Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:35 AM GMT

PDB ID	:	2XLP
Title	:	JOINT-FUNCTIONS OF PROTEIN RESIDUES AND NADP(H) IN OXYGEN-ACTIVATION BY FLAVIN-CONTAINING MONOOXYGENASE: ASN78SER MUTANT
Authors	:	Orru, R.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2010-07-21
Resolution	:	2.80 Å(reported)

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

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

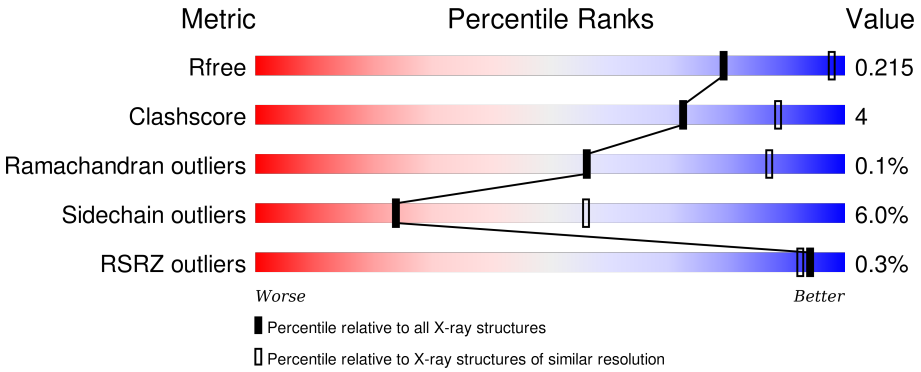
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	461	82% 12%
1	B	461	81% 14%
1	C	461	82% 13%
1	D	461	84% 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
4	EPE	A	1453	-	-	-	X
4	EPE	B	1452	-	-	-	X
4	EPE	C	1452	-	-	-	X
4	EPE	D	1453	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15209 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3658	2347	606	685	20			
1	B	445	Total	C	N	O	S	0	0	0
			3649	2341	604	684	20			
1	C	445	Total	C	N	O	S	0	0	0
			3649	2341	604	684	20			
1	D	446	Total	C	N	O	S	0	0	0
			3658	2347	606	685	20			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
A	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
A	3	MET	-	EXPRESSION TAG	UNP Q83XK4
A	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
A	5	SER	-	EXPRESSION TAG	UNP Q83XK4
A	78	SER	ASN	ENGINEERED MUTATION	UNP Q83XK4
A	158	ALA	GLU	CONFLICT	UNP Q83XK4
A	159	ALA	GLU	CONFLICT	UNP Q83XK4
B	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
B	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
B	3	MET	-	EXPRESSION TAG	UNP Q83XK4
B	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
B	5	SER	-	EXPRESSION TAG	UNP Q83XK4
B	78	SER	ASN	ENGINEERED MUTATION	UNP Q83XK4
B	158	ALA	GLU	CONFLICT	UNP Q83XK4
B	159	ALA	GLU	CONFLICT	UNP Q83XK4
C	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
C	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
C	3	MET	-	EXPRESSION TAG	UNP Q83XK4
C	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
C	5	SER	-	EXPRESSION TAG	UNP Q83XK4

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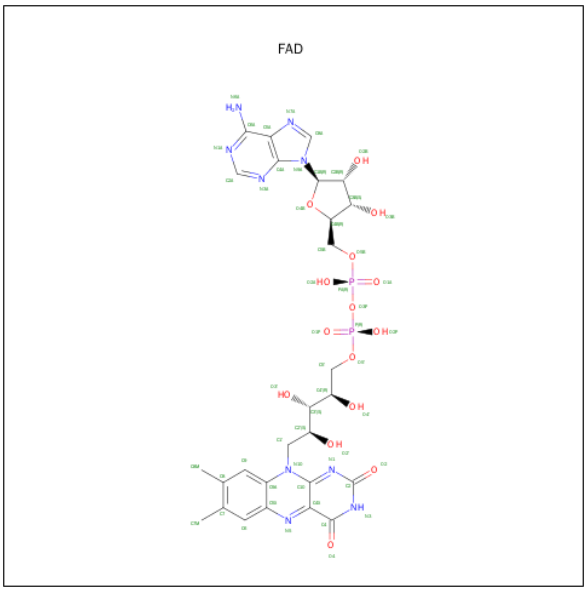
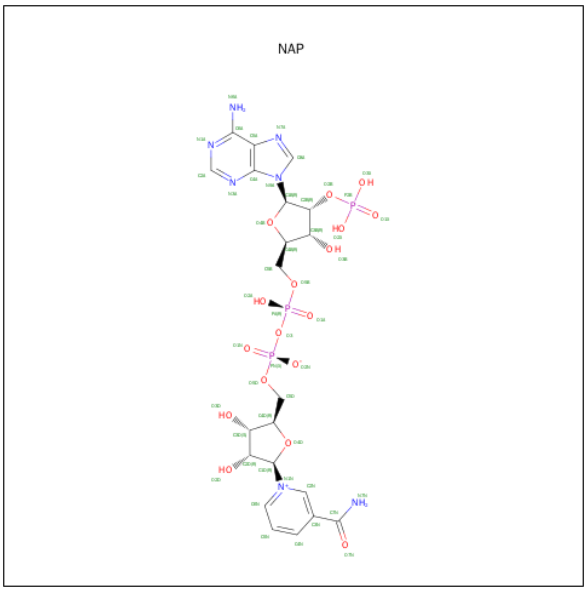
Chain	Residue	Modelled	Actual	Comment	Reference
C	78	SER	ASN	ENGINEERED MUTATION	UNP Q83XK4
C	158	ALA	GLU	CONFLICT	UNP Q83XK4
C	159	ALA	GLU	CONFLICT	UNP Q83XK4
D	1	GLY	-	EXPRESSION TAG	UNP Q83XK4
D	2	ALA	-	EXPRESSION TAG	UNP Q83XK4
D	3	MET	-	EXPRESSION TAG	UNP Q83XK4
D	4	GLY	-	EXPRESSION TAG	UNP Q83XK4
D	5	SER	-	EXPRESSION TAG	UNP Q83XK4
D	78	SER	ASN	ENGINEERED MUTATION	UNP Q83XK4
D	158	ALA	GLU	CONFLICT	UNP Q83XK4
D	159	ALA	GLU	CONFLICT	UNP Q83XK4

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



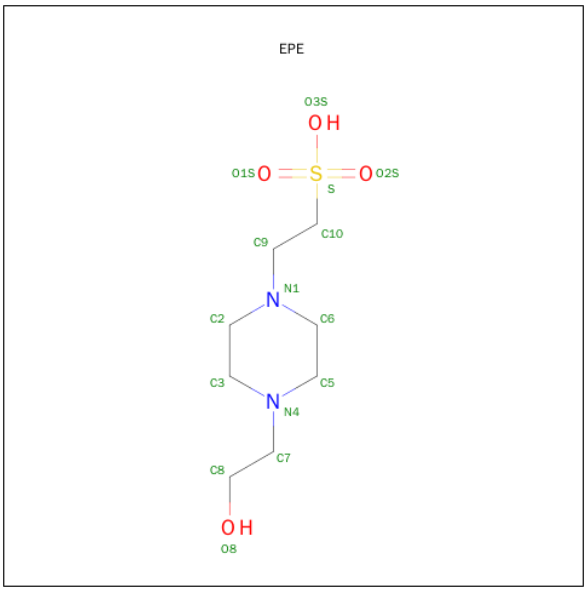
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



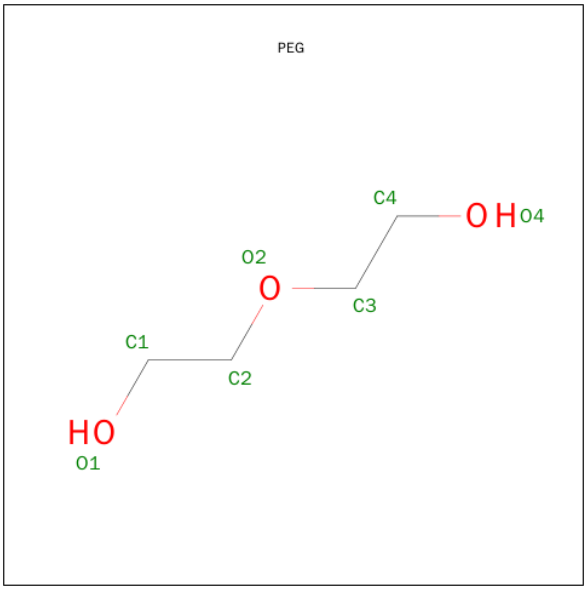
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	24	Total	O	0	0
			24	24		

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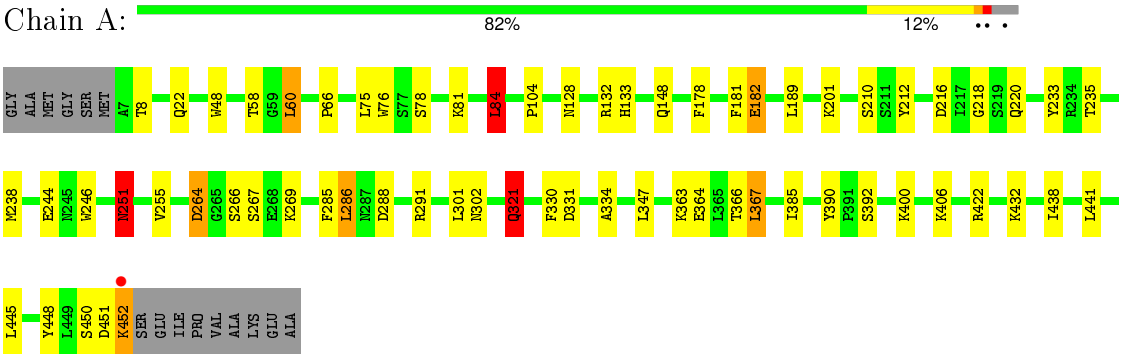
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	30	Total O 30 30	0	0
6	C	24	Total O 24 24	0	0
6	D	18	Total O 18 18	0	0

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.

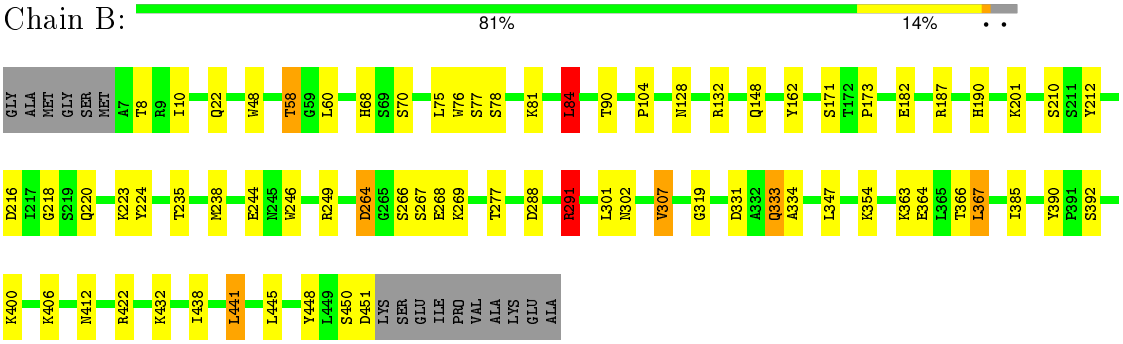
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain A:



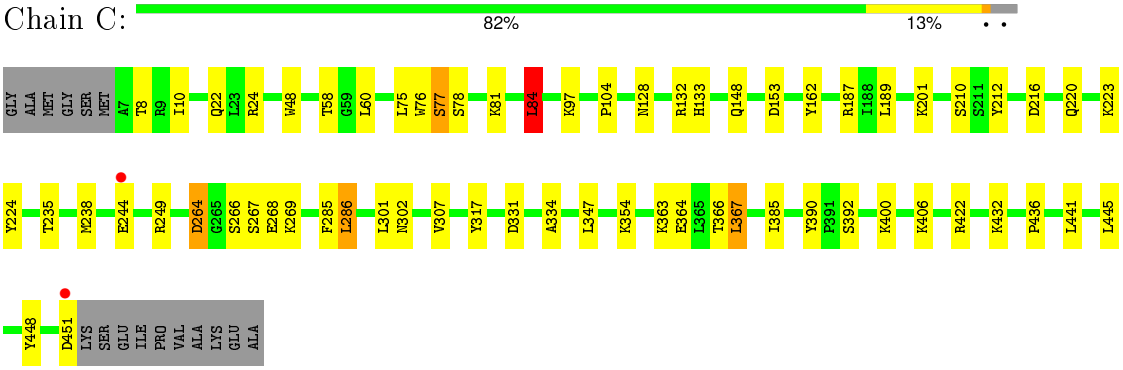
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain B:



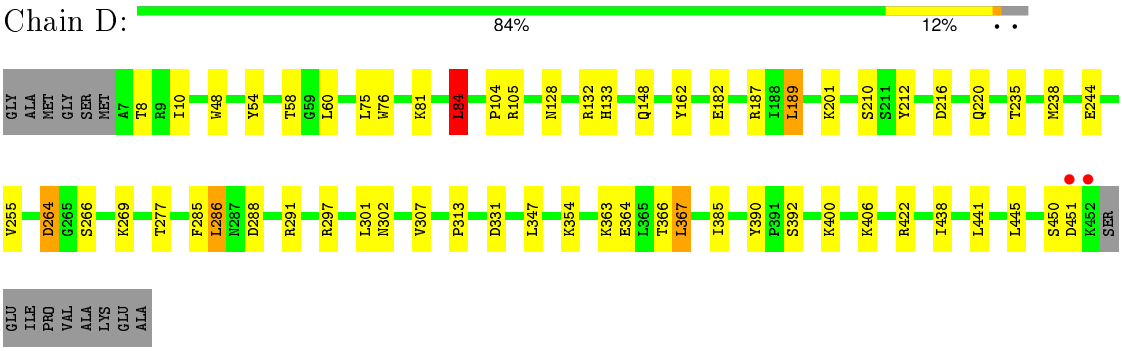
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain C:



• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	219.71Å 219.71Å 131.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.12 – 2.80 62.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (62.12-2.80) 99.6 (62.12-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0078	Depositor
R, R_{free}	0.193 , 0.214 0.194 , 0.215	Depositor DCC
R_{free} test set	4410 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.5	EDS
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 88333 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15209	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: PEG, NAP, EPE, 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	0.82	3/3772 (0.1%)	0.79	4/5121 (0.1%)
1	B	0.83	3/3763 (0.1%)	0.80	5/5110 (0.1%)
1	C	0.80	0/3763	0.79	4/5110 (0.1%)
1	D	0.81	1/3772 (0.0%)	0.78	3/5121 (0.1%)
All	All	0.81	7/15070 (0.0%)	0.79	16/20462 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	VAL	CB-CG2	-6.64	1.39	1.52
1	A	321	GLN	CD-NE2	-6.11	1.17	1.32
1	D	307	VAL	CB-CG1	-5.42	1.41	1.52
1	B	333	GLN	CD-OE1	-5.37	1.12	1.24
1	A	321	GLN	CD-OE1	-5.25	1.12	1.24
1	A	182	GLU	CB-CG	5.23	1.62	1.52
1	B	307	VAL	CB-CG1	-5.06	1.42	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	GLU	OE1-CD-OE2	-7.61	114.17	123.30
1	C	445	LEU	CA-CB-CG	6.81	130.97	115.30
1	B	445	LEU	CA-CB-CG	6.69	130.69	115.30
1	D	445	LEU	CA-CB-CG	6.69	130.68	115.30
1	C	84	LEU	CA-CB-CG	6.65	130.60	115.30
1	B	307	VAL	CB-CA-C	-6.64	98.78	111.40
1	A	84	LEU	CA-CB-CG	6.29	129.77	115.30
1	D	84	LEU	CA-CB-CG	6.26	129.70	115.30
1	B	84	LEU	CA-CB-CG	6.23	129.63	115.30
1	A	445	LEU	CA-CB-CG	6.02	129.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	249	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	251	ASN	CB-CA-C	5.69	121.78	110.40
1	C	24	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	291	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	D	297	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	C	249	ARG	NE-CZ-NH2	-5.09	117.75	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	3658	0	3449	35	0
1	B	3649	0	3436	39	1
1	C	3649	0	3436	27	1
1	D	3658	0	3449	24	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	48	0	25	2	0
3	B	48	0	25	2	0
3	C	48	0	25	2	0
3	D	48	0	25	2	0
4	A	15	0	17	0	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	15	0	17	1	0
5	A	7	0	10	1	0
5	B	21	0	30	0	0
5	D	7	0	10	0	0
6	A	24	0	0	0	0
6	B	30	0	0	1	0
6	C	24	0	0	1	0
6	D	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15209	0	14112	124	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (124) 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:321:GLN:HE21	1:A:321:GLN:N	1.52	1.07
1:C:264:ASP:HB3	1:C:266:SER:H	1.38	0.87
1:B:264:ASP:HB3	1:B:266:SER:H	1.40	0.85
1:A:264:ASP:HB3	1:A:266:SER:H	1.44	0.82
1:D:264:ASP:HB3	1:D:266:SER:H	1.44	0.82
1:A:321:GLN:HE21	1:A:321:GLN:H	1.25	0.79
1:C:285:PHE:CD1	1:C:286:LEU:HD13	2.23	0.73
1:A:285:PHE:CD1	1:A:286:LEU:HD13	2.24	0.72
1:A:363:LYS:HG2	5:A:1454:PEG:H41	1.72	0.71
1:A:321:GLN:N	1:A:321:GLN:NE2	2.35	0.70
1:A:321:GLN:H	1:A:321:GLN:NE2	1.90	0.68
1:D:285:PHE:CD1	1:D:286:LEU:HD13	2.29	0.67
1:A:452:LYS:HB2	1:A:452:LYS:NZ	2.14	0.63
1:B:216:ASP:O	1:B:220:GLN:HG2	1.99	0.63
1:D:363:LYS:O	1:D:366:THR:HB	1.99	0.62
1:B:22:GLN:OE1	1:B:22:GLN:HA	2.00	0.62
1:A:132:ARG:HH21	1:A:148:GLN:NE2	2.01	0.58
1:C:363:LYS:O	1:C:366:THR:HB	2.03	0.58
1:B:363:LYS:O	1:B:366:THR:HB	2.03	0.57
1:D:216:ASP:O	1:D:220:GLN:HG2	2.05	0.57
1:A:363:LYS:O	1:A:366:THR:HB	2.05	0.56
1:D:132:ARG:HH21	1:D:148:GLN:NE2	2.03	0.56
1:C:132:ARG:HH21	1:C:148:GLN:NE2	2.03	0.56
1:B:319:GLY:H	1:B:333:GLN:HE22	1.52	0.56
1:B:132:ARG:HH21	1:B:148:GLN:NE2	2.03	0.56
1:C:331:ASP:HB3	1:C:390:TYR:CE1	2.40	0.55
1:D:75:LEU:HD11	2:D:500:FAD:H6	1.87	0.55
1:C:364:GLU:HA	1:C:367:LEU:HD22	1.89	0.55
1:D:132:ARG:HH21	1:D:148:GLN:HE21	1.55	0.54
1:C:285:PHE:HD1	1:C:286:LEU:HD13	1.70	0.54
1:C:132:ARG:HH21	1:C:148:GLN:HE21	1.55	0.54
1:D:331:ASP:HB3	1:D:390:TYR:CE1	2.43	0.53
1:D:385:ILE:HD12	1:D:392:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:HB3	1:B:390:TYR:CE1	2.44	0.53
1:A:210:SER:HB2	1:A:238:MET:HG3	1.91	0.52
1:D:81:LYS:HA	1:D:84:LEU:HD22	1.92	0.52
1:A:364:GLU:HA	1:A:367:LEU:HD22	1.92	0.52
1:B:75:LEU:HD11	2:B:500:FAD:H6	1.91	0.51
1:B:132:ARG:HH21	1:B:148:GLN:HE21	1.58	0.51
1:B:212:TYR:CD2	3:B:501:NAP:H3D	2.45	0.51
1:C:81:LYS:HA	1:C:84:LEU:HD22	1.92	0.51
1:A:216:ASP:O	1:A:220:GLN:HG2	2.11	0.50
1:D:438:ILE:HG13	1:D:438:ILE:O	2.11	0.50
1:B:22:GLN:OE1	1:B:334:ALA:HB1	2.10	0.50
1:C:307:VAL:HG23	1:C:317:TYR:O	2.12	0.50
1:D:212:TYR:CD2	3:D:501:NAP:H3D	2.48	0.49
1:B:364:GLU:HA	1:B:367:LEU:HD22	1.94	0.49
1:D:187:ARG:HG2	1:D:189:LEU:HD22	1.94	0.49
1:A:212:TYR:CD2	3:A:501:NAP:H3D	2.48	0.49
1:A:81:LYS:HA	1:A:84:LEU:HD22	1.93	0.49
1:C:210:SER:HB2	1:C:238:MET:HG3	1.95	0.49
1:A:132:ARG:HH21	1:A:148:GLN:HE21	1.58	0.49
1:A:331:ASP:HB3	1:A:390:TYR:CE1	2.48	0.48
1:C:216:ASP:O	1:C:220:GLN:HG2	2.14	0.48
1:B:90:THR:HG23	6:B:2009:HOH:O	2.12	0.48
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.76	0.48
1:D:76:TRP:HA	1:D:104:PRO:HA	1.96	0.47
1:A:75:LEU:HD11	2:A:500:FAD:H6	1.96	0.47
1:A:385:ILE:HD12	1:A:392:SER:HA	1.95	0.47
1:A:233:TYR:O	1:A:251:ASN:HB3	2.13	0.47
1:D:288:ASP:OD1	1:D:291:ARG:NH1	2.46	0.47
1:C:76:TRP:O	1:C:77:SER:C	2.52	0.47
1:B:438:ILE:HG13	1:B:438:ILE:O	2.14	0.47
1:A:76:TRP:HA	1:A:104:PRO:HA	1.98	0.46
1:C:187:ARG:HG2	1:C:189:LEU:HD22	1.96	0.46
1:B:319:GLY:H	1:B:333:GLN:NE2	2.13	0.46
1:D:450:SER:OG	1:D:451:ASP:N	2.48	0.46
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.77	0.46
1:D:10:ILE:HD12	1:D:162:TYR:HB2	1.98	0.46
1:D:301:LEU:O	1:D:302:ASN:CB	2.63	0.45
1:D:182:GLU:N	1:D:182:GLU:OE1	2.42	0.45
1:B:81:LYS:HA	1:B:84:LEU:HD22	1.98	0.45
1:B:210:SER:HB2	1:B:238:MET:HG3	1.99	0.45
1:B:68:HIS:CE1	1:B:171:SER:OG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:O	1:C:302:ASN:CB	2.64	0.45
1:A:78:SER:HB3	3:A:501:NAP:C7N	2.47	0.45
1:C:385:ILE:HD12	1:C:392:SER:HA	1.98	0.45
1:B:385:ILE:HD12	1:B:392:SER:HA	1.98	0.45
1:D:364:GLU:HA	1:D:367:LEU:HD22	1.99	0.45
1:B:78:SER:HB3	3:B:501:NAP:C7N	2.48	0.44
1:C:75:LEU:HD11	2:C:500:FAD:H6	1.99	0.44
1:B:291:ARG:NH2	1:C:153:ASP:OD1	2.49	0.44
1:A:301:LEU:O	1:A:302:ASN:CB	2.65	0.44
1:B:450:SER:OG	1:B:451:ASP:N	2.49	0.44
1:C:104:PRO:HD3	1:C:448:TYR:CE1	2.52	0.44
1:B:10:ILE:HD12	1:B:162:TYR:HB2	2.00	0.44
1:C:22:GLN:HA	1:C:334:ALA:HB1	1.99	0.44
1:A:438:ILE:O	1:A:438:ILE:HG13	2.16	0.44
1:B:301:LEU:O	1:B:302:ASN:CB	2.65	0.44
1:B:223:LYS:HE2	1:B:224:TYR:CE1	2.53	0.44
1:C:267:SER:O	1:C:268:GLU:HB3	2.17	0.44
1:B:76:TRP:HA	1:B:104:PRO:HA	1.99	0.44
1:C:212:TYR:CD2	3:C:501:NAP:H3D	2.53	0.44
1:A:452:LYS:HB2	1:A:452:LYS:HZ3	1.83	0.43
1:B:288:ASP:OD1	1:B:291:ARG:NH1	2.48	0.43
1:A:266:SER:O	1:A:267:SER:HB3	2.19	0.43
1:A:60:LEU:HD12	1:A:66:PRO:HA	2.01	0.43
1:B:58:THR:HG23	6:C:2019:HOH:O	2.19	0.43
1:B:301:LEU:O	1:B:302:ASN:HB2	2.18	0.43
1:B:104:PRO:HD3	1:B:448:TYR:CE1	2.54	0.42
1:A:450:SER:OG	1:A:451:ASP:N	2.52	0.42
1:A:330:PHE:CZ	2:A:500:FAD:H5'2	2.55	0.42
1:D:210:SER:HB2	1:D:238:MET:HG3	2.01	0.42
1:B:187:ARG:HD2	1:C:187:ARG:NH1	2.35	0.42
1:A:288:ASP:OD1	1:A:291:ARG:NH1	2.51	0.42
1:B:76:TRP:O	1:B:77:SER:C	2.57	0.42
1:B:218:GLY:HA3	1:B:246:TRP:CH2	2.55	0.42
1:A:22:GLN:HA	1:A:334:ALA:HB1	2.02	0.42
1:B:267:SER:O	1:B:268:GLU:HB3	2.20	0.42
1:B:70:SER:HB2	2:B:500:FAD:HM82	2.01	0.42
1:B:182:GLU:OE1	1:B:182:GLU:N	2.41	0.41
1:A:218:GLY:HA3	1:A:246:TRP:CH2	2.55	0.41
1:C:76:TRP:HA	1:C:104:PRO:HA	2.02	0.41
1:B:173:PRO:HB3	1:B:190:HIS:CE1	2.55	0.41
1:B:68:HIS:CD2	2:B:500:FAD:H3B	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PRO:HD3	1:A:448:TYR:CE1	2.56	0.41
1:C:78:SER:HB3	3:C:501:NAP:C7N	2.51	0.41
1:A:178:PHE:HB2	1:A:181:PHE:CZ	2.55	0.41
1:C:223:LYS:HE2	1:C:224:TYR:CE1	2.56	0.41
1:D:277:THR:HA	3:D:501:NAP:O4B	2.21	0.40
1:C:10:ILE:HD12	1:C:162:TYR:HB2	2.03	0.40
1:B:223:LYS:HE3	1:B:441:LEU:HD12	2.03	0.40
1:D:54:TYR:HB2	1:D:105:ARG:CZ	2.52	0.40
4:D:1453:EPE:H101	4:D:1453:EPE:H61	1.66	0.40

All (1) 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:B:412:ASN:ND2	1:C:451:ASP:OD2[2_775]	2.13	0.07

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	444/461 (96%)	412 (93%)	32 (7%)	0	100	100
1	B	443/461 (96%)	411 (93%)	32 (7%)	0	100	100
1	C	443/461 (96%)	414 (94%)	28 (6%)	1 (0%)	52	84
1	D	444/461 (96%)	410 (92%)	33 (7%)	1 (0%)	52	84
All	All	1774/1844 (96%)	1647 (93%)	125 (7%)	2 (0%)	56	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	77	SER

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Mol	Chain	Res	Type
1	D	313	PRO

5.3.2 Protein sidechains

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	387/397 (98%)	361 (93%)	26 (7%)	20 50
1	B	386/397 (97%)	364 (94%)	22 (6%)	25 58
1	C	386/397 (97%)	363 (94%)	23 (6%)	24 56
1	D	387/397 (98%)	365 (94%)	22 (6%)	25 58
All	All	1546/1588 (97%)	1453 (94%)	93 (6%)	24 56

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	48	TRP
1	A	58	THR
1	A	60	LEU
1	A	84	LEU
1	A	128	ASN
1	A	133	HIS
1	A	182	GLU
1	A	189	LEU
1	A	201	LYS
1	A	235	THR
1	A	244	GLU
1	A	251	ASN
1	A	255	VAL
1	A	264	ASP
1	A	269	LYS
1	A	286	LEU
1	A	321	GLN
1	A	347	LEU
1	A	367	LEU

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Mol	Chain	Res	Type
1	A	400	LYS
1	A	406	LYS
1	A	422	ARG
1	A	432	LYS
1	A	441	LEU
1	A	452	LYS
1	B	8	THR
1	B	48	TRP
1	B	58	THR
1	B	60	LEU
1	B	84	LEU
1	B	128	ASN
1	B	201	LYS
1	B	235	THR
1	B	244	GLU
1	B	264	ASP
1	B	269	LYS
1	B	277	THR
1	B	291	ARG
1	B	307	VAL
1	B	347	LEU
1	B	354	LYS
1	B	367	LEU
1	B	400	LYS
1	B	406	LYS
1	B	422	ARG
1	B	432	LYS
1	B	441	LEU
1	C	8	THR
1	C	48	TRP
1	C	58	THR
1	C	60	LEU
1	C	84	LEU
1	C	97	LYS
1	C	128	ASN
1	C	133	HIS
1	C	201	LYS
1	C	235	THR
1	C	244	GLU
1	C	264	ASP
1	C	269	LYS
1	C	286	LEU

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Mol	Chain	Res	Type
1	C	347	LEU
1	C	354	LYS
1	C	367	LEU
1	C	400	LYS
1	C	406	LYS
1	C	422	ARG
1	C	432	LYS
1	C	436	PRO
1	C	441	LEU
1	D	8	THR
1	D	48	TRP
1	D	58	THR
1	D	60	LEU
1	D	84	LEU
1	D	128	ASN
1	D	133	HIS
1	D	189	LEU
1	D	201	LYS
1	D	235	THR
1	D	244	GLU
1	D	255	VAL
1	D	264	ASP
1	D	269	LYS
1	D	286	LEU
1	D	347	LEU
1	D	354	LYS
1	D	367	LEU
1	D	400	LYS
1	D	406	LYS
1	D	422	ARG
1	D	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	63	ASN
1	A	128	ASN
1	A	133	HIS
1	A	148	GLN
1	A	321	GLN
1	A	433	HIS

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Mol	Chain	Res	Type
1	B	45	GLN
1	B	63	ASN
1	B	128	ASN
1	B	133	HIS
1	B	148	GLN
1	B	333	GLN
1	C	45	GLN
1	C	128	ASN
1	C	148	GLN
1	D	45	GLN
1	D	63	ASN
1	D	128	ASN
1	D	148	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

17 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	$\#\|Z\| > 2$
4	EPE	A	1453	-	14,15,15	0.51	0	18,20,20	2.48	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	A	1454	-	6,6,6	0.69	0	5,5,5	0.82	0
2	FAD	A	500	-	48,58,58	1.32	5 (10%)	54,89,89	2.11	12 (22%)
3	NAP	A	501	-	42,52,52	1.80	7 (16%)	54,80,80	2.35	16 (29%)
4	EPE	B	1452	-	14,15,15	0.56	0	18,20,20	2.75	9 (50%)
5	PEG	B	1453	-	6,6,6	0.72	0	5,5,5	1.08	0
5	PEG	B	1454	-	6,6,6	0.55	0	5,5,5	0.88	0
5	PEG	B	1455	-	6,6,6	0.64	0	5,5,5	0.50	0
2	FAD	B	500	-	48,58,58	1.33	6 (12%)	54,89,89	2.13	13 (24%)
3	NAP	B	501	-	42,52,52	1.80	7 (16%)	54,80,80	2.23	15 (27%)
4	EPE	C	1452	-	14,15,15	0.55	0	18,20,20	2.95	8 (44%)
2	FAD	C	500	-	48,58,58	1.37	5 (10%)	54,89,89	2.29	9 (16%)
3	NAP	C	501	-	42,52,52	1.75	6 (14%)	54,80,80	2.12	17 (31%)
4	EPE	D	1453	-	14,15,15	0.39	0	18,20,20	2.54	5 (27%)
5	PEG	D	1454	-	6,6,6	0.51	0	5,5,5	0.78	0
2	FAD	D	500	-	48,58,58	1.46	6 (12%)	54,89,89	2.10	12 (22%)
3	NAP	D	501	-	42,52,52	1.72	7 (16%)	54,80,80	2.26	16 (29%)

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
4	EPE	A	1453	-	-	0/9/19/19	0/1/1/1
5	PEG	A	1454	-	-	0/4/4/4	0/0/0/0
2	FAD	A	500	-	-	0/30/50/50	0/6/6/6
3	NAP	A	501	-	-	0/27/67/67	0/5/5/5
4	EPE	B	1452	-	-	0/9/19/19	0/1/1/1
5	PEG	B	1453	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1454	-	-	0/4/4/4	0/0/0/0
5	PEG	B	1455	-	-	0/4/4/4	0/0/0/0
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
3	NAP	B	501	-	-	0/27/67/67	0/5/5/5
4	EPE	C	1452	-	-	0/9/19/19	0/1/1/1
2	FAD	C	500	-	-	0/30/50/50	0/6/6/6
3	NAP	C	501	-	-	0/27/67/67	0/5/5/5
4	EPE	D	1453	-	-	0/9/19/19	0/1/1/1
5	PEG	D	1454	-	-	0/4/4/4	0/0/0/0
2	FAD	D	500	-	-	0/30/50/50	0/6/6/6
3	NAP	D	501	-	-	0/27/67/67	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C4X-C10	-2.27	1.36	1.41
2	C	500	FAD	C10-N10	-2.03	1.36	1.39
2	B	500	FAD	C10-N1	2.04	1.39	1.35
2	D	500	FAD	C10-N1	2.19	1.39	1.35
3	B	501	NAP	C4N-C3N	2.25	1.43	1.39
2	B	500	FAD	C2A-N1A	2.38	1.38	1.33
3	B	501	NAP	P2B-O3X	2.44	1.63	1.54
3	A	501	NAP	C4N-C3N	2.50	1.43	1.39
3	D	501	NAP	C4N-C3N	2.59	1.43	1.39
2	B	500	FAD	C4-N3	2.66	1.38	1.33
2	D	500	FAD	C1'-N10	2.68	1.51	1.48
2	A	500	FAD	C2A-N1A	2.70	1.39	1.33
2	B	500	FAD	C1'-N10	2.75	1.51	1.48
3	C	501	NAP	P2B-O3X	2.75	1.64	1.54
2	D	500	FAD	C2A-N1A	2.80	1.39	1.33
2	D	500	FAD	C4-N3	2.94	1.38	1.33
3	D	501	NAP	P2B-O3X	3.01	1.65	1.54
3	A	501	NAP	P2B-O3X	3.03	1.65	1.54
2	C	500	FAD	C1'-N10	3.13	1.51	1.48
3	D	501	NAP	C7N-N7N	3.18	1.39	1.33
2	A	500	FAD	C1'-N10	3.18	1.51	1.48
3	D	501	NAP	P2B-O1X	3.20	1.61	1.51
3	B	501	NAP	C7N-N7N	3.27	1.39	1.33
3	A	501	NAP	C7N-N7N	3.31	1.39	1.33
3	C	501	NAP	C7N-N7N	3.32	1.39	1.33
2	C	500	FAD	C4-N3	3.33	1.39	1.33
3	B	501	NAP	P2B-O1X	3.38	1.62	1.51
2	C	500	FAD	C4X-N5	3.38	1.38	1.33
2	A	500	FAD	C4X-N5	3.40	1.38	1.33
3	D	501	NAP	O4B-C1B	3.53	1.45	1.41
2	C	500	FAD	C2A-N3A	3.59	1.38	1.32
3	C	501	NAP	P2B-O1X	3.64	1.63	1.51
2	A	500	FAD	C2A-N3A	3.71	1.38	1.32
3	A	501	NAP	O4B-C1B	3.76	1.46	1.41
2	B	500	FAD	C2A-N3A	4.10	1.39	1.32
2	B	500	FAD	C4X-N5	4.11	1.39	1.33
3	C	501	NAP	C2N-C3N	4.12	1.45	1.39
3	A	501	NAP	P2B-O1X	4.24	1.65	1.51
3	C	501	NAP	O4B-C1B	4.31	1.46	1.41
3	A	501	NAP	C2N-C3N	4.44	1.45	1.39
3	D	501	NAP	C2N-C3N	4.45	1.45	1.39
3	B	501	NAP	C2N-C3N	4.52	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FAD	C4X-N5	4.55	1.40	1.33
3	A	501	NAP	O4D-C1D	4.56	1.47	1.41
2	D	500	FAD	C2A-N3A	4.65	1.40	1.32
3	B	501	NAP	O4B-C1B	4.83	1.47	1.41
3	B	501	NAP	O4D-C1D	4.95	1.47	1.41
3	C	501	NAP	O4D-C1D	5.02	1.47	1.41
3	D	501	NAP	O4D-C1D	5.03	1.47	1.41

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	FAD	N3A-C2A-N1A	-10.79	120.63	128.89
2	A	500	FAD	N3A-C2A-N1A	-9.81	121.39	128.89
2	D	500	FAD	N3A-C2A-N1A	-9.78	121.41	128.89
2	B	500	FAD	N3A-C2A-N1A	-9.71	121.46	128.89
3	A	501	NAP	N3A-C2A-N1A	-7.89	122.85	128.89
3	B	501	NAP	N3A-C2A-N1A	-6.80	123.69	128.89
3	D	501	NAP	N3A-C2A-N1A	-5.77	124.48	128.89
3	C	501	NAP	N3A-C2A-N1A	-4.69	125.30	128.89
2	C	500	FAD	C4A-C5A-N7A	-4.56	105.28	109.48
2	B	500	FAD	C4A-C5A-N7A	-4.31	105.51	109.48
3	B	501	NAP	PN-O3-PA	-4.06	121.32	132.73
3	C	501	NAP	PN-O3-PA	-3.77	122.13	132.73
3	D	501	NAP	PN-O3-PA	-3.74	122.24	132.73
2	B	500	FAD	P-O3P-PA	-3.61	122.60	132.73
2	D	500	FAD	P-O3P-PA	-3.50	122.91	132.73
3	D	501	NAP	O7N-C7N-N7N	-3.49	117.68	122.59
2	C	500	FAD	P-O3P-PA	-3.49	122.92	132.73
3	A	501	NAP	PN-O3-PA	-3.49	122.93	132.73
2	A	500	FAD	P-O3P-PA	-3.44	123.06	132.73
3	A	501	NAP	O5B-C5B-C4B	-3.40	96.59	109.12
2	A	500	FAD	C4A-C5A-N7A	-3.35	106.39	109.48
3	A	501	NAP	P2B-O2B-C2B	-3.30	113.64	121.56
3	D	501	NAP	O3X-P2B-O1X	-3.30	99.96	110.58
3	B	501	NAP	O5B-C5B-C4B	-3.27	97.06	109.12
3	A	501	NAP	O7N-C7N-N7N	-3.27	118.00	122.59
3	C	501	NAP	O7N-C7N-C3N	-3.16	116.14	119.59
2	D	500	FAD	C4A-C5A-N7A	-3.15	106.58	109.48
3	C	501	NAP	O7N-C7N-N7N	-3.05	118.30	122.59
3	C	501	NAP	C3B-C2B-C1B	-3.05	96.83	102.73
2	C	500	FAD	O2'-C2'-C1'	-3.04	102.48	109.94
3	C	501	NAP	O5B-C5B-C4B	-2.98	98.12	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	NAP	O7N-C7N-N7N	-2.90	118.51	122.59
3	A	501	NAP	O2B-C2B-C1B	-2.89	98.76	110.02
3	D	501	NAP	C4B-O4B-C1B	-2.86	106.58	109.72
3	D	501	NAP	O5B-C5B-C4B	-2.81	98.76	109.12
3	B	501	NAP	O7N-C7N-C3N	-2.80	116.53	119.59
3	B	501	NAP	P2B-O2B-C2B	-2.71	115.06	121.56
4	D	1453	EPE	O3S-S-O2S	-2.70	105.33	111.61
3	B	501	NAP	O2B-C2B-C1B	-2.61	99.84	110.02
3	D	501	NAP	C3B-C2B-C1B	-2.59	97.72	102.73
3	A	501	NAP	O7N-C7N-C3N	-2.57	116.78	119.59
3	C	501	NAP	O2B-C2B-C1B	-2.56	100.06	110.02
4	B	1452	EPE	C9-N1-C6	-2.50	104.85	111.27
2	B	500	FAD	O2'-C2'-C1'	-2.48	103.85	109.94
3	A	501	NAP	C4B-O4B-C1B	-2.47	107.01	109.72
3	C	501	NAP	C4B-O4B-C1B	-2.44	107.04	109.72
3	C	501	NAP	O3X-P2B-O1X	-2.43	102.77	110.58
2	C	500	FAD	C4X-C4-N3	-2.41	120.29	123.59
3	D	501	NAP	O7N-C7N-C3N	-2.35	117.02	119.59
2	B	500	FAD	C4X-C4-N3	-2.33	120.41	123.59
2	A	500	FAD	O2'-C2'-C1'	-2.26	104.40	109.94
2	D	500	FAD	O2'-C2'-C1'	-2.23	104.47	109.94
3	D	501	NAP	O2B-C2B-C1B	-2.21	101.41	110.02
3	A	501	NAP	O3X-P2B-O1X	-2.21	103.47	110.58
2	A	500	FAD	C9A-C5X-N5	-2.19	119.12	122.36
2	D	500	FAD	C9A-C5X-N5	-2.17	119.14	122.36
3	B	501	NAP	C3B-C2B-C1B	-2.16	98.55	102.73
2	D	500	FAD	C4-C4X-C10	-2.09	118.60	119.94
2	B	500	FAD	O3'-C3'-C4'	-2.07	103.53	108.75
3	C	501	NAP	P2B-O2B-C2B	-2.03	116.69	121.56
2	A	500	FAD	C6-C5X-C9A	2.06	121.69	118.98
4	B	1452	EPE	C3-C2-N1	2.08	114.35	110.63
2	B	500	FAD	C5X-C9A-N10	2.09	119.21	117.62
4	B	1452	EPE	C6-C5-N4	2.09	114.37	110.63
2	B	500	FAD	C6-C5X-C9A	2.15	121.81	118.98
2	B	500	FAD	O4B-C1B-N9A	2.17	112.64	108.10
3	A	501	NAP	O3-PA-O5B	2.17	108.70	102.94
2	A	500	FAD	O4B-C1B-N9A	2.18	112.66	108.10
3	C	501	NAP	O2B-C2B-C3B	2.20	120.08	111.51
4	B	1452	EPE	C6-N1-C2	2.21	113.69	108.90
3	C	501	NAP	O2B-P2B-O1X	2.26	112.75	107.11
3	A	501	NAP	O2A-PA-O3	2.26	115.35	105.09
3	B	501	NAP	O2A-PA-O3	2.27	115.41	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	FAD	C4-C4X-N5	2.28	121.49	118.72
3	C	501	NAP	O2A-PA-O3	2.33	115.68	105.09
2	D	500	FAD	O3P-PA-O5B	2.40	109.29	102.94
4	C	1452	EPE	C3-C2-N1	2.42	114.97	110.63
2	D	500	FAD	C6-C5X-C9A	2.45	122.21	118.98
3	D	501	NAP	O2B-C2B-C3B	2.46	121.07	111.51
4	C	1452	EPE	C7-N4-C3	2.53	117.76	111.27
3	D	501	NAP	O4B-C1B-N9A	2.57	113.48	108.10
3	B	501	NAP	O4B-C1B-N9A	2.58	113.49	108.10
4	C	1452	EPE	C5-C6-N1	2.58	115.25	110.63
3	B	501	NAP	O3-PA-O5B	2.59	109.80	102.94
4	B	1452	EPE	C7-N4-C3	2.63	118.00	111.27
4	A	1453	EPE	C9-C10-S	2.64	120.69	112.51
2	B	500	FAD	O3P-PA-O5B	2.68	110.06	102.94
3	D	501	NAP	O3-PA-O5B	2.70	110.10	102.94
2	C	500	FAD	C5X-C9A-N10	2.73	119.69	117.62
2	A	500	FAD	C5X-C9A-N10	2.75	119.71	117.62
3	A	501	NAP	O4B-C1B-N9A	2.82	114.00	108.10
4	D	1453	EPE	C7-N4-C3	3.00	118.95	111.27
4	A	1453	EPE	C7-N4-C5	3.13	119.31	111.27
4	B	1452	EPE	C7-N4-C5	3.14	119.31	111.27
2	C	500	FAD	C4X-N5-C5X	3.21	120.45	116.76
3	C	501	NAP	O4B-C1B-N9A	3.22	114.85	108.10
4	D	1453	EPE	C7-N4-C5	3.27	119.66	111.27
2	B	500	FAD	C4X-N5-C5X	3.41	120.68	116.76
2	D	500	FAD	C4X-N5-C5X	3.42	120.69	116.76
4	C	1452	EPE	C7-N4-C5	3.43	120.05	111.27
3	B	501	NAP	O2B-P2B-O1X	3.50	115.86	107.11
4	A	1453	EPE	C7-N4-C3	3.53	120.31	111.27
3	A	501	NAP	O2B-P2B-O1X	3.53	115.92	107.11
2	A	500	FAD	C1'-N10-C9A	3.56	122.86	118.86
3	D	501	NAP	O2B-P2B-O1X	3.57	116.01	107.11
3	C	501	NAP	O3-PN-O5D	3.65	112.62	102.94
2	D	500	FAD	C5X-C9A-N10	3.85	120.55	117.62
2	B	500	FAD	C1'-N10-C9A	3.86	123.19	118.86
2	A	500	FAD	C4X-N5-C5X	3.86	121.20	116.76
4	B	1452	EPE	O1S-S-C10	3.95	110.28	106.91
3	D	501	NAP	O3-PN-O5D	4.13	113.89	102.94
4	C	1452	EPE	C6-N1-C2	4.17	117.93	108.90
4	B	1452	EPE	C5-N4-C3	4.32	118.25	108.90
3	B	501	NAP	O4D-C1D-N1N	4.37	112.93	108.13
3	A	501	NAP	O3-PN-O5D	4.38	114.57	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	FAD	C1'-N10-C9A	4.50	123.92	118.86
4	A	1453	EPE	C5-N4-C3	4.61	118.89	108.90
3	B	501	NAP	O3-PN-O5D	4.66	115.30	102.94
3	C	501	NAP	O4D-C1D-N1N	4.68	113.27	108.13
4	C	1452	EPE	C5-N4-C3	4.69	119.07	108.90
2	D	500	FAD	C4-N3-C2	4.74	119.34	115.25
4	C	1452	EPE	O2S-S-C10	4.94	111.12	106.91
3	A	501	NAP	O4D-C1D-N1N	5.15	113.78	108.13
2	C	500	FAD	C1'-N10-C9A	5.16	124.65	118.86
4	D	1453	EPE	C5-N4-C3	5.32	120.42	108.90
3	D	501	NAP	O4D-C1D-N1N	5.37	114.03	108.13
2	C	500	FAD	C4-N3-C2	5.45	119.96	115.25
2	B	500	FAD	C4-N3-C2	5.89	120.34	115.25
2	A	500	FAD	C4-N3-C2	5.95	120.39	115.25
3	B	501	NAP	C3N-C7N-N7N	6.53	124.96	117.82
3	A	501	NAP	C3N-C7N-N7N	6.76	125.22	117.82
4	D	1453	EPE	O1S-S-C10	6.79	112.70	106.91
3	D	501	NAP	C3N-C7N-N7N	6.83	125.29	117.82
4	A	1453	EPE	O1S-S-C10	6.85	112.75	106.91
4	C	1452	EPE	O1S-S-C10	6.88	112.78	106.91
3	C	501	NAP	C3N-C7N-N7N	7.08	125.56	117.82
4	B	1452	EPE	O2S-S-C10	7.58	113.37	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1454	PEG	1	0
2	A	500	FAD	2	0
3	A	501	NAP	2	0
2	B	500	FAD	3	0
3	B	501	NAP	2	0
2	C	500	FAD	1	0
3	C	501	NAP	2	0
4	D	1453	EPE	1	0
2	D	500	FAD	1	0
3	D	501	NAP	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	446/461 (96%)	-0.44	1 (0%) 95 94	24, 39, 58, 70	0
1	B	445/461 (96%)	-0.36	0 100 100	24, 39, 58, 65	0
1	C	445/461 (96%)	-0.34	2 (0%) 93 90	24, 39, 58, 65	0
1	D	446/461 (96%)	-0.38	2 (0%) 93 90	25, 39, 58, 70	0
All	All	1782/1844 (96%)	-0.38	5 (0%) 94 92	24, 39, 58, 70	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	451	ASP	3.0
1	A	452	LYS	2.7
1	C	451	ASP	2.3
1	C	244	GLU	2.2
1	D	452	LYS	2.1

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
4	EPE	A	1453	15/15	0.93	0.21	6.01	70,78,87,88	0
4	EPE	C	1452	15/15	0.91	0.22	2.81	72,80,89,89	0
4	EPE	B	1452	15/15	0.93	0.19	2.55	71,78,86,87	0
4	EPE	D	1453	15/15	0.92	0.21	2.18	79,86,98,100	0
3	NAP	B	501	48/48	0.94	0.17	0.85	50,53,73,74	0
3	NAP	C	501	48/48	0.96	0.18	0.58	50,53,73,75	0
3	NAP	D	501	48/48	0.96	0.18	0.56	50,53,73,75	0
3	NAP	A	501	48/48	0.94	0.17	0.44	50,53,73,75	0
5	PEG	B	1453	7/7	0.87	0.17	0.03	39,43,47,48	0
2	FAD	C	500	53/53	0.98	0.15	-0.17	21,27,37,41	0
2	FAD	A	500	53/53	0.99	0.14	-0.27	20,27,37,41	0
2	FAD	D	500	53/53	0.98	0.13	-0.65	20,27,37,41	0
2	FAD	B	500	53/53	0.98	0.14	-0.69	20,27,37,41	0
5	PEG	B	1454	7/7	0.89	0.17	-	46,48,59,59	0
5	PEG	A	1454	7/7	0.93	0.33	-	51,54,58,58	0
5	PEG	D	1454	7/7	0.94	0.12	-	56,58,60,60	0
5	PEG	B	1455	7/7	0.89	0.16	-	50,52,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.