Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:04 AM GMT

PDB ID	:	3D9E
Title	:	Nitroalkane oxidase: active site mutant D402N crystallized with 1-nitrooctane
Authors	:	Heroux, A.; Bozinovski, D.M.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.
Deposited on	:	2008-05-27
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references (i)) 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		4.3%
RSRZ outliers		1.9%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
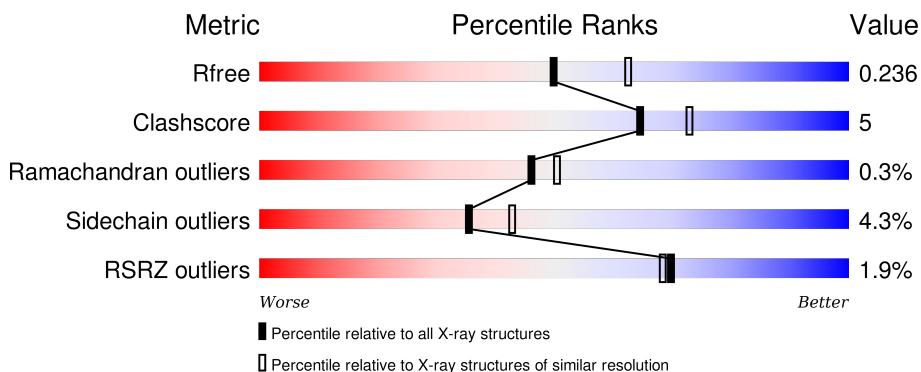
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	438	2% — 86% ... 11% ..
1	B	438	5% — 85% ... 11% ..
1	C	438	88% ... 9% ..
1	D	438	% — 85% ... 12% ..
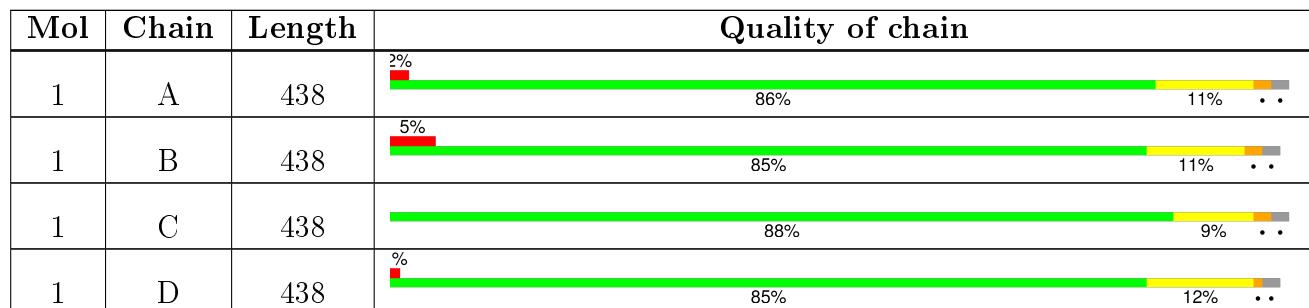
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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	N8C	A	600	-	-	-	X
3	N8C	B	600	-	-	X	-
3	N8C	C	600	-	-	-	X
3	N8C	D	600	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13772 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 Nitroalkane oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total 3306	C 2095	N 566	O 625	S 20	0	0	0
1	B	431	Total 3306	C 2095	N 566	O 625	S 20	0	0	0
1	C	430	Total 3301	C 2092	N 565	O 624	S 20	0	0	0
1	D	431	Total 3306	C 2095	N 566	O 625	S 20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	ASN	ASP	ENGINEERED	UNP Q8X1D8
B	402	ASN	ASP	ENGINEERED	UNP Q8X1D8
C	402	ASN	ASP	ENGINEERED	UNP Q8X1D8
D	402	ASN	ASP	ENGINEERED	UNP Q8X1D8

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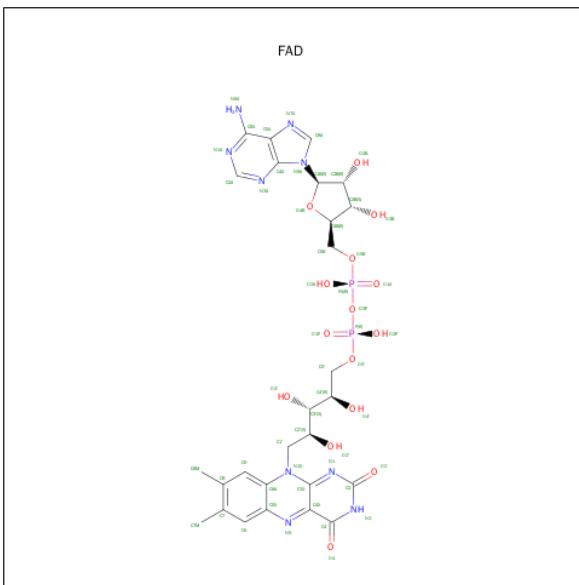
FAD

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		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 1-NITROOCTANE (three-letter code: N8C) (formula: $C_8H_{17}NO_2$).

N8C
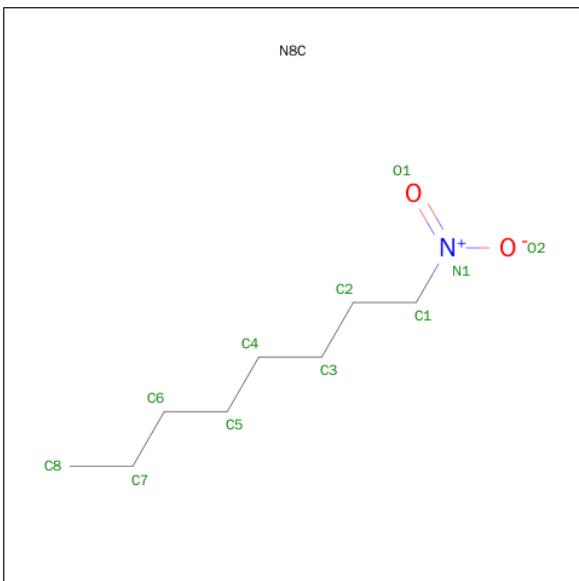
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 11	C 8	N 1	O 2	0	0
3	B	1	Total 11	C 8	N 1	O 2	0	0
3	C	1	Total 11	C 8	N 1	O 2	0	0
3	D	1	Total 11	C 8	N 1	O 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
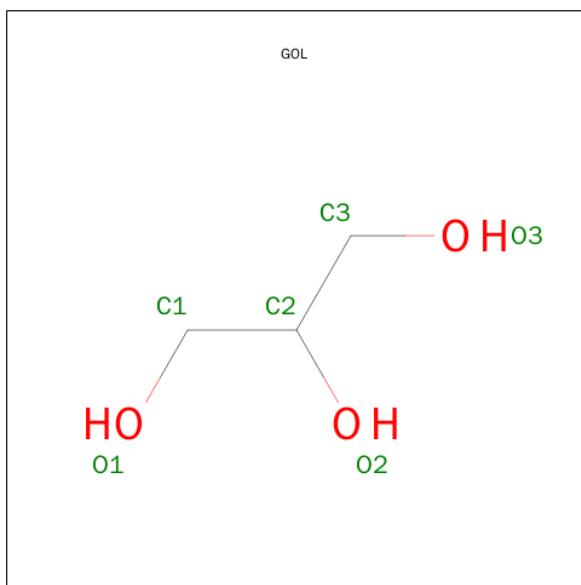
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	47	Total 47	O 47	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	83	Total 83	O 83	0	0
5	D	82	Total 82	O 82	0	0

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: Nitroalkane oxidase
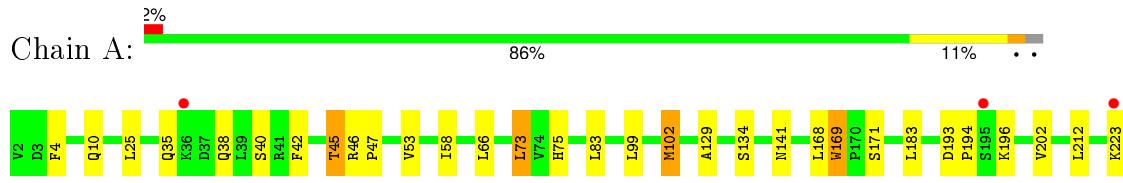
Chain A:

- Molecule 1: Nitroalkane oxidase

Chain B:

- Molecule 1: Nitroalkane oxidase

Chain C:

- Molecule 1: Nitroalkane oxidase

Chain D:
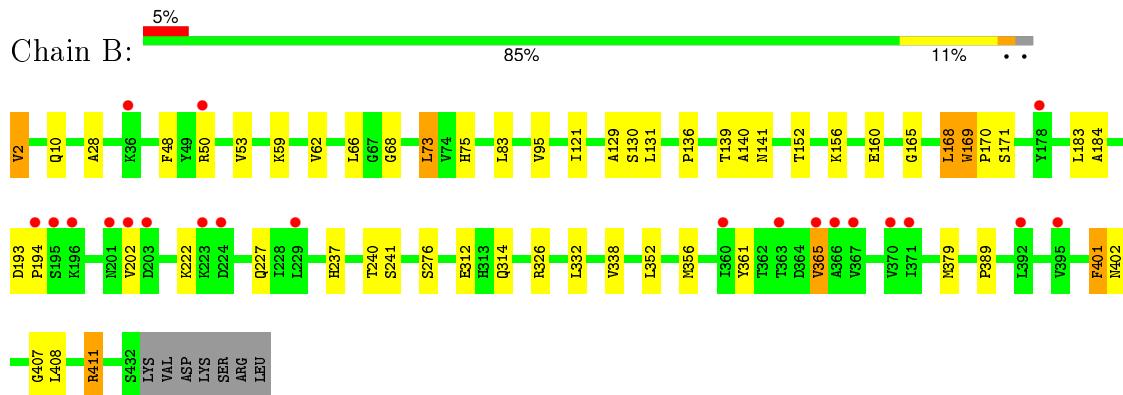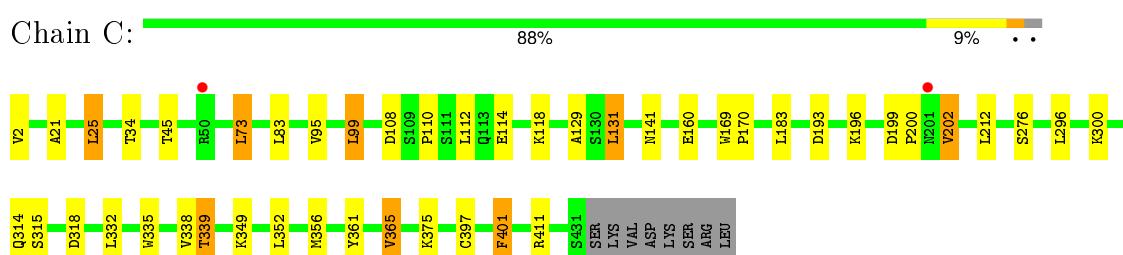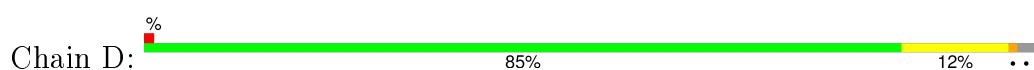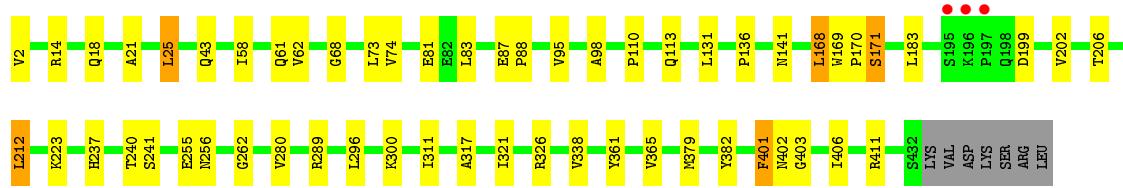
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.00Å 108.00Å 338.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.20 48.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.20) 93.9 (48.71-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.233 0.196 , 0.236	Depositor DCC
R_{free} test set	5515 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 28.6	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 110225 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13772	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FAD, N8C

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	0.55	0/3375	0.66	3/4581 (0.1%)
1	B	0.53	0/3375	0.63	0/4581
1	C	0.57	0/3370	0.64	0/4574
1	D	0.55	0/3375	0.64	0/4581
All	All	0.55	0/13495	0.64	3/18317 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	331	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	410	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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	3306	0	3312	44	0
1	B	3306	0	3312	44	0
1	C	3301	0	3310	30	0
1	D	3306	0	3312	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	3	0
2	B	53	0	31	11	0
2	C	53	0	31	5	0
2	D	53	0	31	3	0
3	A	11	0	17	2	0
3	B	11	0	17	7	0
3	C	11	0	17	2	0
3	D	11	0	17	2	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	61	0	0	0	0
5	B	47	0	0	0	0
5	C	83	0	0	0	0
5	D	82	0	0	1	0
All	All	13772	0	13470	138	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:MET:HE1	1:B:401:PHE:CA	1.99	0.93
1:A:379:MET:CE	1:B:401:PHE:HA	2.00	0.91
1:B:73:LEU:HB3	1:B:338:VAL:HB	1.57	0.87
1:A:379:MET:HE1	1:B:401:PHE:HA	1.56	0.85
1:D:141:ASN:HD21	2:D:500:FAD:H61A	1.27	0.82
1:C:73:LEU:HB3	1:C:338:VAL:HB	1.63	0.80
1:A:4:PHE:HD1	1:C:339:THR:HG21	1.49	0.77
1:A:73:LEU:HB3	1:A:338:VAL:HB	1.66	0.77
1:B:141:ASN:HD21	2:B:500:FAD:H61A	1.32	0.76
1:A:38:GLN:HG3	1:A:232:PRO:O	1.90	0.71
1:A:141:ASN:HD21	2:A:500:FAD:H61A	1.41	0.68
1:C:296:LEU:O	1:C:300:LYS:HG3	1.94	0.67
1:B:95:VAL:HG13	3:B:600:N8C:H5A	1.77	0.67
1:A:326:ARG:HB3	1:A:365:VAL:HG13	1.76	0.67
1:C:141:ASN:HD21	2:C:500:FAD:H61A	1.42	0.65
1:C:193:ASP:HB3	1:C:196:LYS:HD2	1.79	0.65
1:C:199:ASP:HB3	1:C:202:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASN:ND2	2:B:500:FAD:H61A	1.97	0.63
1:B:314:GLN:HE21	1:C:315:SER:H	1.47	0.62
1:A:99:LEU:HA	1:A:102:MET:HE2	1.81	0.62
1:A:53:VAL:HG22	1:A:58:ILE:HG13	1.82	0.62
1:B:276:SER:HB2	3:B:600:N8C:H6A	1.81	0.62
1:D:326:ARG:HB3	1:D:365:VAL:HG13	1.81	0.62
1:C:199:ASP:HB3	1:C:202:VAL:HG13	1.83	0.60
1:A:379:MET:HE3	2:B:500:FAD:H2'	1.84	0.60
1:D:141:ASN:ND2	2:D:500:FAD:H61A	1.97	0.60
1:B:407:GLY:O	1:B:411:ARG:HG2	2.02	0.59
1:A:379:MET:HE1	1:B:401:PHE:N	2.17	0.59
1:C:375:LYS:HB3	1:D:406:ILE:CD1	2.32	0.59
1:B:59:LYS:HG3	1:B:121:ILE:HA	1.84	0.59
1:C:95:VAL:HB	3:C:600:N8C:H6A	1.84	0.58
1:C:335:TRP:O	1:C:339:THR:HB	2.04	0.58
1:C:99:LEU:HD22	1:C:131:LEU:HD23	1.85	0.57
1:B:136:PRO:HA	1:B:168:LEU:HD12	1.86	0.57
1:A:42:PHE:O	1:A:45:THR:HB	2.05	0.56
1:A:271:THR:O	1:A:275:MET:HG3	2.06	0.56
1:C:361:TYR:O	1:C:365:VAL:HB	2.06	0.55
1:A:379:MET:HE1	1:B:401:PHE:CB	2.37	0.55
1:A:193:ASP:OD1	1:A:196:LYS:HG3	2.06	0.55
1:A:379:MET:HE2	2:B:500:FAD:H3'	1.90	0.53
1:C:108:ASP:O	1:C:110:PRO:HD3	2.08	0.53
1:B:401:PHE:C	1:B:401:PHE:CD2	2.81	0.53
1:A:141:ASN:ND2	2:A:500:FAD:H61A	2.06	0.53
1:C:170:PRO:HA	2:C:500:FAD:C4	2.38	0.53
1:A:379:MET:SD	2:B:500:FAD:HM81	2.49	0.53
1:A:4:PHE:CD1	1:C:339:THR:HG21	2.37	0.52
1:B:95:VAL:CG1	3:B:600:N8C:H5A	2.39	0.52
1:D:183:LEU:HD11	1:D:212:LEU:HG	1.91	0.52
1:C:141:ASN:ND2	2:C:500:FAD:H61A	2.07	0.52
1:B:171:SER:HA	1:B:241:SER:O	2.09	0.51
1:A:276:SER:HB2	3:A:600:N8C:H6A	1.92	0.51
1:B:314:GLN:NE2	1:C:315:SER:H	2.08	0.51
1:B:152:THR:HA	1:B:165:GLY:HA3	1.93	0.51
1:D:296:LEU:O	1:D:300:LYS:HG3	2.11	0.51
1:C:21:ALA:HA	1:C:25:LEU:HB2	1.93	0.51
1:A:38:GLN:HE22	1:A:238:ILE:HA	1.77	0.50
1:B:2:VAL:HG11	1:D:74:VAL:HG11	1.94	0.50
1:B:95:VAL:HG13	3:B:600:N8C:H7A	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:HB3	1:B:365:VAL:HG13	1.93	0.50
1:D:255:GLU:HG2	5:D:715:HOH:O	2.11	0.50
1:D:199:ASP:HB3	1:D:202:VAL:CG1	2.42	0.49
1:B:10:GLN:HG3	1:B:75:HIS:CE1	2.46	0.49
1:A:99:LEU:HD12	1:A:102:MET:CE	2.42	0.49
1:A:35:GLN:HB3	1:A:40:SER:HB2	1.94	0.49
1:D:171:SER:HA	1:D:241:SER:O	2.11	0.49
1:B:314:GLN:HB2	1:C:314:GLN:HB2	1.95	0.49
1:A:183:LEU:HD11	1:A:212:LEU:HG	1.94	0.49
1:D:21:ALA:HA	1:D:25:LEU:HB2	1.94	0.48
1:A:229:LEU:HD11	1:A:246:ARG:HB2	1.95	0.48
1:C:397:CYS:HB2	1:D:382:TYR:CZ	2.48	0.48
1:B:402:ASN:HA	3:B:600:N8C:O2	2.13	0.48
1:B:168:LEU:C	1:B:170:PRO:HD3	2.34	0.48
1:D:110:PRO:HA	1:D:113:GLN:HE21	1.80	0.47
1:B:95:VAL:HG13	3:B:600:N8C:C5	2.44	0.47
1:A:379:MET:CE	2:B:500:FAD:H3'	2.44	0.47
1:D:14:ARG:O	1:D:18:GLN:HG3	2.14	0.47
1:D:401:PHE:C	1:D:401:PHE:CD2	2.88	0.47
1:A:304:ARG:HD2	2:B:500:FAD:H51A	1.97	0.47
2:C:500:FAD:O2P	2:C:500:FAD:H52A	2.15	0.47
1:D:168:LEU:C	1:D:170:PRO:HD3	2.36	0.46
1:D:199:ASP:HB3	1:D:202:VAL:HG12	1.97	0.46
1:B:62:VAL:HB	1:B:68:GLY:HA3	1.97	0.46
1:A:10:GLN:HG3	1:A:75:HIS:CE1	2.51	0.46
1:D:206:THR:O	1:D:262:GLY:HA2	2.15	0.46
1:D:136:PRO:HA	1:D:168:LEU:HD12	1.98	0.45
2:D:500:FAD:H52A	2:D:500:FAD:O2P	2.15	0.45
1:C:375:LYS:HB3	1:D:406:ILE:HD11	1.97	0.45
1:A:379:MET:HE3	2:B:500:FAD:C2'	2.46	0.45
1:C:401:PHE:CD2	1:C:401:PHE:C	2.88	0.45
1:A:129:ALA:HA	1:A:183:LEU:O	2.16	0.45
1:D:73:LEU:HB3	1:D:338:VAL:HB	1.99	0.45
1:A:304:ARG:CD	2:B:500:FAD:H51A	2.47	0.45
1:D:62:VAL:O	1:D:68:GLY:HA3	2.17	0.45
1:A:134:SER:HB2	1:A:168:LEU:O	2.16	0.45
2:A:500:FAD:HM81	1:B:379:MET:CE	2.47	0.44
3:B:600:N8C:H1A	3:B:600:N8C:H4A	1.65	0.44
1:A:253:PRO:HB2	1:A:255:GLU:HG2	1.98	0.44
1:C:193:ASP:CB	1:C:196:LYS:HD2	2.47	0.44
1:D:58:ILE:N	1:D:58:ILE:HD12	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ALA:HA	1:C:183:LEU:O	2.18	0.44
1:B:361:TYR:O	1:B:365:VAL:HB	2.17	0.44
1:B:129:ALA:HA	1:B:183:LEU:O	2.18	0.44
1:B:28:ALA:HA	1:B:48:PHE:CZ	2.53	0.44
2:C:500:FAD:HM81	1:D:379:MET:CE	2.48	0.43
1:A:379:MET:HE2	2:B:500:FAD:C3'	2.48	0.43
1:C:183:LEU:HD11	1:C:212:LEU:HG	1.98	0.43
1:D:95:VAL:HB	3:D:600:N8C:H6A	2.01	0.43
1:D:361:TYR:O	1:D:365:VAL:HB	2.18	0.43
1:A:168:LEU:O	1:A:169:TRP:HB2	2.19	0.43
1:D:61:GLN:HE21	1:D:98:ALA:HB2	1.83	0.43
1:B:140:ALA:HA	1:B:408:LEU:HD21	2.01	0.42
1:B:130:SER:O	1:B:184:ALA:HA	2.19	0.42
1:D:402:ASN:HA	3:D:600:N8C:O1	2.20	0.42
1:B:237:HIS:O	1:B:240:THR:HG22	2.19	0.42
1:B:50:ARG:HH21	1:B:53:VAL:HB	1.83	0.42
1:B:352:LEU:O	1:B:356:MET:HG2	2.20	0.42
1:D:43:GLN:HE21	1:D:43:GLN:HB2	1.68	0.42
1:C:276:SER:HB2	3:C:600:N8C:H5	2.02	0.41
1:B:222:LYS:HB3	1:B:222:LYS:HE2	1.83	0.41
1:B:407:GLY:O	1:B:411:ARG:CG	2.67	0.41
1:D:62:VAL:HB	1:D:68:GLY:HA3	2.03	0.41
1:A:193:ASP:HA	1:A:194:PRO:HD2	1.86	0.41
1:A:361:TYR:O	1:A:365:VAL:HB	2.21	0.41
1:B:156:LYS:HD2	1:B:160:GLU:O	2.20	0.41
1:A:410:ARG:HH21	1:C:318:ASP:HA	1.84	0.41
1:C:199:ASP:HA	1:C:200:PRO:HD2	1.93	0.41
1:B:169:TRP:N	1:B:170:PRO:CD	2.83	0.41
1:A:401:PHE:CE1	3:A:600:N8C:H2	2.56	0.41
1:A:379:MET:CE	2:B:500:FAD:C3'	2.99	0.41
1:D:317:ALA:O	1:D:321:ILE:HG13	2.21	0.41
1:A:235:ALA:HB2	1:B:389:PRO:HB3	2.03	0.40
1:D:237:HIS:O	1:D:240:THR:HG22	2.21	0.40
1:B:193:ASP:HA	1:B:194:PRO:HD2	1.91	0.40
1:A:379:MET:CE	1:B:401:PHE:CA	2.71	0.40
1:D:81:GLU:OE1	1:D:289:ARG:NH1	2.51	0.40
1:A:46:ARG:HB3	1:A:47:PRO:HD3	2.03	0.40
1:D:87:GLU:HA	1:D:88:PRO:HD3	1.88	0.40
1:C:352:LEU:O	1:C:356:MET:HG2	2.21	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	429/438 (98%)	421 (98%)	7 (2%)	1 (0%)	52	59
1	B	429/438 (98%)	418 (97%)	10 (2%)	1 (0%)	52	59
1	C	428/438 (98%)	419 (98%)	8 (2%)	1 (0%)	52	59
1	D	429/438 (98%)	422 (98%)	5 (1%)	2 (0%)	34	35
All	All	1715/1752 (98%)	1680 (98%)	30 (2%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TRP
1	B	169	TRP
1	C	169	TRP
1	D	169	TRP
1	D	403	GLY

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	354/363 (98%)	339 (96%)	15 (4%)	36	44
1	B	354/363 (98%)	340 (96%)	14 (4%)	38	47
1	C	354/363 (98%)	335 (95%)	19 (5%)	27	31
1	D	354/363 (98%)	341 (96%)	13 (4%)	41	50
All	All	1416/1452 (98%)	1355 (96%)	61 (4%)	35	43

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	45	THR
1	A	66	LEU
1	A	73	LEU
1	A	83	LEU
1	A	102	MET
1	A	171	SER
1	A	202	VAL
1	A	223	LYS
1	A	256	ASN
1	A	332	LEU
1	A	365	VAL
1	A	401	PHE
1	A	409	ARG
1	A	411	ARG
1	B	2	VAL
1	B	66	LEU
1	B	73	LEU
1	B	83	LEU
1	B	131	LEU
1	B	139	THR
1	B	168	LEU
1	B	202	VAL
1	B	227	GLN
1	B	312	GLU
1	B	332	LEU
1	B	365	VAL
1	B	401	PHE
1	B	411	ARG
1	C	2	VAL
1	C	25	LEU
1	C	34	THR
1	C	45	THR
1	C	73	LEU
1	C	83	LEU
1	C	99	LEU
1	C	112	LEU
1	C	114	GLU
1	C	118	LYS
1	C	131	LEU
1	C	160	GLU
1	C	202	VAL

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Mol	Chain	Res	Type
1	C	332	LEU
1	C	339	THR
1	C	349	LYS
1	C	365	VAL
1	C	401	PHE
1	C	411	ARG
1	D	2	VAL
1	D	25	LEU
1	D	83	LEU
1	D	131	LEU
1	D	168	LEU
1	D	171	SER
1	D	212	LEU
1	D	223	LYS
1	D	256	ASN
1	D	280	VAL
1	D	311	ILE
1	D	401	PHE
1	D	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	22	ASN
1	A	38	GLN
1	A	113	GLN
1	A	137	ASN
1	A	141	ASN
1	A	256	ASN
1	A	414	GLN
1	B	18	GLN
1	B	38	GLN
1	B	137	ASN
1	B	141	ASN
1	B	144	GLN
1	B	227	GLN
1	B	256	ASN
1	B	266	GLN
1	B	314	GLN
1	C	22	ASN
1	C	43	GLN

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Mol	Chain	Res	Type
1	C	113	GLN
1	C	137	ASN
1	C	141	ASN
1	C	198	GLN
1	C	256	ASN
1	C	266	GLN
1	C	357	GLN
1	C	402	ASN
1	D	18	GLN
1	D	43	GLN
1	D	113	GLN
1	D	137	ASN
1	D	141	ASN
1	D	144	GLN
1	D	198	GLN
1	D	227	GLN
1	D	256	ASN
1	D	266	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 ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	FAD	A	500	-	48,58,58	1.44	6 (12%)	54,89,89	2.18	9 (16%)
3	N8C	A	600	-	8,10,10	0.42	0	7,10,10	0.32	0
4	GOL	A	700	-	5,5,5	0.44	0	5,5,5	0.59	0
2	FAD	B	500	-	48,58,58	1.43	6 (12%)	54,89,89	2.14	7 (12%)
3	N8C	B	600	-	8,10,10	0.42	0	7,10,10	0.64	0
4	GOL	B	700	-	5,5,5	0.35	0	5,5,5	0.43	0
2	FAD	C	500	-	48,58,58	1.44	5 (10%)	54,89,89	2.45	8 (14%)
3	N8C	C	600	-	8,10,10	0.35	0	7,10,10	0.60	0
4	GOL	C	700	-	5,5,5	0.28	0	5,5,5	0.36	0
2	FAD	D	500	-	48,58,58	1.46	6 (12%)	54,89,89	2.04	7 (12%)
3	N8C	D	600	-	8,10,10	0.33	0	7,10,10	0.48	0
4	GOL	D	700	-	5,5,5	0.26	0	5,5,5	0.53	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	500	-	-	0/30/50/50	0/6/6/6
3	N8C	A	600	-	-	0/7/8/8	0/0/0/0
4	GOL	A	700	-	-	0/4/4/4	0/0/0/0
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
3	N8C	B	600	-	-	0/7/8/8	0/0/0/0
4	GOL	B	700	-	-	0/4/4/4	0/0/0/0
2	FAD	C	500	-	-	0/30/50/50	0/6/6/6
3	N8C	C	600	-	-	0/7/8/8	0/0/0/0
4	GOL	C	700	-	-	0/4/4/4	0/0/0/0
2	FAD	D	500	-	-	0/30/50/50	0/6/6/6
3	N8C	D	600	-	-	0/7/8/8	0/0/0/0
4	GOL	D	700	-	-	0/4/4/4	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C10-N1	2.18	1.39	1.35
2	B	500	FAD	C2A-N3A	2.30	1.36	1.32
2	A	500	FAD	C2A-N1A	2.33	1.38	1.33
2	D	500	FAD	C5X-N5	2.34	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C4-N3	2.37	1.37	1.33
2	A	500	FAD	C5X-N5	2.48	1.39	1.35
2	B	500	FAD	C5X-N5	2.56	1.39	1.35
2	D	500	FAD	C2A-N1A	2.61	1.38	1.33
2	C	500	FAD	C10-N1	2.74	1.40	1.35
2	D	500	FAD	C4-N3	2.90	1.38	1.33
2	D	500	FAD	C2A-N3A	3.14	1.37	1.32
2	B	500	FAD	C4-N3	3.15	1.38	1.33
2	D	500	FAD	C4X-N5	3.34	1.38	1.33
2	C	500	FAD	C2A-N3A	3.36	1.38	1.32
2	C	500	FAD	C4X-N5	3.49	1.38	1.33
2	A	500	FAD	C2A-N3A	3.88	1.39	1.32
2	A	500	FAD	C4X-N5	3.88	1.39	1.33
2	A	500	FAD	C4-N3	3.94	1.40	1.33
2	B	500	FAD	C4X-N5	4.26	1.40	1.33
2	A	500	FAD	C1'-N10	4.39	1.53	1.48
2	B	500	FAD	C1'-N10	4.79	1.53	1.48
2	C	500	FAD	C1'-N10	5.63	1.54	1.48
2	D	500	FAD	C1'-N10	6.23	1.55	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	N3A-C2A-N1A	-14.19	118.03	128.89
2	A	500	FAD	N3A-C2A-N1A	-12.56	119.27	128.89
2	B	500	FAD	N3A-C2A-N1A	-11.96	119.73	128.89
2	D	500	FAD	N3A-C2A-N1A	-11.18	120.33	128.89
2	D	500	FAD	C4X-C4-N3	-3.59	118.68	123.59
2	C	500	FAD	C4X-C4-N3	-3.52	118.78	123.59
2	B	500	FAD	C4X-C4-N3	-3.13	119.31	123.59
2	A	500	FAD	C4X-C4-N3	-3.01	119.48	123.59
2	C	500	FAD	C2B-C1B-N9A	-2.60	110.32	114.29
2	A	500	FAD	C4A-C5A-N7A	-2.44	107.23	109.48
2	D	500	FAD	P-O3P-PA	-2.23	126.47	132.73
2	A	500	FAD	C2B-C1B-N9A	-2.22	110.91	114.29
2	A	500	FAD	O4'-C4'-C5'	-2.14	105.54	110.19
2	B	500	FAD	P-O3P-PA	-2.08	126.90	132.73
2	D	500	FAD	O2A-PA-O3P	2.12	114.73	105.09
2	A	500	FAD	C4X-N5-C5X	2.15	119.23	116.76
2	C	500	FAD	C4-C4X-C10	2.33	121.43	119.94
2	C	500	FAD	C6-C5X-C9A	2.34	122.06	118.98
2	B	500	FAD	O3P-P-O5'	2.38	109.24	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	FAD	C1'-N10-C9A	2.49	121.66	118.86
2	A	500	FAD	O3P-PA-O5B	2.49	109.55	102.94
2	D	500	FAD	C5X-C9A-N10	2.74	119.70	117.62
2	C	500	FAD	C5X-C9A-N10	3.16	120.02	117.62
2	B	500	FAD	C4X-N5-C5X	3.21	120.46	116.76
2	A	500	FAD	C5X-C9A-N10	3.31	120.13	117.62
2	D	500	FAD	C4X-N5-C5X	3.60	120.90	116.76
2	C	500	FAD	C4X-N5-C5X	3.61	120.92	116.76
2	A	500	FAD	C4-N3-C2	4.26	118.93	115.25
2	B	500	FAD	C4-N3-C2	5.29	119.82	115.25
2	D	500	FAD	C4-N3-C2	5.46	119.97	115.25
2	C	500	FAD	C4-N3-C2	6.16	120.57	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	3	0
3	A	600	N8C	2	0
2	B	500	FAD	11	0
3	B	600	N8C	7	0
2	C	500	FAD	5	0
3	C	600	N8C	2	0
2	D	500	FAD	3	0
3	D	600	N8C	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	431/438 (98%)	-0.13	7 (1%)	74	73	29, 42, 55, 65	0
1	B	431/438 (98%)	0.12	21 (4%)	33	33	30, 47, 62, 72	1 (0%)
1	C	430/438 (98%)	-0.31	2 (0%)	91	91	27, 38, 54, 66	1 (0%)
1	D	431/438 (98%)	-0.28	3 (0%)	89	88	29, 38, 53, 60	2 (0%)
All	All	1723/1752 (98%)	-0.15	33 (1%)	70	68	27, 41, 57, 72	4 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	VAL	3.9
1	A	195	SER	3.8
1	B	196	LYS	3.7
1	B	367	VAL	3.3
1	A	224	ASP	3.3
1	B	224	ASP	3.3
1	B	36	LYS	3.3
1	A	367	VAL	3.2
1	B	195	SER	3.2
1	A	371	ILE	3.0
1	D	195	SER	2.9
1	D	197	PRO	2.8
1	B	202	VAL	2.7
1	D	196	LYS	2.6
1	B	194	PRO	2.6
1	C	201	ASN	2.6
1	B	223	LYS	2.5
1	B	371	ILE	2.5
1	C	50	ARG	2.5
1	B	363	THR	2.4
1	A	365	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	395	VAL	2.4
1	B	178	TYR	2.3
1	A	223	LYS	2.3
1	B	392	LEU	2.3
1	B	203	ASP	2.3
1	B	201	ASN	2.3
1	B	229	LEU	2.3
1	B	366	ALA	2.2
1	B	370	VAL	2.2
1	B	50	ARG	2.1
1	A	36	LYS	2.0
1	B	360	ILE	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	N8C	A	600	11/11	0.91	0.22	5.16	59,60,60,61	0
3	N8C	C	600	11/11	0.87	0.21	3.47	62,63,64,64	0
3	N8C	D	600	11/11	0.94	0.16	2.18	54,55,58,58	0
3	N8C	B	600	11/11	0.91	0.18	1.44	59,60,61,62	0
4	GOL	B	700	6/6	0.97	0.14	1.25	50,51,52,52	0
4	GOL	A	700	6/6	0.94	0.11	0.05	40,43,44,45	0
2	FAD	C	500	53/53	0.97	0.12	-0.20	29,32,36,37	0
2	FAD	B	500	53/53	0.96	0.10	-0.40	30,36,42,42	0
4	GOL	D	700	6/6	0.97	0.09	-0.40	38,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	D	500	53/53	0.97	0.09	-0.45	28,32,37,37	0
2	FAD	A	500	53/53	0.97	0.11	-0.67	29,34,36,37	0
4	GOL	C	700	6/6	0.98	0.10	-0.93	41,41,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.