



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:23 PM GMT

PDB ID : 2JBT
Title : STRUCTURE OF THE MONOOXYGENASE COMPONENT OF P-HYDROXYPHENYLACETATE HYDROXYLASE FROM ACINETOBACTER BAUMANNII
Authors : Alfieri, A.; Mattevi, A.
Deposited on : 2006-12-11
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

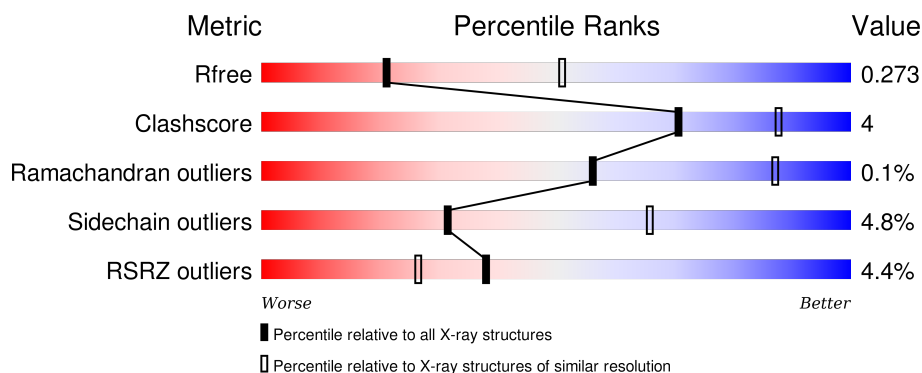
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	422	<div> <div>84%</div> <div>9% • 5%</div> </div>
1	B	422	<div> <div>85%</div> <div>8% • 5%</div> </div>
1	C	422	<div> <div>2%</div> <div>83%</div> <div>10% • 5%</div> </div>
1	D	422	<div> <div>14%</div> <div>84%</div> <div>9% • 5%</div> </div>

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	FMN	D	1423	-	-	-	X
3	4HP	A	1424	-	-	-	X
3	4HP	B	1424	-	-	-	X
3	4HP	C	1424	-	-	-	X
3	4HP	D	1424	-	-	-	X

2 Entry composition [i](#)

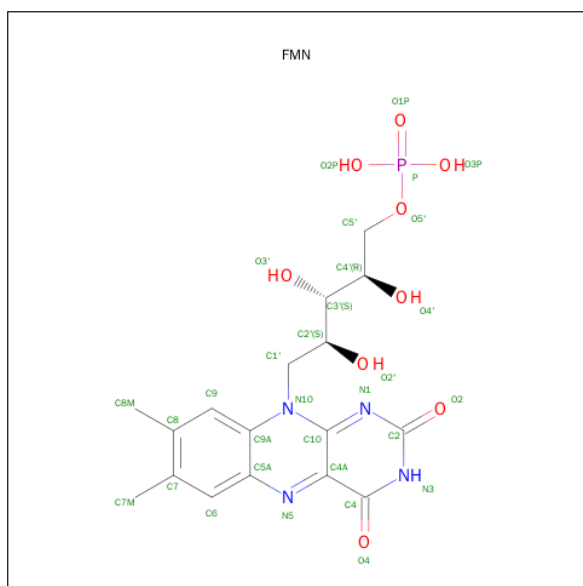
There are 4 unique types of molecules in this entry. The entry contains 12685 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P-HYDROXYPHENYLACETATE HYDROXYLASE C2\;OXYGENASE COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3129	1986	539	583	21			
1	B	399	Total	C	N	O	S	0	0	0
			3121	1980	538	582	21			
1	C	399	Total	C	N	O	S	0	0	0
			3121	1980	538	582	21			
1	D	399	Total	C	N	O	S	0	0	0
			3121	1980	538	582	21			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



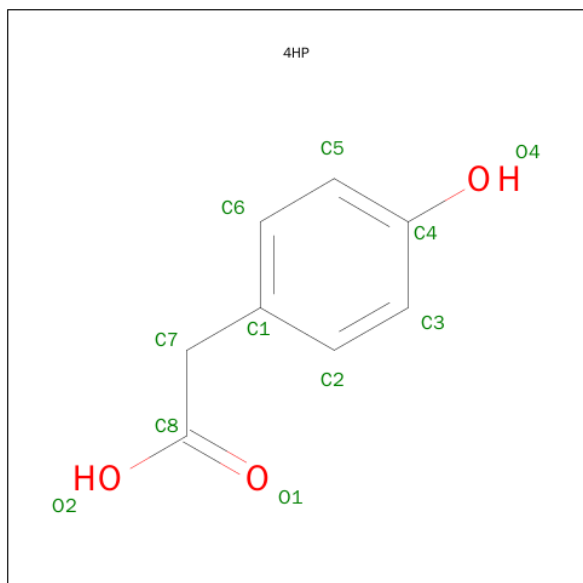
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 4-HYDROXYPHENYLACETATE (three-letter code: 4HP) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	8	3		
3	B	1	Total	C	O	0	0
			11	8	3		
3	C	1	Total	C	O	0	0
			11	8	3		
3	D	1	Total	C	O	0	0
			11	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	10	Total	O	0	0
			10	10		
4	C	6	Total	O	0	0
			6	6		

Continued on next page...


Continued from previous page...

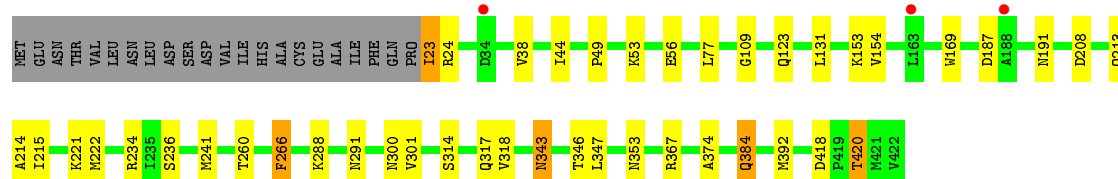
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	O	0	0
			2	2		

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.

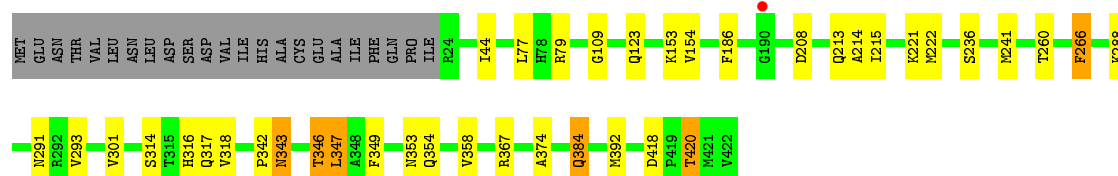
- Molecule 1: P-HYDROXYPHENYLACETATE HYDROXYLASE C2\ :OXYGENASE COMPONENT

Chain A: 




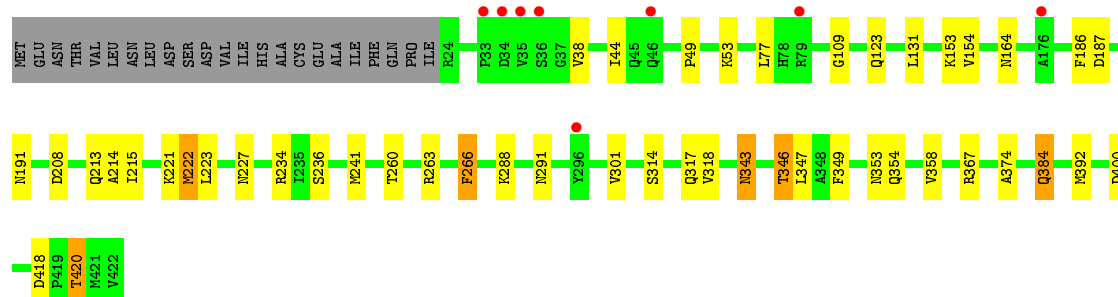
- Molecule 1: P-HYDROXYPHENYLACETATE HYDROXYLASE C2\ :OXYGENASE COMPONENT

Chain B: 



- Molecule 1: P-HYDROXYPHENYLACETATE HYDROXYLASE C2\ :OXYGENASE COMPONENT

Chain C: 



- Molecule 1: P-HYDROXYPHENYLACETATE HYDROXYLASE C2\ :OXYGENASE COMPONENT

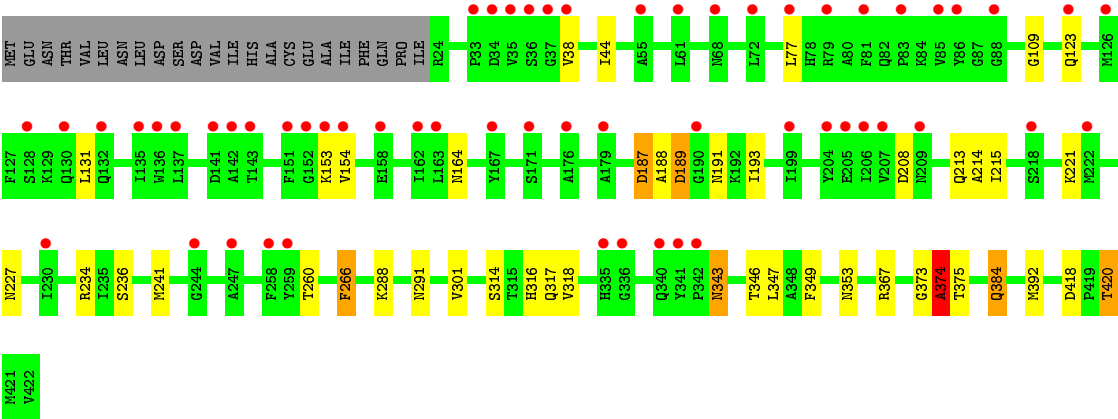
Chain D:

14%

84%

9%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.99Å 181.26Å 286.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.51 – 2.80 84.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (84.51-2.80) 100.0 (84.42-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.235 0.254 , 0.273	Depositor DCC
R_{free} test set	616 reflections (1.05%)	DCC
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 59267 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12685	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: FMN, 4HP

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	0.45	0/3201	0.54	0/4329
1	B	0.45	0/3193	0.55	0/4318
1	C	0.41	0/3193	0.52	0/4318
1	D	0.71	7/3193 (0.2%)	0.72	15/4318 (0.3%)
All	All	0.52	7/12780 (0.1%)	0.59	15/17283 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	187	ASP	CG-OD1	-18.73	0.82	1.25
1	D	189	ASP	CG-OD2	13.70	1.56	1.25
1	D	187	ASP	CG-OD2	11.77	1.52	1.25
1	D	374	ALA	C-N	-11.69	1.07	1.34
1	D	374	ALA	N-CA	10.43	1.67	1.46
1	D	373	GLY	C-N	6.75	1.49	1.34
1	D	189	ASP	CG-OD1	6.61	1.40	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	ASP	CB-CA-C	-11.86	86.67	110.40
1	D	187	ASP	CB-CG-OD2	10.93	128.13	118.30
1	D	188	ALA	N-CA-CB	-9.36	97.00	110.10
1	D	187	ASP	OD1-CG-OD2	-8.57	107.01	123.30
1	D	189	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	D	187	ASP	N-CA-CB	-7.97	96.25	110.60
1	D	373	GLY	O-C-N	7.77	135.13	122.70
1	D	187	ASP	N-CA-C	-7.61	90.46	111.00
1	D	373	GLY	C-N-CA	-7.33	103.39	121.70
1	D	374	ALA	N-CA-CB	-6.77	100.62	110.10
1	D	375	THR	O-C-N	6.40	132.93	122.70
1	D	373	GLY	CA-C-N	-6.25	103.44	117.20
1	D	374	ALA	C-N-CA	6.22	137.25	121.70
1	D	187	ASP	CB-CG-OD1	6.16	123.84	118.30
1	D	375	THR	CA-C-N	-5.53	105.02	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	186	PHE	Peptide
1	C	186	PHE	Peptide
1	D	374	ALA	Mainchain

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	3129	0	3071	29	0
1	B	3121	0	3060	29	0
1	C	3121	0	3060	34	0
1	D	3121	0	3059	30	0
2	A	31	0	19	2	0
2	B	31	0	19	2	0
2	C	31	0	19	1	0
2	D	31	0	19	1	0
3	A	11	0	6	2	0
3	B	11	0	6	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	11	0	6	3	0
3	D	11	0	7	2	0
4	A	7	0	0	0	0
4	B	10	0	0	3	0
4	C	6	0	0	0	0
4	D	2	0	0	1	0
All	All	12685	0	12351	110	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 4.

All (110) 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:D:187:ASP:CB	1:D:187:ASP:OD1	2.05	1.04
1:D:187:ASP:OD1	1:D:187:ASP:CG	0.82	1.01
1:D:187:ASP:OD2	1:D:187:ASP:OD1	1.93	0.87
1:A:23:ILE:O	1:A:23:ILE:HG13	1.81	0.81
1:D:123:GLN:HG2	1:D:241:MET:HE1	1.62	0.80
1:B:384:GLN:HG3	1:C:213:GLN:HG3	1.66	0.77
1:A:384:GLN:HG3	1:D:213:GLN:HG3	1.69	0.75
1:B:384:GLN:CG	1:C:213:GLN:HG3	2.17	0.74
1:B:213:GLN:HG3	1:C:384:GLN:HG3	1.69	0.74
1:A:213:GLN:HG3	1:D:384:GLN:HG3	1.70	0.73
1:A:123:GLN:HG2	1:A:241:MET:CE	2.19	0.72
1:B:213:GLN:HG3	1:C:384:GLN:CG	2.21	0.71
1:D:123:GLN:HG2	1:D:241:MET:CE	2.21	0.70
1:A:384:GLN:CG	1:D:213:GLN:HG3	2.21	0.70
1:A:213:GLN:HG3	1:D:384:GLN:CG	2.22	0.69
1:B:123:GLN:HG2	1:B:241:MET:CE	2.25	0.67
1:A:317:GLN:OE1	1:A:367:ARG:NH2	2.25	0.67
1:A:123:GLN:HG2	1:A:241:MET:HE1	1.74	0.67
1:B:123:GLN:HG2	1:B:241:MET:HE1	1.75	0.67
1:B:79:ARG:HD2	4:B:2001:HOH:O	1.96	0.64
1:C:317:GLN:OE1	1:C:367:ARG:NH2	2.26	0.62
1:C:123:GLN:HG2	1:C:241:MET:CE	2.30	0.61
1:B:346:THR:HB	4:B:2007:HOH:O	2.03	0.59
1:C:123:GLN:HG2	1:C:241:MET:HE1	1.85	0.57
1:D:189:ASP:OD2	1:D:189:ASP:N	2.37	0.57
1:C:208:ASP:HA	1:C:221:LYS:HG2	1.87	0.57
1:B:418:ASP:OD1	1:B:420:THR:HB	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:SER:O	1:D:318:VAL:HG13	2.05	0.56
1:A:314:SER:O	1:A:318:VAL:HG13	2.05	0.56
1:B:317:GLN:OE1	1:B:367:ARG:NH2	2.29	0.56
1:A:418:ASP:OD1	1:A:420:THR:HB	2.05	0.56
1:A:214:ALA:HB3	1:A:392:MET:HB2	1.88	0.55
1:C:214:ALA:HB3	1:C:392:MET:HB2	1.88	0.55
1:D:109:GLY:HA2	1:D:215:ILE:HG23	1.88	0.55
1:C:314:SER:O	1:C:318:VAL:HG13	2.07	0.54
1:C:418:ASP:OD1	1:C:420:THR:HB	2.08	0.54
1:A:109:GLY:HA2	1:A:215:ILE:HG23	1.89	0.54
1:D:187:ASP:HB2	1:D:191:ASN:O	2.08	0.54
1:D:208:ASP:HA	1:D:221:LYS:HG2	1.88	0.54
1:A:208:ASP:HA	1:A:221:LYS:HG2	1.89	0.54
1:D:418:ASP:OD1	1:D:420:THR:HB	2.08	0.53
1:C:109:GLY:HA2	1:C:215:ILE:HG23	1.90	0.53
1:C:215:ILE:HG22	1:C:215:ILE:O	2.09	0.53
1:A:266:PHE:CD2	3:A:1424:4HP:C3	2.92	0.53
1:B:109:GLY:HA2	1:B:215:ILE:HG23	1.90	0.53
1:D:317:GLN:OE1	1:D:367:ARG:NH2	2.30	0.52
1:D:266:PHE:CD2	3:D:1424:4HP:C3	2.93	0.52
1:A:123:GLN:HG2	1:A:241:MET:HE2	1.90	0.52
1:B:266:PHE:CD2	3:B:1424:4HP:C3	2.93	0.52
1:B:208:ASP:HA	1:B:221:LYS:HG2	1.91	0.52
1:D:44:ILE:HD11	1:D:77:LEU:HD22	1.92	0.51
1:B:314:SER:O	1:B:318:VAL:HG13	2.10	0.51
1:B:346:THR:HG21	4:B:2009:HOH:O	2.10	0.51
1:A:215:ILE:HG22	1:A:215:ILE:O	2.11	0.51
1:B:215:ILE:HG22	1:B:215:ILE:O	2.11	0.51
1:A:44:ILE:HD11	1:A:77:LEU:HD22	1.93	0.50
1:C:266:PHE:CD2	3:C:1424:4HP:C3	2.93	0.50
1:B:44:ILE:HD11	1:B:77:LEU:HD22	1.93	0.50
1:C:343:ASN:HD22	1:C:343:ASN:C	2.14	0.50
1:B:343:ASN:HD22	1:B:343:ASN:C	2.15	0.50
1:A:343:ASN:HD22	1:A:343:ASN:C	2.15	0.50
1:A:23:ILE:O	1:A:23:ILE:CG1	2.57	0.50
1:C:44:ILE:HD11	1:C:77:LEU:HD22	1.94	0.50
1:A:214:ALA:CB	1:A:392:MET:HB2	2.41	0.49
1:C:214:ALA:CB	1:C:392:MET:HB2	2.42	0.49
1:D:215:ILE:O	1:D:215:ILE:HG22	2.12	0.49
1:D:214:ALA:HB3	1:D:392:MET:HB2	1.94	0.48
1:B:374:ALA:N	2:C:1423:FMN:O1P	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ALA:N	2:D:1423:FMN:O1P	2.47	0.47
1:B:354:GLN:O	1:B:358:VAL:HG23	2.15	0.47
1:B:349:PHE:HD2	1:B:353:ASN:HD21	1.62	0.46
1:B:214:ALA:HB3	1:B:392:MET:HB2	1.97	0.45
1:C:354:GLN:O	1:C:358:VAL:HG23	2.16	0.45
2:B:1423:FMN:O1P	1:C:374:ALA:N	2.49	0.45
1:D:214:ALA:CB	1:D:392:MET:HB2	2.46	0.45
1:A:187:ASP:HB2	1:A:191:ASN:H	1.80	0.45
1:A:187:ASP:HB2	1:A:191:ASN:N	2.31	0.45
1:B:214:ALA:CB	1:B:392:MET:HB2	2.47	0.44
1:C:346:THR:HB	4:D:2001:HOH:O	2.16	0.44
1:A:353:ASN:HD22	1:B:316:HIS:CD2	2.35	0.44
1:C:164:ASN:ND2	1:C:227:ASN:H	2.16	0.43
1:C:400:ASP:OD1	1:C:400:ASP:C	2.57	0.43
1:D:343:ASN:C	1:D:343:ASN:HD22	2.20	0.43
1:C:123:GLN:HG2	1:C:241:MET:HE2	1.99	0.43
1:D:131:LEU:HD13	1:D:234:ARG:HD2	2.01	0.43
1:A:266:PHE:CD2	3:A:1424:4HP:C2	3.02	0.43
1:B:342:PRO:HG2	1:B:347:LEU:HD22	2.01	0.43
1:D:349:PHE:HD2	1:D:353:ASN:HD21	1.68	0.42
1:C:131:LEU:HD13	1:C:234:ARG:HD2	2.02	0.42
1:C:187:ASP:OD2	1:C:191:ASN:HB2	2.18	0.42
1:A:187:ASP:CB	1:A:191:ASN:H	2.32	0.42
1:D:187:ASP:OD2	1:D:193:ILE:HD11	2.20	0.42
1:B:213:GLN:HG3	1:C:384:GLN:CD	2.40	0.42
1:B:266:PHE:CD2	3:B:1424:4HP:C2	3.03	0.41
1:D:314:SER:HA	1:D:367:ARG:HH21	1.85	0.41
1:B:384:GLN:CD	1:C:213:GLN:HG3	2.39	0.41
1:C:349:PHE:HD2	1:C:353:ASN:HD21	1.69	0.41
2:B:1423:FMN:H4'	2:B:1423:FMN:H1'2	1.89	0.41
1:A:131:LEU:HD13	1:A:234:ARG:HD2	2.03	0.41
1:C:266:PHE:CD2	3:C:1424:4HP:C2	3.04	0.41
1:C:263:ARG:HE	3:C:1424:4HP:C8	2.34	0.41
2:A:1423:FMN:O1P	1:D:374:ALA:N	2.53	0.41
1:C:222:MET:HG2	1:C:223:LEU:N	2.36	0.41
1:D:164:ASN:ND2	1:D:227:ASN:H	2.19	0.41
1:A:169:TRP:O	2:A:1423:FMN:C4	2.70	0.40
1:C:49:PRO:O	1:C:53:LYS:HG2	2.22	0.40
1:C:353:ASN:HD22	1:D:316:HIS:CD2	2.39	0.40
1:B:384:GLN:HG3	1:C:213:GLN:CG	2.46	0.40
1:D:266:PHE:CD2	3:D:1424:4HP:C2	3.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PRO:O	1:A:53:LYS:HG2	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	398/422 (94%)	389 (98%)	8 (2%)	1 (0%)	46	79
1	B	397/422 (94%)	386 (97%)	11 (3%)	0	100	100
1	C	397/422 (94%)	386 (97%)	11 (3%)	0	100	100
1	D	397/422 (94%)	384 (97%)	13 (3%)	0	100	100
All	All	1589/1688 (94%)	1545 (97%)	43 (3%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	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	325/345 (94%)	307 (94%)	18 (6%)	27	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	324/345 (94%)	309 (95%)	15 (5%)	33	67
1	C	324/345 (94%)	309 (95%)	15 (5%)	33	67
1	D	324/345 (94%)	310 (96%)	14 (4%)	35	70
All	All	1297/1380 (94%)	1235 (95%)	62 (5%)	31	66

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	38	VAL
1	A	56	GLU
1	A	153	LYS
1	A	154	VAL
1	A	222	MET
1	A	236	SER
1	A	260	THR
1	A	266	PHE
1	A	288	LYS
1	A	291	ASN
1	A	300	ASN
1	A	301	VAL
1	A	343	ASN
1	A	346	THR
1	A	347	LEU
1	A	384	GLN
1	A	420	THR
1	B	153	LYS
1	B	154	VAL
1	B	222	MET
1	B	236	SER
1	B	260	THR
1	B	266	PHE
1	B	288	LYS
1	B	291	ASN
1	B	293	VAL
1	B	301	VAL
1	B	343	ASN
1	B	346	THR
1	B	347	LEU
1	B	384	GLN
1	B	420	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	38	VAL
1	C	153	LYS
1	C	154	VAL
1	C	222	MET
1	C	236	SER
1	C	260	THR
1	C	266	PHE
1	C	288	LYS
1	C	291	ASN
1	C	301	VAL
1	C	343	ASN
1	C	346	THR
1	C	347	LEU
1	C	384	GLN
1	C	420	THR
1	D	38	VAL
1	D	153	LYS
1	D	154	VAL
1	D	236	SER
1	D	260	THR
1	D	266	PHE
1	D	288	LYS
1	D	291	ASN
1	D	301	VAL
1	D	343	ASN
1	D	346	THR
1	D	347	LEU
1	D	384	GLN
1	D	420	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	164	ASN
1	A	184	ASN
1	A	227	ASN
1	A	343	ASN
1	A	353	ASN
1	B	46	GLN
1	B	164	ASN
1	B	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	191	ASN
1	B	227	ASN
1	B	340	GLN
1	B	343	ASN
1	B	353	ASN
1	C	46	GLN
1	C	164	ASN
1	C	184	ASN
1	C	227	ASN
1	C	340	GLN
1	C	343	ASN
1	C	353	ASN
1	D	46	GLN
1	D	164	ASN
1	D	184	ASN
1	D	191	ASN
1	D	227	ASN
1	D	340	GLN
1	D	343	ASN
1	D	353	ASN

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](#)

8 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	FMN	A	1423	-	32,33,33	2.78	7 (21%)	34,50,50	1.88	8 (23%)
3	4HP	A	1424	-	8,11,11	0.55	0	11,14,14	0.65	0
2	FMN	B	1423	-	32,33,33	1.20	3 (9%)	34,50,50	1.66	6 (17%)
3	4HP	B	1424	-	8,11,11	0.47	0	11,14,14	0.60	0
2	FMN	C	1423	-	32,33,33	1.23	2 (6%)	34,50,50	1.65	6 (17%)
3	4HP	C	1424	-	8,11,11	0.64	0	11,14,14	0.77	0
2	FMN	D	1423	-	32,33,33	1.24	4 (12%)	34,50,50	1.72	6 (17%)
3	4HP	D	1424	-	8,11,11	0.56	0	11,14,14	0.61	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	FMN	A	1423	-	-	0/18/18/18	0/3/3/3
3	4HP	A	1424	-	-	0/2/4/4	0/1/1/1
2	FMN	B	1423	-	-	0/18/18/18	0/3/3/3
3	4HP	B	1424	-	-	0/2/4/4	0/1/1/1
2	FMN	C	1423	-	-	0/18/18/18	0/3/3/3
3	4HP	C	1424	-	-	0/2/4/4	0/1/1/1
2	FMN	D	1423	-	-	0/18/18/18	0/3/3/3
3	4HP	D	1424	-	-	0/2/4/4	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1423	FMN	P-O2P	-9.57	1.21	1.54
2	A	1423	FMN	P-O3P	-9.39	1.22	1.54
2	A	1423	FMN	P-O1P	-4.24	1.37	1.50
2	B	1423	FMN	C5A-N5	2.03	1.38	1.35
2	A	1423	FMN	C1'-N10	2.09	1.50	1.48
2	D	1423	FMN	C1'-N10	2.25	1.50	1.48
2	A	1423	FMN	C5A-N5	2.33	1.39	1.35
2	D	1423	FMN	C5A-N5	2.41	1.39	1.35
2	C	1423	FMN	C4-N3	3.26	1.38	1.33
2	B	1423	FMN	C4-N3	3.41	1.39	1.33
2	D	1423	FMN	C4-N3	3.44	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1423	FMN	C4-N3	3.50	1.39	1.33
2	D	1423	FMN	C4A-N5	3.63	1.38	1.33
2	B	1423	FMN	C4A-N5	3.71	1.39	1.33
2	A	1423	FMN	C4A-N5	3.86	1.39	1.33
2	C	1423	FMN	C4A-N5	3.87	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1423	FMN	N3-C2-N1	-4.76	119.68	127.69
2	A	1423	FMN	N3-C2-N1	-4.61	119.92	127.69
2	C	1423	FMN	N3-C2-N1	-4.60	119.94	127.69
2	B	1423	FMN	N3-C2-N1	-4.22	120.58	127.69
2	B	1423	FMN	C4A-C4-N3	-2.95	119.67	123.52
2	A	1423	FMN	C4A-C4-N3	-2.81	119.85	123.52
2	D	1423	FMN	C4A-C4-N3	-2.78	119.89	123.52
2	C	1423	FMN	C4A-C4-N3	-2.61	120.12	123.52
2	C	1423	FMN	C4-C4A-N5	2.07	121.21	118.70
2	B	1423	FMN	C4-C4A-N5	2.07	121.22	118.70
2	D	1423	FMN	C4-C4A-N5	2.27	121.46	118.70
2	A	1423	FMN	C4-C4A-N5	2.31	121.51	118.70
2	B	1423	FMN	C4A-N5-C5A	2.42	119.57	116.72
2	C	1423	FMN	C4A-N5-C5A	2.48	119.65	116.72
2	D	1423	FMN	C5A-C9A-N10	2.52	119.47	117.58
2	A	1423	FMN	O2P-P-O1P	2.62	119.18	110.63
2	A	1423	FMN	C4A-N5-C5A	2.67	119.87	116.72
2	A	1423	FMN	C5A-C9A-N10	2.86	119.72	117.58
2	D	1423	FMN	C4A-N5-C5A	3.03	120.30	116.72
2	C	1423	FMN	C5A-C9A-N10	3.15	119.94	117.58
2	B	1423	FMN	C5A-C9A-N10	3.17	119.95	117.58
2	A	1423	FMN	O2P-P-O5'	3.42	116.70	106.72
2	B	1423	FMN	C4-N3-C2	5.78	119.98	115.16
2	C	1423	FMN	C4-N3-C2	5.82	120.01	115.16
2	A	1423	FMN	C4-N3-C2	6.06	120.21	115.16
2	D	1423	FMN	C4-N3-C2	6.10	120.25	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1423	FMN	2	0
3	A	1424	4HP	2	0
2	B	1423	FMN	2	0
3	B	1424	4HP	2	0
2	C	1423	FMN	1	0
3	C	1424	4HP	3	0
2	D	1423	FMN	1	0
3	D	1424	4HP	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	400/422 (94%)	0.13	3 (0%) 87 81	43, 56, 75, 85	0
1	B	399/422 (94%)	0.19	1 (0%) 94 92	43, 56, 72, 83	0
1	C	399/422 (94%)	0.24	8 (2%) 68 58	43, 56, 74, 84	0
1	D	399/422 (94%)	0.77	58 (14%) 3 2	43, 56, 72, 83	0
All	All	1597/1688 (94%)	0.33	70 (4%) 38 26	43, 56, 74, 85	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	ASP	5.5
1	C	33	PRO	5.3
1	D	130	GLN	5.0
1	D	136	TRP	4.7
1	D	36	SER	4.3
1	D	35	VAL	4.3
1	D	152	GLY	4.3
1	D	151	PHE	4.2
1	D	247	ALA	4.1
1	D	34	ASP	4.1
1	D	81	PHE	4.0
1	D	123	GLN	4.0
1	D	38	VAL	3.8
1	D	190	GLY	3.6
1	C	36	SER	3.5
1	A	34	ASP	3.5
1	D	126	MET	3.4
1	D	222	MET	3.3
1	D	258	PHE	3.3
1	D	153	LYS	3.1
1	D	142	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	206	ILE	3.0
1	D	259	TYR	3.0
1	D	158	GLU	3.0
1	D	72	LEU	2.9
1	C	79	ARG	2.8
1	D	137	LEU	2.8
1	D	132	GLN	2.7
1	D	55	ALA	2.7
1	D	205	GLU	2.7
1	D	230	ILE	2.7
1	D	33	PRO	2.7
1	D	179	ALA	2.7
1	D	341	TYR	2.6
1	D	154	VAL	2.6
1	D	204	TYR	2.6
1	C	46	GLN	2.6
1	D	163	LEU	2.6
1	D	209	ASN	2.5
1	C	35	VAL	2.5
1	D	85	VAL	2.5
1	D	207	VAL	2.5
1	D	199	ILE	2.4
1	D	86	TYR	2.4
1	C	296	TYR	2.4
1	D	128	SER	2.4
1	D	336	GLY	2.4
1	D	37	GLY	2.4
1	D	135	ILE	2.4
1	D	340	GLN	2.3
1	A	163	LEU	2.3
1	D	61	LEU	2.3
1	B	190	GLY	2.3
1	D	143	THR	2.3
1	D	335	HIS	2.3
1	D	79	ARG	2.2
1	D	218	SER	2.2
1	D	83	PRO	2.2
1	C	176	ALA	2.2
1	A	188	ALA	2.2
1	D	342	PRO	2.2
1	D	244	GLY	2.1
1	D	171	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	68	ASN	2.1
1	D	162	ILE	2.1
1	D	88	GLY	2.1
1	D	167	TYR	2.0
1	D	176	ALA	2.0
1	D	141	ASP	2.0
1	D	77	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	4HP	C	1424	11/11	0.85	0.55	10.88	78,79,81,82	0
3	4HP	A	1424	11/11	0.78	0.49	7.54	78,79,81,82	0
3	4HP	D	1424	11/11	0.81	0.48	4.47	78,79,81,82	0
3	4HP	B	1424	11/11	0.90	0.47	4.20	78,79,81,82	0
2	FMN	D	1423	31/31	0.87	0.41	2.54	70,71,81,82	0
2	FMN	B	1423	31/31	0.92	0.27	1.11	70,71,80,83	0
2	FMN	C	1423	31/31	0.92	0.23	0.62	70,71,80,83	0
2	FMN	A	1423	31/31	0.93	0.19	-0.48	70,71,80,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.