



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:56 AM UTC

PDB ID : 6YA3 / pdb_00006ya3
Title : Crystal structure of PnrA from *S. pneumoniae* in complex with guanosine
Authors : Batuecas, M.T.; Hermoso, J.A.
Deposited on : 2020-03-11
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

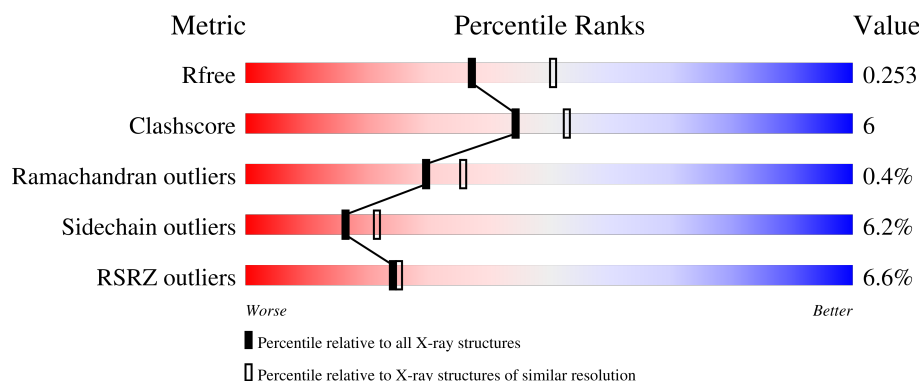
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	331	5% 87% 10% ..
1	B	331	3% 83% 15% ..
1	C	331	3% 84% 15% ..
1	D	331	14% 85% 13% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10419 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 Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	331	Total	C	N	O	S	0	2	0
			2488	1556	424	507	1			
1	A	331	Total	C	N	O	S	0	1	0
			2486	1554	426	505	1			
1	B	331	Total	C	N	O	S	0	1	0
			2486	1554	426	505	1			
1	D	330	Total	C	N	O	S	0	1	0
			2475	1548	422	504	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	SER	-	expression tag	UNP A0A0H2UPF3
C	4	SER	-	expression tag	UNP A0A0H2UPF3
C	5	HIS	-	expression tag	UNP A0A0H2UPF3
C	6	HIS	-	expression tag	UNP A0A0H2UPF3
C	7	HIS	-	expression tag	UNP A0A0H2UPF3
C	8	HIS	-	expression tag	UNP A0A0H2UPF3
C	9	HIS	-	expression tag	UNP A0A0H2UPF3
C	10	HIS	-	expression tag	UNP A0A0H2UPF3
C	11	MET	-	expression tag	UNP A0A0H2UPF3
C	12	SER	-	expression tag	UNP A0A0H2UPF3
C	13	GLY	-	expression tag	UNP A0A0H2UPF3
C	14	GLU	-	expression tag	UNP A0A0H2UPF3
C	15	ASN	-	expression tag	UNP A0A0H2UPF3
C	16	LEU	-	expression tag	UNP A0A0H2UPF3
C	17	TYR	-	expression tag	UNP A0A0H2UPF3
C	18	PHE	-	expression tag	UNP A0A0H2UPF3
C	19	GLN	-	expression tag	UNP A0A0H2UPF3
C	20	GLY	-	expression tag	UNP A0A0H2UPF3
C	21	ALA	-	expression tag	UNP A0A0H2UPF3
C	22	SER	-	expression tag	UNP A0A0H2UPF3
A	3	SER	-	expression tag	UNP A0A0H2UPF3

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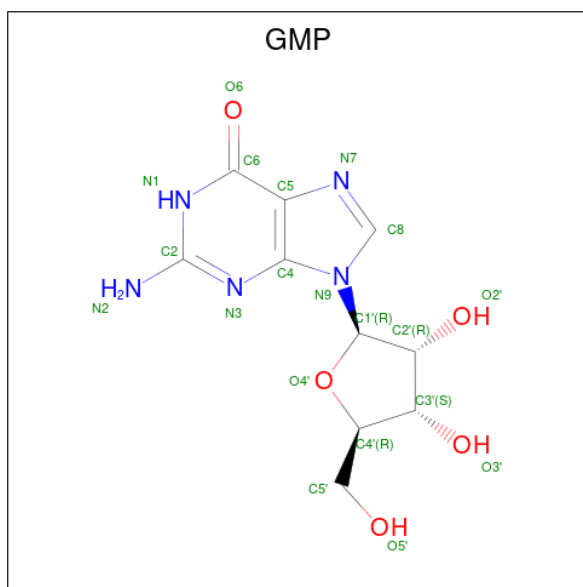
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	expression tag	UNP A0A0H2UPF3
A	5	HIS	-	expression tag	UNP A0A0H2UPF3
A	6	HIS	-	expression tag	UNP A0A0H2UPF3
A	7	HIS	-	expression tag	UNP A0A0H2UPF3
A	8	HIS	-	expression tag	UNP A0A0H2UPF3
A	9	HIS	-	expression tag	UNP A0A0H2UPF3
A	10	HIS	-	expression tag	UNP A0A0H2UPF3
A	11	MET	-	expression tag	UNP A0A0H2UPF3
A	12	SER	-	expression tag	UNP A0A0H2UPF3
A	13	GLY	-	expression tag	UNP A0A0H2UPF3
A	14	GLU	-	expression tag	UNP A0A0H2UPF3
A	15	ASN	-	expression tag	UNP A0A0H2UPF3
A	16	LEU	-	expression tag	UNP A0A0H2UPF3
A	17	TYR	-	expression tag	UNP A0A0H2UPF3
A	18	PHE	-	expression tag	UNP A0A0H2UPF3
A	19	GLN	-	expression tag	UNP A0A0H2UPF3
A	20	GLY	-	expression tag	UNP A0A0H2UPF3
A	21	ALA	-	expression tag	UNP A0A0H2UPF3
A	22	SER	-	expression tag	UNP A0A0H2UPF3
B	3	SER	-	expression tag	UNP A0A0H2UPF3
B	4	SER	-	expression tag	UNP A0A0H2UPF3
B	5	HIS	-	expression tag	UNP A0A0H2UPF3
B	6	HIS	-	expression tag	UNP A0A0H2UPF3
B	7	HIS	-	expression tag	UNP A0A0H2UPF3
B	8	HIS	-	expression tag	UNP A0A0H2UPF3
B	9	HIS	-	expression tag	UNP A0A0H2UPF3
B	10	HIS	-	expression tag	UNP A0A0H2UPF3
B	11	MET	-	expression tag	UNP A0A0H2UPF3
B	12	SER	-	expression tag	UNP A0A0H2UPF3
B	13	GLY	-	expression tag	UNP A0A0H2UPF3
B	14	GLU	-	expression tag	UNP A0A0H2UPF3
B	15	ASN	-	expression tag	UNP A0A0H2UPF3
B	16	LEU	-	expression tag	UNP A0A0H2UPF3
B	17	TYR	-	expression tag	UNP A0A0H2UPF3
B	18	PHE	-	expression tag	UNP A0A0H2UPF3
B	19	GLN	-	expression tag	UNP A0A0H2UPF3
B	20	GLY	-	expression tag	UNP A0A0H2UPF3
B	21	ALA	-	expression tag	UNP A0A0H2UPF3
B	22	SER	-	expression tag	UNP A0A0H2UPF3
D	3	SER	-	expression tag	UNP A0A0H2UPF3
D	4	SER	-	expression tag	UNP A0A0H2UPF3
D	5	HIS	-	expression tag	UNP A0A0H2UPF3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	6	HIS	-	expression tag	UNP A0A0H2UPF3
D	7	HIS	-	expression tag	UNP A0A0H2UPF3
D	8	HIS	-	expression tag	UNP A0A0H2UPF3
D	9	HIS	-	expression tag	UNP A0A0H2UPF3
D	10	HIS	-	expression tag	UNP A0A0H2UPF3
D	11	MET	-	expression tag	UNP A0A0H2UPF3
D	12	SER	-	expression tag	UNP A0A0H2UPF3
D	13	GLY	-	expression tag	UNP A0A0H2UPF3
D	14	GLU	-	expression tag	UNP A0A0H2UPF3
D	15	ASN	-	expression tag	UNP A0A0H2UPF3
D	16	LEU	-	expression tag	UNP A0A0H2UPF3
D	17	TYR	-	expression tag	UNP A0A0H2UPF3
D	18	PHE	-	expression tag	UNP A0A0H2UPF3
D	19	GLN	-	expression tag	UNP A0A0H2UPF3
D	20	GLY	-	expression tag	UNP A0A0H2UPF3
D	21	ALA	-	expression tag	UNP A0A0H2UPF3
D	22	SER	-	expression tag	UNP A0A0H2UPF3

- Molecule 2 is GUANOSINE (CCD ID: GMP) (formula: C₁₀H₁₃N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			20	10	5	5		
2	A	1	Total	C	N	O	0	0
			20	10	5	5		
2	B	1	Total	C	N	O	0	0
			20	10	5	5		

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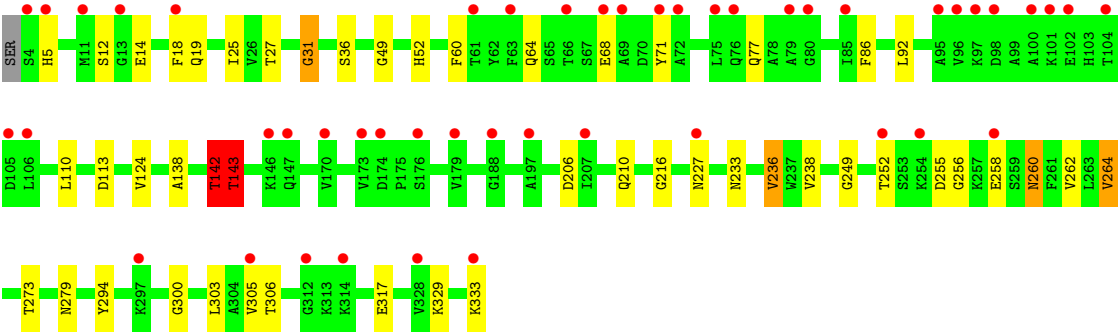
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			20	10	5	5		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total	Ni	0	0
			3	3		
3	A	2	Total	Ni	0	0
			2	2		
3	B	2	Total	Ni	0	0
			2	2		
3	D	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	127	Total	O	0	0
			127	127		
4	A	122	Total	O	0	0
			122	122		
4	B	111	Total	O	0	0
			111	111		
4	D	36	Total	O	0	0
			36	36		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.78Å 304.92Å 128.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.28 49.18 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.18-2.28) 99.6 (49.18-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.29Å)	Xtriage
Refinement program	REFMAC 7.0.078	Depositor
R, R_{free}	0.210 , 0.250 0.213 , 0.253	Depositor DCC
R_{free} test set	3519 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10419	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.19% 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: NI, GMP

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	1.06	0/2531	1.45	4/3417 (0.1%)
1	B	1.02	0/2531	1.45	9/3417 (0.3%)
1	C	1.09	2/2536 (0.1%)	1.47	12/3425 (0.4%)
1	D	1.02	0/2520	1.46	5/3403 (0.1%)
All	All	1.05	2/10118 (0.0%)	1.46	30/13662 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252[A]	THR	C-O	7.11	1.32	1.24
1	C	252[B]	THR	C-O	7.11	1.32	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252[A]	THR	CA-C-O	9.76	130.90	120.36
1	C	252[B]	THR	CA-C-O	9.76	130.90	120.36
1	B	31	GLY	CA-C-O	-7.25	116.42	122.29
1	D	5	HIS	CB-CA-C	7.05	122.08	110.17
1	C	252[A]	THR	O-C-N	-6.85	115.15	123.30
1	C	252[B]	THR	O-C-N	-6.85	115.15	123.30
1	D	31	GLY	CA-C-O	-5.99	117.44	122.29
1	C	287	PRO	CA-C-N	5.68	125.38	119.92
1	C	287	PRO	C-N-CA	5.68	125.38	119.92
1	B	142	THR	CB-CA-C	5.58	117.83	109.13
1	C	36	SER	CA-C-N	5.53	128.47	120.79
1	C	36	SER	C-N-CA	5.53	128.47	120.79
1	A	287	PRO	CA-C-N	5.49	125.19	119.92
1	A	287	PRO	C-N-CA	5.49	125.19	119.92
1	B	12	SER	CA-C-N	5.46	125.28	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	SER	C-N-CA	5.46	125.28	120.10
1	C	143	THR	CB-CA-C	-5.43	101.69	109.84
1	C	142	THR	CB-CA-C	5.43	117.61	109.13
1	D	143	THR	CB-CA-C	-5.29	101.65	109.90
1	C	48	TRP	CA-C-N	5.22	125.89	119.99
1	C	48	TRP	C-N-CA	5.22	125.89	119.99
1	D	18	PHE	CB-CA-C	5.22	118.75	109.72
1	D	142	THR	CB-CA-C	5.19	117.23	109.13
1	A	142	THR	CB-CA-C	5.18	117.22	109.13
1	B	28	ASP	CA-C-N	5.17	127.46	120.38
1	B	28	ASP	C-N-CA	5.17	127.46	120.38
1	B	287	PRO	CA-C-N	5.13	124.84	119.92
1	B	287	PRO	C-N-CA	5.13	124.84	119.92
1	A	143	THR	CB-CA-C	-5.03	102.06	109.90
1	B	143	THR	CB-CA-C	-5.02	102.07	109.90

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	2486	0	2408	33	0
1	B	2486	0	2408	28	0
1	C	2488	0	2410	32	0
1	D	2475	0	2395	27	0
2	A	20	0	13	0	0
2	B	20	0	13	0	0
2	C	20	0	13	0	0
2	D	20	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	122	0	0	10	2
4	B	111	0	0	3	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	127	0	0	8	0
4	D	36	0	0	0	0
All	All	10419	0	9673	118	2

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 (118) 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:282:GLU:OE2	4:C:501:HOH:O	1.66	1.10
1:A:11:MET:HE2	1:A:16:LEU:HD21	1.53	0.91
1:B:252:THR:HG22	1:B:258:GLU:HG3	1.64	0.80
1:D:227:ASN:HD21	1:D:236:VAL:H	1.33	0.76
1:B:227:ASN:HD21	1:B:236:VAL:H	1.31	0.74
1:C:227:ASN:HD21	1:C:236:VAL:H	1.35	0.74
1:B:5:HIS:HA	4:B:506:HOH:O	1.87	0.74
1:A:11:MET:CE	1:A:16:LEU:HD21	2.17	0.74
1:A:227:ASN:HD21	1:A:236:VAL:H	1.33	0.74
1:C:31:GLY:HA2	1:C:64:GLN:HE21	1.58	0.69
1:A:158:VAL:HG23	4:A:569:HOH:O	1.96	0.66
1:C:180[A]:GLN:OE1	4:C:502:HOH:O	2.15	0.65
1:B:322:LYS:HB3	1:B:328:VAL:HG23	1.79	0.65
1:A:264:VAL:HG13	1:A:303:LEU:HD11	1.78	0.65
1:D:110:LEU:HD21	1:D:113:ASP:HB3	1.80	0.63
1:D:68:GLU:HG3	1:D:71:TYR:CE2	2.34	0.63
1:C:264:VAL:HG13	1:C:303:LEU:HD11	1.80	0.62
1:B:264:VAL:HG13	1:B:303:LEU:HD11	1.82	0.62
1:D:252:THR:HG22	1:D:258:GLU:HG2	1.81	0.60
1:C:325:ASP:OD1	1:C:327:SER:HB3	2.01	0.59
1:D:264:VAL:HG13	1:D:303:LEU:HD11	1.85	0.59
1:A:180:GLN:OE1	4:A:501:HOH:O	2.17	0.58
1:C:28:ASP:HB2	4:C:504:HOH:O	2.03	0.57
1:B:227:ASN:ND2	1:B:236:VAL:H	2.02	0.57
1:A:227:ASN:HD21	1:A:236:VAL:N	2.03	0.56
1:C:31:GLY:CA	1:C:64:GLN:HE21	2.18	0.56
1:C:244:ASP:HB3	1:A:53:ASN:HD21	1.69	0.56
1:D:31:GLY:CA	1:D:64:GLN:HE21	2.19	0.56
1:C:313:LYS:NZ	4:C:506:HOH:O	2.38	0.56
1:B:255:ASP:OD1	1:B:255:ASP:N	2.36	0.55
1:B:227:ASN:HD21	1:B:236:VAL:N	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:HIS:HE1	1:D:279:ASN:OD1	1.91	0.54
1:C:227:ASN:ND2	1:C:236:VAL:H	2.04	0.54
1:A:12:SER:HB3	1:A:14:GLU:HG2	1.91	0.53
1:C:14:GLU:HG3	1:A:310:GLU:HG2	1.90	0.53
1:C:52:HIS:CD2	4:C:501:HOH:O	2.62	0.53
1:A:52:HIS:HE1	1:A:279:ASN:OD1	1.92	0.53
1:A:260:ASN:ND2	1:A:262:VAL:H	2.07	0.53
1:C:260:ASN:ND2	1:C:262:VAL:H	2.08	0.52
1:D:227:ASN:ND2	1:D:236:VAL:H	2.03	0.52
1:C:97:LYS:HD2	4:C:556:HOH:O	2.08	0.52
1:B:305:VAL:CG1	1:B:313:LYS:HG2	2.39	0.52
1:D:31:GLY:HA2	1:D:64:GLN:HE21	1.74	0.52
1:B:52:HIS:HE1	1:B:279:ASN:OD1	1.92	0.52
1:C:138:ALA:O	1:C:142:THR:CG2	2.59	0.51
1:B:260:ASN:ND2	1:B:262:VAL:H	2.09	0.51
1:D:260:ASN:ND2	1:D:262:VAL:H	2.08	0.51
1:B:66:THR:OG1	1:B:70:ASP:OD2	2.27	0.51
1:A:110:LEU:HD21	1:A:113:ASP:HB3	1.91	0.50
1:D:227:ASN:HD21	1:D:236:VAL:N	2.05	0.50
1:A:28:ASP:HB2	4:A:502:HOH:O	2.10	0.50
1:B:257:LYS:HA	4:B:543:HOH:O	2.10	0.50
1:A:138:ALA:O	1:A:142:THR:CG2	2.60	0.50
1:D:252:THR:HG22	1:D:258:GLU:CG	2.41	0.50
1:B:31:GLY:CA	1:B:64:GLN:HE21	2.25	0.50
1:D:138:ALA:O	1:D:142:THR:CG2	2.59	0.50
1:A:264:VAL:CG1	1:A:303:LEU:HD11	2.42	0.50
1:C:52:HIS:HE1	1:C:279:ASN:OD1	1.94	0.50
1:A:53:ASN:ND2	4:A:506:HOH:O	2.45	0.49
1:B:138:ALA:O	1:B:142:THR:CG2	2.60	0.49
1:D:294:TYR:HB3	1:D:300:GLY:HA3	1.94	0.49
1:A:294:TYR:HB3	1:A:300:GLY:HA3	1.94	0.49
1:B:31:GLY:HA2	1:B:64:GLN:HE21	1.77	0.48
1:D:255:ASP:N	1:D:255:ASP:OD1	2.32	0.48
1:A:50:LYS:CE	4:A:600:HOH:O	2.61	0.48
1:C:264:VAL:CG1	1:C:303:LEU:HD11	2.43	0.47
1:A:227:ASN:ND2	1:A:236:VAL:H	2.04	0.47
1:C:138:ALA:O	1:C:142:THR:HG23	2.15	0.47
1:C:227:ASN:HD21	1:C:236:VAL:N	2.06	0.47
1:A:31:GLY:HA2	1:A:64:GLN:NE2	2.30	0.47
1:B:138:ALA:O	1:B:142:THR:HG23	2.14	0.47
1:D:138:ALA:O	1:D:142:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:HA2	1:A:64:GLN:HE21	1.80	0.46
1:A:124:VAL:HG11	1:A:273:THR:HG21	1.97	0.46
1:B:294:TYR:HB3	1:B:300:GLY:HA3	1.96	0.46
1:A:50:LYS:HE2	4:A:600:HOH:O	2.15	0.46
1:A:11:MET:CE	1:A:16:LEU:CD2	2.90	0.46
1:B:264:VAL:CG1	1:B:303:LEU:HD11	2.45	0.46
1:A:25:ILE:HG22	1:A:86:PHE:HB2	1.99	0.45
1:A:138:ALA:O	1:A:142:THR:HG23	2.16	0.45
1:D:110:LEU:CD2	1:D:113:ASP:HB3	2.47	0.44
1:A:161:ARG:HD2	4:A:520:HOH:O	2.18	0.44
1:B:124:VAL:HG11	1:B:273:THR:HG21	1.99	0.44
1:C:158:VAL:HG23	4:C:588:HOH:O	2.16	0.44
1:C:294:TYR:HB3	1:C:300:GLY:HA3	1.98	0.44
1:D:25:ILE:HG22	1:D:86:PHE:HB2	1.99	0.44
1:B:25:ILE:HG22	1:B:86:PHE:HB2	1.99	0.43
1:D:124:VAL:HG11	1:D:273:THR:HG21	2.00	0.43
1:D:249:GLY:O	1:D:260:ASN:HA	2.18	0.43
1:A:92:LEU:HD12	4:A:577:HOH:O	2.18	0.43
1:B:305:VAL:HG13	1:B:313:LYS:HG2	2.00	0.43
1:B:119:LYS:HG3	4:B:536:HOH:O	2.18	0.42
1:A:249:GLY:O	1:A:260:ASN:HA	2.19	0.42
1:B:249:GLY:O	1:B:260:ASN:HA	2.19	0.42
1:C:25:ILE:HG22	1:C:86:PHE:HB2	2.01	0.42
1:C:302:ASP:OD2	4:C:503:HOH:O	2.21	0.42
1:B:110:LEU:HD21	1:B:113:ASP:HB3	2.00	0.42
1:B:143:THR:CG2	1:B:206:ASP:OD1	2.67	0.42
1:D:210:GLN:H	1:D:210:GLN:HG3	1.69	0.42
1:C:110:LEU:HD21	1:C:113:ASP:HB3	2.00	0.42
1:C:124:VAL:HG11	1:C:273:THR:HG21	2.01	0.42
1:C:249:GLY:O	1:C:260:ASN:HA	2.19	0.42
1:D:68:GLU:HG3	1:D:71:TYR:CD2	2.55	0.42
1:C:220:PHE:CE2	1:C:248:GLU:HB2	2.55	0.41
1:D:210:GLN:OE1	1:D:216:GLY:HA3	2.20	0.41
1:C:143:THR:CG2	1:C:206:ASP:OD1	2.68	0.41
1:A:143:THR:CG2	1:A:206:ASP:OD1	2.68	0.41
1:D:143:THR:CG2	1:D:206:ASP:OD1	2.69	0.41
1:A:50:LYS:HE3	4:A:600:HOH:O	2.21	0.41
1:C:84:LEU:CD2	1:C:278:SER:HA	2.51	0.41
1:B:23:ALA:O	1:B:60:PHE:HA	2.21	0.41
1:B:126:PHE:HB2	1:B:268:LYS:HE3	2.03	0.41
1:D:49:GLY:HA3	1:D:60:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASN:HD22	1:C:262:VAL:H	1.68	0.41
1:A:283[A]:ARG:NH1	4:A:503:HOH:O	2.28	0.40
1:D:264:VAL:CG1	1:D:303:LEU:HD11	2.48	0.40
1:C:133:TYR:HA	1:C:165:GLY:O	2.22	0.40
1:D:260:ASN:HD22	1:D:262:VAL:H	1.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:570:HOH:O	4:B:520:HOH:O[6_555]	2.11	0.09
4:A:618:HOH:O	4:B:610:HOH:O[6_555]	2.12	0.08

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	330/331 (100%)	312 (94%)	17 (5%)	1 (0%)	36	44
1	B	330/331 (100%)	314 (95%)	15 (4%)	1 (0%)	36	44
1	C	331/331 (100%)	311 (94%)	19 (6%)	1 (0%)	36	44
1	D	329/331 (99%)	310 (94%)	17 (5%)	2 (1%)	21	25
All	All	1320/1324 (100%)	1247 (94%)	68 (5%)	5 (0%)	30	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	306	THR
1	A	306	THR
1	B	306	THR
1	D	256	GLY

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Mol	Chain	Res	Type
1	D	306	THR

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	256/255 (100%)	244 (95%)	12 (5%)	23	33
1	B	256/255 (100%)	236 (92%)	20 (8%)	11	14
1	C	257/255 (101%)	244 (95%)	13 (5%)	21	29
1	D	255/255 (100%)	236 (92%)	19 (8%)	12	15
All	All	1024/1020 (100%)	960 (94%)	64 (6%)	16	21

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	LEU
1	C	27	THR
1	C	29	THR
1	C	77	GLN
1	C	119	LYS
1	C	142	THR
1	C	143	THR
1	C	236	VAL
1	C	238	VAL
1	C	254	LYS
1	C	260	ASN
1	C	264	VAL
1	C	285	GLU
1	A	11	MET
1	A	12	SER
1	A	27	THR
1	A	29	THR
1	A	50	LYS
1	A	92	LEU
1	A	142	THR

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Mol	Chain	Res	Type
1	A	143	THR
1	A	236	VAL
1	A	264	VAL
1	A	305	VAL
1	A	332	GLU
1	B	3	SER
1	B	4	SER
1	B	12	SER
1	B	27	THR
1	B	68	GLU
1	B	77	GLN
1	B	97	LYS
1	B	142	THR
1	B	143	THR
1	B	230	ARG
1	B	233	ASN
1	B	236	VAL
1	B	238	VAL
1	B	246	GLU
1	B	254	LYS
1	B	255	ASP
1	B	258	GLU
1	B	264	VAL
1	B	310	GLU
1	B	317	GLU
1	D	12	SER
1	D	14	GLU
1	D	19	GLN
1	D	27	THR
1	D	36[A]	SER
1	D	36[B]	SER
1	D	77	GLN
1	D	92	LEU
1	D	142	THR
1	D	143	THR
1	D	233	ASN
1	D	236	VAL
1	D	238	VAL
1	D	260	ASN
1	D	264	VAL
1	D	305	VAL
1	D	317	GLU

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Mol	Chain	Res	Type
1	D	329	LYS
1	D	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	19	GLN
1	C	46	GLN
1	C	52	HIS
1	C	64	GLN
1	C	227	ASN
1	C	233	ASN
1	C	260	ASN
1	A	7	HIS
1	A	8	HIS
1	A	46	GLN
1	A	52	HIS
1	A	53	ASN
1	A	64	GLN
1	A	227	ASN
1	A	233	ASN
1	A	260	ASN
1	B	8	HIS
1	B	46	GLN
1	B	52	HIS
1	B	64	GLN
1	B	227	ASN
1	B	260	ASN
1	D	8	HIS
1	D	46	GLN
1	D	52	HIS
1	D	64	GLN
1	D	73	ASN
1	D	227	ASN
1	D	233	ASN
1	D	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GMP	D	401	-	22,22,22	0.45	0	33,33,33	0.45	0
2	GMP	C	401	-	22,22,22	0.39	0	33,33,33	0.46	0
2	GMP	A	401	-	22,22,22	0.37	0	33,33,33	0.40	0
2	GMP	B	401	-	22,22,22	0.41	0	33,33,33	0.39	0

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	GMP	D	401	-	-	0/6/22/22	0/3/3/3
2	GMP	C	401	-	-	0/6/22/22	0/3/3/3
2	GMP	A	401	-	-	0/6/22/22	0/3/3/3
2	GMP	B	401	-	-	0/6/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	331/331 (100%)	0.28	18 (5%) 31 32	19, 38, 75, 93	1 (0%)
1	B	331/331 (100%)	0.34	11 (3%) 49 51	19, 41, 77, 103	1 (0%)
1	C	331/331 (100%)	0.18	11 (3%) 49 51	19, 37, 63, 87	2 (0%)
1	D	330/331 (99%)	1.11	47 (14%) 6 6	27, 61, 95, 110	1 (0%)
All	All	1323/1324 (99%)	0.48	87 (6%) 24 25	19, 44, 84, 110	5 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	LYS	5.5
1	A	333	LYS	3.9
1	C	333	LYS	3.7
1	C	29	THR	3.6
1	D	11	MET	3.6
1	D	96	VAL	3.5
1	A	11	MET	3.5
1	A	29	THR	3.4
1	A	297	LYS	3.4
1	D	5	HIS	3.4
1	B	11	MET	3.3
1	D	4	SER	3.3
1	C	16	LEU	3.2
1	D	61	THR	3.2
1	D	305	VAL	3.2
1	D	179	VAL	3.1
1	A	256	GLY	3.1
1	B	333	LYS	2.9
1	B	254	LYS	2.9
1	D	68	GLU	2.8
1	D	69	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	97	LYS	2.8
1	D	76	GLN	2.7
1	B	3	SER	2.7
1	D	80	GLY	2.7
1	D	297	LYS	2.7
1	C	11	MET	2.7
1	D	72	ALA	2.7
1	D	18	PHE	2.7
1	A	252	THR	2.7
1	A	310	GLU	2.6
1	D	174	ASP	2.6
1	D	252	THR	2.6
1	C	117	ASP	2.6
1	B	328	VAL	2.6
1	D	104	THR	2.5
1	B	314	LYS	2.5
1	D	170	VAL	2.5
1	C	14	GLU	2.5
1	D	13	GLY	2.5
1	D	75	LEU	2.5
1	B	231	PRO	2.5
1	D	71	TYR	2.4
1	A	233	ASN	2.4
1	D	85	ILE	2.4
1	D	328	VAL	2.4
1	D	254	LYS	2.4
1	D	176	SER	2.3
1	A	317	GLU	2.3
1	D	79	ALA	2.3
1	D	100	ALA	2.3
1	D	258	GLU	2.3
1	D	106	LEU	2.3
1	D	66	THR	2.3
1	C	6	HIS	2.3
1	A	314	LYS	2.3
1	D	101	LYS	2.3
1	D	146	LYS	2.3
1	D	95	ALA	2.3
1	A	258	GLU	2.3
1	C	318	ASP	2.2
1	D	98	ASP	2.2
1	D	105	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	17	TYR	2.2
1	B	29	THR	2.2
1	A	30	GLY	2.2
1	D	314	LYS	2.2
1	A	305	VAL	2.2
1	D	227	ASN	2.2
1	A	248	GLU	2.2
1	B	173	VAL	2.2
1	D	147	GLN	2.2
1	D	188	GLY	2.2
1	A	328	VAL	2.1
1	A	257	LYS	2.1
1	D	102	GLU	2.1
1	D	207	ILE	2.1
1	D	312	GLY	2.1
1	B	236	VAL	2.1
1	D	63	PHE	2.1
1	C	23	ALA	2.0
1	A	325	ASP	2.0
1	B	276	ASP	2.0
1	D	173	VAL	2.0
1	C	297	LYS	2.0
1	A	250	LYS	2.0
1	D	197	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GMP	D	401	20/20	0.95	0.07	36,40,47,47	0
2	GMP	B	401	20/20	0.96	0.05	24,27,30,31	0
2	GMP	A	401	20/20	0.96	0.06	23,25,27,29	0
2	GMP	C	401	20/20	0.97	0.05	22,25,31,32	0
3	NI	C	402	1/1	0.98	0.05	74,74,74,74	0
3	NI	C	403	1/1	0.99	0.03	41,41,41,41	0
3	NI	A	402	1/1	0.99	0.08	80,80,80,80	0
3	NI	A	403	1/1	0.99	0.02	20,20,20,20	0
3	NI	B	402	1/1	0.99	0.02	18,18,18,18	0
3	NI	B	403	1/1	0.99	0.01	25,25,25,25	0
3	NI	D	402	1/1	0.99	0.03	49,49,49,49	0
3	NI	C	404	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.