



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

PDB ID : 2GNA
Title : Crystal structure of UDP-GlcNAc inverting 4,6-dehydratase in complex with NADP and UDP-Gal
Authors : Ishiyama, N.; Creuzenet, C.; Lam, J.S.; Berghuis, A.M.
Deposited on : 2006-04-09
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

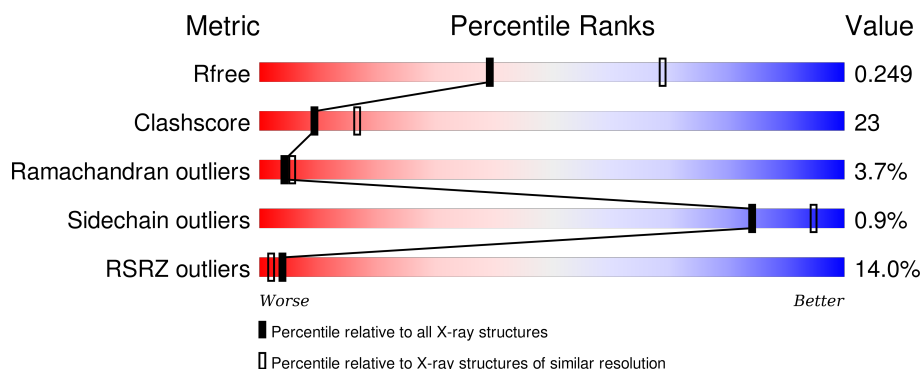
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	344	<div> <div>15%</div> <div>53%</div> <div>41%</div> <div>• •</div> </div>
1	B	344	<div> <div>11%</div> <div>57%</div> <div>35%</div> <div>• 5%</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	MES	B	336	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5516 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.

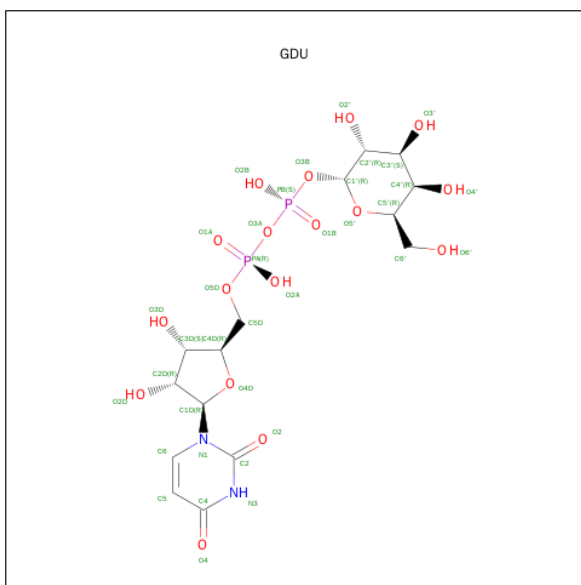
- Molecule 1 is a protein called UDP-GlcNAc C6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2590	1656	440	479	15			
1	B	327	Total	C	N	O	S	0	0	0
			2573	1647	436	475	15			

There are 22 discrepancies between the modelled and reference sequences:

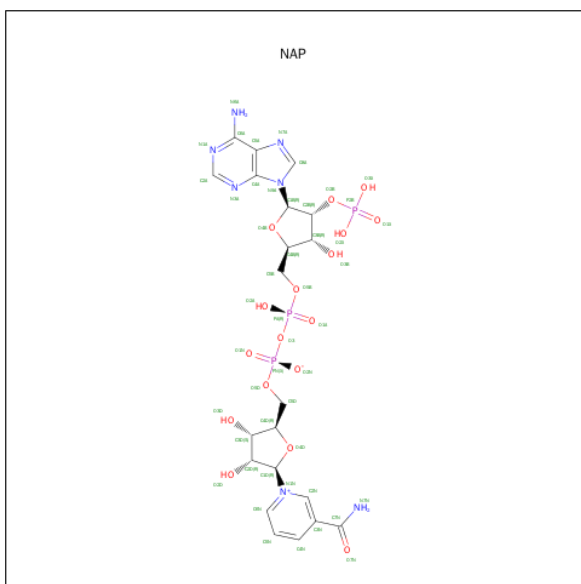
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	CLONING ARTIFACT	UNP O25511
A	-9	HIS	-	EXPRESSION TAG	UNP O25511
A	-8	HIS	-	EXPRESSION TAG	UNP O25511
A	-7	HIS	-	EXPRESSION TAG	UNP O25511
A	-6	HIS	-	EXPRESSION TAG	UNP O25511
A	-5	HIS	-	EXPRESSION TAG	UNP O25511
A	-4	HIS	-	EXPRESSION TAG	UNP O25511
A	-3	GLY	-	CLONING ARTIFACT	UNP O25511
A	-2	SER	-	CLONING ARTIFACT	UNP O25511
A	-1	MET	-	CLONING ARTIFACT	UNP O25511
A	0	SER	-	CLONING ARTIFACT	UNP O25511
B	-10	MET	-	CLONING ARTIFACT	UNP O25511
B	-9	HIS	-	EXPRESSION TAG	UNP O25511
B	-8	HIS	-	EXPRESSION TAG	UNP O25511
B	-7	HIS	-	EXPRESSION TAG	UNP O25511
B	-6	HIS	-	EXPRESSION TAG	UNP O25511
B	-5	HIS	-	EXPRESSION TAG	UNP O25511
B	-4	HIS	-	EXPRESSION TAG	UNP O25511
B	-3	GLY	-	CLONING ARTIFACT	UNP O25511
B	-2	SER	-	CLONING ARTIFACT	UNP O25511
B	-1	MET	-	CLONING ARTIFACT	UNP O25511
B	0	SER	-	CLONING ARTIFACT	UNP O25511

- Molecule 2 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 15	N 2	O 17	P 2	0	0
2	B	1	Total 36	C 15	N 2	O 17	P 2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



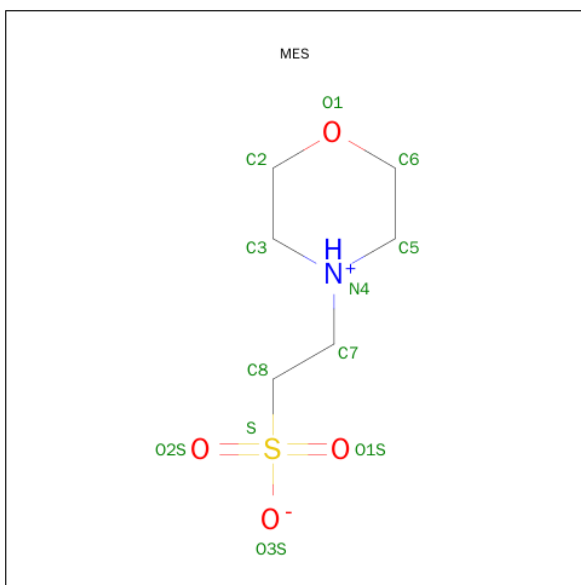
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

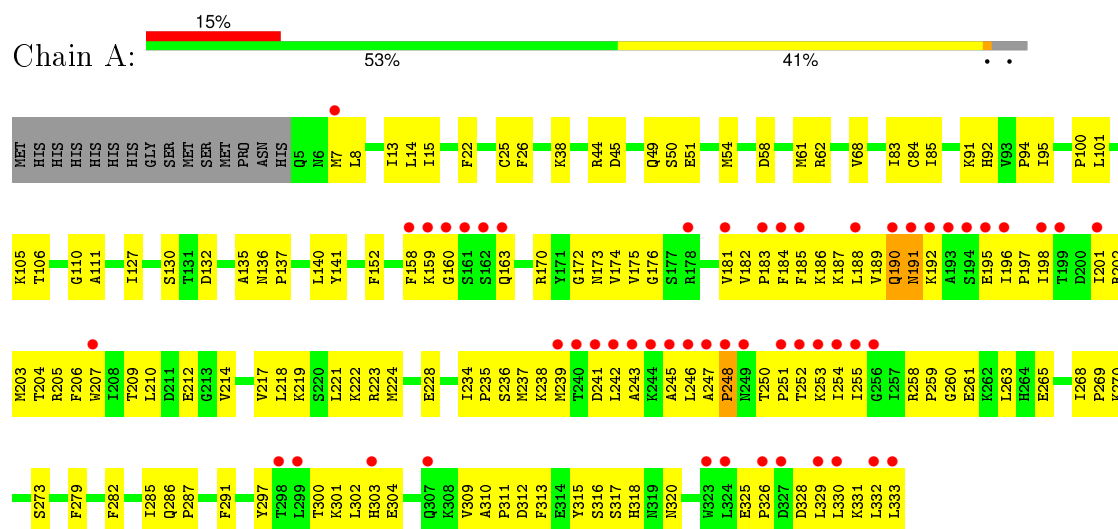
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		
5	B	91	Total	O	0	0
			91	91		

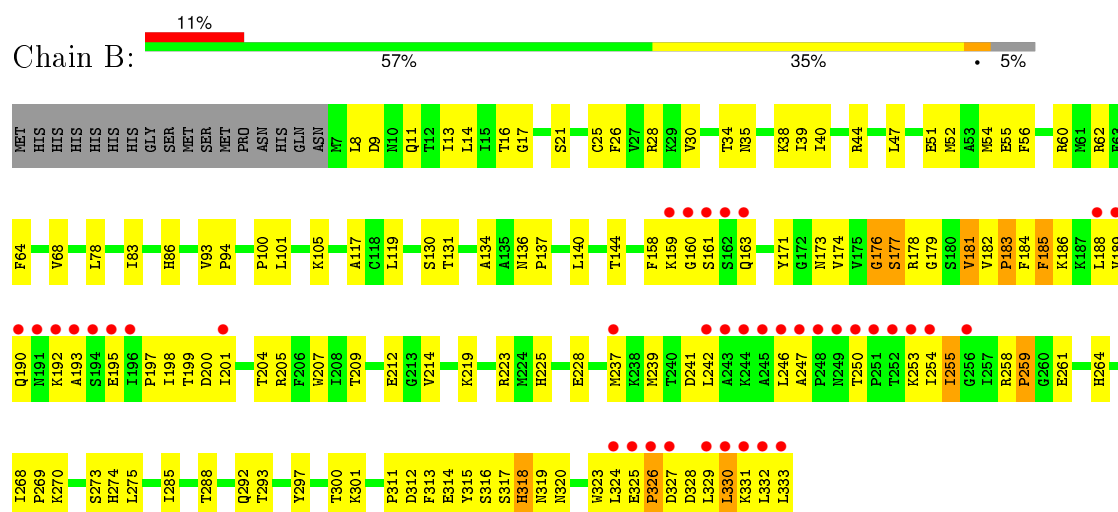
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: UDP-GlcNAc C6 dehydratase



• Molecule 1: UDP-GlcNAc C6 dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	112.22Å 112.22Å 107.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 44.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.60) 97.6 (44.27-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.250 0.195 , 0.249	Depositor DCC
R_{free} test set	2284 reflections (9.89%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.1	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23639 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, GDU, MES

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	0.34	0/2641	0.59	0/3568
1	B	0.35	0/2624	0.61	0/3545
All	All	0.35	0/5265	0.60	0/7113

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	2590	0	2641	123	0
1	B	2573	0	2627	120	0
2	A	36	0	22	0	0
2	B	36	0	22	0	0
3	A	48	0	25	5	0
3	B	48	0	25	5	0
4	B	12	0	13	0	0
5	A	82	0	0	3	0
5	B	91	0	0	3	0
All	All	5516	0	5375	243	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 23.

All (243) 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:204:THR:HG22	1:B:264:HIS:ND1	1.81	0.96
1:A:8:LEU:HD11	1:A:13:ILE:HD11	1.51	0.92
1:A:174:VAL:HG11	1:A:210:LEU:HD12	1.51	0.88
1:A:223:ARG:HB2	1:A:300:THR:HB	1.59	0.85
1:B:181:VAL:HG13	1:B:182:VAL:H	1.41	0.83
1:B:9:ASP:HB3	1:B:35:ASN:HB2	1.59	0.82
1:B:159:LYS:HG2	1:B:163:GLN:HE22	1.44	0.82
1:B:330:LEU:HD22	1:B:330:LEU:H	1.44	0.82
1:A:173:ASN:HD21	1:A:205:ARG:HD2	1.46	0.80
1:A:92:HIS:HD2	1:A:95:ILE:H	1.28	0.80
1:B:186:LYS:HZ2	1:B:333:LEU:HD23	1.49	0.77
1:A:189:VAL:HG21	1:A:247:ALA:HA	1.66	0.77
1:A:253:LYS:HG2	1:A:254:ILE:H	1.51	0.76
1:A:325:GLU:HG2	1:A:328:ASP:OD2	1.87	0.74
1:A:25:CYS:SG	1:A:214:VAL:HG21	2.27	0.73
1:B:258:ARG:HB2	1:B:261:GLU:HG3	1.71	0.71
1:A:181:VAL:HG21	1:A:239:MET:HE1	1.73	0.70
1:A:92:HIS:NE2	1:A:94:PRO:HG2	2.05	0.70
1:B:186:LYS:NZ	1:B:333:LEU:HD23	2.06	0.70
1:B:181:VAL:HG21	1:B:239:MET:HE1	1.73	0.70
1:A:243:ALA:O	1:A:247:ALA:HB3	1.92	0.69
1:A:196:ILE:HB	1:A:252:THR:HG22	1.74	0.69
1:B:8:LEU:HD12	1:B:34:THR:HG21	1.74	0.69
1:B:38:LYS:NZ	1:B:62:ARG:HH11	1.91	0.69
1:B:176:GLY:HA2	1:B:183:PRO:HD3	1.75	0.68
1:A:223:ARG:HA	1:A:301:LYS:HB2	1.76	0.68
1:A:182:VAL:HB	1:A:183:PRO:HD3	1.76	0.68
1:A:173:ASN:ND2	1:A:205:ARG:HD2	2.08	0.68
1:A:245:ALA:HB3	1:A:329:LEU:HD23	1.75	0.67
1:B:93:VAL:HB	1:B:94:PRO:HD3	1.75	0.67
1:A:242:LEU:HD12	1:A:329:LEU:HD21	1.78	0.66
1:B:119:LEU:HD22	1:B:158:PHE:CD2	2.30	0.66
1:B:171:TYR:O	3:B:334:NAP:H5N	1.95	0.65
1:B:199:THR:HA	1:B:255:ILE:HG13	1.79	0.65
1:B:179:GLY:HA2	1:B:184:PHE:CE1	2.32	0.64
1:B:38:LYS:HE2	1:B:40:ILE:HD11	1.80	0.64
1:A:316:SER:C	1:A:318:HIS:H	1.99	0.64
1:B:136:ASN:HD21	1:B:269:PRO:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:MET:CE	1:B:242:LEU:HD23	2.29	0.63
1:B:9:ASP:CB	1:B:35:ASN:HB2	2.27	0.62
1:B:140:LEU:O	1:B:144:THR:HG23	1.99	0.62
1:B:209:THR:HG22	1:B:332:LEU:HD13	1.81	0.62
1:B:8:LEU:HD22	1:B:13:ILE:HD11	1.82	0.62
1:A:309:VAL:HG12	1:A:310:ALA:N	2.14	0.61
1:B:30:VAL:HG12	1:B:39:ILE:HD11	1.83	0.61
1:B:181:VAL:HG13	1:B:182:VAL:N	2.15	0.61
1:B:204:THR:O	1:B:205:ARG:HG2	2.00	0.61
1:B:239:MET:HE3	1:B:242:LEU:HD23	1.81	0.60
1:B:325:GLU:HB3	1:B:326:PRO:HD2	1.82	0.60
1:B:270:LYS:HE3	1:B:312:ASP:HB2	1.83	0.60
1:A:159:LYS:HG2	1:A:163:GLN:OE1	2.02	0.59
1:B:130:SER:O	3:B:334:NAP:H6N	2.03	0.59
1:B:159:LYS:HE3	1:B:292:GLN:HB2	1.84	0.59
1:A:242:LEU:CD1	1:A:329:LEU:HD21	2.32	0.59
1:A:255:ILE:HG22	1:A:255:ILE:O	2.03	0.58
1:A:186:LYS:HG2	1:A:246:LEU:HD11	1.85	0.58
1:A:223:ARG:HA	1:A:301:LYS:CB	2.34	0.58
1:B:189:VAL:CG2	1:B:247:ALA:HB2	2.34	0.58
1:A:101:LEU:HG	1:A:105:LYS:HE3	1.84	0.58
1:A:175:VAL:HA	1:A:207:TRP:CZ3	2.38	0.58
1:A:175:VAL:HA	1:A:207:TRP:HZ3	1.69	0.57
1:B:8:LEU:HA	1:B:11:GLN:HG3	1.87	0.56
1:A:286:GLN:HE21	1:A:297:TYR:HD1	1.52	0.56
1:B:318:HIS:CE1	1:B:319:ASN:HB3	2.40	0.56
1:B:55:GLU:HG3	1:B:56:PHE:CD1	2.40	0.56
1:A:241:ASP:HB3	1:A:326:PRO:HG3	1.86	0.56
1:B:316:SER:HB2	1:B:319:ASN:OD1	2.05	0.56
1:B:189:VAL:HG22	1:B:247:ALA:HB2	1.88	0.56
1:B:209:THR:OG1	1:B:212:GLU:HG3	2.06	0.56
1:B:219:LYS:O	1:B:223:ARG:HG2	2.04	0.56
1:A:185:PHE:HB3	1:A:246:LEU:HG	1.87	0.56
1:A:92:HIS:CD2	1:A:94:PRO:HG2	2.40	0.55
1:A:91:LYS:HA	1:A:141:TYR:CE1	2.41	0.55
1:A:92:HIS:HD2	1:A:95:ILE:N	2.02	0.55
1:A:159:LYS:HA	1:A:163:GLN:OE1	2.07	0.54
1:A:245:ALA:O	1:A:330:LEU:HD21	2.07	0.54
1:A:175:VAL:CG2	1:A:209:THR:HG22	2.36	0.54
1:A:224:MET:O	1:A:301:LYS:HD3	2.08	0.54
1:B:159:LYS:NZ	1:B:293:THR:HB	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:HA	1:A:320:ASN:HD21	1.73	0.54
1:B:293:THR:HG23	1:B:293:THR:O	2.08	0.54
1:A:189:VAL:CG2	1:A:247:ALA:HA	2.37	0.54
1:B:207:TRP:HD1	1:B:237:MET:HB3	1.73	0.54
1:B:181:VAL:O	1:B:185:PHE:HB2	2.07	0.53
1:A:15:ILE:HA	1:A:85:ILE:O	2.08	0.53
1:B:204:THR:CG2	1:B:264:HIS:ND1	2.63	0.53
1:A:175:VAL:HG22	5:A:389:HOH:O	2.08	0.53
1:A:100:PRO:HA	1:A:140:LEU:CD2	2.38	0.53
1:B:159:LYS:HE2	1:B:293:THR:HG22	1.90	0.53
1:B:38:LYS:HZ1	1:B:62:ARG:HH11	1.55	0.53
1:A:239:MET:CE	1:A:242:LEU:HD23	2.39	0.53
1:B:223:ARG:HB2	1:B:300:THR:HB	1.89	0.53
1:A:175:VAL:HG21	1:A:209:THR:HG22	1.90	0.52
1:B:51:GLU:HA	1:B:54:MET:HE3	1.90	0.52
1:A:38:LYS:HD2	1:A:62:ARG:HG3	1.91	0.52
1:A:270:LYS:HA	1:A:313:PHE:O	2.09	0.52
1:B:270:LYS:HB2	1:B:314:GLU:OE1	2.10	0.52
1:B:159:LYS:NZ	1:B:292:GLN:HB2	2.25	0.52
1:A:268:ILE:HG12	1:A:285:ILE:HD11	1.92	0.52
1:B:159:LYS:CE	1:B:292:GLN:HB2	2.39	0.51
1:B:101:LEU:HG	1:B:105:LYS:HE3	1.93	0.51
1:A:228:GLU:HG3	1:A:297:TYR:CD2	2.44	0.51
1:A:22:PHE:CZ	1:A:217:VAL:HG21	2.46	0.51
1:A:68:VAL:HG22	3:A:334:NAP:N1A	2.25	0.51
1:A:45:ASP:O	1:A:49:GLN:HG3	2.11	0.51
1:A:91:LYS:HZ2	3:A:334:NAP:H72N	1.59	0.50
1:A:309:VAL:HG12	1:A:310:ALA:H	1.76	0.50
1:B:30:VAL:CG1	1:B:39:ILE:HD11	2.41	0.50
1:B:189:VAL:HG11	1:B:246:LEU:O	2.11	0.50
1:A:250:THR:CG2	1:A:251:PRO:HD2	2.42	0.50
1:A:219:LYS:O	1:A:223:ARG:HG2	2.11	0.50
1:B:8:LEU:CD2	1:B:83:ILE:HD12	2.42	0.50
1:A:198:ILE:O	1:A:254:ILE:HA	2.11	0.49
1:B:197:PRO:O	1:B:198:ILE:HD13	2.12	0.49
1:B:325:GLU:HB3	1:B:326:PRO:CD	2.42	0.49
1:A:287:PRO:HG2	1:A:291:PHE:CE2	2.47	0.49
1:A:310:ALA:C	1:A:312:ASP:H	2.16	0.49
1:B:325:GLU:O	1:B:328:ASP:HB2	2.12	0.49
1:B:173:ASN:HD22	1:B:173:ASN:N	2.11	0.49
1:A:235:PRO:HA	1:A:320:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:C	1:A:333:LEU:HD23	2.33	0.49
1:B:225:HIS:ND1	1:B:301:LYS:HE2	2.27	0.49
1:A:91:LYS:NZ	3:A:334:NAP:H72N	2.11	0.49
1:B:329:LEU:O	1:B:330:LEU:C	2.51	0.49
1:B:159:LYS:HZ1	1:B:293:THR:N	2.11	0.48
1:B:207:TRP:CD1	1:B:237:MET:HB3	2.48	0.48
1:A:45:ASP:HB2	5:A:395:HOH:O	2.13	0.48
1:B:68:VAL:HG22	3:B:334:NAP:N1A	2.28	0.48
1:B:185:PHE:O	1:B:188:LEU:HB2	2.13	0.48
1:A:202:ARG:HA	1:A:238:LYS:HE3	1.95	0.48
1:A:313:PHE:CE2	1:A:315:TYR:HB2	2.48	0.48
1:B:38:LYS:HZ2	1:B:62:ARG:HH11	1.61	0.48
1:B:38:LYS:HE2	1:B:40:ILE:CD1	2.43	0.47
1:A:316:SER:C	1:A:318:HIS:N	2.67	0.47
1:B:242:LEU:HD12	1:B:242:LEU:O	2.14	0.47
1:A:176:GLY:HA2	1:A:182:VAL:HB	1.96	0.47
1:B:209:THR:HG21	1:B:332:LEU:HD22	1.96	0.47
1:B:159:LYS:HZ3	1:B:293:THR:HB	1.79	0.47
1:A:204:THR:O	1:A:205:ARG:HG2	2.13	0.47
1:B:25:CYS:SG	1:B:214:VAL:HG21	2.53	0.47
1:A:58:ASP:HB3	1:A:61:MET:HG2	1.95	0.47
1:A:176:GLY:H	1:A:182:VAL:HG21	1.80	0.47
1:A:330:LEU:C	1:A:332:LEU:H	2.18	0.47
1:B:288:THR:HG22	5:B:400:HOH:O	2.14	0.47
1:A:228:GLU:HG3	1:A:297:TYR:CE2	2.50	0.47
1:A:136:ASN:HD21	1:A:269:PRO:HB3	1.79	0.47
1:A:190:GLN:HG2	1:A:191:ASN:N	2.30	0.47
1:A:51:GLU:HA	1:A:54:MET:HE3	1.96	0.47
1:B:159:LYS:CE	1:B:293:THR:HG22	2.45	0.46
1:B:176:GLY:O	1:B:177:SER:C	2.54	0.46
1:B:137:PRO:HA	5:B:410:HOH:O	2.14	0.46
1:B:223:ARG:HA	1:B:301:LYS:HB2	1.97	0.46
1:A:273:SER:HB2	1:A:313:PHE:HB3	1.97	0.46
1:A:175:VAL:HG12	1:A:207:TRP:HE3	1.80	0.46
1:B:324:LEU:HD12	1:B:328:ASP:HB3	1.97	0.46
1:B:40:ILE:CG2	1:B:64:PHE:HD2	2.29	0.46
1:A:127:ILE:HD12	1:A:221:LEU:HG	1.98	0.46
1:B:253:LYS:O	1:B:255:ILE:HG23	2.15	0.46
1:A:182:VAL:HG13	1:A:246:LEU:HD22	1.96	0.45
1:A:50:SER:O	1:A:54:MET:HG3	2.16	0.45
1:B:228:GLU:HG3	1:B:297:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:HG21	1:B:246:LEU:O	2.17	0.45
1:A:186:LYS:HE2	1:A:246:LEU:HD13	1.99	0.45
1:B:26:PHE:O	1:B:30:VAL:HG23	2.16	0.45
1:A:91:LYS:NZ	3:A:334:NAP:N7N	2.64	0.45
1:A:258:ARG:NE	1:A:261:GLU:OE1	2.49	0.45
1:A:189:VAL:HG21	1:A:246:LEU:O	2.16	0.45
1:B:52:MET:HA	1:B:55:GLU:HG2	1.98	0.45
1:A:250:THR:HG23	1:A:251:PRO:HD2	1.97	0.45
1:A:197:PRO:O	1:A:198:ILE:HD13	2.17	0.45
1:B:195:GLU:OE2	1:B:253:LYS:HE2	2.16	0.45
1:B:268:ILE:HG12	1:B:285:ILE:HD11	1.98	0.45
1:B:28:ARG:O	1:B:28:ARG:HD3	2.16	0.45
1:B:327:ASP:HA	1:B:330:LEU:HD23	2.00	0.44
1:B:258:ARG:HB3	1:B:259:PRO:HD2	1.99	0.44
1:A:245:ALA:HB2	1:A:326:PRO:HB3	2.00	0.44
1:B:17:GLY:HA2	3:B:334:NAP:H1B	2.00	0.44
1:A:209:THR:OG1	1:A:212:GLU:HG3	2.17	0.44
1:A:234:ILE:HA	1:A:235:PRO:HD3	1.82	0.44
1:A:130:SER:HB3	1:A:170:ARG:HB2	2.00	0.44
1:A:182:VAL:HA	1:A:246:LEU:CD2	2.48	0.44
1:A:309:VAL:CG1	1:A:310:ALA:N	2.80	0.44
1:A:7:MET:SD	1:A:222:LYS:HA	2.57	0.44
1:A:258:ARG:HB3	1:A:259:PRO:CD	2.48	0.44
1:A:201:ILE:HG22	1:A:201:ILE:O	2.18	0.44
1:A:183:PRO:O	1:A:187:LYS:HG3	2.18	0.43
1:A:135:ALA:HA	5:A:358:HOH:O	2.17	0.43
1:B:159:LYS:HZ1	1:B:292:GLN:C	2.22	0.43
1:A:189:VAL:HG11	1:A:248:PRO:HD2	2.00	0.43
1:A:242:LEU:O	1:A:246:LEU:HB3	2.18	0.43
1:B:8:LEU:CD1	1:B:34:THR:HG21	2.44	0.43
1:B:78:LEU:HD12	1:B:117:ALA:CB	2.49	0.43
1:A:44:ARG:NH1	1:B:44:ARG:HB3	2.33	0.43
1:B:204:THR:HG23	1:B:317:SER:OG	2.18	0.43
1:A:175:VAL:HG12	1:A:207:TRP:CE3	2.53	0.43
1:B:241:ASP:HB3	1:B:326:PRO:HD3	2.01	0.43
1:A:184:PHE:O	1:A:188:LEU:HG	2.18	0.43
1:A:195:GLU:CG	1:A:253:LYS:HB2	2.49	0.43
1:B:130:SER:OG	1:B:131:THR:N	2.51	0.43
3:B:334:NAP:H8A	5:B:369:HOH:O	2.18	0.43
1:B:100:PRO:HA	1:B:140:LEU:CD2	2.49	0.43
1:A:174:VAL:HG11	1:A:210:LEU:CD1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLU:HG3	1:B:56:PHE:HD1	1.83	0.42
1:A:206:PHE:CD1	1:A:317:SER:HB3	2.54	0.42
1:A:207:TRP:HD1	1:A:237:MET:HB3	1.84	0.42
1:B:47:LEU:O	1:B:51:GLU:HG3	2.19	0.42
1:B:320:ASN:O	1:B:323:TRP:NE1	2.48	0.42
1:A:203:MET:SD	1:A:263:LEU:HA	2.59	0.42
1:B:228:GLU:HG3	1:B:297:TYR:CD1	2.54	0.42
1:A:8:LEU:HD13	1:A:83:ILE:HD12	2.02	0.42
1:A:253:LYS:HG2	1:A:254:ILE:N	2.28	0.42
1:A:214:VAL:O	1:A:218:LEU:HD23	2.19	0.42
1:B:190:GLN:HG2	1:B:190:GLN:O	2.20	0.42
1:B:189:VAL:HG21	1:B:247:ALA:HB2	2.02	0.42
1:B:174:VAL:O	1:B:177:SER:HB2	2.20	0.42
1:A:111:ALA:HB1	1:A:152:PHE:CE2	2.55	0.42
1:A:302:LEU:O	1:A:304:GLU:HG3	2.20	0.42
1:B:200:ASP:OD1	1:B:201:ILE:N	2.52	0.42
1:B:134:ALA:O	1:B:137:PRO:HD3	2.20	0.42
1:B:192:LYS:O	1:B:193:ALA:C	2.57	0.42
1:B:188:LEU:C	1:B:190:GLN:H	2.24	0.41
1:B:247:ALA:HB1	1:B:250:THR:HB	2.02	0.41
1:A:132:ASP:OD2	1:A:265:GLU:HB3	2.21	0.41
1:A:313:PHE:CZ	1:A:315:TYR:HB2	2.54	0.41
1:A:136:ASN:N	1:A:137:PRO:CD	2.83	0.41
1:A:279:PHE:HB2	1:A:282:PHE:O	2.19	0.41
1:A:172:GLY:O	3:A:334:NAP:H4N	2.21	0.41
1:B:16:THR:OG1	1:B:86:HIS:HA	2.21	0.41
1:A:14:LEU:O	1:A:84:CYS:HA	2.20	0.41
1:B:186:LYS:HZ1	1:B:333:LEU:C	2.24	0.41
1:A:26:PHE:CZ	1:A:85:ILE:HG13	2.56	0.41
1:B:182:VAL:HG13	1:B:246:LEU:HD11	2.03	0.41
1:B:100:PRO:HB3	1:B:140:LEU:HD22	2.03	0.41
1:A:258:ARG:HB3	1:A:259:PRO:HD2	2.02	0.41
1:B:14:LEU:C	1:B:14:LEU:HD23	2.41	0.41
1:B:186:LYS:HZ2	1:B:333:LEU:CD2	2.26	0.40
1:B:181:VAL:HG13	1:B:182:VAL:HG23	2.04	0.40
1:B:273:SER:OG	1:B:313:PHE:HB3	2.21	0.40
1:B:274:HIS:CE1	1:B:275:LEU:HG	2.55	0.40
1:B:181:VAL:CG1	1:B:182:VAL:H	2.23	0.40
1:A:236:SER:H	1:A:320:ASN:HD22	1.69	0.40
1:A:242:LEU:HA	1:A:329:LEU:CD2	2.52	0.40
1:A:106:THR:O	1:A:110:GLY:HA3	2.21	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	327/344 (95%)	286 (88%)	31 (10%)	10 (3%)	5	8
1	B	325/344 (94%)	286 (88%)	25 (8%)	14 (4%)	3	4
All	All	652/688 (95%)	572 (88%)	56 (9%)	24 (4%)	4	5

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	PRO
1	B	161	SER
1	B	254	ILE
1	A	158	PHE
1	A	160	GLY
1	A	190	GLN
1	B	177	SER
1	B	178	ARG
1	B	330	LEU
1	A	191	ASN
1	A	260	GLY
1	A	303	HIS
1	B	183	PRO
1	B	255	ILE
1	B	331	LYS
1	A	192	LYS
1	A	331	LYS
1	B	160	GLY
1	B	311	PRO
1	B	326	PRO
1	A	311	PRO
1	B	181	VAL

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Mol	Chain	Res	Type
1	B	176	GLY
1	B	259	PRO

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	290/304 (95%)	290 (100%)	0	100	100
1	B	288/304 (95%)	283 (98%)	5 (2%)	68	88
All	All	578/608 (95%)	573 (99%)	5 (1%)	84	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	SER
1	B	60	ARG
1	B	185	PHE
1	B	315	TYR
1	B	318	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	125	GLN
1	A	136	ASN
1	A	165	GLN
1	A	173	ASN
1	A	190	GLN
1	A	274	HIS
1	A	286	GLN
1	A	318	HIS
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	322	GLN
1	B	75	ASN
1	B	136	ASN
1	B	163	GLN
1	B	165	GLN
1	B	173	ASN
1	B	191	ASN
1	B	286	GLN
1	B	320	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAP	A	334	-	42,52,52	1.57	11 (26%)	54,80,80	1.49	9 (16%)
2	GDU	A	335	-	29,38,38	1.32	3 (10%)	43,58,58	2.28	3 (6%)
3	NAP	B	334	-	42,52,52	1.56	9 (21%)	54,80,80	1.47	8 (14%)
2	GDU	B	335	-	29,38,38	1.35	3 (10%)	43,58,58	2.27	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	B	336	-	11,12,12	0.58	0	14,16,16	1.46	2 (14%)

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	NAP	A	334	-	-	0/27/67/67	0/5/5/5
2	GDU	A	335	-	-	0/19/59/59	0/3/3/3
3	NAP	B	334	-	-	0/27/67/67	0/5/5/5
2	GDU	B	335	-	-	0/19/59/59	0/3/3/3
4	MES	B	336	-	-	0/6/14/14	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	334	NAP	C2D-C3D	-2.03	1.47	1.53
3	A	334	NAP	C7N-N7N	2.04	1.37	1.33
3	A	334	NAP	P2B-O2X	2.06	1.62	1.54
3	B	334	NAP	C5N-C4N	2.07	1.43	1.38
3	A	334	NAP	C5N-C4N	2.20	1.43	1.38
3	B	334	NAP	C2N-C3N	2.29	1.42	1.39
3	B	334	NAP	C7N-N7N	2.29	1.37	1.33
3	A	334	NAP	C2A-N3A	2.30	1.36	1.32
3	A	334	NAP	C4A-N3A	2.51	1.39	1.35
3	B	334	NAP	C4A-N3A	2.53	1.39	1.35
3	A	334	NAP	C4N-C3N	2.53	1.43	1.39
3	B	334	NAP	PN-O1N	2.56	1.60	1.51
3	A	334	NAP	PN-O1N	2.69	1.61	1.51
3	B	334	NAP	C4N-C3N	2.77	1.44	1.39
3	A	334	NAP	PA-O1A	2.90	1.61	1.51
2	A	335	GDU	PB-O1B	2.91	1.61	1.51
3	B	334	NAP	PA-O1A	2.94	1.61	1.51
2	B	335	GDU	PA-O1A	2.95	1.61	1.51
2	A	335	GDU	PA-O1A	3.03	1.62	1.51
2	B	335	GDU	PB-O1B	3.06	1.62	1.51
3	B	334	NAP	P2B-O1X	3.19	1.61	1.51
3	B	334	NAP	C2A-N1A	3.33	1.40	1.33
3	A	334	NAP	P2B-O1X	3.38	1.62	1.51
3	A	334	NAP	C2A-N1A	3.48	1.40	1.33
2	A	335	GDU	C4-N3	3.57	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	GDU	C4-N3	3.68	1.39	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	335	GDU	O5'-C1'-O3B	-6.68	102.55	111.36
2	A	335	GDU	O5'-C1'-O3B	-6.61	102.64	111.36
3	B	334	NAP	C3N-C2N-N1N	-3.95	115.81	120.36
3	A	334	NAP	C3N-C2N-N1N	-3.83	115.95	120.36
3	A	334	NAP	C3N-C7N-N7N	-3.68	113.79	117.82
4	B	336	MES	O2S-S-C8	-3.33	104.06	106.91
2	B	335	GDU	C5-C4-N3	-3.29	114.69	123.12
3	B	334	NAP	C3N-C7N-N7N	-3.23	114.28	117.82
2	A	335	GDU	C5-C4-N3	-3.22	114.86	123.12
3	B	334	NAP	C1B-N9A-C4A	-2.92	122.54	126.94
4	B	336	MES	C7-C8-S	-2.55	104.61	112.51
3	A	334	NAP	C1B-N9A-C4A	-2.49	123.19	126.94
3	B	334	NAP	N3A-C2A-N1A	-2.47	127.00	128.89
3	A	334	NAP	N3A-C2A-N1A	-2.36	127.08	128.89
3	A	334	NAP	C5N-C6N-N1N	-2.17	116.72	120.47
3	B	334	NAP	C5N-C6N-N1N	-2.02	116.97	120.47
3	B	334	NAP	O2B-P2B-O1X	2.04	112.20	107.11
3	A	334	NAP	C4A-C5A-N7A	2.12	111.43	109.48
3	B	334	NAP	N6A-C6A-N1A	2.21	123.95	119.20
3	A	334	NAP	O2B-P2B-O1X	2.35	112.98	107.11
3	A	334	NAP	N6A-C6A-N1A	2.38	124.30	119.20
3	B	334	NAP	O7N-C7N-C3N	3.70	123.62	119.59
3	A	334	NAP	O7N-C7N-C3N	4.04	124.00	119.59
2	B	335	GDU	C4-N3-C2	11.70	125.73	114.14
2	A	335	GDU	C4-N3-C2	11.74	125.77	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	334	NAP	5	0
3	B	334	NAP	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	329/344 (95%)	0.56	53 (16%)	3 1	10, 40, 80, 80	0
1	B	327/344 (95%)	0.38	39 (11%)	6 4	12, 35, 80, 80	0
All	All	656/688 (95%)	0.47	92 (14%)	4 2	10, 37, 80, 80	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	SER	10.6
1	B	161	SER	8.5
1	A	162	SER	8.1
1	A	196	ILE	7.9
1	B	193	ALA	7.3
1	A	249	ASN	6.5
1	A	184	PHE	6.2
1	A	324	LEU	6.0
1	B	162	SER	6.0
1	B	249	ASN	6.0
1	A	188	LEU	6.0
1	B	248	PRO	5.8
1	B	192	LYS	5.6
1	B	189	VAL	5.2
1	B	190	GLN	5.2
1	B	196	ILE	5.2
1	B	160	GLY	5.1
1	A	329	LEU	5.1
1	A	194	SER	5.0
1	A	243	ALA	5.0
1	B	188	LEU	4.8
1	A	330	LEU	4.6
1	B	331	LYS	4.6
1	B	191	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	332	LEU	4.4
1	B	246	LEU	4.4
1	B	247	ALA	4.3
1	B	330	LEU	4.1
1	B	195	GLU	4.1
1	A	333	LEU	4.0
1	B	194	SER	4.0
1	A	254	ILE	4.0
1	B	159	LYS	3.9
1	A	239	MET	3.8
1	A	195	GLU	3.8
1	A	201	ILE	3.8
1	A	247	ALA	3.7
1	A	326	PRO	3.6
1	A	158	PHE	3.6
1	B	245	ALA	3.5
1	A	252	THR	3.5
1	B	252	THR	3.5
1	B	324	LEU	3.4
1	A	253	LYS	3.4
1	A	244	LYS	3.4
1	B	254	ILE	3.4
1	A	256	GLY	3.4
1	B	201	ILE	3.2
1	B	253	LYS	3.2
1	A	255	ILE	3.2
1	A	248	PRO	3.2
1	A	193	ALA	3.1
1	B	250	THR	3.1
1	B	326	PRO	3.1
1	B	333	LEU	3.1
1	B	329	LEU	3.0
1	A	246	LEU	3.0
1	A	192	LYS	2.9
1	A	323	TRP	2.9
1	B	243	ALA	2.9
1	A	199	THR	2.9
1	A	245	ALA	2.9
1	A	207	TRP	2.8
1	A	299	LEU	2.8
1	B	251	PRO	2.8
1	A	7	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	2.7
1	A	183	PRO	2.7
1	A	307	GLN	2.7
1	A	241	ASP	2.6
1	B	244	LYS	2.6
1	A	159	LYS	2.6
1	A	240	THR	2.6
1	A	190	GLN	2.5
1	A	178	ARG	2.5
1	A	327	ASP	2.4
1	B	332	LEU	2.4
1	A	185	PHE	2.4
1	A	298	THR	2.3
1	A	251	PRO	2.3
1	A	163	GLN	2.3
1	B	327	ASP	2.3
1	A	198	ILE	2.3
1	B	237	MET	2.2
1	B	242	LEU	2.2
1	B	163	GLN	2.2
1	B	325	GLU	2.2
1	A	242	LEU	2.1
1	A	181	VAL	2.1
1	A	303	HIS	2.1
1	B	256	GLY	2.0
1	A	191	ASN	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	MES	B	336	12/12	0.91	0.20	2.80	60,61,61,61	0
3	NAP	A	334	48/48	0.96	0.19	0.59	18,36,62,66	0
3	NAP	B	334	48/48	0.97	0.18	0.44	14,31,67,71	0
2	GDU	A	335	36/36	0.77	0.23	-0.17	77,79,80,80	0
2	GDU	B	335	36/36	0.85	0.20	-0.34	59,68,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.