Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:19 PM GMT

PDB ID	:	1T2A
Title	:	Crystal structure of human GDP-D-mannose 4,6-dehydratase
Authors	:	Walker, J.R.; Vedadi, M.; Sharma, S.; Houston, S.; Wasney, G.; Loppnau, P.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; Oppermann, U.
Deposited on	:	2004-04-20
Resolution	:	1.84 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

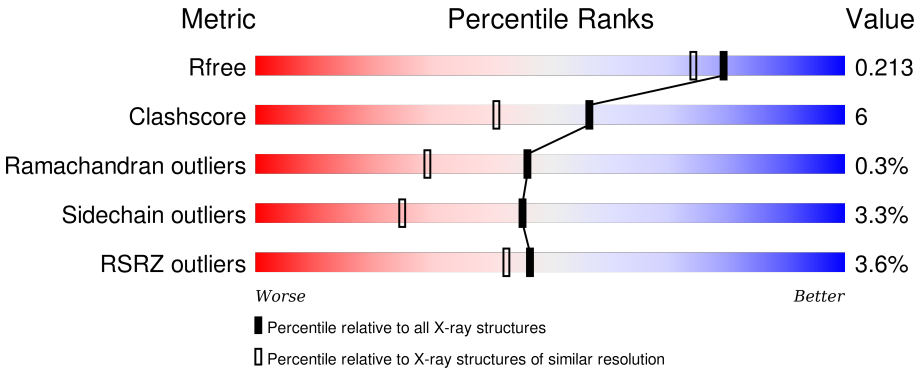
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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 <=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	375	2% 76% 12% • 10%
1	B	375	3% 77% 11% • 10%
1	C	375	6% 74% 15% • 10%
1	D	375	2% 79% 9% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12166 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 GDP-mannose 4,6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2718	1735	467	506	10			
1	B	338	Total	C	N	O	S	0	0	0
			2718	1735	467	506	10			
1	C	338	Total	C	N	O	S	0	0	0
			2718	1735	467	506	10			
1	D	337	Total	C	N	O	S	0	0	0
			2710	1731	465	504	10			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	CLONING ARTIFACT	UNP O60547
A	1	GLY	-	CLONING ARTIFACT	UNP O60547
A	3	SER	-	CLONING ARTIFACT	UNP O60547
A	3	SER	-	CLONING ARTIFACT	UNP O60547
A	5	HIS	-	CLONING ARTIFACT	UNP O60547
A	6	HIS	-	CLONING ARTIFACT	UNP O60547
A	7	HIS	-	CLONING ARTIFACT	UNP O60547
A	8	HIS	-	CLONING ARTIFACT	UNP O60547
A	9	HIS	-	CLONING ARTIFACT	UNP O60547
A	9	HIS	-	CLONING ARTIFACT	UNP O60547
A	11	SER	-	CLONING ARTIFACT	UNP O60547
A	11	SER	-	CLONING ARTIFACT	UNP O60547
A	12	GLY	-	CLONING ARTIFACT	UNP O60547
A	13	ARG	-	CLONING ARTIFACT	UNP O60547
A	14	GLU	-	CLONING ARTIFACT	UNP O60547
A	15	ASN	-	CLONING ARTIFACT	UNP O60547
A	16	LYS	-	CLONING ARTIFACT	UNP O60547
A	17	TYR	-	CLONING ARTIFACT	UNP O60547
A	18	PHE	-	CLONING ARTIFACT	UNP O60547
A	19	GLN	-	CLONING ARTIFACT	UNP O60547
A	20	GLY	-	CLONING ARTIFACT	UNP O60547

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	HIS	-	CLONING ARTIFACT	UNP O60547
A	22	MET	-	CLONING ARTIFACT	UNP O60547
A	373	GLY	-	CLONING ARTIFACT	UNP O60547
A	374	SER	-	CLONING ARTIFACT	UNP O60547
B	0	MET	-	CLONING ARTIFACT	UNP O60547
B	1	GLY	-	CLONING ARTIFACT	UNP O60547
B	3	SER	-	CLONING ARTIFACT	UNP O60547
B	3	SER	-	CLONING ARTIFACT	UNP O60547
B	5	HIS	-	CLONING ARTIFACT	UNP O60547
B	6	HIS	-	CLONING ARTIFACT	UNP O60547
B	7	HIS	-	CLONING ARTIFACT	UNP O60547
B	8	HIS	-	CLONING ARTIFACT	UNP O60547
B	9	HIS	-	CLONING ARTIFACT	UNP O60547
B	9	HIS	-	CLONING ARTIFACT	UNP O60547
B	11	SER	-	CLONING ARTIFACT	UNP O60547
B	11	SER	-	CLONING ARTIFACT	UNP O60547
B	12	GLY	-	CLONING ARTIFACT	UNP O60547
B	13	ARG	-	CLONING ARTIFACT	UNP O60547
B	14	GLU	-	CLONING ARTIFACT	UNP O60547
B	15	ASN	-	CLONING ARTIFACT	UNP O60547
B	16	LYS	-	CLONING ARTIFACT	UNP O60547
B	17	TYR	-	CLONING ARTIFACT	UNP O60547
B	18	PHE	-	CLONING ARTIFACT	UNP O60547
B	19	GLN	-	CLONING ARTIFACT	UNP O60547
B	20	GLY	-	CLONING ARTIFACT	UNP O60547
B	21	HIS	-	CLONING ARTIFACT	UNP O60547
B	22	MET	-	CLONING ARTIFACT	UNP O60547
B	373	GLY	-	CLONING ARTIFACT	UNP O60547
B	374	SER	-	CLONING ARTIFACT	UNP O60547
C	0	MET	-	CLONING ARTIFACT	UNP O60547
C	1	GLY	-	CLONING ARTIFACT	UNP O60547
C	3	SER	-	CLONING ARTIFACT	UNP O60547
C	3	SER	-	CLONING ARTIFACT	UNP O60547
C	5	HIS	-	CLONING ARTIFACT	UNP O60547
C	6	HIS	-	CLONING ARTIFACT	UNP O60547
C	7	HIS	-	CLONING ARTIFACT	UNP O60547
C	8	HIS	-	CLONING ARTIFACT	UNP O60547
C	9	HIS	-	CLONING ARTIFACT	UNP O60547
C	9	HIS	-	CLONING ARTIFACT	UNP O60547
C	11	SER	-	CLONING ARTIFACT	UNP O60547
C	11	SER	-	CLONING ARTIFACT	UNP O60547
C	12	GLY	-	CLONING ARTIFACT	UNP O60547

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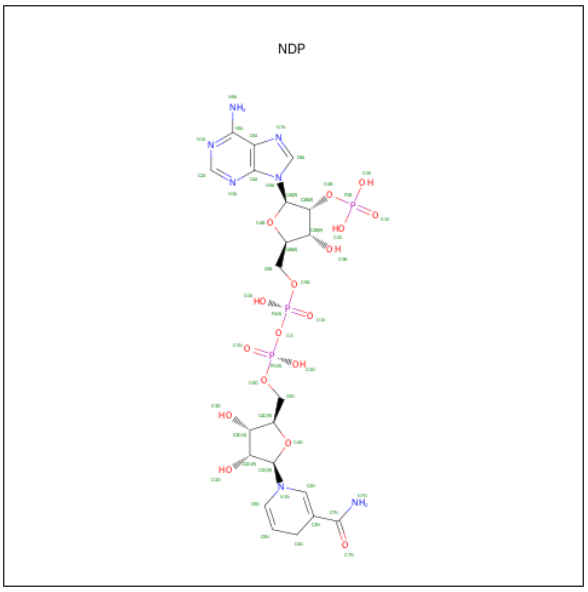
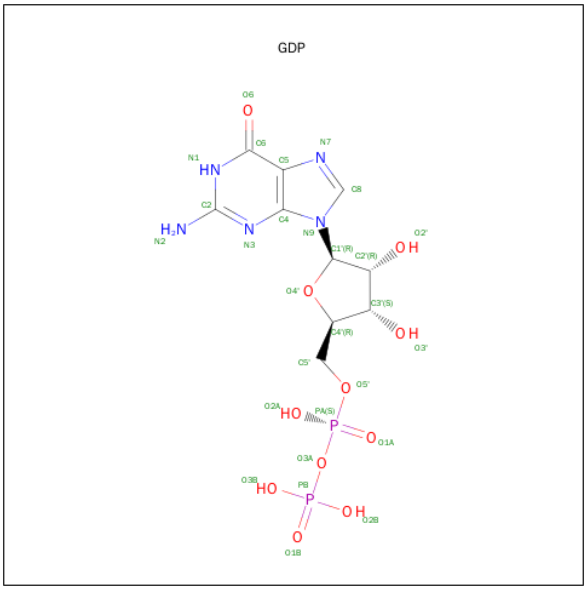
Chain	Residue	Modelled	Actual	Comment	Reference
C	13	ARG	-	CLONING ARTIFACT	UNP O60547
C	14	GLU	-	CLONING ARTIFACT	UNP O60547
C	15	ASN	-	CLONING ARTIFACT	UNP O60547
C	16	LYS	-	CLONING ARTIFACT	UNP O60547
C	17	TYR	-	CLONING ARTIFACT	UNP O60547
C	18	PHE	-	CLONING ARTIFACT	UNP O60547
C	19	GLN	-	CLONING ARTIFACT	UNP O60547
C	20	GLY	-	CLONING ARTIFACT	UNP O60547
C	21	HIS	-	CLONING ARTIFACT	UNP O60547
C	22	MET	-	CLONING ARTIFACT	UNP O60547
C	373	GLY	-	CLONING ARTIFACT	UNP O60547
C	374	SER	-	CLONING ARTIFACT	UNP O60547
D	0	MET	-	CLONING ARTIFACT	UNP O60547
D	1	GLY	-	CLONING ARTIFACT	UNP O60547
D	3	SER	-	CLONING ARTIFACT	UNP O60547
D	3	SER	-	CLONING ARTIFACT	UNP O60547
D	5	HIS	-	CLONING ARTIFACT	UNP O60547
D	6	HIS	-	CLONING ARTIFACT	UNP O60547
D	7	HIS	-	CLONING ARTIFACT	UNP O60547
D	8	HIS	-	CLONING ARTIFACT	UNP O60547
D	9	HIS	-	CLONING ARTIFACT	UNP O60547
D	9	HIS	-	CLONING ARTIFACT	UNP O60547
D	11	SER	-	CLONING ARTIFACT	UNP O60547
D	11	SER	-	CLONING ARTIFACT	UNP O60547
D	12	GLY	-	CLONING ARTIFACT	UNP O60547
D	13	ARG	-	CLONING ARTIFACT	UNP O60547
D	14	GLU	-	CLONING ARTIFACT	UNP O60547
D	15	ASN	-	CLONING ARTIFACT	UNP O60547
D	16	LYS	-	CLONING ARTIFACT	UNP O60547
D	17	TYR	-	CLONING ARTIFACT	UNP O60547
D	18	PHE	-	CLONING ARTIFACT	UNP O60547
D	19	GLN	-	CLONING ARTIFACT	UNP O60547
D	20	GLY	-	CLONING ARTIFACT	UNP O60547
D	21	HIS	-	CLONING ARTIFACT	UNP O60547
D	22	MET	-	CLONING ARTIFACT	UNP O60547
D	373	GLY	-	CLONING ARTIFACT	UNP O60547
D	374	SER	-	CLONING ARTIFACT	UNP O60547

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is water.

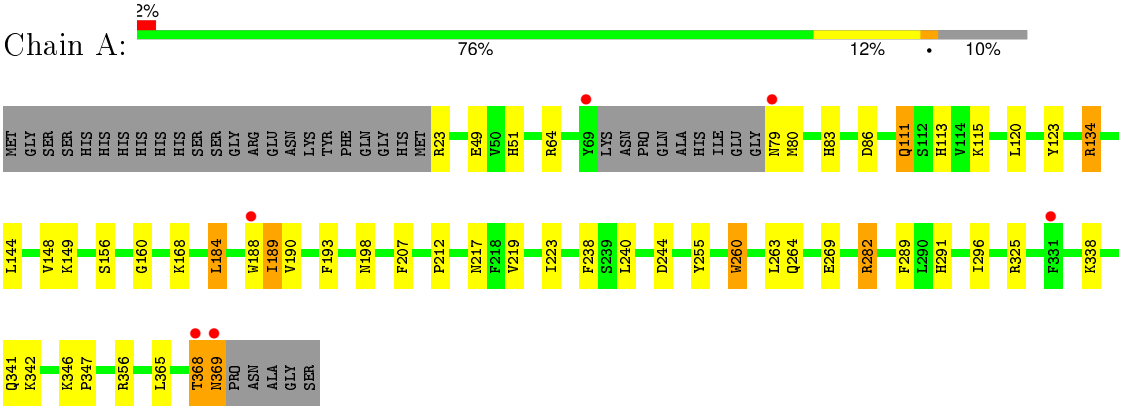
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	285	Total	O	0	0
			285	285		
4	B	256	Total	O	0	0
			256	256		
4	C	199	Total	O	0	0
			199	199		
4	D	258	Total	O	0	0
			258	258		

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.

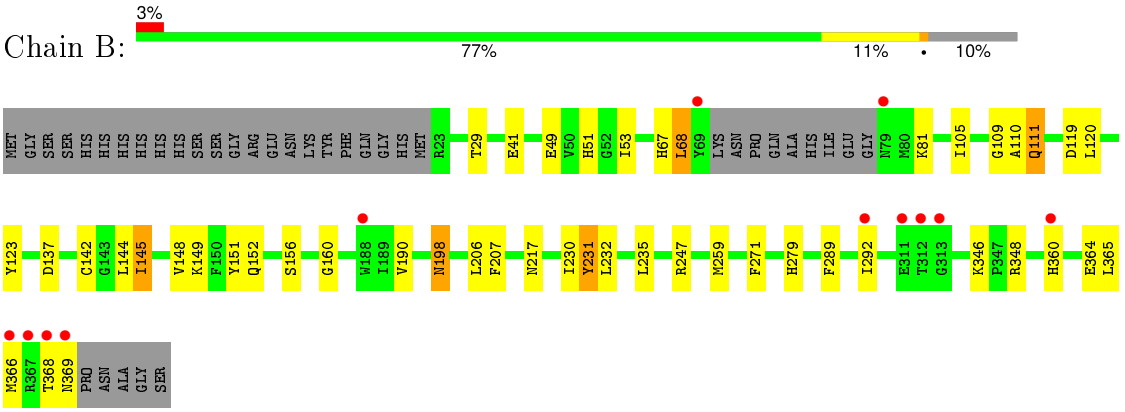
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain A:



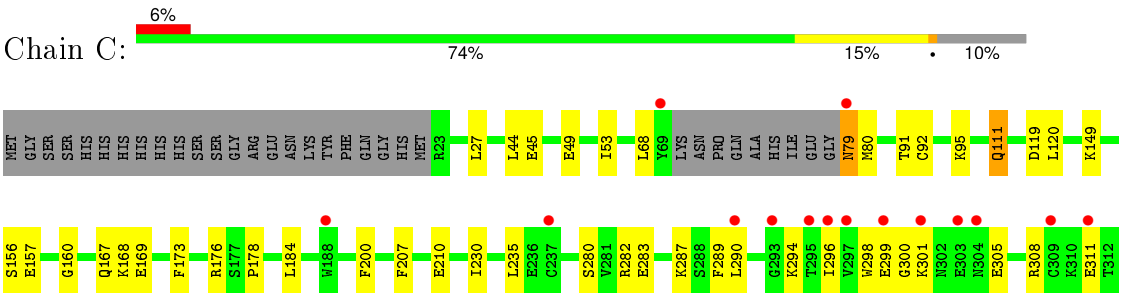
- Molecule 1: GDP-mannose 4,6 dehydratase

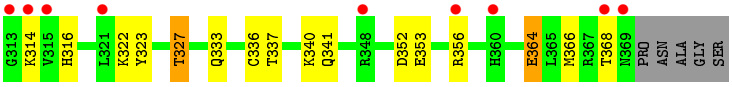
Chain B:



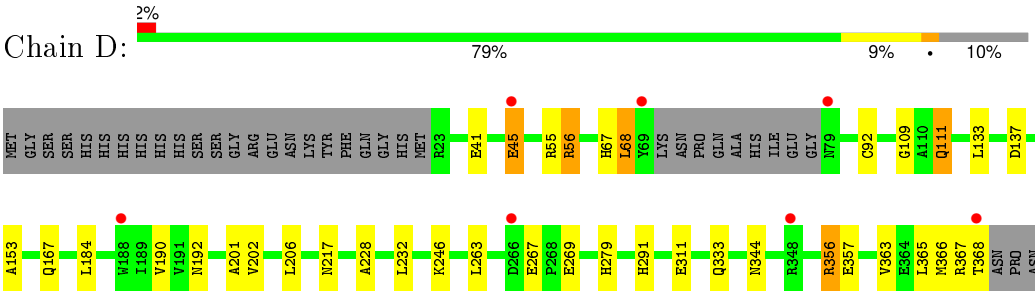
- Molecule 1: GDP-mannose 4,6 dehydratase

Chain C:





• Molecule 1: GDP-mannose 4,6 dehydratase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.59Å 122.06Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.93 – 1.84 35.75 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (24.93-1.84) 98.3 (35.75-1.84)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.173 , 0.212 0.173 , 0.213	Depositor DCC
R_{free} test set	6496 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 59.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 129273 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12166	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.375 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: GDP, NDP

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	1.16	3/2777 (0.1%)	1.21	11/3755 (0.3%)
1	B	1.09	3/2777 (0.1%)	1.20	6/3755 (0.2%)
1	C	0.97	2/2777 (0.1%)	0.90	2/3755 (0.1%)
1	D	1.15	4/2769 (0.1%)	0.96	4/3744 (0.1%)
All	All	1.10	12/11100 (0.1%)	1.08	23/15009 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	GLU	CD-OE1	6.46	1.32	1.25
1	D	357	GLU	CD-OE2	-6.34	1.18	1.25
1	A	260	TRP	CE3-CZ3	6.07	1.48	1.38
1	D	311	GLU	CG-CD	5.91	1.60	1.51
1	A	134	ARG	CD-NE	-5.89	1.36	1.46
1	D	228	ALA	CA-CB	5.41	1.63	1.52
1	B	110	ALA	CA-CB	5.29	1.63	1.52
1	C	169	GLU	CG-CD	5.23	1.59	1.51
1	A	190	VAL	CB-CG2	5.19	1.63	1.52
1	D	153	ALA	CA-CB	5.17	1.63	1.52
1	B	247	ARG	CD-NE	-5.08	1.37	1.46
1	B	271	PHE	CD1-CE1	5.03	1.49	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	ARG	NE-CZ-NH2	-32.81	103.90	120.30
1	A	134	ARG	NE-CZ-NH1	31.96	136.28	120.30
1	B	247	ARG	NE-CZ-NH1	30.76	135.68	120.30
1	A	134	ARG	NE-CZ-NH2	-29.80	105.40	120.30
1	B	247	ARG	CD-NE-CZ	10.43	138.21	123.60
1	A	134	ARG	CD-NE-CZ	9.56	136.98	123.60
1	B	247	ARG	CG-CD-NE	-8.19	94.59	111.80
1	D	55	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	325	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	111	GLN	N-CA-C	-6.86	92.48	111.00
1	A	111	GLN	N-CA-C	-6.37	93.79	111.00
1	C	111	GLN	N-CA-C	-6.28	94.05	111.00
1	A	134	ARG	CG-CD-NE	-6.04	99.12	111.80
1	D	111	GLN	N-CA-C	-6.02	94.73	111.00
1	A	282	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	D	356	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	C	49	GLU	N-CA-C	-5.37	96.50	111.00
1	B	49	GLU	N-CA-C	-5.32	96.63	111.00
1	A	149	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	49	GLU	N-CA-C	-5.19	97.00	111.00
1	A	86	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	A	64	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	56	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	231	TYR	Sidechain

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	2718	0	2687	35	0
1	B	2718	0	2687	30	0
1	C	2718	0	2687	42	0
1	D	2710	0	2681	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	26	0	0
2	B	48	0	26	2	0
2	C	48	0	26	0	0
2	D	48	0	26	2	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	285	0	0	5	0
4	B	256	0	0	7	0
4	C	199	0	0	1	0
4	D	258	0	0	7	0
All	All	12166	0	10894	134	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 6.

All (134) 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:C:327:THR:HG21	1:D:192:ASN:HD21	1.29	0.95
1:D:145:ILE:HD12	1:D:145:ILE:H	1.40	0.87
1:A:244:ASP:OD1	1:A:282:ARG:NH1	2.07	0.87
1:D:167:GLN:HE22	1:D:333:GLN:H	1.21	0.85
1:C:27:LEU:HD11	1:C:53:ILE:HD11	1.58	0.84
1:D:217:ASN:ND2	4:D:1391:HOH:O	2.05	0.84
1:C:167:GLN:HE22	1:C:333:GLN:H	1.30	0.80
1:A:341:GLN:HG3	4:A:1148:HOH:O	1.83	0.79
1:C:27:LEU:HD11	1:C:53:ILE:CD1	2.13	0.78
1:D:140:LYS:HA	1:D:145:ILE:HG13	1.67	0.77
1:C:353:GLU:HG3	1:C:356:ARG:NH2	2.01	0.76
1:A:189:ILE:HD13	1:A:189:ILE:O	1.86	0.75
1:B:149:LYS:HE2	4:B:1212:HOH:O	1.85	0.74
1:C:294:LYS:HE2	1:C:316:HIS:NE2	2.03	0.74
1:A:346:LYS:HG3	1:A:347:PRO:HD2	1.70	0.73
1:A:368:THR:O	1:A:369:ASN:HB2	1.91	0.70
1:C:300:GLY:O	1:C:301:LYS:HD3	1.92	0.70
1:C:91:THR:HG22	1:C:95:LYS:NZ	2.07	0.70
1:D:145:ILE:CD1	1:D:145:ILE:H	2.05	0.69
1:A:223:ILE:HD11	1:A:240:LEU:HD11	1.73	0.69
1:B:120:LEU:HG	1:B:123:TYR:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASP:HB2	4:B:1317:HOH:O	1.94	0.68
1:C:282:ARG:NH1	1:C:305:GLU:OE2	2.27	0.67
1:C:176:ARG:O	1:C:327:THR:HG23	1.94	0.67
1:D:217:ASN:OD1	4:D:1560:HOH:O	2.12	0.67
1:C:327:THR:HG21	1:D:192:ASN:ND2	2.08	0.66
1:C:149:LYS:HD2	1:C:200:PHE:CG	2.31	0.66
1:C:322:LYS:HE3	1:C:323:TYR:CZ	2.33	0.63
1:B:231:TYR:HB2	1:B:292:ILE:CG1	2.30	0.62
1:A:120:LEU:HG	1:A:123:TYR:HB3	1.82	0.61
1:A:134:ARG:HD3	4:B:1161:HOH:O	2.00	0.61
1:D:202:VAL:HG13	1:D:269:GLU:O	2.00	0.61
1:A:144:LEU:HB3	1:A:148:VAL:HG13	1.82	0.60
1:A:51:HIS:ND1	1:A:83:HIS:HE1	1.99	0.60
1:C:280:SER:OG	1:C:283:GLU:HG3	2.01	0.60
1:A:269:GLU:OE1	4:A:1161:HOH:O	2.17	0.60
1:D:140:LYS:HG3	1:D:145:ILE:HG12	1.84	0.59
1:C:91:THR:HG22	1:C:95:LYS:HZ3	1.67	0.59
1:A:291:HIS:HE1	4:A:1196:HOH:O	1.86	0.58
1:C:337:THR:O	1:C:341:GLN:HG3	2.05	0.57
1:C:336:CYS:SG	1:C:340:LYS:HE3	2.46	0.56
1:A:189:ILE:C	1:A:189:ILE:HD13	2.25	0.55
1:A:368:THR:O	1:A:369:ASN:CB	2.54	0.55
4:B:1156:HOH:O	1:C:120:LEU:HD11	2.06	0.55
1:B:151:TYR:CZ	1:B:259:MET:HG2	2.42	0.54
1:D:356:ARG:NH1	4:D:1446:HOH:O	2.41	0.54
1:A:219:VAL:O	1:A:223:ILE:HG12	2.09	0.53
1:B:368:THR:HG22	1:B:368:THR:O	2.09	0.53
1:D:246:LYS:HE3	4:D:1415:HOH:O	2.09	0.53
1:C:168:LYS:HE2	4:C:1360:HOH:O	2.09	0.52
1:C:282:ARG:HH12	1:C:305:GLU:CD	2.12	0.52
1:C:287:LYS:HE2	1:C:352:ASP:OD1	2.10	0.52
1:C:230:ILE:HA	1:C:235:LEU:O	2.09	0.52
1:D:140:LYS:HA	1:D:145:ILE:CG1	2.39	0.52
1:D:167:GLN:NE2	1:D:333:GLN:H	1.99	0.52
1:A:223:ILE:CD1	1:A:240:LEU:HD11	2.37	0.51
1:C:176:ARG:O	1:C:327:THR:CG2	2.57	0.51
1:D:45:GLU:HG3	4:D:1496:HOH:O	2.11	0.51
1:B:145:ILE:HB	4:B:1272:HOH:O	2.11	0.50
1:C:149:LYS:HD2	1:C:200:PHE:CD1	2.47	0.50
1:B:198:ASN:ND2	4:B:1323:HOH:O	2.45	0.50
1:A:189:ILE:HD11	1:A:193:PHE:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HD11	1:A:193:PHE:CE1	2.47	0.49
1:C:91:THR:HG22	1:C:95:LYS:HZ2	1.77	0.49
1:C:364:GLU:O	1:C:368:THR:HG23	2.11	0.49
1:B:109:GLY:HA2	2:B:1101:NDP:O4B	2.11	0.49
1:B:67:HIS:NE2	1:B:68:LEU:HD13	2.28	0.48
1:C:353:GLU:HG3	1:C:356:ARG:HH22	1.75	0.48
1:B:41:GLU:HG2	1:B:68:LEU:HD11	1.95	0.48
1:B:152:GLN:HB2	1:B:190:VAL:HG21	1.96	0.48
1:D:291:HIS:HD2	4:D:1326:HOH:O	1.97	0.47
1:A:184:LEU:HD22	1:A:188:TRP:CD1	2.50	0.47
1:B:279:HIS:HD2	4:B:1120:HOH:O	1.97	0.47
1:A:346:LYS:HG3	1:A:347:PRO:CD	2.41	0.47
1:B:156:SER:HB3	1:B:207:PHE:CG	2.50	0.47
1:C:176:ARG:CZ	1:C:327:THR:OG1	2.63	0.46
1:D:232:LEU:CD1	1:D:366:MET:HB2	2.45	0.46
1:B:105:ILE:HG13	1:B:148:VAL:HG21	1.96	0.46
1:D:67:HIS:CD2	1:D:68:LEU:HD13	2.51	0.46
1:D:190:VAL:HG13	1:D:201:ALA:HB1	1.98	0.46
1:C:299:GLU:O	1:C:305:GLU:HA	2.16	0.46
1:C:308:ARG:HA	1:C:314:LYS:O	2.16	0.46
1:B:289:PHE:O	1:B:292:ILE:HG22	2.15	0.45
1:C:156:SER:HB3	1:C:207:PHE:CG	2.51	0.45
1:C:167:GLN:NE2	1:C:333:GLN:H	2.06	0.45
1:A:113:HIS:CE1	1:A:115:LYS:HB3	2.51	0.45
1:A:223:ILE:HD11	1:A:240:LEU:HD21	1.98	0.45
1:A:168:LYS:HE3	4:A:1242:HOH:O	2.15	0.45
1:A:289:PHE:CD1	1:A:296:ILE:HG13	2.51	0.45
1:D:184:LEU:HD13	1:D:184:LEU:C	2.37	0.45
1:C:290:LEU:HA	1:C:290:LEU:HD12	1.81	0.44
1:C:298:TRP:C	1:C:299:GLU:HG2	2.38	0.44
1:B:346:LYS:HE3	1:B:348:ARG:NH1	2.33	0.44
1:C:289:PHE:CB	1:C:296:ILE:HD13	2.48	0.44
1:C:53:ILE:HD12	1:C:53:ILE:N	2.33	0.43
1:B:231:TYR:HB2	1:B:292:ILE:HG12	1.98	0.43
1:B:206:LEU:O	2:B:1101:NDP:H5N	2.18	0.43
1:D:232:LEU:HD12	1:D:366:MET:HB2	2.00	0.43
1:C:44:LEU:HD22	1:C:79:ASN:HB3	2.01	0.43
1:C:366:MET:CE	1:C:366:MET:HA	2.48	0.43
1:B:29:THR:HG22	1:B:53:ILE:HD12	2.00	0.43
1:B:360:HIS:O	1:B:364:GLU:HG2	2.18	0.42
1:B:67:HIS:CD2	1:B:68:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LYS:HG2	1:A:342:LYS:HD2	2.01	0.42
1:B:232:LEU:HD12	1:B:366:MET:CB	2.49	0.42
1:C:173:PHE:CD2	1:C:184:LEU:HD13	2.55	0.42
1:B:156:SER:OG	1:B:207:PHE:HA	2.20	0.42
1:D:279:HIS:HD2	4:D:1357:HOH:O	2.01	0.42
1:D:133:LEU:HD12	1:D:137:ASP:OD1	2.20	0.42
1:B:365:LEU:HD22	1:B:366:MET:CE	2.50	0.42
1:A:212:PRO:HA	4:A:1162:HOH:O	2.20	0.42
1:D:206:LEU:O	2:D:1301:NDP:H5N	2.19	0.42
1:B:230:ILE:HA	1:B:235:LEU:O	2.20	0.41
1:C:27:LEU:CD1	1:C:53:ILE:CD1	2.91	0.41
1:B:142:CYS:O	1:B:144:LEU:HD13	2.20	0.41
1:D:133:LEU:CD1	1:D:137:ASP:OD1	2.68	0.41
1:D:109:GLY:HA2	2:D:1301:NDP:O4B	2.19	0.41
1:A:223:ILE:HD13	1:A:238:PHE:HE1	1.86	0.41
1:B:232:LEU:HD12	1:B:366:MET:HB3	2.03	0.41
1:C:327:THR:HG23	1:C:327:THR:O	2.21	0.41
1:A:184:LEU:HD22	1:A:188:TRP:HD1	1.85	0.41
1:D:41:GLU:HG2	1:D:68:LEU:HD11	2.02	0.41
1:A:255:TYR:HD1	1:A:255:TYR:N	2.19	0.41
1:A:369:ASN:HA	1:A:369:ASN:HD22	1.64	0.41
1:A:255:TYR:N	1:A:255:TYR:CD1	2.89	0.41
1:A:260:TRP:O	1:A:264:GLN:HG2	2.21	0.41
1:D:56:ARG:HD3	1:D:56:ARG:C	2.41	0.41
1:B:366:MET:O	1:B:369:ASN:HB2	2.21	0.41
1:D:363:VAL:O	1:D:367:ARG:HG3	2.22	0.40
1:A:291:HIS:CD2	1:A:356:ARG:HG3	2.56	0.40
1:B:51:HIS:HA	1:B:81:LYS:O	2.21	0.40
1:A:156:SER:HB3	1:A:207:PHE:CG	2.56	0.40
1:A:223:ILE:HD13	1:A:238:PHE:CE1	2.56	0.40
1:C:27:LEU:CD1	1:C:53:ILE:HD11	2.41	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	334/375 (89%)	327 (98%)	5 (2%)	2 (1%)	30 14
1	B	334/375 (89%)	325 (97%)	8 (2%)	1 (0%)	46 29
1	C	334/375 (89%)	325 (97%)	8 (2%)	1 (0%)	46 29
1	D	333/375 (89%)	326 (98%)	7 (2%)	0	100 100
All	All	1335/1500 (89%)	1303 (98%)	28 (2%)	4 (0%)	46 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	THR
1	A	160	GLY
1	C	160	GLY
1	B	160	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	293/323 (91%)	282 (96%)	11 (4%)	40 19
1	B	293/323 (91%)	287 (98%)	6 (2%)	63 47
1	C	293/323 (91%)	281 (96%)	12 (4%)	37 16
1	D	292/323 (90%)	282 (97%)	10 (3%)	44 23
All	All	1171/1292 (91%)	1132 (97%)	39 (3%)	45 25

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	79	ASN
1	A	80	MET
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	184	LEU
1	A	189	ILE
1	A	198	ASN
1	A	217	ASN
1	A	263	LEU
1	A	365	LEU
1	A	369	ASN
1	B	68	LEU
1	B	111	GLN
1	B	137	ASP
1	B	145	ILE
1	B	198	ASN
1	B	217	ASN
1	C	68	LEU
1	C	79	ASN
1	C	80	MET
1	C	92	CYS
1	C	111	GLN
1	C	119	ASP
1	C	157	GLU
1	C	178	PRO
1	C	210	GLU
1	C	311	GLU
1	C	327	THR
1	C	364	GLU
1	D	45	GLU
1	D	68	LEU
1	D	92	CYS
1	D	111	GLN
1	D	145	ILE
1	D	263	LEU
1	D	267	GLU
1	D	344	ASN
1	D	365	LEU
1	D	368	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	83	HIS
1	A	198	ASN

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	333	GLN
1	A	341	GLN
1	A	369	ASN
1	B	198	ASN
1	B	217	ASN
1	B	279	HIS
1	B	304	ASN
1	B	333	GLN
1	B	344	ASN
1	B	369	ASN
1	C	167	GLN
1	C	279	HIS
1	C	291	HIS
1	C	333	GLN
1	C	369	ASN
1	D	167	GLN
1	D	192	ASN
1	D	279	HIS
1	D	291	HIS
1	D	333	GLN
1	D	344	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	NDP	A	1001	-	42,52,52	0.78	2 (4%)	55,80,80	1.01	4 (7%)
3	GDP	A	1002	-	23,30,30	1.04	1 (4%)	30,47,47	2.27	4 (13%)
2	NDP	B	1101	-	42,52,52	0.75	2 (4%)	55,80,80	1.01	4 (7%)
3	GDP	B	1102	-	23,30,30	1.04	1 (4%)	30,47,47	2.27	4 (13%)
2	NDP	C	1201	-	42,52,52	0.78	2 (4%)	55,80,80	1.01	4 (7%)
3	GDP	C	1202	-	23,30,30	1.03	1 (4%)	30,47,47	2.28	4 (13%)
2	NDP	D	1301	-	42,52,52	0.75	2 (4%)	55,80,80	1.01	4 (7%)
3	GDP	D	1302	-	23,30,30	1.05	1 (4%)	30,47,47	2.28	4 (13%)

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	NDP	A	1001	-	-	0/30/77/77	0/5/5/5
3	GDP	A	1002	-	-	0/12/32/32	0/3/3/3
2	NDP	B	1101	-	-	0/30/77/77	0/5/5/5
3	GDP	B	1102	-	-	0/12/32/32	0/3/3/3
2	NDP	C	1201	-	-	0/30/77/77	0/5/5/5
3	GDP	C	1202	-	-	0/12/32/32	0/3/3/3
2	NDP	D	1301	-	-	0/30/77/77	0/5/5/5
3	GDP	D	1302	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NDP	P2B-O2B	-2.51	1.52	1.60
2	C	1201	NDP	P2B-O2B	-2.47	1.52	1.60
2	B	1101	NDP	P2B-O2B	-2.30	1.53	1.60
2	D	1301	NDP	P2B-O2B	-2.27	1.53	1.60
2	D	1301	NDP	C4N-C5N	2.11	1.53	1.49
2	B	1101	NDP	C4N-C5N	2.13	1.53	1.49
2	C	1201	NDP	C4N-C5N	2.17	1.53	1.49
2	A	1001	NDP	C4N-C5N	2.18	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	GDP	C6-N1	3.61	1.39	1.33
3	C	1202	GDP	C6-N1	3.64	1.39	1.33
3	D	1302	GDP	C6-N1	3.64	1.39	1.33
3	A	1002	GDP	C6-N1	3.70	1.40	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1302	GDP	C5-C6-N1	-8.82	111.53	123.59
3	B	1102	GDP	C5-C6-N1	-8.79	111.57	123.59
3	C	1202	GDP	C5-C6-N1	-8.75	111.63	123.59
3	A	1002	GDP	C5-C6-N1	-8.74	111.63	123.59
2	D	1301	NDP	O2B-P2B-O1X	-2.91	99.83	107.11
2	B	1101	NDP	O2B-P2B-O1X	-2.91	99.85	107.11
2	C	1201	NDP	O2B-P2B-O1X	-2.83	100.03	107.11
2	A	1001	NDP	O2B-P2B-O1X	-2.82	100.08	107.11
3	C	1202	GDP	N3-C2-N1	-2.32	123.92	127.44
3	B	1102	GDP	N3-C2-N1	-2.28	123.97	127.44
3	A	1002	GDP	N3-C2-N1	-2.27	123.99	127.44
3	D	1302	GDP	N3-C2-N1	-2.26	124.01	127.44
2	A	1001	NDP	O4B-C1B-C2B	-2.24	102.56	106.60
2	C	1201	NDP	O4B-C1B-C2B	-2.23	102.56	106.60
2	B	1101	NDP	C3B-C2B-C1B	-2.16	98.56	102.73
2	D	1301	NDP	C3B-C2B-C1B	-2.15	98.56	102.73
2	A	1001	NDP	O3X-P2B-O2X	2.02	115.06	107.38
2	C	1201	NDP	O3X-P2B-O2X	2.03	115.09	107.38
2	B	1101	NDP	O3X-P2B-O2X	2.08	115.30	107.38
2	D	1301	NDP	O3X-P2B-O2X	2.08	115.32	107.38
3	A	1002	GDP	O3B-PB-O2B	2.46	116.75	107.38
3	C	1202	GDP	O3B-PB-O2B	2.47	116.79	107.38
3	B	1102	GDP	O3B-PB-O2B	2.49	116.85	107.38
3	D	1302	GDP	O3B-PB-O2B	2.49	116.86	107.38
2	B	1101	NDP	C2D-C1D-N1N	2.60	120.36	113.34
2	D	1301	NDP	C2D-C1D-N1N	2.61	120.38	113.34
2	A	1001	NDP	C2D-C1D-N1N	2.80	120.90	113.34
2	C	1201	NDP	C2D-C1D-N1N	2.80	120.91	113.34
3	A	1002	GDP	C6-N1-C2	6.47	124.92	115.94
3	D	1302	GDP	C6-N1-C2	6.50	124.96	115.94
3	C	1202	GDP	C6-N1-C2	6.51	124.98	115.94
3	B	1102	GDP	C6-N1-C2	6.52	124.99	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	NDP	2	0
2	D	1301	NDP	2	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, 95^{th} 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	338/375 (90%)	-0.28	6 (1%) 71 69	7, 18, 35, 62	1 (0%)
1	B	338/375 (90%)	-0.12	12 (3%) 46 42	7, 21, 43, 64	1 (0%)
1	C	338/375 (90%)	0.20	24 (7%) 19 17	9, 26, 47, 63	1 (0%)
1	D	337/375 (89%)	-0.10	7 (2%) 67 64	11, 21, 37, 55	1 (0%)
All	All	1351/1500 (90%)	-0.08	49 (3%) 46 42	7, 21, 43, 64	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	TYR	8.5
1	D	188	TRP	8.4
1	B	188	TRP	8.1
1	C	188	TRP	7.9
1	A	368	THR	7.8
1	A	188	TRP	7.3
1	C	69	TYR	7.3
1	A	69	TYR	6.9
1	D	69	TYR	6.9
1	B	368	THR	5.6
1	C	368	THR	5.4
1	B	369	ASN	5.3
1	A	331	PHE	4.9
1	A	369	ASN	4.1
1	C	369	ASN	4.0
1	C	313	GLY	3.8
1	D	368	THR	3.7
1	C	79	ASN	3.5
1	C	304	ASN	3.4
1	C	297	VAL	3.4
1	C	309	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	266	ASP	3.1
1	B	367	ARG	3.1
1	C	299	GLU	3.1
1	C	311	GLU	3.0
1	C	290	LEU	2.9
1	B	312	THR	2.9
1	C	321	LEU	2.9
1	C	315	VAL	2.9
1	A	79	ASN	2.7
1	B	311	GLU	2.7
1	C	314	LYS	2.7
1	C	301	LYS	2.7
1	B	366	MET	2.7
1	C	360	HIS	2.6
1	D	79	ASN	2.5
1	C	296	ILE	2.5
1	B	313	GLY	2.5
1	D	45	GLU	2.4
1	B	292	ILE	2.4
1	C	295	THR	2.4
1	C	348	ARG	2.4
1	B	360	HIS	2.3
1	C	293	GLY	2.3
1	C	356	ARG	2.2
1	C	237	CYS	2.1
1	D	348	ARG	2.1
1	C	303	GLU	2.1
1	B	79	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NDP	D	1301	48/48	0.94	0.16	1.64	11,13,17,17	0
2	NDP	A	1001	48/48	0.95	0.12	1.46	10,13,17,17	0
3	GDP	B	1102	28/28	0.92	0.12	1.37	16,18,23,25	0
2	NDP	B	1101	48/48	0.92	0.12	1.34	11,13,17,17	0
3	GDP	A	1002	28/28	0.94	0.10	0.99	14,15,21,23	0
3	GDP	D	1302	28/28	0.97	0.09	-0.11	15,17,22,24	0
2	NDP	C	1201	48/48	0.96	0.10	-0.44	10,13,17,17	0
3	GDP	C	1202	28/28	0.95	0.09	-0.65	14,15,21,23	0

6.5 Other polymers (i)

There are no such residues in this entry.