



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:15 am GMT

PDB ID : 4HS4  
Title : Crystal structure of a putative chromate reductase from *Gluconacetobacter hansenii*, Gh-ChrR, containing a Y129N substitution.  
Authors : Zhang, Y.; Robinson, H.; Buchko, G.W.  
Deposited on : 2012-10-29  
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

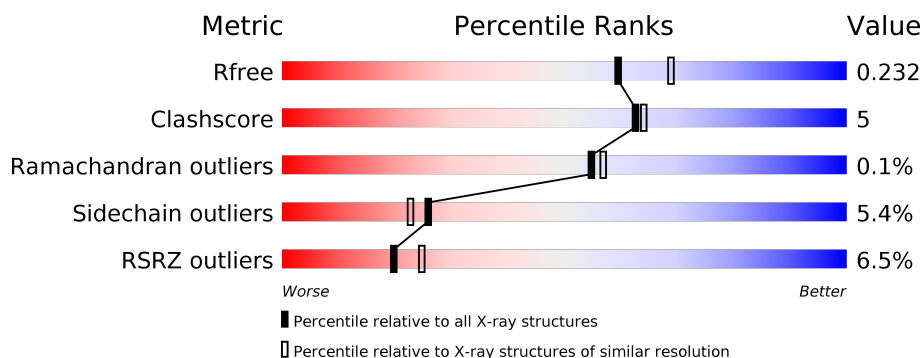
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	199	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>••</div> <div>8%</div> </div> </div>
1	B	199	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>••</div> <div>8%</div> </div> </div>
1	C	199	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>••</div> <div>8%</div> </div> </div>
1	D	199	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>8%</div> </div> </div>
1	E	199	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>••</div> <div>8%</div> </div> </div>
1	F	199	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>••</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	199	
1	H	199	

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	FMN	B	201	-	-	-	X
2	FMN	H	201	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11687 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 Chromate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	B	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	C	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	D	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	E	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	F	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	G	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			
1	H	184	Total	C	N	O	S	0	0	0
			1372	876	237	256	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
A	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
A	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
A	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
A	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
A	198	HIS	-	EXPRESSION TAG	UNP D5QFC5
A	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
B	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
B	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
B	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
B	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
B	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
B	198	HIS	-	EXPRESSION TAG	UNP D5QFC5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
C	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
C	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
C	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
C	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
C	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
C	198	HIS	-	EXPRESSION TAG	UNP D5QFC5
C	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
D	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
D	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
D	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
D	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
D	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
D	198	HIS	-	EXPRESSION TAG	UNP D5QFC5
D	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
E	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
E	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
E	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
E	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
E	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
E	198	HIS	-	EXPRESSION TAG	UNP D5QFC5
E	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
F	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
F	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
F	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
F	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
F	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
F	198	HIS	-	EXPRESSION TAG	UNP D5QFC5
F	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
G	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
G	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
G	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
G	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
G	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
G	198	HIS	-	EXPRESSION TAG	UNP D5QFC5
G	199	HIS	-	EXPRESSION TAG	UNP D5QFC5
H	129	ASN	TYR	ENGINEERED MUTATION	UNP D5QFC5
H	194	HIS	-	EXPRESSION TAG	UNP D5QFC5
H	195	HIS	-	EXPRESSION TAG	UNP D5QFC5
H	196	HIS	-	EXPRESSION TAG	UNP D5QFC5
H	197	HIS	-	EXPRESSION TAG	UNP D5QFC5
H	198	HIS	-	EXPRESSION TAG	UNP D5QFC5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	199	HIS	-	EXPRESSION TAG	UNP D5QFC5

- # FMN
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- The image displays the chemical structure of Flavin Mononucleotide (FMN). The structure consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms) attached to a ribityl chain. The ribityl chain is a three-carbon chain with hydroxyl groups at the 2' and 3' positions. The 3' carbon is linked to a phosphate group, which is further linked to a ribose sugar (a five-membered ring with an oxygen atom at the top) and a phosphate group. The ribose sugar is also linked to a phosphate group. The structure is labeled with various atoms and bonds, including carbon (C), nitrogen (N), oxygen (O), and phosphorus (P). The ribityl chain is shown in a 3D representation with wedged and dashed bonds. The phosphate groups are shown in a 2D representation. The ribose sugar is shown in a 2D representation. The structure is labeled with various atoms and bonds, including carbon (C), nitrogen (N), oxygen (O), and phosphorus (P).
- O=P([O-])([O-])O[C@H]1O[C@H](COP(=O)(O)O)[C@H](O)[C@@H]1O

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

- | Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | A     | 117      | Total O<br>117 117 | 0       | 0       |
| 3   | B     | 90       | Total O<br>90 90   | 0       | 0       |
| 3   | C     | 79       | Total O<br>79 79   | 0       | 0       |
| 3   | D     | 85       | Total O<br>85 85   | 0       | 0       |
| 3   | E     | 61       | Total O<br>61 61   | 0       | 0       |
| 3   | F     | 86       | Total O<br>86 86   | 0       | 0       |

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

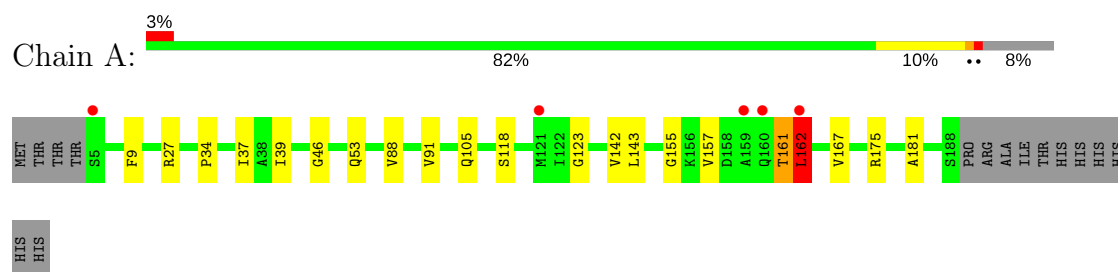
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	57	Total	O	0	0
			57	57		
3	H	43	Total	O	0	0
			43	43		

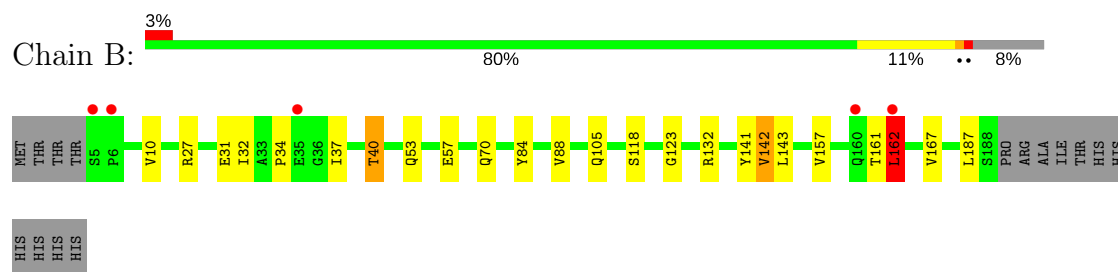
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

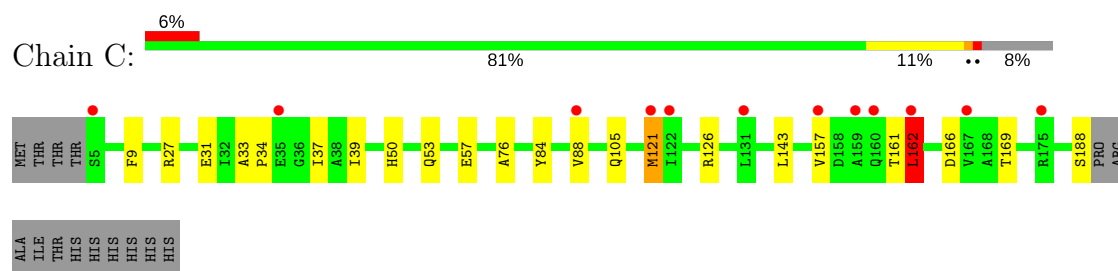
#### • Molecule 1: Chromate reductase



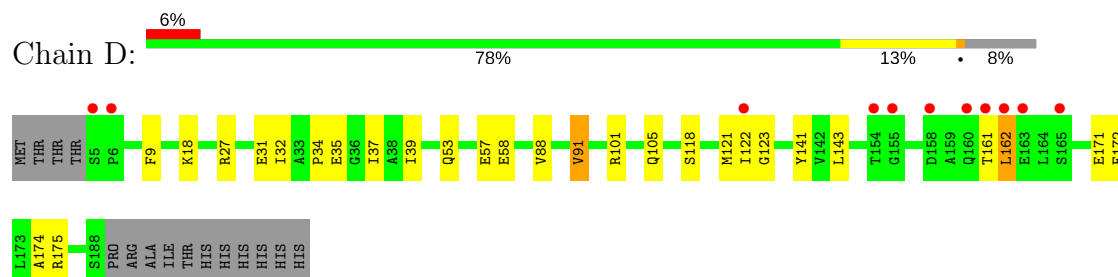
#### • Molecule 1: Chromate reductase



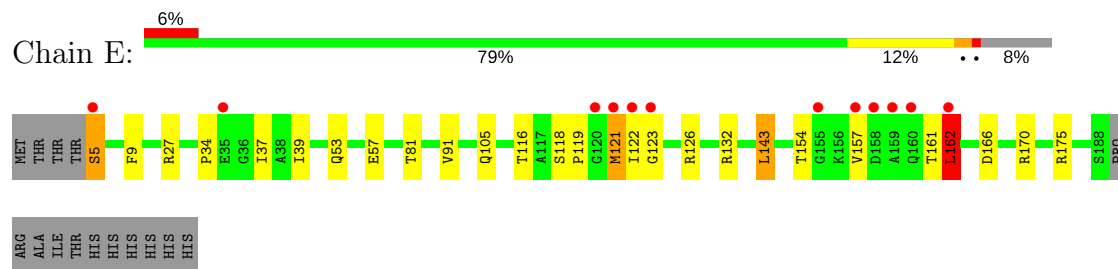
#### • Molecule 1: Chromate reductase



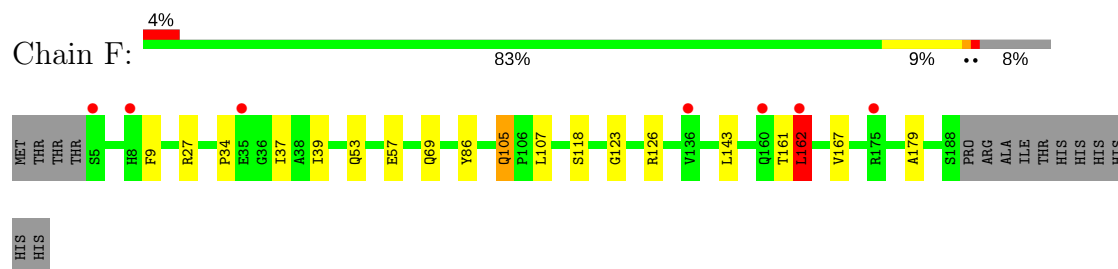
#### • Molecule 1: Chromate reductase



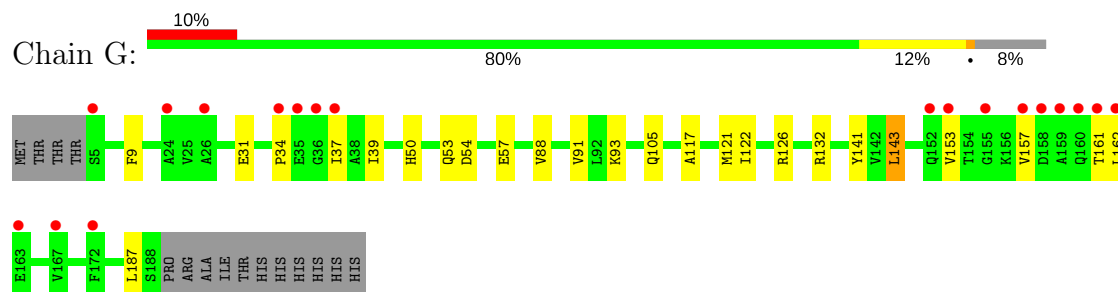
- Molecule 1: Chromate reductase



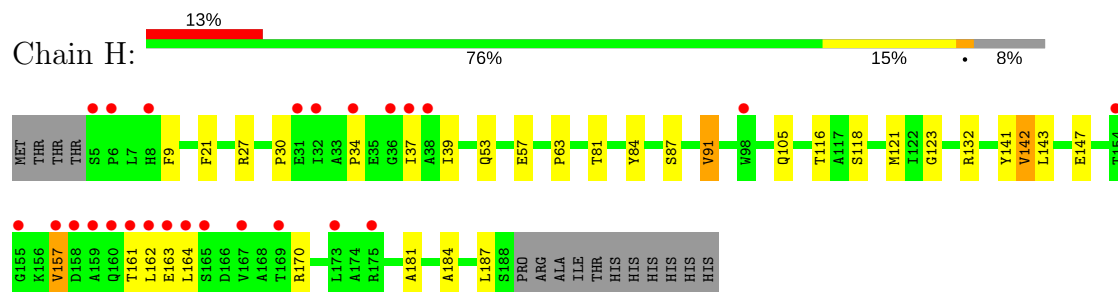
- Molecule 1: Chromate reductase



- Molecule 1: Chromate reductase



- Molecule 1: Chromate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.42Å 92.15Å 188.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.96 – 2.10 44.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.96-2.10) 99.6 (44.96-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, $R_{free}$	0.208 , 0.232 0.205 , 0.232	Depositor DCC
$R_{free}$ test set	1996 reflections (2.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.43	0/1400	0.60	1/1915 (0.1%)
1	B	0.41	0/1400	0.60	1/1915 (0.1%)
1	C	0.39	0/1400	0.58	1/1915 (0.1%)
1	D	0.39	0/1400	0.58	0/1915
1	E	0.35	0/1400	0.57	1/1915 (0.1%)
1	F	0.39	0/1400	0.59	1/1915 (0.1%)
1	G	0.35	0/1400	0.58	0/1915
1	H	0.32	0/1400	0.54	0/1915
All	All	0.38	0/11200	0.58	5/15320 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	LEU	CA-CB-CG	6.12	129.38	115.30
1	F	162	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	162	LEU	CA-CB-CG	5.68	128.37	115.30
1	E	162	LEU	CA-CB-CG	5.65	128.30	115.30
1	C	162	LEU	CA-CB-CG	5.27	127.42	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	1372	0	1402	14	0
1	B	1372	0	1402	16	0
1	C	1372	0	1402	12	0
1	D	1372	0	1402	19	0
1	E	1372	0	1402	17	0
1	F	1372	0	1402	10	1
1	G	1372	0	1402	11	0
1	H	1372	0	1402	20	1
2	B	31	0	19	2	0
2	C	31	0	19	3	0
2	H	31	0	19	2	0
3	A	117	0	0	6	1
3	B	90	0	0	8	0
3	C	79	0	0	1	0
3	D	85	0	0	4	1
3	E	61	0	0	1	0
3	F	86	0	0	3	0
3	G	57	0	0	1	0
3	H	43	0	0	4	0
All	All	11687	0	11273	112	2

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

All (112) 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:H:63:PRO:O	3:H:323:HOH:O	1.86	0.93
1:F:179:ALA:O	3:F:259:HOH:O	1.91	0.88
1:D:58:GLU:OE1	3:D:283:HOH:O	1.92	0.88
1:D:171:GLU:OE2	1:D:175:ARG:NH1	2.12	0.83
1:D:141:TYR:OH	3:D:274:HOH:O	1.95	0.82
1:A:34:PRO:HG2	1:A:37:ILE:HD12	1.63	0.79
1:C:34:PRO:HG2	1:C:37:ILE:HD12	1.64	0.77
1:B:70:GLN:NE2	3:B:343:HOH:O	2.16	0.77
1:C:126:ARG:NH1	3:C:325:HOH:O	2.19	0.75
1:H:34:PRO:HG2	1:H:37:ILE:HD12	1.70	0.73
1:B:70:GLN:NE2	3:B:375:HOH:O	2.22	0.72
1:E:34:PRO:HG2	1:E:37:ILE:HD12	1.72	0.71
1:A:27:ARG:NH2	1:A:162:LEU:HG	2.06	0.70
1:A:27:ARG:HH21	1:A:162:LEU:HG	1.56	0.69
1:C:53:GLN:O	1:C:57:GLU:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:PRO:HG2	1:D:37:ILE:HD12	1.74	0.69
1:H:184:ALA:O	3:H:337:HOH:O	2.10	0.69
1:B:70:GLN:OE1	3:B:305:HOH:O	2.12	0.68
1:G:54:ASP:OD1	3:G:217:HOH:O	2.10	0.67
1:F:34:PRO:HG2	1:F:37:ILE:HD12	1.77	0.66
1:A:155:GLY:N	1:B:57:GLU:OE1	2.29	0.65
1:D:121:MET:HG3	1:E:121:MET:HG3	1.80	0.64
1:E:9:PHE:HB2	1:E:39:ILE:HG12	1.80	0.62
1:G:34:PRO:HG2	1:G:37:ILE:HD12	1.83	0.61
2:B:201:FMN:O2'	3:B:310:HOH:O	2.15	0.61
1:E:27:ARG:NH2	1:E:162:LEU:HG	2.15	0.60
1:D:9:PHE:HB2	1:D:39:ILE:HG12	1.84	0.59
1:G:53:GLN:O	1:G:57:GLU:HG2	2.02	0.59
1:F:27:ARG:HH21	1:F:162:LEU:HG	1.67	0.59
1:B:53:GLN:O	1:B:57:GLU:HG2	2.02	0.59
1:C:9:PHE:HB2	1:C:39:ILE:HG12	1.84	0.59
1:G:132:ARG:NH2	1:G:143:LEU:O	2.35	0.58
1:F:53:GLN:O	1:F:57:GLU:HG2	2.03	0.58
1:H:27:ARG:NH1	3:H:341:HOH:O	2.23	0.58
1:H:163:GLU:OE2	1:H:170:ARG:NH2	2.36	0.57
1:A:175:ARG:NE	3:A:300:HOH:O	1.98	0.56
1:H:9:PHE:HB2	1:H:39:ILE:HG12	1.87	0.56
1:B:40:THR:HG23	3:B:348:HOH:O	2.07	0.55
1:B:34:PRO:HG2	1:B:37:ILE:HD12	1.88	0.55
1:E:118:SER:HB3	1:E:123:GLY:HA2	1.89	0.54
1:D:53:GLN:O	1:D:57:GLU:HG2	2.06	0.54
1:H:118:SER:HB3	1:H:123:GLY:HA2	1.88	0.54
1:H:141:TYR:CD2	1:H:187:LEU:HD13	2.43	0.53
1:C:27:ARG:NH2	1:C:162:LEU:HG	2.23	0.53
1:C:27:ARG:HH21	1:C:162:LEU:HG	1.73	0.53
1:G:9:PHE:HB2	1:G:39:ILE:HG12	1.90	0.53
1:A:155:GLY:HA2	3:A:249:HOH:O	2.08	0.53
1:E:53:GLN:O	1:E:57:GLU:HG2	2.10	0.52
1:E:81:THR:O	1:E:116:THR:HG22	2.09	0.52
1:H:53:GLN:O	1:H:57:GLU:HG2	2.10	0.52
1:B:70:GLN:CD	3:B:343:HOH:O	2.46	0.51
1:H:157:VAL:HG12	1:H:164:LEU:HA	1.91	0.51
1:F:126:ARG:NH2	3:F:239:HOH:O	2.42	0.51
1:D:121:MET:CG	1:E:121:MET:HG3	2.41	0.51
1:G:141:TYR:CD2	1:G:187:LEU:HD13	2.46	0.50
1:G:93:LYS:HE3	1:H:87:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:FMN:HM82	1:D:101:ARG:HD3	1.93	0.50
1:G:117:ALA:HB1	1:G:153:VAL:HG21	1.94	0.50
1:F:9:PHE:HB2	1:F:39:ILE:HG12	1.93	0.49
1:E:27:ARG:HH21	1:E:162:LEU:HG	1.77	0.49
1:F:27:ARG:NH2	1:F:162:LEU:HG	2.26	0.49
1:F:118:SER:HB3	1:F:123:GLY:HA2	1.94	0.49
1:A:37:ILE:HD11	1:A:181:ALA:HB2	1.94	0.49
1:D:172:PHE:HD2	1:D:175:ARG:HH21	1.60	0.49
1:B:118:SER:HB3	1:B:123:GLY:HA2	1.95	0.48
1:E:5:SER:O	1:E:5:SER:OG	2.32	0.47
1:B:27:ARG:HH21	1:B:162:LEU:HG	1.79	0.47
1:A:9:PHE:HB2	1:A:39:ILE:HG12	1.96	0.47
1:B:84:TYR:HA	2:B:201:FMN:C5A	2.45	0.47
1:H:21:PHE:HD1	1:H:157:VAL:HG21	1.80	0.46
1:D:118:SER:HB3	1:D:123:GLY:HA2	1.97	0.45
1:H:21:PHE:CD1	1:H:157:VAL:HG21	2.50	0.45
1:A:53:GLN:OE1	3:A:301:HOH:O	2.21	0.45
1:E:91:VAL:HG23	3:E:202:HOH:O	2.16	0.45
1:F:105:GLN:NE2	1:F:107:LEU:H	2.15	0.45
1:F:69:GLN:NE2	3:F:249:HOH:O	2.50	0.45
1:E:166:ASP:O	1:E:170:ARG:HG3	2.17	0.44
1:A:46:GLY:O	3:A:280:HOH:O	2.21	0.44
1:H:84:TYR:HA	2:H:201:FMN:C5A	2.47	0.44
1:C:84:TYR:HA	2:C:201:FMN:C5A	2.47	0.44
1:H:30:PRO:HB3	1:H:39:ILE:O	2.17	0.44
1:C:50:HIS:CG	1:D:91:VAL:HG13	2.53	0.44
1:B:141:TYR:CD2	1:B:187:LEU:HD13	2.53	0.44
1:A:118:SER:HB3	1:A:123:GLY:HA2	2.00	0.44
1:C:84:TYR:HA	2:C:201:FMN:N5	2.33	0.43
1:B:10:VAL:HA	1:B:40:THR:O	2.19	0.43
1:C:33:ALA:HA	1:C:34:PRO:HD2	1.81	0.43
1:D:32:ILE:HG23	1:D:174:ALA:HB2	2.00	0.43
1:G:50:HIS:CG	1:H:91:VAL:HG13	2.54	0.43
1:D:122:ILE:HG23	1:E:122:ILE:HD12	2.01	0.42
1:E:122:ILE:HG13	1:E:126:ARG:HH22	1.85	0.42
1:G:91:VAL:HG23	3:H:310:HOH:O	2.18	0.42
1:D:121:MET:HG2	1:E:121:MET:CE	2.49	0.42
1:D:35:GLU:OE1	1:D:35:GLU:HA	2.19	0.42
1:G:122:ILE:HG13	1:G:126:ARG:NH2	2.35	0.42
1:B:132:ARG:NH1	1:B:142:VAL:HG22	2.34	0.42
1:A:91:VAL:HG23	3:A:201:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:THR:O	1:H:116:THR:HG22	2.20	0.42
1:H:84:TYR:HA	2:H:201:FMN:N5	2.35	0.42
1:C:9:PHE:CD1	1:C:76:ALA:HB3	2.56	0.41
1:C:166:ASP:OD2	1:C:169:THR:N	2.45	0.41
1:A:167:VAL:HG12	3:A:304:HOH:O	2.21	0.41
1:D:27:ARG:NH1	3:D:278:HOH:O	2.36	0.41
1:E:118:SER:HA	1:E:119:PRO:HD3	1.93	0.41
1:D:18:LYS:O	3:D:249:HOH:O	2.22	0.41
1:H:132:ARG:NH1	1:H:142:VAL:HG22	2.36	0.40
1:H:37:ILE:HD11	1:H:181:ALA:HB2	2.02	0.40
1:A:161:THR:O	1:A:161:THR:OG1	2.38	0.40
1:B:32:ILE:O	3:B:372:HOH:O	2.22	0.40
1:B:70:GLN:OE1	3:B:343:HOH:O	2.21	0.40
1:D:27:ARG:NH2	1:D:162:LEU:HG	2.37	0.40
1:E:132:ARG:NH2	1:E:143:LEU:O	2.49	0.40

All (2) 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)
3:A:316:HOH:O	3:D:265:HOH:O[3_445]	1.80	0.40
1:F:86:TYR:OH	1:H:147:GLU:OE1[1_455]	2.14	0.06

## 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	182/199 (92%)	179 (98%)	3 (2%)	0	100	100
1	B	182/199 (92%)	178 (98%)	4 (2%)	0	100	100
1	C	182/199 (92%)	177 (97%)	4 (2%)	1 (0%)	32	28
1	D	182/199 (92%)	179 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	182/199 (92%)	178 (98%)	4 (2%)	0	100	100
1	F	182/199 (92%)	178 (98%)	4 (2%)	0	100	100
1	G	182/199 (92%)	177 (97%)	5 (3%)	0	100	100
1	H	182/199 (92%)	177 (97%)	5 (3%)	0	100	100
All	All	1456/1592 (92%)	1423 (98%)	32 (2%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	121	MET

### 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	145/159 (91%)	138 (95%)	7 (5%)	30	27
1	B	145/159 (91%)	135 (93%)	10 (7%)	18	14
1	C	145/159 (91%)	136 (94%)	9 (6%)	21	18
1	D	145/159 (91%)	138 (95%)	7 (5%)	30	27
1	E	145/159 (91%)	136 (94%)	9 (6%)	21	18
1	F	145/159 (91%)	140 (97%)	5 (3%)	42	43
1	G	145/159 (91%)	137 (94%)	8 (6%)	25	22
1	H	145/159 (91%)	137 (94%)	8 (6%)	25	22
All	All	1160/1272 (91%)	1097 (95%)	63 (5%)	26	23

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	105	GLN
1	A	142	VAL

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Mol	Chain	Res	Type
1	A	143	LEU
1	A	157	VAL
1	A	161	THR
1	A	162	LEU
1	B	31	GLU
1	B	40	THR
1	B	88	VAL
1	B	105	GLN
1	B	142	VAL
1	B	143	LEU
1	B	157	VAL
1	B	161	THR
1	B	162	LEU
1	B	167	VAL
1	C	31	GLU
1	C	88	VAL
1	C	105	GLN
1	C	121	MET
1	C	143	LEU
1	C	157	VAL
1	C	161	THR
1	C	162	LEU
1	C	188	SER
1	D	31	GLU
1	D	88	VAL
1	D	91	VAL
1	D	105	GLN
1	D	143	LEU
1	D	161	THR
1	D	162	LEU
1	E	5	SER
1	E	105	GLN
1	E	121	MET
1	E	143	LEU
1	E	154	THR
1	E	157	VAL
1	E	161	THR
1	E	162	LEU
1	E	175	ARG
1	F	105	GLN
1	F	143	LEU
1	F	161	THR

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Mol	Chain	Res	Type
1	F	162	LEU
1	F	167	VAL
1	G	31	GLU
1	G	88	VAL
1	G	105	GLN
1	G	121	MET
1	G	143	LEU
1	G	157	VAL
1	G	161	THR
1	G	162	LEU
1	H	91	VAL
1	H	105	GLN
1	H	121	MET
1	H	142	VAL
1	H	143	LEU
1	H	157	VAL
1	H	161	THR
1	H	162	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	105	GLN
1	C	105	GLN
1	E	105	GLN
1	G	85	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

3 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	B	201	-	31,33,33	1.36	4 (12%)	38,50,50	1.58	5 (13%)
2	FMN	C	201	-	31,33,33	1.41	4 (12%)	38,50,50	1.70	7 (18%)
2	FMN	H	201	-	31,33,33	1.41	5 (16%)	38,50,50	1.57	4 (10%)

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	B	201	-	-	0/16/18/18	0/3/3/3
2	FMN	C	201	-	-	0/16/18/18	0/3/3/3
2	FMN	H	201	-	-	0/16/18/18	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	FMN	C5A-N5	2.18	1.38	1.35
2	B	201	FMN	C5A-N5	2.25	1.38	1.35
2	C	201	FMN	C5A-N5	2.53	1.39	1.35
2	H	201	FMN	C1'-N10	2.76	1.51	1.48
2	H	201	FMN	C4-N3	3.02	1.38	1.33
2	B	201	FMN	C4-N3	3.07	1.38	1.33
2	C	201	FMN	C4-N3	3.17	1.38	1.33
2	B	201	FMN	C4A-N5	3.60	1.38	1.33
2	C	201	FMN	C10-N1	3.65	1.38	1.33
2	H	201	FMN	C10-N1	3.82	1.38	1.33
2	H	201	FMN	C4A-N5	3.90	1.38	1.33
2	B	201	FMN	C10-N1	3.98	1.38	1.33
2	C	201	FMN	C4A-N5	4.27	1.39	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	FMN	C4A-C4-N3	-2.81	119.48	123.48
2	C	201	FMN	C4A-C4-N3	-2.77	119.55	123.48
2	H	201	FMN	C4A-C4-N3	-2.63	119.74	123.48
2	C	201	FMN	C9A-C5A-N5	-2.17	119.00	122.24
2	C	201	FMN	C1'-N10-C9A	2.22	120.38	118.35
2	B	201	FMN	C5A-C9A-N10	2.47	119.49	117.66
2	C	201	FMN	C4-C4A-N5	2.77	121.72	118.68
2	B	201	FMN	C1'-N10-C9A	3.04	121.13	118.35
2	C	201	FMN	C5A-C9A-N10	3.23	120.06	117.66
2	H	201	FMN	C5A-C9A-N10	3.65	120.37	117.66
2	H	201	FMN	C4A-N5-C5A	4.00	120.98	116.76
2	C	201	FMN	C4A-N5-C5A	4.08	121.07	116.76
2	B	201	FMN	C4A-N5-C5A	4.20	121.19	116.76
2	H	201	FMN	C4-N3-C2	5.60	120.06	115.16
2	B	201	FMN	C4-N3-C2	5.99	120.40	115.16
2	C	201	FMN	C4-N3-C2	6.48	120.83	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	FMN	2	0
2	C	201	FMN	3	0
2	H	201	FMN	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<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	184/199 (92%)	0.03	5 (2%)	55	61	23, 32, 62, 89	0
1	B	184/199 (92%)	0.08	5 (2%)	55	61	23, 34, 68, 87	0
1	C	184/199 (92%)	0.38	12 (6%)	20	25	24, 36, 75, 101	0
1	D	184/199 (92%)	0.28	11 (5%)	23	28	25, 38, 69, 98	0
1	E	184/199 (92%)	0.25	12 (6%)	20	25	23, 39, 75, 106	0
1	F	184/199 (92%)	0.19	7 (3%)	41	48	24, 39, 65, 82	0
1	G	184/199 (92%)	0.66	19 (10%)	7	9	30, 44, 88, 112	0
1	H	184/199 (92%)	0.87	25 (13%)	3	5	31, 54, 87, 114	0
All	All	1472/1592 (92%)	0.34	96 (6%)	20	25	23, 39, 80, 114	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	160	GLN	6.7
1	D	162	LEU	6.6
1	H	160	GLN	6.4
1	H	155	GLY	6.2
1	E	160	GLN	6.1
1	C	160	GLN	6.0
1	H	158	ASP	5.9
1	A	162	LEU	5.9
1	G	160	GLN	5.7
1	H	164	LEU	5.5
1	B	162	LEU	5.4
1	H	162	LEU	5.4
1	H	159	ALA	5.3
1	G	157	VAL	5.3
1	E	162	LEU	4.9
1	A	5	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	5	SER	4.5
1	H	161	THR	4.4
1	D	165	SER	4.4
1	G	172	PHE	4.2
1	D	158	ASP	4.1
1	G	158	ASP	4.1
1	E	159	ALA	4.1
1	B	5	SER	4.0
1	H	163	GLU	3.9
1	G	162	LEU	3.9
1	B	160	GLN	3.9
1	H	167	VAL	3.9
1	D	161	THR	3.8
1	A	160	GLN	3.8
1	H	154	THR	3.7
1	C	159	ALA	3.7
1	H	6	PRO	3.7
1	E	121	MET	3.7
1	C	162	LEU	3.7
1	G	161	THR	3.7
1	E	122	ILE	3.7
1	C	122	ILE	3.5
1	H	38	ALA	3.4
1	H	165	SER	3.3
1	G	167	VAL	3.2
1	G	159	ALA	3.1
1	H	32	ILE	3.1
1	D	154	THR	3.1
1	H	157	VAL	3.1
1	H	173	LEU	3.0
1	H	8	HIS	3.0
1	F	162	LEU	3.0
1	G	36	GLY	2.9
1	D	163	GLU	2.9
1	B	35	GLU	2.9
1	C	35	GLU	2.9
1	D	5	SER	2.9
1	E	155	GLY	2.8
1	H	169	THR	2.8
1	G	153	VAL	2.8
1	G	163	GLU	2.8
1	A	159	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	36	GLY	2.8
1	C	121	MET	2.8
1	F	5	SER	2.8
1	H	5	SER	2.7
1	E	158	ASP	2.7
1	E	123	GLY	2.7
1	B	6	PRO	2.7
1	F	8	HIS	2.7
1	G	37	ILE	2.6
1	G	24	ALA	2.5
1	H	34	PRO	2.5
1	F	136	VAL	2.5
1	G	152	GLN	2.5
1	F	160	GLN	2.5
1	D	6	PRO	2.4
1	F	35	GLU	2.4
1	C	175	ARG	2.4
1	G	35	GLU	2.4
1	F	175	ARG	2.3
1	D	122	ILE	2.3
1	E	120	GLY	2.3
1	E	35	GLU	2.3
1	E	5	SER	2.3
1	G	34	PRO	2.2
1	D	155	GLY	2.2
1	G	26	ALA	2.1
1	C	167	VAL	2.1
1	E	157	VAL	2.1
1	G	155	GLY	2.1
1	C	131	LEU	2.1
1	G	5	SER	2.1
1	A	121	MET	2.1
1	C	88	VAL	2.1
1	H	175	ARG	2.1
1	H	98	TRP	2.0
1	H	37	ILE	2.0
1	C	157	VAL	2.0
1	H	31	GLU	2.0

## 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 [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( $\text{\AA}^2$ )	Q<0.9
2	FMN	B	201	31/31	0.90	0.20	2.50	34,62,70,74	0
2	FMN	H	201	31/31	0.90	0.21	2.20	43,67,74,77	0
2	FMN	C	201	31/31	0.91	0.19	1.36	29,45,62,68	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.