Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:05 AM GMT

PDB ID	:	2PDT
Title	:	2.3 Angstrom Structure of Phosphodiesterase treated Vivid
Authors	:	Zoltowski, B.D.; Crane, B.R.; Bilwes, A.M.
Deposited on	:	2007-04-01
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

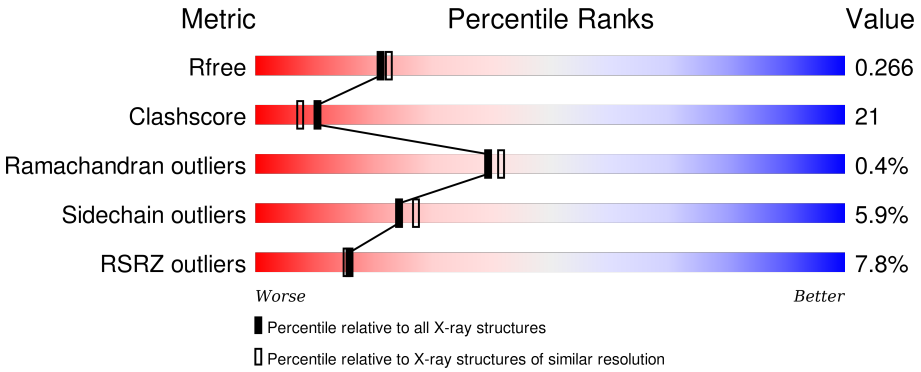
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 <=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	149	4% 64% 31%
1	B	149	7% 54% 36% 6%
1	C	149	3% 70% 24% 5%
1	D	149	15% 56% 34% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5269 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.

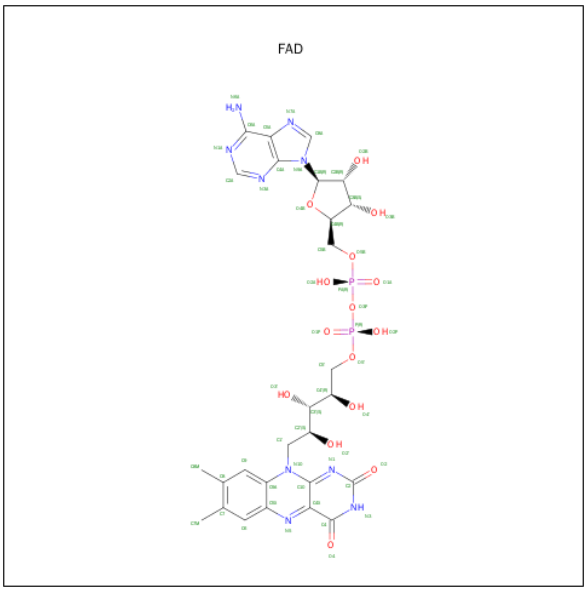
- Molecule 1 is a protein called Vivid PAS protein VVD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	1	0
			1170	737	199	222	12			
1	B	140	Total	C	N	O	S	0	1	0
			1123	706	192	213	12			
1	C	147	Total	C	N	O	S	0	1	0
			1170	737	199	222	12			
1	D	140	Total	C	N	O	S	0	0	0
			1122	706	192	213	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	MET	-	INITIATING METHIONINE	UNP Q9C3Y6
B	36	MET	-	INITIATING METHIONINE	UNP Q9C3Y6
C	36	MET	-	INITIATING METHIONINE	UNP Q9C3Y6
D	36	MET	-	INITIATING METHIONINE	UNP Q9C3Y6

- 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	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	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		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

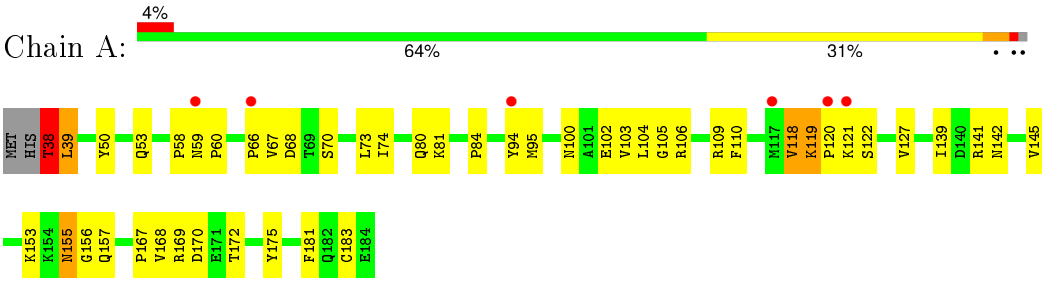
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	117	Total	O	0	0
			117	117		
3	C	165	Total	O	0	0
			165	165		
3	D	109	Total	O	0	0
			109	109		

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.

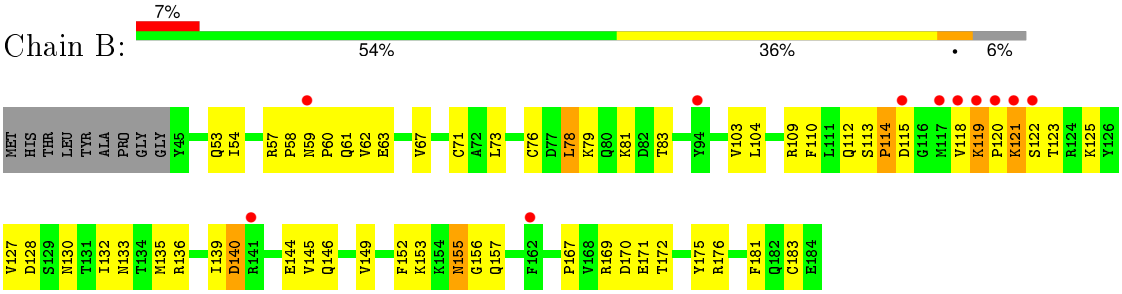
- Molecule 1: Vivid PAS protein VVD

Chain A:



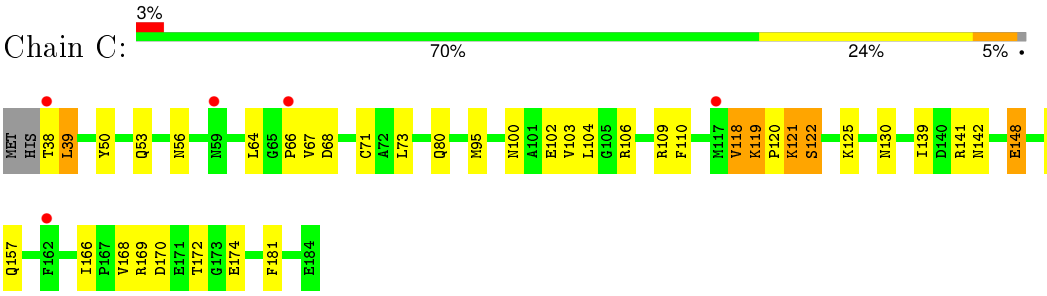
- Molecule 1: Vivid PAS protein VVD

Chain B:



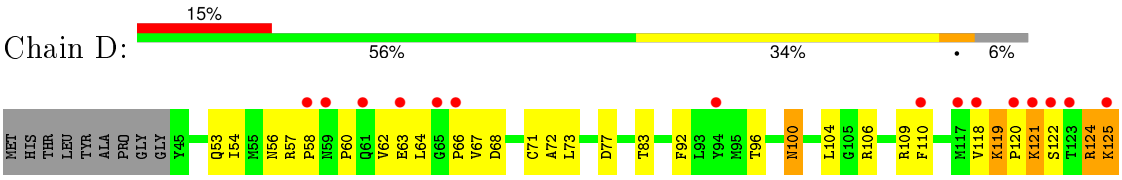
- Molecule 1: Vivid PAS protein VVD

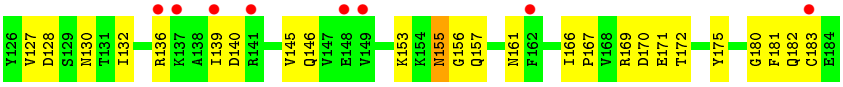
Chain C:



- Molecule 1: Vivid PAS protein VVD

Chain D:




Y126
V127
D128
S129
N130
T131
I132
R136
K137
A138
I139
D140
R141
V145
Q146
Y147
E148
V149
K153
K154
N155
G156
Q157
N161
F162
I166
P167
Y168
R169
D170
E171
T172
Y175
G180
F181
Q182
C183
E184

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.12Å 80.57Å 64.11Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 45.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.20) 99.0 (45.34-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.266 0.236 , 0.266	Depositor DCC
R_{free} test set	2897 reflections (8.74%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.6	EDS
Estimated twinning fraction	0.015 for -l,k,h 0.477 for -h,-k,l 0.017 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 37779 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5269	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.78 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0149e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.45	0/1197	0.67	1/1616 (0.1%)
1	B	0.35	0/1148	0.59	0/1548
1	C	0.51	2/1197 (0.2%)	0.67	1/1616 (0.1%)
1	D	0.34	0/1142	0.56	0/1540
All	All	0.42	2/4684 (0.0%)	0.62	2/6320 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	GLU	CD-OE2	-6.11	1.19	1.25
1	C	148	GLU	CG-CD	-5.24	1.44	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	148	GLU	CG-CD-OE1	5.68	129.66	118.30
1	A	38	THR	N-CA-CB	-5.58	99.69	110.30

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	1170	0	1160	48	2
1	B	1123	0	1115	59	0
1	C	1170	0	1160	49	2
1	D	1122	0	1114	48	0
2	A	31	0	19	3	0
2	B	31	0	19	1	0
2	C	31	0	19	1	0
2	D	31	0	19	2	0
3	A	169	0	0	3	0
3	B	117	0	0	5	0
3	C	165	0	0	2	0
3	D	109	0	0	3	0
All	All	5269	0	4625	200	2

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 21.

All (200) 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:119:LYS:H	1:D:119:LYS:HE2	1.14	1.11
1:C:38:THR:HG23	1:C:80:GLN:NE2	1.68	1.08
1:C:119:LYS:HE2	1:C:119:LYS:H	1.12	1.08
1:A:119:LYS:H	1:A:119:LYS:HE2	1.18	1.05
1:B:119:LYS:HE2	1:B:119:LYS:H	1.19	1.04
1:A:39:LEU:H	1:A:80:GLN:HE22	1.08	0.97
1:B:53:GLN:HE22	1:B:169:ARG:H	1.13	0.93
1:C:155:ASN:ND2	1:C:157:GLN:H	1.64	0.93
1:A:59:ASN:HA	3:A:475:HOH:O	1.68	0.92
1:C:39:LEU:H	1:C:80:GLN:HE22	1.18	0.90
1:D:53:GLN:HE22	1:D:169:ARG:H	1.17	0.89
1:A:155:ASN:ND2	1:A:157:GLN:H	1.71	0.88
1:B:81:LYS:HA	3:B:609:HOH:O	1.77	0.85
1:D:155:ASN:ND2	1:D:157:GLN:H	1.73	0.84
1:A:53:GLN:HE22	1:A:169:ARG:H	1.27	0.83
1:A:119:LYS:H	1:A:119:LYS:CE	1.94	0.81
1:B:155:ASN:HD22	1:B:156:GLY:H	1.29	0.80
1:A:39:LEU:H	1:A:80:GLN:NE2	1.78	0.80
1:B:155:ASN:ND2	1:B:157:GLN:H	1.80	0.79
1:C:53:GLN:HE22	1:C:169:ARG:H	1.30	0.79
1:A:39:LEU:N	1:A:80:GLN:HE22	1.82	0.78
1:B:155:ASN:HD22	1:B:156:GLY:N	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HG2	1:B:122:SER:HB3	1.66	0.78
1:C:119:LYS:CE	1:C:119:LYS:H	1.92	0.78
1:A:155:ASN:HD22	1:A:156:GLY:N	1.82	0.77
1:A:38:THR:HA	1:A:80:GLN:NE2	2.00	0.77
1:D:155:ASN:HD22	1:D:156:GLY:N	1.82	0.77
1:C:155:ASN:HD22	1:C:156:GLY:N	1.83	0.76
1:C:119:LYS:N	1:C:119:LYS:HE2	1.97	0.76
1:D:155:ASN:HD22	1:D:156:GLY:H	1.32	0.76
1:A:38:THR:HG21	1:A:105:GLY:HA2	1.68	0.75
1:D:119:LYS:H	1:D:119:LYS:CE	1.97	0.73
1:C:39:LEU:H	1:C:80:GLN:NE2	1.86	0.73
1:D:153:LYS:HB2	1:D:155:ASN:ND2	2.03	0.72
1:C:119:LYS:HG2	1:C:122:SER:HB2	1.71	0.72
1:B:119:LYS:CE	1:B:119:LYS:H	1.98	0.72
1:C:39:LEU:N	1:C:80:GLN:HE22	1.89	0.71
1:B:110:PHE:HA	1:B:118:VAL:HG12	1.73	0.69
1:B:153:LYS:HB2	1:B:155:ASN:ND2	2.08	0.69
1:B:78:LEU:HB2	1:B:176:ARG:O	1.93	0.69
1:C:38:THR:HG23	1:C:80:GLN:HE22	1.59	0.68
1:D:155:ASN:ND2	1:D:156:GLY:N	2.41	0.68
1:D:110:PHE:HA	1:D:118:VAL:HG12	1.76	0.67
1:A:119:LYS:N	1:A:119:LYS:HE2	2.02	0.67
1:D:110:PHE:HA	1:D:118:VAL:CG1	2.24	0.67
1:B:109:ARG:HG3	1:B:118:VAL:HG13	1.77	0.66
1:A:70:SER:HB2	1:B:123:THR:O	1.96	0.66
1:C:38:THR:HG23	1:C:80:GLN:CD	2.17	0.65
1:C:38:THR:CG2	1:C:80:GLN:NE2	2.53	0.65
1:A:119:LYS:HG2	1:A:122:SER:HB3	1.77	0.65
1:D:119:LYS:HE2	1:D:119:LYS:N	1.99	0.65
1:C:155:ASN:HD21	1:C:157:GLN:HB3	1.60	0.64
1:C:155:ASN:HD21	1:C:157:GLN:H	1.42	0.64
1:C:130:ASN:HB2	3:C:695:HOH:O	1.97	0.64
1:A:183:CYS:HB2	3:A:545:HOH:O	1.96	0.64
1:B:119:LYS:HE2	1:B:119:LYS:N	2.03	0.64
1:A:110:PHE:HA	1:A:118:VAL:CG1	2.29	0.63
1:B:109:ARG:O	1:B:118:VAL:HG11	1.99	0.63
1:B:155:ASN:ND2	1:B:156:GLY:N	2.46	0.62
1:D:67:VAL:HG23	1:D:71:CYS:SG	2.40	0.62
1:D:155:ASN:HD21	1:D:157:GLN:H	1.46	0.61
1:B:167:PRO:HB2	1:B:175:TYR:CD1	2.35	0.61
1:B:120:PRO:HB3	1:B:121:LYS:NZ	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:PRO:HB2	1:D:175:TYR:CD1	2.36	0.60
1:D:125:LYS:HD3	3:D:438:HOH:O	2.01	0.59
1:D:119:LYS:HG2	1:D:122:SER:HB3	1.84	0.59
1:C:170:ASP:OD1	1:C:172:THR:HB	2.03	0.58
1:C:66:PRO:HB2	1:D:56:ASN:OD1	2.03	0.57
1:C:56:ASN:OD1	1:D:66:PRO:HB2	2.05	0.57
1:C:110:PHE:HA	1:C:118:VAL:CG1	2.35	0.57
1:B:58:PRO:O	1:B:60:PRO:HD2	2.04	0.57
1:C:155:ASN:HD22	1:C:155:ASN:C	2.06	0.56
1:A:38:THR:HG21	1:A:105:GLY:CA	2.34	0.56
1:C:109:ARG:O	1:C:118:VAL:HG11	2.06	0.56
1:D:161:ASN:HD21	1:D:182:GLN:HG2	1.70	0.56
1:D:153:LYS:HB2	1:D:155:ASN:HD21	1.70	0.56
1:D:124:ARG:NH1	2:D:204:FAD:O2P	2.35	0.56
1:C:67:VAL:HG21	1:C:181:PHE:CE1	2.40	0.55
1:B:153:LYS:HB2	1:B:155:ASN:HD21	1.70	0.55
1:A:109:ARG:O	1:A:118:VAL:HG11	2.07	0.55
1:A:155:ASN:HD21	1:A:157:GLN:HB3	1.71	0.55
1:B:121:LYS:N	1:B:121:LYS:HE3	2.22	0.55
1:C:38:THR:CG2	1:C:80:GLN:HE22	2.16	0.55
1:A:170:ASP:OD1	1:A:172:THR:HB	2.07	0.54
1:C:67:VAL:HG23	1:C:71:CYS:SG	2.48	0.54
1:A:38:THR:HA	1:A:80:GLN:HE22	1.73	0.54
1:A:155:ASN:HD21	1:A:157:GLN:H	1.51	0.53
1:C:38:THR:HG22	1:C:39:LEU:N	2.23	0.53
1:C:102:GLU:O	1:C:106:ARG:HD2	2.09	0.52
1:B:67:VAL:HG21	1:B:181:PHE:CE1	2.44	0.52
1:D:67:VAL:HG21	1:D:181:PHE:CE1	2.45	0.52
1:B:120:PRO:HB3	1:B:121:LYS:HZ1	1.73	0.51
1:B:67:VAL:HG23	1:B:71:CYS:SG	2.49	0.51
1:D:120:PRO:HB3	1:D:121:LYS:NZ	2.25	0.51
1:B:109:ARG:HG3	1:B:118:VAL:CG1	2.41	0.51
1:B:132:ILE:O	1:B:136:ARG:HG2	2.11	0.51
1:D:73:LEU:HD12	1:D:73:LEU:C	2.31	0.51
1:A:155:ASN:C	1:A:155:ASN:HD22	2.12	0.51
1:C:155:ASN:ND2	1:C:155:ASN:C	2.64	0.51
1:C:109:ARG:NH2	1:C:120:PRO:HG3	2.25	0.51
1:A:58:PRO:O	1:A:60:PRO:HD2	2.11	0.51
1:B:73:LEU:HD12	1:B:73:LEU:C	2.31	0.51
1:C:172:THR:HG22	1:C:174:GLU:HG3	1.94	0.50
1:C:38:THR:HG22	1:C:39:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLU:HG3	3:B:487:HOH:O	2.11	0.50
1:B:136:ARG:O	1:B:140:ASP:HB2	2.12	0.50
1:D:128:ASP:OD1	1:D:130:ASN:N	2.45	0.50
1:C:73:LEU:C	1:C:73:LEU:HD12	2.32	0.50
1:A:81:LYS:O	1:A:84:PRO:HD3	2.12	0.49
1:A:94:TYR:CE2	1:B:121:LYS:HD3	2.47	0.49
1:B:61:GLN:HA	1:B:61:GLN:HE21	1.78	0.49
1:A:66:PRO:HD2	3:A:801:HOH:O	2.13	0.49
1:D:120:PRO:HB3	1:D:121:LYS:HZ1	1.77	0.49
1:A:102:GLU:O	1:A:106:ARG:HD2	2.13	0.49
1:B:54:ILE:O	1:B:57:ARG:HG2	2.13	0.49
1:D:106:ARG:CZ	3:D:576:HOH:O	2.61	0.48
1:C:119:LYS:HG2	1:C:122:SER:CB	2.43	0.48
1:D:54:ILE:O	1:D:57:ARG:HG2	2.13	0.48
1:A:139:ILE:HD13	2:A:201:FAD:HM81	1.94	0.48
1:D:183:CYS:HB3	3:D:429:HOH:O	2.14	0.48
1:C:139:ILE:HD13	2:C:203:FAD:HM81	1.94	0.48
1:B:110:PHE:HA	1:B:118:VAL:CG1	2.44	0.47
1:A:73:LEU:HD12	1:A:73:LEU:C	2.35	0.47
1:A:155:ASN:ND2	1:A:156:GLY:N	2.58	0.47
1:B:120:PRO:C	1:B:121:LYS:HG2	2.35	0.47
1:D:72:ALA:HB3	1:D:182:GLN:O	2.15	0.47
1:C:38:THR:CG2	1:C:39:LEU:N	2.77	0.47
1:B:109:ARG:O	1:B:112:GLN:HB2	2.15	0.47
1:A:167:PRO:HB2	1:A:175:TYR:CD1	2.50	0.47
1:D:145:VAL:HG22	1:D:146:GLN:N	2.30	0.47
1:D:64:LEU:HD22	1:D:166:ILE:HD12	1.97	0.47
1:D:139:ILE:HD13	2:D:204:FAD:HM81	1.97	0.46
1:C:130:ASN:HB3	3:C:624:HOH:O	2.16	0.46
1:B:135:MET:O	1:B:139:ILE:HG13	2.15	0.46
1:A:39:LEU:HD12	1:A:39:LEU:HA	1.74	0.46
1:D:171:GLU:HA	1:D:171:GLU:OE2	2.15	0.46
1:B:127:VAL:HB	1:B:132:ILE:HD11	1.98	0.46
1:D:121:LYS:N	1:D:121:LYS:HE3	2.31	0.46
1:D:73:LEU:HA	1:D:180:GLY:O	2.16	0.46
1:A:74:ILE:HD11	2:A:201:FAD:C6	2.46	0.46
1:D:64:LEU:HD22	1:D:166:ILE:CD1	2.45	0.46
1:B:170:ASP:OD1	1:B:172:THR:HB	2.15	0.46
1:D:62:VAL:HG12	1:D:63:GLU:N	2.30	0.46
1:A:155:ASN:ND2	1:A:155:ASN:C	2.69	0.46
1:B:133:ASN:HA	1:B:136:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ARG:O	1:D:118:VAL:HG11	2.16	0.45
1:D:67:VAL:HG22	1:D:68:ASP:N	2.32	0.45
1:A:127:VAL:HG13	1:A:149:VAL:HG23	1.99	0.45
1:C:64:LEU:HD22	1:C:166:ILE:CD1	2.47	0.45
1:B:103:VAL:HG23	1:B:104:LEU:N	2.32	0.45
1:B:145:VAL:HG22	1:B:146:GLN:N	2.32	0.45
1:B:128:ASP:O	1:B:132:ILE:HG13	2.16	0.45
1:A:118:VAL:O	1:A:118:VAL:HG22	2.16	0.45
1:B:114:PRO:HD3	1:B:152:PHE:CE2	2.52	0.44
1:B:113:SER:C	1:B:115:ASP:H	2.19	0.44
1:A:145:VAL:HG22	1:A:146:GLN:N	2.32	0.44
1:B:183:CYS:HB3	3:B:492:HOH:O	2.16	0.44
1:B:127:VAL:HG13	1:B:149:VAL:HG23	1.99	0.44
1:C:119:LYS:O	1:C:122:SER:HB2	2.17	0.44
1:B:128:ASP:OD1	1:B:130:ASN:N	2.51	0.44
1:A:67:VAL:HG21	1:A:181:PHE:CE1	2.53	0.43
1:A:103:VAL:HG23	1:A:104:LEU:N	2.32	0.43
1:D:77:ASP:O	1:D:83:THR:HA	2.17	0.43
1:B:172:THR:HG21	3:B:794:HOH:O	2.17	0.43
1:C:121:LYS:N	1:C:121:LYS:HE3	2.34	0.43
1:B:171:GLU:OE2	1:B:171:GLU:HA	2.19	0.42
1:C:103:VAL:HG23	1:C:104:LEU:N	2.33	0.42
1:C:102:GLU:OE1	1:C:154:LYS:HE3	2.19	0.42
1:D:67:VAL:HG21	1:D:181:PHE:HE1	1.84	0.42
1:B:171:GLU:HB2	3:B:718:HOH:O	2.18	0.42
1:A:67:VAL:HG21	1:A:181:PHE:CD1	2.55	0.42
1:D:155:ASN:HD22	1:D:155:ASN:N	2.18	0.42
1:B:62:VAL:HG12	1:B:63:GLU:N	2.35	0.42
1:D:92:PHE:CZ	1:D:96:THR:HG21	2.55	0.41
1:D:170:ASP:OD1	1:D:172:THR:HB	2.21	0.41
1:C:95:MET:O	1:C:153:LYS:HE2	2.20	0.41
1:B:112:GLN:HG2	1:B:127:VAL:HG21	2.01	0.41
1:B:155:ASN:HD22	1:B:155:ASN:N	2.17	0.41
1:C:67:VAL:HG22	1:C:68:ASP:N	2.34	0.41
1:C:103:VAL:CG2	1:C:104:LEU:N	2.83	0.41
1:A:50:TYR:CG	1:A:168:VAL:HG11	2.56	0.41
1:B:118:VAL:O	1:B:118:VAL:HG13	2.20	0.41
1:B:57:ARG:HG2	1:B:57:ARG:HH11	1.85	0.41
1:C:155:ASN:HD21	1:C:157:GLN:CB	2.30	0.41
1:A:155:ASN:HD22	1:A:156:GLY:H	1.62	0.41
1:A:109:ARG:NH2	1:A:120:PRO:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:HE	1:B:144:GLU:CD	2.22	0.41
1:A:141:ARG:O	1:A:142:ASN:HB2	2.20	0.41
1:D:100:ASN:ND2	1:D:104:LEU:HD13	2.36	0.41
1:C:64:LEU:HD22	1:C:166:ILE:HD11	2.03	0.40
1:B:76:CYS:HB3	1:B:83:THR:HG22	2.03	0.40
1:D:58:PRO:O	1:D:60:PRO:HD2	2.22	0.40
1:C:141:ARG:O	1:C:142:ASN:HB2	2.21	0.40
1:B:61:GLN:HA	1:B:61:GLN:NE2	2.35	0.40
1:B:139:ILE:HD13	2:B:202:FAD:HM81	2.03	0.40
1:A:95:MET:O	1:A:153:LYS:HE2	2.20	0.40
1:D:127:VAL:HB	1:D:132:ILE:HD11	2.03	0.40
1:A:74:ILE:HD11	2:A:201:FAD:H6	2.02	0.40
1:A:67:VAL:HG22	1:A:68:ASP:N	2.37	0.40
1:C:50:TYR:CG	1:C:168:VAL:HG11	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:N	1:C:148:GLU:OE2[2_755]	1.82	0.38
1:A:148:GLU:OE2	1:C:38:THR:N[2_756]	2.06	0.14

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	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
1	B	139/149 (93%)	134 (96%)	3 (2%)	2 (1%)	14	10
1	C	146/149 (98%)	142 (97%)	4 (3%)	0	100	100
1	D	138/149 (93%)	128 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	569/596 (96%)	546 (96%)	21 (4%)	2 (0%)	39 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	ASN
1	B	114	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	131/132 (99%)	124 (95%)	7 (5%)	28 32
1	B	127/132 (96%)	120 (94%)	7 (6%)	27 30
1	C	131/132 (99%)	123 (94%)	8 (6%)	23 26
1	D	126/132 (96%)	118 (94%)	8 (6%)	22 24
All	All	515/528 (98%)	485 (94%)	30 (6%)	24 28

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	39	LEU
1	A	100	ASN
1	A	118	VAL
1	A	119	LYS
1	A	121	LYS
1	A	155	ASN
1	B	78	LEU
1	B	79	LYS
1	B	119	LYS
1	B	121	LYS
1	B	125	LYS
1	B	140	ASP

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Mol	Chain	Res	Type
1	B	155	ASN
1	C	39	LEU
1	C	100	ASN
1	C	118	VAL
1	C	119	LYS
1	C	121	LYS
1	C	122	SER
1	C	125	LYS
1	C	155	ASN
1	D	100	ASN
1	D	119	LYS
1	D	121	LYS
1	D	124	ARG
1	D	125	LYS
1	D	136	ARG
1	D	140	ASP
1	D	155	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	56	ASN
1	A	61	GLN
1	A	80	GLN
1	A	100	ASN
1	A	155	ASN
1	A	157	GLN
1	B	53	GLN
1	B	61	GLN
1	B	100	ASN
1	B	133	ASN
1	B	155	ASN
1	B	157	GLN
1	C	53	GLN
1	C	61	GLN
1	C	80	GLN
1	C	100	ASN
1	C	155	ASN
1	C	157	GLN
1	D	53	GLN
1	D	61	GLN

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Mol	Chain	Res	Type
1	D	100	ASN
1	D	133	ASN
1	D	155	ASN
1	D	157	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	201	-	30,33,58	2.12	5 (16%)	33,50,89	2.25	3 (9%)
2	FAD	B	202	-	30,33,58	2.04	6 (20%)	33,50,89	2.39	3 (9%)
2	FAD	C	203	-	30,33,58	2.02	6 (20%)	33,50,89	2.42	3 (9%)
2	FAD	D	204	-	30,33,58	2.15	6 (20%)	33,50,89	2.40	3 (9%)

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	201	-	-	0/18/18/50	0/3/3/6
2	FAD	B	202	-	-	0/18/18/50	0/3/3/6
2	FAD	C	203	-	-	0/18/18/50	0/3/3/6
2	FAD	D	204	-	-	0/18/18/50	0/3/3/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	FAD	C4X-C10	2.01	1.44	1.41
2	C	203	FAD	P-O3P	2.07	1.62	1.54
2	D	204	FAD	C4X-C10	2.14	1.45	1.41
2	D	204	FAD	C9-C8	2.51	1.44	1.37
2	C	203	FAD	C9-C8	2.54	1.44	1.37
2	B	202	FAD	C9-C8	2.55	1.44	1.37
2	A	201	FAD	C9-C8	2.55	1.44	1.37
2	B	202	FAD	C5X-N5	2.99	1.40	1.35
2	D	204	FAD	C5X-N5	3.45	1.40	1.35
2	C	203	FAD	C5X-N5	3.52	1.41	1.35
2	A	201	FAD	C5X-N5	3.75	1.41	1.35
2	B	202	FAD	C4-N3	4.07	1.40	1.33
2	C	203	FAD	C4-N3	4.20	1.40	1.33
2	D	204	FAD	C4-N3	4.32	1.41	1.33
2	A	201	FAD	C4-N3	4.83	1.42	1.33
2	C	203	FAD	C4X-N5	5.14	1.41	1.33
2	C	203	FAD	C9A-N10	5.29	1.46	1.38
2	A	201	FAD	C9A-N10	5.30	1.46	1.38
2	B	202	FAD	C9A-N10	5.51	1.46	1.38
2	D	204	FAD	C9A-N10	5.70	1.46	1.38
2	B	202	FAD	C4X-N5	5.77	1.42	1.33
2	A	201	FAD	C4X-N5	5.94	1.42	1.33
2	D	204	FAD	C4X-N5	6.25	1.43	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	203	FAD	C4X-C4-N3	-6.11	115.24	123.59
2	A	201	FAD	C4X-C4-N3	-6.11	115.24	123.59
2	D	204	FAD	C4X-C4-N3	-6.02	115.36	123.59
2	B	202	FAD	C4X-C4-N3	-6.02	115.36	123.59
2	A	201	FAD	C1'-N10-C9A	2.84	122.05	118.86
2	B	202	FAD	C1'-N10-C9A	2.96	122.18	118.86
2	D	204	FAD	C1'-N10-C9A	2.98	122.21	118.86
2	C	203	FAD	C1'-N10-C9A	3.26	122.52	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	FAD	C4-N3-C2	10.19	124.06	115.25
2	D	204	FAD	C4-N3-C2	11.08	124.83	115.25
2	B	202	FAD	C4-N3-C2	11.10	124.84	115.25
2	C	203	FAD	C4-N3-C2	11.19	124.92	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	FAD	3	0
2	B	202	FAD	1	0
2	C	203	FAD	1	0
2	D	204	FAD	2	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

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^{th} 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	147/149 (98%)	-0.03	6 (4%) 41 39	15, 30, 57, 65	0
1	B	140/149 (93%)	0.45	11 (7%) 15 15	22, 47, 79, 88	0
1	C	147/149 (98%)	-0.02	5 (3%) 49 47	15, 30, 58, 68	0
1	D	140/149 (93%)	0.78	23 (16%) 2 2	26, 51, 78, 97	0
All	All	574/596 (96%)	0.29	45 (7%) 16 15	15, 39, 71, 97	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	MET	7.1
1	C	38	THR	5.6
1	B	94	TYR	5.2
1	D	118	VAL	4.8
1	B	59	ASN	4.6
1	D	94	TYR	4.5
1	D	162	PHE	4.4
1	C	59	ASN	4.3
1	B	121	LYS	4.1
1	D	141	ARG	4.0
1	D	120	PRO	3.6
1	D	183	CYS	3.6
1	D	65	GLY	3.5
1	B	117	MET	3.5
1	D	66	PRO	3.5
1	D	59	ASN	3.5
1	A	66	PRO	3.4
1	B	118	VAL	3.3
1	D	122	SER	3.2
1	D	61	GLN	3.1
1	B	119	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	117	MET	3.0
1	A	121	LYS	2.9
1	A	59	ASN	2.9
1	C	162	PHE	2.9
1	B	141	ARG	2.8
1	B	162	PHE	2.8
1	B	120	PRO	2.8
1	B	122	SER	2.7
1	D	121	LYS	2.7
1	C	66	PRO	2.4
1	D	58	PRO	2.3
1	B	115	ASP	2.3
1	A	117	MET	2.2
1	A	120	PRO	2.2
1	D	110	PHE	2.2
1	D	123	THR	2.2
1	D	139	ILE	2.1
1	D	125	LYS	2.1
1	D	136	ARG	2.1
1	A	94	TYR	2.1
1	D	149	VAL	2.1
1	D	63	GLU	2.0
1	D	148	GLU	2.0
1	D	137	LYS	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^{th} 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
2	FAD	C	203	31/53	0.95	0.11	-0.19	12,18,24,27	0
2	FAD	A	201	31/53	0.96	0.11	-0.22	12,18,25,25	0
2	FAD	B	202	31/53	0.92	0.11	-0.64	31,37,46,48	0
2	FAD	D	204	31/53	0.91	0.12	-0.69	32,36,53,56	0

6.5 Other polymers (i)

There are no such residues in this entry.