



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:01 PM GMT

PDB ID : 3SGZ  
Title : High resolution crystal structure of rat long chain hydroxy acid oxidase in complex with the inhibitor 4-carboxy-5-[(4-chlorophenyl)sulfanyl]-1, 2, 3-thiadiazole.  
Authors : Chen, Z.; Vignaud, C.; Jaafar, A.; Gueritte, F.; Guenard, D.; Lederer, F.; Mathews, F.S.  
Deposited on : 2011-06-15  
Resolution : 1.35 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

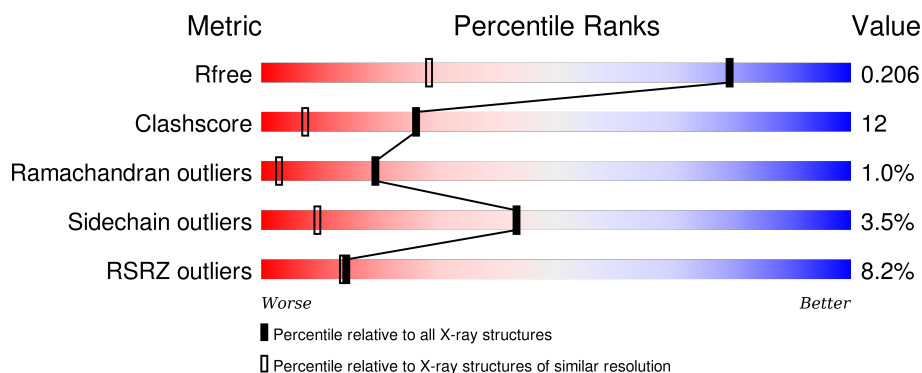
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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	2199 (1.40-1.32)
Clashscore	102246	2337 (1.40-1.32)
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)
RSRZ outliers	91569	2199 (1.40-1.32)

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	352	<div> <div>7%</div> <div>81%13%.. 5%</div> </div>
1	B	352	<div> <div>7%</div> <div>81%12%• 5%</div> </div>
1	C	352	<div> <div>10%</div> <div>79%14%.. 5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9157 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 Hydroxyacid oxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	5	0
			2646	1674	464	492	16			
1	B	334	Total	C	N	O	S	0	4	0
			2620	1659	458	487	16			
1	C	336	Total	C	N	O	S	0	5	0
			2646	1674	464	492	16			

There are 12 discrepancies between the modelled and reference sequences:

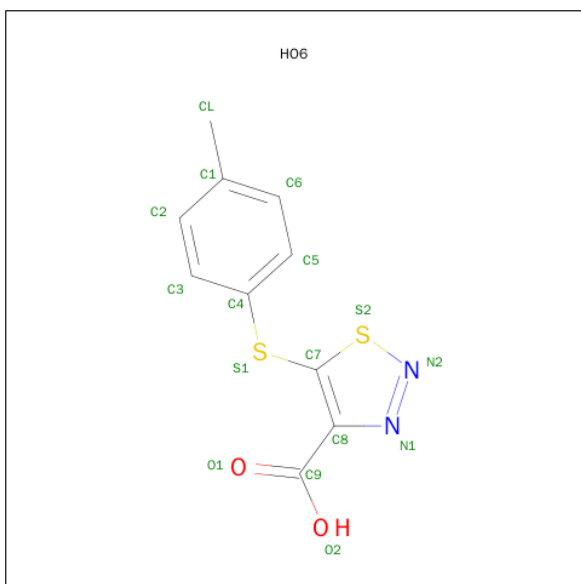
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	LYS	LEU	CONFLICT	UNP Q07523
A	181	ALA	LYS	CONFLICT	UNP Q07523
A	182	ALA	ASP	CONFLICT	UNP Q07523
A	198	LEU	SER	CONFLICT	UNP Q07523
B	180	LYS	LEU	CONFLICT	UNP Q07523
B	181	ALA	LYS	CONFLICT	UNP Q07523
B	182	ALA	ASP	CONFLICT	UNP Q07523
B	198	LEU	SER	CONFLICT	UNP Q07523
C	180	LYS	LEU	CONFLICT	UNP Q07523
C	181	ALA	LYS	CONFLICT	UNP Q07523
C	182	ALA	ASP	CONFLICT	UNP Q07523
C	198	LEU	SER	CONFLICT	UNP Q07523

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 3 is 5-[(4-METHYLPHENYL)SULFANYL]-1,2,3-THIADIAZOLE-4-CARBOXYLIC ACID (three-letter code: HO6) (formula: C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			16	10	2	2	2		
3	B	1	Total	C	N	O	S	0	0
			16	10	2	2	2		
3	C	1	Total	C	N	O	S	0	0
			16	10	2	2	2		

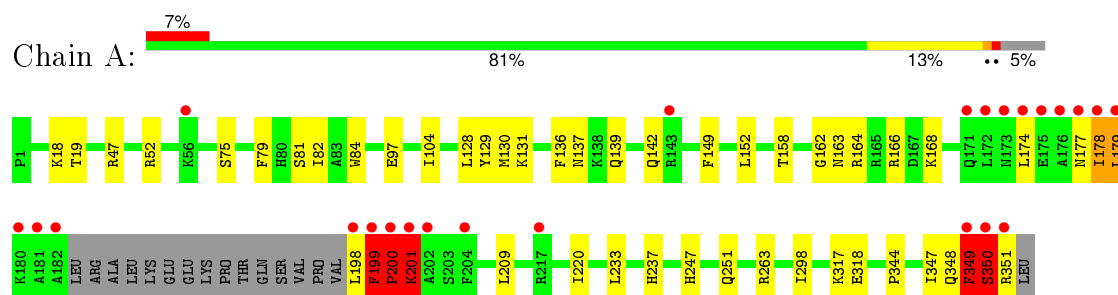
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	391	Total	O	0	0
			391	391		
4	B	344	Total	O	0	0
			344	344		
4	C	369	Total	O	0	0
			369	369		

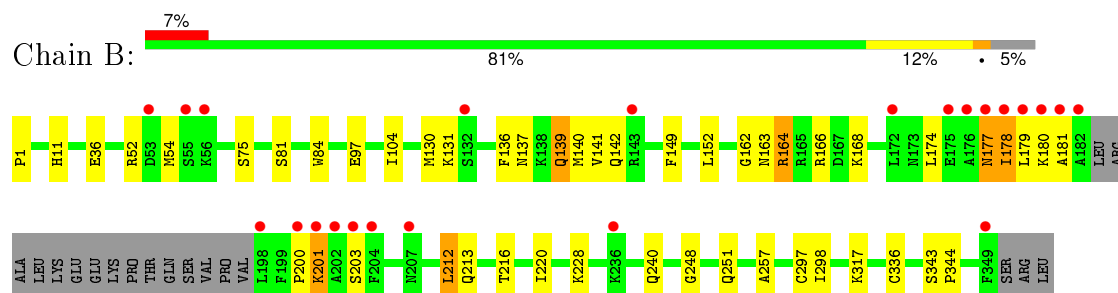
### 3 Residue-property plots [i](#)

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.

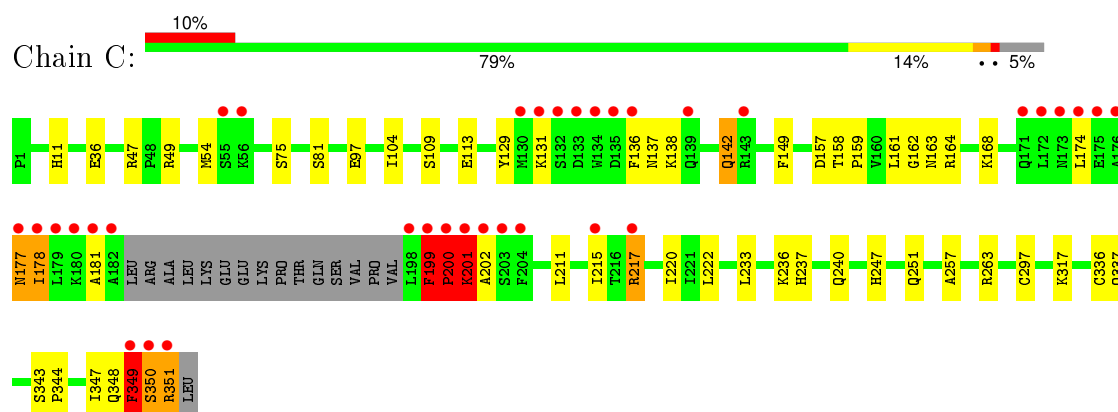
#### • Molecule 1: Hydroxyacid oxidase 2



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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.45Å 108.45Å 491.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.35 39.91 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.91-1.35) 98.3 (39.91-1.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.35Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.203 0.188 , 0.206	Depositor DCC
$R_{free}$ test set	15480 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.4	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 311329 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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, HO6

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	0.63	1/2691 (0.0%)	0.88	10/3637 (0.3%)
1	B	0.59	1/2664 (0.0%)	0.76	2/3599 (0.1%)
1	C	0.65	1/2691 (0.0%)	0.82	2/3637 (0.1%)
All	All	0.62	3/8046 (0.0%)	0.82	14/10873 (0.1%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	GLN	C-N	-12.10	1.06	1.34
1	C	142	GLN	C-N	-9.31	1.12	1.34
1	A	142	GLN	C-N	-6.71	1.18	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	SER	N-CA-C	-10.65	82.25	111.00
1	A	199	PHE	N-CA-C	9.91	137.77	111.00
1	A	201	LYS	N-CA-C	8.42	133.74	111.00
1	A	199	PHE	N-CA-CB	-7.15	97.73	110.60
1	A	198	LEU	C-N-CA	6.75	138.57	121.70
1	C	200	PRO	C-N-CA	6.29	137.43	121.70
1	C	199	PHE	C-N-CD	-6.13	107.11	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	199	PHE	C-N-CD	-5.68	108.10	120.60
1	A	199	PHE	C-N-CA	5.49	145.07	122.00
1	B	200	PRO	N-CA-CB	5.47	109.86	103.30
1	A	47	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	198	LEU	CA-C-N	-5.21	105.74	117.20
1	A	200	PRO	CA-N-CD	-5.02	104.47	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	199	PHE	Peptide

## 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	2646	0	2678	70	0
1	B	2620	0	2647	40	0
1	C	2646	0	2678	89	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
2	C	31	0	19	0	0
3	A	16	0	7	0	0
3	B	16	0	7	1	0
3	C	16	0	7	1	0
4	A	391	0	0	11	0
4	B	344	0	0	9	0
4	C	369	0	0	9	0
All	All	9157	0	8081	199	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 12.

All (199) 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:C:344:PRO:O	1:C:351:ARG:HB2	1.21	1.33
1:C:199:PHE:HB3	1:C:200:PRO:CB	1.72	1.19
1:C:199:PHE:HB3	1:C:200:PRO:HB3	1.23	1.16
1:C:351:ARG:HH21	1:C:351:ARG:HG2	1.02	1.16
1:C:347:ILE:O	1:C:351:ARG:HB3	1.45	1.15
1:A:263:ARG:HH12	1:A:350:SER:HB3	1.00	1.10
1:C:263:ARG:NH1	1:C:350:SER:HB3	1.69	1.08
1:C:199:PHE:CE2	1:C:201:LYS:HE3	1.89	1.07
1:A:344:PRO:O	1:A:351:ARG:HG2	1.54	1.07
1:C:263:ARG:HH12	1:C:350:SER:HB3	0.96	1.06
1:A:349:PHE:HD1	1:A:349:PHE:O	1.36	1.06
1:C:199:PHE:HE2	1:C:201:LYS:HE3	1.15	1.05
1:A:347:ILE:O	1:A:351:ARG:HG3	1.58	1.02
1:C:263:ARG:HH12	1:C:350:SER:CB	1.73	1.01
1:C:351:ARG:HG3	4:C:1187:HOH:O	1.58	1.01
1:C:344:PRO:O	1:C:351:ARG:CB	2.09	1.00
1:C:351:ARG:HH21	1:C:351:ARG:CG	1.77	0.97
1:A:263:ARG:HH12	1:A:350:SER:CB	1.76	0.97
1:C:351:ARG:HG2	1:C:351:ARG:NH2	1.62	0.97
1:A:263:ARG:NH1	1:A:350:SER:HB3	1.78	0.96
1:A:19:THR:HG21	1:A:179:LEU:HD23	1.48	0.95
1:A:131:LYS:H	1:A:137:ASN:HD21	1.15	0.93
1:C:217:ARG:HD2	1:C:217:ARG:H	1.33	0.93
1:A:18:LYS:NZ	1:A:166:ARG:HH12	1.67	0.93
1:A:349:PHE:CD1	1:A:349:PHE:O	2.24	0.91
1:C:168:LYS:HE3	4:C:1350:HOH:O	1.71	0.91
1:C:344:PRO:HB2	1:C:351:ARG:O	1.72	0.90
1:B:131:LYS:H	1:B:137:ASN:HD21	1.08	0.90
1:A:168:LYS:HE3	4:A:888:HOH:O	1.72	0.89
1:A:201:LYS:HD3	4:A:743:HOH:O	1.74	0.87
1:C:349:PHE:O	1:C:349:PHE:HD1	1.57	0.87
1:C:174:LEU:HD22	1:C:178:ILE:HD11	1.55	0.87
1:C:199:PHE:CB	1:C:200:PRO:HB3	2.03	0.86
1:A:129:TYR:HB3	1:A:201:LYS:HE3	1.57	0.84
1:C:158[A]:THR:HB	1:C:201:LYS:HZ1	1.45	0.81
1:A:18:LYS:HZ1	1:A:166:ARG:HH12	1.26	0.81
1:C:220:ILE:H	1:C:240:GLN:HE21	1.28	0.80
1:A:129:TYR:HB3	1:A:201:LYS:CE	2.15	0.77
1:C:199:PHE:HB3	1:C:200:PRO:CG	2.15	0.75
1:A:201:LYS:HG2	4:A:872:HOH:O	1.85	0.74
1:A:350:SER:O	1:A:351:ARG:HB2	1.86	0.74
1:C:158[B]:THR:OG1	1:C:201:LYS:NZ	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HB3	4:A:688:HOH:O	1.88	0.73
1:C:199:PHE:CE2	1:C:201:LYS:CE	2.69	0.73
1:A:351:ARG:NH2	4:A:653:HOH:O	2.21	0.73
1:A:129:TYR:CB	1:A:201:LYS:HE3	2.19	0.73
1:A:199:PHE:HB3	1:A:200:PRO:HA	1.69	0.72
1:B:220:ILE:H	1:B:240:GLN:HE21	1.36	0.71
1:C:347:ILE:O	1:C:351:ARG:CB	2.34	0.71
1:C:199:PHE:CD2	1:C:200:PRO:HB3	2.26	0.70
1:B:174:LEU:HD22	1:B:178:ILE:HD11	1.73	0.69
1:C:349:PHE:O	1:C:349:PHE:CD1	2.42	0.69
1:A:19:THR:HG21	1:A:179:LEU:CD2	2.22	0.68
1:C:217:ARG:HD2	1:C:217:ARG:N	2.06	0.67
1:A:347:ILE:O	1:A:351:ARG:CG	2.39	0.66
1:A:201:LYS:HB2	4:A:743:HOH:O	1.97	0.65
1:B:213:GLN:HG2	1:B:220:ILE:HD12	1.79	0.65
1:C:162:GLY:H	1:C:251:GLN:HE22	1.46	0.64
1:C:158[B]:THR:HG21	1:C:247:HIS:CE1	2.33	0.63
1:C:199:PHE:HB3	1:C:200:PRO:CA	2.24	0.63
1:B:97:GLU:HG2	1:B:317:LYS:HE3	1.80	0.62
1:C:54[B]:MET:HE1	1:C:336:CYS:C	2.19	0.62
1:B:104[B]:ILE:HD12	1:B:104[B]:ILE:N	2.14	0.62
1:A:348:GLN:O	1:A:349:PHE:C	2.38	0.62
1:A:347:ILE:HG22	1:A:350:SER:HB2	1.82	0.61
1:A:201:LYS:NZ	1:A:201:LYS:CB	2.63	0.61
1:C:131:LYS:H	1:C:137:ASN:HD21	1.48	0.61
1:C:129:TYR:CE2	1:C:201:LYS:NZ	2.68	0.61
1:A:18:LYS:NZ	1:A:166:ARG:NH1	2.45	0.61
1:C:104[B]:ILE:N	1:C:104[B]:ILE:HD12	2.16	0.61
1:B:343:SER:HB2	1:B:344:PRO:HD2	1.83	0.60
1:C:199:PHE:HD2	1:C:200:PRO:HB3	1.65	0.60
1:C:97:GLU:HG2	1:C:317:LYS:HE3	1.84	0.59
1:C:36:GLU:HG3	1:C:257:ALA:HB2	1.84	0.59
1:A:164:ARG:HH21	1:A:251:GLN:HE21	1.49	0.59
1:A:162:GLY:H	1:A:251:GLN:HE22	1.50	0.59
1:B:164:ARG:HH21	1:B:251:GLN:HE21	1.49	0.59
1:A:201:LYS:HZ2	1:A:201:LYS:HB2	1.68	0.59
1:B:139:GLN:HG3	1:B:140:MET:N	2.17	0.58
1:C:164:ARG:HH21	1:C:251:GLN:HE21	1.50	0.58
1:C:158[B]:THR:O	1:C:201:LYS:NZ	2.36	0.58
1:A:131:LYS:HE2	1:A:136:PHE:CE1	2.39	0.58
1:C:104[A]:ILE:HD12	1:C:149:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:H	1:B:251:GLN:HE22	1.49	0.58
1:A:104[A]:ILE:HD12	1:A:149:PHE:CE2	2.38	0.57
1:B:164:ARG:HD2	4:B:834:HOH:O	2.04	0.56
1:C:131:LYS:HE2	1:C:136:PHE:CE1	2.40	0.56
1:C:162:GLY:H	1:C:251:GLN:NE2	2.03	0.56
1:A:19:THR:CG2	1:A:179:LEU:HD23	2.32	0.55
1:B:162:GLY:H	1:B:251:GLN:NE2	2.05	0.55
1:A:174:LEU:HD22	1:A:178:ILE:HD11	1.88	0.55
1:A:18:LYS:HZ2	1:A:166:ARG:HH12	1.50	0.55
1:A:158[B]:THR:HG21	1:A:247:HIS:CE1	2.41	0.55
1:A:199:PHE:HB3	1:A:200:PRO:CA	2.36	0.55
1:C:129:TYR:CD2	1:C:201:LYS:HE2	2.42	0.54
1:A:104[B]:ILE:HD12	1:A:104[B]:ILE:N	2.23	0.54
1:C:158[A]:THR:O	1:C:201:LYS:NZ	2.40	0.54
1:C:343:SER:HB2	1:C:344:PRO:HD2	1.90	0.53
1:B:164:ARG:HH12	3:B:402:HO6:C9	2.20	0.53
1:C:158[B]:THR:O	1:C:201:LYS:HE3	2.09	0.53
1:A:163:ASN:HD21	1:A:168:LYS:NZ	2.06	0.53
1:A:130:MET:O	1:A:201:LYS:HE2	2.08	0.53
1:A:233:LEU:O	1:A:237:HIS:HD2	1.91	0.53
1:A:18:LYS:HZ2	1:A:166:ARG:NH1	2.06	0.53
1:C:349:PHE:H	1:C:351:ARG:NH1	2.07	0.52
1:C:158[A]:THR:O	1:C:201:LYS:HE3	2.09	0.52
1:A:174:LEU:HD13	1:A:178:ILE:HD11	1.90	0.52
1:C:344:PRO:CB	1:C:351:ARG:O	2.49	0.52
1:A:348:GLN:O	1:A:349:PHE:O	2.27	0.52
1:B:228:LYS:NZ	4:B:820:HOH:O	2.42	0.52
1:B:164:ARG:HD3	4:B:844:HOH:O	2.10	0.52
1:A:19:THR:CG2	1:A:179:LEU:CD2	2.87	0.52
1:B:180:LYS:HE2	4:B:751:HOH:O	2.09	0.52
1:A:174:LEU:HD22	1:A:178:ILE:CD1	2.40	0.52
1:C:158[B]:THR:O	1:C:201:LYS:CE	2.58	0.52
1:A:162:GLY:H	1:A:251:GLN:NE2	2.06	0.52
1:C:199:PHE:HB3	1:C:200:PRO:CD	2.37	0.51
1:C:161:LEU:HD11	3:C:402:HO6:H3	1.92	0.51
1:A:351:ARG:HD3	4:A:688:HOH:O	2.09	0.51
1:A:128:LEU:HD23	1:A:130:MET:CE	2.41	0.51
1:C:158[A]:THR:O	1:C:201:LYS:CE	2.60	0.50
1:C:104[A]:ILE:HD12	1:C:149:PHE:CZ	2.47	0.50
1:C:217:ARG:CD	1:C:217:ARG:H	2.03	0.50
1:C:237:HIS:HE1	4:C:1205:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:HD21	1:B:168:LYS:NZ	2.10	0.50
1:C:199:PHE:CG	1:C:200:PRO:HB3	2.45	0.50
1:B:220:ILE:H	1:B:240:GLN:NE2	2.08	0.49
1:C:129:TYR:HE2	1:C:201:LYS:HZ3	1.54	0.49
1:A:349:PHE:O	1:A:350:SER:OG	2.24	0.49
1:B:177:ASN:O	1:B:181:ALA:HB3	2.12	0.49
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.77	0.49
1:B:36:GLU:HG3	1:B:257:ALA:HB2	1.95	0.49
1:A:201:LYS:HB2	4:A:891:HOH:O	2.13	0.49
1:A:79:PHE:HB2	1:A:82:ILE:HD12	1.94	0.49
1:C:349:PHE:O	1:C:350:SER:OG	2.14	0.48
1:A:104[A]:ILE:HD12	1:A:149:PHE:HE2	1.78	0.48
1:C:54[B]:MET:HE1	1:C:337:GLN:N	2.28	0.48
1:B:201:LYS:HG3	1:B:201:LYS:O	2.14	0.48
1:C:211:LEU:N	1:C:211:LEU:HD12	2.28	0.48
1:C:215:ILE:HG22	4:C:1248:HOH:O	2.13	0.48
1:C:201:LYS:NZ	4:C:1083:HOH:O	2.45	0.48
1:C:11:HIS:HE1	4:C:1351:HOH:O	1.96	0.48
1:A:344:PRO:HB3	1:A:351:ARG:HA	1.96	0.47
1:C:348:GLN:O	1:C:349:PHE:C	2.53	0.47
1:B:104[B]:ILE:CD1	1:B:104[B]:ILE:N	2.77	0.47
1:B:104[A]:ILE:HD12	1:B:149:PHE:CE2	2.50	0.47
1:B:130:MET:CE	1:B:212:LEU:HG	2.44	0.47
1:B:1:PRO:HD2	4:B:635:HOH:O	2.15	0.47
1:B:298:ILE:C	1:B:298:ILE:HD12	2.34	0.47
1:A:131:LYS:HE2	1:A:136:PHE:CD1	2.50	0.46
1:A:158[A]:THR:O	1:A:199:PHE:HE2	1.98	0.46
1:B:141:VAL:HG11	1:B:216:THR:HB	1.98	0.46
1:C:157:ASP:OD2	1:C:158[B]:THR:HG23	2.16	0.46
1:C:220:ILE:H	1:C:240:GLN:NE2	2.05	0.46
1:B:203:SER:HA	4:B:760:HOH:O	2.16	0.45
1:B:11:HIS:HE1	4:B:815:HOH:O	2.00	0.45
1:C:236:LYS:HD2	4:C:1134:HOH:O	2.16	0.45
1:C:349:PHE:HA	1:C:351:ARG:HH22	1.80	0.45
1:A:158[A]:THR:HG22	1:A:199:PHE:CE2	2.52	0.45
1:C:159:PRO:HB2	1:C:202:ALA:HA	1.99	0.45
1:C:81[A]:SER:HB2	1:C:109:SER:HG	1.82	0.45
1:A:318:GLU:HG3	4:A:847:HOH:O	2.17	0.45
1:C:47:ARG:CD	1:C:351:ARG:HE	2.30	0.44
1:B:177:ASN:O	1:B:181:ALA:CB	2.65	0.44
1:C:158[B]:THR:HG22	1:C:251:GLN:CD	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104[A]:ILE:HD12	1:A:149:PHE:CZ	2.52	0.44
1:C:113:GLU:CD	1:C:113:GLU:H	2.20	0.44
1:A:350:SER:C	1:A:351:ARG:O	2.55	0.44
1:A:201:LYS:NZ	4:A:891:HOH:O	2.24	0.43
1:C:104[B]:ILE:N	1:C:104[B]:ILE:CD1	2.81	0.43
1:A:97:GLU:HG2	1:A:317:LYS:HE3	2.01	0.43
1:C:163:ASN:HD21	1:C:168:LYS:NZ	2.16	0.43
1:A:158[B]:THR:O	1:A:199:PHE:HE2	1.99	0.43
1:A:52:ARG:HB2	4:A:886:HOH:O	2.18	0.43
1:A:152:LEU:HB2	1:A:220:ILE:HD13	2.00	0.43
1:C:138:LYS:O	1:C:142:GLN:HG3	2.19	0.43
1:C:177:ASN:O	1:C:181:ALA:CB	2.66	0.43
1:C:104[A]:ILE:HD12	1:C:149:PHE:HE2	1.82	0.43
1:C:199:PHE:CB	1:C:200:PRO:CA	2.96	0.43
1:C:131:LYS:HE2	1:C:136:PHE:CZ	2.53	0.43
1:B:180:LYS:CE	4:B:751:HOH:O	2.66	0.43
1:A:128:LEU:HD23	1:A:130:MET:HE2	1.99	0.42
1:A:163:ASN:HD21	1:A:168:LYS:HZ2	1.67	0.42
1:A:81[A]:SER:HA	1:A:84:TRP:O	2.20	0.42
1:B:54[B]:MET:HE1	1:B:336:CYS:C	2.39	0.42
1:B:248:GLY:CA	2:B:401:FMN:H5'2	2.50	0.42
1:B:166:ARG:HG2	1:B:166:ARG:NH1	2.35	0.41
1:C:233:LEU:O	1:C:237:HIS:HD2	2.03	0.41
1:B:81[A]:SER:HA	1:B:84:TRP:O	2.20	0.41
1:C:159:PRO:CB	1:C:202:ALA:HA	2.50	0.41
1:B:131:LYS:HD2	1:B:136:PHE:CD1	2.54	0.41
1:C:351:ARG:O	4:C:1294:HOH:O	2.20	0.41
1:B:52:ARG:HB2	4:B:708:HOH:O	2.21	0.41
1:A:298:ILE:C	1:A:298:ILE:HD12	2.40	0.41
1:C:49:ARG:HD3	4:C:1169:HOH:O	2.21	0.40
1:B:97:GLU:HG2	1:B:317:LYS:CE	2.47	0.40
1:C:211:LEU:CD1	1:C:211:LEU:N	2.85	0.40
1:B:201:LYS:CG	1:B:201:LYS:O	2.69	0.40
1:C:138:LYS:HE3	1:C:138:LYS:HB2	1.86	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	337/352 (96%)	325 (96%)	7 (2%)	5 (2%)	13	1
1	B	334/352 (95%)	324 (97%)	10 (3%)	0	100	100
1	C	337/352 (96%)	321 (95%)	11 (3%)	5 (2%)	13	1
All	All	1008/1056 (96%)	970 (96%)	28 (3%)	10 (1%)	19	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PHE
1	A	200	PRO
1	A	201	LYS
1	A	349	PHE
1	A	350	SER
1	C	199	PHE
1	C	200	PRO
1	C	349	PHE
1	C	350	SER
1	C	201	LYS

### 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	283/294 (96%)	273 (96%)	10 (4%)	43	9
1	B	279/294 (95%)	269 (96%)	10 (4%)	42	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	283/294 (96%)	272 (96%)	11 (4%)	39 7
All	All	845/882 (96%)	814 (96%)	31 (4%)	43 8

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	A	139	GLN
1	A	177	ASN
1	A	178	ILE
1	A	179	LEU
1	A	199	PHE
1	A	200	PRO
1	A	201	LYS
1	A	209	LEU
1	A	349	PHE
1	B	75	SER
1	B	139	GLN
1	B	152	LEU
1	B	177	ASN
1	B	178	ILE
1	B	179	LEU
1	B	201	LYS
1	B	212	LEU
1	B	297[A]	CYS
1	B	297[B]	CYS
1	C	75	SER
1	C	177	ASN
1	C	178	ILE
1	C	199	PHE
1	C	201	LYS
1	C	217	ARG
1	C	222	LEU
1	C	297[A]	CYS
1	C	297[B]	CYS
1	C	349	PHE
1	C	351	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	64	GLN
1	A	96	GLN
1	A	99	ASN
1	A	137	ASN
1	A	163	ASN
1	A	173	ASN
1	A	237	HIS
1	A	251	GLN
1	B	64	GLN
1	B	99	ASN
1	B	137	ASN
1	B	163	ASN
1	B	173	ASN
1	B	240	GLN
1	B	251	GLN
1	C	64	GLN
1	C	99	ASN
1	C	137	ASN
1	C	163	ASN
1	C	173	ASN
1	C	237	HIS
1	C	240	GLN
1	C	251	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 ⓘ

6 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	401	-	32,33,33	1.98	8 (25%)	34,50,50	3.52	7 (20%)
3	HO6	A	402	-	10,17,17	2.46	2 (20%)	11,23,23	0.96	0
2	FMN	B	401	-	32,33,33	2.05	9 (28%)	34,50,50	3.46	7 (20%)
3	HO6	B	402	-	10,17,17	2.27	2 (20%)	11,23,23	0.91	0
2	FMN	C	401	-	32,33,33	2.06	8 (25%)	34,50,50	3.75	8 (23%)
3	HO6	C	402	-	10,17,17	2.25	2 (20%)	11,23,23	0.97	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	401	-	-	0/18/18/18	0/3/3/3
3	HO6	A	402	-	-	0/2/8/8	0/1/2/2
2	FMN	B	401	-	-	0/18/18/18	0/3/3/3
3	HO6	B	402	-	-	0/2/8/8	0/1/2/2
2	FMN	C	401	-	-	0/18/18/18	0/3/3/3
3	HO6	C	402	-	-	0/2/8/8	0/1/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C1'-N10	-5.20	1.42	1.48
2	B	401	FMN	C1'-N10	-5.05	1.43	1.48
2	C	401	FMN	C1'-N10	-5.03	1.43	1.48
2	C	401	FMN	C4'-C3'	-4.40	1.44	1.53
2	A	401	FMN	C4'-C3'	-3.98	1.45	1.53
2	B	401	FMN	C4'-C3'	-3.35	1.46	1.53
2	B	401	FMN	P-O3P	-2.69	1.45	1.54
2	A	401	FMN	P-O3P	-2.10	1.47	1.54
2	C	401	FMN	C9A-N10	2.04	1.41	1.38
2	C	401	FMN	C5A-N5	2.46	1.39	1.35
2	A	401	FMN	C9A-N10	2.53	1.42	1.38
2	C	401	FMN	O3'-C3'	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FMN	O3'-C3'	2.66	1.49	1.43
2	B	401	FMN	C2-N3	2.67	1.43	1.38
2	A	401	FMN	C5A-N5	2.78	1.39	1.35
2	B	401	FMN	C9A-N10	3.07	1.43	1.38
2	A	401	FMN	C4-N3	3.12	1.38	1.33
2	C	401	FMN	C2-N3	3.17	1.44	1.38
2	B	401	FMN	C5A-N5	3.40	1.40	1.35
2	A	401	FMN	O3'-C3'	3.49	1.51	1.43
3	C	402	HO6	C8-N1	4.03	1.43	1.34
3	B	402	HO6	C8-N1	4.04	1.43	1.34
2	B	401	FMN	C4A-N5	4.09	1.39	1.33
2	C	401	FMN	C4-N3	4.19	1.40	1.33
2	A	401	FMN	C4A-N5	4.36	1.40	1.33
2	B	401	FMN	C4-N3	4.40	1.41	1.33
2	C	401	FMN	C4A-N5	4.85	1.40	1.33
3	B	402	HO6	CL-C1	4.86	1.69	1.51
3	A	402	HO6	C8-N1	4.99	1.44	1.34
3	C	402	HO6	CL-C1	5.06	1.70	1.51
3	A	402	HO6	CL-C1	5.14	1.70	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FMN	N3-C2-N1	-8.64	113.14	127.69
2	C	401	FMN	C4A-C4-N3	-8.52	112.38	123.52
2	B	401	FMN	C4A-C4-N3	-8.29	112.68	123.52
2	A	401	FMN	N3-C2-N1	-8.13	113.99	127.69
2	B	401	FMN	N3-C2-N1	-8.07	114.09	127.69
2	A	401	FMN	C4A-C4-N3	-8.05	113.00	123.52
2	C	401	FMN	C4-C4A-N5	-3.75	114.13	118.70
2	A	401	FMN	C4-C4A-N5	-3.21	114.79	118.70
2	B	401	FMN	C4-C4A-N5	-3.07	114.96	118.70
2	C	401	FMN	C6-C5A-C9A	2.04	121.36	119.11
2	B	401	FMN	C5A-C9A-N10	2.07	119.13	117.58
2	A	401	FMN	C5A-C9A-N10	2.67	119.58	117.58
2	A	401	FMN	C1'-N10-C9A	3.43	122.81	118.83
2	B	401	FMN	C1'-N10-C9A	3.51	122.90	118.83
2	C	401	FMN	C5A-C9A-N10	3.65	120.31	117.58
2	C	401	FMN	C1'-N10-C9A	3.65	123.06	118.83
2	C	401	FMN	C4-C4A-C10	4.11	122.57	119.94
2	A	401	FMN	C4-C4A-C10	4.21	122.64	119.94
2	B	401	FMN	C4-C4A-C10	4.90	123.08	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FMN	C4-N3-C2	14.12	126.94	115.16
2	A	401	FMN	C4-N3-C2	14.71	127.43	115.16
2	C	401	FMN	C4-N3-C2	15.57	128.15	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FMN	1	0
3	B	402	HO6	1	0
3	C	402	HO6	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	336/352 (95%)	0.35	24 (7%)	19 18	8, 14, 43, 63	0
1	B	334/352 (94%)	0.22	23 (6%)	20 20	11, 18, 41, 62	0
1	C	336/352 (95%)	0.47	35 (10%)	8 9	8, 15, 50, 63	0
All	All	1006/1056 (95%)	0.35	82 (8%)	14 14	8, 15, 45, 63	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	20.3
1	A	198	LEU	14.2
1	C	182	ALA	12.6
1	C	198	LEU	12.6
1	A	178	ILE	12.3
1	B	198	LEU	11.7
1	B	182	ALA	10.4
1	A	200	PRO	9.7
1	A	349	PHE	9.0
1	C	349	PHE	9.0
1	C	178	ILE	8.9
1	C	201	LYS	8.8
1	B	200	PRO	8.6
1	C	200	PRO	8.5
1	C	181	ALA	8.3
1	A	179	LEU	8.2
1	C	177	ASN	7.9
1	A	175	GLU	7.3
1	A	351	ARG	7.2
1	A	181	ALA	7.2
1	A	177	ASN	7.0
1	A	176	ALA	6.9
1	C	202	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	174	LEU	6.8
1	C	176	ALA	6.8
1	B	178	ILE	6.7
1	A	180	LYS	6.2
1	A	199	PHE	6.2
1	C	175	GLU	6.1
1	C	351	ARG	6.0
1	A	201	LYS	5.4
1	C	180	LYS	5.3
1	C	132	SER	5.3
1	C	134	TRP	5.1
1	C	350	SER	5.1
1	B	349	PHE	5.1
1	C	136	PHE	4.8
1	C	179	LEU	4.7
1	B	179	LEU	4.7
1	A	202	ALA	4.4
1	C	135	ASP	4.4
1	B	56	LYS	4.4
1	A	174	LEU	4.4
1	A	350	SER	4.4
1	C	203	SER	4.3
1	C	56	LYS	4.1
1	C	173	ASN	4.0
1	B	181	ALA	3.9
1	C	55	SER	3.8
1	B	177	ASN	3.8
1	C	143	ARG	3.7
1	C	217	ARG	3.7
1	C	172	LEU	3.7
1	C	215	ILE	3.7
1	A	171	GLN	3.6
1	B	175	GLU	3.5
1	C	171	GLN	3.4
1	C	139	GLN	3.3
1	B	207	ASN	3.2
1	A	143	ARG	3.0
1	C	131	LYS	2.9
1	A	56	LYS	2.8
1	A	172	LEU	2.8
1	B	172	LEU	2.8
1	B	202	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	173	ASN	2.7
1	B	55	SER	2.6
1	B	176	ALA	2.6
1	B	53	ASP	2.6
1	B	143	ARG	2.6
1	A	217	ARG	2.3
1	A	204	PHE	2.3
1	C	133	ASP	2.3
1	C	199	PHE	2.3
1	B	201	LYS	2.3
1	B	236	LYS	2.2
1	C	204	PHE	2.2
1	B	180	LYS	2.2
1	B	132	SER	2.1
1	B	204	PHE	2.1
1	C	130	MET	2.1
1	B	203	SER	2.1

## 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	FMN	A	401	31/31	0.99	0.09	0.50	7,9,12,13	0
2	FMN	B	401	31/31	0.98	0.08	0.34	10,12,15,16	0
3	HO6	B	402	16/16	0.93	0.08	-0.19	11,17,24,24	0
2	FMN	C	401	31/31	0.99	0.08	-0.28	8,10,14,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HO6	A	402	16/16	0.95	0.08	-0.40	11,16,23,26	0
3	HO6	C	402	16/16	0.96	0.07	-0.45	12,18,25,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.