



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 11:05 AM EDT

PDB ID : 4GQA  
Title : Crystal structure of NAD binding oxidoreductase from *Klebsiella pneumoniae*  
Authors : Osinski, S.; Majorek, K.A.; Niedzialkowska, E.; Osinski, T.; Porebski, P.J.; Nawar, A.; Hammonds, J.; Hillerich, B.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; Minor, W.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2012-08-22  
Resolution : 2.42 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

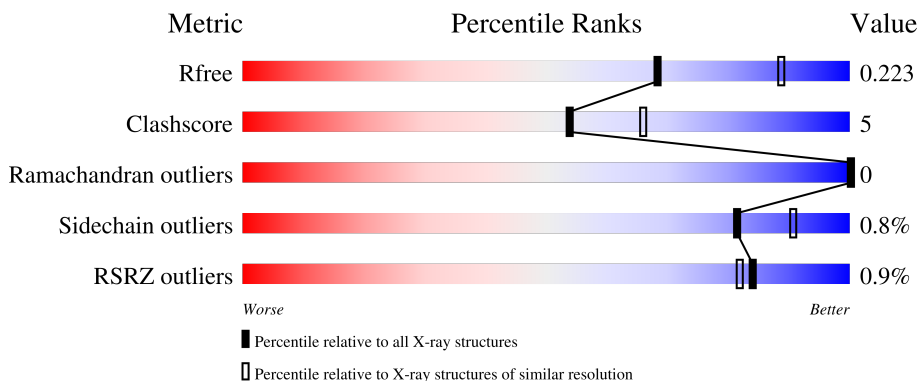
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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  $\geq 3$ , 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	412	 83% 8% 9%
1	B	412	 82% 9% 9%
1	C	412	 83% 9% 8%
1	D	412	 81% 10% 9%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12033 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 NAD binding Oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	376	2920	1846	525	533	6	10	0	5	0
1	B	375	2903	1835	512	540	6	10	0	5	0
1	C	377	2911	1842	517	536	6	10	0	4	0
1	D	376	2912	1841	522	533	6	10	0	4	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	expression tag	UNP B5Y097
A	-20	HIS	-	expression tag	UNP B5Y097
A	-19	HIS	-	expression tag	UNP B5Y097
A	-18	HIS	-	expression tag	UNP B5Y097
A	-17	HIS	-	expression tag	UNP B5Y097
A	-16	HIS	-	expression tag	UNP B5Y097
A	-15	HIS	-	expression tag	UNP B5Y097
A	-14	SER	-	expression tag	UNP B5Y097
A	-13	SER	-	expression tag	UNP B5Y097
A	-12	GLY	-	expression tag	UNP B5Y097
A	-11	VAL	-	expression tag	UNP B5Y097
A	-10	ASP	-	expression tag	UNP B5Y097
A	-9	LEU	-	expression tag	UNP B5Y097
A	-8	GLY	-	expression tag	UNP B5Y097
A	-7	THR	-	expression tag	UNP B5Y097
A	-6	GLU	-	expression tag	UNP B5Y097
A	-5	ASN	-	expression tag	UNP B5Y097
A	-4	LEU	-	expression tag	UNP B5Y097
A	-3	TYR	-	expression tag	UNP B5Y097
A	-2	PHE	-	expression tag	UNP B5Y097
A	-1	GLN	-	expression tag	UNP B5Y097

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP B5Y097
A	49	MSE	LEU	cloning artifact	UNP B5Y097
B	-21	MSE	-	expression tag	UNP B5Y097
B	-20	HIS	-	expression tag	UNP B5Y097
B	-19	HIS	-	expression tag	UNP B5Y097
B	-18	HIS	-	expression tag	UNP B5Y097
B	-17	HIS	-	expression tag	UNP B5Y097
B	-16	HIS	-	expression tag	UNP B5Y097
B	-15	HIS	-	expression tag	UNP B5Y097
B	-14	SER	-	expression tag	UNP B5Y097
B	-13	SER	-	expression tag	UNP B5Y097
B	-12	GLY	-	expression tag	UNP B5Y097
B	-11	VAL	-	expression tag	UNP B5Y097
B	-10	ASP	-	expression tag	UNP B5Y097
B	-9	LEU	-	expression tag	UNP B5Y097
B	-8	GLY	-	expression tag	UNP B5Y097
B	-7	THR	-	expression tag	UNP B5Y097
B	-6	GLU	-	expression tag	UNP B5Y097
B	-5	ASN	-	expression tag	UNP B5Y097
B	-4	LEU	-	expression tag	UNP B5Y097
B	-3	TYR	-	expression tag	UNP B5Y097
B	-2	PHE	-	expression tag	UNP B5Y097
B	-1	GLN	-	expression tag	UNP B5Y097
B	0	SER	-	expression tag	UNP B5Y097
B	49	MSE	LEU	cloning artifact	UNP B5Y097
C	-21	MSE	-	expression tag	UNP B5Y097
C	-20	HIS	-	expression tag	UNP B5Y097
C	-19	HIS	-	expression tag	UNP B5Y097
C	-18	HIS	-	expression tag	UNP B5Y097
C	-17	HIS	-	expression tag	UNP B5Y097
C	-16	HIS	-	expression tag	UNP B5Y097
C	-15	HIS	-	expression tag	UNP B5Y097
C	-14	SER	-	expression tag	UNP B5Y097
C	-13	SER	-	expression tag	UNP B5Y097
C	-12	GLY	-	expression tag	UNP B5Y097
C	-11	VAL	-	expression tag	UNP B5Y097
C	-10	ASP	-	expression tag	UNP B5Y097
C	-9	LEU	-	expression tag	UNP B5Y097
C	-8	GLY	-	expression tag	UNP B5Y097
C	-7	THR	-	expression tag	UNP B5Y097
C	-6	GLU	-	expression tag	UNP B5Y097
C	-5	ASN	-	expression tag	UNP B5Y097

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	LEU	-	expression tag	UNP B5Y097
C	-3	TYR	-	expression tag	UNP B5Y097
C	-2	PHE	-	expression tag	UNP B5Y097
C	-1	GLN	-	expression tag	UNP B5Y097
C	0	SER	-	expression tag	UNP B5Y097
C	49	MSE	LEU	cloning artifact	UNP B5Y097
D	-21	MSE	-	expression tag	UNP B5Y097
D	-20	HIS	-	expression tag	UNP B5Y097
D	-19	HIS	-	expression tag	UNP B5Y097
D	-18	HIS	-	expression tag	UNP B5Y097
D	-17	HIS	-	expression tag	UNP B5Y097
D	-16	HIS	-	expression tag	UNP B5Y097
D	-15	HIS	-	expression tag	UNP B5Y097
D	-14	SER	-	expression tag	UNP B5Y097
D	-13	SER	-	expression tag	UNP B5Y097
D	-12	GLY	-	expression tag	UNP B5Y097
D	-11	VAL	-	expression tag	UNP B5Y097
D	-10	ASP	-	expression tag	UNP B5Y097
D	-9	LEU	-	expression tag	UNP B5Y097
D	-8	GLY	-	expression tag	UNP B5Y097
D	-7	THR	-	expression tag	UNP B5Y097
D	-6	GLU	-	expression tag	UNP B5Y097
D	-5	ASN	-	expression tag	UNP B5Y097
D	-4	LEU	-	expression tag	UNP B5Y097
D	-3	TYR	-	expression tag	UNP B5Y097
D	-2	PHE	-	expression tag	UNP B5Y097
D	-1	GLN	-	expression tag	UNP B5Y097
D	0	SER	-	expression tag	UNP B5Y097
D	49	MSE	LEU	cloning artifact	UNP B5Y097

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



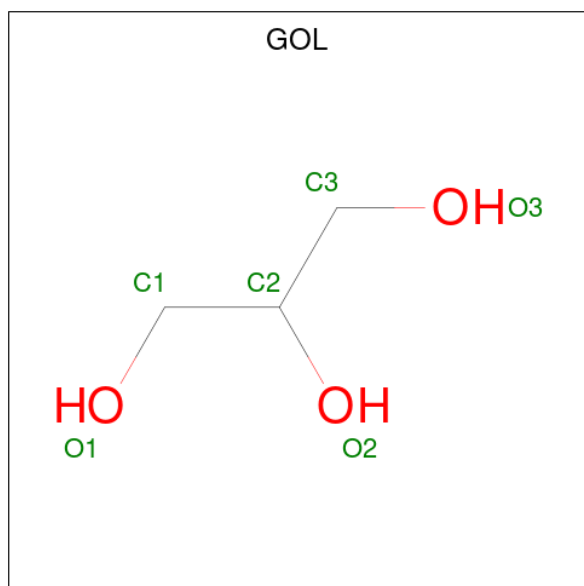
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			8	5	3		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			9	6	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

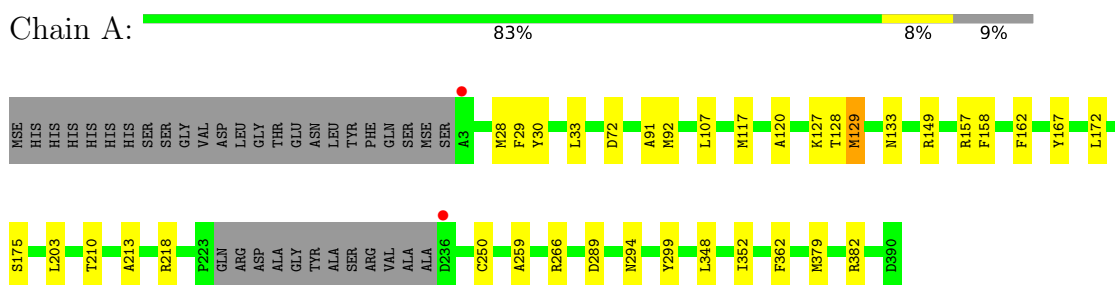
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	B	79	Total O 79 79	0	1
5	C	84	Total O 84 84	0	0
5	D	106	Total O 106 106	0	1

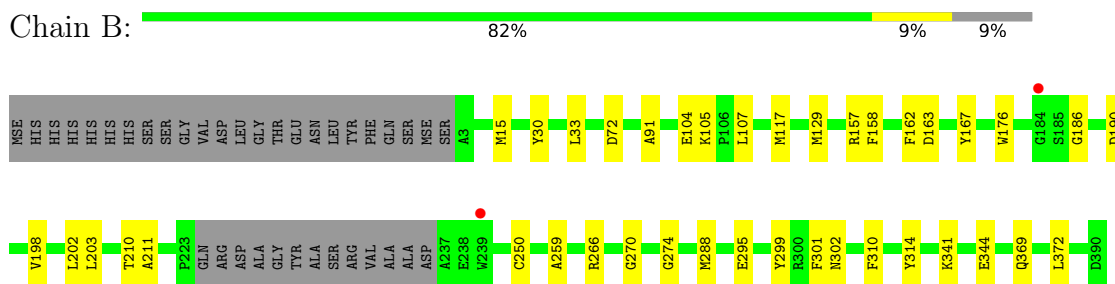
### 3 Residue-property plots [i](#)

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

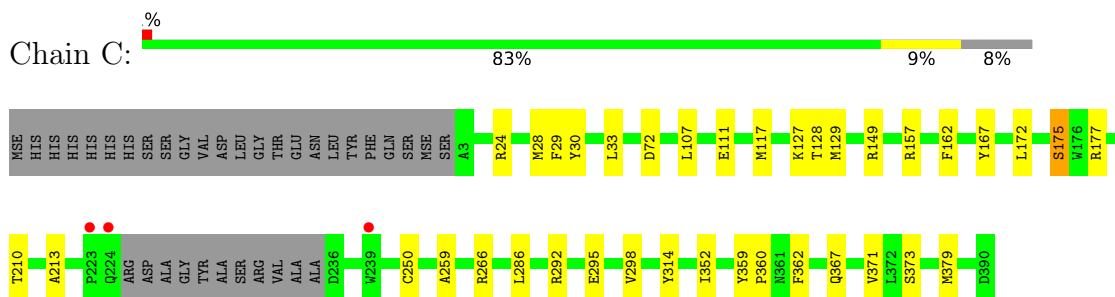
- Molecule 1: NAD binding Oxidoreductase



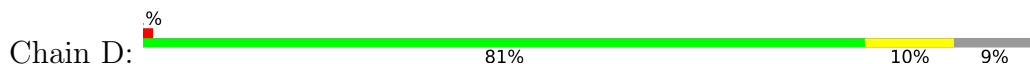
- Molecule 1: NAD binding Oxidoreductase



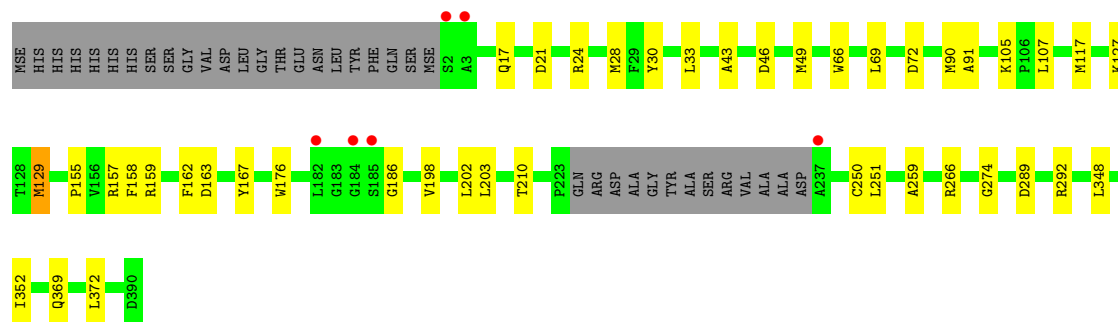
- Molecule 1: NAD binding Oxidoreductase



- Molecule 1: NAD binding Oxidoreductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.42Å 113.03Å 132.17Å 90.00° 90.54° 90.00°	Depositor
Resolution (Å)	50.00 – 2.42 42.95 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.42) 96.7 (42.95-2.42)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.186 , 0.230 0.185 , 0.223	Depositor DCC
$R_{free}$ test set	3279 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 21.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.002 for -k,-h,-l 0.409 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, GOL, PG4

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	0.80	0/2993	0.87	5/4035 (0.1%)
1	B	0.86	1/2979 (0.0%)	0.86	2/4018 (0.0%)
1	C	0.80	0/2979	0.86	1/4020 (0.0%)
1	D	0.83	1/2978 (0.0%)	0.85	5/4013 (0.1%)
All	All	0.82	2/11929 (0.0%)	0.86	13/16086 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	176	TRP	CD2-CE2	5.18	1.47	1.41
1	B	176	TRP	CD2-CE2	5.14	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	MSE	CG-SE-CE	5.73	111.50	98.90
1	D	28	MSE	CG-SE-CE	5.65	111.33	98.90
1	D	129	MSE	CA-CB-CG	-5.49	103.97	113.30
1	D	159	ARG	CB-CG-CD	5.44	125.75	111.60
1	A	382	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	129	MSE	CG-SE-CE	-5.33	87.17	98.90
1	C	149	ARG	CG-CD-NE	5.32	122.98	111.80
1	D	289	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	251	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	A	149	ARG	CG-CD-NE	5.14	122.59	111.80
1	A	129	MSE	CA-CB-CG	-5.07	104.68	113.30
1	B	341	LYS	CD-CE-NZ	5.04	123.30	111.70
1	A	289	ASP	CB-CG-OD1	5.02	122.82	118.30

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	2920	0	2789	25	0
1	B	2903	0	2768	28	0
1	C	2911	0	2764	37	0
1	D	2912	0	2797	43	0
2	B	12	0	13	3	0
2	C	4	0	4	0	0
2	D	9	0	11	0	0
3	B	4	0	5	0	0
4	D	12	0	16	0	0
5	A	77	0	0	1	0
5	B	79	0	0	1	0
5	C	84	0	0	0	0
5	D	106	0	0	1	0
All	All	12033	0	11167	121	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 5.

All (121) 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:24[B]:ARG:NH1	1:D:24[B]:ARG:HB3	1.22	1.48
1:C:24[B]:ARG:HH11	1:D:24[B]:ARG:CB	1.48	1.25
1:C:28:MSE:HE1	1:D:21:ASP:HB2	1.29	1.11
1:C:24[B]:ARG:NH1	1:D:24[B]:ARG:CB	2.18	0.96
1:D:129:MSE:CE	1:D:348:LEU:HA	2.03	0.88
1:B:301[B]:PHE:O	1:B:302[B]:ASN:HB2	1.77	0.82
1:C:129:MSE:HE2	1:C:360:PRO:HD2	1.63	0.81
1:C:286:LEU:CD2	1:C:298:VAL:HG22	2.10	0.81
1:D:129:MSE:HE1	1:D:348:LEU:CA	2.11	0.80
1:D:129:MSE:CE	1:D:348:LEU:CA	2.60	0.80
1:A:129:MSE:HE2	1:A:348:LEU:HD13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24[B]:ARG:HH12	1:D:24[B]:ARG:HB3	1.48	0.76
1:D:129:MSE:HE1	1:D:348:LEU:N	2.02	0.73
1:D:129:MSE:HE3	1:D:348:LEU:HB2	1.69	0.72
1:C:286:LEU:HD23	1:C:298:VAL:HG22	1.75	0.68
1:D:129:MSE:HE1	1:D:348:LEU:HA	1.74	0.67
1:A:92:MSE:HE1	1:A:120:ALA:HB2	1.76	0.67
1:D:129:MSE:HE2	1:D:348:LEU:HA	1.75	0.66
1:B:301[B]:PHE:O	1:B:302[B]:ASN:CB	2.43	0.64
1:C:129:MSE:CE	1:C:359:TYR:O	2.46	0.64
1:C:28:MSE:HE3	1:D:17:GLN:HG2	1.81	0.62
1:A:129:MSE:HE1	1:A:348:LEU:HB2	1.80	0.62
1:C:213:ALA:HB3	1:C:379:MSE:HE3	1.81	0.62
1:B:198:VAL:HG12	1:B:202:LEU:HD12	1.80	0.62
1:C:107:LEU:HD22	1:C:117:MSE:HE2	1.82	0.61
1:A:158:PHE:HB2	1:A:203:LEU:HD13	1.82	0.61
1:C:24[B]:ARG:HH11	1:D:24[B]:ARG:CG	2.12	0.61
1:D:186:GLY:HA2	5:D:590:HOH:O	2.03	0.58
1:C:175:SER:OG	1:C:177:ARG:NH2	2.36	0.58
1:D:198:VAL:HG12	1:D:202:LEU:HD12	1.86	0.57
1:A:172:LEU:HD23	1:A:172:LEU:C	2.25	0.57
1:B:190:ASP:OD2	2:B:403:PG4:H72	2.04	0.56
1:D:129:MSE:CE	1:D:348:LEU:CB	2.83	0.56
1:A:218[B]:ARG:HH11	1:A:218[B]:ARG:HG3	1.71	0.55
1:C:172:LEU:C	1:C:172:LEU:HD23	2.26	0.55
1:D:46:ASP:OD2	1:D:49:MSE:HE3	2.07	0.55
1:D:129:MSE:HE3	1:D:348:LEU:CB	2.37	0.54
1:C:24[B]:ARG:HE	1:D:24[B]:ARG:HD3	1.72	0.54
1:A:107:LEU:HD22	1:A:117:MSE:HE2	1.90	0.54
1:B:158:PHE:HB2	1:B:203:LEU:HD13	1.90	0.54
1:C:28:MSE:HE2	1:C:29:PHE:HE1	1.73	0.54
1:D:129:MSE:CE	1:D:348:LEU:HB2	2.35	0.53
1:C:24[B]:ARG:HG3	1:C:24[B]:ARG:NH2	2.23	0.53
1:B:369:GLN:HA	1:B:372:LEU:HD12	1.90	0.53
1:D:107:LEU:HD22	1:D:117:MSE:HE2	1.90	0.52
1:A:218[B]:ARG:HG3	1:A:218[B]:ARG:NH1	2.23	0.52
1:B:299:TYR:HB2	1:B:310:PHE:CD1	2.44	0.52
1:A:30:TYR:HB3	1:A:33:LEU:HG	1.92	0.52
1:C:107:LEU:HD22	1:C:117:MSE:CE	2.39	0.51
1:B:91:ALA:CB	1:B:117:MSE:HE3	2.40	0.51
1:B:129:MSE:HE3	1:B:344:GLU:HG2	1.93	0.51
1:D:30:TYR:HB3	1:D:33:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:THR:O	1:D:250:CYS:HB2	2.11	0.51
1:B:186:GLY:HA2	5:B:553:HOH:O	2.10	0.50
1:C:30:TYR:HB3	1:C:33:LEU:HG	1.94	0.50
1:B:299:TYR:HB2	1:B:310:PHE:CE1	2.46	0.50
1:A:210:THR:O	1:A:250:CYS:HB2	2.12	0.50
1:C:210:THR:O	1:C:250:CYS:HB2	2.12	0.50
1:B:210:THR:O	1:B:250:CYS:HB2	2.12	0.49
1:C:28:MSE:HE2	1:C:29:PHE:CE1	2.48	0.49
1:D:155:PRO:HB2	1:D:203:LEU:HD22	1.93	0.49
1:D:167:TYR:HB2	1:D:266:ARG:O	2.13	0.49
1:A:28:MSE:HE2	1:A:29:PHE:HE1	1.77	0.48
1:B:266:ARG:CD	2:B:403:PG4:H82	2.44	0.48
1:A:28:MSE:HE2	1:A:29:PHE:CE1	2.49	0.48
1:A:213:ALA:HB3	1:A:379:MSE:HE3	1.94	0.48
1:B:30:TYR:HB3	1:B:33:LEU:HG	1.95	0.48
1:B:72:ASP:C	1:B:72:ASP:OD2	2.52	0.48
1:B:107:LEU:HD22	1:B:117:MSE:HE2	1.95	0.48
1:D:155:PRO:HB3	1:D:203:LEU:HD21	1.96	0.48
1:C:213:ALA:CB	1:C:379:MSE:HE3	2.44	0.48
1:D:91:ALA:CB	1:D:117:MSE:HE3	2.45	0.47
1:C:24[B]:ARG:NH2	1:C:24[B]:ARG:CG	2.77	0.47
1:D:155:PRO:CB	1:D:203:LEU:CD2	2.93	0.46
1:A:72:ASP:C	1:A:72:ASP:OD2	2.54	0.46
1:C:127:LYS:HD3	1:C:352:ILE:HA	1.97	0.46
1:C:167:TYR:HB2	1:C:266:ARG:O	2.16	0.46
1:B:167:TYR:HB2	1:B:266:ARG:O	2.15	0.46
1:C:72:ASP:OD1	1:C:72:ASP:C	2.55	0.46
1:D:72:ASP:OD2	1:D:72:ASP:C	2.54	0.46
1:B:15[A]:MSE:HE3	1:B:104:GLU:OE2	2.16	0.46
1:C:128:THR:HB	1:C:362:PHE:CD1	2.50	0.46
1:B:266:ARG:HD2	2:B:403:PG4:H82	1.99	0.45
1:A:91:ALA:CB	1:A:117:MSE:HE3	2.47	0.45
1:A:167:TYR:HB2	1:A:266:ARG:O	2.16	0.45
1:D:369:GLN:HA	1:D:372:LEU:HD12	1.97	0.45
1:D:43:ALA:HB2	1:D:69:LEU:HD13	1.98	0.45
1:C:111[B]:GLU:CG	1:C:373:SER:OG	2.64	0.45
1:A:127:LYS:HD3	1:A:352:ILE:HA	1.97	0.45
1:A:218[B]:ARG:HH11	1:A:218[B]:ARG:CG	2.30	0.45
1:A:128:THR:HB	1:A:362:PHE:CD2	2.52	0.44
1:B:299:TYR:CD2	1:B:299:TYR:C	2.91	0.44
1:D:66:TRP:CG	1:D:90:MSE:HE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:CG1	1:D:202:LEU:HD12	2.48	0.44
1:D:157:ARG:HA	1:D:259:ALA:O	2.18	0.43
1:A:299:TYR:CE1	1:B:270:GLY:HA2	2.52	0.43
1:B:157:ARG:HA	1:B:259:ALA:O	2.18	0.43
1:B:211:ALA:CB	1:B:250:CYS:HB3	2.48	0.43
1:D:158:PHE:HB2	1:D:203:LEU:HD12	2.00	0.43
1:D:127:LYS:HD3	1:D:352:ILE:HA	2.00	0.42
1:A:129:MSE:HE2	1:A:348:LEU:CD1	2.43	0.42
1:A:157:ARG:HA	1:A:259:ALA:O	2.19	0.42
1:B:295:GLU:CG	1:B:314:TYR:CE2	3.02	0.42
1:C:24[B]:ARG:HH11	1:D:24[B]:ARG:HB3	0.65	0.42
1:C:157:ARG:HA	1:C:259:ALA:O	2.19	0.42
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.76	0.42
1:C:24[B]:ARG:NE	1:D:24[B]:ARG:HD3	2.33	0.42
1:D:107:LEU:HD23	1:D:107:LEU:HA	1.78	0.42
1:B:129:MSE:HE1	1:B:344:GLU:O	2.19	0.41
1:A:213:ALA:CB	1:A:379:MSE:HE3	2.50	0.41
1:A:294:ASN:HB2	5:A:444:HOH:O	2.21	0.41
1:C:129:MSE:HE1	1:C:359:TYR:O	2.20	0.41
1:B:163:ASP:O	1:B:274:GLY:HA3	2.20	0.41
1:C:295:GLU:CG	1:C:314:TYR:CE2	3.03	0.41
1:C:367:GLN:O	1:C:371:VAL:HG23	2.20	0.41
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.93	0.41
1:B:211:ALA:HB2	1:B:250:CYS:CB	2.51	0.40
1:D:155:PRO:CB	1:D:203:LEU:HD22	2.51	0.40
1:A:129:MSE:CE	1:A:348:LEU:HB2	2.47	0.40
1:C:292:ARG:NH2	1:D:292:ARG:NH1	2.68	0.40
1:D:163:ASP:O	1:D:274:GLY:HA3	2.20	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	377/412 (92%)	370 (98%)	7 (2%)	0	100	100
1	B	376/412 (91%)	367 (98%)	9 (2%)	0	100	100
1	C	377/412 (92%)	370 (98%)	7 (2%)	0	100	100
1	D	376/412 (91%)	368 (98%)	8 (2%)	0	100	100
All	All	1506/1648 (91%)	1475 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	284/310 (92%)	281 (99%)	3 (1%)	73	86
1	B	287/310 (93%)	285 (99%)	2 (1%)	84	92
1	C	283/310 (91%)	281 (99%)	2 (1%)	84	92
1	D	285/310 (92%)	283 (99%)	2 (1%)	84	92
All	All	1139/1240 (92%)	1130 (99%)	9 (1%)	81	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	162	PHE
1	A	175	SER
1	B	105	LYS
1	B	162	PHE
1	C	162	PHE
1	C	175	SER
1	D	105	LYS
1	D	162	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:



Mol	Chain	Res	Type
1	B	85	HIS
1	C	85	HIS
1	D	145	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

7 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	PG4	D	401	-	8,8,12	1.21	0	7,7,11	1.75	1 (14%)
2	PG4	C	401	-	3,3,12	0.73	0	2,2,11	0.11	0
2	PG4	B	401	-	7,7,12	0.97	0	6,6,11	1.09	1 (16%)
4	GOL	D	402	-	5,5,5	0.41	0	5,5,5	0.20	0
4	GOL	D	403	-	5,5,5	0.61	0	5,5,5	0.72	0
3	PEG	B	402	-	3,3,6	0.62	0	2,2,5	0.16	0
2	PG4	B	403	-	3,3,12	1.21	0	2,2,11	0.97	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	PG4	D	401	-	-	3/6/6/10	-
2	PG4	C	401	-	-	1/1/1/10	-
2	PG4	B	401	-	-	5/5/5/10	-
4	GOL	D	402	-	-	2/4/4/4	-
4	GOL	D	403	-	-	4/4/4/4	-
3	PEG	B	402	-	-	0/1/1/4	-
2	PG4	B	403	-	-	0/1/1/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PG4	C4-O3-C5	3.44	125.24	112.90
2	B	401	PG4	C5-O3-C4	2.19	122.76	113.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	GOL	O1-C1-C2-C3
4	D	403	GOL	O1-C1-C2-C3
2	B	401	PG4	O3-C5-C6-O4
2	B	401	PG4	O2-C3-C4-O3
4	D	403	GOL	C1-C2-C3-O3
4	D	402	GOL	O1-C1-C2-O2
4	D	403	GOL	O2-C2-C3-O3
2	D	401	PG4	O3-C5-C6-O4
4	D	403	GOL	O1-C1-C2-O2
2	B	401	PG4	C3-C4-O3-C5
2	D	401	PG4	C8-C7-O4-C6
2	B	401	PG4	C4-C3-O2-C2
2	D	401	PG4	C5-C6-O4-C7
2	B	401	PG4	C6-C5-O3-C4
2	C	401	PG4	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	PG4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/412 (89%)	-0.47	2 (0%) 91 89	29, 48, 79, 125	0
1	B	366/412 (88%)	-0.37	2 (0%) 91 89	23, 47, 91, 114	0
1	C	368/412 (89%)	-0.43	3 (0%) 86 84	30, 48, 82, 127	0
1	D	367/412 (89%)	-0.39	6 (1%) 72 69	23, 47, 94, 116	0
All	All	1468/1648 (89%)	-0.42	13 (0%) 84 82	23, 47, 88, 127	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	GLY	4.3
1	D	2	SER	3.9
1	C	223	PRO	3.8
1	A	236	ASP	3.4
1	D	3	ALA	3.0
1	D	184	GLY	2.9
1	A	3	ALA	2.8
1	C	224	GLN	2.7
1	D	182	LEU	2.4
1	C	239	TRP	2.2
1	D	237	ALA	2.2
1	D	185	SER	2.1
1	B	239	TRP	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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	PG4	D	401	9/13	0.74	0.23	35,51,55,62	0
2	PG4	B	401	8/13	0.82	0.18	40,47,58,59	0
2	PG4	B	403	4/13	0.84	0.27	54,54,55,58	0
4	GOL	D	403	6/6	0.86	0.28	68,74,81,85	0
4	GOL	D	402	6/6	0.93	0.22	65,68,69,69	0
3	PEG	B	402	4/7	0.94	0.18	63,64,67,68	0
2	PG4	C	401	4/13	0.97	0.10	34,36,37,42	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.