



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2016 – 12:40 AM EDT

PDB ID : 5IN4
Title : Crystal Structure of GDP-mannose 4,6 dehydratase bound to a GDP-fucose based inhibitor
Authors : Sickmier, E.A.
Deposited on : 2016-03-07
Resolution : 1.60 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

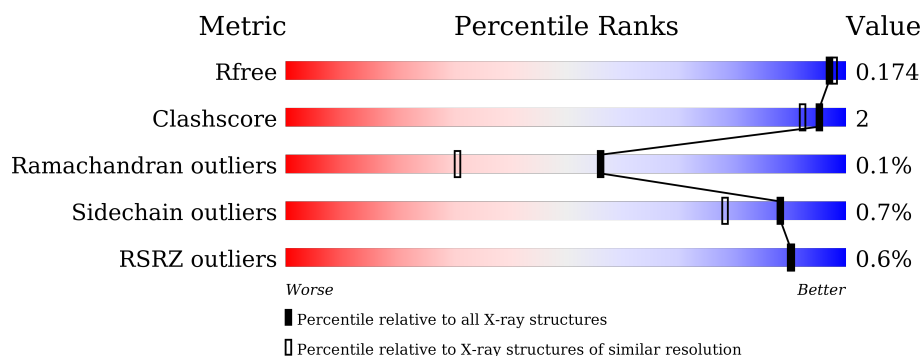
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	364	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	364	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>
1	C	364	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>
1	D	364	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13235 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	355	Total	C	N	O	S	0	2	0
			2864	1827	492	534	11			
1	B	351	Total	C	N	O	S	0	4	0
			2832	1803	488	529	12			
1	C	351	Total	C	N	O	S	0	3	0
			2824	1799	486	528	11			
1	D	351	Total	C	N	O	S	0	3	0
			2827	1800	487	528	12			

There are 56 discrepancies between the modelled and reference sequences:

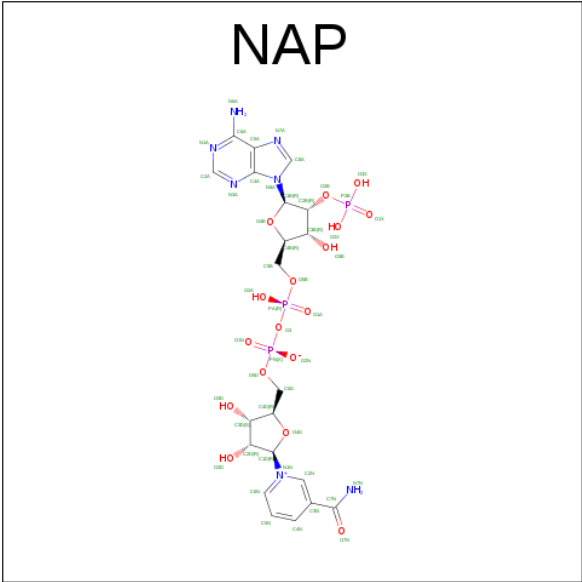
Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP O60547
A	-34	HIS	-	expression tag	UNP O60547
A	-33	HIS	-	expression tag	UNP O60547
A	-32	HIS	-	expression tag	UNP O60547
A	-31	HIS	-	expression tag	UNP O60547
A	-30	HIS	-	expression tag	UNP O60547
A	-29	HIS	-	expression tag	UNP O60547
A	-28	GLU	-	expression tag	UNP O60547
A	-27	ASN	-	expression tag	UNP O60547
A	-26	LEU	-	expression tag	UNP O60547
A	-25	TYR	-	expression tag	UNP O60547
A	-24	PHE	-	expression tag	UNP O60547
A	-23	GLN	-	expression tag	UNP O60547
A	-22	GLY	-	expression tag	UNP O60547
B	-35	MET	-	expression tag	UNP O60547
B	-34	HIS	-	expression tag	UNP O60547
B	-33	HIS	-	expression tag	UNP O60547
B	-32	HIS	-	expression tag	UNP O60547
B	-31	HIS	-	expression tag	UNP O60547
B	-30	HIS	-	expression tag	UNP O60547
B	-29	HIS	-	expression tag	UNP O60547

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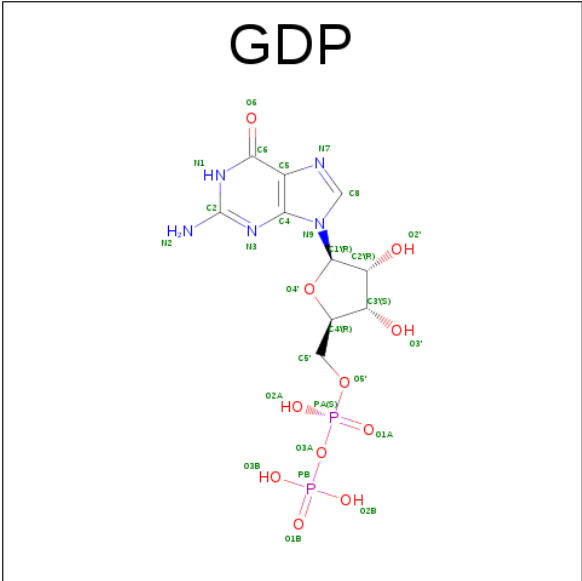
Chain	Residue	Modelled	Actual	Comment	Reference
B	-28	GLU	-	expression tag	UNP O60547
B	-27	ASN	-	expression tag	UNP O60547
B	-26	LEU	-	expression tag	UNP O60547
B	-25	TYR	-	expression tag	UNP O60547
B	-24	PHE	-	expression tag	UNP O60547
B	-23	GLN	-	expression tag	UNP O60547
B	-22	GLY	-	expression tag	UNP O60547
C	-35	MET	-	expression tag	UNP O60547
C	-34	HIS	-	expression tag	UNP O60547
C	-33	HIS	-	expression tag	UNP O60547
C	-32	HIS	-	expression tag	UNP O60547
C	-31	HIS	-	expression tag	UNP O60547
C	-30	HIS	-	expression tag	UNP O60547
C	-29	HIS	-	expression tag	UNP O60547
C	-28	GLU	-	expression tag	UNP O60547
C	-27	ASN	-	expression tag	UNP O60547
C	-26	LEU	-	expression tag	UNP O60547
C	-25	TYR	-	expression tag	UNP O60547
C	-24	PHE	-	expression tag	UNP O60547
C	-23	GLN	-	expression tag	UNP O60547
C	-22	GLY	-	expression tag	UNP O60547
D	-35	MET	-	expression tag	UNP O60547
D	-34	HIS	-	expression tag	UNP O60547
D	-33	HIS	-	expression tag	UNP O60547
D	-32	HIS	-	expression tag	UNP O60547
D	-31	HIS	-	expression tag	UNP O60547
D	-30	HIS	-	expression tag	UNP O60547
D	-29	HIS	-	expression tag	UNP O60547
D	-28	GLU	-	expression tag	UNP O60547
D	-27	ASN	-	expression tag	UNP O60547
D	-26	LEU	-	expression tag	UNP O60547
D	-25	TYR	-	expression tag	UNP O60547
D	-24	PHE	-	expression tag	UNP O60547
D	-23	GLN	-	expression tag	UNP O60547
D	-22	GLY	-	expression tag	UNP O60547

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



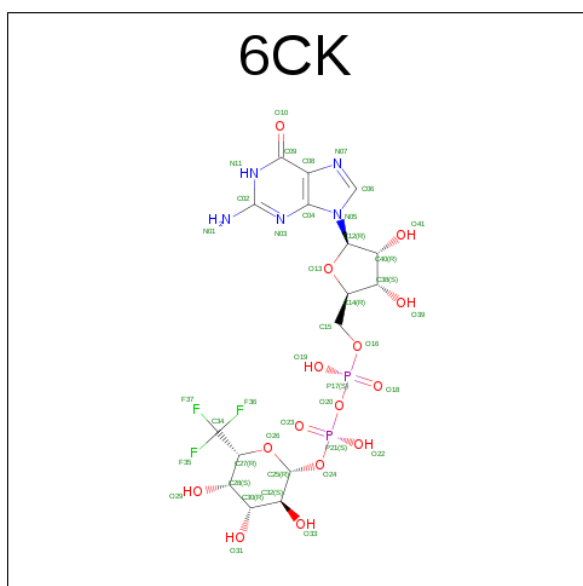
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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 [(2R,3S,4R,5R)-5-(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4R,5S,6R)-3,4,5-trihydroxy-6-(trifluoromethyl)tetrahydro-2H-pyran-2-yl dihydrogen diphosphate (non-preferred name) (three-letter code: 6CK) (formula: C₁₆H₂₂F₃N₅O₁₅P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 41	C 16	F 3	N 5	O 15	P 2	0	0
4	B	1	Total 41	C 16	F 3	N 5	O 15	P 2	0	0
4	C	1	Total 41	C 16	F 3	N 5	O 15	P 2	0	0
4	D	1	Total 41	C 16	F 3	N 5	O 15	P 2	0	0

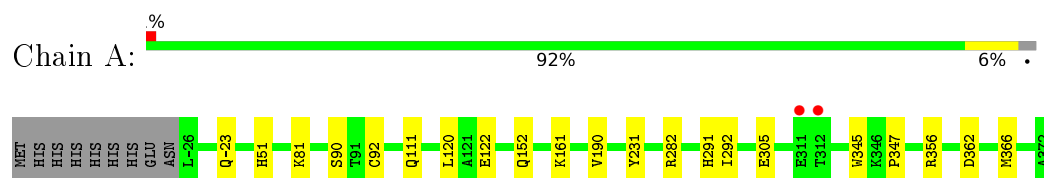
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	338	Total 338	O 338	0	0
5	B	337	Total 337	O 337	0	0
5	C	360	Total 360	O 360	0	0
5	D	385	Total 385	O 385	0	0

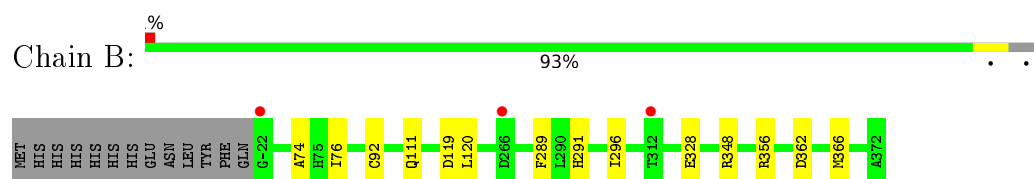
3 Residue-property plots [i](#)

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.

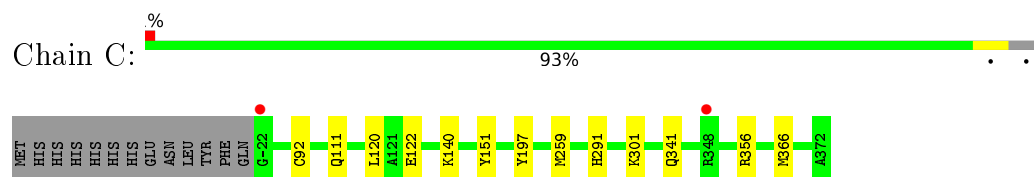
- Molecule 1: GDP-mannose 4,6 dehydratase



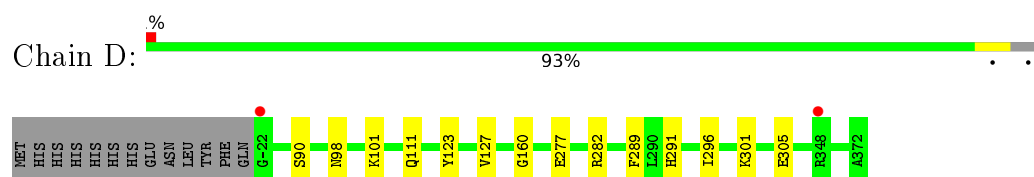
- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.03 Å 140.08 Å 85.95 Å 90.00° 106.24° 90.00°	Depositor
Resolution (Å)	29.57 – 1.60 29.57 – 1.59	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.57-1.60) 86.1 (29.57-1.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.58 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.146 , 0.176 0.145 , 0.174	Depositor DCC
R_{free} test set	8110 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13235	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, NAP, 6CK

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	0.44	0/2932	0.61	0/3966
1	B	0.44	0/2904	0.61	0/3928
1	C	0.46	0/2896	0.61	0/3917
1	D	0.47	0/2896	0.62	0/3917
All	All	0.45	0/11628	0.61	0/15728

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 [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	2864	0	2825	11	0
1	B	2832	0	2799	9	0
1	C	2824	0	2794	9	0
1	D	2827	0	2793	9	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
4	A	41	0	0	0	0
4	B	41	0	0	0	0
4	C	41	0	0	0	0
4	D	41	0	0	0	0
5	A	338	0	0	4	0
5	B	337	0	0	4	0
5	C	360	0	0	5	0
5	D	385	0	0	5	0
All	All	13235	0	11359	38	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 2.

All (38) 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:D:282:ARG:NH1	1:D:305:GLU:OE2	2.18	0.75
1:C:366:MET:SD	5:C:1173:HOH:O	2.51	0.69
1:A:-23:GLN:NE2	5:A:1105:HOH:O	2.29	0.64
1:A:282:ARG:NH1	1:A:305:GLU:OE2	2.26	0.64
1:B:119:ASP:OD1	5:B:501:HOH:O	2.16	0.60
1:B:328:GLU:HG3	5:B:798:HOH:O	2.01	0.60
1:C:122[A]:GLU:OE2	5:C:1101:HOH:O	2.18	0.56
5:A:1176:HOH:O	1:B:120:LEU:HD11	2.07	0.55
1:D:98:ASN:O	1:D:101:LYS:NZ	2.39	0.55
1:D:301:LYS:NZ	5:D:506:HOH:O	2.28	0.53
1:A:122[B]:GLU:OE1	5:A:1101:HOH:O	2.19	0.52
1:A:291:HIS:CE1	1:A:356:ARG:HB2	2.46	0.50
1:B:291:HIS:NE2	1:B:356:ARG:HB2	2.26	0.49
1:D:282:ARG:HH12	1:D:305:GLU:CD	2.15	0.48
1:A:120:LEU:HD11	5:B:606:HOH:O	2.13	0.48
1:B:291:HIS:CE1	1:B:356:ARG:HB2	2.47	0.48
1:C:151:TYR:CZ	1:C:259:MET:HG2	2.49	0.47
1:C:356:ARG:HD3	5:C:1150:HOH:O	2.14	0.46
1:B:348:ARG:NH1	5:B:517:HOH:O	2.47	0.46
1:C:120:LEU:HD11	5:D:596:HOH:O	2.14	0.46
1:A:362:ASP:O	1:A:366:MET:HG2	2.18	0.43
1:D:277:GLU:OE1	5:D:502:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:HB3	1:B:76:ILE:HG12	2.01	0.43
1:B:362:ASP:O	1:B:366:MET:HG2	2.18	0.43
1:C:301:LYS:NZ	5:C:1102:HOH:O	2.21	0.43
1:A:161:LYS:NZ	5:A:1123:HOH:O	2.52	0.42
1:D:289:PHE:CD2	1:D:296:ILE:HG13	2.55	0.42
1:D:291:HIS:HE1	5:D:628:HOH:O	2.03	0.41
1:C:341:GLN:OE1	5:C:1103:HOH:O	2.22	0.41
1:D:90:SER:OG	5:D:501:HOH:O	2.19	0.41
1:D:123:TYR:CZ	1:D:127:VAL:HG21	2.55	0.41
1:A:345:TRP:CZ3	1:A:347:PRO:HD3	2.55	0.41
1:C:291:HIS:CE1	1:C:356:ARG:HB2	2.56	0.41
1:A:231:TYR:CD1	1:A:292:ILE:HB	2.56	0.40
1:A:51:HIS:HA	1:A:81:LYS:O	2.21	0.40
1:B:289:PHE:CD2	1:B:296:ILE:HG13	2.56	0.40
1:C:140:LYS:HE3	1:C:197:TYR:CZ	2.56	0.40
1:A:152:GLN:HB2	1:A:190:VAL:HG21	2.03	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	355/364 (98%)	349 (98%)	6 (2%)	0	100	100
1	B	353/364 (97%)	347 (98%)	6 (2%)	0	100	100
1	C	352/364 (97%)	345 (98%)	7 (2%)	0	100	100
1	D	352/364 (97%)	345 (98%)	6 (2%)	1 (0%)	46	23
All	All	1412/1456 (97%)	1386 (98%)	25 (2%)	1 (0%)	56	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	160	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/315 (98%)	304 (99%)	4 (1%)	76	56
1	B	306/315 (97%)	303 (99%)	3 (1%)	82	67
1	C	305/315 (97%)	303 (99%)	2 (1%)	88	78
1	D	305/315 (97%)	304 (100%)	1 (0%)	94	90
All	All	1224/1260 (97%)	1214 (99%)	10 (1%)	88	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	92[A]	CYS
1	A	92[B]	CYS
1	A	111	GLN
1	B	92[A]	CYS
1	B	92[B]	CYS
1	B	111	GLN
1	C	92	CYS
1	C	111	GLN
1	D	111	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	73	GLN
1	D	198	ASN
1	D	291	HIS
1	D	360	HIS

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 ⓘ

12 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	NAP	A	1001	-	45,52,52	1.91	10 (22%)	55,80,80	1.77	10 (18%)
3	GDP	A	1002	-	24,30,30	1.09	2 (8%)	26,47,47	2.06	4 (15%)
4	6CK	A	1003	-	38,44,44	2.22	11 (28%)	47,70,70	1.88	9 (19%)
4	6CK	B	401	-	38,44,44	2.08	14 (36%)	47,70,70	1.80	7 (14%)
2	NAP	B	402	-	45,52,52	1.88	9 (20%)	55,80,80	1.93	13 (23%)
3	GDP	B	403	-	24,30,30	1.07	2 (8%)	26,47,47	1.96	4 (15%)
2	NAP	C	1001	-	45,52,52	1.90	9 (20%)	55,80,80	1.70	9 (16%)
3	GDP	C	1002	-	24,30,30	1.04	2 (8%)	26,47,47	1.99	4 (15%)
4	6CK	C	1003	-	38,44,44	2.06	9 (23%)	47,70,70	1.84	6 (12%)
4	6CK	D	401	-	38,44,44	2.09	11 (28%)	47,70,70	1.86	8 (17%)
2	NAP	D	402	-	45,52,52	1.84	8 (17%)	55,80,80	1.78	10 (18%)
3	GDP	D	403	-	24,30,30	1.05	2 (8%)	26,47,47	1.77	4 (15%)

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	NAP	A	1001	-	-	0/27/67/67	0/5/5/5
3	GDP	A	1002	-	-	0/12/32/32	0/3/3/3
4	6CK	A	1003	-	-	0/23/63/63	0/4/4/4
4	6CK	B	401	-	-	0/23/63/63	0/4/4/4
2	NAP	B	402	-	-	0/27/67/67	0/5/5/5
3	GDP	B	403	-	-	0/12/32/32	0/3/3/3
2	NAP	C	1001	-	-	0/27/67/67	0/5/5/5
3	GDP	C	1002	-	-	0/12/32/32	0/3/3/3
4	6CK	C	1003	-	-	0/23/63/63	0/4/4/4
4	6CK	D	401	-	-	0/23/63/63	0/4/4/4
2	NAP	D	402	-	-	0/27/67/67	0/5/5/5
3	GDP	D	403	-	-	0/12/32/32	0/3/3/3

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	6CK	O26-C27	-4.29	1.35	1.43
4	B	401	6CK	O26-C27	-3.39	1.37	1.43
2	B	402	NAP	C3N-C7N	-3.37	1.45	1.50
4	A	1003	6CK	O26-C27	-2.92	1.38	1.43
2	D	402	NAP	C3N-C7N	-2.86	1.46	1.50
2	B	402	NAP	C6N-C5N	-2.80	1.32	1.38
4	D	401	6CK	O26-C27	-2.78	1.38	1.43
2	C	1001	NAP	C3N-C7N	-2.51	1.46	1.50
2	A	1001	NAP	C3N-C7N	-2.43	1.46	1.50
2	A	1001	NAP	O2B-C2B	-2.43	1.36	1.44
4	B	401	6CK	O24-C25	-2.33	1.30	1.42
2	C	1001	NAP	C6N-C5N	-2.24	1.33	1.38
2	A	1001	NAP	C6N-C5N	-2.24	1.33	1.38
2	C	1001	NAP	O2B-C2B	-2.20	1.37	1.44
2	D	402	NAP	C2N-C3N	-2.09	1.35	1.39
4	B	401	6CK	O16-C15	-2.05	1.36	1.44
4	B	401	6CK	P17-O19	-2.03	1.46	1.55
4	B	401	6CK	O39-C38	-2.02	1.38	1.43
4	C	1003	6CK	C32-C30	2.01	1.57	1.52
2	C	1001	NAP	C6N-N1N	2.02	1.41	1.35
4	D	401	6CK	C04-N03	2.03	1.39	1.35
2	A	1001	NAP	C4A-N3A	2.04	1.38	1.35
2	B	402	NAP	C6N-N1N	2.05	1.41	1.35
4	A	1003	6CK	C38-C14	2.06	1.58	1.53
2	A	1001	NAP	C2D-C1D	2.12	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	6CK	C25-C32	2.18	1.59	1.52
2	A	1001	NAP	O4D-C1D	2.19	1.44	1.41
2	B	402	NAP	C3D-C4D	2.21	1.58	1.53
4	D	401	6CK	C28-C27	2.22	1.57	1.53
4	B	401	6CK	C15-C14	2.23	1.58	1.51
4	C	1003	6CK	P17-O16	2.25	1.68	1.59
4	A	1003	6CK	C04-N03	2.25	1.39	1.35
4	B	401	6CK	P17-O16	2.26	1.68	1.59
2	D	402	NAP	C6N-N1N	2.33	1.42	1.35
2	B	402	NAP	PN-O5D	2.43	1.69	1.59
4	D	401	6CK	P17-O16	2.45	1.69	1.59
4	D	401	6CK	O13-C12	2.46	1.44	1.41
2	B	402	NAP	C7N-N7N	2.50	1.38	1.33
4	B	401	6CK	O13-C12	2.54	1.44	1.41
4	B	401	6CK	C04-N03	2.56	1.39	1.35
4	C	1003	6CK	C02-N01	2.56	1.39	1.34
3	C	1002	GDP	C5-C4	2.58	1.46	1.40
3	D	403	GDP	C6-C5	2.66	1.46	1.41
3	B	403	GDP	C6-C5	2.67	1.46	1.41
3	C	1002	GDP	C6-C5	2.68	1.46	1.41
4	A	1003	6CK	O13-C12	2.70	1.45	1.41
4	A	1003	6CK	P21-O24	2.76	1.68	1.60
2	C	1001	NAP	C2D-C1D	2.79	1.58	1.53
3	A	1002	GDP	C6-C5	2.84	1.47	1.41
2	A	1001	NAP	C7N-N7N	2.85	1.38	1.33
4	D	401	6CK	C02-N01	2.87	1.40	1.34
4	A	1003	6CK	P17-O16	2.88	1.71	1.59
3	D	403	GDP	C5-C4	2.92	1.47	1.40
4	D	401	6CK	O26-C25	2.93	1.49	1.41
4	C	1003	6CK	C02-N11	2.94	1.40	1.35
3	A	1002	GDP	C5-C4	3.04	1.47	1.40
4	A	1003	6CK	C02-N11	3.08	1.41	1.35
3	B	403	GDP	C5-C4	3.15	1.47	1.40
4	B	401	6CK	C02-N11	3.16	1.41	1.35
4	D	401	6CK	C02-N11	3.17	1.41	1.35
2	D	402	NAP	C7N-N7N	3.27	1.39	1.33
2	A	1001	NAP	C2N-N1N	3.48	1.40	1.35
2	D	402	NAP	O4D-C1D	3.54	1.46	1.41
4	A	1003	6CK	C02-N01	3.69	1.41	1.34
4	B	401	6CK	P21-O24	3.73	1.70	1.60
2	D	402	NAP	C5N-C4N	3.82	1.46	1.38
2	B	402	NAP	C5N-C4N	3.85	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	NAP	C7N-N7N	3.88	1.40	1.33
4	B	401	6CK	C02-N01	3.90	1.42	1.34
4	C	1003	6CK	O13-C12	3.94	1.46	1.41
4	C	1003	6CK	P21-O24	4.19	1.71	1.60
2	A	1001	NAP	C5N-C4N	4.26	1.47	1.38
4	B	401	6CK	C34-C27	4.27	1.56	1.51
2	D	402	NAP	C2N-N1N	4.47	1.41	1.35
2	C	1001	NAP	C5N-C4N	4.55	1.47	1.38
2	B	402	NAP	C2N-N1N	4.84	1.42	1.35
4	D	401	6CK	P21-O24	4.98	1.73	1.60
4	D	401	6CK	C09-N11	5.15	1.42	1.33
4	C	1003	6CK	C34-C27	5.16	1.57	1.51
4	D	401	6CK	C34-C27	5.18	1.57	1.51
2	C	1001	NAP	C2N-N1N	5.21	1.42	1.35
4	B	401	6CK	C09-N11	5.21	1.42	1.33
4	C	1003	6CK	C09-N11	5.69	1.43	1.33
4	A	1003	6CK	C09-N11	5.74	1.43	1.33
2	C	1001	NAP	C4N-C3N	6.14	1.49	1.39
2	D	402	NAP	C4N-C3N	6.29	1.49	1.39
2	B	402	NAP	C4N-C3N	7.00	1.50	1.39
4	A	1003	6CK	C34-C27	7.15	1.59	1.51
2	A	1001	NAP	C4N-C3N	7.61	1.51	1.39

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	NAP	C5N-C4N-C3N	-7.08	111.90	120.35
4	A	1003	6CK	O26-C25-O24	-6.61	102.65	111.36
4	B	401	6CK	O26-C25-O24	-6.53	102.75	111.36
2	A	1001	NAP	C5N-C4N-C3N	-6.12	113.05	120.35
4	D	401	6CK	O26-C25-O24	-6.08	103.34	111.36
4	C	1003	6CK	O26-C25-O24	-5.82	103.69	111.36
2	D	402	NAP	C5N-C4N-C3N	-5.80	113.43	120.35
3	C	1002	GDP	C5-C6-N1	-5.59	116.22	123.52
3	A	1002	GDP	C5-C6-N1	-5.37	116.50	123.52
2	C	1001	NAP	C5N-C4N-C3N	-5.25	114.08	120.35
4	C	1003	6CK	C30-C28-C27	-4.88	103.52	111.27
2	D	402	NAP	O4D-C1D-N1N	-4.80	102.92	108.10
4	C	1003	6CK	C08-C09-N11	-4.79	117.25	123.52
2	B	402	NAP	O4D-C1D-N1N	-4.77	102.95	108.10
3	B	403	GDP	C5-C6-N1	-4.71	117.36	123.52
2	A	1001	NAP	O2B-P2B-O1X	-4.61	96.48	107.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	6CK	C08-C09-N11	-4.56	117.56	123.52
2	B	402	NAP	O2B-P2B-O1X	-4.41	96.95	107.48
4	B	401	6CK	C08-C09-N11	-4.39	117.78	123.52
3	D	403	GDP	C5-C6-N1	-4.37	117.81	123.52
2	C	1001	NAP	O2B-P2B-O1X	-4.20	97.44	107.48
2	C	1001	NAP	O4D-C1D-N1N	-4.20	103.57	108.10
4	A	1003	6CK	C30-C28-C27	-4.16	104.66	111.27
4	A	1003	6CK	N03-C02-N11	-4.06	122.03	127.56
4	B	401	6CK	C30-C28-C27	-3.86	105.13	111.27
2	D	402	NAP	O2B-P2B-O1X	-3.71	98.63	107.48
4	D	401	6CK	F37-C34-C27	-3.62	107.56	111.92
3	D	403	GDP	N3-C2-N1	-3.53	122.75	127.56
4	C	1003	6CK	N03-C02-N11	-3.48	122.82	127.56
3	B	403	GDP	N3-C2-N1	-3.46	122.85	127.56
4	A	1003	6CK	C08-C09-N11	-3.44	119.02	123.52
4	D	401	6CK	C30-C28-C27	-3.40	105.87	111.27
3	A	1002	GDP	N3-C2-N1	-3.37	122.97	127.56
4	B	401	6CK	N03-C02-N11	-3.31	123.06	127.56
2	A	1001	NAP	O4D-C1D-N1N	-3.21	104.64	108.10
2	A	1001	NAP	O7N-C7N-N7N	-3.20	118.02	122.58
4	D	401	6CK	N03-C02-N11	-3.14	123.29	127.56
3	D	403	GDP	C6-C5-C4	-3.03	117.39	120.86
3	C	1002	GDP	N3-C2-N1	-3.01	123.46	127.56
4	B	401	6CK	F36-C34-C27	-2.99	108.32	111.92
2	C	1001	NAP	C3B-C2B-C1B	-2.87	97.14	102.63
2	B	402	NAP	C3B-C2B-C1B	-2.85	97.18	102.63
3	A	1002	GDP	C6-C5-C4	-2.84	117.61	120.86
3	B	403	GDP	C6-C5-C4	-2.81	117.65	120.86
4	A	1003	6CK	F36-C34-C27	-2.80	108.55	111.92
4	A	1003	6CK	C09-C08-C04	-2.73	117.73	120.86
2	C	1001	NAP	O7N-C7N-N7N	-2.68	118.77	122.58
3	C	1002	GDP	C6-C5-C4	-2.61	117.87	120.86
2	A	1001	NAP	C3B-C2B-C1B	-2.60	97.65	102.63
2	D	402	NAP	O7N-C7N-N7N	-2.55	118.95	122.58
2	B	402	NAP	C4B-O4B-C1B	-2.54	106.95	109.64
2	D	402	NAP	C3B-C2B-C1B	-2.46	97.91	102.63
4	D	401	6CK	C09-C08-C04	-2.44	118.07	120.86
2	B	402	NAP	O7N-C7N-N7N	-2.42	119.12	122.58
4	A	1003	6CK	C12-N05-C04	-2.36	124.17	126.81
2	B	402	NAP	O5B-C5B-C4B	-2.34	100.64	109.09
4	A	1003	6CK	F37-C34-C27	-2.22	109.24	111.92
2	D	402	NAP	C2A-N1A-C6A	-2.11	114.99	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	6CK	O33-C32-C25	-2.09	105.38	110.01
2	A	1001	NAP	C4B-O4B-C1B	-2.08	107.43	109.64
2	D	402	NAP	C4N-C3N-C7N	-2.08	115.58	121.11
2	B	402	NAP	C4N-C3N-C7N	-2.05	115.67	121.11
4	C	1003	6CK	C09-C08-C04	-2.02	118.55	120.86
2	A	1001	NAP	O2N-PN-O3	2.04	114.00	105.27
2	B	402	NAP	O2N-PN-O3	2.04	114.00	105.27
2	C	1001	NAP	O2N-PN-O1N	2.04	123.18	112.56
2	B	402	NAP	O2N-PN-O1N	2.06	123.29	112.56
2	C	1001	NAP	O3X-P2B-O2X	2.12	115.24	107.44
2	B	402	NAP	O2X-P2B-O1X	2.16	117.67	110.63
2	D	402	NAP	O7N-C7N-C3N	2.18	122.01	119.60
4	B	401	6CK	F37-C34-F35	2.18	111.89	106.84
2	A	1001	NAP	O7N-C7N-C3N	2.20	122.03	119.60
2	A	1001	NAP	O3X-P2B-O2X	2.34	116.03	107.44
2	C	1001	NAP	O2N-PN-O3	2.49	115.95	105.27
2	B	402	NAP	C6N-C5N-C4N	2.59	123.36	119.43
2	D	402	NAP	N3A-C2A-N1A	2.61	130.92	128.87
4	A	1003	6CK	C09-N11-C02	2.89	119.27	115.88
2	C	1001	NAP	C2N-C3N-C4N	3.12	121.80	118.27
4	D	401	6CK	C09-N11-C02	3.45	119.92	115.88
2	A	1001	NAP	C2N-C3N-C4N	3.47	122.20	118.27
4	C	1003	6CK	C09-N11-C02	3.70	120.22	115.88
4	B	401	6CK	C09-N11-C02	3.75	120.27	115.88
2	D	402	NAP	C2N-C3N-C4N	3.82	122.60	118.27
2	B	402	NAP	C2N-C3N-C4N	4.18	123.00	118.27
3	D	403	GDP	C6-N1-C2	5.33	122.12	115.88
3	B	403	GDP	C6-N1-C2	6.27	123.23	115.88
3	A	1002	GDP	C6-N1-C2	6.30	123.27	115.88
3	C	1002	GDP	C6-N1-C2	6.45	123.44	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/364 (97%)	-0.39	2 (0%) 90 90	7, 16, 35, 51	0
1	B	351/364 (96%)	-0.40	3 (0%) 85 85	8, 15, 34, 50	0
1	C	351/364 (96%)	-0.48	2 (0%) 90 90	7, 14, 29, 52	0
1	D	351/364 (96%)	-0.50	2 (0%) 90 90	8, 14, 32, 58	0
All	All	1408/1456 (96%)	-0.44	9 (0%) 90 90	7, 15, 32, 58	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-22	GLY	5.3
1	B	-22	GLY	3.9
1	B	266	ASP	2.8
1	A	311	GLU	2.6
1	C	348	ARG	2.3
1	A	312	THR	2.2
1	B	312	THR	2.2
1	D	348	ARG	2.1
1	D	-22	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
3	GDP	B	403	28/28	0.93	0.09	1.19	11,16,28,34	0
3	GDP	A	1002	28/28	0.94	0.09	0.89	11,18,26,34	0
2	NAP	B	402	48/48	0.98	0.08	0.00	6,10,12,13	0
3	GDP	D	403	28/28	0.96	0.07	-0.06	7,13,23,29	0
3	GDP	C	1002	28/28	0.96	0.07	-0.24	8,13,18,26	0
2	NAP	C	1001	48/48	0.99	0.07	-0.31	6,9,13,15	0
2	NAP	D	402	48/48	0.99	0.06	-0.65	7,10,12,13	0
2	NAP	A	1001	48/48	0.99	0.07	-0.67	7,9,12,13	0
4	6CK	D	401	41/41	0.98	0.05	-1.01	8,12,14,17	0
4	6CK	C	1003	41/41	0.98	0.05	-1.12	9,12,16,18	0
4	6CK	A	1003	41/41	0.98	0.05	-1.12	9,13,16,18	0
4	6CK	B	401	41/41	0.98	0.05	-1.15	9,13,15,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.