1:B:163:VAL:HG23	2.01	0.42
1:B:286:ILE:HG21	1:B:308:LEU:HG	1.99	0.42
1:A:150:ASN:HA	1:A:200:ASN:ND2	2.35	0.42
1:A:246:ASN:HB2	3:A:723:HOH:O	2.20	0.42
1:A:373:LYS:HA	1:A:489:LYS:HD3	2.01	0.42
1:A:167:ASP:O	1:A:171:ARG:HG3	2.20	0.42
1:A:309:ALA:O	1:A:313:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PHE:HE2	1:B:251:VAL:HG12	1.84	0.42
1:B:354:ASN:OD1	1:B:356:ASP:HB3	2.20	0.42
1:A:150:ASN:HD22	1:A:152:ALA:H	1.66	0.42
1:A:337:VAL:HG21	1:A:380:ILE:HG22	2.02	0.42
1:B:187:TYR:OH	1:B:219:HIS:HD2	2.02	0.42
1:B:319:ASP:HB3	1:B:490:ALA:HB3	2.01	0.42
1:B:381:ILE:HG13	1:B:388:TYR:CD2	2.55	0.42
1:A:71:ILE:HG21	1:A:243:TRP:CZ3	2.54	0.42
1:B:353:GLY:CA	1:B:406:LYS:HA	2.49	0.42
1:A:11:SER:OG	1:B:44:ARG:HG2	2.20	0.42
1:B:483:PHE:HB3	1:B:510:LEU:HD21	2.01	0.42
1:A:352:LEU:N	1:A:352:LEU:CD2	2.83	0.42
1:B:302:VAL:HB	1:B:303:PRO:HD2	2.02	0.41
1:A:200:ASN:H	1:A:200:ASN:ND2	2.18	0.41
1:B:254:SER:HA	1:B:255:PRO:HD3	1.96	0.41
1:B:272:HIS:HE1	1:B:274:GLU:HG3	1.85	0.41
1:B:378:ASP:O	1:B:382:ALA:HB2	2.20	0.41
1:A:426:GLY:HA3	1:B:440:LEU:HD13	2.01	0.41
1:A:184:SER:O	1:A:202:CYS:HA	2.21	0.41
1:A:246:ASN:HD22	1:A:246:ASN:N	2.19	0.41
1:B:327:LYS:HG2	1:B:503:LEU:CD2	2.49	0.41
1:A:441:LEU:HA	1:A:441:LEU:HD23	1.92	0.41
1:B:134:LEU:HD11	1:B:517:LEU:HB3	2.03	0.41
1:B:352:LEU:HD23	1:B:352:LEU:H	1.86	0.41
1:A:452:MET:HG3	1:A:487:TRP:HH2	1.86	0.41
1:A:467:VAL:O	1:A:467:VAL:HG23	2.21	0.41
1:B:23:ASP:O	1:B:24:ASN:HB2	2.21	0.41
1:A:310:GLU:HA	1:A:479:PRO:HG2	2.01	0.41
1:B:40:THR:HG21	1:B:44:ARG:NH1	2.36	0.41
1:B:189:ASP:OD1	1:B:249:ARG:NH2	2.54	0.40
1:B:265:LEU:HD11	1:B:308:LEU:HD13	2.03	0.40
1:B:147:TRP:CD2	1:B:281:PHE:HE2	2.40	0.40
1:B:59:ASP:O	1:B:458:ARG:HD2	2.21	0.40
1:A:166:TYR:O	1:A:170:GLN:HG2	2.21	0.40
1:A:480:VAL:HG13	1:A:492:LEU:HD23	2.03	0.40
1:B:201:ASN:HD22	1:B:201:ASN:HA	1.73	0.40
1:B:208:LYS:HB2	1:B:210:ASN:HD22	1.86	0.40
1:B:369:LYS:O	1:B:371:ILE:N	2.54	0.40
1:B:350:ASN:HB2	1:B:402:ILE:HD13	2.03	0.40
1:A:37:VAL:HG22	1:A:47:VAL:HG22	2.04	0.40
1:B:351:HIS:HA	1:B:403:LYS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LEU:CD2	1:B:445:LEU:C	2.90	0.40
2:B:660:NAI:N7N	2:B:660:NAI:O1N	2.54	0.40
1:A:327:LYS:HG2	1:A:503:LEU:HD22	2.03	0.40
1:B:194:ASN:ND2	1:B:195:GLN:HG2	2.36	0.40
1:B:515:ARG:NH2	1:B:521:PRO:O	2.52	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	523/533 (98%)	489 (94%)	27 (5%)	7 (1%)	14	8
1	B	506/533 (95%)	473 (94%)	25 (5%)	8 (2%)	11	5
All	All	1029/1066 (96%)	962 (94%)	52 (5%)	15 (2%)	12	6

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	ASP
1	B	319	ASP
1	A	375	SER
1	A	472	GLY
1	B	322	LYS
1	B	370	GLU
1	B	478	TYR
1	A	468	LYS
1	A	207	GLU
1	B	477	PHE
1	B	479	PRO
1	A	320	ASP
1	A	470	ASP

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Mol	Chain	Res	Type
1	B	320	ASP
1	B	502	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	464/471 (98%)	452 (97%)	12 (3%)	51	55
1	B	453/471 (96%)	433 (96%)	20 (4%)	33	31
All	All	917/942 (97%)	885 (96%)	32 (4%)	41	42

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	122	GLU
1	A	188	PRO
1	A	197	GLU
1	A	200	ASN
1	A	208	LYS
1	A	246	ASN
1	A	258	ASN
1	A	298	GLN
1	A	352	LEU
1	A	473	LYS
1	A	483	PHE
1	B	13	LYS
1	B	16	THR
1	B	34	ASN
1	B	44	ARG
1	B	52	GLN
1	B	53	ASP
1	B	95	GLN
1	B	113	SER
1	B	158	MET

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Mol	Chain	Res	Type
1	B	194	ASN
1	B	201	ASN
1	B	249	ARG
1	B	258	ASN
1	B	299	ASN
1	B	319	ASP
1	B	352	LEU
1	B	438	ASP
1	B	460	SER
1	B	479	PRO
1	B	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	77	ASN
1	A	88	ASN
1	A	90	HIS
1	A	104	ASN
1	A	111	GLN
1	A	150	ASN
1	A	151	ASN
1	A	169	GLN
1	A	200	ASN
1	A	201	ASN
1	A	221	GLN
1	A	228	GLN
1	A	229	ASN
1	A	258	ASN
1	A	266	GLN
1	A	270	ASN
1	A	272	HIS
1	A	294	ASN
1	A	298	GLN
1	A	325	GLN
1	A	350	ASN
1	A	365	GLN
1	A	501	ASN
1	A	504	ASN
1	A	512	ASN
1	A	523	GLN

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Mol	Chain	Res	Type
1	B	34	ASN
1	B	52	GLN
1	B	91	ASN
1	B	95	GLN
1	B	124	ASN
1	B	140	ASN
1	B	159	GLN
1	B	194	ASN
1	B	195	GLN
1	B	201	ASN
1	B	210	ASN
1	B	219	HIS
1	B	228	GLN
1	B	258	ASN
1	B	263	ASN
1	B	266	GLN
1	B	270	ASN
1	B	299	ASN
1	B	334	GLN
1	B	351	HIS
1	B	355	ASN
1	B	427	HIS
1	B	428	ASN
1	B	498	HIS
1	B	504	ASN
1	B	506	GLN
1	B	523	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	NAI	A	650	-	40,48,48	1.39	3 (7%)	41,73,73	1.08	3 (7%)
2	NAI	B	660	-	40,48,48	1.39	5 (12%)	41,73,73	1.20	2 (4%)

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	NAI	A	650	-	-	0/25/72/72	0/5/5/5
2	NAI	B	660	-	-	0/25/72/72	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	NAI	C4A-N3A	2.01	1.38	1.35
2	B	660	NAI	C1D-N1N	2.33	1.53	1.46
2	B	660	NAI	C6N-N1N	3.37	1.46	1.37
2	A	650	NAI	C6N-N1N	3.64	1.47	1.37
2	B	660	NAI	C6N-C5N	3.74	1.40	1.33
2	A	650	NAI	C2A-N1A	4.00	1.41	1.33
2	B	660	NAI	C2A-N1A	4.09	1.41	1.33
2	A	650	NAI	C6N-C5N	4.41	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	650	NAI	C1D-N1N-C2N	-2.46	116.91	121.09
2	A	650	NAI	O4D-C4D-C3D	2.37	109.87	105.17
2	A	650	NAI	C4A-C5A-N7A	2.45	111.78	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	660	NAI	C4A-C5A-N7A	3.00	112.31	109.41
2	B	660	NAI	O4D-C1D-N1N	3.19	114.49	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	650	NAI	1	0
2	B	660	NAI	4	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	525/533 (98%)	0.45	42 (8%) 13 17	20, 39, 68, 70	0
1	B	512/533 (96%)	0.71	70 (13%) 3 4	20, 40, 70, 70	0
All	All	1037/1066 (97%)	0.58	112 (10%) 6 8	20, 40, 70, 70	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	PHE	10.2
1	A	41	ALA	6.6
1	B	371	ILE	6.6
1	A	533	LEU	6.2
1	B	41	ALA	5.7
1	B	477	PHE	5.6
1	B	500	VAL	5.6
1	A	9	ILE	5.3
1	B	358	TYR	5.2
1	B	366	PHE	5.2
1	B	360	LEU	5.2
1	A	209	GLY	5.1
1	B	361	SER	5.0
1	B	362	ALA	5.0
1	B	484	LEU	4.8
1	B	478	TYR	4.8
1	A	121	ALA	4.8
1	B	363	PRO	4.7
1	B	498	HIS	4.7
1	B	495	PRO	4.7
1	B	496	GLY	4.5
1	A	208	LYS	4.4
1	A	40	THR	4.4
1	B	194	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	499	PRO	4.2
1	B	370	GLU	4.1
1	A	371	ILE	4.0
1	B	479	PRO	3.9
1	B	494	ARG	3.8
1	A	207	GLU	3.8
1	B	321	LEU	3.8
1	B	376	VAL	3.8
1	A	193	ALA	3.8
1	B	207	GLU	3.7
1	B	487	TRP	3.7
1	B	40	THR	3.6
1	B	43	GLY	3.6
1	B	392	LEU	3.6
1	B	22	LYS	3.5
1	B	42	SER	3.5
1	B	488	LEU	3.4
1	B	398	HIS	3.4
1	A	42	SER	3.4
1	B	315	PHE	3.4
1	A	362	ALA	3.3
1	B	390	ASP	3.2
1	B	364	LYS	3.2
1	B	404	TYR	3.2
1	B	23	ASP	3.2
1	B	394	LYS	3.1
1	A	321	LEU	3.1
1	B	208	LYS	3.0
1	A	363	PRO	3.0
1	B	473	LYS	3.0
1	B	481	LEU	3.0
1	B	122	GLU	3.0
1	B	486	TYR	3.0
1	A	374	SER	3.0
1	B	381	ILE	3.0
1	B	369	LYS	2.8
1	A	486	TYR	2.8
1	B	493	THR	2.8
1	B	21	TYR	2.7
1	B	483	PHE	2.7
1	B	254	SER	2.7
1	A	318	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	379	ASP	2.7
1	B	319	ASP	2.7
1	B	533	LEU	2.7
1	B	408	VAL	2.6
1	A	43	GLY	2.6
1	B	367	ARG	2.6
1	B	255	PRO	2.6
1	A	323	SER	2.6
1	A	496	GLY	2.5
1	A	394	LYS	2.5
1	B	393	GLY	2.5
1	B	378	ASP	2.5
1	A	255	PRO	2.5
1	A	358	TYR	2.5
1	A	44	ARG	2.5
1	A	378	ASP	2.5
1	B	243	TRP	2.5
1	A	390	ASP	2.5
1	B	253	VAL	2.4
1	A	375	SER	2.4
1	B	242	LEU	2.4
1	B	318	GLY	2.4
1	B	395	LYS	2.4
1	B	24	ASN	2.4
1	A	210	ASN	2.3
1	A	324	GLY	2.3
1	A	361	SER	2.3
1	B	490	ALA	2.3
1	A	472	GLY	2.2
1	A	381	ILE	2.2
1	B	482	THR	2.2
1	A	242	LEU	2.2
1	B	256	GLY	2.2
1	B	252	GLU	2.2
1	A	449	LEU	2.1
1	A	364	LYS	2.1
1	A	446	ILE	2.1
1	A	445	LEU	2.1
1	A	441	LEU	2.1
1	B	15	VAL	2.1
1	B	399	CYS	2.1
1	A	377	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	197	GLU	2.0
1	A	214	ARG	2.0
1	B	396	VAL	2.0
1	B	209	GLY	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( $\text{\AA}^2$ )	Q<0.9
2	NAI	A	650	44/44	0.94	0.16	0.12	25,35,68,73	0
2	NAI	B	660	44/44	0.95	0.17	-0.12	25,34,75,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.