



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 PM GMT

PDB ID : 4GI5  
Title : Crystal Structure Of a Putative quinone reductase from Klebsiella pneumoniae (Target PSI-013613)  
Authors : Kumar, P.R.; Ahmed, M.; Banu, N.; Bhosle, R.; Bonanno, J.; Chamala, S.; Chowdhury, S.; Gizzi, A.; Glen, S.; Hammonds, J.; Hillerich, B.; Love, J.D.; Seidel, R.; Stead, M.; Toro, R.; Washington, E.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2012-08-08  
Resolution : 1.75 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

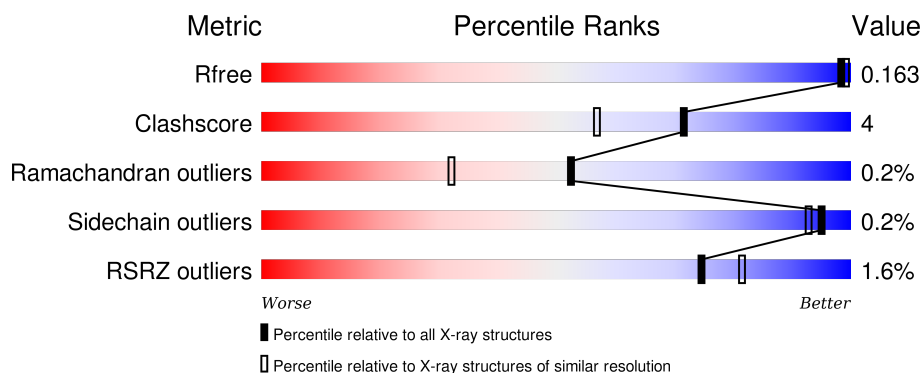
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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  $\geq 3$ , 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	280	 82% 9% • 8%
1	B	280	 81% 11% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	A	302	-	-	-	X
3	UNL	B	302	-	-	-	X
4	GOL	A	303	-	-	-	X
4	GOL	B	303	-	-	-	X
4	GOL	B	304	-	-	X	X
4	GOL	B	305	-	-	-	X
4	GOL	B	307	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4787 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 quinone reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	Se	0	4	0
			2103	1362	360	374	1	6			
1	B	261	Total	C	N	O	S	Se	0	1	0
			2093	1355	359	372	1	6			

There are 48 discrepancies between the modelled and reference sequences:

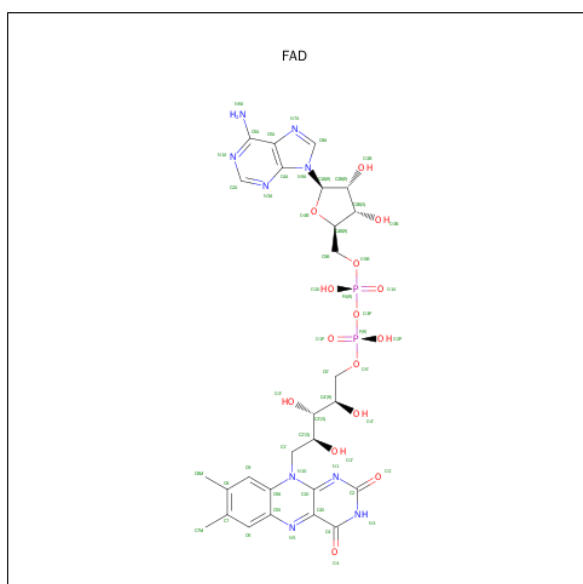
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	EXPRESSION TAG	UNP A6THR9
A	-20	HIS	-	EXPRESSION TAG	UNP A6THR9
A	-19	HIS	-	EXPRESSION TAG	UNP A6THR9
A	-18	HIS	-	EXPRESSION TAG	UNP A6THR9
A	-17	HIS	-	EXPRESSION TAG	UNP A6THR9
A	-16	HIS	-	EXPRESSION TAG	UNP A6THR9
A	-15	HIS	-	EXPRESSION TAG	UNP A6THR9
A	-14	SER	-	EXPRESSION TAG	UNP A6THR9
A	-13	SER	-	EXPRESSION TAG	UNP A6THR9
A	-12	GLY	-	EXPRESSION TAG	UNP A6THR9
A	-11	VAL	-	EXPRESSION TAG	UNP A6THR9
A	-10	ASP	-	EXPRESSION TAG	UNP A6THR9
A	-9	LEU	-	EXPRESSION TAG	UNP A6THR9
A	-8	GLY	-	EXPRESSION TAG	UNP A6THR9
A	-7	THR	-	EXPRESSION TAG	UNP A6THR9
A	-6	GLU	-	EXPRESSION TAG	UNP A6THR9
A	-5	ASN	-	EXPRESSION TAG	UNP A6THR9
A	-4	LEU	-	EXPRESSION TAG	UNP A6THR9
A	-3	TYR	-	EXPRESSION TAG	UNP A6THR9
A	-2	PHE	-	EXPRESSION TAG	UNP A6THR9
A	-1	GLN	-	EXPRESSION TAG	UNP A6THR9
A	0	SER	-	EXPRESSION TAG	UNP A6THR9
A	1	MSE	-	EXPRESSION TAG	UNP A6THR9
A	258	ALA	-	EXPRESSION TAG	UNP A6THR9
B	-21	MSE	-	EXPRESSION TAG	UNP A6THR9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	EXPRESSION TAG	UNP A6THR9
B	-19	HIS	-	EXPRESSION TAG	UNP A6THR9
B	-18	HIS	-	EXPRESSION TAG	UNP A6THR9
B	-17	HIS	-	EXPRESSION TAG	UNP A6THR9
B	-16	HIS	-	EXPRESSION TAG	UNP A6THR9
B	-15	HIS	-	EXPRESSION TAG	UNP A6THR9
B	-14	SER	-	EXPRESSION TAG	UNP A6THR9
B	-13	SER	-	EXPRESSION TAG	UNP A6THR9
B	-12	GLY	-	EXPRESSION TAG	UNP A6THR9
B	-11	VAL	-	EXPRESSION TAG	UNP A6THR9
B	-10	ASP	-	EXPRESSION TAG	UNP A6THR9
B	-9	LEU	-	EXPRESSION TAG	UNP A6THR9
B	-8	GLY	-	EXPRESSION TAG	UNP A6THR9
B	-7	THR	-	EXPRESSION TAG	UNP A6THR9
B	-6	GLU	-	EXPRESSION TAG	UNP A6THR9
B	-5	ASN	-	EXPRESSION TAG	UNP A6THR9
B	-4	LEU	-	EXPRESSION TAG	UNP A6THR9
B	-3	TYR	-	EXPRESSION TAG	UNP A6THR9
B	-2	PHE	-	EXPRESSION TAG	UNP A6THR9
B	-1	GLN	-	EXPRESSION TAG	UNP A6THR9
B	0	SER	-	EXPRESSION TAG	UNP A6THR9
B	1	MSE	-	EXPRESSION TAG	UNP A6THR9
B	258	ALA	-	EXPRESSION TAG	UNP A6THR9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

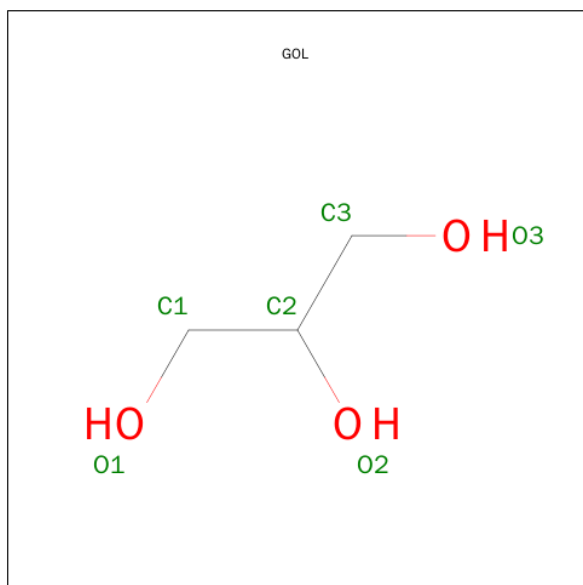


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			9	7	2		
3	A	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	A	2	Total 2	Cl 2	0	0

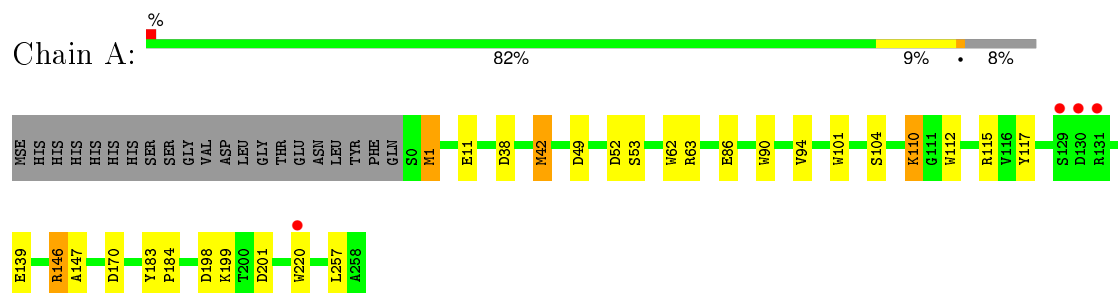
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total 220	O 220	0	0
6	B	214	Total 214	O 214	0	0

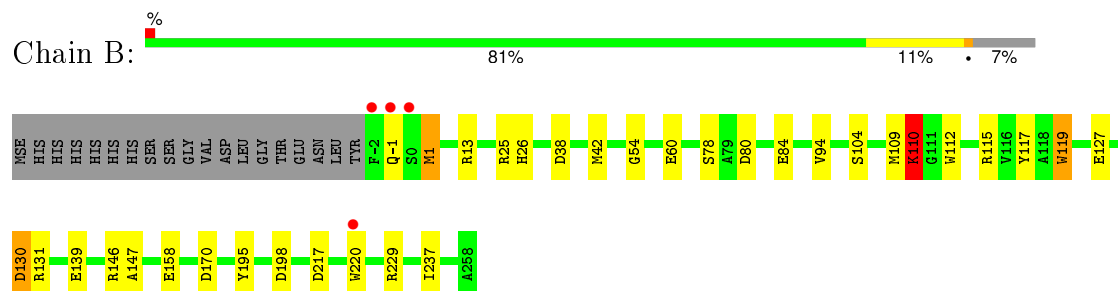
### 3 Residue-property plots [i](#)

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: quinone reductase



- Molecule 1: quinone reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.83Å 106.57Å 109.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 1.75 48.64 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.69-1.75) 100.0 (48.64-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.77 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.144 , 0.163 0.143 , 0.163	Depositor DCC
$R_{free}$ test set	5040 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.6	EDS
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 101073 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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, 0.375 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: GOL, UNL, FAD, CL

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	1.26	5/2168 (0.2%)	1.21	15/2943 (0.5%)
1	B	1.32	11/2157 (0.5%)	1.25	16/2926 (0.5%)
All	All	1.29	16/4325 (0.4%)	1.23	31/5869 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	TYR	CE1-CZ	-8.25	1.27	1.38
1	B	78	SER	CB-OG	-6.32	1.34	1.42
1	B	84	GLU	CD-OE2	6.14	1.32	1.25
1	B	158	GLU	CG-CD	5.98	1.60	1.51
1	A	11	GLU	CD-OE2	5.97	1.32	1.25
1	A	90	TRP	CG-CD1	5.85	1.45	1.36
1	B	119	TRP	CG-CD1	5.68	1.44	1.36
1	B	127	GLU	CG-CD	5.68	1.60	1.51
1	A	112	TRP	CD2-CE2	5.59	1.48	1.41
1	A	62	TRP	CE3-CZ3	5.58	1.48	1.38
1	B	139	GLU	CD-OE1	-5.51	1.19	1.25
1	B	112	TRP	CG-CD1	5.36	1.44	1.36
1	B	60	GLU	CG-CD	-5.31	1.44	1.51
1	B	117	TYR	CE1-CZ	5.12	1.45	1.38
1	A	101	TRP	CD1-NE1	5.06	1.46	1.38
1	B	13	ARG	CZ-NH1	-5.06	1.26	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	MSE	CG-SE-CE	-14.35	67.33	98.90
1	A	201	ASP	CB-CG-OD1	8.60	126.04	118.30
1	A	170	ASP	CB-CG-OD1	8.20	125.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	38	ASP	CB-CG-OD1	7.86	125.38	118.30
1	B	110	LYS	CD-CE-NZ	7.86	129.77	111.70
1	B	80	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	115	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	115	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	170	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	42	MSE	CG-SE-CE	-7.01	83.47	98.90
1	B	229	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	B	146	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	109	MSE	CG-SE-CE	-6.83	83.87	98.90
1	B	130	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	146	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	110	LYS	CD-CE-NZ	6.23	126.02	111.70
1	B	170	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	1	MSE	CG-SE-CE	5.72	111.48	98.90
1	B	170	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	38	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	195	TYR	CD1-CE1-CZ	5.57	124.81	119.80
1	A	63	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	117	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	49	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	52	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	131	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	115	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	1	MSE	CG-SE-CE	5.14	110.20	98.90
1	A	139	GLU	CB-CA-C	-5.13	100.14	110.40
1	B	109	MSE	CB-CG-SE	-5.07	97.50	112.70

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	2103	0	2010	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2093	0	2005	18	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
4	A	6	0	8	0	0
4	B	24	0	32	12	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	220	0	0	4	1
6	B	214	0	0	10	0
All	All	4787	0	4117	36	1

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 4.

All (36) 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:A:198:ASP:OD1	6:A:613:HOH:O	1.85	0.94
1:A:104[A]:SER:OG	1:B:110:LYS:HE3	1.67	0.94
1:B:130:ASP:O	4:B:304:GOL:C3	2.19	0.91
1:B:130:ASP:O	4:B:304:GOL:H32	1.71	0.90
1:A:110:LYS:HE3	1:B:104[A]:SER:OG	1.72	0.87
1:B:130:ASP:OD1	4:B:304:GOL:H31	1.78	0.84
1:B:25:ARG:NH1	6:B:549:HOH:O	2.06	0.83
4:B:307:GOL:H32	6:B:464:HOH:O	1.88	0.72
1:B:237:ILE:O	4:B:304:GOL:H2	1.93	0.69
1:B:130:ASP:O	4:B:304:GOL:H31	1.94	0.68
2:A:301:FAD:HM72	6:B:552:HOH:O	1.96	0.65
1:B:237:ILE:O	4:B:304:GOL:C2	2.47	0.63
1:B:26:HIS:HE1	1:B:217:ASP:OD1	1.83	0.60
1:A:1:MSE:HG3	1:A:220[B]:TRP:CE2	2.41	0.55
4:B:305:GOL:C3	6:B:474:HOH:O	2.55	0.54
1:A:146:ARG:HD2	1:A:220[A]:TRP:CD2	2.44	0.53
1:B:26:HIS:HD2	6:B:488:HOH:O	1.90	0.52
1:B:237:ILE:O	4:B:304:GOL:C3	2.60	0.50
6:A:478:HOH:O	2:B:301:FAD:HM72	2.11	0.50
1:B:94:VAL:O	1:B:147:ALA:HA	2.14	0.48
4:B:305:GOL:H32	6:B:474:HOH:O	2.14	0.48
1:A:86[A]:GLU:OE1	6:A:604:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HE2	1:A:220[B]:TRP:CD1	2.49	0.47
1:B:54:GLY:N	6:B:561:HOH:O	2.47	0.47
1:A:183:TYR:HB3	1:A:184:PRO:HD3	1.99	0.44
1:B:1:MSE:HB3	1:B:220:TRP:CZ2	2.52	0.44
1:B:198:ASP:OD1	6:B:568:HOH:O	2.21	0.44
1:A:94:VAL:O	1:A:147:ALA:HA	2.18	0.44
1:A:257:LEU:N	1:A:257:LEU:HD12	2.33	0.43
1:A:199:LYS:HD3	1:A:199:LYS:HA	1.94	0.43
4:B:304:GOL:H2	6:B:562:HOH:O	2.18	0.42
1:A:53:SER:HB3	6:A:563:HOH:O	2.19	0.42
4:B:307:GOL:C3	6:B:464:HOH:O	2.57	0.42
1:B:1:MSE:CB	1:B:220:TRP:CZ2	3.03	0.41
1:A:42:MSE:HB2	1:A:42:MSE:HE3	1.89	0.40
1:B:119:TRP:CD1	1:B:119:TRP:C	2.95	0.40

All (1) 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)
6:A:532:HOH:O	6:A:534:HOH:O[3_746]	2.08	0.12

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/280 (93%)	257 (98%)	4 (2%)	0	100	100
1	B	260/280 (93%)	251 (96%)	8 (3%)	1 (0%)	39	19
All	All	521/560 (93%)	508 (98%)	12 (2%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-1	GLN

### 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	212/220 (96%)	212 (100%)	0	100	100
1	B	211/220 (96%)	210 (100%)	1 (0%)	92	87
All	All	423/440 (96%)	422 (100%)	1 (0%)	95	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	B	26	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are unknown and 3 are monoatomic - leaving 7 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	FAD	A	301	-	48,58,58	1.72	8 (16%)	54,89,89	2.73	13 (24%)
4	GOL	A	303	-	5,5,5	1.19	0	5,5,5	1.42	1 (20%)
2	FAD	B	301	-	48,58,58	2.03	8 (16%)	54,89,89	2.64	20 (37%)
4	GOL	B	303	-	5,5,5	0.51	0	5,5,5	0.48	0
4	GOL	B	304	-	5,5,5	2.36	2 (40%)	5,5,5	2.30	1 (20%)
4	GOL	B	305	-	5,5,5	0.62	0	5,5,5	1.48	2 (40%)
4	GOL	B	307	-	5,5,5	0.41	0	5,5,5	1.39	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	FAD	A	301	-	-	0/30/50/50	0/6/6/6
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	FAD	B	301	-	-	0/30/50/50	0/6/6/6
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0
4	GOL	B	304	-	-	0/4/4/4	0/0/0/0
4	GOL	B	305	-	-	0/4/4/4	0/0/0/0
4	GOL	B	307	-	-	0/4/4/4	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FAD	C6-C5X	-6.65	1.31	1.41
2	A	301	FAD	C4A-N3A	-4.60	1.28	1.35
2	B	301	FAD	C4A-N3A	-4.42	1.29	1.35
2	A	301	FAD	C1'-N10	-3.16	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	C5A-N7A	-2.09	1.32	1.39
2	B	301	FAD	PA-O2A	-2.09	1.46	1.54
2	B	301	FAD	C4X-N5	2.39	1.37	1.33
2	B	301	FAD	C5'-C4'	2.61	1.55	1.51
2	A	301	FAD	C5'-C4'	2.67	1.55	1.51
4	B	304	GOL	O2-C2	2.73	1.51	1.43
2	A	301	FAD	C9A-N10	2.95	1.42	1.38
4	B	304	GOL	O3-C3	3.76	1.58	1.42
2	B	301	FAD	C2A-N3A	3.99	1.39	1.32
2	A	301	FAD	C5X-N5	4.06	1.41	1.35
2	A	301	FAD	C2A-N3A	4.28	1.39	1.32
2	A	301	FAD	C4X-N5	4.45	1.40	1.33
2	B	301	FAD	C5X-N5	4.50	1.42	1.35
2	B	301	FAD	O4B-C1B	6.48	1.49	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FAD	N3A-C2A-N1A	-10.94	120.51	128.89
2	B	301	FAD	N3A-C2A-N1A	-10.35	120.97	128.89
2	A	301	FAD	C4X-C10-N10	-7.38	116.17	120.52
2	A	301	FAD	C4-C4X-C10	-6.95	115.50	119.94
2	B	301	FAD	C4X-C4-N3	-4.67	117.20	123.59
2	B	301	FAD	C4X-C10-N10	-4.43	117.91	120.52
2	B	301	FAD	C1B-N9A-C4A	-3.70	121.36	126.94
2	A	301	FAD	C2B-C1B-N9A	-3.38	109.12	114.29
2	A	301	FAD	O3B-C3B-C4B	-3.24	101.34	111.05
2	B	301	FAD	C4-C4X-C10	-3.05	117.99	119.94
2	A	301	FAD	O3P-P-O5'	-2.89	95.26	102.94
2	B	301	FAD	O3P-PA-O5B	-2.82	95.46	102.94
4	A	303	GOL	O2-C2-C1	-2.65	96.52	108.65
2	B	301	FAD	C4B-O4B-C1B	-2.44	107.04	109.72
2	B	301	FAD	C9A-C5X-N5	-2.42	118.78	122.36
2	A	301	FAD	C1B-N9A-C4A	-2.30	123.47	126.94
2	B	301	FAD	O3P-P-O5'	-2.29	96.86	102.94
2	B	301	FAD	C2B-C1B-N9A	-2.27	110.83	114.29
2	B	301	FAD	O3'-C3'-C2'	-2.15	103.33	108.75
2	A	301	FAD	C4X-C4-N3	-2.05	120.78	123.59
4	B	305	GOL	O3-C3-C2	2.01	119.91	110.18
2	A	301	FAD	O4B-C1B-N9A	2.10	112.50	108.10
2	B	301	FAD	O2A-PA-O1A	2.33	125.16	112.53
2	A	301	FAD	C5X-C9A-N10	2.39	119.44	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FAD	C4X-N5-C5X	2.43	119.56	116.76
2	B	301	FAD	O2'-C2'-C1'	2.57	116.27	109.94
4	B	305	GOL	O2-C2-C1	2.63	120.70	108.65
2	B	301	FAD	C1'-N10-C9A	2.69	121.88	118.86
2	B	301	FAD	N6A-C6A-N1A	2.73	125.07	119.20
2	B	301	FAD	O4B-C4B-C3B	2.90	110.99	105.15
2	B	301	FAD	C5X-C9A-N10	2.92	119.84	117.62
2	A	301	FAD	N6A-C6A-N1A	4.21	128.23	119.20
4	B	304	GOL	O2-C2-C1	4.57	129.61	108.65
2	A	301	FAD	C4-N3-C2	4.95	119.53	115.25
2	B	301	FAD	C4A-C5A-N7A	5.83	114.84	109.48
2	A	301	FAD	C4A-C5A-N7A	6.15	115.14	109.48
2	B	301	FAD	C4-N3-C2	7.64	121.85	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FAD	1	0
2	B	301	FAD	1	0
4	B	304	GOL	8	0
4	B	305	GOL	2	0
4	B	307	GOL	2	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	253/280 (90%)	-0.13	4 (1%) 74 81	12, 19, 36, 61	0
1	B	255/280 (91%)	-0.23	4 (1%) 74 81	12, 19, 33, 74	0
All	All	508/560 (90%)	-0.18	8 (1%) 74 81	12, 19, 35, 74	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-2	PHE	11.2
1	B	-1	GLN	6.1
1	A	130	ASP	4.1
1	B	220	TRP	3.9
1	A	131	ARG	3.6
1	B	0	SER	2.9
1	A	220[A]	TRP	2.3
1	A	129	SER	2.3

### 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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	307	6/6	0.86	0.29	16.17	37,49,52,57	0
4	GOL	B	304	6/6	0.78	0.26	15.16	19,33,38,44	0
3	UNL	B	302	9/-	0.85	0.17	6.85	27,31,45,45	0
3	UNL	A	302	9/-	0.86	0.14	5.67	26,32,42,51	0
4	GOL	A	303	6/6	0.95	0.14	5.53	21,30,38,45	0
4	GOL	B	305	6/6	0.94	0.16	4.74	18,38,39,43	0
4	GOL	B	303	6/6	0.95	0.17	3.00	29,42,48,53	0
2	FAD	A	301	53/53	0.99	0.09	-0.17	11,14,24,30	0
2	FAD	B	301	53/53	0.98	0.07	-0.42	11,15,26,28	0
5	CL	A	305	1/1	0.98	0.04	-1.42	29,29,29,29	0
5	CL	B	306	1/1	0.99	0.04	-3.76	28,28,28,28	0
5	CL	A	304	1/1	0.98	0.05	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.