



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 AM GMT

PDB ID : 2IVD  
Title : STRUCTURE OF PROTOPORPHYRINOGEN OXIDASE FROM MYXOCOCCLUS XANTHUS WITH ACIFLUORFEN  
Authors : Corradi, H.R.; Corrigall, A.V.; Boix, E.; Mohan, C.G.; Sturrock, E.D.; Meissner, P.N.; Acharya, K.R.  
Deposited on : 2006-06-12  
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

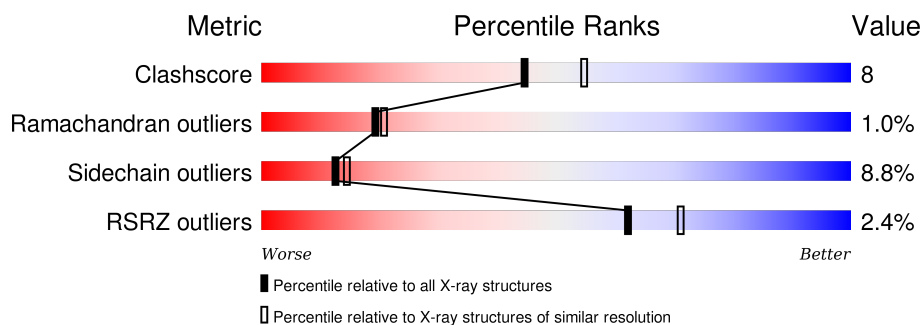
# 1 Overall quality at a glance

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))
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	478	
1	B	478	

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
2	ACJ	A	1465	-	-	-	X
2	ACJ	B	1468	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1467	-	-	-	X
5	TWN	B	1472	-	-	-	X

## 2 Entry composition [i](#)

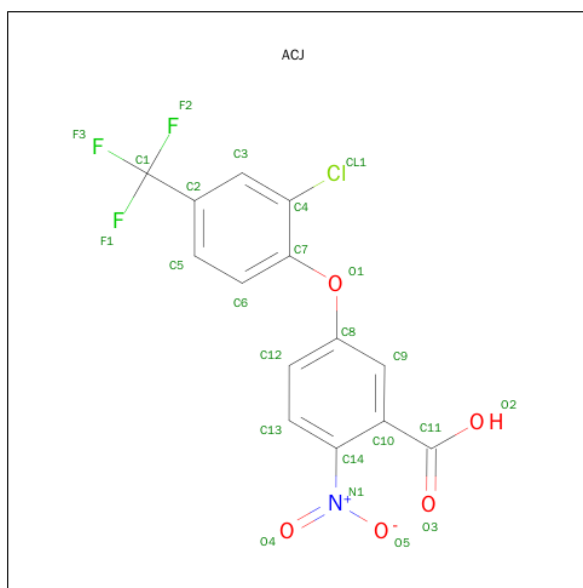
There are 6 unique types of molecules in this entry. The entry contains 7129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTOPORPHYRINOGEN OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	20	0	0
			3313	2085	627	595	6			
1	B	449	Total	C	N	O	S	28	0	0
			3319	2087	627	599	6			

- Molecule 2 is 5-[2-CHLORO-4-(TRIFLUOROMETHYL)PHENOXY]-2-NITROBENZOIC ACID (three-letter code: ACJ) (formula:  $C_{14}H_7ClF_3NO_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0
			24	14	1	3	1	5	
2	B	1	Total	C	Cl	F	N	O	0
			24	14	1	3	1	5	

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

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



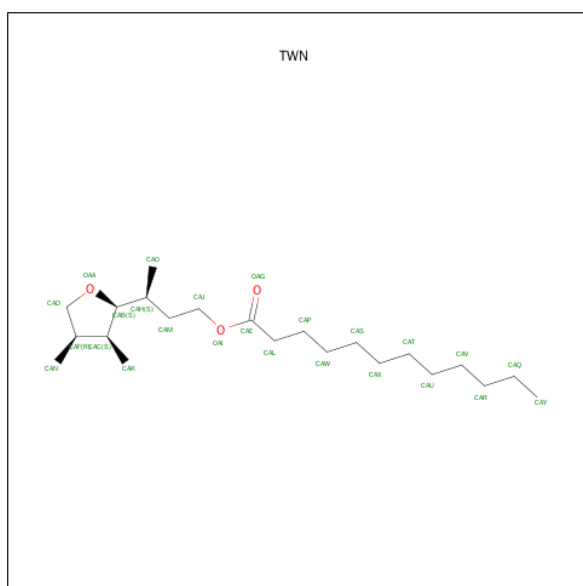
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 (3S)-3-[(2S,3S,4R)-3,4-DIMETHYLTETRAHYDROFURAN-2-YL]BUTYL LAURATE (three-letter code: TWN) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			25	22	3		

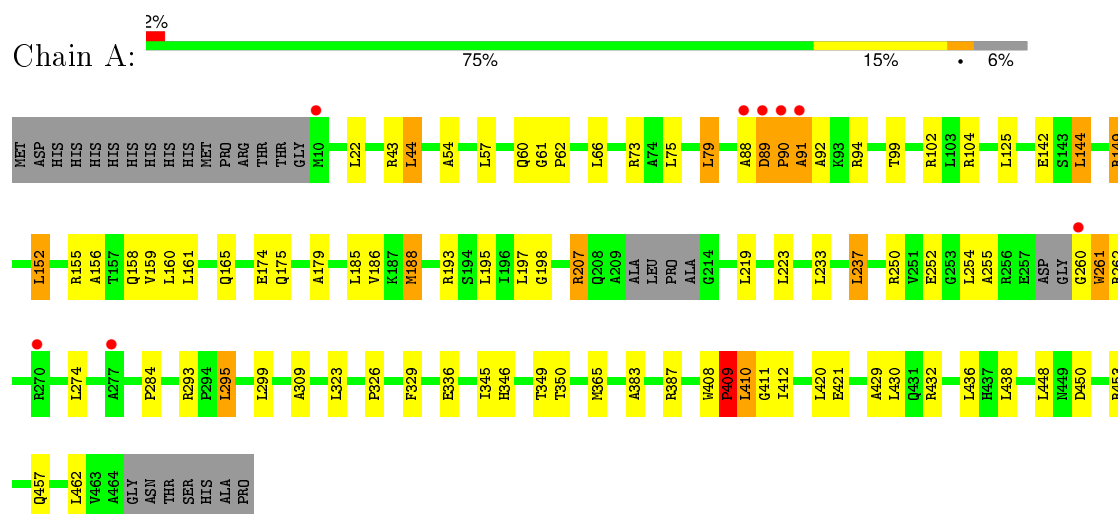
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	146	Total	O	0	0
			146	146		
6	B	142	Total	O	0	0
			142	142		

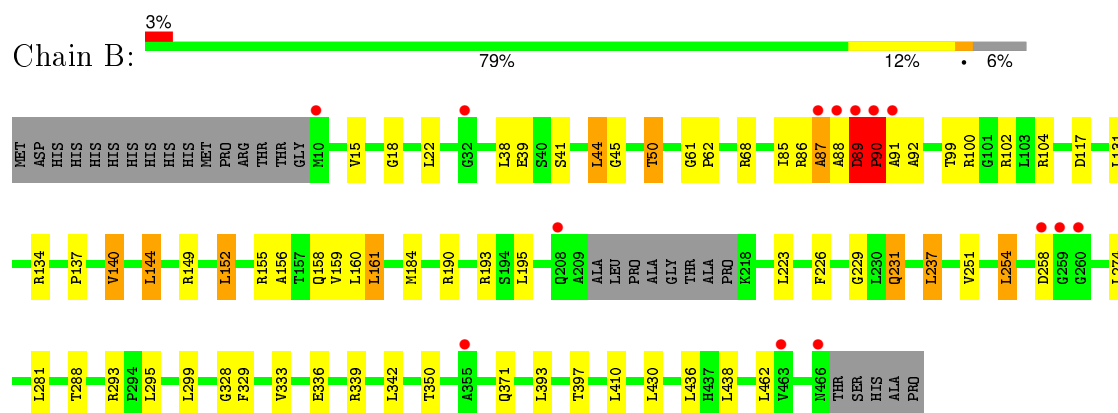
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: PROTOPORPHYRINOGEN OXIDASE



#### • Molecule 1: PROTOPORPHYRINOGEN OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.92Å 148.92Å 131.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.30 49.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (49.39-2.30) 86.3 (49.37-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.234 , 0.283 0.238 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 95815 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, TWN, FAD, ACJ

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	0.47	0/3370	0.69	1/4574 (0.0%)
1	B	0.46	0/3376	0.67	4/4580 (0.1%)
All	All	0.46	0/6746	0.68	5/9154 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	149	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	89	ASP	C-N-CD	-5.75	107.95	120.60
1	B	89	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	149	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	409	PRO	Peptide
1	A	410	LEU	Peptide
1	B	87	ALA	Peptide
1	B	89	ASP	Peptide
1	B	90	PRO	Peptide
1	B	91	ALA	Peptide

## 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	3313	0	3367	53	0
1	B	3319	0	3375	48	0
2	A	24	0	6	1	0
2	B	24	0	6	1	0
3	A	53	0	31	4	0
3	B	53	0	31	2	0
4	A	12	0	16	2	0
4	B	18	0	24	1	0
5	B	25	0	42	12	0
6	A	146	0	0	3	0
6	B	142	0	0	1	0
All	All	7129	0	6898	107	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 8.

All (107) 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:B:134:ARG:HE	5:B:1472:TWN:HAF	0.98	1.10
1:B:18:GLY:HA2	1:B:45:GLY:O	1.51	1.09
1:B:134:ARG:NE	5:B:1472:TWN:HAF	1.69	1.05
1:A:309:ALA:O	1:A:411:GLY:HA3	1.58	1.04
1:B:134:ARG:HH11	5:B:1472:TWN:HAN1	1.20	1.02
1:A:155:ARG:O	1:A:159:VAL:HG13	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLY:O	1:A:261:TRP:CD1	2.18	0.97
5:B:1472:TWN:HAK2	5:B:1472:TWN:HAO3	1.51	0.90
1:A:260:GLY:O	1:A:261:TRP:CG	2.33	0.81
1:B:155:ARG:O	1:B:159:VAL:HG13	1.81	0.80
1:B:134:ARG:HH11	5:B:1472:TWN:CAN	1.95	0.79
1:B:50:THR:H	1:B:231:GLN:HG3	1.49	0.78
1:A:89:ASP:CB	1:A:90:PRO:HD2	2.15	0.77
5:B:1472:TWN:HAO1	5:B:1472:TWN:HAD2	1.66	0.76
1:B:158:GLN:HG2	1:B:336:GLU:OE1	1.84	0.75
1:A:158:GLN:HG2	1:A:336:GLU:OE1	1.88	0.73
1:B:158:GLN:CG	1:B:336:GLU:OE1	2.36	0.72
1:B:50:THR:H	1:B:231:GLN:CG	2.05	0.70
1:A:89:ASP:CB	1:A:350:THR:O	2.40	0.70
1:A:193:ARG:HH21	4:A:1468:GOL:H32	1.59	0.68
1:A:329:PHE:O	1:A:346:HIS:HB2	1.93	0.67
5:B:1472:TWN:CAK	5:B:1472:TWN:HAO3	2.26	0.66
1:B:89:ASP:HA	1:B:90:PRO:O	1.97	0.64
1:B:131:LEU:O	1:B:193:ARG:NH2	2.32	0.63
1:A:188:MET:HE2	1:A:195:LEU:HA	1.79	0.63
1:A:188:MET:CE	1:A:198:GLY:HA3	2.30	0.62
1:B:137:PRO:HB2	1:B:140:VAL:HG13	1.80	0.62
1:A:144:LEU:HD22	1:A:161:LEU:HD21	1.82	0.62
1:A:156:ALA:O	1:A:160:LEU:HB2	2.00	0.60
1:A:188:MET:CE	1:A:195:LEU:HA	2.32	0.60
1:A:61:GLY:HA2	3:A:1466:FAD:HM72	1.84	0.59
1:A:411:GLY:O	1:A:412:ILE:HD13	2.03	0.59
1:A:155:ARG:O	1:A:159:VAL:CG1	2.43	0.59
1:A:450:ASP:OD2	1:A:453:ARG:NH2	2.36	0.59
1:B:134:ARG:HE	5:B:1472:TWN:CAF	1.92	0.58
1:B:430:LEU:HD11	1:B:438:LEU:HG	1.86	0.57
1:A:158:GLN:CG	1:A:336:GLU:OE1	2.53	0.57
1:A:188:MET:HE1	1:A:198:GLY:HA3	1.86	0.56
1:A:22:LEU:HD21	1:A:44:LEU:HG	1.88	0.55
1:B:158:GLN:HG3	1:B:336:GLU:OE1	2.06	0.54
5:B:1472:TWN:CAO	5:B:1472:TWN:HAK2	2.31	0.54
1:A:149:ARG:NH2	1:A:174:GLU:OE2	2.41	0.53
1:A:88:ALA:HB2	1:A:223:LEU:O	2.08	0.53
1:A:412:ILE:HD11	3:A:1466:FAD:C8	2.39	0.52
1:A:102:ARG:HD2	6:A:2034:HOH:O	2.10	0.52
1:B:87:ALA:HA	1:B:223:LEU:O	2.11	0.51
1:B:134:ARG:NH1	5:B:1472:TWN:HAN1	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:HB1	1:B:350:THR:CG2	2.41	0.51
1:B:137:PRO:HB2	1:B:140:VAL:CG1	2.40	0.50
1:B:88:ALA:HB1	1:B:350:THR:HG23	1.92	0.50
1:A:159:VAL:HG22	1:A:160:LEU:HG	1.94	0.50
1:B:152:LEU:HB3	1:B:156:ALA:HB3	1.92	0.50
1:A:89:ASP:CB	1:A:90:PRO:CD	2.86	0.50
1:A:309:ALA:O	1:A:411:GLY:CA	2.46	0.49
1:B:134:ARG:CZ	5:B:1472:TWN:HAF	2.41	0.49
1:B:22:LEU:HB3	1:B:237:LEU:HG	1.95	0.49
1:A:383:ALA:O	1:A:387:ARG:HG3	2.12	0.49
1:B:22:LEU:HD21	1:B:44:LEU:HD13	1.95	0.48
1:A:299:LEU:HD13	1:A:429:ALA:HB3	1.96	0.48
1:A:430:LEU:HD11	1:A:438:LEU:HG	1.95	0.48
1:B:62:PRO:HA	3:B:1469:FAD:N5	2.29	0.48
1:A:73:ARG:HG3	1:A:219:LEU:HD21	1.96	0.47
1:B:61:GLY:HA2	3:B:1469:FAD:HM72	1.96	0.47
1:B:18:GLY:CA	1:B:45:GLY:O	2.43	0.47
1:A:62:PRO:HA	3:A:1466:FAD:N5	2.29	0.47
1:A:75:LEU:CD1	1:A:233:LEU:HD11	2.44	0.47
1:B:223:LEU:HD21	1:B:329:PHE:CE1	2.51	0.46
1:A:91:ALA:O	1:A:92:ALA:HB3	2.15	0.46
1:B:15:VAL:HG22	1:B:251:VAL:HG21	1.97	0.46
1:A:89:ASP:CB	1:A:349:THR:O	2.64	0.46
1:B:226:PHE:HB2	1:B:229:GLY:O	2.16	0.46
1:A:197:LEU:CD1	4:A:1468:GOL:H12	2.46	0.45
1:A:99:THR:HG23	1:A:104:ARG:HD3	1.99	0.45
1:B:159:VAL:CG2	1:B:160:LEU:N	2.77	0.45
1:B:159:VAL:HG22	1:B:160:LEU:N	2.31	0.45
1:B:144:LEU:HD22	1:B:161:LEU:HD11	1.99	0.45
1:B:39:GLU:OE1	1:B:41:SER:HB2	2.17	0.45
1:A:149:ARG:HH22	1:A:174:GLU:CD	2.21	0.44
1:A:207:ARG:O	1:A:207:ARG:HG2	2.17	0.44
1:B:193:ARG:NE	4:B:1467:GOL:H2	2.33	0.43
5:B:1472:TWN:HAO1	5:B:1472:TWN:CAD	2.44	0.43
1:A:179:ALA:HA	1:A:186:VAL:HG21	2.01	0.43
1:B:254:LEU:HD13	1:B:295:LEU:HD11	2.00	0.43
1:B:339:ARG:HA	1:B:339:ARG:HD3	1.63	0.43
1:B:92:ALA:HB1	1:B:328:GLY:H	1.82	0.42
1:A:408:TRP:N	1:A:409:PRO:HD3	2.33	0.42
1:A:188:MET:HB3	1:A:188:MET:HE2	1.95	0.42
1:B:161:LEU:HA	1:B:161:LEU:HD23	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:MET:HG3	2:A:1465:ACJ:C7	2.50	0.41
1:B:155:ARG:NH2	1:B:158:GLN:HG2	2.35	0.41
1:A:79:LEU:HD21	1:A:237:LEU:HD13	2.01	0.41
1:B:339:ARG:HG3	1:B:393:LEU:HD21	2.03	0.41
1:B:85:ILE:C	1:B:86:ARG:HG2	2.39	0.41
1:B:99:THR:HG23	1:B:104:ARG:HD2	2.02	0.41
1:A:152:LEU:HB3	1:A:156:ALA:HB3	2.01	0.41
1:A:326:PRO:HB2	1:A:346:HIS:CE1	2.56	0.41
1:A:88:ALA:HB2	1:A:223:LEU:HB3	2.01	0.41
1:B:281:LEU:HD13	1:B:288:THR:HG23	2.02	0.41
1:B:158:GLN:NE2	6:B:2049:HOH:O	2.53	0.41
1:B:156:ALA:O	1:B:160:LEU:HB2	2.21	0.41
1:A:175:GLN:NE2	6:A:2077:HOH:O	2.37	0.41
2:B:1468:ACJ:O4	2:B:1468:ACJ:C11	2.69	0.41
1:A:255:ALA:HA	1:A:295:LEU:HD11	2.03	0.41
1:A:54:ALA:HB1	6:A:2009:HOH:O	2.20	0.41
1:A:22:LEU:HB3	1:A:237:LEU:HG	2.03	0.40
1:B:100:ARG:NH2	1:B:117:ASP:O	2.55	0.40
1:A:284:PRO:HD3	3:A:1466:FAD:H51A	2.04	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	443/478 (93%)	423 (96%)	15 (3%)	5 (1%)	17	18
1	B	445/478 (93%)	431 (97%)	10 (2%)	4 (1%)	21	24
All	All	888/956 (93%)	854 (96%)	25 (3%)	9 (1%)	19	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	PRO
1	B	258	ASP
1	A	90	PRO
1	A	91	ALA
1	A	261	TRP
1	B	44	LEU
1	A	89	ASP
1	B	89	ASP
1	A	409	PRO

### 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	317/344 (92%)	285 (90%)	32 (10%)	9	11
1	B	319/344 (93%)	295 (92%)	24 (8%)	17	21
All	All	636/688 (92%)	580 (91%)	56 (9%)	12	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	44	LEU
1	A	57	LEU
1	A	60	GLN
1	A	66	LEU
1	A	79	LEU
1	A	94	ARG
1	A	125	LEU
1	A	142	GLU
1	A	144	LEU
1	A	152	LEU
1	A	165	GLN
1	A	185	LEU
1	A	188	MET
1	A	207	ARG

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Mol	Chain	Res	Type
1	A	237	LEU
1	A	250	ARG
1	A	252	GLU
1	A	254	LEU
1	A	262	ARG
1	A	274	LEU
1	A	293	ARG
1	A	295	LEU
1	A	323	LEU
1	A	410	LEU
1	A	420	LEU
1	A	421	GLU
1	A	432	ARG
1	A	436	LEU
1	A	448	LEU
1	A	457	GLN
1	A	462	LEU
1	B	38	LEU
1	B	50	THR
1	B	68	ARG
1	B	102	ARG
1	B	140	VAL
1	B	144	LEU
1	B	152	LEU
1	B	161	LEU
1	B	184	MET
1	B	190	ARG
1	B	195	LEU
1	B	231	GLN
1	B	237	LEU
1	B	254	LEU
1	B	274	LEU
1	B	293	ARG
1	B	299	LEU
1	B	333	VAL
1	B	342	LEU
1	B	371	GLN
1	B	397	THR
1	B	410	LEU
1	B	436	LEU
1	B	462	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	315	HIS
1	A	346	HIS
1	A	416	ASN
1	B	158	GLN
1	B	431	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	ACJ	A	1465	-	20,25,25	2.97	4 (20%)	28,37,37	1.06	1 (3%)
3	FAD	A	1466	-	48,58,58	1.22	6 (12%)	54,89,89	2.36	9 (16%)
4	GOL	A	1467	-	5,5,5	0.34	0	5,5,5	0.53	0
4	GOL	A	1468	-	5,5,5	0.47	0	5,5,5	0.79	0
4	GOL	B	1467	-	5,5,5	0.41	0	5,5,5	0.60	0
2	ACJ	B	1468	-	20,25,25	3.04	4 (20%)	28,37,37	2.77	7 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	B	1469	-	48,58,58	1.18	6 (12%)	54,89,89	2.33	7 (12%)
4	GOL	B	1470	-	5,5,5	0.26	0	5,5,5	0.65	0
4	GOL	B	1471	-	5,5,5	0.32	0	5,5,5	0.41	0
5	TWN	B	1472	-	25,25,25	0.53	0	23,30,30	1.31	3 (13%)

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	ACJ	A	1465	-	-	0/13/18/18	0/2/2/2
3	FAD	A	1466	-	-	0/30/50/50	0/6/6/6
4	GOL	A	1467	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1468	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1467	-	-	0/4/4/4	0/0/0/0
2	ACJ	B	1468	-	-	0/13/18/18	0/2/2/2
3	FAD	B	1469	-	-	0/30/50/50	0/6/6/6
4	GOL	B	1470	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1471	-	-	0/4/4/4	0/0/0/0
5	TWN	B	1472	-	-	0/21/34/34	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1469	FAD	C10-N1	2.14	1.39	1.35
2	A	1465	ACJ	C4-CL1	2.25	1.79	1.73
2	B	1468	ACJ	C4-CL1	2.32	1.79	1.73
3	A	1466	FAD	C10-N1	2.38	1.39	1.35
3	B	1469	FAD	C1'-N10	2.38	1.50	1.48
3	A	1466	FAD	C2A-N1A	2.48	1.38	1.33
3	B	1469	FAD	C2A-N1A	2.57	1.38	1.33
3	A	1466	FAD	C4-N3	2.67	1.38	1.33
3	A	1466	FAD	C1'-N10	2.68	1.51	1.48
3	B	1469	FAD	C4X-N5	2.74	1.37	1.33
3	B	1469	FAD	C4-N3	3.04	1.38	1.33
3	A	1466	FAD	C4X-N5	3.34	1.38	1.33
3	B	1469	FAD	C2A-N3A	3.47	1.38	1.32
3	A	1466	FAD	C2A-N3A	3.74	1.38	1.32
2	B	1468	ACJ	C7-C4	4.89	1.48	1.39
2	A	1465	ACJ	C7-C4	5.32	1.49	1.39
2	A	1465	ACJ	C10-C14	8.07	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1468	ACJ	C10-C14	8.38	1.50	1.40
2	A	1465	ACJ	O4-N1	8.48	1.39	1.22
2	B	1468	ACJ	O4-N1	8.84	1.40	1.22

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1466	FAD	N3A-C2A-N1A	-12.56	119.28	128.89
3	B	1469	FAD	N3A-C2A-N1A	-12.28	119.49	128.89
2	B	1468	ACJ	F3-C1-C2	-7.85	96.16	112.95
2	B	1468	ACJ	F2-C1-C2	-6.77	98.48	112.95
2	B	1468	ACJ	F1-C1-C2	-6.59	98.85	112.95
3	B	1469	FAD	C4X-C4-N3	-3.79	118.41	123.59
3	A	1466	FAD	C4X-C4-N3	-3.55	118.73	123.59
5	B	1472	TWN	CAJ-OAI-CAE	-3.36	107.61	117.02
3	B	1469	FAD	C4B-O4B-C1B	-2.46	107.01	109.72
3	A	1466	FAD	C4X-C10-N10	-2.37	119.12	120.52
3	B	1469	FAD	C1B-N9A-C4A	-2.34	123.42	126.94
3	A	1466	FAD	C9A-C5X-N5	-2.10	119.25	122.36
5	B	1472	TWN	OAI-CAE-OAG	-2.06	118.18	123.49
3	A	1466	FAD	C8M-C8-C9	-2.01	114.81	120.28
2	A	1465	ACJ	C3-C4-CL1	2.27	121.99	118.50
3	A	1466	FAD	O4B-C1B-N9A	2.58	113.49	108.10
2	B	1468	ACJ	C3-C4-CL1	2.68	122.63	118.50
3	B	1469	FAD	C5X-C9A-N10	2.75	119.71	117.62
5	B	1472	TWN	OAI-CAE-CAL	2.89	120.70	111.90
2	B	1468	ACJ	F3-C1-F2	3.24	117.42	105.71
2	B	1468	ACJ	F2-C1-F1	3.26	117.47	105.71
3	A	1466	FAD	C4X-N5-C5X	3.47	120.76	116.76
3	B	1469	FAD	C4X-N5-C5X	3.67	120.98	116.76
2	B	1468	ACJ	F3-C1-F1	3.86	119.64	105.71
3	A	1466	FAD	C5X-C9A-N10	4.03	120.68	117.62
3	A	1466	FAD	C4-N3-C2	6.77	121.10	115.25
3	B	1469	FAD	C4-N3-C2	7.15	121.43	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1465	ACJ	1	0
3	A	1466	FAD	4	0
4	A	1468	GOL	2	0
4	B	1467	GOL	1	0
2	B	1468	ACJ	1	0
3	B	1469	FAD	2	0
5	B	1472	TWN	12	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

### 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, 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	449/478 (93%)	0.02	8 (1%) 71 78	17, 34, 50, 62	6 (1%)
1	B	449/478 (93%)	-0.03	14 (3%) 52 62	16, 34, 50, 62	8 (1%)
All	All	898/956 (93%)	-0.00	22 (2%) 62 71	16, 34, 50, 62	14 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLY	4.8
1	A	10	MET	4.5
1	A	91	ALA	4.4
1	A	260	GLY	4.0
1	B	466	ASN	3.9
1	A	270	ARG	3.6
1	B	90	PRO	3.4
1	B	10	MET	3.4
1	A	90	PRO	3.4
1	B	87	ALA	3.2
1	A	88	ALA	3.1
1	B	258	ASP	2.7
1	B	260	GLY	2.7
1	B	355	ALA	2.7
1	B	88	ALA	2.6
1	B	208	GLN	2.6
1	B	89	ASP	2.4
1	A	89	ASP	2.3
1	B	91	ALA	2.1
1	B	463	VAL	2.1
1	A	277	ALA	2.0
1	B	32	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	TWN	B	1472	25/25	0.79	0.22	4.30	63,65,66,67	0
2	ACJ	B	1468	24/24	0.84	0.22	4.05	52,53,54,56	0
4	GOL	A	1467	6/6	0.90	0.17	3.92	32,34,36,37	0
2	ACJ	A	1465	24/24	0.91	0.20	2.61	49,50,51,52	0
4	GOL	A	1468	6/6	0.90	0.14	1.72	23,29,31,33	0
4	GOL	B	1471	6/6	0.91	0.15	1.14	32,35,37,39	0
4	GOL	B	1467	6/6	0.82	0.15	0.71	42,42,43,43	0
4	GOL	B	1470	6/6	0.95	0.13	0.44	28,29,29,29	0
3	FAD	B	1469	53/53	0.96	0.12	-0.09	25,28,32,32	0
3	FAD	A	1466	53/53	0.96	0.12	-0.56	23,26,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.