



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 AM GMT

PDB ID : 2WET  
Title : CRYSTAL STRUCTURE OF TRYPTOPHAN 5-HALOGENASE (PYRH)  
COMPLEX WITH FAD (TRYPTOPHAN)  
Authors : De Laurentis, W.; Zhu, X.; Naismith, J.H.  
Deposited on : 2009-04-01  
Resolution : 2.40 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

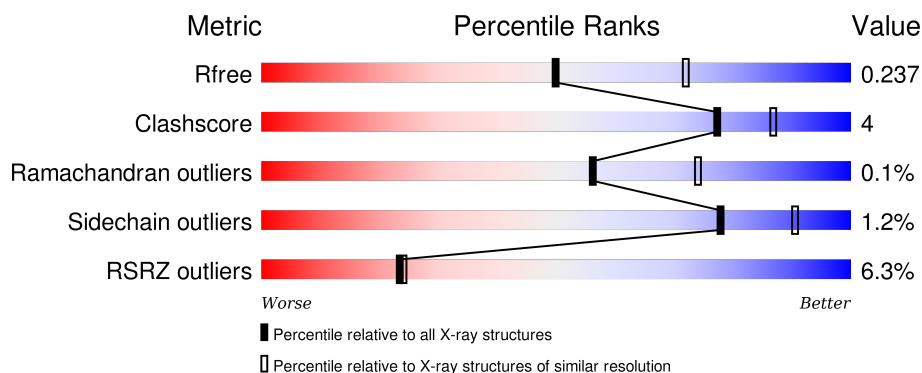
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	511	<div> <div></div> <div>88% 9% .</div> </div>
1	B	511	<div> <div>2%</div> <div>85% 12% ..</div> </div>
1	C	511	<div> <div>5%</div> <div>89% 8% .</div> </div>
1	D	511	<div> <div>17%</div> <div>90% 6% .</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
3	CL	B	1653	-	-	-	X

## 2 Entry composition [i](#)

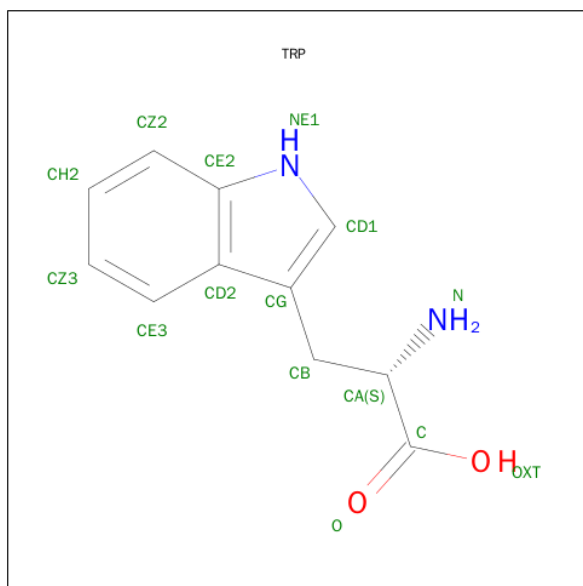
There are 6 unique types of molecules in this entry. The entry contains 17003 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPTOPHAN 5-HALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	2	0
			4008	2547	708	734	19			
1	B	501	Total	C	N	O	S	0	3	0
			4052	2574	716	743	19			
1	C	494	Total	C	N	O	S	0	1	0
			3983	2533	701	730	19			
1	D	494	Total	C	N	O	S	0	0	0
			3974	2528	699	728	19			

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).

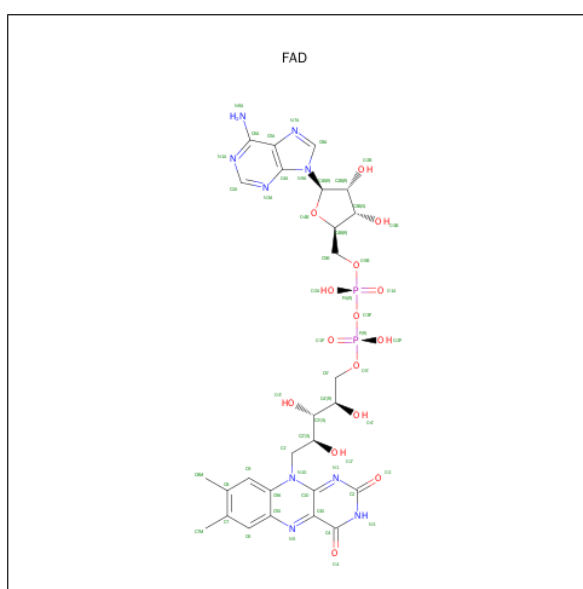


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		
3	D	2	Total	Cl	0	0
			2	2		
3	C	2	Total	Cl	0	0
			2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

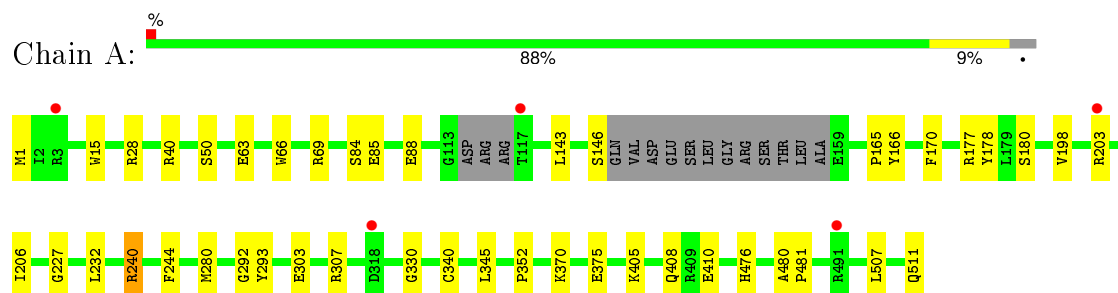
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total	O	0	0
			251	251		
6	B	207	Total	O	0	0
			207	207		
6	C	183	Total	O	0	0
			183	183		
6	D	105	Total	O	0	0
			105	105		

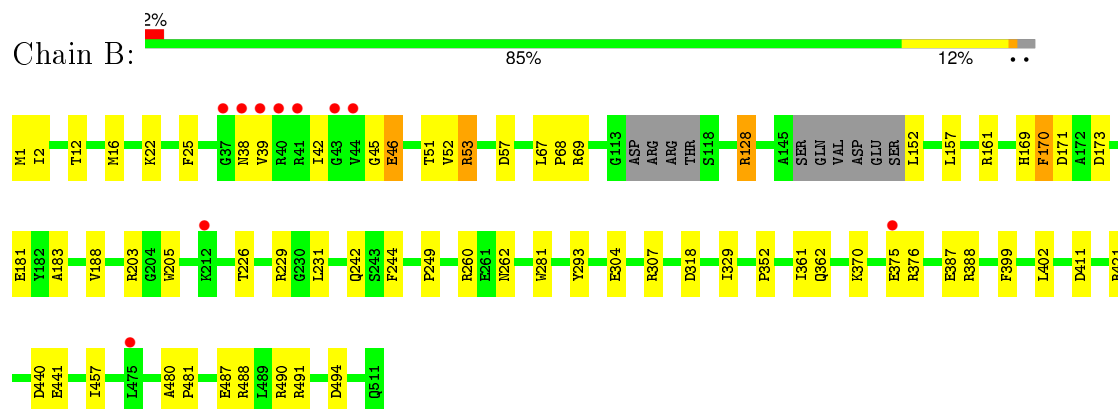
### 3 Residue-property plots [i](#)

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.

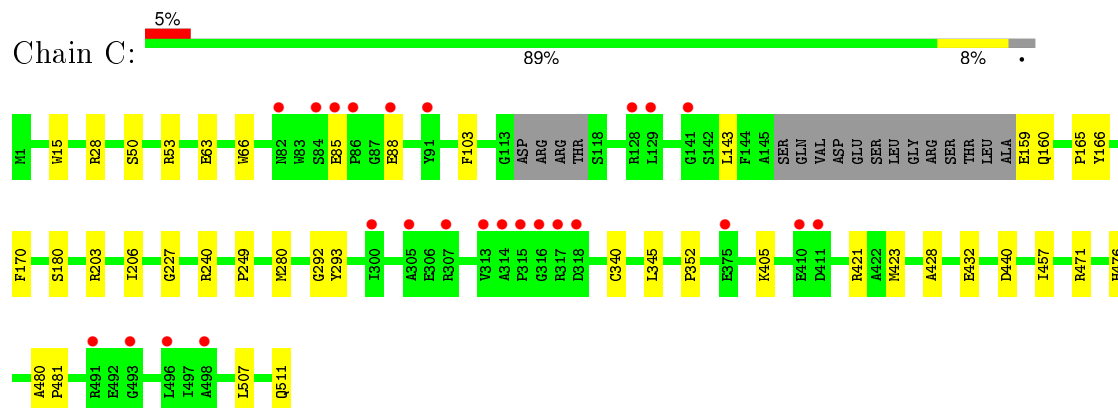
#### • Molecule 1: TRYPTOPHAN 5-HALOGENASE



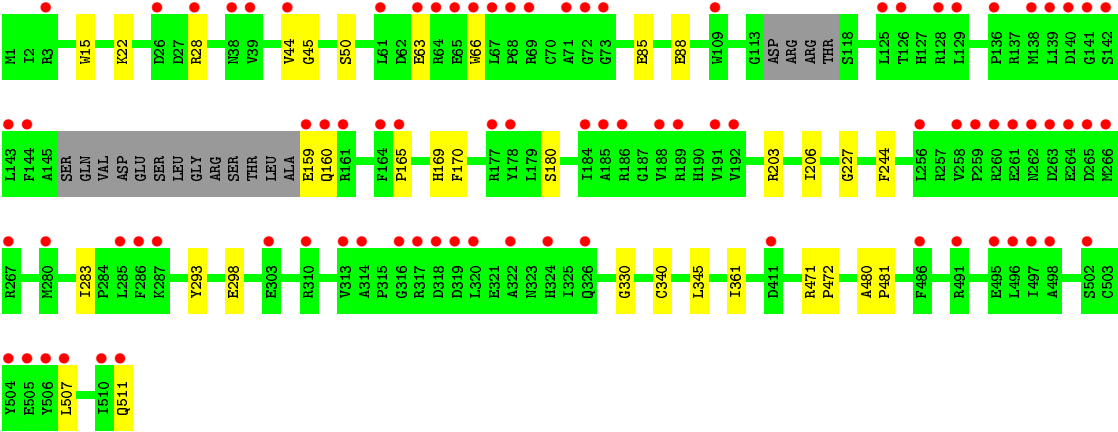
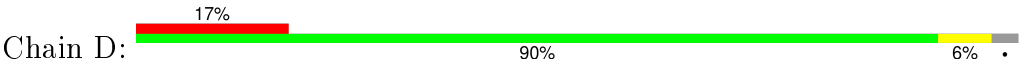
#### • Molecule 1: TRYPTOPHAN 5-HALOGENASE



#### • Molecule 1: TRYPTOPHAN 5-HALOGENASE



#### • Molecule 1: TRYPTOPHAN 5-HALOGENASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.53Å 137.53Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.40 48.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.06-2.40) 98.3 (48.07-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.196 , 0.234 0.203 , 0.237	Depositor DCC
$R_{free}$ test set	5779 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 113763 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17003	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 1.68% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.69	1/4116 (0.0%)	0.73	3/5579 (0.1%)
1	B	0.66	0/4159	0.69	1/5636 (0.0%)
1	C	0.62	0/4090	0.66	2/5544 (0.0%)
1	D	0.54	0/4081	0.64	2/5532 (0.0%)
All	All	0.63	1/16446 (0.0%)	0.68	8/22291 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	GLU	CB-CG	-5.29	1.42	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	D	203	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	A	203	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	C	203	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	D	203	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	C	203	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	240	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	440	ASP	CB-CG-OD1	5.50	123.25	118.30

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	4008	0	3844	29	1
1	B	4052	0	3893	51	0
1	C	3983	0	3821	28	0
1	D	3974	0	3814	20	1
2	B	15	0	9	0	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
3	C	2	0	0	1	0
3	D	2	0	0	0	0
4	A	53	0	31	0	0
4	B	53	0	31	2	0
4	C	53	0	31	0	0
4	D	53	0	31	4	0
5	C	5	0	0	1	0
6	A	251	0	0	2	0
6	B	207	0	0	4	0
6	C	183	0	0	2	0
6	D	105	0	0	1	0
All	All	17003	0	15505	118	1

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

All (118) 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:50:SER:HB2	1:C:165:PRO:HB2	1.81	0.62
1:B:51:THR:HB	1:B:157:LEU:HD23	1.81	0.62
1:D:85:GLU:HB2	1:D:88:GLU:HG3	1.84	0.60
1:A:410:GLU:HB3	1:B:262:ASN:HD21	1.66	0.59
1:B:361:ILE:HD11	4:B:1652:FAD:H5'1	1.83	0.59
1:C:85:GLU:HB2	1:C:88:GLU:HG3	1.84	0.59
1:A:307:ARG:HD3	1:B:490:ARG:NH2	2.17	0.59
1:B:2:ILE:O	1:B:2:ILE:HG13	2.03	0.58
1:B:57:ASP:OD2	1:B:152:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:H3	1:A:375:GLU:HB3	1.70	0.57
1:B:488:ARG:HG2	1:B:491:ARG:NH2	2.20	0.56
1:B:128[B]:ARG:HG3	1:B:128[B]:ARG:HH11	1.71	0.56
1:A:307:ARG:HD3	1:B:490:ARG:CZ	2.35	0.56
1:B:388:ARG:NH2	1:C:440:ASP:OD2	2.34	0.55
1:D:85:GLU:CB	1:D:88:GLU:HG3	2.36	0.55
1:A:85:GLU:HB2	1:A:88:GLU:HG3	1.87	0.55
1:C:85:GLU:CB	1:C:88:GLU:HG3	2.36	0.55
1:B:352:PRO:HA	3:B:700:CL:CL	2.44	0.55
1:A:1:MET:N	1:A:375:GLU:HB3	2.22	0.54
1:A:206:ILE:HD12	1:A:340:CYS:HB2	1.89	0.54
1:A:50:SER:HB2	1:A:165:PRO:HB2	1.89	0.54
1:D:50:SER:HB2	1:D:165:PRO:HB2	1.89	0.54
1:B:260:ARG:HD3	6:B:2077:HOH:O	2.06	0.54
1:B:488:ARG:HG2	1:B:491:ARG:HH22	1.73	0.53
1:A:480:ALA:HB3	1:A:481:PRO:HD3	1.89	0.53
1:B:128[B]:ARG:HG3	1:B:128[B]:ARG:NH1	2.22	0.53
1:B:457:ILE:HD11	6:B:2162:HOH:O	2.08	0.53
1:D:206:ILE:HD12	1:D:340:CYS:HB2	1.91	0.51
1:B:128[A]:ARG:NH2	1:B:494:ASP:OD1	2.42	0.51
4:D:1513:FAD:H51A	6:D:2104:HOH:O	2.10	0.51
1:C:457:ILE:HD11	6:C:2157:HOH:O	2.10	0.51
1:B:1:MET:N	1:B:375:GLU:OE2	2.37	0.50
1:B:25:PHE:CD1	1:C:476:HIS:HB2	2.46	0.50
1:B:25:PHE:CD1	1:C:476:HIS:CB	2.95	0.50
1:C:206:ILE:HD12	1:C:340:CYS:HB2	1.94	0.49
1:B:12:THR:HG22	1:B:16:MET:SD	2.52	0.49
1:A:85:GLU:CB	1:A:88:GLU:HG3	2.42	0.49
1:C:240:ARG:HD3	5:C:1514:SO4:O2	2.13	0.48
1:C:249:PRO:HG3	1:C:421:ARG:CZ	2.42	0.48
1:B:370:LYS:O	1:C:471:ARG:HD3	2.12	0.48
1:B:370:LYS:HE3	1:C:103:PHE:CE2	2.48	0.48
1:D:507:LEU:O	1:D:511:GLN:HG2	2.13	0.48
1:A:50:SER:HB3	1:A:165:PRO:O	2.13	0.48
1:B:318:ASP:N	1:B:318:ASP:OD1	2.42	0.48
1:B:411:ASP:OD1	1:B:411:ASP:N	2.45	0.48
1:B:229:ARG:HB2	6:B:2050:HOH:O	2.13	0.48
1:A:143:LEU:O	1:A:146:SER:HB3	2.14	0.47
1:B:53:ARG:HB3	1:B:53:ARG:HH11	1.79	0.47
1:B:67:LEU:HB3	1:B:68:PRO:HD3	1.96	0.47
1:A:84:SER:HB3	1:A:408:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:OD1	1:B:173:ASP:HB2	2.14	0.47
1:B:128[B]:ARG:HH22	1:B:490:ARG:HG3	1.80	0.47
1:B:69:ARG:NH1	1:B:181:GLU:OE1	2.32	0.47
1:B:203:ARG:HG3	1:B:205:TRP:CD1	2.50	0.47
1:D:45:GLY:HA2	4:D:1513:FAD:C4X	2.45	0.47
1:C:405:LYS:HE3	1:C:423:MET:HG2	1.97	0.47
1:C:15:TRP:CE3	1:C:180:SER:HA	2.50	0.46
1:D:480:ALA:HB3	1:D:481:PRO:HD3	1.97	0.46
1:B:25:PHE:CG	1:C:476:HIS:HB3	2.50	0.46
1:A:198:VAL:HG21	1:A:232:LEU:HD22	1.98	0.46
1:A:476:HIS:NE2	6:A:2234:HOH:O	2.36	0.46
1:A:370:LYS:O	1:D:471:ARG:HD3	2.16	0.46
1:A:507:LEU:O	1:A:511:GLN:HG2	2.17	0.45
1:C:53:ARG:HD2	6:C:2015:HOH:O	2.15	0.44
1:B:244:PHE:HB2	1:B:329:ILE:HG22	1.99	0.44
1:C:63:GLU:HA	1:C:66:TRP:CD1	2.53	0.44
1:D:44:VAL:HG21	4:D:1513:FAD:C7	2.47	0.44
1:A:15:TRP:CE3	1:A:180:SER:HA	2.52	0.44
1:B:46:GLU:O	1:B:169:HIS:HA	2.18	0.44
1:A:227:GLY:HA2	1:A:345:LEU:HB2	1.99	0.44
1:A:280:MET:HA	1:A:292:GLY:O	2.17	0.44
1:B:46:GLU:HB3	1:B:170:PHE:O	2.16	0.44
1:C:507:LEU:O	1:C:511:GLN:HG2	2.18	0.44
1:C:428:ALA:O	1:C:432:GLU:HG3	2.17	0.44
1:B:441:GLU:CD	1:B:441:GLU:H	2.20	0.44
1:B:304:GLU:HG3	1:B:307:ARG:NH2	2.33	0.43
1:B:242:GLN:NE2	6:B:2052:HOH:O	2.39	0.43
1:D:15:TRP:CE3	1:D:180:SER:HA	2.54	0.43
1:D:361:ILE:HD11	4:D:1513:FAD:H5'1	2.00	0.43
1:B:480:ALA:HB3	1:B:481:PRO:HD3	2.01	0.43
1:B:25:PHE:CD1	1:C:476:HIS:HB3	2.54	0.42
1:B:226:THR:HG21	1:B:231:LEU:HB3	2.00	0.42
1:B:487:GLU:HA	1:B:487:GLU:OE2	2.19	0.42
1:A:244:PHE:CD2	1:A:330:GLY:HA2	2.55	0.42
1:C:480:ALA:HB3	1:C:481:PRO:HD3	2.01	0.42
1:D:159:GLU:HG3	1:D:160:GLN:H	1.84	0.42
1:B:51:THR:HB	1:B:157:LEU:CD2	2.49	0.42
1:D:471:ARG:HA	1:D:472:PRO:HD3	1.93	0.42
1:C:457:ILE:HG21	1:C:457:ILE:HD13	1.79	0.42
1:B:399:PHE:O	1:B:402:LEU:HB3	2.20	0.42
1:B:183:ALA:HB1	1:B:188:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:GLY:HA2	1:C:345:LEU:HB2	2.02	0.41
1:B:52:VAL:HA	1:B:362:GLN:OE1	2.20	0.41
1:B:22:LYS:HA	1:B:22:LYS:HD3	1.81	0.41
1:D:227:GLY:HA2	1:D:345:LEU:HB2	2.03	0.41
1:C:280:MET:HA	1:C:292:GLY:O	2.20	0.41
1:A:352:PRO:HA	3:A:700:CL:CL	2.57	0.41
1:A:40[A]:ARG:NH1	1:A:40[A]:ARG:HG3	2.35	0.41
1:D:50:SER:HB3	1:D:165:PRO:O	2.20	0.41
1:B:249:PRO:HG3	1:B:421:ARG:CZ	2.51	0.41
1:D:244:PHE:CD2	1:D:330:GLY:HA2	2.56	0.41
1:C:159:GLU:HG3	1:C:160:GLN:H	1.86	0.41
1:C:159:GLU:HG3	1:C:160:GLN:N	2.36	0.41
1:C:143:LEU:HD11	1:C:166:TYR:HE1	1.85	0.41
1:D:22:LYS:HA	1:D:22:LYS:HD3	1.95	0.41
1:A:405:LYS:HD3	1:A:405:LYS:HA	1.91	0.41
1:B:42:ILE:HA	1:B:42:ILE:HD12	1.95	0.41
4:B:1652:FAD:HO2'	4:B:1652:FAD:HO4'	1.69	0.40
1:A:63:GLU:HA	1:A:66:TRP:CD1	2.57	0.40
1:D:169:HIS:CD2	1:D:283:ILE:HG23	2.56	0.40
1:B:161:ARG:HD3	1:B:161:ARG:HA	1.82	0.40
1:A:307:ARG:HD2	1:B:494:ASP:OD2	2.20	0.40
1:D:471:ARG:HH11	1:D:471:ARG:HD3	1.78	0.40
1:A:177:ARG:HD3	6:A:2067:HOH:O	2.20	0.40
1:C:352:PRO:HA	3:C:700:CL:CL	2.59	0.40
1:A:69:ARG:HG2	1:A:178:TYR:CE1	2.57	0.40
1:A:143:LEU:HD11	1:A:166:TYR:HE1	1.86	0.40
1:D:63:GLU:HA	1:D:66:TRP:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:NH2	1:D:298:GLU:O[7_555]	1.84	0.36

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/511 (96%)	474 (96%)	18 (4%)	0	100	100
1	B	498/511 (98%)	478 (96%)	18 (4%)	2 (0%)	39	56
1	C	489/511 (96%)	472 (96%)	17 (4%)	0	100	100
1	D	488/511 (96%)	472 (97%)	16 (3%)	0	100	100
All	All	1967/2044 (96%)	1896 (96%)	69 (4%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	VAL
1	B	45	GLY

### 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	413/424 (97%)	410 (99%)	3 (1%)	88	95
1	B	417/424 (98%)	407 (98%)	10 (2%)	57	76
1	C	410/424 (97%)	407 (99%)	3 (1%)	88	95
1	D	409/424 (96%)	406 (99%)	3 (1%)	88	95
All	All	1649/1696 (97%)	1630 (99%)	19 (1%)	78	90

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	170	PHE
1	A	293	TYR
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	46	GLU
1	B	53	ARG
1	B	128[A]	ARG
1	B	128[B]	ARG
1	B	170	PHE
1	B	281	TRP
1	B	293	TYR
1	B	376	ARG
1	B	387	GLU
1	C	28	ARG
1	C	170	PHE
1	C	293	TYR
1	D	28	ARG
1	D	170	PHE
1	D	293	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	197	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	FAD	A	1513	-	48,58,58	1.22	5 (10%)	54,89,89	2.35	11 (20%)
4	FAD	B	1652	-	48,58,58	1.32	7 (14%)	54,89,89	2.29	8 (14%)
2	TRP	B	650	-	12,16,16	0.87	0	7,22,22	1.01	0
4	FAD	C	1513	-	48,58,58	1.24	5 (10%)	54,89,89	2.30	9 (16%)
5	SO4	C	1514	-	4,4,4	0.42	0	6,6,6	0.50	0
4	FAD	D	1513	-	48,58,58	1.33	6 (12%)	54,89,89	2.08	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	A	1513	-	-	0/30/50/50	0/6/6/6
4	FAD	B	1652	-	-	0/30/50/50	0/6/6/6
2	TRP	B	650	-	-	0/3/8/8	0/2/2/2
4	FAD	C	1513	-	-	0/30/50/50	0/6/6/6
5	SO4	C	1514	-	-	0/0/0/0	0/0/0/0
4	FAD	D	1513	-	-	0/30/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1513	FAD	C6-C5X	-2.11	1.38	1.41
4	A	1513	FAD	C2A-N1A	2.09	1.37	1.33
4	B	1652	FAD	C5'-C4'	2.20	1.55	1.51
4	C	1513	FAD	C2A-N1A	2.26	1.38	1.33
4	A	1513	FAD	C4-N3	2.34	1.37	1.33
4	D	1513	FAD	C2A-N1A	2.45	1.38	1.33
4	B	1652	FAD	C5X-N5	2.49	1.39	1.35
4	D	1513	FAD	C5X-N5	2.56	1.39	1.35
4	B	1652	FAD	C2A-N1A	2.61	1.38	1.33
4	C	1513	FAD	C1'-N10	2.66	1.51	1.48
4	B	1652	FAD	C4-N3	2.92	1.38	1.33
4	A	1513	FAD	C2A-N3A	3.12	1.37	1.32
4	D	1513	FAD	C4-N3	3.28	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1652	FAD	C1'-N10	3.30	1.51	1.48
4	C	1513	FAD	C4X-N5	3.31	1.38	1.33
4	B	1652	FAD	C4X-N5	3.33	1.38	1.33
4	D	1513	FAD	C1'-N10	3.37	1.52	1.48
4	C	1513	FAD	C2A-N3A	3.38	1.38	1.32
4	C	1513	FAD	C4-N3	3.43	1.39	1.33
4	D	1513	FAD	C2A-N3A	3.47	1.38	1.32
4	B	1652	FAD	C2A-N3A	3.55	1.38	1.32
4	A	1513	FAD	C4X-N5	3.72	1.39	1.33
4	D	1513	FAD	C4X-N5	4.01	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1513	FAD	N3A-C2A-N1A	-13.35	118.67	128.89
4	C	1513	FAD	N3A-C2A-N1A	-13.00	118.94	128.89
4	B	1652	FAD	N3A-C2A-N1A	-11.78	119.88	128.89
4	D	1513	FAD	N3A-C2A-N1A	-11.61	120.01	128.89
4	B	1652	FAD	C4X-C4-N3	-3.09	119.36	123.59
4	C	1513	FAD	C4X-C4-N3	-2.76	119.81	123.59
4	A	1513	FAD	C4-C4X-C10	-2.73	118.19	119.94
4	D	1513	FAD	C4X-C4-N3	-2.72	119.86	123.59
4	D	1513	FAD	C4A-C5A-N7A	-2.51	107.17	109.48
4	C	1513	FAD	O3B-C3B-C4B	-2.41	103.81	111.05
4	A	1513	FAD	C4X-C4-N3	-2.34	120.39	123.59
4	C	1513	FAD	C4A-C5A-N7A	-2.29	107.37	109.48
4	A	1513	FAD	C4A-C5A-N7A	-2.23	107.43	109.48
4	C	1513	FAD	C1B-N9A-C4A	-2.12	123.75	126.94
4	A	1513	FAD	C1B-N9A-C4A	-2.05	123.84	126.94
4	B	1652	FAD	C4A-C5A-N7A	-2.01	107.63	109.48
4	B	1652	FAD	O2A-PA-O3P	2.13	114.77	105.09
4	D	1513	FAD	C4-C4X-N5	2.15	121.33	118.72
4	C	1513	FAD	C5X-C9A-N10	2.20	119.29	117.62
4	D	1513	FAD	C5X-C9A-N10	2.27	119.34	117.62
4	C	1513	FAD	C4-C4X-N5	2.38	121.61	118.72
4	D	1513	FAD	C1'-N10-C9A	2.40	121.56	118.86
4	A	1513	FAD	O4B-C1B-N9A	2.40	113.13	108.10
4	A	1513	FAD	C1'-N10-C9A	2.57	121.75	118.86
4	B	1652	FAD	C4-C4X-N5	2.63	121.91	118.72
4	A	1513	FAD	C5X-C9A-N10	2.68	119.66	117.62
4	A	1513	FAD	C4X-N5-C5X	2.83	120.02	116.76
4	A	1513	FAD	C4-C4X-N5	2.84	122.16	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1652	FAD	C1'-N10-C9A	3.05	122.28	118.86
4	D	1513	FAD	C4X-N5-C5X	3.29	120.54	116.76
4	C	1513	FAD	C4X-N5-C5X	3.45	120.74	116.76
4	B	1652	FAD	C4X-N5-C5X	3.77	121.09	116.76
4	D	1513	FAD	C4-N3-C2	5.80	120.26	115.25
4	C	1513	FAD	C4-N3-C2	6.32	120.71	115.25
4	A	1513	FAD	C4-N3-C2	6.34	120.73	115.25
4	B	1652	FAD	C4-N3-C2	7.82	122.00	115.25

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
4	B	1652	FAD	2	0
5	C	1514	SO4	1	0
4	D	1513	FAD	4	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	496/511 (97%)	0.03	5 (1%) 84 83	15, 19, 26, 32	0
1	B	501/511 (98%)	0.05	10 (1%) 68 68	11, 20, 32, 53	0
1	C	494/511 (96%)	0.23	25 (5%) 32 32	15, 19, 25, 33	0
1	D	494/511 (96%)	0.76	85 (17%) 2 2	15, 19, 26, 32	0
All	All	1985/2044 (97%)	0.26	125 (6%) 23 24	11, 19, 28, 53	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	LYS	6.2
1	D	286	PHE	5.3
1	D	510	ILE	5.0
1	B	39	VAL	4.8
1	D	498	ALA	4.8
1	D	263	ASP	4.8
1	D	507	LEU	4.5
1	D	259	PRO	4.4
1	D	69	ARG	4.0
1	D	504	TYR	3.9
1	D	63	GLU	3.9
1	D	261	GLU	3.9
1	D	144	PHE	3.9
1	B	43	GLY	3.9
1	B	41	ARG	3.9
1	D	314	ALA	3.8
1	D	264	GLU	3.8
1	D	140	ASP	3.7
1	D	316	GLY	3.7
1	D	262	ASN	3.7
1	D	136	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	496	LEU	3.6
1	B	44	VAL	3.6
1	D	141	GLY	3.5
1	D	164	PHE	3.5
1	D	66	TRP	3.5
1	D	491	ARG	3.3
1	D	126	THR	3.3
1	D	189	ARG	3.3
1	D	73	GLY	3.2
1	D	61	LEU	3.2
1	D	318	ASP	3.1
1	D	258	VAL	3.1
1	C	493	GLY	3.1
1	B	37	GLY	3.1
1	D	322	ALA	3.1
1	D	184	ILE	3.0
1	D	186	ARG	3.0
1	B	38	ASN	3.0
1	D	139	LEU	3.0
1	C	316	GLY	3.0
1	D	138	MET	2.9
1	D	285	LEU	2.9
1	D	411	ASP	2.9
1	D	64	ARG	2.9
1	D	165	PRO	2.9
1	C	84	SER	2.9
1	D	188	VAL	2.9
1	C	141	GLY	2.9
1	C	85	GLU	2.9
1	D	3	ARG	2.9
1	D	72	GLY	2.8
1	A	491	ARG	2.8
1	A	117	THR	2.8
1	D	128	ARG	2.8
1	C	375	GLU	2.8
1	C	313	VAL	2.8
1	C	86	PRO	2.7
1	D	71	ALA	2.7
1	D	256	LEU	2.7
1	D	497	ILE	2.7
1	D	39	VAL	2.7
1	D	303	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	300	ILE	2.6
1	C	318	ASP	2.6
1	D	260	ARG	2.6
1	D	310	ARG	2.6
1	D	129	LEU	2.6
1	C	88	GLU	2.6
1	D	159	GLU	2.6
1	D	511	GLN	2.6
1	C	91	TYR	2.5
1	D	506	TYR	2.5
1	C	317	ARG	2.5
1	D	496	LEU	2.5
1	D	280	MET	2.5
1	C	491	ARG	2.5
1	D	67	LEU	2.5
1	D	320	LEU	2.5
1	A	203	ARG	2.5
1	D	505	GLU	2.5
1	D	313	VAL	2.4
1	C	128	ARG	2.4
1	C	410	GLU	2.4
1	C	307	ARG	2.4
1	C	129	LEU	2.4
1	D	495	GLU	2.4
1	D	143	LEU	2.4
1	D	319	ASP	2.4
1	D	267	ARG	2.3
1	D	192	VAL	2.3
1	C	314	ALA	2.2
1	C	498	ALA	2.2
1	D	177	ARG	2.2
1	D	502	SER	2.2
1	A	318	ASP	2.2
1	D	160	GLN	2.2
1	D	317	ARG	2.2
1	D	68	PRO	2.2
1	D	26	ASP	2.2
1	D	266	MET	2.2
1	B	475	LEU	2.1
1	D	142	SER	2.1
1	D	191	VAL	2.1
1	D	109	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	185	ALA	2.1
1	C	82	ASN	2.1
1	D	161	ARG	2.1
1	D	265	ASP	2.1
1	D	38	ASN	2.1
1	D	28	ARG	2.1
1	B	375	GLU	2.1
1	D	486	PHE	2.1
1	C	411	ASP	2.1
1	B	40	ARG	2.1
1	D	125	LEU	2.0
1	A	3	ARG	2.0
1	B	212	LYS	2.0
1	D	44	VAL	2.0
1	D	324	HIS	2.0
1	D	178	TYR	2.0
1	D	326	GLN	2.0
1	D	65	GLU	2.0
1	C	305	ALA	2.0
1	C	315	PRO	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
3	CL	B	1653	1/1	0.99	0.35	4.92	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FAD	A	1513	53/53	0.98	0.18	0.29	15,21,27,27	0
4	FAD	C	1513	53/53	0.97	0.15	-0.03	15,22,27,27	0
3	CL	A	700	1/1	0.99	0.16	-0.21	35,35,35,35	0
4	FAD	B	1652	53/53	0.92	0.17	-0.40	16,23,27,27	0
2	TRP	B	650	15/15	0.94	0.17	-0.43	41,44,47,47	0
4	FAD	D	1513	53/53	0.94	0.12	-1.15	16,22,27,27	0
3	CL	B	700	1/1	0.94	0.15	-1.56	50,50,50,50	0
5	SO4	C	1514	5/5	0.94	0.13	-1.82	41,49,51,53	0
3	CL	D	700	1/1	0.96	0.10	-3.31	39,39,39,39	0
3	CL	C	700	1/1	0.99	0.10	-3.71	37,37,37,37	0
3	CL	A	1514	1/1	0.98	0.34	-	50,50,50,50	0
3	CL	D	1514	1/1	0.95	0.39	-	49,49,49,49	0
3	CL	C	1515	1/1	0.99	0.30	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.