Full wwPDB X-ray Structure Validation Report (i)

Mar 31, 2016 – 07:58 PM EDT

PDB ID	:	4CCQ
Title	:	Crystal structure of the thioredoxin reductase from Entamoeba histolytica with NADP
Authors	:	Parsonage, D.; Kells, P.M.; Hirata, K.; Debnath, A.; Poole, L.B.; McKerrow, J.H.; Reed, S.L.; Podust, L.M.
Deposited on	:	2013-10-24
Resolution	:	1.50 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:

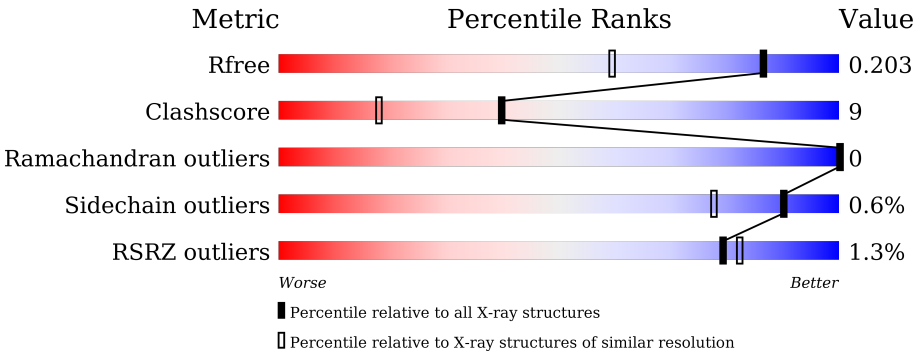
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	314	87% 12%
1	B	314	85% 13%

2 Entry composition

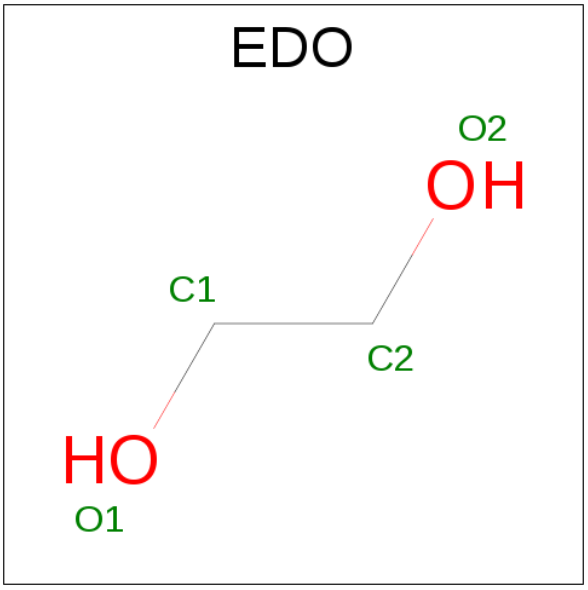
There are 6 unique types of molecules in this entry. The entry contains 6002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THIOREDOXIN REDUCTASE.

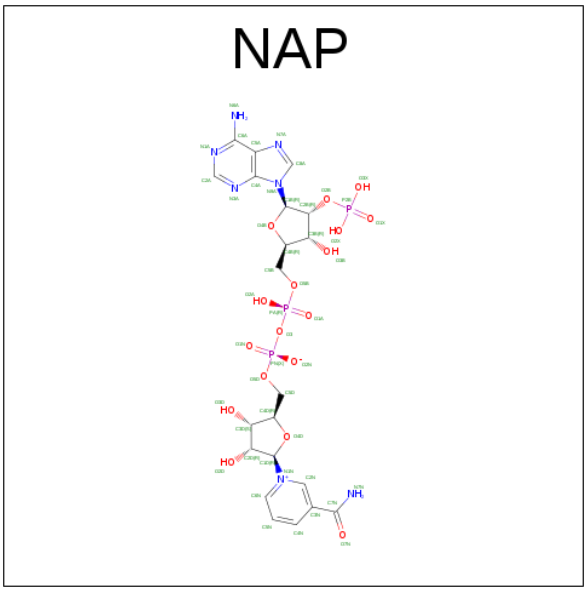
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	10	0
			2422	1529	410	465	18			
1	B	312	Total	C	N	O	S	0	19	0
			2506	1574	435	477	20			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



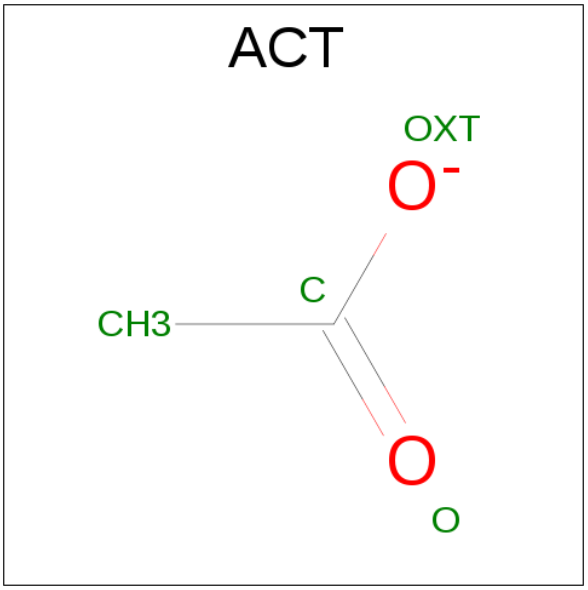
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

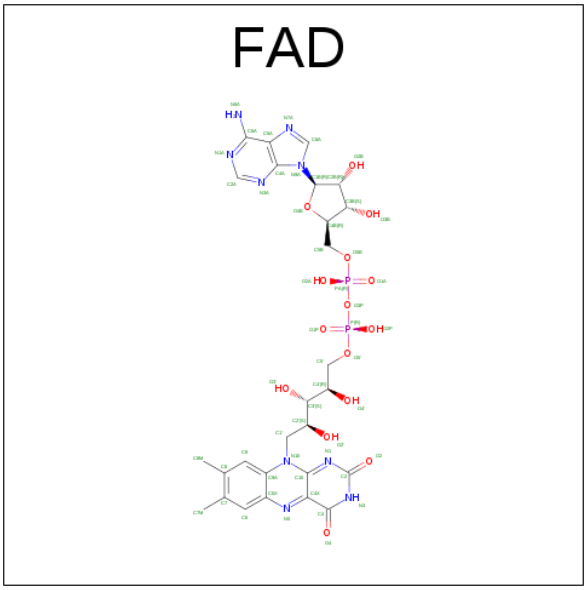
- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

$C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is water.

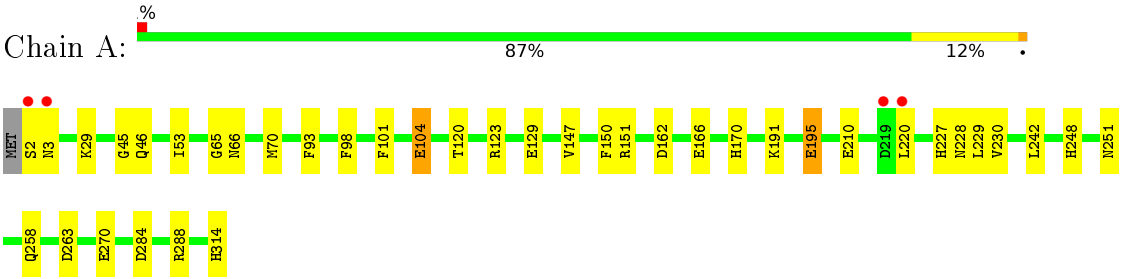
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	454	Total	O	0	0
			454	454		
6	B	410	Total	O	0	0
			410	410		

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.

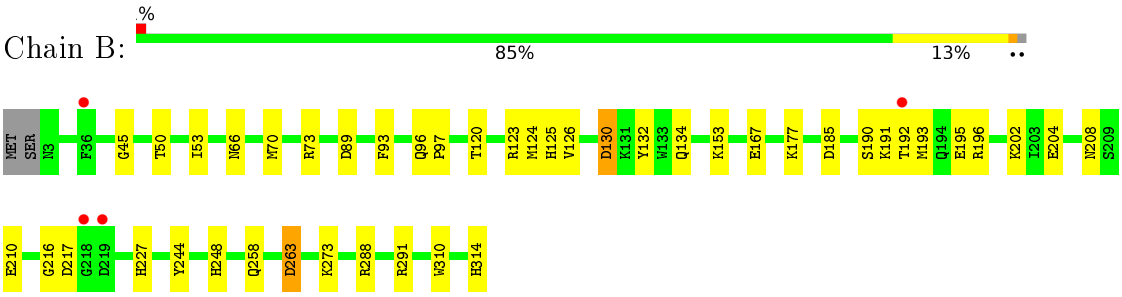
- Molecule 1: THIOREDOXIN REDUCTASE

Chain A:



- Molecule 1: THIOREDOXIN REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.76Å 92.22Å 103.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.52 – 1.50 40.67 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (103.52-1.50) 95.5 (40.67-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.172 , 0.207 0.168 , 0.203	Depositor DCC
R_{free} test set	4857 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 96720 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6002	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAP, EDO, FAD, ACT

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	1.25	5/2468 (0.2%)	1.11	6/3341 (0.2%)
1	B	1.17	1/2552 (0.0%)	1.16	8/3450 (0.2%)
All	All	1.21	6/5020 (0.1%)	1.14	14/6791 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLU	CD-OE2	-6.03	1.19	1.25
1	A	98	PHE	CD2-CE2	5.26	1.49	1.39
1	B	202	LYS	CE-NZ	5.26	1.62	1.49
1	A	104	GLU	CB-CG	-5.24	1.42	1.52
1	A	101	PHE	CE1-CZ	5.18	1.47	1.37
1	A	288	ARG	CG-CD	5.13	1.64	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	263[A]	ASP	CB-CG-OD2	13.93	130.83	118.30
1	B	263[B]	ASP	CB-CG-OD2	13.93	130.83	118.30
1	B	89[A]	ASP	CB-CG-OD1	11.76	128.89	118.30
1	B	89[B]	ASP	CB-CG-OD1	11.76	128.89	118.30
1	B	130	ASP	CB-CG-OD1	6.88	124.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	3	ASN	N-CA-C	-6.67	92.99	111.00
1	A	284	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	89[A]	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	89[B]	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	151	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	229[A]	LEU	CA-CB-CG	-5.07	103.63	115.30
1	A	229[B]	LEU	CA-CB-CG	-5.07	103.63	115.30
1	A	162	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	SER	Peptide

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	2422	0	2376	23	0
1	B	2506	0	2472	66	1
2	A	4	0	6	0	0
2	B	8	0	12	2	0
3	A	48	0	25	1	0
3	B	40	0	19	4	0
4	A	4	0	3	1	0
5	A	53	0	31	2	0
5	B	53	0	31	1	0
6	A	454	0	0	10	5
6	B	410	0	0	17	6
All	All	6002	0	4975	89	7

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 9.

All (89) 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:96[B]:GLN:NE2	1:B:97:PRO:HA	1.25	1.39
1:A:314:HIS:C	6:A:2221:HOH:O	1.92	1.05
1:B:193[A]:MET:HE3	1:B:196[A]:ARG:NH1	1.72	1.04
1:B:96[B]:GLN:NE2	1:B:97:PRO:CA	2.20	1.04
1:B:96[B]:GLN:HE21	1:B:97:PRO:CA	1.70	1.02
1:A:220:LEU:HB2	6:A:2334:HOH:O	1.59	0.99
1:B:291[B]:ARG:NH2	3:B:1315:NAP:O2N	1.98	0.95
1:B:124[A]:MET:HE3	1:B:244:TYR:CE1	2.03	0.93
1:B:193[A]:MET:CE	1:B:196[A]:ARG:NH1	2.31	0.92
1:B:96[B]:GLN:HE22	1:B:97:PRO:HA	1.29	0.87
1:B:248:HIS:ND1	1:B:291[B]:ARG:NE	2.22	0.87
1:B:134:GLN:HG3	6:B:2197:HOH:O	1.73	0.86
1:B:124[A]:MET:HE3	1:B:244:TYR:HE1	1.40	0.83
1:B:248:HIS:CE1	1:B:291[B]:ARG:HE	1.99	0.79
1:B:93:PHE:H	1:B:258:GLN:HE21	1.34	0.76
1:B:120[A]:THR:HG22	6:B:2050:HOH:O	1.85	0.74
1:B:96[B]:GLN:HE21	1:B:97:PRO:HA	0.92	0.74
1:B:193[A]:MET:HE3	1:B:196[A]:ARG:HH11	1.52	0.73
1:B:248:HIS:CE1	1:B:291[B]:ARG:NE	2.56	0.73
1:B:193[A]:MET:CE	1:B:196[A]:ARG:HH11	1.99	0.73
1:B:210:GLU:OE2	1:B:227:HIS:HD2	1.72	0.71
1:B:120[A]:THR:CG2	6:B:2050:HOH:O	2.38	0.71
1:A:120:THR:HB	1:A:251:ASN:HD21	1.55	0.71
1:B:93:PHE:H	1:B:258:GLN:NE2	1.89	0.69
1:B:273:LYS:HE3	6:B:2391:HOH:O	1.92	0.68
1:B:124[A]:MET:CE	1:B:244:TYR:CE1	2.78	0.67
1:B:248:HIS:ND1	1:B:291[B]:ARG:CZ	2.58	0.66
1:B:288[B]:ARG:NH2	6:B:2377:HOH:O	2.29	0.65
1:A:93:PHE:H	1:A:258:GLN:NE2	1.93	0.65
1:B:96[B]:GLN:HE21	1:B:96[B]:GLN:HA	1.62	0.63
1:A:93:PHE:H	1:A:258:GLN:HE21	1.45	0.62
1:A:210:GLU:OE2	1:A:227:HIS:HD2	1.82	0.61
1:B:263[A]:ASP:OD1	6:B:2347:HOH:O	2.16	0.61
1:B:124[A]:MET:CE	1:B:244:TYR:HE1	2.12	0.60
1:B:291[B]:ARG:HD2	6:B:2327:HOH:O	2.00	0.60
1:A:248:HIS:HD2	6:A:2361:HOH:O	1.85	0.58
1:B:70[B]:MET:CE	6:B:2104:HOH:O	2.51	0.58
1:B:50:THR:HG21	1:B:53:ILE:HD11	1.86	0.58
1:A:147:VAL:HG22	1:A:150:PHE:CD2	2.40	0.57
1:B:167[B]:GLU:OE2	6:B:2200:HOH:O	2.17	0.56
1:A:66:ASN:O	1:A:70[A]:MET:HG3	2.05	0.56
1:B:96[B]:GLN:HE21	1:B:96[B]:GLN:CA	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HG2	6:A:2152:HOH:O	2.06	0.55
1:B:310:TRP:O	1:B:314:HIS:HD2	1.89	0.55
1:A:53:ILE:HD11	1:A:65:GLY:HA2	1.90	0.54
1:B:248:HIS:CE1	1:B:291[B]:ARG:HH21	2.25	0.53
1:B:227:HIS:HE1	6:B:2306:HOH:O	1.91	0.53
1:B:193[A]:MET:HE3	1:B:196[A]:ARG:HH12	1.65	0.53
1:B:185:ASP:HB3	1:B:208:ASN:HD21	1.74	0.53
1:B:192:THR:O	1:B:196[B]:ARG:HG3	2.09	0.52
1:A:170:HIS:HE1	6:A:2251:HOH:O	1.93	0.52
1:B:248:HIS:CE1	1:B:291[B]:ARG:NH2	2.78	0.52
1:A:46:GLN:HE21	5:A:1318:FAD:HM81	1.75	0.50
1:B:177:LYS:HE2	1:B:204:GLU:OE1	2.10	0.50
1:B:45:GLY:HA2	5:B:1318:FAD:O3B	2.12	0.50
1:B:66:ASN:O	1:B:70[A]:MET:HG3	2.12	0.50
1:A:166:GLU:CG	3:A:1316:NAP:O7N	2.60	0.49
1:B:248:HIS:HE1	1:B:291[B]:ARG:HH21	1.60	0.49
1:B:70[B]:MET:HE1	6:B:2104:HOH:O	2.11	0.49
1:A:191:LYS:O	1:A:195[B]:GLU:HG3	2.12	0.49
1:A:270[A]:GLU:HG2	4:A:1317:ACT:H1	1.95	0.49
1:B:291[B]:ARG:HH22	3:B:1315:NAP:PN	2.36	0.48
1:A:45:GLY:HA2	5:A:1318:FAD:O3B	2.13	0.48
1:B:70[B]:MET:HE3	6:B:2104:HOH:O	2.14	0.47
1:B:153:LYS:HE2	6:B:2212:HOH:O	2.15	0.47
1:B:248:HIS:CE1	1:B:291[B]:ARG:CZ	2.98	0.47
1:B:191[B]:LYS:HG2	1:B:195:GLU:OE2	2.15	0.47
1:B:291[B]:ARG:NH2	3:B:1315:NAP:PN	2.87	0.47
1:B:288[B]:ARG:HD3	6:B:2378:HOH:O	2.15	0.46
1:B:288[B]:ARG:CZ	6:B:2377:HOH:O	2.64	0.46
1:A:228:ASN:OD1	1:A:230:VAL:HG22	2.15	0.45
1:B:96[A]:GLN:NE2	6:B:2155:HOH:O	2.48	0.45
6:A:2039:HOH:O	1:B:192:THR:HB	2.14	0.45
1:A:263:ASP:HB2	6:A:2384:HOH:O	2.17	0.45
1:B:190:SER:OG	1:B:193[B]:MET:HG2	2.17	0.45
1:B:288[B]:ARG:NH1	6:B:2377:HOH:O	2.49	0.45
1:B:132:TYR:CZ	1:B:216:GLY:HA3	2.52	0.45
1:A:120:THR:CG2	6:A:2227:HOH:O	2.64	0.44
1:B:123:ARG:NH2	1:B:130:ASP:OD1	2.51	0.43
1:B:288[A]:ARG:O	1:B:291[A]:ARG:CZ	2.68	0.42
1:A:29:LYS:HE3	6:A:2040:HOH:O	2.18	0.42
1:B:193[A]:MET:HE1	1:B:196[A]:ARG:NH1	2.25	0.42
1:B:70[B]:MET:HE3	1:B:73:ARG:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HD2	2:B:1316:EDO:H11	2.02	0.42
1:A:53:ILE:CD1	1:A:65:GLY:HA2	2.49	0.41
1:B:124[A]:MET:HG2	1:B:126:VAL:HG13	2.03	0.41
1:A:120:THR:HG23	6:A:2227:HOH:O	2.20	0.40
1:B:291[A]:ARG:NH2	3:B:1315:NAP:H52N	2.36	0.40
1:B:70[A]:MET:HA	2:B:1316:EDO:H22	2.02	0.40

All (7) 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)
6:B:2034:HOH:O	6:B:2219:HOH:O[4_555]	1.31	0.89
6:A:2155:HOH:O	6:B:2101:HOH:O[3_544]	1.94	0.26
1:B:125:HIS:NE2	6:A:2384:HOH:O[3_554]	2.09	0.11
6:A:2384:HOH:O	6:B:2181:HOH:O[3_544]	2.11	0.09
6:B:2293:HOH:O	6:B:2403:HOH:O[3_554]	2.13	0.07
6:A:2235:HOH:O	6:B:2377:HOH:O[3_544]	2.18	0.02
6:A:2387:HOH:O	6:B:2330:HOH:O[3_544]	2.19	0.01

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	321/314 (102%)	313 (98%)	8 (2%)	0	100	100
1	B	329/314 (105%)	323 (98%)	6 (2%)	0	100	100
All	All	650/628 (104%)	636 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	256/251 (102%)	252 (98%)	4 (2%)	70 41
1	B	267/251 (106%)	267 (100%)	0	100 100
All	All	523/502 (104%)	519 (99%)	4 (1%)	90 70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	195[A]	GLU
1	A	195[B]	GLU
1	A	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	ASN
1	A	194	GLN
1	A	208	ASN
1	A	227	HIS
1	A	248	HIS
1	A	251	ASN
1	A	258	GLN
1	A	292	GLN
1	B	61	ASN
1	B	66	ASN
1	B	194	GLN
1	B	208	ASN
1	B	227	HIS
1	B	258	GLN
1	B	314	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	EDO	A	1315	-	3,3,3	0.68	0	2,2,2	1.09	0
3	NAP	A	1316	-	45,52,52	1.18	4 (8%)	55,80,80	1.38	8 (14%)
4	ACT	A	1317	-	0,3,3	0.00	-	0,3,3	0.00	-
5	FAD	A	1318	-	52,58,58	1.70	9 (17%)	52,89,89	1.98	10 (19%)
3	NAP	B	1315	-	37,43,52	1.19	2 (5%)	45,67,80	1.82	7 (15%)
2	EDO	B	1316	-	3,3,3	0.48	0	2,2,2	0.82	0
2	EDO	B	1317	-	3,3,3	0.84	0	2,2,2	0.14	0
5	FAD	B	1318	-	52,58,58	1.43	9 (17%)	52,89,89	2.11	10 (19%)

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	EDO	A	1315	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	A	1316	-	-	0/27/67/67	0/5/5/5
4	ACT	A	1317	-	-	0/0/0/0	0/0/0/0
5	FAD	A	1318	-	-	0/30/50/50	0/6/6/6
3	NAP	B	1315	-	-	0/23/59/67	0/4/4/5
2	EDO	B	1316	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1317	-	-	0/1/1/1	0/0/0/0
5	FAD	B	1318	-	-	0/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1318	FAD	C2-N1	-3.46	1.31	1.38
5	A	1318	FAD	P-O2P	-3.17	1.41	1.55
5	B	1318	FAD	P-O2P	-2.85	1.43	1.55
5	A	1318	FAD	PA-O2A	-2.57	1.44	1.55
5	B	1318	FAD	C4A-N3A	2.24	1.38	1.35
3	A	1316	NAP	C4N-C3N	2.29	1.43	1.39
3	A	1316	NAP	C2N-C3N	2.31	1.42	1.39
5	B	1318	FAD	C10-N1	2.33	1.39	1.35
5	B	1318	FAD	C2A-N3A	2.36	1.36	1.32
3	A	1316	NAP	C3N-C7N	2.39	1.54	1.50
5	A	1318	FAD	C2A-N3A	2.44	1.36	1.32
5	B	1318	FAD	C1'-N10	2.49	1.51	1.48
5	B	1318	FAD	C2A-N1A	2.65	1.39	1.33
3	B	1315	NAP	O4D-C1D	2.71	1.46	1.41
3	B	1315	NAP	C5A-C4A	2.79	1.46	1.40
5	A	1318	FAD	C5X-N5	3.00	1.40	1.35
5	A	1318	FAD	C10-N1	3.08	1.40	1.35
5	B	1318	FAD	C4-N3	3.20	1.38	1.33
5	B	1318	FAD	C5X-N5	3.22	1.40	1.35
3	A	1316	NAP	O4D-C1D	3.31	1.46	1.41
5	A	1318	FAD	C4-N3	3.53	1.39	1.33
5	A	1318	FAD	C1'-N10	3.99	1.52	1.48
5	B	1318	FAD	C4X-N5	4.44	1.40	1.33
5	A	1318	FAD	C4X-N5	4.88	1.40	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1315	NAP	N3A-C2A-N1A	-7.70	122.82	128.87
5	B	1318	FAD	N3A-C2A-N1A	-5.70	124.39	128.87
5	A	1318	FAD	C4X-C4-N3	-4.62	117.48	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1318	FAD	C4X-C4-N3	-4.49	117.66	123.52
5	A	1318	FAD	N3-C2-N1	-4.44	120.21	127.69
5	A	1318	FAD	C1B-N9A-C4A	-3.27	123.16	126.81
5	B	1318	FAD	O2'-C2'-C1'	-3.08	102.33	109.93
5	B	1318	FAD	N3-C2-N1	-3.00	122.63	127.69
5	A	1318	FAD	O4B-C4B-C3B	-2.91	99.27	105.16
3	A	1316	NAP	N3A-C2A-N1A	-2.83	126.65	128.87
5	A	1318	FAD	O2'-C2'-C1'	-2.48	103.81	109.93
3	A	1316	NAP	O5B-C5B-C4B	-2.40	100.45	109.09
5	B	1318	FAD	O3'-C3'-C4'	-2.34	102.66	108.73
3	B	1315	NAP	O2B-C2B-C1B	-2.21	101.44	110.12
5	A	1318	FAD	N3A-C2A-N1A	-2.21	127.14	128.87
5	B	1318	FAD	O2B-C2B-C1B	-2.15	104.90	111.61
3	A	1316	NAP	O7N-C7N-N7N	-2.10	119.59	122.58
5	B	1318	FAD	O3B-C3B-C4B	2.03	117.07	111.01
5	A	1318	FAD	C4-C4X-N5	2.05	121.19	118.70
3	B	1315	NAP	O2A-PA-O3	2.26	114.97	105.27
3	A	1316	NAP	O2A-PA-O3	2.31	115.15	105.27
3	B	1315	NAP	O2A-PA-O1A	2.36	124.86	112.56
3	A	1316	NAP	O2N-PN-O1N	2.41	125.12	112.56
3	B	1315	NAP	C2A-N1A-C6A	2.45	123.14	118.77
5	A	1318	FAD	C4X-N5-C5X	2.53	119.70	116.72
3	B	1315	NAP	O2N-PN-O5D	2.67	120.96	108.24
5	B	1318	FAD	C5X-C9A-N10	2.68	119.59	117.58
3	A	1316	NAP	O4D-C1D-N1N	2.98	111.32	108.10
3	A	1316	NAP	N6A-C6A-N1A	3.06	123.65	118.52
5	A	1318	FAD	C1'-N10-C9A	3.32	122.67	118.83
3	B	1315	NAP	N6A-C6A-N1A	3.70	124.72	118.52
3	A	1316	NAP	C4D-O4D-C1D	3.73	113.59	109.64
5	B	1318	FAD	C1'-N10-C9A	5.42	125.11	118.83
5	B	1318	FAD	C4-N3-C2	7.86	121.71	115.16
5	A	1318	FAD	C4-N3-C2	8.50	122.25	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1316	NAP	1	0
4	A	1317	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1318	FAD	2	0
3	B	1315	NAP	4	0
2	B	1316	EDO	2	0
5	B	1318	FAD	1	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	313/314 (99%)	-0.01	4 (1%)	79	82	9, 16, 28, 41	0
1	B	312/314 (99%)	0.01	4 (1%)	79	82	10, 16, 30, 38	0
All	All	625/628 (99%)	0.00	8 (1%)	79	82	9, 16, 30, 41	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.5
1	B	36	PHE	3.9
1	A	3	ASN	3.3
1	A	220	LEU	3.2
1	A	219	ASP	2.8
1	B	218	GLY	2.8
1	B	219[A]	ASP	2.5
1	B	192	THR	2.2

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

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	EDO	B	1316	4/4	0.91	0.13	1.31	32,36,37,43	0
2	EDO	B	1317	4/4	0.76	0.13	0.91	37,38,38,40	0
2	EDO	A	1315	4/4	0.92	0.11	0.84	24,24,24,25	0
5	FAD	B	1318	53/53	0.95	0.11	0.41	14,18,26,28	0
3	NAP	B	1315	40/48	0.93	0.10	0.04	14,20,52,52	0
4	ACT	A	1317	4/4	0.88	0.10	-0.08	47,48,48,48	0
3	NAP	A	1316	48/48	0.97	0.08	-0.27	11,18,50,58	0
5	FAD	A	1318	53/53	0.96	0.08	-0.81	10,14,21,22	0

6.5 Other polymers (i)

There are no such residues in this entry.