



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:22 pm GMT

PDB ID : 1RM0
Title : Crystal Structure of Myo-Inositol 1-Phosphate Synthase From *Saccharomyces cerevisiae* In Complex With NAD⁺ and 2-deoxy-D-glucitol 6-(E)-vinylhomophosphate
Authors : Jin, X.; Foley, K.M.; Geiger, J.H.
Deposited on : 2003-11-26
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

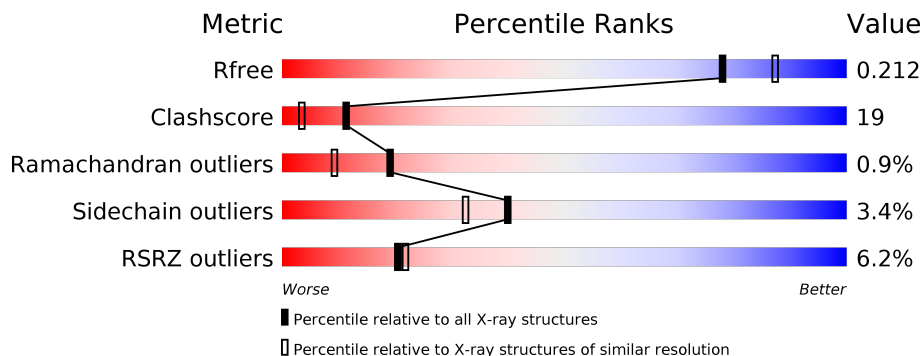
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	111664	1449 (2.04-2.04)
Clashscore	122126	1524 (2.04-2.04)
Ramachandran outliers	120053	1512 (2.04-2.04)
Sidechain outliers	120020	1512 (2.04-2.04)
RSRZ outliers	108989	1429 (2.04-2.04)

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 ≥ 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>4%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	B	533	<div> <div>8%</div> <div>61%</div> <div>33%</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
4	NAI	B	660	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8687 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.

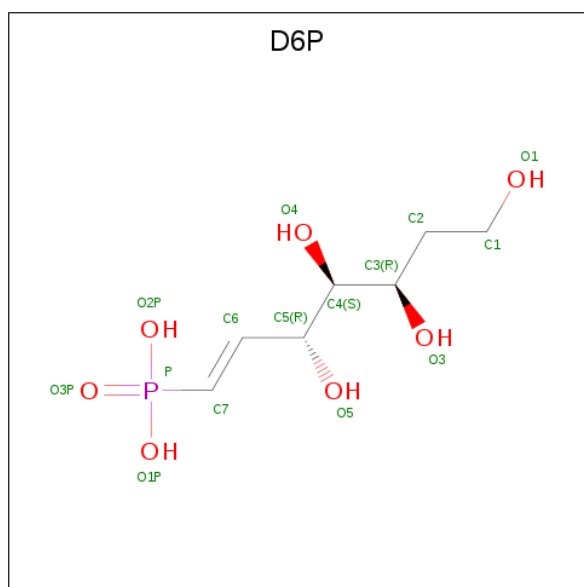
- Molecule 1 is a protein called myo-inositol-phosphate synthase.

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	516	Total	C	N	O	S	0	0	0
			4073	2592	685	780	16			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

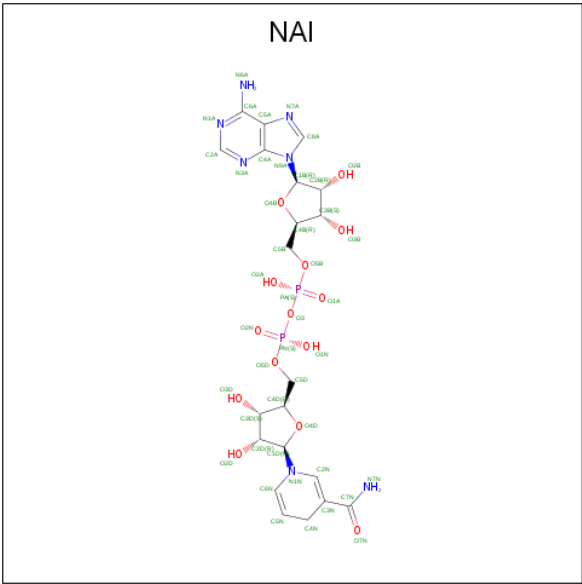
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is (3,4,5,7-TETRAHYDROXY-HEPT-1-ENYL)-PHOSPHONIC ACID (three-letter code: D6P) (formula: C₇H₁₅O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			15	7	7	1		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

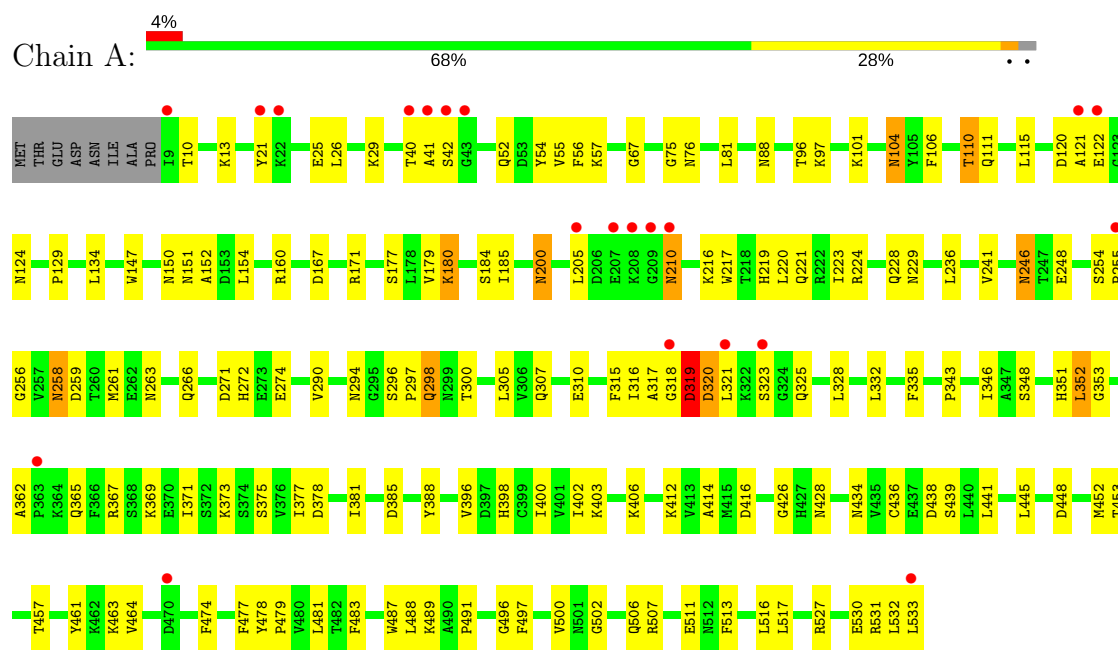
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	0
			197	197		
5	B	175	Total	O	0	0
			175	175		

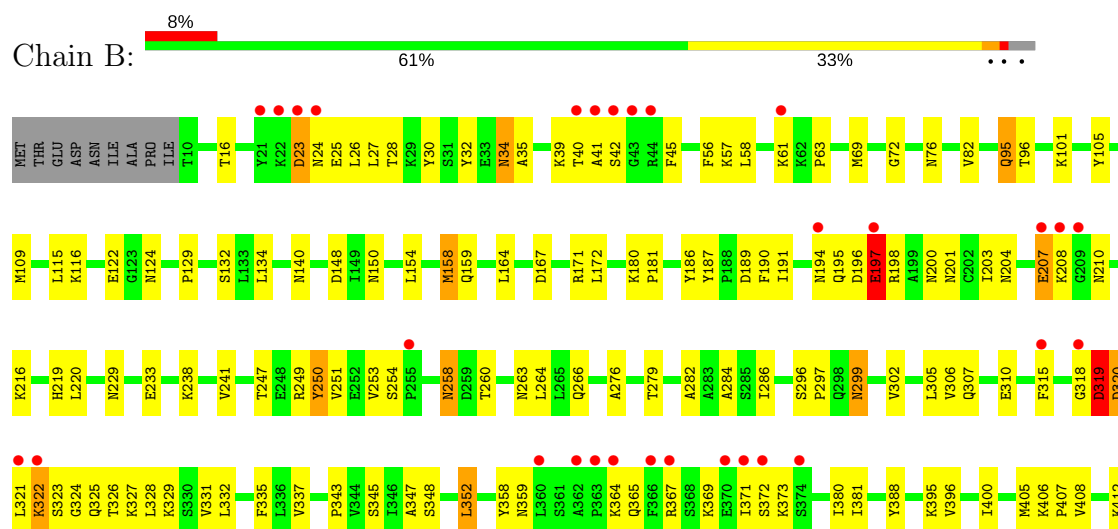
3 Residue-property plots

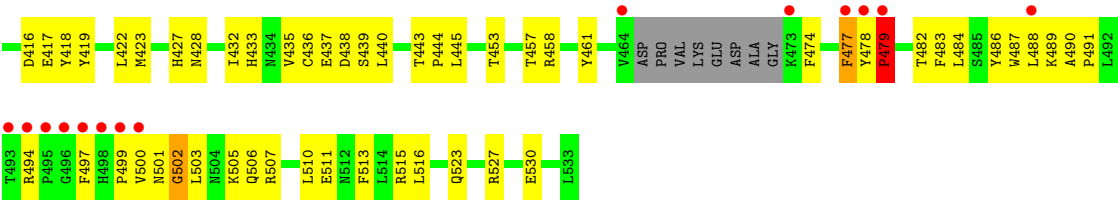
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: myo-inositol-phosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.81Å 97.78Å 122.29Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	35.00 – 2.05 35.83 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.05) 97.9 (35.83-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.244 0.212 , 0.212	Depositor DCC
R_{free} test set	5539 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8687	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, D6P, MN

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	0.35	0/4219	0.62	0/5719
1	B	0.35	0/4152	0.60	0/5626
All	All	0.35	0/8371	0.61	0/11345

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	4138	0	4147	147	0
1	B	4073	0	4084	184	0
2	A	1	0	0	0	0
3	A	15	0	13	4	0
4	A	44	0	26	5	0
4	B	44	0	27	4	0
5	A	197	0	0	5	0
5	B	175	0	0	9	0
All	All	8687	0	8297	315	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 19.

All (315) 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:115:LEU:HD22	1:B:511:GLU:HG3	1.48	0.96
1:B:322:LYS:HA	1:B:489:LYS:HG3	1.47	0.95
1:B:323:SER:HB2	5:B:760:HOH:O	1.75	0.85
1:A:104:ASN:HD22	1:A:106:PHE:H	1.29	0.81
1:A:110:THR:HB	1:A:448:ASP:OD1	1.80	0.81
1:B:373:LYS:HG2	1:B:489:LYS:HD2	1.61	0.80
1:A:150:ASN:ND2	1:A:160:ARG:HH12	1.81	0.79
1:A:110:THR:CG2	1:A:111:GLN:HE21	1.96	0.77
1:B:25:GLU:OE1	1:B:57:LYS:HD3	1.84	0.77
1:A:104:ASN:ND2	1:A:106:PHE:H	1.82	0.77
1:B:158:MET:HE2	1:B:164:LEU:HD12	1.65	0.77
1:B:395:LYS:HD3	1:B:396:VAL:H	1.49	0.77
1:B:310:GLU:HG2	1:B:479:PRO:HG2	1.67	0.76
1:A:373:LYS:HG2	1:A:489:LYS:HE2	1.68	0.76
1:B:109:MET:HE2	1:B:507:ARG:HE	1.51	0.75
1:A:151:ASN:H	1:A:200:ASN:HD21	1.35	0.72
1:B:395:LYS:HD3	1:B:396:VAL:N	2.04	0.72
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.25	0.72
1:A:104:ASN:HD21	1:B:423:MET:HA	1.54	0.72
1:A:272:HIS:CD2	1:A:274:GLU:H	2.08	0.71
1:B:445:LEU:HD21	1:B:487:TRP:HB3	1.73	0.70
1:B:251:VAL:H	1:B:299:ASN:HD21	1.39	0.69
1:B:249:ARG:O	1:B:249:ARG:HD2	1.93	0.68
1:B:318:GLY:O	1:B:319:ASP:HB2	1.94	0.68
1:A:527:ARG:CZ	1:B:500:VAL:HG21	2.24	0.67
1:B:373:LYS:HE2	1:B:489:LYS:NZ	2.10	0.67
1:B:299:ASN:HD22	1:B:299:ASN:N	1.91	0.66
1:B:299:ASN:HD22	1:B:299:ASN:H	1.43	0.66
1:B:220:LEU:HD12	1:B:284:ALA:HB2	1.76	0.66
1:A:210:ASN:N	1:A:210:ASN:HD22	1.94	0.66
1:B:412:LYS:HE3	1:B:438:ASP:OD1	1.96	0.66
1:A:266:GLN:HA	1:A:266:GLN:NE2	2.11	0.66
1:A:110:THR:HG22	1:A:111:GLN:HE21	1.61	0.65
1:A:500:VAL:HG21	1:B:527:ARG:NH2	2.11	0.65
1:A:258:ASN:H	1:A:258:ASN:HD22	1.44	0.65
1:A:272:HIS:CD2	1:A:274:GLU:HB2	2.32	0.65
1:A:369:LYS:HD3	3:A:1520:D6P:H3	1.78	0.64
1:A:436:CYS:HB3	1:B:428:ASN:HD22	1.61	0.64
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.28	0.64
1:B:372:SER:HB3	1:B:490:ALA:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:THR:HG21	1:B:489:LYS:HG2	1.79	0.64
1:B:348:SER:HB2	1:B:400:ILE:HD13	1.80	0.63
1:A:200:ASN:HD22	1:A:200:ASN:C	2.02	0.63
1:B:329:LYS:HG3	1:B:418:TYR:OH	1.99	0.63
1:A:318:GLY:O	1:A:319:ASP:HB2	1.99	0.63
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.34	0.62
1:B:321:LEU:HD22	1:B:445:LEU:HD22	1.81	0.62
1:B:40:THR:HG22	1:B:41:ALA:N	2.15	0.62
1:B:515:ARG:HD2	5:B:764:HOH:O	1.99	0.62
1:A:261:MET:H	1:A:307:GLN:NE2	1.97	0.62
1:A:502:GLY:O	1:A:506:GLN:HG3	1.99	0.61
1:A:40:THR:HG22	1:A:42:SER:H	1.64	0.61
1:B:109:MET:HE2	1:B:507:ARG:NE	2.14	0.61
1:A:402:ILE:HD13	3:A:1520:D6P:H11	1.83	0.61
1:B:72:GLY:HA2	4:B:660:NAI:O2B	2.01	0.61
1:A:272:HIS:HD2	1:A:274:GLU:H	1.49	0.61
1:A:205:LEU:HA	1:A:210:ASN:O	2.01	0.60
1:B:329:LYS:NZ	1:B:400:ILE:HD11	2.16	0.60
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.15	0.60
1:A:348:SER:HB2	1:A:400:ILE:HD13	1.84	0.60
1:A:154:LEU:HD22	1:A:179:VAL:HG11	1.83	0.59
1:A:224:ARG:O	1:A:228:GLN:HG3	2.01	0.59
1:B:352:LEU:HD23	1:B:352:LEU:N	2.17	0.59
1:A:254:SER:H	1:A:258:ASN:HD21	1.50	0.59
1:B:247:THR:HG23	1:B:297:PRO:HG2	1.83	0.59
1:B:95:GLN:HA	1:B:95:GLN:HE21	1.68	0.59
1:A:21:TYR:CZ	1:A:26:LEU:HD13	2.37	0.59
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.38	0.59
1:A:310:GLU:HA	1:A:479:PRO:HG2	1.85	0.58
1:B:34:ASN:ND2	1:B:35:ALA:H	2.02	0.58
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.33	0.58
1:B:367:ARG:O	1:B:371:ILE:HG13	2.03	0.58
1:A:13:LYS:HG3	5:A:933:HOH:O	2.02	0.58
1:B:26:LEU:O	1:B:57:LYS:HA	2.03	0.58
1:B:352:LEU:HD23	1:B:352:LEU:H	1.68	0.58
1:B:315:PHE:CD2	1:B:457:THR:HG22	2.39	0.57
1:A:266:GLN:HE21	1:A:266:GLN:HA	1.68	0.57
1:B:158:MET:CE	1:B:164:LEU:HD12	2.35	0.57
1:B:129:PRO:HB2	1:B:132:SER:HB3	1.86	0.57
1:B:203:ILE:HG13	1:B:204:ASN:N	2.20	0.57
1:B:189:ASP:HB2	5:B:936:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLU:HG3	1:B:497:PHE:CD2	2.40	0.57
1:A:272:HIS:HD2	1:A:274:GLU:HB2	1.67	0.57
1:B:372:SER:CB	1:B:490:ALA:HB2	2.34	0.57
1:B:373:LYS:HE2	1:B:489:LYS:HZ3	1.69	0.56
4:B:660:NAI:H52A	4:B:660:NAI:O2B	2.05	0.56
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.05	0.56
1:B:494:ARG:HD2	1:B:497:PHE:HE2	1.71	0.56
1:B:432:ILE:HG22	1:B:433:HIS:N	2.20	0.56
1:B:187:TYR:OH	1:B:219:HIS:HD2	1.88	0.56
1:B:189:ASP:HB3	5:B:961:HOH:O	2.06	0.56
1:A:351:HIS:HA	1:A:403:LYS:O	2.06	0.55
1:B:494:ARG:HD2	1:B:497:PHE:CE2	2.41	0.55
1:A:246:ASN:ND2	4:A:650:NAI:H51A	2.21	0.55
1:B:310:GLU:CG	1:B:479:PRO:HG2	2.35	0.55
1:B:477:PHE:O	1:B:478:TYR:C	2.45	0.55
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.88	0.55
1:B:299:ASN:ND2	1:B:299:ASN:H	2.05	0.55
1:B:319:ASP:HB3	1:B:490:ALA:HB3	1.88	0.54
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.90	0.54
1:A:256:GLY:HA2	1:A:263:ASN:OD1	2.07	0.54
1:A:323:SER:HB3	1:A:445:LEU:HD12	1.88	0.54
1:B:116:LYS:HB3	1:B:523:GLN:HE22	1.72	0.54
1:B:158:MET:HE3	1:B:172:LEU:HD12	1.90	0.54
1:B:453:THR:O	1:B:457:THR:HG23	2.07	0.54
1:B:258:ASN:HD22	1:B:258:ASN:H	1.54	0.54
1:A:104:ASN:HD22	1:A:104:ASN:C	2.11	0.54
1:A:246:ASN:HD22	1:A:246:ASN:N	2.04	0.54
1:B:477:PHE:HZ	1:B:513:PHE:CZ	2.26	0.54
1:A:184:SER:OG	1:A:185:ILE:N	2.42	0.53
1:A:29:LYS:HE3	5:A:893:HOH:O	2.08	0.53
1:B:207:GLU:CD	1:B:207:GLU:H	2.11	0.53
1:A:294:ASN:ND2	1:A:296:SER:H	2.07	0.53
1:A:412:LYS:HE3	1:A:414:ALA:HB2	1.89	0.53
1:A:97:LYS:HG2	5:A:881:HOH:O	2.08	0.53
1:B:486:TYR:HA	1:B:506:GLN:HE21	1.74	0.53
1:A:241:VAL:HG23	1:A:290:VAL:HG11	1.91	0.53
1:A:258:ASN:ND2	1:A:258:ASN:H	2.08	0.52
1:B:115:LEU:HD22	1:B:511:GLU:CG	2.31	0.52
1:A:533:LEU:HD23	1:B:461:TYR:OH	2.09	0.52
1:B:254:SER:H	1:B:258:ASN:HD21	1.55	0.52
1:B:321:LEU:O	1:B:489:LYS:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.90	0.52
1:B:324:GLY:O	1:B:327:LYS:HB3	2.09	0.52
1:A:167:ASP:O	1:A:171:ARG:HG3	2.09	0.52
1:B:343:PRO:HD2	1:B:388:TYR:OH	2.10	0.52
1:B:167:ASP:O	1:B:171:ARG:HG3	2.09	0.52
1:B:95:GLN:CA	1:B:95:GLN:HE21	2.20	0.52
1:B:489:LYS:C	1:B:491:PRO:HD3	2.31	0.51
1:A:318:GLY:HA2	1:A:488:LEU:CD1	2.41	0.51
1:A:52:GLN:NE2	1:A:463:LYS:HD3	2.26	0.51
1:B:30:TYR:HE1	1:B:32:TYR:HB2	1.76	0.51
1:B:63:PRO:HG3	1:B:238:LYS:HD2	1.93	0.51
1:A:362:ALA:HB3	1:A:365:GLN:HE21	1.76	0.51
1:A:436:CYS:HB3	1:B:428:ASN:ND2	2.25	0.51
1:A:258:ASN:ND2	1:A:258:ASN:N	2.56	0.51
1:B:258:ASN:HD22	1:B:258:ASN:N	2.08	0.51
1:B:197:GLU:OE1	1:B:197:GLU:N	2.44	0.51
1:A:120:ASP:OD1	1:A:124:ASN:N	2.42	0.50
1:A:453:THR:O	1:A:457:THR:HG23	2.11	0.50
1:A:25:GLU:OE1	1:A:57:LYS:HD3	2.11	0.50
1:B:318:GLY:HA2	1:B:488:LEU:CD1	2.41	0.50
1:A:10:THR:HG21	1:A:129:PRO:HD2	1.91	0.50
1:B:190:PHE:CE2	1:B:276:ALA:HB2	2.47	0.50
1:B:405:MET:O	1:B:408:VAL:HG22	2.12	0.50
1:B:95:GLN:HA	1:B:95:GLN:NE2	2.25	0.50
1:A:255:PRO:HA	1:A:259:ASP:OD1	2.11	0.50
1:B:266:GLN:HA	1:B:266:GLN:NE2	2.27	0.50
1:B:327:LYS:O	1:B:331:VAL:HG23	2.11	0.50
1:A:507:ARG:HD3	5:B:941:HOH:O	2.11	0.50
1:A:200:ASN:ND2	1:A:200:ASN:C	2.64	0.50
1:A:497:PHE:CD2	1:B:530:GLU:HB2	2.47	0.50
1:A:315:PHE:CD1	1:A:481:LEU:HD11	2.47	0.50
1:A:375:SER:HA	1:A:378:ASP:OD2	2.11	0.50
1:A:477:PHE:HZ	1:A:513:PHE:CZ	2.28	0.50
1:A:217:TRP:O	1:A:221:GLN:HG2	2.12	0.49
1:A:328:LEU:C	1:A:328:LEU:HD23	2.33	0.49
1:B:296:SER:HB3	1:B:297:PRO:HD2	1.93	0.49
1:A:248:GLU:H	1:A:298:GLN:NE2	2.11	0.49
1:B:299:ASN:ND2	1:B:299:ASN:N	2.60	0.49
1:B:445:LEU:CD2	1:B:487:TRP:HB3	2.42	0.49
1:A:122:GLU:N	1:A:122:GLU:OE1	2.45	0.49
1:A:121:ALA:HB3	1:A:122:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:ND2	5:A:673:HOH:O	2.44	0.49
1:A:318:GLY:HA2	1:A:488:LEU:HD13	1.94	0.49
1:B:502:GLY:HA3	1:B:505:LYS:CE	2.42	0.49
1:B:264:LEU:HD21	1:B:305:LEU:HD13	1.95	0.49
1:B:322:LYS:NZ	1:B:506:GLN:HE22	2.11	0.49
1:A:377:ILE:O	1:A:381:ILE:HG12	2.13	0.48
1:B:318:GLY:CA	1:B:488:LEU:HD13	2.43	0.48
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.14	0.48
1:A:343:PRO:O	1:A:396:VAL:HG22	2.14	0.48
1:B:76:ASN:HB3	1:B:439:SER:OG	2.13	0.48
1:B:487:TRP:CH2	1:B:510:LEU:HD11	2.49	0.48
1:A:210:ASN:N	1:A:210:ASN:ND2	2.62	0.48
1:B:325:GLN:OE1	1:B:348:SER:HB3	2.14	0.48
1:A:489:LYS:O	1:A:491:PRO:HD3	2.14	0.47
1:B:82:VAL:HG21	1:B:154:LEU:CD1	2.44	0.47
1:B:40:THR:HG22	1:B:42:SER:H	1.79	0.47
1:A:436:CYS:SG	1:A:441:LEU:HD12	2.55	0.47
1:A:55:VAL:HG23	1:A:464:VAL:CG2	2.44	0.47
1:B:445:LEU:HG	1:B:487:TRP:HD1	1.79	0.47
1:A:96:THR:OG1	1:A:101:LYS:HE3	2.15	0.47
1:A:385:ASP:HA	1:A:388:TYR:O	2.15	0.47
1:B:318:GLY:HA2	1:B:488:LEU:HD13	1.96	0.47
1:B:58:LEU:HD22	1:B:134:LEU:HD13	1.95	0.47
1:A:110:THR:CG2	1:A:111:GLN:NE2	2.73	0.47
1:B:229:ASN:O	1:B:233:GLU:HB2	2.15	0.47
1:A:461:TYR:O	1:A:474:PHE:HA	2.15	0.47
1:A:258:ASN:HD22	1:A:258:ASN:N	2.03	0.47
1:A:532:LEU:C	1:B:494:ARG:HH22	2.17	0.46
1:B:247:THR:CG2	1:B:297:PRO:HG2	2.45	0.46
1:B:34:ASN:ND2	1:B:35:ALA:N	2.63	0.46
1:A:246:ASN:HD22	4:A:650:NAI:H51A	1.78	0.46
1:A:516:LEU:C	1:A:516:LEU:HD12	2.36	0.46
1:B:23:ASP:N	1:B:23:ASP:OD2	2.48	0.46
1:A:352:LEU:H	1:A:352:LEU:HD23	1.81	0.46
1:B:445:LEU:O	1:B:445:LEU:HD23	2.16	0.46
1:A:531:ARG:HG2	1:B:482:THR:OG1	2.16	0.46
1:B:484:LEU:HA	1:B:487:TRP:CZ3	2.51	0.46
1:B:150:ASN:HA	1:B:200:ASN:OD1	2.16	0.45
1:A:332:LEU:HD13	1:B:328:LEU:HD11	1.98	0.45
1:B:435:VAL:O	1:B:436:CYS:HB3	2.16	0.45
1:B:282:ALA:O	1:B:286:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:CE	1:B:489:LYS:NZ	2.77	0.45
1:A:266:GLN:HE21	1:A:266:GLN:CA	2.27	0.45
1:A:115:LEU:HD22	1:A:511:GLU:HG3	1.99	0.45
1:B:196:ASP:C	1:B:198:ARG:H	2.19	0.45
1:A:369:LYS:O	1:A:373:LYS:HG3	2.17	0.45
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.29	0.45
1:B:276:ALA:O	1:B:279:THR:HB	2.17	0.45
1:B:432:ILE:CG2	1:B:433:HIS:N	2.80	0.45
1:A:369:LYS:HD3	3:A:1520:D6P:O5	2.17	0.44
1:A:500:VAL:HG21	1:B:527:ARG:CZ	2.46	0.44
1:A:75:GLY:HA3	4:A:650:NAI:O5B	2.17	0.44
1:B:260:THR:HG22	1:B:307:GLN:HE22	1.83	0.44
1:B:427:HIS:HE1	5:B:709:HOH:O	2.00	0.44
1:B:186:TYR:HE1	1:B:191:ILE:HD11	1.82	0.44
1:B:247:THR:O	1:B:365:GLN:HG3	2.17	0.44
1:A:369:LYS:HG2	1:A:402:ILE:CD1	2.48	0.44
1:B:445:LEU:HD23	1:B:445:LEU:C	2.38	0.44
1:A:321:LEU:HB2	4:A:650:NAI:C5N	2.47	0.44
1:A:369:LYS:HG2	1:A:402:ILE:HD11	1.99	0.44
1:A:52:GLN:HG3	1:A:54:TYR:CE1	2.53	0.44
1:B:96:THR:OG1	1:B:101:LYS:HE3	2.17	0.44
1:A:428:ASN:HD22	1:B:436:CYS:HB3	1.82	0.44
1:B:369:LYS:HD3	1:B:373:LYS:HE3	2.00	0.44
1:A:104:ASN:C	1:A:104:ASN:ND2	2.70	0.44
1:B:373:LYS:HG2	1:B:489:LYS:CD	2.41	0.44
1:B:40:THR:CG2	1:B:41:ALA:N	2.80	0.44
1:A:426:GLY:HA3	1:B:440:LEU:HD13	2.00	0.44
1:B:502:GLY:HA3	1:B:505:LYS:HE2	2.00	0.44
1:A:110:THR:HG22	1:A:111:GLN:HG2	2.00	0.43
1:A:177:SER:O	1:A:180:LYS:HE2	2.17	0.43
1:A:216:LYS:HA	1:A:219:HIS:ND1	2.33	0.43
1:A:296:SER:HB3	1:A:297:PRO:HD2	2.00	0.43
1:A:300:THR:O	1:A:305:LEU:HD12	2.18	0.43
5:A:669:HOH:O	1:B:422:LEU:HB3	2.19	0.43
1:B:23:ASP:O	1:B:24:ASN:HB2	2.17	0.43
1:B:249:ARG:HB2	1:B:364:LYS:HE3	2.01	0.43
1:B:347:ALA:O	1:B:416:ASP:HA	2.18	0.43
1:B:437:GLU:HB2	1:B:440:LEU:HD12	2.00	0.43
1:B:320:ASP:O	1:B:488:LEU:HA	2.18	0.43
1:B:445:LEU:HG	1:B:487:TRP:CD1	2.54	0.43
1:A:352:LEU:N	1:A:352:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:HB2	1:B:124:ASN:ND2	2.32	0.43
1:B:27:LEU:HD22	1:B:27:LEU:N	2.34	0.43
1:A:316:ILE:O	1:A:317:ALA:HB2	2.18	0.43
1:A:318:GLY:CA	1:A:488:LEU:HD13	2.48	0.43
1:B:109:MET:HE3	1:B:486:TYR:CZ	2.53	0.43
1:B:208:LYS:HG2	1:B:210:ASN:ND2	2.34	0.43
1:B:491:PRO:HB2	1:B:499:PRO:HB2	1.99	0.43
1:B:105:TYR:OH	1:B:140:ASN:ND2	2.51	0.43
1:B:180:LYS:HA	1:B:181:PRO:HD3	1.90	0.43
1:B:195:GLN:OE1	1:B:359:ASN:HB2	2.19	0.43
1:A:513:PHE:O	1:A:516:LEU:HG	2.18	0.43
1:B:258:ASN:ND2	1:B:258:ASN:N	2.66	0.43
1:B:406:LYS:HB3	1:B:407:PRO:HD3	2.01	0.43
1:B:58:LEU:HD12	1:B:458:ARG:O	2.19	0.43
1:A:353:GLY:HA3	1:A:406:LYS:HA	2.01	0.43
1:B:369:LYS:CG	1:B:373:LYS:HE3	2.49	0.43
1:A:328:LEU:O	1:A:328:LEU:HD23	2.19	0.42
1:B:115:LEU:CD2	1:B:511:GLU:HG3	2.34	0.42
1:A:414:ALA:HB3	1:A:434:ASN:HB3	2.00	0.42
1:A:497:PHE:CD1	1:A:497:PHE:N	2.88	0.42
1:B:251:VAL:HG22	1:B:299:ASN:HD21	1.84	0.42
1:B:260:THR:OG1	1:B:263:ASN:ND2	2.53	0.42
1:B:57:LYS:HE3	1:B:474:PHE:CD2	2.54	0.42
1:B:69:MET:HB2	1:B:241:VAL:HG22	2.01	0.42
1:A:57:LYS:HB2	1:A:474:PHE:CE2	2.54	0.42
1:B:494:ARG:HB3	1:B:497:PHE:HD2	1.85	0.42
1:B:501:ASN:O	1:B:503:LEU:N	2.52	0.42
1:B:352:LEU:CD2	1:B:352:LEU:N	2.82	0.42
1:B:194:ASN:ND2	1:B:358:TYR:CD1	2.87	0.42
1:B:477:PHE:CZ	1:B:513:PHE:CZ	3.07	0.42
1:B:56:PHE:CD2	1:B:461:TYR:HB3	2.55	0.42
1:A:150:ASN:ND2	1:A:152:ALA:H	2.17	0.42
1:A:367:ARG:O	1:A:371:ILE:HG13	2.20	0.42
1:B:28:THR:HG21	1:B:516:LEU:O	2.20	0.42
1:B:327:LYS:HD2	5:B:795:HOH:O	2.18	0.42
1:B:72:GLY:CA	4:B:660:NAI:O2B	2.66	0.42
1:A:297:PRO:HG3	1:A:369:LYS:HE3	2.02	0.42
1:A:320:ASP:OD1	4:A:650:NAI:H6N	2.20	0.42
1:B:345:SER:HB3	1:B:419:TYR:HB3	2.02	0.42
1:B:148:ASP:CG	4:B:660:NAI:H2B	2.40	0.42
1:A:452:MET:HG3	1:A:487:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:N	1:B:444:PRO:HD2	2.35	0.41
1:A:533:LEU:HD23	1:B:461:TYR:HH	1.85	0.41
1:A:81:LEU:HD23	1:A:81:LEU:C	2.40	0.41
1:B:250:TYR:CE1	1:B:299:ASN:HB3	2.55	0.41
1:A:320:ASP:OD2	1:A:369:LYS:HE2	2.20	0.41
1:A:76:ASN:HB3	1:A:439:SER:OG	2.20	0.41
1:A:56:PHE:CD1	1:A:461:TYR:HB3	2.55	0.41
1:B:30:TYR:CE1	1:B:32:TYR:HB2	2.54	0.41
1:B:109:MET:HE2	1:B:507:ARG:CD	2.50	0.41
1:A:67:GLY:HA3	1:A:236:LEU:HD13	2.02	0.41
1:B:253:VAL:HA	1:B:258:ASN:HD21	1.86	0.41
1:A:298:GLN:HE21	1:A:298:GLN:HB3	1.62	0.41
1:A:346:ILE:O	1:A:398:HIS:HA	2.21	0.41
1:A:220:LEU:HD12	1:A:221:GLN:HE21	1.85	0.41
1:B:381:ILE:HD11	1:B:396:VAL:HG23	2.03	0.41
1:A:325:GLN:N	3:A:1520:D6P:O2P	2.54	0.40
1:A:496:GLY:HA3	5:B:929:HOH:O	2.22	0.40
1:B:207:GLU:CD	1:B:207:GLU:N	2.75	0.40
1:B:39:LYS:HE2	1:B:45:PHE:CZ	2.56	0.40
1:A:219:HIS:O	1:A:223:ILE:HG12	2.21	0.40
1:A:40:THR:HG22	1:A:41:ALA:N	2.36	0.40
1:A:448:ASP:HB3	1:A:487:TRP:CE2	2.56	0.40
1:A:497:PHE:CE2	1:B:530:GLU:HB2	2.56	0.40
1:B:328:LEU:O	1:B:332:LEU:HG	2.21	0.40
1:A:335:PHE:HE1	1:B:503:LEU:CD2	2.34	0.40
1:B:306:VAL:O	1:B:310:GLU:HG3	2.22	0.40
1:A:373:LYS:HG2	1:A:489:LYS:CE	2.42	0.40
1:B:159:GLN:HG2	5:B:956:HOH:O	2.20	0.40
1:B:253:VAL:HG22	1:B:302:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/533 (98%)	502 (96%)	19 (4%)	2 (0%)	36	26
1	B	512/533 (96%)	476 (93%)	29 (6%)	7 (1%)	12	4
All	All	1035/1066 (97%)	978 (94%)	48 (5%)	9 (1%)	19	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	ASP
1	B	319	ASP
1	B	250	TYR
1	B	322	LYS
1	A	320	ASP
1	B	197	GLU
1	B	479	PRO
1	B	502	GLY
1	B	320	ASP

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%)	451 (97%)	13 (3%)	47	40
1	B	457/471 (97%)	439 (96%)	18 (4%)	35	27
All	All	921/942 (98%)	890 (97%)	31 (3%)	40	32

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	110	THR
1	A	180	LYS
1	A	200	ASN
1	A	210	ASN
1	A	246	ASN
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	298	GLN
1	A	319	ASP
1	A	352	LEU
1	A	416	ASP
1	A	438	ASP
1	A	483	PHE
1	B	16	THR
1	B	23	ASP
1	B	34	ASN
1	B	61	LYS
1	B	95	GLN
1	B	158	MET
1	B	197	GLU
1	B	201	ASN
1	B	207	GLU
1	B	258	ASN
1	B	299	ASN
1	B	319	ASP
1	B	335	PHE
1	B	352	LEU
1	B	417	GLU
1	B	477	PHE
1	B	479	PRO
1	B	483	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
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	159	GLN
1	A	169	GLN
1	A	170	GLN
1	A	200	ASN
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	221	GLN
1	A	229	ASN
1	A	246	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	307	GLN
1	A	365	GLN
1	A	501	ASN
1	A	512	ASN
1	A	523	GLN
1	B	34	ASN
1	B	95	GLN
1	B	140	ASN
1	B	159	GLN
1	B	194	ASN
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	307	GLN
1	B	325	GLN
1	B	355	ASN
1	B	427	HIS
1	B	428	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	D6P	A	1520	-	13,14,14	6.63	5 (38%)	12,19,19	0.75	0
4	NAI	A	650	2	41,48,48	1.29	3 (7%)	45,73,73	1.12	4 (8%)
4	NAI	B	660	-	41,48,48	1.47	6 (14%)	45,73,73	1.34	5 (11%)

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
3	D6P	A	1520	-	-	0/13/17/17	0/0/0/0
4	NAI	A	650	2	-	0/25/72/72	0/5/5/5
4	NAI	B	660	-	2/2/13/16	0/25/72/72	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1520	D6P	P-C7	-21.01	1.48	1.76
3	A	1520	D6P	C5-C6	-4.15	1.42	1.50
4	B	660	NAI	C7N-C3N	2.08	1.53	1.48
4	B	660	NAI	C2N-C3N	2.17	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	660	NAI	C4A-N3A	2.52	1.39	1.35
4	A	650	NAI	C6N-N1N	2.98	1.45	1.37
4	B	660	NAI	C6N-N1N	3.14	1.46	1.37
4	A	650	NAI	C2A-N1A	3.84	1.41	1.33
4	A	650	NAI	C6N-C5N	3.91	1.40	1.33
4	B	660	NAI	C6N-C5N	3.95	1.40	1.33
4	B	660	NAI	C2A-N1A	4.06	1.41	1.33
3	A	1520	D6P	P-O2P	5.14	1.61	1.54
3	A	1520	D6P	P-O1P	5.59	1.62	1.54
3	A	1520	D6P	P-O3P	6.74	1.60	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	C1D-N1N-C2N	-3.23	115.64	121.10
4	B	660	NAI	O4B-C4B-C3B	-3.22	98.77	105.15
4	B	660	NAI	N3A-C2A-N1A	-2.57	126.67	128.86
4	A	650	NAI	N3A-C2A-N1A	-2.20	126.98	128.86
4	A	650	NAI	O4D-C4D-C3D	2.10	109.31	105.15
4	B	660	NAI	C4B-O4B-C1B	2.25	112.17	109.83
4	B	660	NAI	O4D-C1D-N1N	2.38	112.78	108.04
4	A	650	NAI	C4A-C5A-N7A	2.59	111.91	109.41
4	B	660	NAI	C4A-C5A-N7A	3.20	112.50	109.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	660	NAI	C1B
4	B	660	NAI	C4B

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1520	D6P	4	0
4	A	650	NAI	5	0
4	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, 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%)	0.04	21 (4%) 38 42	18, 32, 61, 70	0
1	B	516/533 (96%)	0.23	44 (8%) 11 11	16, 34, 69, 70	0
All	All	1041/1066 (97%)	0.13	65 (6%) 20 22	16, 33, 67, 70	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ALA	7.5
1	B	497	PHE	7.3
1	B	371	ILE	7.0
1	B	41	ALA	5.8
1	A	9	ILE	5.8
1	A	533	LEU	5.3
1	B	496	GLY	5.2
1	B	194	ASN	4.8
1	A	208	LYS	4.7
1	B	366	PHE	4.5
1	B	362	ALA	4.4
1	A	207	GLU	3.9
1	A	209	GLY	3.9
1	A	40	THR	3.9
1	B	500	VAL	3.9
1	B	207	GLU	3.8
1	B	477	PHE	3.8
1	B	23	ASP	3.7
1	B	21	TYR	3.7
1	B	473	LYS	3.6
1	B	494	ARG	3.6
1	B	321	LEU	3.6
1	B	318	GLY	3.5
1	B	372	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	367	ARG	3.4
1	A	42	SER	3.3
1	B	360	LEU	3.3
1	B	478	TYR	3.2
1	A	121	ALA	3.1
1	B	495	PRO	3.1
1	B	498	HIS	3.0
1	B	208	LYS	3.0
1	B	42	SER	3.0
1	B	24	ASN	3.0
1	B	374	SER	2.9
1	A	323	SER	2.9
1	B	363	PRO	2.9
1	B	479	PRO	2.9
1	A	21	TYR	2.9
1	A	363	PRO	2.8
1	B	364	LYS	2.8
1	B	499	PRO	2.8
1	B	209	GLY	2.8
1	A	205	LEU	2.8
1	B	22	LYS	2.7
1	A	22	LYS	2.7
1	B	40	THR	2.7
1	A	122	GLU	2.6
1	B	44	ARG	2.6
1	A	318	GLY	2.5
1	B	464	VAL	2.5
1	B	61	LYS	2.4
1	B	255	PRO	2.4
1	A	210	ASN	2.3
1	B	370	GLU	2.3
1	B	315	PHE	2.3
1	A	255	PRO	2.3
1	B	488	LEU	2.2
1	B	493	THR	2.2
1	A	321	LEU	2.2
1	B	43	GLY	2.1
1	B	197	GLU	2.0
1	A	43	GLY	2.0
1	A	470	ASP	2.0
1	B	322	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 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. 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(\AA^2)	Q<0.9
3	D6P	A	1520	15/15	0.84	0.41	30,39,42,42	15
2	MN	A	630	1/1	0.89	0.47	44,44,44,44	0
4	NAI	B	660	44/44	0.91	0.19	29,47,57,62	0
4	NAI	A	650	44/44	0.97	0.11	20,26,47,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.