Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2016 – 05:18 AM EDT

PDB ID	:	5HEI
Title	:	Structure of B. megaterium NfrA2
Authors	:	Vigouroux, A.; Morera, S.
Deposited on	:	2016-01-06
Resolution	:	2.84 Å(reported)

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

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

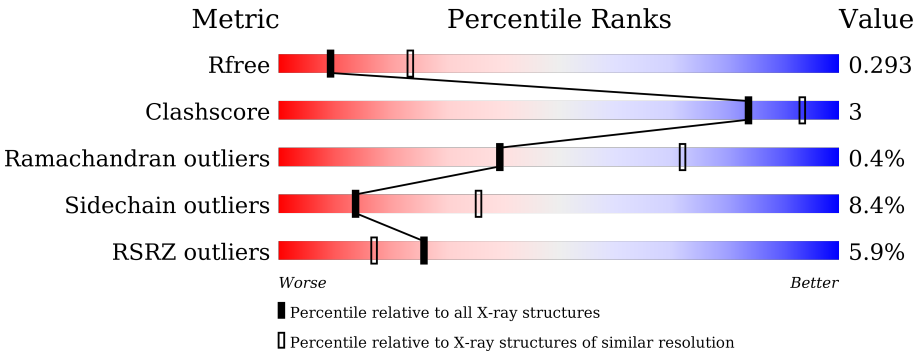
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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	253	8% 82% 15%
1	B	253	5% 82% 15%
1	C	253	4% 83% 14%
1	D	253	2% 83% 13%
1	E	253	15% 85% 11%
1	F	253	9% 83% 13%

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Mol	Chain	Length	Quality of chain
1	G	253	2% 85% 11%
1	H	253	% 80% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15833 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 NfrA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			
1	B	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			
1	C	245	Total	C	N	O	S	0	0	0
			1905	1197	331	373	4			
1	D	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			
1	E	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			
1	F	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			
1	G	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			
1	H	246	Total	C	N	O	S	0	0	0
			1913	1202	332	374	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	LYS	-	expression tag	UNP A0A0K0VJM8
A	247	GLY	-	expression tag	UNP A0A0K0VJM8
A	248	HIS	-	expression tag	UNP A0A0K0VJM8
A	249	HIS	-	expression tag	UNP A0A0K0VJM8
A	250	HIS	-	expression tag	UNP A0A0K0VJM8
A	251	HIS	-	expression tag	UNP A0A0K0VJM8
A	252	HIS	-	expression tag	UNP A0A0K0VJM8
A	253	HIS	-	expression tag	UNP A0A0K0VJM8
B	246	LYS	-	expression tag	UNP A0A0K0VJM8
B	247	GLY	-	expression tag	UNP A0A0K0VJM8
B	248	HIS	-	expression tag	UNP A0A0K0VJM8
B	249	HIS	-	expression tag	UNP A0A0K0VJM8
B	250	HIS	-	expression tag	UNP A0A0K0VJM8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	251	HIS	-	expression tag	UNP A0A0K0VJM8
B	252	HIS	-	expression tag	UNP A0A0K0VJM8
B	253	HIS	-	expression tag	UNP A0A0K0VJM8
C	246	LYS	-	expression tag	UNP A0A0K0VJM8
C	247	GLY	-	expression tag	UNP A0A0K0VJM8
C	248	HIS	-	expression tag	UNP A0A0K0VJM8
C	249	HIS	-	expression tag	UNP A0A0K0VJM8
C	250	HIS	-	expression tag	UNP A0A0K0VJM8
C	251	HIS	-	expression tag	UNP A0A0K0VJM8
C	252	HIS	-	expression tag	UNP A0A0K0VJM8
C	253	HIS	-	expression tag	UNP A0A0K0VJM8
D	246	LYS	-	expression tag	UNP A0A0K0VJM8
D	247	GLY	-	expression tag	UNP A0A0K0VJM8
D	248	HIS	-	expression tag	UNP A0A0K0VJM8
D	249	HIS	-	expression tag	UNP A0A0K0VJM8
D	250	HIS	-	expression tag	UNP A0A0K0VJM8
D	251	HIS	-	expression tag	UNP A0A0K0VJM8
D	252	HIS	-	expression tag	UNP A0A0K0VJM8
D	253	HIS	-	expression tag	UNP A0A0K0VJM8
E	246	LYS	-	expression tag	UNP A0A0K0VJM8
E	247	GLY	-	expression tag	UNP A0A0K0VJM8
E	248	HIS	-	expression tag	UNP A0A0K0VJM8
E	249	HIS	-	expression tag	UNP A0A0K0VJM8
E	250	HIS	-	expression tag	UNP A0A0K0VJM8
E	251	HIS	-	expression tag	UNP A0A0K0VJM8
E	252	HIS	-	expression tag	UNP A0A0K0VJM8
E	253	HIS	-	expression tag	UNP A0A0K0VJM8
F	246	LYS	-	expression tag	UNP A0A0K0VJM8
F	247	GLY	-	expression tag	UNP A0A0K0VJM8
F	248	HIS	-	expression tag	UNP A0A0K0VJM8
F	249	HIS	-	expression tag	UNP A0A0K0VJM8
F	250	HIS	-	expression tag	UNP A0A0K0VJM8
F	251	HIS	-	expression tag	UNP A0A0K0VJM8
F	252	HIS	-	expression tag	UNP A0A0K0VJM8
F	253	HIS	-	expression tag	UNP A0A0K0VJM8
G	246	LYS	-	expression tag	UNP A0A0K0VJM8
G	247	GLY	-	expression tag	UNP A0A0K0VJM8
G	248	HIS	-	expression tag	UNP A0A0K0VJM8
G	249	HIS	-	expression tag	UNP A0A0K0VJM8
G	250	HIS	-	expression tag	UNP A0A0K0VJM8
G	251	HIS	-	expression tag	UNP A0A0K0VJM8
G	252	HIS	-	expression tag	UNP A0A0K0VJM8

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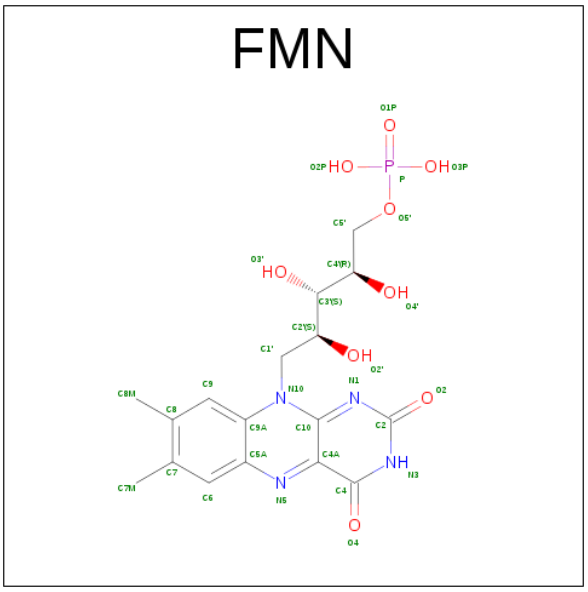
Chain	Residue	Modelled	Actual	Comment	Reference
G	253	HIS	-	expression tag	UNP A0A0K0VJM8
H	246	LYS	-	expression tag	UNP A0A0K0VJM8
H	247	GLY	-	expression tag	UNP A0A0K0VJM8
H	248	HIS	-	expression tag	UNP A0A0K0VJM8
H	249	HIS	-	expression tag	UNP A0A0K0VJM8
H	250	HIS	-	expression tag	UNP A0A0K0VJM8
H	251	HIS	-	expression tag	UNP A0A0K0VJM8
H	252	HIS	-	expression tag	UNP A0A0K0VJM8
H	253	HIS	-	expression tag	UNP A0A0K0VJM8

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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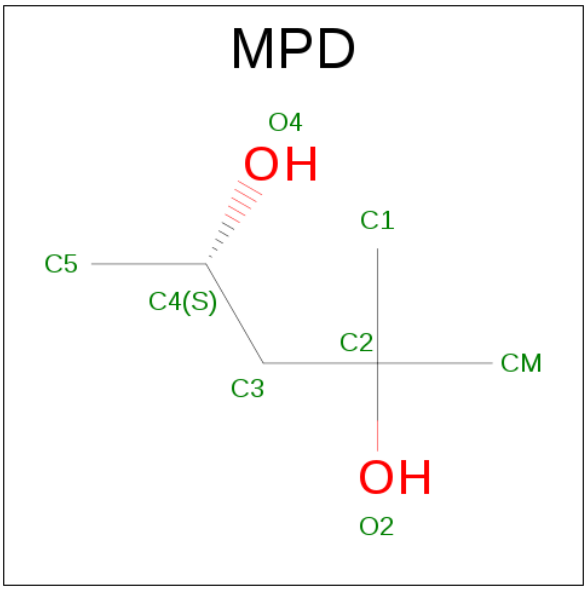
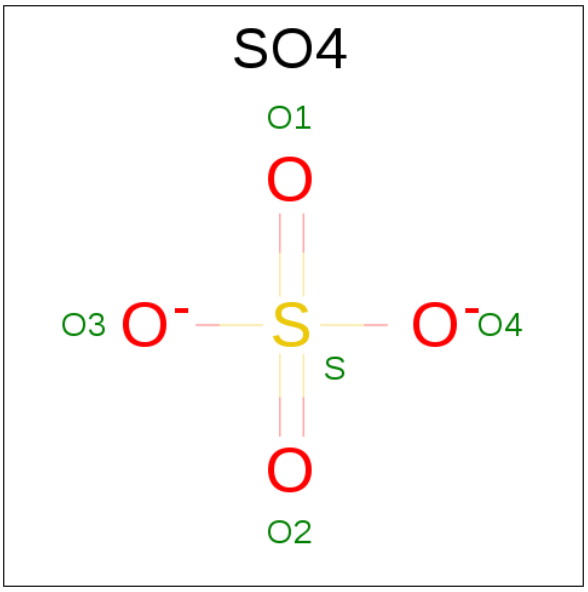
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O		0	0
			8	6	2			
3	H	1	Total	C	O		0	0
			8	6	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	26	Total O 26 26	0	0
5	C	41	Total O 41 41	0	0
5	D	40	Total O 40 40	0	0
5	E	19	Total O 19 19	0	0
5	F	16	Total O 16 16	0	0
5	G	36	Total O 36 36	0	0

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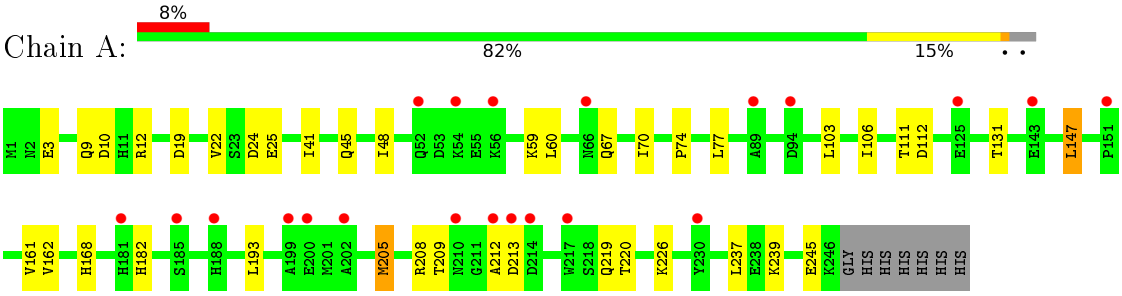
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	47	Total	O	0	0
			47	47		

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.

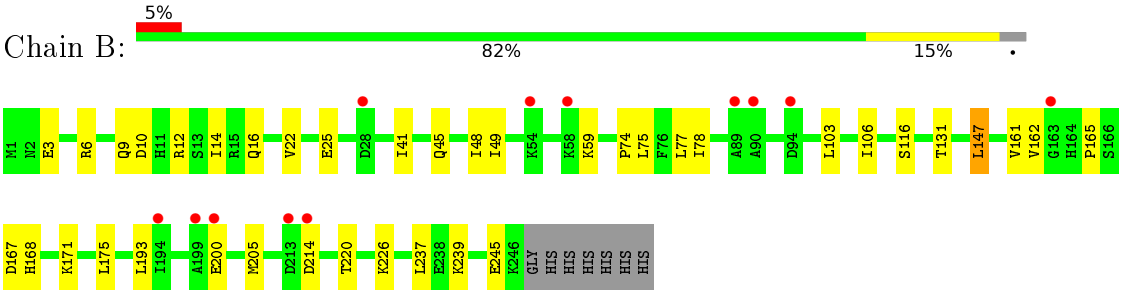
- Molecule 1: NfrA2

Chain A:



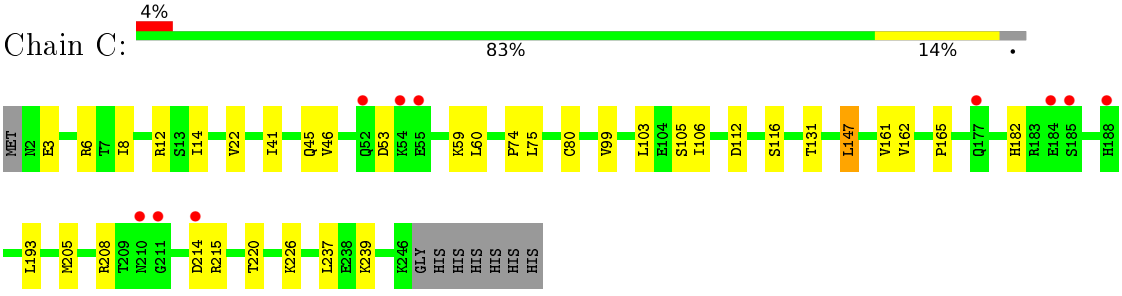
- Molecule 1: NfrA2

Chain B:



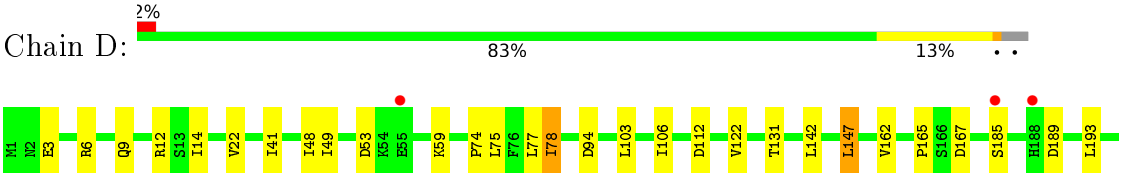
- Molecule 1: NfrA2

Chain C:

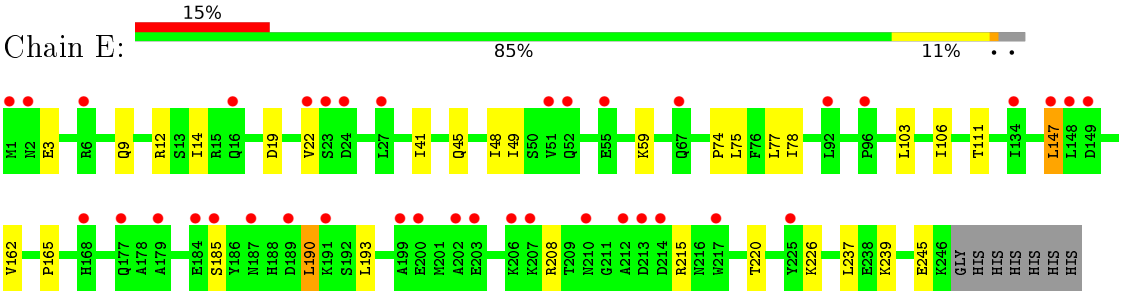


- Molecule 1: NfrA2

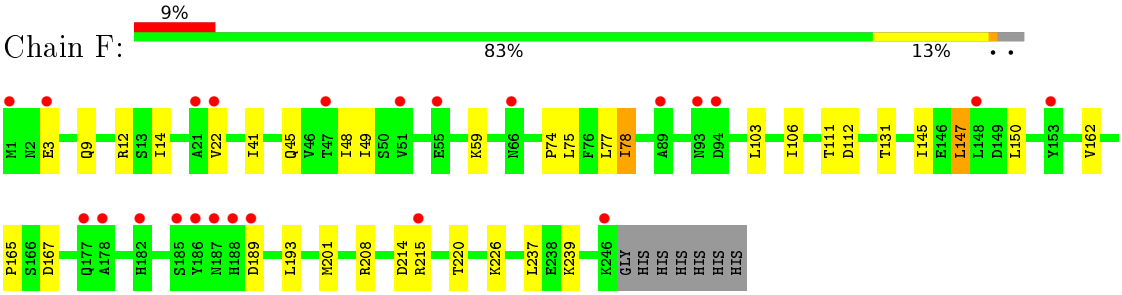
Chain D:



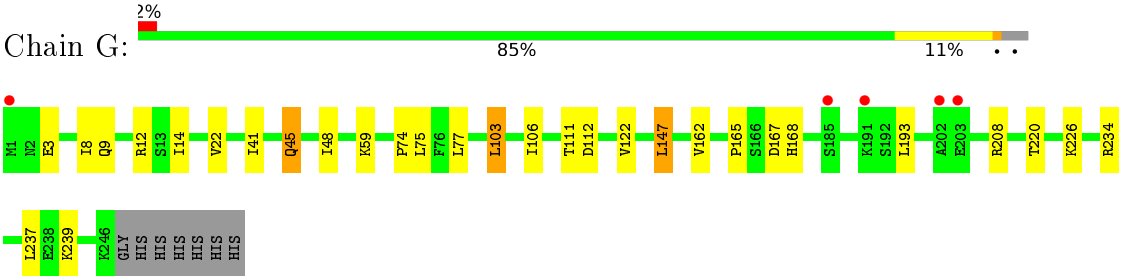
• Molecule 1: NfrA2



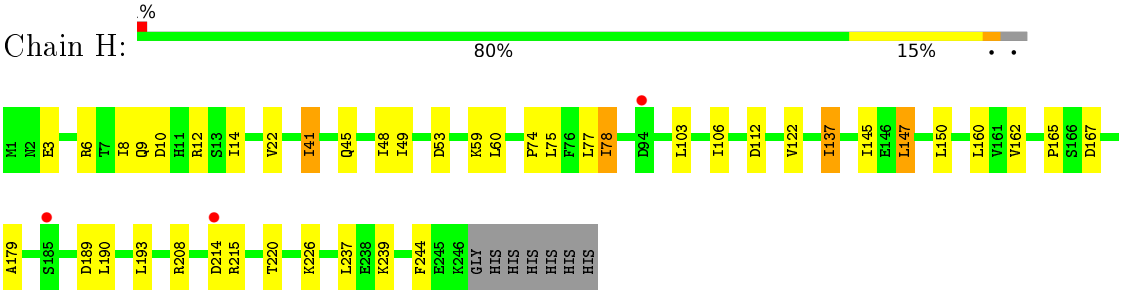
• Molecule 1: NfrA2



• Molecule 1: NfrA2



• Molecule 1: NfrA2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.44Å 158.19Å 103.86Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	28.63 – 2.84 48.33 – 2.84	Depositor EDS
% Data completeness (in resolution range)	97.2 (28.63-2.84) 97.3 (48.33-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.247 0.244 , 0.293	Depositor DCC
R_{free} test set	2218 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15833	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4182e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, MPD, SO4

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	0.41	0/1947	0.63	0/2636
1	B	0.41	0/1947	0.63	0/2636
1	C	0.42	0/1939	0.64	0/2626
1	D	0.41	0/1947	0.64	0/2636
1	E	0.41	0/1947	0.65	1/2636 (0.0%)
1	F	0.40	0/1947	0.62	0/2636
1	G	0.42	0/1947	0.63	0/2636
1	H	0.41	0/1947	0.63	0/2636
All	All	0.41	0/15568	0.63	1/21078 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	190	LEU	CA-CB-CG	6.03	129.17	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1913	0	1906	16	0
1	B	1913	0	1906	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1905	0	1894	11	0
1	D	1913	0	1906	12	0
1	E	1913	0	1906	9	0
1	F	1913	0	1906	11	0
1	G	1913	0	1906	13	0
1	H	1913	0	1906	20	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
3	C	8	0	14	0	0
3	H	8	0	14	1	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	A	23	0	0	0	0
5	B	26	0	0	0	0
5	C	41	0	0	0	0
5	D	40	0	0	0	0
5	E	19	0	0	0	0
5	F	16	0	0	0	0
5	G	36	0	0	0	0
5	H	47	0	0	0	0
All	All	15833	0	15416	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (92) 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:E:3:GLU:HB3	1:F:3:GLU:HB3	1.63	0.80
1:G:103:LEU:HD11	1:H:244:PHE:CZ	2.19	0.77
1:D:48:ILE:HD11	1:D:77:LEU:HB3	1.66	0.76
1:H:48:ILE:HD11	1:H:77:LEU:HB3	1.67	0.76
1:C:14:ILE:HG21	1:C:165:PRO:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:HD11	1:E:77:LEU:HB3	1.67	0.76
1:G:48:ILE:HD11	1:G:77:LEU:HB3	1.67	0.75
1:F:48:ILE:HD11	1:F:77:LEU:HB3	1.68	0.73
1:A:48:ILE:HD11	1:A:77:LEU:HB3	1.68	0.73
1:G:103:LEU:HD11	1:H:244:PHE:HZ	1.52	0.72
1:A:3:GLU:HB3	1:B:3:GLU:HB3	1.72	0.71
1:A:205:MET:O	1:A:209:THR:HG22	1.89	0.71
1:G:3:GLU:HB3	1:H:3:GLU:HB3	1.74	0.68
1:B:48:ILE:HD11	1:B:77:LEU:HB3	1.76	0.67
1:A:209:THR:HG21	1:A:213:ASP:H	1.60	0.66
1:D:106:ILE:HD12	1:D:237:LEU:HD22	1.77	0.65
1:H:106:ILE:HD12	1:H:237:LEU:HD22	1.78	0.64
1:D:49:ILE:HB	1:D:78:ILE:HG23	1.79	0.64
1:F:49:ILE:HB	1:F:78:ILE:HG23	1.80	0.63
1:C:106:ILE:HD12	1:C:237:LEU:HD22	1.80	0.63
1:H:41:ILE:HG22	3:H:302:MPD:H32	1.81	0.63
1:H:49:ILE:HB	1:H:78:ILE:HG23	1.80	0.62
1:F:106:ILE:HD12	1:F:237:LEU:HD22	1.82	0.62
1:G:106:ILE:HD12	1:G:237:LEU:HD22	1.82	0.62
1:A:106:ILE:HD12	1:A:237:LEU:HD22	1.82	0.61
1:B:106:ILE:HD12	1:B:237:LEU:HD22	1.82	0.61
1:E:106:ILE:HD12	1:E:237:LEU:HD22	1.82	0.61
1:A:209:THR:OG1	1:A:212:ALA:HB3	2.01	0.60
1:G:122:VAL:HG23	1:H:8:ILE:HD11	1.84	0.59
1:C:8:ILE:HD11	1:D:122:VAL:HG23	1.84	0.58
1:A:209:THR:CG2	1:A:213:ASP:H	2.17	0.58
1:G:8:ILE:HD11	1:H:122:VAL:HG23	1.86	0.58
1:E:49:ILE:HB	1:E:78:ILE:HG23	1.87	0.57
1:G:75:LEU:HD23	1:G:162:VAL:HB	1.89	0.55
1:B:12:ARG:HD2	1:B:168:HIS:O	2.07	0.54
1:B:49:ILE:HB	1:B:78:ILE:HG23	1.89	0.54
1:C:75:LEU:HD23	1:C:162:VAL:HB	1.90	0.54
1:F:75:LEU:HD23	1:F:162:VAL:HB	1.91	0.53
1:E:75:LEU:HD23	1:E:162:VAL:HB	1.91	0.53
1:D:75:LEU:HD23	1:D:162:VAL:HB	1.91	0.53
1:C:3:GLU:HB3	1:D:3:GLU:HB3	1.91	0.52
1:H:75:LEU:HD23	1:H:162:VAL:HB	1.91	0.52
1:H:78:ILE:HD13	1:H:137:ILE:HG12	1.91	0.52
1:B:75:LEU:HD23	1:B:162:VAL:HB	1.91	0.52
1:H:14:ILE:HG21	1:H:165:PRO:HB3	1.92	0.52
1:E:14:ILE:HG21	1:E:165:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:HG21	1:B:165:PRO:HB3	1.93	0.51
1:D:14:ILE:HG21	1:D:165:PRO:HB3	1.92	0.51
1:G:14:ILE:HG21	1:G:165:PRO:HB3	1.93	0.51
1:F:14:ILE:HG21	1:F:165:PRO:HB3	1.93	0.50
1:C:59:LYS:HB3	1:C:147:LEU:HD11	1.92	0.50
1:A:59:LYS:HB3	1:A:147:LEU:HD11	1.93	0.49
1:F:145:ILE:HG23	1:F:150:LEU:HB2	1.95	0.49
1:A:209:THR:HG21	1:A:213:ASP:N	2.27	0.49
1:D:59:LYS:HB3	1:D:147:LEU:HD11	1.95	0.48
1:B:10:ASP:HA	1:B:171:LYS:HD2	1.96	0.48
1:B:59:LYS:HB3	1:B:147:LEU:HD11	1.95	0.48
1:G:59:LYS:HB3	1:G:147:LEU:HD11	1.94	0.48
1:H:77:LEU:HB2	1:H:160:LEU:HB3	1.96	0.48
1:F:59:LYS:HB3	1:F:147:LEU:HD11	1.96	0.47
1:C:99:VAL:HG22	1:C:105:SER:HB3	1.98	0.46
1:A:131:THR:HG22	1:A:162:VAL:HG22	1.97	0.46
1:H:59:LYS:HB3	1:H:147:LEU:HD11	1.97	0.46
1:C:215:ARG:HD2	1:C:220:THR:HG22	1.97	0.46
1:E:59:LYS:HB3	1:E:147:LEU:HD11	1.97	0.45
1:E:215:ARG:HD2	1:E:220:THR:HG22	1.97	0.45
1:A:209:THR:HG23	1:A:212:ALA:H	1.82	0.45
1:A:209:THR:HG1	1:A:212:ALA:HB3	1.81	0.44
1:A:67:GLN:HB2	1:A:70:ILE:HD12	1.98	0.44
1:H:215:ARG:HD2	1:H:220:THR:HG22	1.99	0.44
1:C:131:THR:HA	1:C:161:VAL:O	2.18	0.44
1:D:208:ARG:HH12	1:H:10:ASP:CG	2.21	0.43
1:H:22:VAL:HG23	1:H:74:PRO:HG2	2.00	0.43
1:D:22:VAL:HG23	1:D:74:PRO:HG2	2.01	0.43
1:F:215:ARG:HD2	1:F:220:THR:HG22	2.00	0.42
1:G:234:ARG:HH11	1:H:244:PHE:HB3	1.84	0.42
1:E:22:VAL:HG23	1:E:74:PRO:HG2	2.01	0.42
1:C:22:VAL:HG23	1:C:74:PRO:HG2	2.01	0.42
1:F:22:VAL:HG23	1:F:74:PRO:HG2	2.01	0.42
1:G:22:VAL:HG23	1:G:74:PRO:HG2	2.02	0.42
1:B:131:THR:HG22	1:B:162:VAL:HG22	2.02	0.41
1:A:22:VAL:HG23	1:A:74:PRO:HG2	2.02	0.41
1:G:45:GLN:HB2	1:G:45:GLN:HE21	1.72	0.41
1:D:131:THR:HG22	1:D:162:VAL:HG22	2.02	0.41
1:F:131:THR:HG22	1:F:162:VAL:HG22	2.02	0.41
1:H:179:ALA:HA	1:H:190:LEU:HD22	2.02	0.41
1:A:131:THR:HA	1:A:161:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:HIS:O	1:B:49:ILE:HA	2.21	0.40
1:C:182:HIS:O	1:D:49:ILE:HA	2.20	0.40
1:H:145:ILE:HG23	1:H:150:LEU:HB2	2.03	0.40
1:B:131:THR:HA	1:B:161:VAL:O	2.22	0.40
1:B:22:VAL:HG23	1:B:74:PRO:HG2	2.02	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	244/253 (96%)	234 (96%)	9 (4%)	1 (0%)	39	72
1	B	244/253 (96%)	234 (96%)	9 (4%)	1 (0%)	39	72
1	C	243/253 (96%)	234 (96%)	8 (3%)	1 (0%)	39	72
1	D	244/253 (96%)	236 (97%)	7 (3%)	1 (0%)	39	72
1	E	244/253 (96%)	236 (97%)	7 (3%)	1 (0%)	39	72
1	F	244/253 (96%)	236 (97%)	7 (3%)	1 (0%)	39	72
1	G	244/253 (96%)	235 (96%)	8 (3%)	1 (0%)	39	72
1	H	244/253 (96%)	235 (96%)	8 (3%)	1 (0%)	39	72
All	All	1951/2024 (96%)	1880 (96%)	63 (3%)	8 (0%)	39	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	B	41	ILE
1	E	41	ILE
1	F	41	ILE
1	H	41	ILE

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Mol	Chain	Res	Type
1	C	41	ILE
1	D	41	ILE
1	G	41	ILE

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	205/211 (97%)	184 (90%)	21 (10%)	9 25
1	B	205/211 (97%)	187 (91%)	18 (9%)	12 33
1	C	204/211 (97%)	187 (92%)	17 (8%)	14 36
1	D	205/211 (97%)	185 (90%)	20 (10%)	10 27
1	E	205/211 (97%)	191 (93%)	14 (7%)	20 47
1	F	205/211 (97%)	189 (92%)	16 (8%)	16 39
1	G	205/211 (97%)	191 (93%)	14 (7%)	20 47
1	H	205/211 (97%)	187 (91%)	18 (9%)	12 33
All	All	1639/1688 (97%)	1501 (92%)	138 (8%)	14 36

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	ASP
1	A	12	ARG
1	A	19	ASP
1	A	24	ASP
1	A	25	GLU
1	A	45	GLN
1	A	60	LEU
1	A	103	LEU
1	A	111	THR
1	A	112	ASP
1	A	147	LEU

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Mol	Chain	Res	Type
1	A	168	HIS
1	A	193	LEU
1	A	205	MET
1	A	208	ARG
1	A	219	GLN
1	A	220	THR
1	A	226	LYS
1	A	239	LYS
1	A	245	GLU
1	B	6	ARG
1	B	9	GLN
1	B	16	GLN
1	B	25	GLU
1	B	45	GLN
1	B	103	LEU
1	B	116	SER
1	B	147	LEU
1	B	167	ASP
1	B	175	LEU
1	B	193	LEU
1	B	200	GLU
1	B	205	MET
1	B	214	ASP
1	B	220	THR
1	B	226	LYS
1	B	239	LYS
1	B	245	GLU
1	C	6	ARG
1	C	12	ARG
1	C	45	GLN
1	C	46	VAL
1	C	53	ASP
1	C	60	LEU
1	C	80	CYS
1	C	103	LEU
1	C	112	ASP
1	C	116	SER
1	C	147	LEU
1	C	193	LEU
1	C	205	MET
1	C	208	ARG
1	C	214	ASP

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Mol	Chain	Res	Type
1	C	226	LYS
1	C	239	LYS
1	D	6	ARG
1	D	9	GLN
1	D	12	ARG
1	D	53	ASP
1	D	78	ILE
1	D	94	ASP
1	D	103	LEU
1	D	112	ASP
1	D	142	LEU
1	D	147	LEU
1	D	167	ASP
1	D	185	SER
1	D	189	ASP
1	D	193	LEU
1	D	203	GLU
1	D	208	ARG
1	D	220	THR
1	D	226	LYS
1	D	239	LYS
1	D	245	GLU
1	E	9	GLN
1	E	12	ARG
1	E	19	ASP
1	E	45	GLN
1	E	103	LEU
1	E	111	THR
1	E	147	LEU
1	E	185	SER
1	E	190	LEU
1	E	193	LEU
1	E	208	ARG
1	E	226	LYS
1	E	239	LYS
1	E	245	GLU
1	F	9	GLN
1	F	12	ARG
1	F	45	GLN
1	F	78	ILE
1	F	103	LEU
1	F	111	THR

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Mol	Chain	Res	Type
1	F	112	ASP
1	F	147	LEU
1	F	167	ASP
1	F	189	ASP
1	F	193	LEU
1	F	201	MET
1	F	208	ARG
1	F	214	ASP
1	F	226	LYS
1	F	239	LYS
1	G	9	GLN
1	G	12	ARG
1	G	45	GLN
1	G	103	LEU
1	G	111	THR
1	G	112	ASP
1	G	147	LEU
1	G	167	ASP
1	G	168	HIS
1	G	193	LEU
1	G	208	ARG
1	G	220	THR
1	G	226	LYS
1	G	239	LYS
1	H	6	ARG
1	H	9	GLN
1	H	12	ARG
1	H	45	GLN
1	H	53	ASP
1	H	60	LEU
1	H	78	ILE
1	H	103	LEU
1	H	112	ASP
1	H	137	ILE
1	H	147	LEU
1	H	167	ASP
1	H	189	ASP
1	H	193	LEU
1	H	208	ARG
1	H	214	ASP
1	H	226	LYS
1	H	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	52	GLN
1	A	188	HIS
1	B	9	GLN
1	B	210	ASN
1	D	9	GLN
1	D	188	HIS
1	D	210	ASN
1	E	9	GLN
1	F	9	GLN
1	F	187	ASN
1	F	210	ASN
1	G	9	GLN
1	H	9	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

15 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	FMN	A	301	-	32,33,33	1.33	5 (15%)	34,50,50	2.92	5 (14%)
2	FMN	B	301	-	32,33,33	1.28	5 (15%)	34,50,50	2.92	5 (14%)
2	FMN	C	301	-	32,33,33	1.33	5 (15%)	34,50,50	2.91	5 (14%)
3	MPD	C	302	-	6,7,7	0.52	0	6,10,10	0.42	0
4	SO4	C	303	-	4,4,4	0.06	0	6,6,6	0.11	0
2	FMN	D	301	-	32,33,33	1.28	5 (15%)	34,50,50	2.90	5 (14%)
4	SO4	D	302	-	4,4,4	0.64	0	6,6,6	0.44	0
4	SO4	D	303	-	4,4,4	0.13	0	6,6,6	0.14	0
2	FMN	E	301	-	32,33,33	1.30	5 (15%)	34,50,50	2.91	5 (14%)
2	FMN	F	301	-	32,33,33	1.31	5 (15%)	34,50,50	2.91	5 (14%)
2	FMN	G	301	-	32,33,33	1.27	5 (15%)	34,50,50	2.92	5 (14%)
4	SO4	G	302	-	4,4,4	0.13	0	6,6,6	0.13	0
2	FMN	H	301	-	32,33,33	1.31	5 (15%)	34,50,50	2.93	5 (14%)
3	MPD	H	302	-	6,7,7	0.43	0	6,10,10	0.48	0
4	SO4	H	303	-	4,4,4	0.18	0	6,6,6	0.10	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	FMN	A	301	-	-	0/18/18/18	0/3/3/3
2	FMN	B	301	-	-	0/18/18/18	0/3/3/3
2	FMN	C	301	-	-	0/18/18/18	0/3/3/3
3	MPD	C	302	-	-	0/5/5/5	0/0/0/0
4	SO4	C	303	-	-	0/0/0/0	0/0/0/0
2	FMN	D	301	-	-	0/18/18/18	0/3/3/3
4	SO4	D	302	-	-	0/0/0/0	0/0/0/0
4	SO4	D	303	-	-	0/0/0/0	0/0/0/0
2	FMN	E	301	-	-	0/18/18/18	0/3/3/3
2	FMN	F	301	-	-	0/18/18/18	0/3/3/3
2	FMN	G	301	-	-	0/18/18/18	0/3/3/3
4	SO4	G	302	-	-	0/0/0/0	0/0/0/0
2	FMN	H	301	-	-	0/18/18/18	0/3/3/3
3	MPD	H	302	-	-	0/5/5/5	0/0/0/0
4	SO4	H	303	-	-	0/0/0/0	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FMN	C9A-N10	2.42	1.42	1.38
2	D	301	FMN	C9A-N10	2.56	1.42	1.38
2	G	301	FMN	C5A-N5	2.59	1.39	1.35
2	F	301	FMN	C9A-N10	2.64	1.42	1.38
2	E	301	FMN	C9A-N10	2.67	1.42	1.38
2	H	301	FMN	C9A-N10	2.68	1.42	1.38
2	A	301	FMN	C9A-N10	2.70	1.42	1.38
2	G	301	FMN	C9A-N10	2.70	1.42	1.38
2	F	301	FMN	C5A-N5	2.76	1.39	1.35
2	D	301	FMN	C5A-N5	2.78	1.39	1.35
2	E	301	FMN	C5A-N5	2.79	1.39	1.35
2	B	301	FMN	C4-C4A	2.80	1.47	1.41
2	C	301	FMN	C9A-N10	2.81	1.42	1.38
2	A	301	FMN	C5A-N5	2.83	1.39	1.35
2	C	301	FMN	C5A-N5	2.84	1.39	1.35
2	H	301	FMN	C5A-N5	2.85	1.39	1.35
2	H	301	FMN	C4-C4A	2.93	1.47	1.41
2	B	301	FMN	C5A-N5	2.94	1.39	1.35
2	G	301	FMN	C4-C4A	2.94	1.47	1.41
2	D	301	FMN	C4-C4A	2.95	1.47	1.41
2	E	301	FMN	C4A-C10	2.99	1.46	1.40
2	G	301	FMN	C4A-C10	2.99	1.46	1.40
2	F	301	FMN	C4-C4A	3.00	1.47	1.41
2	B	301	FMN	C4A-C10	3.07	1.46	1.40
2	C	301	FMN	C4-C4A	3.09	1.47	1.41
2	A	301	FMN	C4-C4A	3.10	1.47	1.41
2	D	301	FMN	C4A-C10	3.11	1.46	1.40
2	D	301	FMN	C4-N3	3.13	1.38	1.33
2	E	301	FMN	C4-N3	3.15	1.38	1.33
2	C	301	FMN	C4A-C10	3.17	1.46	1.40
2	H	301	FMN	C4-N3	3.18	1.38	1.33
2	A	301	FMN	C4A-C10	3.23	1.46	1.40
2	C	301	FMN	C4-N3	3.25	1.38	1.33
2	F	301	FMN	C4-N3	3.26	1.38	1.33
2	G	301	FMN	C4-N3	3.27	1.38	1.33
2	E	301	FMN	C4-C4A	3.29	1.47	1.41
2	B	301	FMN	C4-N3	3.29	1.39	1.33
2	F	301	FMN	C4A-C10	3.30	1.46	1.40
2	H	301	FMN	C4A-C10	3.38	1.47	1.40
2	A	301	FMN	C4-N3	3.38	1.39	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	FMN	C4A-C4-N3	-7.36	113.89	123.52
2	A	301	FMN	C4A-C4-N3	-7.34	113.92	123.52
2	C	301	FMN	C4A-C4-N3	-7.34	113.92	123.52
2	G	301	FMN	C4A-C4-N3	-7.34	113.92	123.52
2	B	301	FMN	C4A-C4-N3	-7.34	113.93	123.52
2	E	301	FMN	C4A-C4-N3	-7.34	113.93	123.52
2	H	301	FMN	C4A-C4-N3	-7.30	113.98	123.52
2	D	301	FMN	C4A-C4-N3	-7.25	114.05	123.52
2	G	301	FMN	C4A-C10-N10	-5.08	116.83	120.52
2	A	301	FMN	C4A-C10-N10	-5.04	116.86	120.52
2	H	301	FMN	C4A-C10-N10	-5.03	116.87	120.52
2	F	301	FMN	C4A-C10-N10	-5.00	116.89	120.52
2	E	301	FMN	C4A-C10-N10	-4.94	116.93	120.52
2	D	301	FMN	C4A-C10-N10	-4.93	116.94	120.52
2	B	301	FMN	C4A-C10-N10	-4.91	116.95	120.52
2	C	301	FMN	C4A-C10-N10	-4.90	116.96	120.52
2	B	301	FMN	N3-C2-N1	-4.66	119.85	127.69
2	H	301	FMN	N3-C2-N1	-4.63	119.90	127.69
2	G	301	FMN	N3-C2-N1	-4.61	119.93	127.69
2	D	301	FMN	N3-C2-N1	-4.58	119.98	127.69
2	C	301	FMN	N3-C2-N1	-4.56	120.01	127.69
2	E	301	FMN	N3-C2-N1	-4.55	120.03	127.69
2	F	301	FMN	N3-C2-N1	-4.52	120.07	127.69
2	A	301	FMN	N3-C2-N1	-4.52	120.08	127.69
2	B	301	FMN	C4-C4A-C10	-3.90	117.44	119.94
2	A	301	FMN	C4-C4A-C10	-3.90	117.44	119.94
2	H	301	FMN	C4-C4A-C10	-3.86	117.47	119.94
2	C	301	FMN	C4-C4A-C10	-3.86	117.47	119.94
2	D	301	FMN	C4-C4A-C10	-3.78	117.52	119.94
2	E	301	FMN	C4-C4A-C10	-3.74	117.55	119.94
2	G	301	FMN	C4-C4A-C10	-3.74	117.55	119.94
2	F	301	FMN	C4-C4A-C10	-3.70	117.58	119.94
2	A	301	FMN	C4-N3-C2	12.82	125.86	115.16
2	C	301	FMN	C4-N3-C2	12.84	125.87	115.16
2	D	301	FMN	C4-N3-C2	12.85	125.88	115.16
2	F	301	FMN	C4-N3-C2	12.86	125.88	115.16
2	B	301	FMN	C4-N3-C2	12.87	125.90	115.16
2	G	301	FMN	C4-N3-C2	12.89	125.91	115.16
2	E	301	FMN	C4-N3-C2	12.90	125.92	115.16
2	H	301	FMN	C4-N3-C2	13.01	126.01	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	MPD	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	246/253 (97%)	0.64	21 (8%) 13 7	50, 70, 91, 105	0
1	B	246/253 (97%)	0.50	12 (4%) 33 23	49, 67, 89, 114	0
1	C	245/253 (96%)	0.19	10 (4%) 41 30	27, 47, 75, 105	0
1	D	246/253 (97%)	0.05	4 (1%) 74 67	30, 44, 69, 85	0
1	E	246/253 (97%)	0.87	38 (15%) 3 2	52, 74, 100, 116	0
1	F	246/253 (97%)	0.65	23 (9%) 11 6	51, 70, 90, 109	0
1	G	246/253 (97%)	0.17	5 (2%) 68 59	28, 47, 76, 93	0
1	H	246/253 (97%)	0.06	3 (1%) 81 74	26, 43, 69, 85	0
All	All	1967/2024 (97%)	0.39	116 (5%) 26 17	26, 61, 89, 116	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	ALA	6.0
1	E	185	SER	4.5
1	B	89	ALA	4.5
1	F	188	HIS	4.2
1	E	147	LEU	4.1
1	C	214	ASP	3.9
1	F	153	TYR	3.9
1	A	200	GLU	3.8
1	A	214	ASP	3.8
1	G	185	SER	3.7
1	F	185	SER	3.7
1	F	177	GLN	3.7
1	E	148	LEU	3.6
1	F	186	TYR	3.5
1	E	168	HIS	3.4
1	E	52	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	213	ASP	3.3
1	E	27	LEU	3.3
1	A	56	LYS	3.3
1	F	94	ASP	3.2
1	F	89	ALA	3.2
1	E	191	LYS	3.2
1	B	90	ALA	3.2
1	A	217	TRP	3.2
1	A	188	HIS	3.1
1	E	187	ASN	3.1
1	D	188	HIS	3.1
1	A	213	ASP	3.1
1	E	210	ASN	3.0
1	B	213	ASP	3.0
1	A	181	HIS	3.0
1	F	178	ALA	3.0
1	E	207	LYS	2.9
1	F	215	ARG	2.9
1	E	55	GLU	2.9
1	F	182	HIS	2.9
1	D	55	GLU	2.8
1	E	200	GLU	2.8
1	H	185	SER	2.8
1	E	6	ARG	2.8
1	E	203	GLU	2.8
1	F	187	ASN	2.8
1	A	89	ALA	2.8
1	E	199	ALA	2.8
1	F	3	GLU	2.7
1	E	92	LEU	2.7
1	E	217	TRP	2.7
1	E	214	ASP	2.7
1	G	191	LYS	2.7
1	E	206	LYS	2.7
1	A	143	GLU	2.7
1	C	54	LYS	2.6
1	E	149	ASP	2.6
1	E	212	ALA	2.6
1	C	188	HIS	2.6
1	E	184	GLU	2.6
1	E	96	PRO	2.6
1	E	24	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	51	VAL	2.5
1	F	189	ASP	2.5
1	E	134	ILE	2.5
1	E	23	SER	2.5
1	F	55	GLU	2.5
1	E	177	GLN	2.5
1	E	2	ASN	2.5
1	A	151	PRO	2.5
1	D	185	SER	2.5
1	G	202	ALA	2.5
1	A	66	ASN	2.4
1	F	22	VAL	2.4
1	B	194	ILE	2.4
1	B	94	ASP	2.4
1	C	184	GLU	2.4
1	F	1	MET	2.4
1	E	189	ASP	2.4
1	H	94	ASP	2.4
1	E	1	MET	2.4
1	E	179	ALA	2.3
1	B	163	GLY	2.3
1	B	214	ASP	2.3
1	A	199	ALA	2.3
1	C	210	ASN	2.3
1	F	148	LEU	2.3
1	F	246	LYS	2.3
1	A	210	ASN	2.3
1	A	54	LYS	2.3
1	B	199	ALA	2.3
1	F	47	THR	2.2
1	B	54	LYS	2.2
1	A	185	SER	2.2
1	C	185	SER	2.2
1	B	28	ASP	2.1
1	F	51	VAL	2.1
1	A	212	ALA	2.1
1	F	93	ASN	2.1
1	G	203	GLU	2.1
1	H	214	ASP	2.1
1	E	16	GLN	2.1
1	E	22	VAL	2.1
1	A	230	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	52	GLN	2.1
1	B	58	LYS	2.1
1	E	202	ALA	2.1
1	G	1	MET	2.1
1	C	211	GLY	2.1
1	F	21	ALA	2.1
1	A	125	GLU	2.1
1	C	52	GLN	2.0
1	C	177	GLN	2.0
1	E	225	TYR	2.0
1	E	67	GLN	2.0
1	C	55	GLU	2.0
1	A	94	ASP	2.0
1	B	200	GLU	2.0
1	D	199	ALA	2.0
1	F	66	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	D	302	5/5	0.91	0.20	0.55	11,16,18,19	0
2	FMN	C	301	31/31	0.94	0.20	0.24	26,35,49,51	0
2	FMN	H	301	31/31	0.94	0.19	0.20	31,39,41,42	0
2	FMN	B	301	31/31	0.90	0.22	0.17	68,73,78,79	0
2	FMN	A	301	31/31	0.92	0.21	0.09	58,68,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FMN	F	301	31/31	0.92	0.20	0.06	61,68,71,72	0
2	FMN	G	301	31/31	0.94	0.19	-0.05	32,44,67,68	0
2	FMN	D	301	31/31	0.95	0.18	-0.12	35,38,44,47	0
2	FMN	E	301	31/31	0.92	0.20	-0.79	47,61,80,82	0
4	SO4	D	303	5/5	0.93	0.17	-0.84	74,74,75,75	0
4	SO4	H	303	5/5	0.93	0.16	-0.95	70,71,72,72	0
4	SO4	G	302	5/5	0.85	0.24	-	82,83,83,84	0
3	MPD	C	302	8/8	0.75	0.31	-	43,47,50,52	0
3	MPD	H	302	8/8	0.69	0.32	-	38,46,49,50	0
4	SO4	C	303	5/5	0.83	0.25	-	86,86,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.