



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:14 PM GMT

PDB ID : 2HAY  
Title : The Crystal Structure of the Putative NAD(P)H-Flavin Oxidoreductase from Streptococcus pyogenes M1 GAS  
Authors : Kim, Y.; Duggan, E.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2006-06-13  
Resolution : 2.11 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](mailto: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.

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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-20026982  
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-20026982

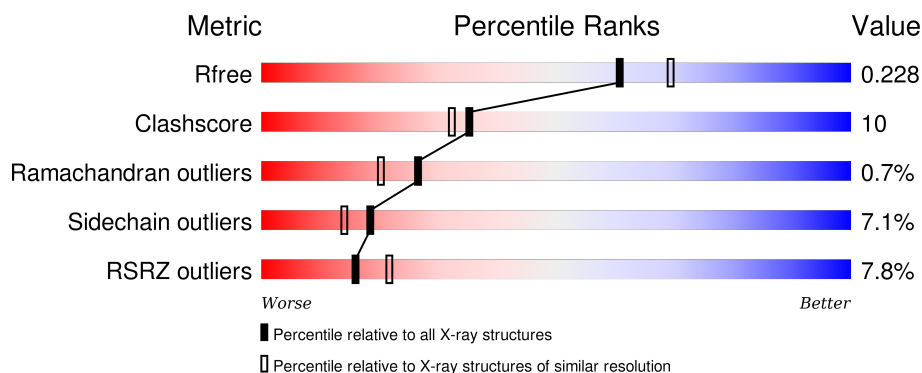
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	224	<div> <div>8%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	B	224	<div> <div>8%</div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	C	224	<div> <div>7%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	D	224	<div> <div>7%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>

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
2	SO4	B	802	-	-	-	X
2	SO4	D	804	-	-	-	X
2	SO4	D	805	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8080 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 Putative NAD(P)H-flavin oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	Se	0	9	0
			1834	1167	327	332	1	7			
1	B	221	Total	C	N	O	S	Se	0	9	0
			1858	1182	321	344	1	10			
1	C	216	Total	C	N	O	S	Se	0	5	0
			1781	1137	311	323	1	9			
1	D	222	Total	C	N	O	S	Se	0	7	0
			1849	1177	325	338	1	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q9A120
A	-1	ASN	-	CLONING ARTIFACT	UNP Q9A120
A	0	ALA	-	CLONING ARTIFACT	UNP Q9A120
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	128	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	130	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	152	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	153	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	154	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	194	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
A	217	MSE	ILE	CONFLICT	UNP Q9A120
B	-2	SER	-	CLONING ARTIFACT	UNP Q9A120
B	-1	ASN	-	CLONING ARTIFACT	UNP Q9A120
B	0	ALA	-	CLONING ARTIFACT	UNP Q9A120
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
B	128	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
B	130	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
B	152	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
B	153	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
B	154	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
B	194	MSE	MET	MODIFIED RESIDUE	UNP Q9A120

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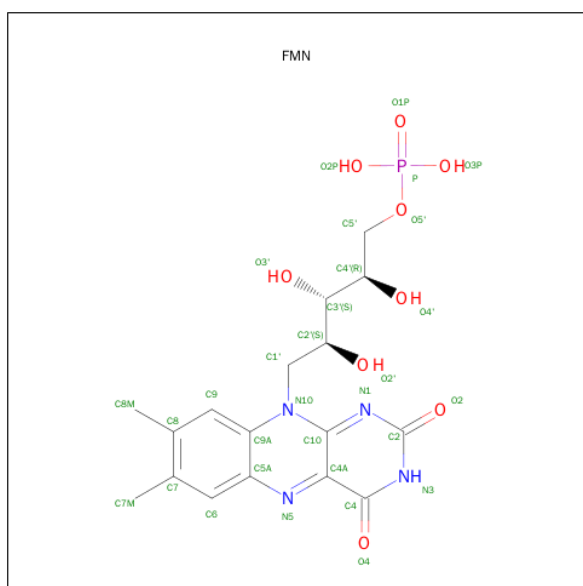
Chain	Residue	Modelled	Actual	Comment	Reference
B	217	MSE	ILE	CONFLICT	UNP Q9A120
C	-2	SER	-	CLONING ARTIFACT	UNP Q9A120
C	-1	ASN	-	CLONING ARTIFACT	UNP Q9A120
C	0	ALA	-	CLONING ARTIFACT	UNP Q9A120
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	128	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	130	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	152	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	153	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	154	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	194	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
C	217	MSE	ILE	CONFLICT	UNP Q9A120
D	-2	SER	-	CLONING ARTIFACT	UNP Q9A120
D	-1	ASN	-	CLONING ARTIFACT	UNP Q9A120
D	0	ALA	-	CLONING ARTIFACT	UNP Q9A120
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	128	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	130	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	152	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	153	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	154	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	194	MSE	MET	MODIFIED RESIDUE	UNP Q9A120
D	217	MSE	ILE	CONFLICT	UNP Q9A120

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	152	Total O 152 152	0	0

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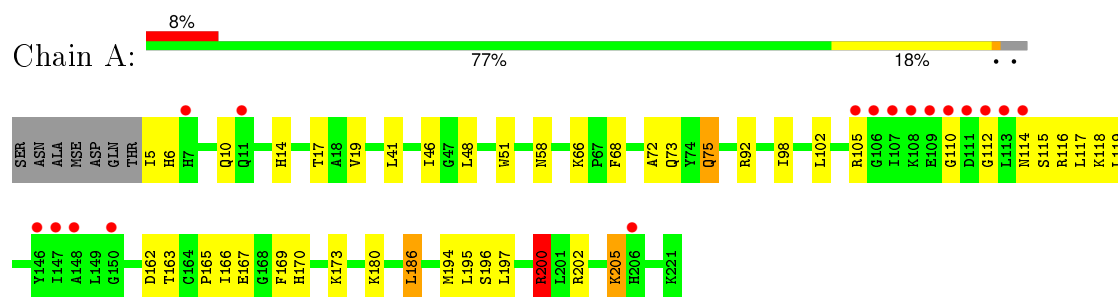
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	161	Total 161	O 161	0	0
4	C	141	Total 141	O 141	0	0
4	D	155	Total 155	O 155	0	0

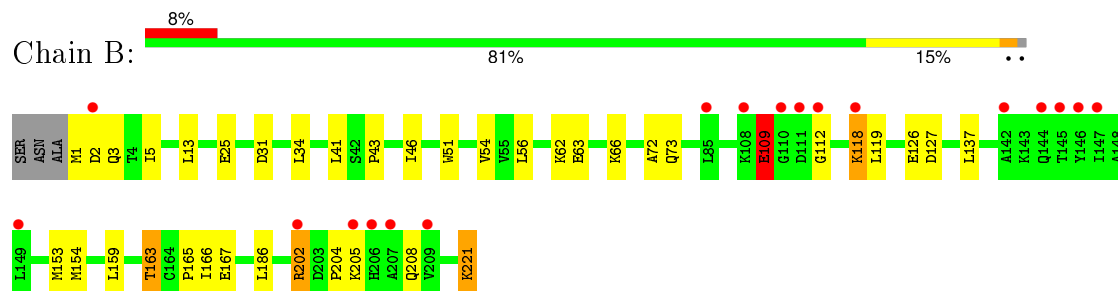
### 3 Residue-property plots [i](#)

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.

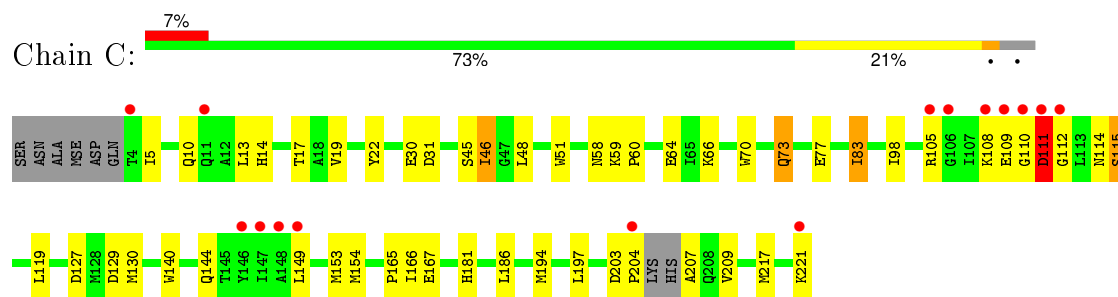
- Molecule 1: Putative NAD(P)H-flavin oxidoreductase



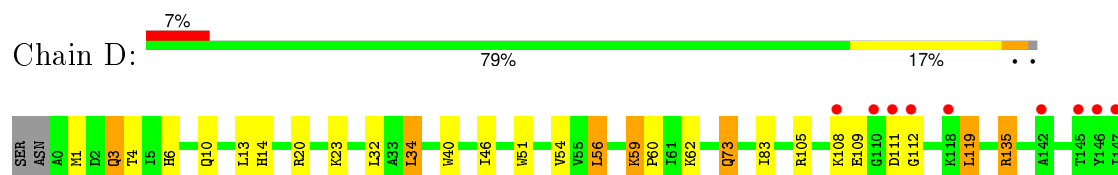
- Molecule 1: Putative NAD(P)H-flavin oxidoreductase



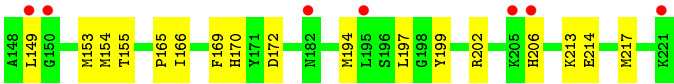
- Molecule 1: Putative NAD(P)H-flavin oxidoreductase



- Molecule 1: Putative NAD(P)H-flavin oxidoreductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.20 Å 91.87 Å 175.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.71 – 2.11 40.71 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.71-2.11) 96.8 (40.71-2.11)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.175 , 0.232 0.171 , 0.228	Depositor DCC
$R_{free}$ test set	5552 reflections (11.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	1.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55132 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, 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	0.60	0/1867	0.72	2/2504 (0.1%)
1	B	0.65	0/1889	0.68	0/2532
1	C	0.61	0/1810	0.71	1/2427 (0.0%)
1	D	0.60	0/1880	0.70	0/2522
All	All	0.61	0/7446	0.70	3/9985 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	200	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	111	ASP	N-CA-C	-5.40	96.41	111.00

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	1834	0	1833	47	0
1	B	1858	0	1858	32	0
1	C	1781	0	1797	42	0
1	D	1849	0	1855	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	D	10	0	0	0	0
3	A	31	0	19	5	0
3	B	31	0	19	3	0
3	C	31	0	19	2	0
3	D	31	0	19	3	0
4	A	152	0	0	6	0
4	B	161	0	0	3	0
4	C	141	0	0	2	0
4	D	155	0	0	4	0
All	All	8080	0	7419	146	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 10.

All (146) 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)
4:A:953:HOH:O	1:B:221:LYS:HB2	1.42	1.20
1:C:59[B]:LYS:H	1:C:59[B]:LYS:HE2	1.30	0.96
1:A:163:THR:HG22	1:A:197:LEU:HD22	1.50	0.93
1:A:205:LYS:H	1:A:205:LYS:CD	1.87	0.83
1:C:83:ILE:HD13	1:C:197:LEU:CD1	2.10	0.81
1:B:159:LEU:HD22	1:D:4:THR:HG21	1.61	0.80
1:D:73[A]:GLN:HE21	1:D:73[A]:GLN:HA	1.49	0.77
1:A:163:THR:HG22	1:A:197:LEU:CD2	2.15	0.76
1:C:59[B]:LYS:HG2	1:C:60:PRO:HD3	1.68	0.75
1:D:166:ILE:HG21	1:D:194:MSE:HE3	1.69	0.74
1:D:59[A]:LYS:HD2	1:D:60:PRO:HD3	1.70	0.74
1:A:110:GLY:O	1:A:114:ASN:HB2	1.89	0.72
1:B:3:GLN:HG2	1:D:199:TYR:CZ	2.25	0.71
1:A:166:ILE:HG21	1:A:194:MSE:HE3	1.72	0.69
1:D:109:GLU:HB2	1:D:111:ASP:OD1	1.92	0.69
1:A:166:ILE:HG21	1:A:194:MSE:CE	2.22	0.68
1:B:163:THR:HG22	4:B:804:HOH:O	1.91	0.68
1:D:109:GLU:HG3	1:D:112:GLY:H	1.57	0.68
1:D:169:PHE:CD1	1:D:194:MSE:HE2	2.32	0.65
1:B:2[A]:ASP:OD2	1:B:5:ILE:HD12	1.96	0.65
1:A:165:PRO:HG2	3:A:702:FMN:C9	2.28	0.64
1:C:10[B]:GLN:NE2	4:C:808:HOH:O	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PRO:HA	2:B:803:SO4:O4	1.99	0.62
1:C:83:ILE:HD13	1:C:197:LEU:HD13	1.80	0.62
1:A:205:LYS:H	1:A:205:LYS:HD3	1.64	0.61
1:A:10:GLN:HE21	1:A:14:HIS:CE1	2.18	0.61
1:A:75[B]:GLN:HE21	1:A:75[B]:GLN:H	1.48	0.61
1:C:83:ILE:HD13	1:C:197:LEU:HD11	1.80	0.61
1:C:217[B]:MSE:SE	1:D:40:TRP:HB2	2.52	0.60
1:A:196:SER:O	1:A:197:LEU:HD23	2.02	0.60
1:A:162:ASP:OD2	1:A:200:ARG:HD2	2.02	0.59
1:D:73[A]:GLN:HE21	1:D:73[A]:GLN:CA	2.14	0.58
1:C:129:ASP:O	1:D:135:ARG:NH1	2.37	0.58
1:C:154[B]:MSE:HG2	1:D:154:MSE:HG2	1.85	0.58
1:D:165:PRO:HG2	3:D:703:FMN:C9	2.33	0.57
1:D:59[A]:LYS:CD	1:D:59[A]:LYS:H	2.16	0.57
1:D:170:HIS:CE1	1:D:172:ASP:HB3	2.39	0.57
1:A:169:PHE:CD1	1:A:194:MSE:HE2	2.39	0.57
1:D:166:ILE:HG21	1:D:194:MSE:CE	2.35	0.56
1:C:31:ASP:OD1	1:D:6:HIS:HE1	1.88	0.56
1:A:10:GLN:HE21	1:A:14:HIS:HE1	1.54	0.55
1:B:13:LEU:CD2	1:B:154[A]:MSE:HE1	2.36	0.55
1:C:45:SER:H	1:C:144:GLN:NE2	2.04	0.55
1:C:13:LEU:CD2	1:C:154[A]:MSE:HE1	2.36	0.54
1:D:166:ILE:CG2	1:D:194:MSE:HE3	2.36	0.54
4:B:807:HOH:O	1:D:4:THR:HG23	2.06	0.54
1:D:170:HIS:HE1	1:D:172:ASP:HB3	1.72	0.54
1:C:144:GLN:HE22	3:D:703:FMN:C7M	2.19	0.54
1:C:73:GLN:O	1:C:77:GLU:HG2	2.07	0.54
1:B:165:PRO:HG2	3:B:701:FMN:C9	2.37	0.54
1:D:20[A]:ARG:NH2	4:D:892:HOH:O	2.40	0.53
1:C:13:LEU:HD23	1:C:154[A]:MSE:HE1	1.89	0.53
1:B:159:LEU:O	1:D:4:THR:HG22	2.09	0.52
1:A:166:ILE:CG2	1:A:194:MSE:CE	2.86	0.52
1:D:10:GLN:O	1:D:14:HIS:HD2	1.93	0.51
1:D:13:LEU:HD21	1:D:154:MSE:HE1	1.92	0.51
1:C:111:ASP:O	1:C:115:SER:HB2	2.11	0.51
1:B:3:GLN:HG2	1:D:199:TYR:CE2	2.45	0.51
1:A:72:ALA:HA	1:A:75[B]:GLN:NE2	2.26	0.51
1:B:72:ALA:HB2	1:B:166:ILE:HG21	1.92	0.50
1:A:163:THR:CG2	1:A:197:LEU:HD22	2.32	0.50
1:C:110:GLY:O	1:C:114:ASN:HB2	2.11	0.50
1:A:66:LYS:O	1:A:73[A]:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ASN:OD1	1:C:60:PRO:HD2	2.12	0.50
1:D:149:LEU:HG	1:D:153:MSE:HE2	1.94	0.49
1:A:68:PHE:CD2	1:A:173:LYS:HD3	2.48	0.49
1:A:205:LYS:H	1:A:205:LYS:HD2	1.74	0.49
3:A:702:FMN:HM81	1:B:43:PRO:HB2	1.94	0.49
1:A:6:HIS:HE1	1:B:31:ASP:OD1	1.96	0.48
1:C:165:PRO:HG2	3:C:704:FMN:C9	2.43	0.48
1:C:166:ILE:HB	1:C:194:MSE:HB2	1.95	0.48
1:B:153:MSE:HG2	1:B:163:THR:HG21	1.96	0.48
1:C:10[A]:GLN:O	1:C:14:HIS:HD2	1.96	0.48
1:A:115:SER:HB2	4:A:912:HOH:O	2.14	0.48
1:A:41:LEU:HD22	1:B:208:GLN:NE2	2.30	0.47
1:D:20[A]:ARG:HG2	4:D:867:HOH:O	2.13	0.47
1:B:63[B]:GLU:OE2	1:B:66:LYS:NZ	2.34	0.47
1:B:118:LYS:HE3	4:B:923:HOH:O	2.15	0.47
1:B:202:ARG:NH2	1:B:205:LYS:NZ	2.61	0.47
1:C:203:ASP:HB3	1:C:204:PRO:HD2	1.96	0.47
3:A:702:FMN:N5	4:A:943:HOH:O	2.35	0.46
1:C:144:GLN:HE22	3:D:703:FMN:HM71	1.81	0.46
1:C:109:GLU:HG2	1:C:111:ASP:H	1.79	0.46
1:D:56:LEU:HD13	1:D:62:LYS:HG2	1.96	0.46
1:A:112:GLY:HA3	4:A:887:HOH:O	2.16	0.46
1:D:59[A]:LYS:H	1:D:59[A]:LYS:HD2	1.81	0.46
1:C:109:GLU:OE1	1:C:112:GLY:HA3	2.16	0.46
1:D:166:ILE:CG2	1:D:194:MSE:CE	2.93	0.46
1:A:170:HIS:HE1	1:B:126[B]:GLU:OE2	1.98	0.46
1:A:10:GLN:NE2	1:A:14:HIS:HE1	2.13	0.46
1:C:30:GLU:HB2	1:D:1:MSE:HE3	1.96	0.46
1:A:6:HIS:CD2	1:B:34:LEU:HD22	2.51	0.45
1:A:72:ALA:HB2	1:A:166:ILE:HG21	1.97	0.45
1:A:5:ILE:N	4:A:940:HOH:O	2.49	0.45
1:B:13:LEU:HD23	1:B:154[A]:MSE:HE1	1.97	0.45
1:B:13:LEU:HD21	1:B:154[A]:MSE:HE1	1.97	0.45
1:D:59[B]:LYS:HG2	4:D:859:HOH:O	2.17	0.45
1:A:169:PHE:O	1:B:127:ASP:HB3	2.17	0.45
1:C:207:ALA:N	4:C:801:HOH:O	2.49	0.45
1:B:56:LEU:O	1:B:62:LYS:HE3	2.16	0.45
1:C:167:GLU:HG3	3:C:704:FMN:H6	1.98	0.44
1:A:166:ILE:CG2	1:A:194:MSE:HE3	2.43	0.44
1:C:59[B]:LYS:H	1:C:59[B]:LYS:CE	2.13	0.44
1:C:221:LYS:HG3	1:D:59[A]:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLU:OE1	1:C:181:HIS:NE2	2.40	0.44
1:C:19:VAL:HG22	1:C:22:TYR:CZ	2.52	0.44
1:A:72:ALA:O	1:A:75[A]:GLN:HG2	2.18	0.44
1:C:46:ILE:HD11	1:C:98:ILE:CD1	2.48	0.44
1:C:130:MSE:HE1	1:C:140:TRP:CD2	2.53	0.44
1:D:166:ILE:HB	1:D:194:MSE:HB2	2.00	0.43
1:B:167:GLU:HG3	3:B:701:FMN:H6	2.00	0.43
1:B:25[B]:GLU:HG2	1:D:3:GLN:OE1	2.18	0.43
1:A:195:LEU:CD2	1:A:197:LEU:HD21	2.49	0.43
1:A:205:LYS:N	1:A:205:LYS:CD	2.69	0.42
1:C:109:GLU:CG	1:C:111:ASP:HB3	2.49	0.42
1:C:109:GLU:HG2	1:C:111:ASP:HB3	2.01	0.42
1:D:83:ILE:HD12	1:D:197:LEU:HD11	2.01	0.42
1:D:3:GLN:HA	1:D:3:GLN:HE21	1.83	0.42
1:A:163:THR:HB	1:A:195:LEU:HD11	2.02	0.42
1:A:167:GLU:HG3	3:A:702:FMN:H6	2.01	0.42
1:D:202:ARG:HD3	4:D:941:HOH:O	2.18	0.42
1:C:149:LEU:HG	1:C:153:MSE:HE2	2.01	0.42
1:B:109:GLU:OE1	1:B:112:GLY:HA3	2.20	0.42
1:A:169:PHE:HD1	1:A:194:MSE:HE2	1.85	0.41
1:C:70:TRP:CE3	1:D:119:LEU:HD11	2.54	0.41
1:D:135:ARG:O	1:D:135:ARG:HG2	2.20	0.41
4:A:944:HOH:O	1:B:1:MSE:HB2	2.20	0.41
1:D:34:LEU:HD13	1:D:155:THR:CG2	2.50	0.41
1:C:83:ILE:HD12	1:C:83:ILE:N	2.35	0.41
1:C:19:VAL:HG22	1:C:22:TYR:CE1	2.56	0.41
1:B:41:LEU:HA	1:B:41:LEU:HD23	1.87	0.41
1:B:165:PRO:O	3:B:701:FMN:C5A	2.68	0.41
1:B:202:ARG:NH2	1:B:205:LYS:HZ2	2.19	0.41
1:A:92:ARG:O	1:A:98:ILE:HG13	2.20	0.41
1:C:127:ASP:HB3	1:D:169:PHE:O	2.20	0.41
1:A:58:ASN:ND2	1:B:221:LYS:HD3	2.36	0.40
1:C:83:ILE:CD1	1:C:83:ILE:N	2.84	0.40
1:A:166:ILE:HA	3:A:702:FMN:N5	2.36	0.40
1:A:75[B]:GLN:NE2	1:A:75[B]:GLN:H	2.15	0.40
1:D:213:LYS:HG2	1:D:217:MSE:HE3	2.03	0.40
1:A:17:THR:HG23	1:A:19:VAL:HG12	2.02	0.40
1:A:186:LEU:HA	1:A:186:LEU:HD23	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	224/224 (100%)	214 (96%)	9 (4%)	1 (0%)	39	36
1	B	228/224 (102%)	220 (96%)	6 (3%)	2 (1%)	21	14
1	C	217/224 (97%)	210 (97%)	5 (2%)	2 (1%)	21	14
1	D	227/224 (101%)	219 (96%)	7 (3%)	1 (0%)	39	36
All	All	896/896 (100%)	863 (96%)	27 (3%)	6 (1%)	26	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	GLU
1	C	111	ASP
1	A	46	ILE
1	B	46	ILE
1	C	46	ILE
1	D	46	ILE

### 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	195/184 (106%)	179 (92%)	16 (8%)	14	10
1	B	199/184 (108%)	188 (94%)	11 (6%)	27	23
1	C	190/184 (103%)	177 (93%)	13 (7%)	20	16
1	D	197/184 (107%)	179 (91%)	18 (9%)	12	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	781/736 (106%)	723 (93%)	58 (7%)	18	13

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	51	TRP
1	A	75[A]	GLN
1	A	75[B]	GLN
1	A	102	LEU
1	A	105[A]	ARG
1	A	105[B]	ARG
1	A	116	ARG
1	A	117	LEU
1	A	118	LYS
1	A	119	LEU
1	A	180	LYS
1	A	186	LEU
1	A	200	ARG
1	A	202	ARG
1	A	205	LYS
1	B	51	TRP
1	B	54	VAL
1	B	73	GLN
1	B	109	GLU
1	B	118	LYS
1	B	119	LEU
1	B	137	LEU
1	B	163	THR
1	B	186	LEU
1	B	202	ARG
1	B	221	LYS
1	C	5	ILE
1	C	17	THR
1	C	48	LEU
1	C	51	TRP
1	C	66	LYS
1	C	73	GLN
1	C	83	ILE
1	C	105	ARG
1	C	108	LYS
1	C	115	SER

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Mol	Chain	Res	Type
1	C	119	LEU
1	C	186	LEU
1	C	209	VAL
1	D	3	GLN
1	D	23	LYS
1	D	32	LEU
1	D	34	LEU
1	D	51	TRP
1	D	54	VAL
1	D	56	LEU
1	D	59[A]	LYS
1	D	59[B]	LYS
1	D	73[A]	GLN
1	D	73[B]	GLN
1	D	105	ARG
1	D	108	LYS
1	D	119	LEU
1	D	135	ARG
1	D	206[A]	HIS
1	D	206[B]	HIS
1	D	214	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	14	HIS
1	A	170	HIS
1	B	73	GLN
1	B	151	ASN
1	B	208	GLN
1	C	11	GLN
1	C	144	GLN
1	C	176	HIS
1	D	6	HIS
1	D	14	HIS
1	D	114	ASN
1	D	151	ASN

### 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 ⓘ

9 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$
3	FMN	A	702	-	32,33,33	1.68	6 (18%)	34,50,50	2.25	7 (20%)
2	SO4	A	801	-	4,4,4	0.19	0	6,6,6	0.07	0
3	FMN	B	701	-	32,33,33	1.57	5 (15%)	34,50,50	2.13	7 (20%)
2	SO4	B	802	-	4,4,4	2.73	2 (50%)	6,6,6	0.52	0
2	SO4	B	803	-	4,4,4	0.18	0	6,6,6	0.12	0
3	FMN	C	704	-	32,33,33	1.62	6 (18%)	34,50,50	2.01	5 (14%)
3	FMN	D	703	-	32,33,33	1.68	5 (15%)	34,50,50	1.87	5 (14%)
2	SO4	D	804	-	4,4,4	0.11	0	6,6,6	0.25	0
2	SO4	D	805	-	4,4,4	0.16	0	6,6,6	0.24	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
3	FMN	A	702	-	-	0/18/18/18	0/3/3/3
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	FMN	B	701	-	-	0/18/18/18	0/3/3/3
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	803	-	-	0/0/0/0	0/0/0/0
3	FMN	C	704	-	-	0/18/18/18	0/3/3/3
3	FMN	D	703	-	-	0/18/18/18	0/3/3/3
2	SO4	D	804	-	-	0/0/0/0	0/0/0/0
2	SO4	D	805	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	FMN	C6-C5A	-2.59	1.37	1.41
3	A	702	FMN	C1'-N10	2.19	1.50	1.48
3	B	701	FMN	C9A-N10	2.42	1.42	1.38
3	A	702	FMN	C9A-N10	2.43	1.42	1.38
3	B	701	FMN	C5A-N5	2.79	1.39	1.35
3	C	704	FMN	C1'-N10	2.79	1.51	1.48
3	D	703	FMN	C1'-N10	2.93	1.51	1.48
3	C	704	FMN	C5A-N5	3.01	1.40	1.35
3	A	702	FMN	C5A-N5	3.10	1.40	1.35
3	A	702	FMN	C10-N1	3.30	1.41	1.35
3	A	702	FMN	C4-N3	3.39	1.39	1.33
2	B	802	SO4	O3-S	3.53	1.60	1.47
3	D	703	FMN	C4-N3	3.62	1.39	1.33
3	C	704	FMN	C10-N1	3.64	1.41	1.35
2	B	802	SO4	O4-S	3.68	1.60	1.47
3	B	701	FMN	C4-N3	3.72	1.39	1.33
3	D	703	FMN	C10-N1	3.81	1.42	1.35
3	C	704	FMN	C4-N3	3.89	1.40	1.33
3	D	703	FMN	C5A-N5	3.91	1.41	1.35
3	B	701	FMN	C10-N1	3.96	1.42	1.35
3	B	701	FMN	C4A-N5	4.27	1.39	1.33
3	C	704	FMN	C4A-N5	4.34	1.40	1.33
3	D	703	FMN	C4A-N5	4.38	1.40	1.33
3	A	702	FMN	C4A-N5	5.18	1.41	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	704	FMN	N3-C2-N1	-5.16	119.00	127.69
3	B	701	FMN	N3-C2-N1	-4.89	119.46	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FMN	C4A-C4-N3	-4.27	117.94	123.52
3	A	702	FMN	N3-C2-N1	-4.25	120.54	127.69
3	D	703	FMN	N3-C2-N1	-4.12	120.75	127.69
3	B	701	FMN	C4A-C10-N10	-3.87	117.71	120.52
3	B	701	FMN	C4A-C4-N3	-3.34	119.16	123.52
3	A	702	FMN	C4A-C10-N10	-3.34	118.09	120.52
3	C	704	FMN	C4A-C4-N3	-2.99	119.61	123.52
3	D	703	FMN	C4A-C10-N10	-2.80	118.49	120.52
3	D	703	FMN	C4A-C4-N3	-2.57	120.16	123.52
3	C	704	FMN	C4-C4A-C10	-2.05	118.63	119.94
3	C	704	FMN	C5A-C9A-N10	2.28	119.29	117.58
3	B	701	FMN	O3P-P-O5'	2.31	113.46	106.72
3	A	702	FMN	O2P-P-O5'	2.42	113.78	106.72
3	B	701	FMN	C5A-C9A-N10	2.59	119.52	117.58
3	B	701	FMN	C4A-N5-C5A	3.05	120.31	116.72
3	A	702	FMN	C5A-C9A-N10	3.34	120.08	117.58
3	A	702	FMN	C4A-N5-C5A	3.80	121.20	116.72
3	D	703	FMN	C5A-C9A-N10	4.20	120.73	117.58
3	D	703	FMN	C4-N3-C2	6.85	120.87	115.16
3	B	701	FMN	C4-N3-C2	8.14	121.95	115.16
3	C	704	FMN	C4-N3-C2	8.27	122.05	115.16
3	A	702	FMN	C4-N3-C2	8.46	122.22	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	FMN	5	0
3	B	701	FMN	3	0
2	B	803	SO4	1	0
3	C	704	FMN	2	0
3	D	703	FMN	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	210/224 (93%)	0.44	17 (8%) 15 20	23, 28, 44, 58	0
1	B	213/224 (95%)	0.49	18 (8%) 13 18	23, 29, 49, 59	0
1	C	209/224 (93%)	0.51	15 (7%) 18 25	24, 29, 39, 50	0
1	D	214/224 (95%)	0.48	16 (7%) 17 23	23, 29, 46, 57	0
All	All	846/896 (94%)	0.48	66 (7%) 16 22	23, 29, 45, 59	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	111	ASP	9.4
1	C	111	ASP	5.7
1	D	112	GLY	5.7
1	B	205	LYS	5.5
1	C	112	GLY	5.5
1	A	110	GLY	5.4
1	D	205	LYS	5.3
1	B	206	HIS	5.1
1	B	147	ILE	4.3
1	C	110	GLY	4.2
1	A	106	GLY	4.1
1	A	111	ASP	4.0
1	A	7	HIS	4.0
1	A	107	ILE	3.9
1	D	206[A]	HIS	3.8
1	A	108	LYS	3.8
1	C	204	PRO	3.7
1	A	109	GLU	3.7
1	B	110	GLY	3.7
1	C	147	ILE	3.4
1	B	146	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	111	ASP	3.3
1	C	108	LYS	3.3
1	D	110	GLY	3.3
1	D	146	TYR	3.2
1	D	108	LYS	3.2
1	D	147	ILE	3.2
1	A	105[A]	ARG	3.1
1	A	146	TYR	3.1
1	C	106	GLY	3.0
1	B	112	GLY	3.0
1	A	113	LEU	3.0
1	C	149	LEU	2.9
1	C	221	LYS	2.9
1	D	221	LYS	2.9
1	A	147	ILE	2.8
1	A	112	GLY	2.8
1	A	206[A]	HIS	2.8
1	B	108	LYS	2.8
1	B	149	LEU	2.8
1	A	114	ASN	2.8
1	C	105	ARG	2.7
1	C	109	GLU	2.7
1	B	142	ALA	2.7
1	C	148	ALA	2.7
1	D	149	LEU	2.7
1	D	145	THR	2.6
1	B	118	LYS	2.5
1	D	118	LYS	2.5
1	D	142	ALA	2.5
1	B	85	LEU	2.4
1	B	207	ALA	2.4
1	B	209	VAL	2.4
1	A	11	GLN	2.3
1	C	146	TYR	2.3
1	D	182	ASN	2.3
1	B	2[A]	ASP	2.3
1	D	195	LEU	2.2
1	B	145	THR	2.2
1	B	202	ARG	2.2
1	B	144	GLN	2.1
1	D	150	GLY	2.1
1	A	150	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	4	THR	2.1
1	C	11	GLN	2.0
1	A	148	ALA	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	D	805	5/5	0.81	0.39	5.68	71,71,73,73	0
2	SO4	B	802	5/5	0.82	0.32	4.64	135,135,136,136	0
2	SO4	D	804	5/5	0.77	0.35	3.95	89,90,90,91	0
3	FMN	A	702	31/31	0.85	0.26	1.37	26,36,42,44	0
3	FMN	C	704	31/31	0.88	0.22	0.85	29,35,39,41	0
3	FMN	B	701	31/31	0.85	0.23	0.78	34,42,45,47	0
3	FMN	D	703	31/31	0.87	0.22	0.65	28,38,44,46	0
2	SO4	B	803	5/5	0.75	0.34	0.27	117,117,118,118	0
2	SO4	A	801	5/5	0.90	0.34	-	91,91,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.