



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:48 AM GMT

PDB ID : 2YG4  
Title : STRUCTURE-BASED REDESIGN OF COFACTOR BINDING IN PUTRESCINE OXIDASE: WILD TYPE BOUND TO PUTRESCINE  
Authors : Kopacz, M.M.; Rovida, S.; Van Duijn, E.; Fraaije, M.W.; Mattevi, A.  
Deposited on : 2011-04-11  
Resolution : 2.30 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

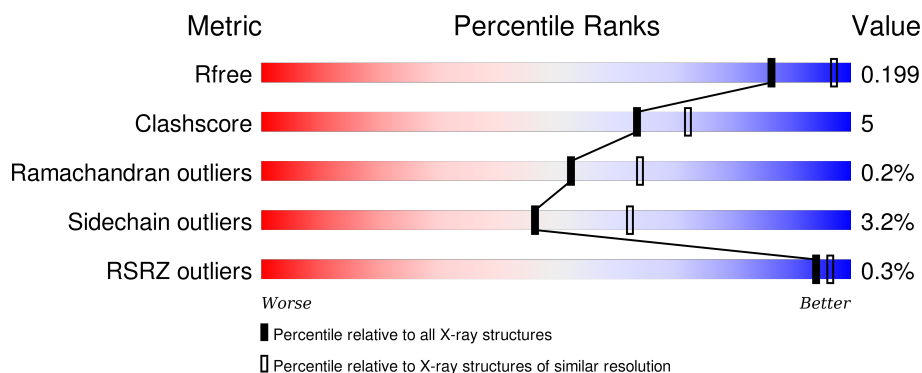
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	453	 84% 13% ...
1	B	453	 88% 11% ..

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	4HA	A	601	-	-	-	X
3	4HA	B	601	-	-	-	X
4	GOL	A	1451	-	-	-	X
4	GOL	A	1452	-	-	-	X
4	GOL	A	1455	-	-	-	X
5	SO4	B	1453	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7773 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 PUTRESCINE OXIDASE.

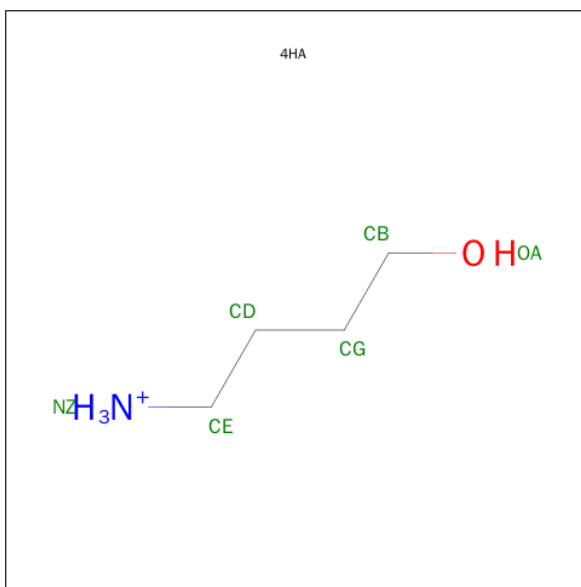
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3450	2157	605	678	10			
1	B	450	Total	C	N	O	S	0	0	0
			3456	2160	606	680	10			

- 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 4-HYDROXYBUTAN-1-AMINIUM (three-letter code: 4HA) (formula:  $C_4H_{12}NO$ ).



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

- 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	A	1	Total	C	O	0	0
			6	3	3		

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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		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

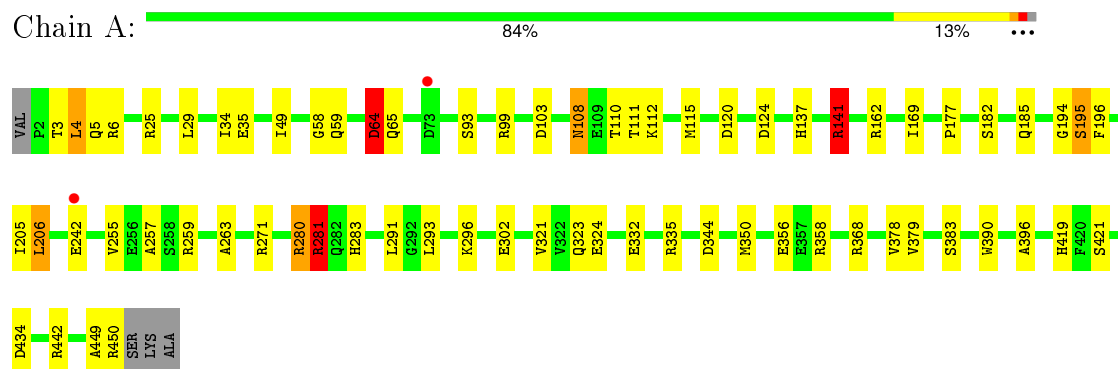
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	399	Total	O	0	0
			399	399		
6	B	306	Total	O	0	0
			306	306		

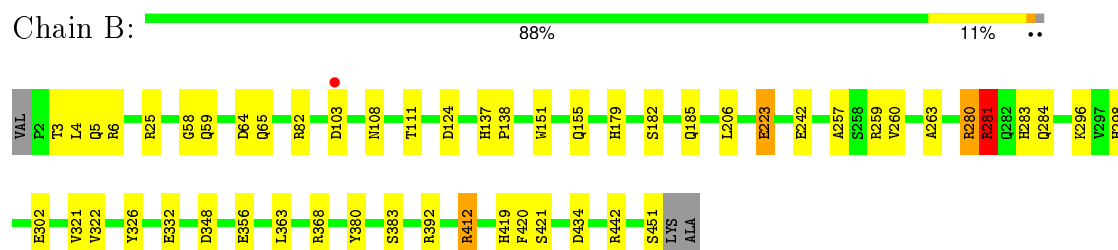
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: PUTRESCINE OXIDASE



#### • Molecule 1: PUTRESCINE OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.59 Å 80.61 Å 92.12 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.61 – 2.30 34.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.61-2.30) 99.7 (34.43-2.30)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.157 , 0.197 0.160 , 0.199	Depositor DCC
$R_{free}$ test set	3327 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 66347 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 4HA, FAD

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	1.13	8/3521 (0.2%)	1.07	21/4781 (0.4%)
1	B	1.14	7/3527 (0.2%)	1.00	11/4789 (0.2%)
All	All	1.13	15/7048 (0.2%)	1.03	32/9570 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	GLU	CG-CD	8.22	1.64	1.51
1	A	302	GLU	CB-CG	7.25	1.66	1.52
1	A	356	GLU	CG-CD	6.40	1.61	1.51
1	A	64	ASP	CB-CG	6.23	1.64	1.51
1	B	242	GLU	CG-CD	6.23	1.61	1.51
1	B	281	ARG	CD-NE	-5.90	1.36	1.46
1	A	242	GLU	CG-CD	5.79	1.60	1.51
1	B	326	TYR	CD1-CE1	5.68	1.47	1.39
1	B	380	TYR	CD2-CE2	5.59	1.47	1.39
1	B	302	GLU	CG-CD	5.48	1.60	1.51
1	A	390	TRP	CE3-CZ3	5.40	1.47	1.38
1	A	35	GLU	CB-CG	5.37	1.62	1.52
1	B	223	GLU	CG-CD	5.14	1.59	1.51
1	A	141	ARG	CB-CG	5.09	1.66	1.52
1	B	356	GLU	CG-CD	5.04	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ARG	NE-CZ-NH2	-14.70	112.95	120.30
1	B	281	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	A	368	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	A	141	ARG	NE-CZ-NH1	-10.65	114.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	MET	CG-SD-CE	-9.95	84.28	100.20
1	A	281	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	B	281	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	B	281	ARG	CG-CD-NE	-7.48	96.09	111.80
1	B	412	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	368	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	335	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	25	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	280	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	348	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	141	ARG	CG-CD-NE	6.38	125.21	111.80
1	A	99	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	281	ARG	CG-CD-NE	-6.25	98.68	111.80
1	B	280	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	25	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	25	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	64	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	259	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	259	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	260	VAL	CB-CA-C	-5.74	100.49	111.40
1	B	82	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	271	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	49	ILE	CG1-CB-CG2	-5.53	99.25	111.40
1	A	442	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	442	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	4	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	120	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	162	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	3450	0	3337	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3456	0	3342	25	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	6	0	11	0	0
3	B	6	0	11	1	0
4	A	18	0	24	3	0
4	B	6	0	8	2	0
5	A	10	0	0	1	0
5	B	10	0	0	2	0
6	A	399	0	0	11	0
6	B	306	0	0	4	0
All	All	7773	0	6795	72	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 (72) 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:64:ASP:HB2	6:A:2076:HOH:O	1.37	1.19
1:B:280:ARG:HD2	5:B:1453:SO4:O3	1.47	1.14
1:A:124:ASP:HB2	6:A:2145:HOH:O	1.58	1.04
1:A:141:ARG:HH11	1:A:141:ARG:CG	1.81	0.93
1:A:449:ALA:O	1:A:450:ARG:HB2	1.69	0.89
1:B:182:SER:H	1:B:185:GLN:HE21	1.26	0.82
1:B:412:ARG:O	4:B:1452:GOL:H32	1.83	0.77
1:A:450:ARG:HH11	1:A:450:ARG:HG2	1.50	0.76
1:A:141:ARG:HH11	1:A:141:ARG:HG3	1.51	0.75
1:B:182:SER:H	1:B:185:GLN:NE2	1.92	0.67
1:B:259:ARG:NH1	6:B:2192:HOH:O	2.29	0.66
4:A:1455:GOL:H31	6:A:2316:HOH:O	1.96	0.65
1:A:59:GLN:HE21	1:A:296:LYS:NZ	1.94	0.65
1:A:59:GLN:HE21	1:A:296:LYS:HZ1	1.48	0.62
1:A:182:SER:H	1:A:185:GLN:HE21	1.46	0.61
1:A:449:ALA:O	1:A:450:ARG:CB	2.46	0.60
1:A:112:LYS:HE3	6:A:2134:HOH:O	2.02	0.59
1:A:450:ARG:HH11	1:A:450:ARG:CG	2.14	0.59
1:A:112:LYS:CE	6:A:2134:HOH:O	2.49	0.58
1:A:263:ALA:HA	1:A:421:SER:O	2.02	0.58
1:A:205:ILE:HG23	1:A:206:LEU:HD13	1.85	0.58
4:A:1455:GOL:C3	6:A:2316:HOH:O	2.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:ND2	1:A:111:THR:H	2.02	0.57
1:B:451:SER:O	6:B:2299:HOH:O	2.17	0.56
1:A:110:THR:HB	6:A:2137:HOH:O	2.05	0.56
1:B:58:GLY:HA2	2:B:600:FAD:C4X	2.36	0.55
1:A:141:ARG:CG	1:A:141:ARG:NH1	2.58	0.55
1:B:108:ASN:ND2	1:B:111:THR:H	2.05	0.54
1:A:450:ARG:NH1	1:A:450:ARG:CG	2.70	0.52
1:A:450:ARG:HG2	1:A:450:ARG:NH1	2.23	0.52
1:A:65:GLN:HG2	1:A:434:ASP:CB	2.39	0.52
1:A:34:ILE:HD11	1:A:255:VAL:HG21	1.90	0.52
1:B:59:GLN:HE21	1:B:296:LYS:NZ	2.08	0.51
1:A:194:GLY:O	1:A:195:SER:HB3	2.10	0.51
1:A:6:ARG:O	1:A:257:ALA:HA	2.10	0.51
1:A:141:ARG:NH1	5:A:1453:SO4:S	2.80	0.51
1:B:419:HIS:HE1	6:B:2203:HOH:O	1.94	0.51
1:A:182:SER:H	1:A:185:GLN:NE2	2.10	0.49
1:B:108:ASN:HD21	1:B:111:THR:H	1.59	0.49
1:B:298:HIS:HE1	1:B:383:SER:OG	1.96	0.48
1:A:59:GLN:NE2	1:A:296:LYS:HZ1	2.10	0.48
1:B:59:GLN:HE21	1:B:296:LYS:HZ1	1.63	0.47
1:A:419:HIS:HD2	4:A:1452:GOL:O2	1.98	0.47
1:A:296:LYS:HB3	1:A:383:SER:HB2	1.97	0.46
1:A:65:GLN:HG2	1:A:434:ASP:HB2	1.98	0.46
1:B:65:GLN:HB3	1:B:434:ASP:HB2	1.99	0.45
1:B:283:HIS:HE1	6:B:2215:HOH:O	1.99	0.45
1:A:29:LEU:N	1:A:29:LEU:HD12	2.32	0.45
1:A:350:MET:HB3	1:A:358:ARG:HG3	1.99	0.45
1:A:293:LEU:HB2	1:B:284:GLN:NE2	2.33	0.44
1:B:420:PHE:O	4:B:1452:GOL:H31	2.18	0.43
1:A:59:GLN:NE2	1:A:296:LYS:NZ	2.65	0.43
1:A:177:PRO:HD3	1:A:344:ASP:HB2	1.99	0.43
1:A:206:LEU:HD11	3:B:601:4HA:HD2	1.99	0.43
1:B:263:ALA:HA	1:B:421:SER:O	2.19	0.43
1:B:281:ARG:NH1	5:B:1453:SO4:O1	2.52	0.43
1:A:29:LEU:CD1	1:A:29:LEU:N	2.81	0.43
1:A:108:ASN:HD22	1:A:108:ASN:C	2.22	0.43
1:A:283:HIS:HE1	6:A:2273:HOH:O	2.01	0.43
1:A:291:LEU:HD23	1:A:396:ALA:C	2.38	0.43
1:A:323:GLN:HG3	1:A:324:GLU:HG3	2.00	0.43
1:A:281:ARG:HD3	6:A:2281:HOH:O	2.18	0.42
1:B:151:TRP:O	1:B:155:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:HA2	2:A:600:FAD:C5X	2.50	0.42
1:A:378:VAL:HG23	1:A:379:VAL:HG23	2.01	0.42
1:B:6:ARG:O	1:B:257:ALA:HA	2.19	0.41
1:B:137:HIS:ND1	1:B:138:PRO:HD2	2.36	0.41
1:B:321:VAL:HG23	1:B:322:VAL:N	2.34	0.41
6:A:2040:HOH:O	1:B:179:HIS:HD2	2.04	0.41
1:B:363:LEU:HA	1:B:363:LEU:HD23	1.88	0.41
1:A:137:HIS:HB2	6:A:2158:HOH:O	2.21	0.41
1:A:169:ILE:CG1	1:A:196:PHE:HE1	2.35	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	447/453 (99%)	430 (96%)	16 (4%)	1 (0%)	52	64
1	B	448/453 (99%)	430 (96%)	17 (4%)	1 (0%)	52	64
All	All	895/906 (99%)	860 (96%)	33 (4%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	B	392	ARG

### 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	357/360 (99%)	344 (96%)	13 (4%)	42	57
1	B	358/360 (99%)	348 (97%)	10 (3%)	51	68
All	All	715/720 (99%)	692 (97%)	23 (3%)	46	62

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	LEU
1	A	5	GLN
1	A	64	ASP
1	A	93	SER
1	A	103	ASP
1	A	108	ASN
1	A	141	ARG
1	A	206	LEU
1	A	280	ARG
1	A	281	ARG
1	A	321	VAL
1	A	332	GLU
1	B	3	THR
1	B	4	LEU
1	B	5	GLN
1	B	64	ASP
1	B	103	ASP
1	B	124	ASP
1	B	206	LEU
1	B	223	GLU
1	B	281	ARG
1	B	332	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	108	ASN
1	A	179	HIS
1	A	185	GLN

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Mol	Chain	Res	Type
1	A	283	HIS
1	A	298	HIS
1	A	328	ASN
1	A	405	HIS
1	A	419	HIS
1	B	59	GLN
1	B	108	ASN
1	B	179	HIS
1	B	185	GLN
1	B	283	HIS
1	B	284	GLN
1	B	298	HIS
1	B	328	ASN
1	B	419	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 [i](#)

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
4	GOL	A	1451	-	5,5,5	0.88	0	5,5,5	1.94	2 (40%)
4	GOL	A	1452	-	5,5,5	0.63	0	5,5,5	1.49	1 (20%)
5	SO4	A	1453	-	4,4,4	0.36	0	6,6,6	0.43	0
5	SO4	A	1454	-	4,4,4	0.99	0	6,6,6	1.03	1 (16%)
4	GOL	A	1455	-	5,5,5	0.61	0	5,5,5	1.86	2 (40%)
2	FAD	A	600	-	48,58,58	1.78	10 (20%)	54,89,89	2.58	12 (22%)
3	4HA	A	601	-	5,5,5	1.49	1 (20%)	4,4,4	1.28	1 (25%)
4	GOL	B	1452	-	5,5,5	0.65	0	5,5,5	1.51	1 (20%)
5	SO4	B	1453	-	4,4,4	1.98	2 (50%)	6,6,6	1.06	0
5	SO4	B	1454	-	4,4,4	0.91	0	6,6,6	1.06	1 (16%)
2	FAD	B	600	-	48,58,58	1.57	7 (14%)	54,89,89	2.53	13 (24%)
3	4HA	B	601	-	5,5,5	1.49	1 (20%)	4,4,4	1.39	1 (25%)

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
4	GOL	A	1451	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1452	-	-	0/4/4/4	0/0/0/0
5	SO4	A	1453	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1454	-	-	0/0/0/0	0/0/0/0
4	GOL	A	1455	-	-	0/4/4/4	0/0/0/0
2	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	4HA	A	601	-	-	0/3/3/3	0/0/0/0
4	GOL	B	1452	-	-	0/4/4/4	0/0/0/0
5	SO4	B	1453	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1454	-	-	0/0/0/0	0/0/0/0
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	4HA	B	601	-	-	0/3/3/3	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	4HA	OA-CB	-3.23	1.24	1.42
3	B	601	4HA	OA-CB	-3.18	1.24	1.42
5	B	1453	SO4	O4-S	2.21	1.55	1.47
2	B	600	FAD	C8A-N7A	2.32	1.39	1.34
2	A	600	FAD	C6-C5X	2.41	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2A-N1A	2.42	1.38	1.33
2	B	600	FAD	C2A-N3A	2.42	1.36	1.32
2	A	600	FAD	C7M-C7	2.46	1.56	1.51
2	B	600	FAD	C4-N3	2.51	1.37	1.33
2	A	600	FAD	C4-N3	2.94	1.38	1.33
2	A	600	FAD	C6-C7	2.97	1.46	1.37
2	B	600	FAD	C10-N1	3.08	1.40	1.35
5	B	1453	SO4	O2-S	3.26	1.58	1.47
2	A	600	FAD	C2A-N3A	3.26	1.38	1.32
2	B	600	FAD	C9A-N10	3.42	1.43	1.38
2	A	600	FAD	C10-N1	3.59	1.41	1.35
2	B	600	FAD	C5X-N5	3.76	1.41	1.35
2	A	600	FAD	C4X-N5	4.16	1.39	1.33
2	A	600	FAD	C5X-N5	4.92	1.43	1.35
2	A	600	FAD	C1'-N10	5.54	1.54	1.48
2	B	600	FAD	C4X-N5	5.56	1.42	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	N3A-C2A-N1A	-11.92	119.77	128.89
2	A	600	FAD	N3A-C2A-N1A	-11.74	119.91	128.89
2	B	600	FAD	C4X-C10-N10	-5.72	117.15	120.52
2	B	600	FAD	C1B-N9A-C4A	-3.66	121.42	126.94
2	A	600	FAD	C4X-C4-N3	-3.33	119.04	123.59
2	B	600	FAD	C9A-C5X-N5	-3.13	117.72	122.36
2	A	600	FAD	C4-C4X-C10	-3.03	118.00	119.94
2	A	600	FAD	C9A-C5X-N5	-3.01	117.91	122.36
2	B	600	FAD	C4-C4X-C10	-2.71	118.20	119.94
2	B	600	FAD	C4X-C4-N3	-2.51	120.16	123.59
4	A	1455	GOL	C3-C2-C1	-2.51	101.29	111.12
2	A	600	FAD	P-O3P-PA	-2.44	125.86	132.73
2	B	600	FAD	P-O3P-PA	-2.37	126.06	132.73
2	A	600	FAD	C4X-C10-N10	-2.36	119.13	120.52
3	A	601	4HA	CD-CG-CB	-2.29	99.39	114.20
2	B	600	FAD	O3B-C3B-C4B	-2.21	104.41	111.05
2	A	600	FAD	O3'-C3'-C4'	-2.18	103.26	108.75
5	A	1454	SO4	O4-S-O3	-2.18	100.13	108.98
2	B	600	FAD	C4A-C5A-N7A	-2.15	107.50	109.48
3	B	601	4HA	CD-CG-CB	-2.15	100.28	114.20
4	B	1452	GOL	C3-C2-C1	-2.10	102.90	111.12
4	A	1455	GOL	O3-C3-C2	-2.05	100.23	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C7M-C7-C8	2.01	125.13	120.73
2	B	600	FAD	C6-C5X-C9A	2.11	121.76	118.98
5	B	1454	SO4	O2-S-O1	2.29	116.77	109.50
2	B	600	FAD	C2A-N1A-C6A	2.42	123.09	118.77
4	A	1452	GOL	O2-C2-C3	2.50	120.09	108.65
4	A	1451	GOL	O3-C3-C2	2.65	123.04	110.18
4	A	1451	GOL	C3-C2-C1	2.91	122.55	111.12
2	A	600	FAD	C6-C5X-N5	3.33	123.24	118.96
2	B	600	FAD	C5X-C9A-N10	3.51	120.29	117.62
2	A	600	FAD	C4-C4X-N5	3.65	123.15	118.72
2	A	600	FAD	C1'-N10-C9A	3.98	123.33	118.86
2	B	600	FAD	C4-N3-C2	7.00	121.30	115.25
2	A	600	FAD	C4-N3-C2	8.84	122.89	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1452	GOL	1	0
5	A	1453	SO4	1	0
4	A	1455	GOL	2	0
2	A	600	FAD	1	0
4	B	1452	GOL	2	0
5	B	1453	SO4	2	0
2	B	600	FAD	1	0
3	B	601	4HA	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	449/453 (99%)	-0.56	2 (0%) 93 95	5, 12, 26, 36	0
1	B	450/453 (99%)	-0.47	1 (0%) 95 97	6, 15, 30, 47	0
All	All	899/906 (99%)	-0.52	3 (0%) 94 96	5, 14, 28, 47	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ASP	2.4
1	A	242	GLU	2.3
1	B	103	ASP	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1453	5/5	0.92	0.44	10.03	37,42,51,52	0
3	4HA	A	601	6/6	0.94	0.33	8.54	14,22,29,30	0
3	4HA	B	601	6/6	0.96	0.32	6.60	18,23,30,31	0
4	GOL	A	1455	6/6	0.93	0.17	6.14	29,33,34,34	0
4	GOL	A	1451	6/6	0.93	0.16	3.11	24,27,28,31	0
4	GOL	A	1452	6/6	0.93	0.11	2.93	13,18,27,29	0
4	GOL	B	1452	6/6	0.93	0.10	1.27	16,23,28,30	0
2	FAD	A	600	53/53	0.98	0.10	-0.18	2,11,17,22	0
2	FAD	B	600	53/53	0.98	0.10	-0.42	2,11,21,24	0
5	SO4	A	1454	5/5	0.86	0.35	-	55,60,60,61	0
5	SO4	B	1454	5/5	0.81	0.35	-	61,62,65,65	0
5	SO4	A	1453	5/5	0.89	0.28	-	58,59,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.