



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4GDP
Title : Yeast polyamine oxidase FMS1, N195A mutant
Authors : Taylor, A.B.; Adachi, M.S.; Hart, P.J.; Fitzpatrick, P.F.
Deposited on : 2012-08-01
Resolution : 2.00 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 (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

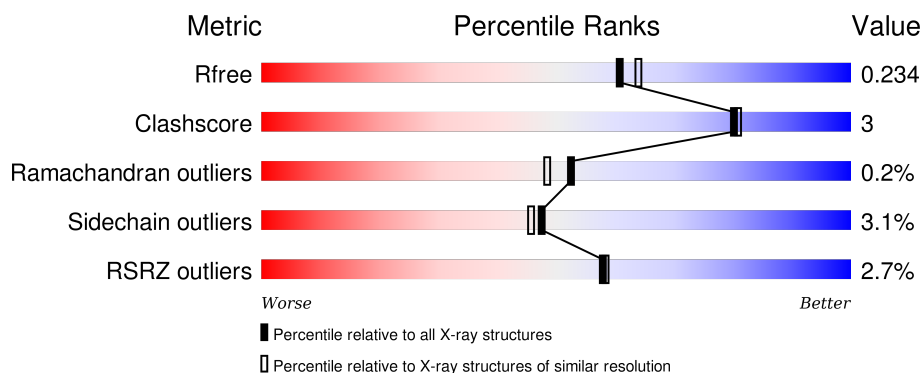
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	516	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	516	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	C	516	<div> <div>2%</div> <div>86%</div> <div>7%</div> <div>5%</div> </div>
1	D	516	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>..</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
3	PG4	D	802	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16892 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 Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3967	2505	689	751	22			
1	B	502	Total	C	N	O	S	0	3	0
			4029	2544	698	763	24			
1	C	488	Total	C	N	O	S	0	1	0
			3916	2474	679	740	23			
1	D	498	Total	C	N	O	S	0	2	0
			3997	2525	693	757	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
A	509	LEU	-	EXPRESSION TAG	UNP P50264
A	510	GLU	-	EXPRESSION TAG	UNP P50264
A	511	HIS	-	EXPRESSION TAG	UNP P50264
A	512	HIS	-	EXPRESSION TAG	UNP P50264
A	513	HIS	-	EXPRESSION TAG	UNP P50264
A	514	HIS	-	EXPRESSION TAG	UNP P50264
A	515	HIS	-	EXPRESSION TAG	UNP P50264
A	516	HIS	-	EXPRESSION TAG	UNP P50264
B	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
B	509	LEU	-	EXPRESSION TAG	UNP P50264
B	510	GLU	-	EXPRESSION TAG	UNP P50264
B	511	HIS	-	EXPRESSION TAG	UNP P50264
B	512	HIS	-	EXPRESSION TAG	UNP P50264
B	513	HIS	-	EXPRESSION TAG	UNP P50264
B	514	HIS	-	EXPRESSION TAG	UNP P50264
B	515	HIS	-	EXPRESSION TAG	UNP P50264
B	516	HIS	-	EXPRESSION TAG	UNP P50264
C	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
C	509	LEU	-	EXPRESSION TAG	UNP P50264
C	510	GLU	-	EXPRESSION TAG	UNP P50264

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	511	HIS	-	EXPRESSION TAG	UNP P50264
C	512	HIS	-	EXPRESSION TAG	UNP P50264
C	513	HIS	-	EXPRESSION TAG	UNP P50264
C	514	HIS	-	EXPRESSION TAG	UNP P50264
C	515	HIS	-	EXPRESSION TAG	UNP P50264
C	516	HIS	-	EXPRESSION TAG	UNP P50264
D	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
D	509	LEU	-	EXPRESSION TAG	UNP P50264
D	510	GLU	-	EXPRESSION TAG	UNP P50264
D	511	HIS	-	EXPRESSION TAG	UNP P50264
D	512	HIS	-	EXPRESSION TAG	UNP P50264
D	513	HIS	-	EXPRESSION TAG	UNP P50264
D	514	HIS	-	EXPRESSION TAG	UNP P50264
D	515	HIS	-	EXPRESSION TAG	UNP P50264
D	516	HIS	-	EXPRESSION TAG	UNP P50264

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



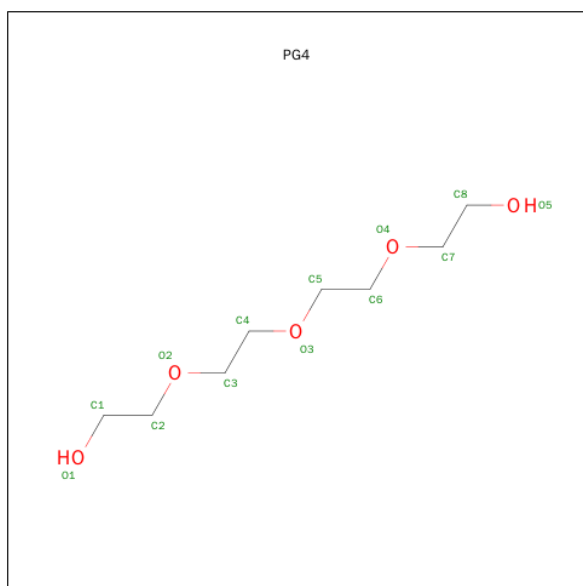
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			11	7	4		
3	C	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			11	8	3		

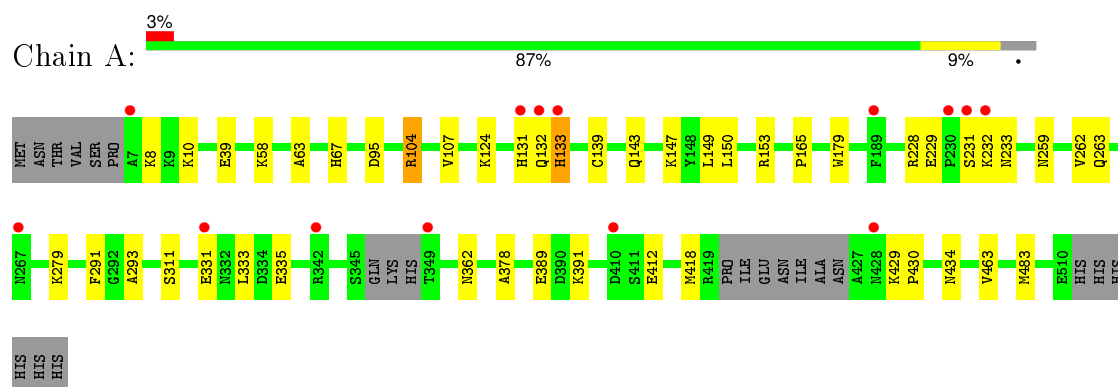
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	199	Total	O	0	0
			199	199		
4	C	161	Total	O	0	0
			161	161		
4	D	200	Total	O	0	0
			200	200		

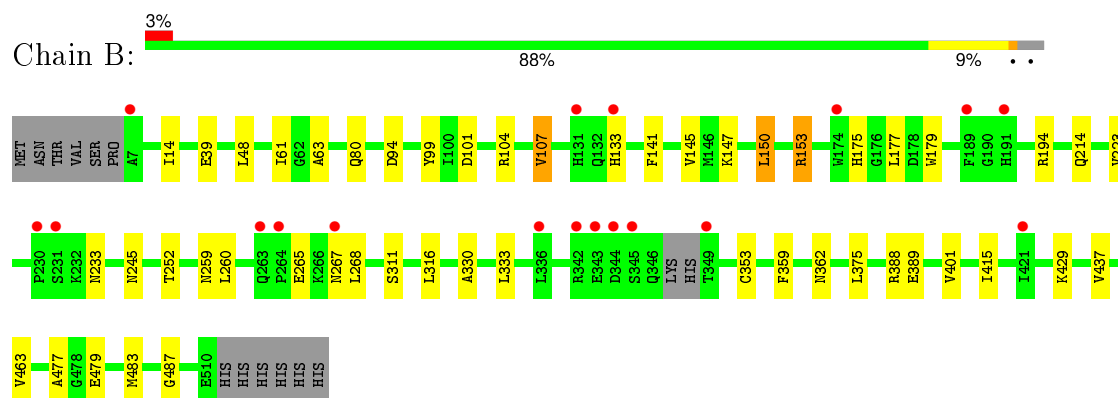
3 Residue-property plots [i](#)

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.

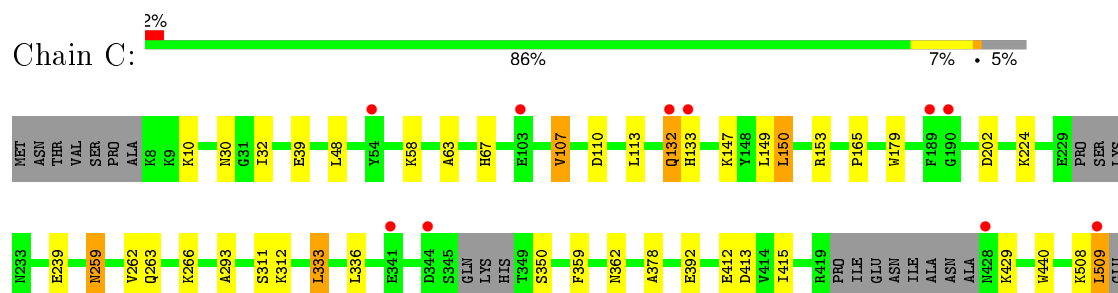
• Molecule 1: Polyamine oxidase FMS1



• Molecule 1: Polyamine oxidase FMS1



• Molecule 1: Polyamine oxidase FMS1



HIS

HIS

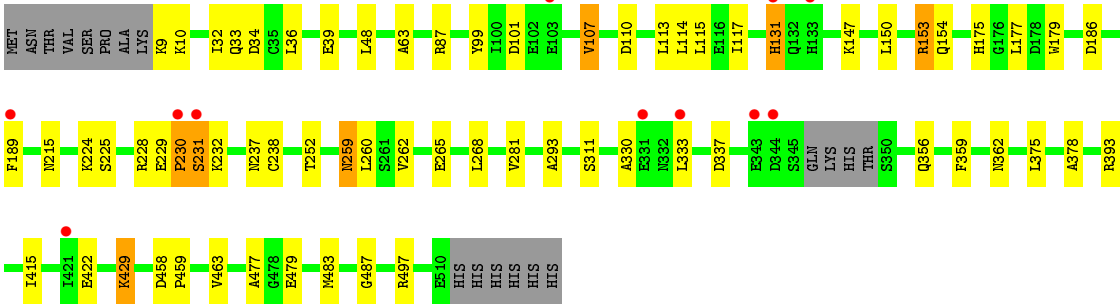
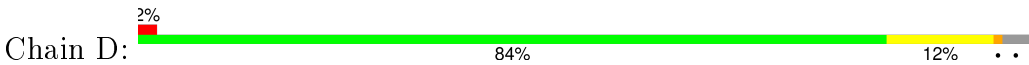
HIS

HIS

HIS

HIS

● Molecule 1: Polyamine oxidase FMS1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.85Å 81.89Å 104.79Å 78.07° 79.51° 78.92°	Depositor
Resolution (Å)	79.07 – 2.00 79.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (79.07-2.00) 85.1 (79.08-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.234 0.202 , 0.234	Depositor DCC
R_{free} test set	1999 reflections (1.35%)	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.5	EDS
Estimated twinning fraction	0.138 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 149579 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16892	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: PG4, 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	0.28	0/4050	0.44	0/5474
1	B	0.28	0/4119	0.44	0/5570
1	C	0.28	0/3996	0.43	0/5399
1	D	0.28	0/4084	0.44	0/5523
All	All	0.28	0/16249	0.44	0/21966

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3967	0	3885	23	0
1	B	4029	0	3955	26	0
1	C	3916	0	3837	24	0
1	D	3997	0	3921	38	0
2	A	53	0	31	4	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	13	0	18	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	13	0	0
3	C	13	0	18	2	0
3	D	11	0	12	0	0
4	A	163	0	0	2	0
4	B	199	0	0	3	0
4	C	161	0	0	1	0
4	D	200	0	0	4	0
All	All	16892	0	15783	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 3.

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:B:14:ILE:HD12	1:B:223:VAL:HG21	1.65	0.78
1:C:412:GLU:HG3	1:C:429:LYS:HE3	1.73	0.70
1:D:229:GLU:O	1:D:231:SER:N	2.22	0.70
1:D:9:LYS:N	1:D:34:ASP:O	2.26	0.68
1:A:133:HIS:O	1:D:393:ARG:NH2	2.29	0.65
1:C:67:HIS:HE1	3:C:802:PG4:H71	1.63	0.64
1:C:149:LEU:HD11	1:C:165:PRO:HG3	1.80	0.62
1:D:153:ARG:NH2	1:D:330:ALA:O	2.31	0.62
1:A:279:LYS:NZ	4:A:1048:HOH:O	2.34	0.61
1:C:150:LEU:HD23	1:C:336:LEU:HD22	1.84	0.60
1:C:10:LYS:HE2	1:C:32:ILE:HG23	1.83	0.59
1:A:149:LEU:HD11	1:A:165:PRO:HG3	1.85	0.58
1:C:39:GLU:OE1	2:C:801:FAD:O2B	2.22	0.58
1:B:80:GLN:NE2	4:B:1009:HOH:O	2.34	0.57
1:C:508:LYS:O	1:C:509:LEU:HB2	2.05	0.57
1:A:39:GLU:OE1	2:A:801:FAD:O2B	2.22	0.56
1:B:99:TYR:HB3	1:B:316:LEU:HD21	1.87	0.56
1:B:147:LYS:HG2	1:B:333:LEU:HD11	1.87	0.56
1:C:67:HIS:CE1	3:C:802:PG4:H71	2.40	0.55
1:D:293:ALA:HB3	1:D:378:ALA:HB2	1.89	0.55
1:C:415:ILE:HD11	1:C:429:LYS:HD3	1.90	0.54
1:A:311:SER:HA	1:A:362:ASN:HB3	1.89	0.54
1:A:10:LYS:NZ	4:A:1007:HOH:O	2.40	0.54
1:C:311:SER:HA	1:C:362:ASN:HB3	1.90	0.54
1:B:214:GLN:NE2	4:B:993:HOH:O	2.40	0.54
1:D:497:ARG:NE	4:D:1069:HOH:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.90	0.53
1:C:293:ALA:HB3	1:C:378:ALA:HB2	1.91	0.53
1:B:39:GLU:OE1	2:B:801:FAD:O2B	2.27	0.53
1:A:8:LYS:HE2	1:A:233:ASN:HD21	1.75	0.52
1:A:139:CYS:HB2	1:A:143:GLN:OE1	2.10	0.52
1:D:131:HIS:ND1	1:D:131:HIS:O	2.44	0.51
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.92	0.51
1:D:147:LYS:HG2	1:D:333:LEU:HD11	1.93	0.50
1:D:39:GLU:OE1	2:D:801:FAD:O2B	2.29	0.49
1:D:224:LYS:NZ	1:D:238:CYS:O	2.45	0.49
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.77	0.49
1:C:147:LYS:HG2	1:C:333:LEU:HD21	1.95	0.49
1:B:48:LEU:HD23	1:B:63:ALA:HB3	1.95	0.49
1:D:479:GLU:OE1	1:D:487:GLY:HA2	2.13	0.48
1:D:359:PHE:HD2	1:D:375:LEU:HD22	1.78	0.48
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.53	0.48
1:B:311:SER:HA	1:B:362:ASN:HB3	1.96	0.48
1:A:147:LYS:HD3	1:A:333:LEU:HD11	1.95	0.48
1:B:133:HIS:HD1	1:D:422:GLU:CD	2.17	0.48
1:D:110:ASP:HB3	1:D:113:LEU:HB2	1.95	0.47
1:C:132:GLN:HG3	1:C:133:HIS:CE1	2.49	0.47
1:D:186:ASP:HB2	4:D:1003:HOH:O	2.14	0.47
1:A:8:LYS:HE2	1:A:233:ASN:ND2	2.29	0.47
1:D:48:LEU:CD2	1:D:63:ALA:HB3	2.45	0.47
1:A:463:VAL:HG11	1:A:483:MET:HG2	1.97	0.47
1:A:67:HIS:HE1	3:A:802:PG4:H21	1.80	0.46
1:D:150:LEU:O	1:D:153:ARG:HD2	2.15	0.46
1:D:229:GLU:HA	1:D:230:PRO:HD3	1.82	0.46
1:D:463:VAL:HG11	1:D:483:MET:HG2	1.96	0.46
1:D:228:ARG:NE	1:D:232:LYS:O	2.35	0.46
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.46	0.46
1:C:58:LYS:NZ	1:C:202:ASP:OD2	2.48	0.45
1:A:228:ARG:HH21	1:A:232:LYS:HA	1.82	0.45
1:D:153:ARG:HG2	1:D:154:GLN:N	2.31	0.45
1:A:132:GLN:HB2	1:A:133:HIS:ND1	2.32	0.45
1:D:311:SER:HA	1:D:362:ASN:HB3	1.98	0.45
1:C:312:LYS:HD2	1:C:359:PHE:CZ	2.52	0.44
1:A:418:MET:HE3	1:A:434:ASN:HA	1.98	0.44
1:D:415:ILE:HD11	1:D:429:LYS:HD3	2.00	0.44
1:C:107:VAL:HG22	1:C:113:LEU:HD13	1.99	0.44
1:C:30:ASN:O	1:C:508:LYS:HE3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD22	1:D:268:LEU:HD13	2.00	0.43
1:A:63:ALA:HA	2:A:801:FAD:C4X	2.48	0.43
1:B:415:ILE:HD11	1:B:429:LYS:HD3	2.00	0.43
1:C:48:LEU:HD22	1:C:63:ALA:HB3	2.00	0.43
1:D:114:LEU:HB3	1:D:117:ILE:HD12	1.99	0.43
1:B:153:ARG:NH2	1:B:330:ALA:O	2.45	0.43
1:D:215:ASN:ND2	4:D:1056:HOH:O	2.33	0.43
1:D:10:LYS:NZ	1:D:33:GLN:H	2.17	0.43
1:A:429:LYS:HA	1:A:430:PRO:HD3	1.89	0.43
1:C:63:ALA:HA	2:C:801:FAD:N5	2.34	0.43
1:D:281:VAL:HG22	4:D:1019:HOH:O	2.18	0.43
1:D:131:HIS:O	1:D:131:HIS:CG	2.72	0.43
1:A:412:GLU:HB3	1:A:429:LYS:HE3	2.01	0.42
1:A:63:ALA:HA	2:A:801:FAD:N5	2.34	0.42
1:D:359:PHE:CD2	1:D:375:LEU:HD22	2.54	0.42
1:C:224:LYS:HE3	1:C:239:GLU:HG2	2.02	0.42
1:D:107:VAL:HG13	1:D:115:LEU:HD12	2.01	0.42
1:D:225:SER:HB2	1:D:237:ASN:HB2	2.01	0.42
1:D:259:ASN:O	1:D:262:VAL:HG22	2.20	0.42
1:B:260:LEU:HD22	1:B:268:LEU:HD13	2.00	0.42
1:C:259:ASN:O	1:C:262:VAL:HG22	2.20	0.42
1:C:413:ASP:O	1:C:429:LYS:HE2	2.20	0.41
1:C:440:TRP:HB2	4:C:981:HOH:O	2.19	0.41
1:B:61:ILE:HA	1:B:61:ILE:HD12	1.88	0.41
1:A:147:LYS:HE2	1:A:147:LYS:HB2	1.60	0.41
1:D:10:LYS:HD2	1:D:32:ILE:HG23	2.03	0.41
1:B:141:PHE:O	1:B:145:VAL:HG23	2.20	0.41
1:A:104:ARG:O	1:A:104:ARG:HG3	2.21	0.41
1:B:94:ASP:OD1	1:B:194:ARG:HB3	2.20	0.41
1:B:104:ARG:HG2	1:B:107:VAL:HG23	2.03	0.41
1:B:487:GLY:O	2:B:801:FAD:O3'	2.38	0.41
1:B:150:LEU:HA	1:B:150:LEU:HD22	1.89	0.41
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.21	0.41
1:A:259:ASN:O	1:A:262:VAL:HG22	2.21	0.40
1:D:252:THR:HG22	1:D:477:ALA:HB3	2.03	0.40
1:B:463:VAL:HG11	1:B:483:MET:HG2	2.02	0.40
1:B:388:ARG:HB2	1:B:437:VAL:HB	2.04	0.40
2:A:801:FAD:N5	3:A:802:PG4:H51	2.36	0.40
1:D:99:TYR:HB2	1:D:107:VAL:HG12	2.04	0.40
1:D:458:ASP:HA	1:D:459:PRO:HD2	1.83	0.40
1:C:110:ASP:HB3	1:C:113:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:HIS:CE1	1:D:189:PHE:HE2	2.40	0.40
1:B:175:HIS:HD2	4:B:955:HOH:O	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	490/516 (95%)	473 (96%)	17 (4%)	0	100	100
1	B	501/516 (97%)	488 (97%)	13 (3%)	0	100	100
1	C	481/516 (93%)	464 (96%)	16 (3%)	1 (0%)	52	48
1	D	496/516 (96%)	480 (97%)	14 (3%)	2 (0%)	39	33
All	All	1968/2064 (95%)	1905 (97%)	60 (3%)	3 (0%)	52	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
1	D	231	SER
1	D	230	PRO

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	437/456 (96%)	419 (96%)	18 (4%)	37	32
1	B	445/456 (98%)	433 (97%)	12 (3%)	52	52
1	C	432/456 (95%)	421 (98%)	11 (2%)	55	55
1	D	441/456 (97%)	428 (97%)	13 (3%)	50	49
All	All	1755/1824 (96%)	1701 (97%)	54 (3%)	47	46

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	95	ASP
1	A	104	ARG
1	A	107	VAL
1	A	124	LYS
1	A	131	HIS
1	A	133	HIS
1	A	150	LEU
1	A	153	ARG
1	A	179	TRP
1	A	229	GLU
1	A	231	SER
1	A	263	GLN
1	A	291	PHE
1	A	331	GLU
1	A	335	GLU
1	A	389	GLU
1	A	391	LYS
1	B	101	ASP
1	B	107	VAL
1	B	150	LEU
1	B	153	ARG
1	B	177	LEU
1	B	179	TRP
1	B	233	ASN
1	B	245	ASN
1	B	259	ASN
1	B	265	GLU
1	B	267	ASN
1	B	389	GLU
1	C	107	VAL
1	C	150	LEU
1	C	153	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	179	TRP
1	C	259	ASN
1	C	263	GLN
1	C	266	LYS
1	C	333	LEU
1	C	350	SER
1	C	392	GLU
1	C	509	LEU
1	D	36	LEU
1	D	87	ARG
1	D	101	ASP
1	D	107	VAL
1	D	131	HIS
1	D	153	ARG
1	D	177	LEU
1	D	179	TRP
1	D	259	ASN
1	D	265	GLU
1	D	337	ASP
1	D	356	GLN
1	D	429	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	233	ASN
1	A	245	ASN
1	B	191	HIS
1	C	67	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	FAD	A	801	-	48,58,58	1.90	10 (20%)	54,89,89	2.44	9 (16%)
3	PG4	A	802	-	12,12,12	0.70	0	11,11,11	1.45	0
2	FAD	B	801	-	48,58,58	1.90	10 (20%)	54,89,89	2.45	9 (16%)
3	PG4	B	802	-	10,10,12	0.68	0	9,9,11	1.33	0
2	FAD	C	801	-	48,58,58	1.90	10 (20%)	54,89,89	2.86	13 (24%)
3	PG4	C	802	-	12,12,12	0.67	0	11,11,11	1.45	0
2	FAD	D	801	-	48,58,58	1.91	9 (18%)	54,89,89	2.45	9 (16%)
3	PG4	D	802	-	10,10,12	0.62	0	9,9,11	1.45	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	801	-	-	0/30/50/50	0/6/6/6
3	PG4	A	802	-	-	0/10/10/10	0/0/0/0
2	FAD	B	801	-	-	0/30/50/50	0/6/6/6
3	PG4	B	802	-	-	0/8/8/10	0/0/0/0
2	FAD	C	801	-	-	0/30/50/50	0/6/6/6
3	PG4	C	802	-	-	0/10/10/10	0/0/0/0
2	FAD	D	801	-	-	0/30/50/50	0/6/6/6
3	PG4	D	802	-	-	0/8/8/10	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C8M-C8	-5.51	1.39	1.51
2	A	801	FAD	C7M-C7	-5.51	1.39	1.51
2	D	801	FAD	C7M-C7	-5.50	1.39	1.51
2	C	801	FAD	C7M-C7	-5.50	1.39	1.51
2	D	801	FAD	C8M-C8	-5.49	1.39	1.51
2	C	801	FAD	C8M-C8	-5.49	1.39	1.51
2	B	801	FAD	C7M-C7	-5.47	1.40	1.51
2	A	801	FAD	C8M-C8	-5.45	1.40	1.51
2	D	801	FAD	C10-N10	-4.06	1.34	1.39
2	B	801	FAD	C10-N10	-4.04	1.34	1.39
2	A	801	FAD	C10-N10	-4.03	1.34	1.39
2	C	801	FAD	C10-N10	-4.02	1.34	1.39
2	A	801	FAD	C5A-C4A	-2.99	1.33	1.40
2	D	801	FAD	C5A-C4A	-2.97	1.33	1.40
2	B	801	FAD	C5A-C4A	-2.97	1.33	1.40
2	C	801	FAD	C5A-C4A	-2.95	1.33	1.40
2	B	801	FAD	C9A-N10	-2.73	1.35	1.38
2	D	801	FAD	C9A-N10	-2.73	1.35	1.38
2	A	801	FAD	C9A-N10	-2.72	1.35	1.38
2	C	801	FAD	C9A-N10	-2.69	1.35	1.38
2	B	801	FAD	O4B-C1B	2.02	1.43	1.41
2	C	801	FAD	O4B-C1B	2.03	1.43	1.41
2	A	801	FAD	O4B-C1B	2.06	1.43	1.41
2	B	801	FAD	C10-N1	2.86	1.40	1.35
2	C	801	FAD	C10-N1	2.86	1.40	1.35
2	A	801	FAD	C10-N1	2.87	1.40	1.35
2	D	801	FAD	C10-N1	2.89	1.40	1.35
2	C	801	FAD	C2A-N1A	3.18	1.39	1.33
2	B	801	FAD	C2A-N1A	3.19	1.40	1.33
2	A	801	FAD	C2A-N1A	3.20	1.40	1.33
2	D	801	FAD	C2A-N1A	3.22	1.40	1.33
2	C	801	FAD	C4-N3	3.93	1.40	1.33
2	D	801	FAD	C4-N3	3.98	1.40	1.33
2	B	801	FAD	C4-N3	3.98	1.40	1.33
2	A	801	FAD	C4-N3	3.99	1.40	1.33
2	B	801	FAD	C2A-N3A	4.48	1.40	1.32
2	D	801	FAD	C2A-N3A	4.48	1.40	1.32
2	A	801	FAD	C2A-N3A	4.49	1.40	1.32
2	C	801	FAD	C2A-N3A	4.50	1.40	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	N3A-C2A-N1A	-14.09	118.10	128.89
2	D	801	FAD	N3A-C2A-N1A	-14.07	118.12	128.89
2	C	801	FAD	N3A-C2A-N1A	-14.05	118.14	128.89
2	A	801	FAD	N3A-C2A-N1A	-13.99	118.18	128.89
2	C	801	FAD	O3P-PA-O5B	-7.57	82.86	102.94
2	C	801	FAD	O5B-PA-O1A	-5.36	88.80	109.62
2	C	801	FAD	C4B-O4B-C1B	-5.09	104.12	109.72
2	D	801	FAD	C4B-O4B-C1B	-4.92	104.32	109.72
2	B	801	FAD	C4B-O4B-C1B	-4.88	104.35	109.72
2	A	801	FAD	C4B-O4B-C1B	-4.86	104.38	109.72
2	C	801	FAD	P-O3P-PA	-4.51	120.06	132.73
2	C	801	FAD	O2A-PA-O5B	-4.43	86.11	108.46
2	B	801	FAD	P-O3P-PA	-4.39	120.41	132.73
2	D	801	FAD	P-O3P-PA	-4.38	120.42	132.73
2	A	801	FAD	P-O3P-PA	-4.38	120.44	132.73
2	A	801	FAD	C4X-C4-N3	-2.79	119.78	123.59
2	D	801	FAD	C4X-C4-N3	-2.75	119.83	123.59
2	B	801	FAD	C4X-C4-N3	-2.73	119.85	123.59
2	C	801	FAD	C4X-C4-N3	-2.72	119.87	123.59
2	D	801	FAD	C2B-C1B-N9A	-2.06	111.14	114.29
2	A	801	FAD	C2B-C1B-N9A	-2.05	111.16	114.29
2	C	801	FAD	C2B-C1B-N9A	-2.05	111.17	114.29
2	B	801	FAD	C2B-C1B-N9A	-2.03	111.19	114.29
2	A	801	FAD	C1'-N10-C9A	2.26	121.40	118.86
2	D	801	FAD	C1'-N10-C9A	2.28	121.42	118.86
2	C	801	FAD	C1'-N10-C9A	2.30	121.44	118.86
2	B	801	FAD	C1'-N10-C9A	2.33	121.47	118.86
2	D	801	FAD	C5X-C9A-N10	2.34	119.40	117.62
2	A	801	FAD	C5X-C9A-N10	2.37	119.42	117.62
2	C	801	FAD	C5X-C9A-N10	2.39	119.43	117.62
2	B	801	FAD	C5X-C9A-N10	2.39	119.44	117.62
2	A	801	FAD	C4X-N5-C5X	2.44	119.58	116.76
2	D	801	FAD	C4X-N5-C5X	2.46	119.60	116.76
2	B	801	FAD	C4X-N5-C5X	2.50	119.64	116.76
2	C	801	FAD	C4X-N5-C5X	2.59	119.74	116.76
2	C	801	FAD	O2A-PA-O3P	2.73	117.48	105.09
2	C	801	FAD	C4-N3-C2	5.49	119.99	115.25
2	D	801	FAD	C4-N3-C2	5.53	120.03	115.25
2	B	801	FAD	C4-N3-C2	5.53	120.03	115.25
2	A	801	FAD	C4-N3-C2	5.57	120.06	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	4	0
3	A	802	PG4	2	0
2	B	801	FAD	2	0
2	C	801	FAD	2	0
3	C	802	PG4	2	0
2	D	801	FAD	1	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	494/516 (95%)	0.22	14 (2%) 56 57	18, 31, 53, 77	0
1	B	502/516 (97%)	0.27	18 (3%) 46 48	19, 31, 57, 80	0
1	C	488/516 (94%)	0.18	10 (2%) 68 69	18, 31, 51, 73	0
1	D	498/516 (96%)	0.25	11 (2%) 65 66	17, 30, 55, 82	0
All	All	1982/2064 (96%)	0.23	53 (2%) 58 58	17, 30, 54, 82	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PRO	4.8
1	D	230	PRO	4.5
1	A	189	PHE	4.3
1	B	231	SER	4.3
1	D	421	ILE	4.3
1	A	132	GLN	4.2
1	B	133	HIS	3.9
1	B	349	THR	3.9
1	B	421	ILE	3.8
1	A	232	LYS	3.7
1	C	133	HIS	3.7
1	C	189	PHE	3.4
1	B	264	PRO	3.3
1	A	131	HIS	3.2
1	C	344	ASP	3.2
1	A	428	ASN	3.1
1	C	428	ASN	3.1
1	A	7	ALA	3.1
1	D	133	HIS	3.0
1	C	132	GLN	2.9
1	B	189	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	131	HIS	2.9
1	D	344	ASP	2.8
1	D	343	GLU	2.8
1	B	230	PRO	2.7
1	D	189	PHE	2.6
1	B	174	TRP	2.6
1	B	7	ALA	2.5
1	B	263	GLN	2.5
1	B	344	ASP	2.5
1	D	103	GLU	2.4
1	C	190	GLY	2.4
1	B	342	ARG	2.4
1	A	133	HIS	2.4
1	C	509	LEU	2.3
1	A	267	ASN	2.3
1	A	342	ARG	2.2
1	B	336	LEU	2.2
1	A	231	SER	2.2
1	D	231	SER	2.2
1	A	410	ASP	2.2
1	D	331	GLU	2.2
1	B	267	ASN	2.1
1	A	331	GLU	2.1
1	C	54	TYR	2.1
1	D	333	LEU	2.1
1	B	343	GLU	2.1
1	C	103	GLU	2.1
1	B	345	SER	2.0
1	B	191	HIS	2.0
1	A	349	THR	2.0
1	C	341	GLU	2.0
1	B	131	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	PG4	D	802	11/13	0.88	0.18	2.80	30,37,43,47	0
2	FAD	D	801	53/53	0.96	0.13	1.56	15,20,25,25	0
3	PG4	C	802	13/13	0.88	0.16	1.54	29,37,46,64	0
3	PG4	A	802	13/13	0.89	0.18	1.25	31,37,46,47	0
2	FAD	B	801	53/53	0.96	0.13	1.25	18,21,25,26	0
2	FAD	A	801	53/53	0.97	0.11	0.91	15,20,23,26	0
3	PG4	B	802	11/13	0.87	0.14	0.84	31,38,45,47	0
2	FAD	C	801	53/53	0.97	0.11	0.75	14,21,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.