Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:16 AM EDT

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*
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:

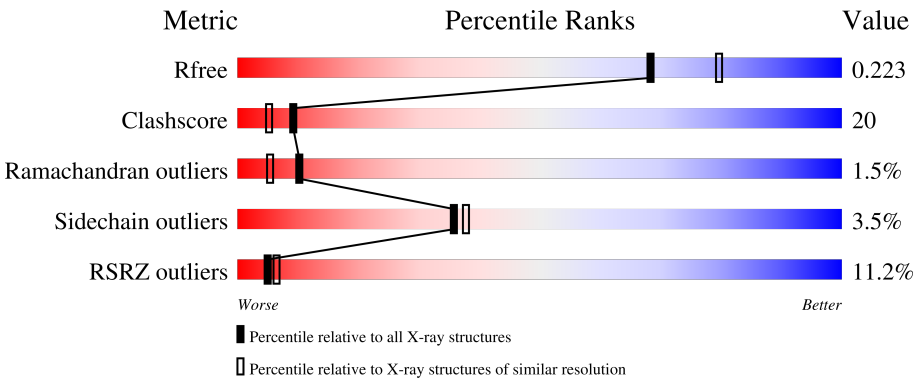
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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% 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	8%, 65%, 32%, • •
1	B	533	14%, 60%, 32%, • •

2 Entry composition (i)

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.

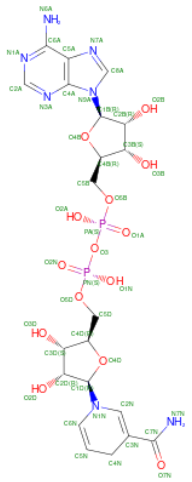
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	525	4138	2632	695	795	16	0	0	0
1	B	512	4046	2577	680	773	16	0	0	0

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: $C_{21}H_{29}N_7O_{14}P_2$).

NAI



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

- Molecule 3 is water.

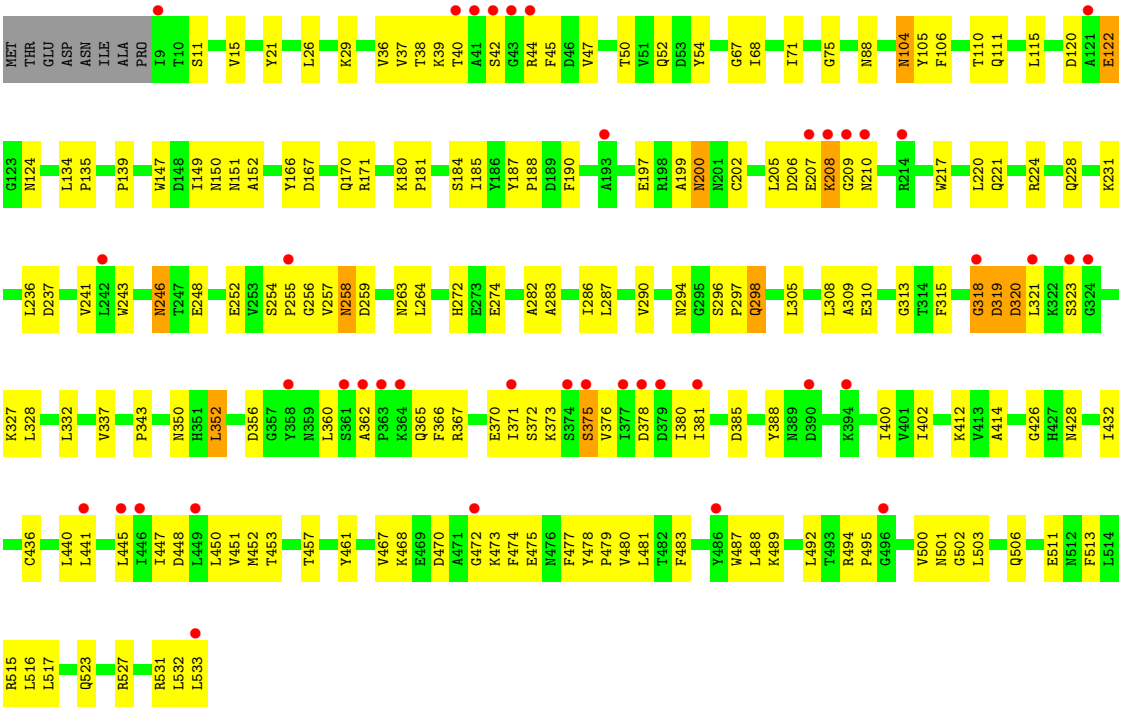
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	99	99	99	0	0
			Total	O		
3	B	79	79	79	0	0

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 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.

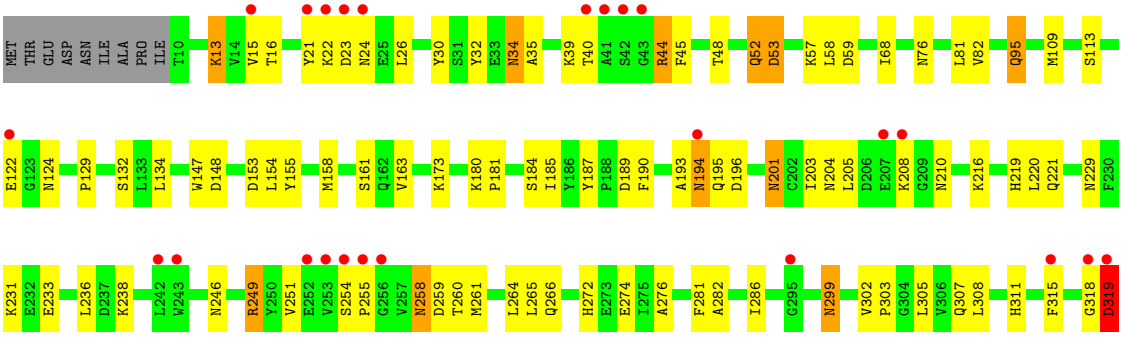
• Molecule 1: Inositol-3-phosphate synthase

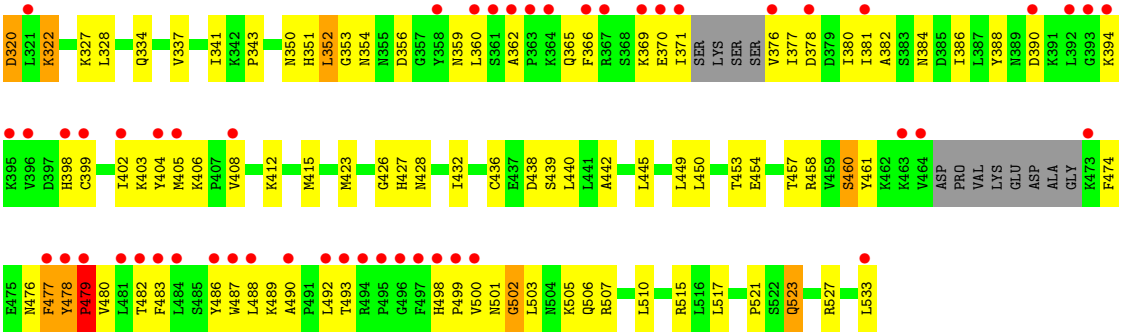
Chain A:



• Molecule 1: Inositol-3-phosphate synthase

Chain B:




D320
L321
K322
K327
L328
Q334
V337
I341
K342
P343
N350
H351
L352
G353
N354
N355
D356
G357
Y358
N359
L360
S361
A362
P363
K364
Q365
F366
R367
S368
K369
E370
I371
SER
LYS
SER
SER
V376
I377
D378
D379
I380
I381
A382
S383
N384
D385
I386
L387
Y388
N389
D390
K391
L392
G393
K394
K396
V396
D397
H398
C399
I402
K403
Y404
M405
K406
P407
V408
K412
M415
M423
G426
H427
N428
I432
C436
E437
D438
S439
L440
L441
A442
L445
L449
L450
T453
E454
T457
R458
V459
S460
Y461
K462
K463
V464
ASP
PRO
VAL
LYS
GLU
ASP
ALA
GLY
K473
F474
E475
N476
F477
Y478
P479
V480
L481
T482
F483
L484
S485
Y486
W487
L488
K489
A490
P491
L492
T493
R494
P495
G496
F497
H498
P499
V500
N501
G502
L503
N504
K505
Q506
R507
L510
R515
L516
L517
P521
S522
Q523
R527
L533

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.34 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.261 0.232 , 0.223	Depositor DCC
R_{free} test set	4136 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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:HG23	1:B:15:VAL:O	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:HD23	1:B:445:LEU:O	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:95:GLN:HE21	1:B:95:GLN:HA	1.65	0.62
1:B:442:ALA:HB2	2:B:660:NAI:H42N	1.82	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:HD23	1:A:352:LEU:H	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:N	1:B:498:HIS:CD2	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:N	1:B:352:LEU:HD23	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:95:GLN:HE21	1:B:95:GLN:CA	2.18	0.54
1:B:122:GLU:HB2	1:B:124:ASN:ND2	2.22	0.54
1:A:258:ASN:HD22	1:A:258:ASN:H	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:68:ILE:HD12	1:A:450:LEU:HD13	1.90	0.54
1:A:208:LYS:H	1:A:208:LYS:HD3	1.73	0.54
1:A:258:ASN:H	1:A:258:ASN:ND2	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:82:VAL:HG21	1:B:154:LEU:CD1	2.39	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:381:ILE:HD11	1:B:394:LYS:O	2.09	0.53
1:B:15:VAL:O	1:B:15:VAL:CG2	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:57:LYS:HE3	1:B:474:PHE:CD2	2.45	0.51
1:B:299:ASN:HD22	1:B:299:ASN:H	1.57	0.51
1:B:109:MET:HE2	1:B:507:ARG:HE	1.75	0.51
1:A:352:LEU:HD23	1:A:352:LEU:N	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:52:GLN:NE2	1:B:53:ASP:N	2.58	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: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:O	1:A:15:VAL:HG13	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:76:ASN:HB3	1:B:439:SER:OG	2.10	0.50
1:B:258:ASN:N	1:B:258:ASN:ND2	2.59	0.50
1:A:52:GLN:HG3	1:A:54:TYR:CE1	2.47	0.50
1:A:294:ASN:ND2	1:A:296:SER:H	2.10	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:40:THR:HG22	1:A:42:SER:N	2.27	0.49
1:A:272:HIS:CD2	1:A:274:GLU:H	2.30	0.49
1:A:531:ARG:CG	1:B:482:THR:HB	2.42	0.49
1:B:205:LEU:HA	1:B:210:ASN:O	2.11	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:C	1:A:200:ASN:HD22	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:81:LEU:C	1:B:81:LEU:HD13	2.34	0.48
1:B:486:TYR:HB2	1:B:506:GLN:HB3	1.95	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:HG3	1:B:249:ARG:O	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:HD22	1:A:200:ASN:H	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:O	1:A:370:GLU:HG2	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:NE2	1:B:266:GLN:HA	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:ND2	1:A:104:ASN:C	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:52:GLN:NE2	1:B:53:ASP:O	2.49	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: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:HE3	1:A:489:LYS:HB2	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:445:LEU:CD2	1:A:487:TRP:HB3	2.44	0.45
1:A:475:GLU:HB3	1:B:533:LEU:HD12	1.98	0.45
1:A:298:GLN:HE21	1:A:298:GLN:HB3	1.62	0.45
1:B:194:ASN:HD22	1:B:194:ASN:C	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:241:VAL:HG23	1:A:290:VAL:HG11	1.98	0.44
1:A:252:GLU:N	1:A:274:GLU:OE1	2.50	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:O5D	2:B:660:NAI:H2N	2.18	0.44
1:A:452:MET:HG3	1:A:487:TRP:CH2	2.53	0.44
1:B:109:MET:HE1	1:B:507:ARG:HD2	1.99	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:A:533:LEU:N	1:B:461:TYR:OH	2.51	0.43
1:A:263:ASN:N	1:A:263:ASN:HD22	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:71:ILE:HG21	1:A:243:TRP:CE3	2.54	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:B:492:LEU:HD13	1:B:493:THR:H	1.80	0.43
1:B:44:ARG:HH11	1:B:44:ARG:HB3	1.82	0.43
1:B:68:ILE:HD12	1:B:450:LEU:HD13	1.99	0.43
1:B:184:SER:OG	1:B:185:ILE:N	2.51	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:88:ASN:HD21	1:A:104:ASN:HA	1.82	0.42
1:A:426:GLY:HA3	1:B:440:LEU:CD1	2.48	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:11:SER:OG	1:B:44:ARG:HG2	2.20	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: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:A:426:GLY:HA3	1:B:440:LEU:HD13	2.01	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:184:SER:O	1:A:202:CYS:HA	2.21	0.41
1:A:246:ASN:N	1:A:246:ASN:HD22	2.19	0.41
1:B:327:LYS:HG2	1:B:503:LEU:CD2	2.49	0.41
1:A:441:LEU:HD23	1:A:441:LEU:HA	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:HG23	1:A:467:VAL:O	2.21	0.41
1:A:310:GLU:HA	1:A:479:PRO:HG2	2.01	0.41
1:B:23:ASP:O	1:B:24:ASN:HB2	2.21	0.41
1:B:40:THR:HG21	1:B:44:ARG:NH1	2.36	0.41
1:B:59:ASP:O	1:B:458:ARG:HD2	2.21	0.40
1:B:147:TRP:CD2	1:B:281:PHE:HE2	2.40	0.40
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: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:350:ASN:HB2	1:B:402:ILE:HD13	2.03	0.40
1:B:369:LYS:O	1:B:371:ILE:N	2.54	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:O1N	2:B:660:NAI:N7N	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%)	12 7
1	B	506/533 (95%)	473 (94%)	25 (5%)	8 (2%)	9 5
All	All	1029/1066 (96%)	962 (94%)	52 (5%)	15 (2%)	10 5

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 (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	464/471 (98%)	452 (97%)	12 (3%)	46	50
1	B	453/471 (96%)	433 (96%)	20 (4%)	28	28
All	All	917/942 (97%)	885 (96%)	32 (4%)	36	38

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

Sometimes 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 (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)

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	B	660	-	43,48,48	1.57	7 (16%)	50,73,73	1.26	5 (10%)
2	NAI	A	650	-	43,48,48	1.43	5 (11%)	50,73,73	1.17	6 (12%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	NAI	PA-O3	-4.72	1.54	1.59
2	B	660	NAI	C2A-N1A	4.31	1.41	1.33
2	A	650	NAI	C6N-N1N	4.24	1.47	1.37
2	A	650	NAI	C2A-N1A	4.21	1.41	1.33
2	B	660	NAI	C6N-N1N	3.93	1.46	1.37
2	A	650	NAI	PN-O3	2.90	1.62	1.59
2	A	650	NAI	C6N-C5N	2.73	1.41	1.33
2	B	660	NAI	C1D-N1N	2.48	1.53	1.46
2	B	660	NAI	C7N-C3N	2.36	1.53	1.48
2	B	660	NAI	C6N-C5N	2.33	1.40	1.33
2	A	650	NAI	C7N-C3N	2.21	1.53	1.48
2	B	660	NAI	C4A-N3A	2.13	1.38	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	660	NAI	O4D-C1D-N1N	3.36	114.49	108.08
2	B	660	NAI	C4A-C5A-N7A	2.81	112.31	109.34
2	A	650	NAI	C1D-N1N-C2N	-2.56	116.91	121.14
2	A	650	NAI	O4D-C4D-C3D	2.38	109.87	105.15
2	B	660	NAI	O2A-PA-O3	2.36	113.66	107.27
2	A	650	NAI	C3N-C7N-N7N	2.32	121.79	117.67
2	A	650	NAI	C4A-C5A-N7A	2.31	111.78	109.34
2	A	650	NAI	C5A-C6A-N6A	2.25	123.74	120.31
2	B	660	NAI	O4B-C1B-N9A	-2.18	105.85	108.75
2	A	650	NAI	O2A-PA-O3	2.08	112.90	107.27
2	B	660	NAI	O5D-PN-O2N	2.02	116.93	108.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	660	NAI	O4D-C1D-N1N-C6N
2	A	650	NAI	O4D-C1D-N1N-C6N
2	B	660	NAI	PN-O3-PA-O5B
2	A	650	NAI	C2N-C3N-C7N-N7N

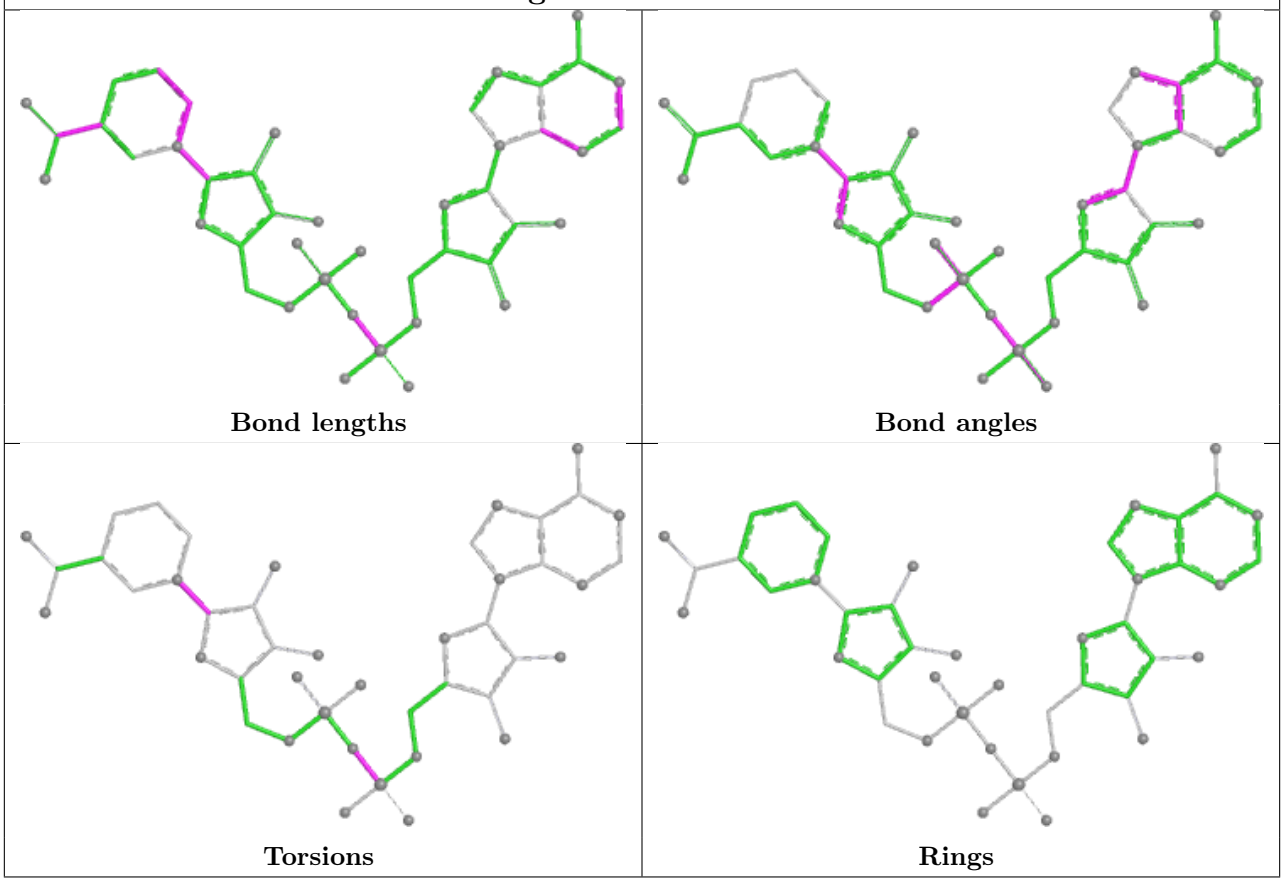
There are no ring outliers.

2 monomers are involved in 5 short contacts:

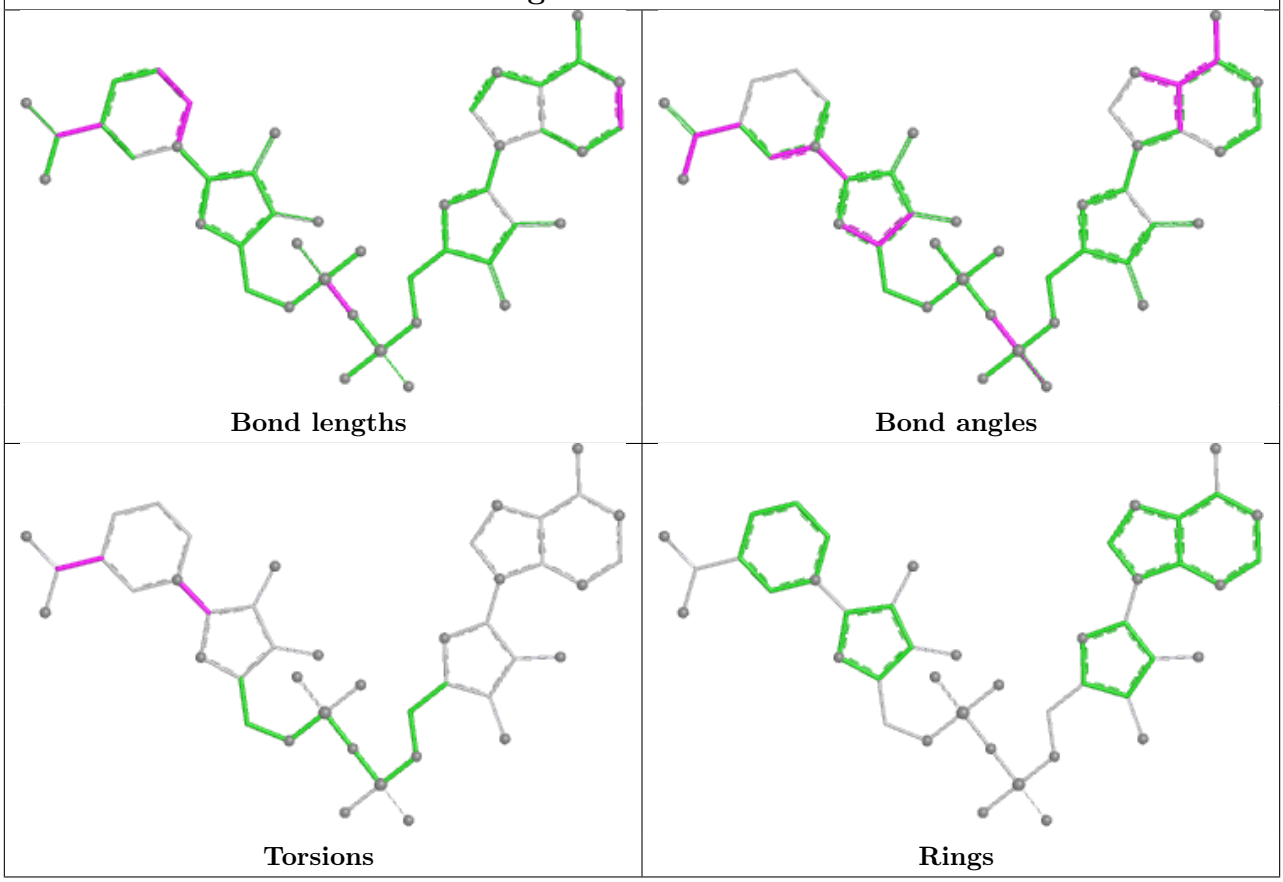
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	660	NAI	4	0
2	A	650	NAI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAI B 660



Ligand NAI A 650



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)

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, 95th 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^2)	Q<0.9
1	A	525/533 (98%)	0.46	41 (7%) 13 17	20, 39, 68, 70	0
1	B	512/533 (96%)	0.72	75 (14%) 2 3	20, 40, 70, 70	0
All	All	1037/1066 (97%)	0.59	116 (11%) 5 6	20, 40, 70, 70	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	PHE	10.2
1	A	41	ALA	6.7
1	B	371	ILE	6.5
1	A	533	LEU	6.2
1	B	477	PHE	5.8
1	B	41	ALA	5.8
1	B	500	VAL	5.6
1	A	9	ILE	5.4
1	B	362	ALA	5.4
1	B	360	LEU	5.4
1	B	361	SER	5.3
1	B	363	PRO	5.1
1	B	358	TYR	5.1
1	B	366	PHE	5.0
1	B	484	LEU	5.0
1	A	121	ALA	5.0
1	A	209	GLY	4.9
1	B	478	TYR	4.9
1	B	498	HIS	4.7
1	B	495	PRO	4.7
1	B	496	GLY	4.6
1	A	40	THR	4.5
1	A	208	LYS	4.5
1	B	499	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	ASN	4.2
1	A	371	ILE	4.1
1	B	479	PRO	4.1
1	B	370	GLU	4.0
1	A	207	GLU	3.9
1	B	494	ARG	3.9
1	B	321	LEU	3.7
1	B	207	GLU	3.6
1	B	42	SER	3.6
1	B	398	HIS	3.6
1	B	40	THR	3.6
1	B	43	GLY	3.6
1	A	193	ALA	3.5
1	B	487	TRP	3.5
1	B	315	PHE	3.5
1	B	22	LYS	3.5
1	B	376	VAL	3.5
1	A	42	SER	3.5
1	B	390	ASP	3.4
1	B	392	LEU	3.4
1	B	488	LEU	3.4
1	B	364	LYS	3.2
1	A	362	ALA	3.2
1	B	23	ASP	3.1
1	B	486	TYR	3.1
1	B	404	TYR	3.1
1	B	122	GLU	3.1
1	B	208	LYS	3.0
1	A	363	PRO	3.0
1	A	321	LEU	3.0
1	B	394	LYS	3.0
1	B	473	LYS	3.0
1	B	381	ILE	3.0
1	A	374	SER	2.9
1	B	493	THR	2.9
1	B	481	LEU	2.9
1	A	486	TYR	2.8
1	B	255	PRO	2.8
1	A	318	GLY	2.8
1	B	533	LEU	2.7
1	B	254	SER	2.7
1	B	319	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	483	PHE	2.7
1	B	490	ALA	2.7
1	B	367	ARG	2.7
1	B	21	TYR	2.6
1	A	43	GLY	2.6
1	B	378	ASP	2.6
1	A	379	ASP	2.6
1	A	358	TYR	2.6
1	A	323	SER	2.6
1	A	390	ASP	2.6
1	B	253	VAL	2.6
1	B	369	LYS	2.5
1	A	375	SER	2.5
1	A	378	ASP	2.5
1	B	408	VAL	2.5
1	A	394	LYS	2.5
1	B	393	GLY	2.5
1	A	361	SER	2.5
1	A	44	ARG	2.5
1	B	318	GLY	2.5
1	B	482	THR	2.5
1	A	496	GLY	2.5
1	B	243	TRP	2.4
1	A	255	PRO	2.4
1	B	242	LEU	2.4
1	B	24	ASN	2.4
1	A	324	GLY	2.4
1	B	395	LYS	2.3
1	A	210	ASN	2.3
1	A	472	GLY	2.3
1	B	402	ILE	2.3
1	A	449	LEU	2.2
1	A	381	ILE	2.2
1	A	242	LEU	2.2
1	B	256	GLY	2.2
1	B	396	VAL	2.2
1	A	441	LEU	2.2
1	B	399	CYS	2.2
1	B	15	VAL	2.1
1	B	252	GLU	2.1
1	A	377	ILE	2.1
1	A	364	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	445	LEU	2.1
1	A	214	ARG	2.1
1	A	446	ILE	2.1
1	B	405	MET	2.0
1	B	464	VAL	2.0
1	B	492	LEU	2.0
1	B	295	GLY	2.0
1	B	463	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

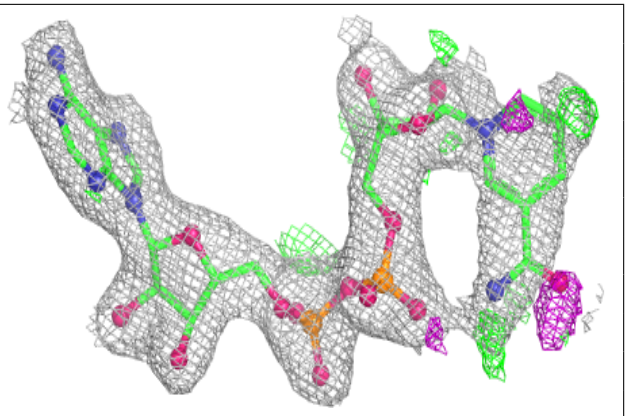
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

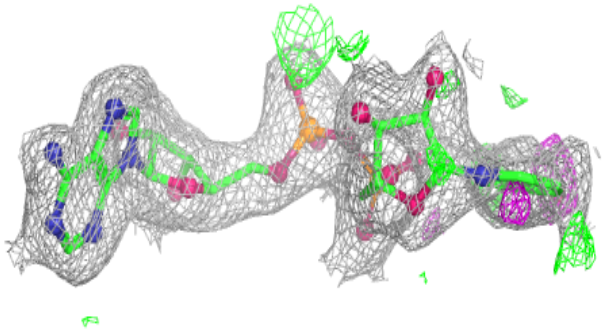
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAI	A	650	44/44	0.94	0.16	25,35,68,73	0
2	NAI	B	660	44/44	0.95	0.17	25,34,75,77	0

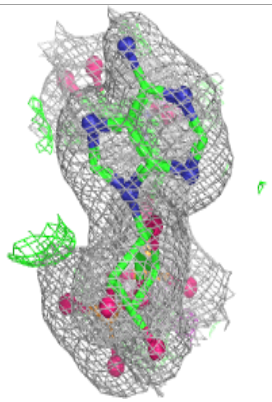
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAI A 650:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

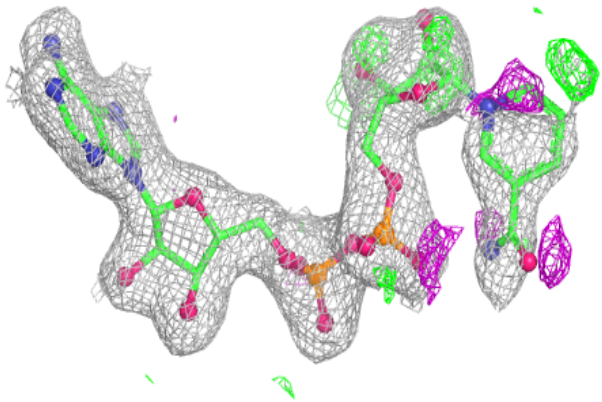


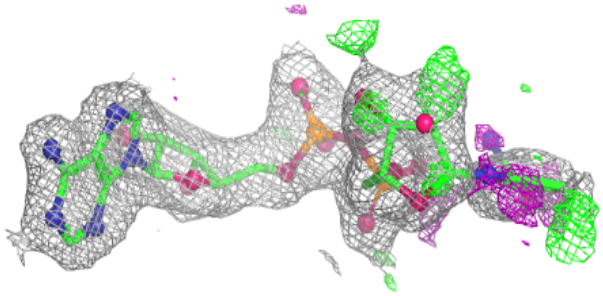


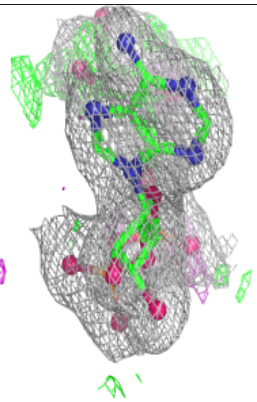


Electron density around NAI B 660:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.