



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:00 pm GMT

PDB ID : 2J4D  
Title : CRYPTOCHROME 3 FROM ARABIDOPSIS THALIANA  
Authors : Klar, T.; Pokorny, R.; Batschauer, A.; Essen, L.-O.  
Deposited on : 2006-08-28  
Resolution : 1.90 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

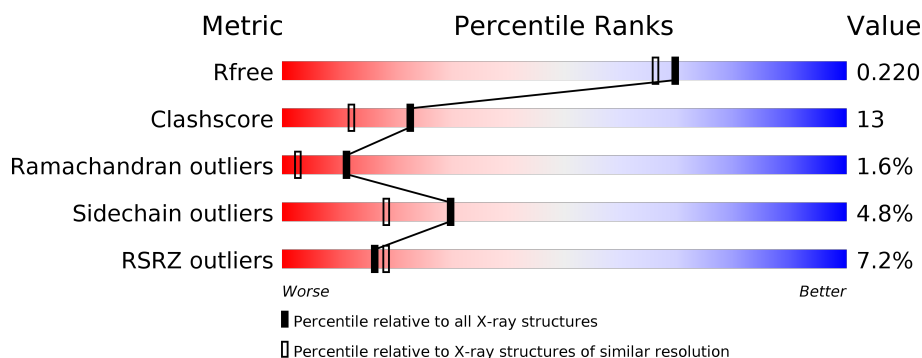
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	525	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•• 6%</div> </div> </div>
1	B	525	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>•• 5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9038 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 CRYPTOCHROME DASH.

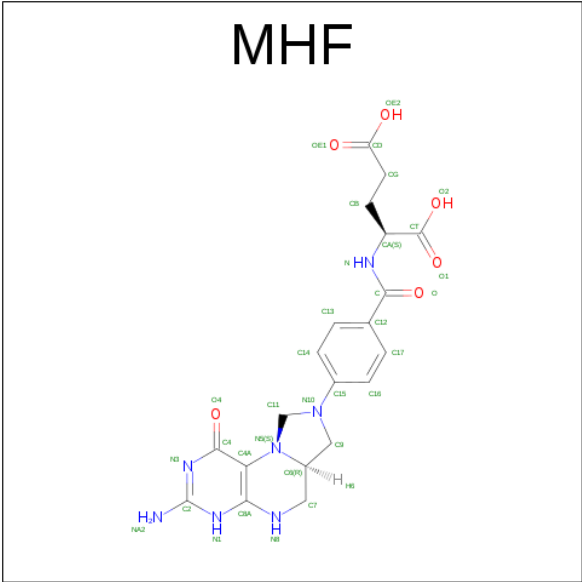
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			4050	2596	702	732	20			
1	B	499	Total	C	N	O	S	9	0	0
			4069	2607	706	736	20			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 3 is 5,10-METHENYL-6,7,8-TRIHYDROFOLIC ACID (three-letter code: MHF) (formula:  $C_{20}H_{23}N_7O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	7	6		
3	B	1	Total	C	N	O	0	0
			33	20	7	6		

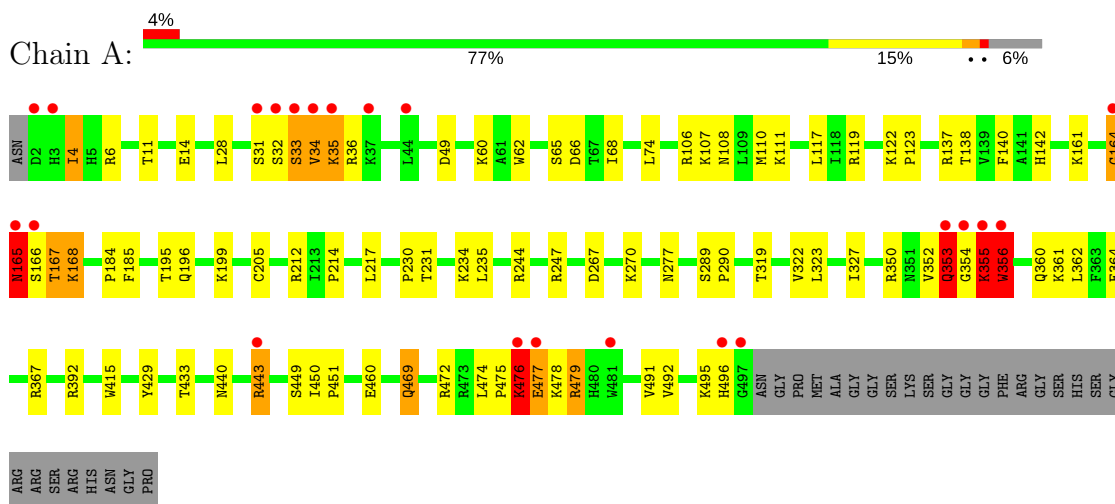
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	437	Total	O	0	0
			437	437		
4	B	310	Total	O	0	0
			310	310		

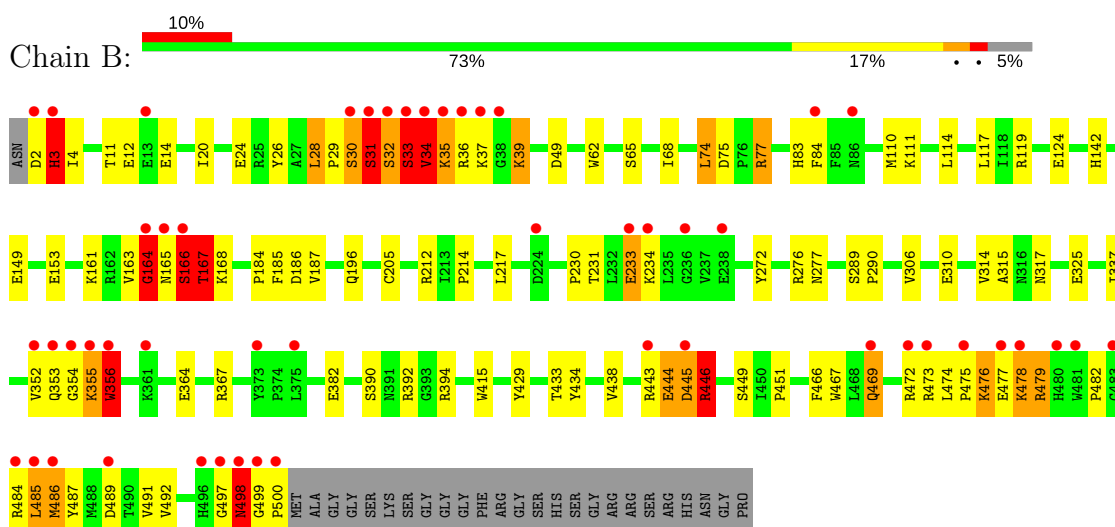
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: CRYPTOCHROME DASH



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.30Å 116.78Å 135.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.3 (19.92-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.221 0.189 , 0.220	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MHF, FAD

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	0.42	1/4162 (0.0%)	0.70	5/5631 (0.1%)
1	B	0.56	1/4182 (0.0%)	0.85	15/5659 (0.3%)
All	All	0.50	2/8344 (0.0%)	0.78	20/11290 (0.2%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	GLY	C-N	-23.64	0.79	1.34
1	A	164	GLY	C-N	-10.54	1.09	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLY	O-C-N	-22.82	86.19	122.70
1	B	33	SER	N-CA-C	-10.92	81.50	111.00
1	B	166	SER	N-CA-C	-9.52	85.29	111.00
1	B	39	LYS	N-CA-C	8.97	135.23	111.00
1	B	445	ASP	CB-CA-C	7.47	125.34	110.40
1	B	445	ASP	N-CA-C	-7.32	91.24	111.00
1	A	356	TRP	N-CA-C	6.85	129.49	111.00
1	B	167	THR	O-C-N	-6.82	111.79	122.70
1	B	32	SER	N-CA-C	-6.61	93.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	TRP	N-CA-C	6.35	128.14	111.00
1	B	164	GLY	CA-C-N	-6.23	103.49	117.20
1	A	355	LYS	N-CA-C	5.92	126.99	111.00
1	A	165	ASN	N-CA-C	-5.90	95.08	111.00
1	B	446	ARG	N-CA-C	5.76	126.55	111.00
1	B	31	SER	N-CA-C	5.64	126.24	111.00
1	B	164	GLY	C-N-CA	-5.42	108.15	121.70
1	A	167	THR	C-N-CA	5.35	135.07	121.70
1	A	165	ASN	CB-CA-C	5.15	120.71	110.40
1	B	354	GLY	CA-C-N	-5.12	105.93	117.20
1	B	353	GLN	C-N-CA	-5.02	111.77	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	GLY	Mainchain

## 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	4050	0	3973	98	0
1	B	4069	0	3989	114	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	33	0	21	0	0
3	B	33	0	21	0	0
4	A	437	0	0	3	0
4	B	310	0	0	6	0
All	All	9038	0	8066	212	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 13.

All (212) 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:B:35:LYS:O	1:B:39:LYS:HE3	1.31	1.30
1:B:32:SER:HA	1:B:34:VAL:CG1	1.63	1.28
1:B:484:ARG:NH1	1:B:489:ASP:OD1	1.78	1.17
1:B:34:VAL:HG22	1:B:35:LYS:H	0.97	1.07
1:B:32:SER:CA	1:B:34:VAL:HG12	1.89	1.01
1:B:486:MET:H	1:B:486:MET:HE2	1.20	1.00
1:B:32:SER:HA	1:B:34:VAL:HG12	0.97	0.97
1:B:34:VAL:CG2	1:B:35:LYS:H	1.76	0.95
1:B:34:VAL:HG23	1:B:36:ARG:HG3	1.49	0.94
1:B:34:VAL:O	1:B:35:LYS:HB2	1.63	0.94
1:B:34:VAL:HG22	1:B:35:LYS:N	1.77	0.93
1:B:34:VAL:CG2	1:B:36:ARG:HG3	1.99	0.93
1:B:36:ARG:HA	1:B:39:LYS:HD2	1.49	0.92
1:A:355:LYS:HG3	1:A:356:TRP:H	1.36	0.91
1:B:35:LYS:O	1:B:39:LYS:CE	2.19	0.89
1:A:495:LYS:HE2	1:A:496:HIS:NE2	1.88	0.88
1:B:498:ASN:HD22	1:B:499:GLY:H	1.19	0.87
1:B:486:MET:N	1:B:486:MET:HE2	1.90	0.85
1:A:355:LYS:CG	1:A:356:TRP:H	1.83	0.81
1:B:497:GLY:O	1:B:498:ASN:HB2	1.78	0.81
1:A:161:LYS:HG3	4:A:2175:HOH:O	1.85	0.77
1:B:34:VAL:CG2	1:B:35:LYS:N	2.38	0.74
1:B:32:SER:O	1:B:33:SER:HB3	1.86	0.73
1:A:49:ASP:OD2	1:A:142:HIS:HD2	1.72	0.72
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.55	0.72
1:B:164:GLY:C	1:B:166:SER:N	2.44	0.71
1:B:498:ASN:ND2	1:B:499:GLY:H	1.88	0.70
1:A:34:VAL:HG11	1:A:62:TRP:CH2	2.26	0.70
1:B:445:ASP:O	1:B:446:ARG:HB2	1.91	0.69
1:B:75:ASP:OD1	1:B:77:ARG:HD2	1.92	0.69
1:A:476:LYS:HA	1:A:479:ARG:HG3	1.73	0.69
1:B:184:PRO:HD3	1:B:205:CYS:SG	2.32	0.69
1:A:165:ASN:O	1:A:166:SER:HB3	1.93	0.69
1:A:244:ARG:NH1	1:A:469:GLN:HE22	1.90	0.69
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.08	0.69
1:B:39:LYS:HB3	1:B:65:SER:HA	1.75	0.68
1:A:355:LYS:HG3	1:A:356:TRP:N	2.09	0.68
1:B:352:VAL:CG1	1:B:438:VAL:HG12	2.25	0.67
1:B:289:SER:OG	1:B:290:PRO:HD3	1.95	0.67
1:B:20:ILE:O	1:B:24:GLU:HG3	1.96	0.66
1:A:74:LEU:HD21	1:A:235:LEU:CD1	2.24	0.66
1:A:352:VAL:CG1	1:A:353:GLN:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ASN:HD22	1:B:499:GLY:N	1.93	0.65
1:B:119:ARG:HD2	4:B:2091:HOH:O	1.97	0.64
1:B:352:VAL:HG11	1:B:438:VAL:HG12	1.79	0.64
1:A:460:GLU:OE2	1:A:476:LYS:HE3	1.98	0.64
1:A:35:LYS:H	1:A:35:LYS:HZ3	1.46	0.64
1:B:49:ASP:OD2	1:B:142:HIS:HD2	1.80	0.64
1:B:28:LEU:HD23	1:B:29:PRO:HD2	1.80	0.63
1:B:196:GLN:HG3	4:B:2053:HOH:O	1.99	0.63
1:A:277:ASN:HD21	1:A:392:ARG:HH21	1.47	0.62
1:A:353:GLN:HG3	1:A:354:GLY:H	1.63	0.62
1:B:477:GLU:H	1:B:477:GLU:CD	2.01	0.62
1:A:138:THR:HG22	1:A:168:LYS:CG	2.29	0.62
1:A:196:GLN:HG3	4:A:2075:HOH:O	1.98	0.62
1:B:478:LYS:HE2	1:B:478:LYS:HA	1.82	0.62
1:A:244:ARG:HH22	1:A:472:ARG:NH2	1.99	0.60
1:A:35:LYS:H	1:A:35:LYS:NZ	1.99	0.59
1:A:352:VAL:CG1	1:A:353:GLN:N	2.64	0.59
1:A:476:LYS:HB2	1:A:477:GLU:OE2	2.02	0.59
1:B:484:ARG:HH11	1:B:489:ASP:CG	2.02	0.59
1:A:231:THR:HG23	1:A:234:LYS:HE3	1.84	0.59
1:A:277:ASN:ND2	1:A:392:ARG:HH21	2.00	0.59
1:A:35:LYS:HG2	1:A:35:LYS:O	2.02	0.58
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.15	0.58
1:B:231:THR:OG1	1:B:234:LYS:HG3	2.02	0.58
1:B:231:THR:HG23	1:B:234:LYS:HE3	1.83	0.58
1:B:434:TYR:HE2	1:B:444:GLU:OE2	1.85	0.58
1:A:62:TRP:HA	1:A:68:ILE:HD11	1.86	0.57
1:A:352:VAL:HG12	1:A:353:GLN:CB	2.34	0.57
1:A:469:GLN:H	1:A:469:GLN:CD	2.07	0.57
1:B:77:ARG:NH2	1:B:124:GLU:OE2	2.36	0.57
1:A:184:PRO:HD3	1:A:205:CYS:SG	2.45	0.56
1:A:450:ILE:N	1:A:451:PRO:HD2	2.20	0.56
1:B:2:ASP:HB3	1:B:466:PHE:HE2	1.70	0.56
1:A:353:GLN:CG	1:A:354:GLY:H	2.18	0.56
1:B:32:SER:CA	1:B:34:VAL:CG1	2.59	0.56
1:A:350:ARG:HB3	1:A:352:VAL:HG23	1.87	0.56
1:B:11:THR:OG1	1:B:14:GLU:HG3	2.05	0.56
1:B:32:SER:HA	1:B:34:VAL:HG13	1.76	0.56
1:A:214:PRO:HG2	1:A:217:LEU:CD2	2.37	0.56
1:A:495:LYS:CE	1:A:496:HIS:NE2	2.66	0.55
1:A:60:LYS:HG3	1:A:140:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:HG3	1:B:415:TRP:CE2	2.42	0.54
1:A:74:LEU:CD2	1:A:235:LEU:HD21	2.36	0.54
1:B:445:ASP:O	1:B:446:ARG:CB	2.52	0.54
1:A:475:PRO:O	1:A:479:ARG:HG2	2.08	0.54
1:A:138:THR:HG22	1:A:168:LYS:HG3	1.90	0.54
1:A:74:LEU:HD21	1:A:235:LEU:HD11	1.88	0.54
1:B:74:LEU:HD13	1:B:230:PRO:HG3	1.89	0.54
1:A:429:TYR:O	1:A:433:THR:HG23	2.07	0.54
1:B:36:ARG:HA	1:B:39:LYS:CD	2.30	0.53
1:B:485:LEU:CD1	1:B:485:LEU:C	2.77	0.53
1:A:360:GLN:O	1:A:364:GLU:HG3	2.08	0.53
1:A:352:VAL:HG13	1:A:353:GLN:HB2	1.90	0.53
1:A:138:THR:HG22	1:A:168:LYS:HG2	1.91	0.53
1:B:26:TYR:O	1:B:212:ARG:HD2	2.09	0.53
1:B:34:VAL:HG23	1:B:36:ARG:CG	2.32	0.53
1:B:289:SER:HB3	2:B:1501:FAD:H5'2	1.90	0.53
1:A:74:LEU:HD22	1:A:230:PRO:HG3	1.90	0.52
1:A:164:GLY:C	1:A:165:ASN:O	2.39	0.52
1:B:434:TYR:CE2	1:B:444:GLU:OE2	2.63	0.52
1:A:108:ASN:HA	1:A:111:LYS:HE2	1.92	0.52
1:B:75:ASP:OD1	1:B:77:ARG:CD	2.58	0.52
1:A:11:THR:OG1	1:A:14:GLU:HG3	2.10	0.51
1:B:382:GLU:HG3	1:B:467:TRP:CZ2	2.45	0.51
1:B:364:GLU:HG2	1:B:367:ARG:NH2	2.25	0.51
1:A:214:PRO:HG2	1:A:217:LEU:HD23	1.92	0.51
1:B:36:ARG:HB3	1:B:65:SER:O	2.10	0.51
1:A:350:ARG:HD2	1:A:352:VAL:CG2	2.40	0.51
1:B:277:ASN:ND2	4:B:2199:HOH:O	2.43	0.51
1:B:485:LEU:HD13	1:B:485:LEU:C	2.31	0.51
1:A:34:VAL:HA	1:A:35:LYS:NZ	2.26	0.51
1:B:29:PRO:O	1:B:30:SER:O	2.30	0.50
1:A:475:PRO:C	1:A:476:LYS:O	2.47	0.50
1:B:111:LYS:NZ	4:B:2085:HOH:O	2.45	0.50
1:B:39:LYS:CB	1:B:65:SER:HA	2.42	0.50
1:A:289:SER:HB3	2:A:1498:FAD:H5'2	1.93	0.49
1:A:319:THR:O	1:A:322:VAL:HG12	2.12	0.49
1:B:276:ARG:HD3	4:B:2193:HOH:O	2.13	0.49
1:B:352:VAL:HG13	1:B:438:VAL:HG12	1.95	0.49
1:B:187:VAL:HG21	1:B:337:ILE:HG21	1.95	0.49
1:A:244:ARG:NH2	1:A:472:ARG:HH22	2.11	0.49
1:B:476:LYS:HG2	1:B:477:GLU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:VAL:HG12	1:A:353:GLN:HB2	1.94	0.48
1:A:195:THR:CG2	1:A:199:LYS:HE2	2.44	0.48
1:A:267:ASP:OD2	1:A:270:LYS:HE3	2.14	0.48
1:B:478:LYS:HE2	1:B:478:LYS:CA	2.42	0.48
1:A:476:LYS:O	1:A:477:GLU:HB2	2.14	0.48
1:B:30:SER:OG	1:B:31:SER:N	2.46	0.48
1:A:367:ARG:HG3	1:A:415:TRP:CE2	2.49	0.48
1:B:83:HIS:CD2	1:B:84:PHE:CZ	3.02	0.47
1:B:28:LEU:CD2	1:B:29:PRO:HD2	2.45	0.47
1:B:110:MET:HA	1:B:114:LEU:O	2.15	0.47
1:A:491:VAL:HG13	1:A:492:VAL:HG22	1.96	0.47
1:B:164:GLY:C	1:B:165:ASN:C	2.37	0.47
1:A:195:THR:HG22	1:A:199:LYS:HE2	1.97	0.47
1:B:364:GLU:HG2	1:B:367:ARG:CZ	2.45	0.47
1:A:165:ASN:O	1:A:166:SER:CB	2.57	0.47
1:A:476:LYS:O	1:A:477:GLU:CB	2.61	0.47
1:B:272:TYR:OH	1:B:325:GLU:HG3	2.15	0.46
1:B:485:LEU:HD13	1:B:485:LEU:O	2.15	0.46
1:B:83:HIS:HD2	1:B:84:PHE:CE2	2.33	0.46
1:B:29:PRO:O	1:B:30:SER:C	2.52	0.46
1:A:244:ARG:NH1	1:A:469:GLN:NE2	2.61	0.46
1:B:164:GLY:C	1:B:166:SER:H	2.19	0.46
1:A:244:ARG:NH2	1:A:472:ARG:NH2	2.62	0.46
1:B:3:HIS:HB3	1:B:4:ILE:H	1.41	0.46
1:A:74:LEU:HD21	1:A:235:LEU:HD13	1.97	0.46
1:B:36:ARG:CA	1:B:39:LYS:HD2	2.34	0.46
1:B:33:SER:O	1:B:34:VAL:O	2.33	0.46
1:B:474:LEU:O	1:B:479:ARG:HD3	2.15	0.46
1:B:482:PRO:HG2	1:B:487:TYR:HB2	1.98	0.46
1:B:355:LYS:C	1:B:356:TRP:CD1	2.89	0.45
1:A:4:ILE:HG12	1:A:4:ILE:H	1.61	0.45
1:A:478:LYS:HD2	1:A:478:LYS:HA	1.72	0.45
1:B:2:ASP:CG	1:B:3:HIS:H	2.20	0.45
1:B:497:GLY:O	1:B:498:ASN:CB	2.56	0.45
1:A:36:ARG:O	1:A:66:ASP:HB3	2.16	0.45
1:B:166:SER:HB2	1:B:167:THR:H	1.14	0.45
1:A:289:SER:OG	1:A:290:PRO:HD3	2.17	0.45
1:B:163:VAL:HG12	1:B:163:VAL:O	2.17	0.45
1:A:107:LYS:O	1:A:111:LYS:HG3	2.16	0.44
1:B:168:LYS:HG2	1:B:168:LYS:H	1.54	0.44
1:A:231:THR:HG23	1:A:234:LYS:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:O	1:B:310:GLU:HG3	2.17	0.44
1:B:277:ASN:HD21	1:B:392:ARG:HH21	1.65	0.44
1:A:137:ARG:O	1:A:168:LYS:HE3	2.17	0.44
1:A:352:VAL:HG13	1:A:353:GLN:N	2.32	0.44
1:B:469:GLN:HB3	1:B:472:ARG:CZ	2.48	0.44
1:A:117:LEU:HD11	1:A:119:ARG:CZ	2.48	0.44
1:B:484:ARG:HD3	1:B:489:ASP:OD2	2.18	0.44
1:A:74:LEU:HD23	1:A:235:LEU:HD21	2.00	0.44
1:A:34:VAL:HA	1:A:35:LYS:HZ2	1.81	0.44
1:B:429:TYR:O	1:B:433:THR:HG23	2.18	0.44
1:B:62:TRP:HA	1:B:68:ILE:HD11	2.00	0.44
1:B:475:PRO:O	1:B:479:ARG:HG2	2.18	0.44
1:A:74:LEU:CD2	1:A:235:LEU:CD2	2.95	0.43
1:A:474:LEU:O	1:A:479:ARG:HD3	2.18	0.43
1:B:149:GLU:O	1:B:153:GLU:HG3	2.18	0.43
1:B:477:GLU:N	1:B:477:GLU:OE1	2.46	0.43
1:B:491:VAL:HG23	1:B:492:VAL:HG13	1.99	0.43
1:A:350:ARG:HA	1:A:440:ASN:HD21	1.83	0.43
1:B:390:SER:O	1:B:394:ARG:HG3	2.18	0.43
1:B:117:LEU:HD11	1:B:119:ARG:NH2	2.33	0.43
1:B:277:ASN:ND2	1:B:392:ARG:HH21	2.17	0.43
1:B:314:VAL:HG22	1:B:315:ALA:N	2.33	0.43
1:A:476:LYS:H	1:A:476:LYS:HD3	1.83	0.43
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.87	0.43
1:B:310:GLU:HB3	1:B:315:ALA:HB2	2.02	0.42
1:B:34:VAL:HG21	1:B:36:ARG:HG3	1.96	0.42
1:B:163:VAL:CG1	1:B:163:VAL:O	2.68	0.42
1:B:161:LYS:HE3	1:B:161:LYS:HB2	1.92	0.42
1:A:6:ARG:NH1	4:A:2003:HOH:O	2.53	0.42
1:B:186:ASP:HB3	4:B:2143:HOH:O	2.19	0.42
1:B:214:PRO:HD2	1:B:217:LEU:HD21	2.02	0.42
1:A:32:SER:OG	1:A:33:SER:N	2.52	0.41
1:A:449:SER:OG	1:A:451:PRO:HG2	2.21	0.41
1:A:460:GLU:HB3	1:A:476:LYS:NZ	2.35	0.41
1:B:449:SER:OG	1:B:451:PRO:HD2	2.21	0.41
1:A:49:ASP:OD2	1:A:142:HIS:CD2	2.63	0.41
1:A:106:ARG:O	1:A:110:MET:HG3	2.21	0.41
1:A:350:ARG:HD2	1:A:352:VAL:HG21	2.02	0.41
1:A:475:PRO:O	1:A:476:LYS:O	2.39	0.41
1:A:122:LYS:HA	1:A:123:PRO:HD3	1.97	0.40
1:A:36:ARG:HB3	1:A:65:SER:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:O	1:A:167:THR:N	2.55	0.40
1:A:323:LEU:O	1:A:327:ILE:HG13	2.22	0.40
1:B:34:VAL:O	1:B:35:LYS:CB	2.48	0.40
1:B:83:HIS:HD2	1:B:84:PHE:CD2	2.40	0.40
1:A:353:GLN:CG	1:A:354:GLY:N	2.85	0.40
1:B:233:GLU:HG2	1:B:233:GLU:H	1.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/525 (94%)	465 (94%)	24 (5%)	5 (1%)	18	7
1	B	497/525 (95%)	458 (92%)	28 (6%)	11 (2%)	8	1
All	All	991/1050 (94%)	923 (93%)	52 (5%)	16 (2%)	11	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	355	LYS
1	B	30	SER
1	B	33	SER
1	B	34	VAL
1	B	35	LYS
1	B	355	LYS
1	B	498	ASN
1	A	356	TRP
1	B	356	TRP
1	A	476	LYS
1	B	3	HIS

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Mol	Chain	Res	Type
1	B	167	THR
1	A	165	ASN
1	B	31	SER
1	B	446	ARG

### 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	439/458 (96%)	422 (96%)	17 (4%)	37	26
1	B	441/458 (96%)	416 (94%)	25 (6%)	24	13
All	All	880/916 (96%)	838 (95%)	42 (5%)	30	18

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	28	LEU
1	A	31	SER
1	A	33	SER
1	A	34	VAL
1	A	35	LYS
1	A	168	LYS
1	A	185	PHE
1	A	212	ARG
1	A	247	ARG
1	A	353	GLN
1	A	361	LYS
1	A	443	ARG
1	A	469	GLN
1	A	476	LYS
1	A	477	GLU
1	A	479	ARG
1	B	3	HIS
1	B	12	GLU

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Mol	Chain	Res	Type
1	B	28	LEU
1	B	34	VAL
1	B	37	LYS
1	B	74	LEU
1	B	77	ARG
1	B	166	SER
1	B	167	THR
1	B	185	PHE
1	B	233	GLU
1	B	317	ASN
1	B	356	TRP
1	B	443	ARG
1	B	444	GLU
1	B	446	ARG
1	B	469	GLN
1	B	473	ARG
1	B	476	LYS
1	B	478	LYS
1	B	479	ARG
1	B	485	LEU
1	B	486	MET
1	B	498	ASN
1	B	500	PRO

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

Mol	Chain	Res	Type
1	A	83	HIS
1	A	142	HIS
1	A	277	ASN
1	A	353	GLN
1	A	440	ASN
1	A	469	GLN
1	B	83	HIS
1	B	142	HIS
1	B	196	GLN
1	B	277	ASN
1	B	353	GLN
1	B	440	ASN
1	B	496	HIS
1	B	498	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 ⓘ

4 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	FAD	A	1498	-	51,58,58	1.53	8 (15%)	54,89,89	1.93	7 (12%)
3	MHF	A	1499	-	25,36,36	1.55	7 (28%)	30,52,52	2.44	11 (36%)
2	FAD	B	1501	-	51,58,58	1.48	8 (15%)	54,89,89	2.02	7 (12%)
3	MHF	B	1502	-	25,36,36	1.68	8 (32%)	30,52,52	2.57	12 (40%)

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	FAD	A	1498	-	-	0/28/50/50	0/6/6/6
3	MHF	A	1499	-	-	0/15/42/42	0/4/4/4
2	FAD	B	1501	-	-	0/28/50/50	0/6/6/6
3	MHF	B	1502	-	-	0/15/42/42	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1502	MHF	C4-N3	2.06	1.36	1.33
3	B	1502	MHF	C9-N10	2.06	1.49	1.46
2	A	1498	FAD	O4B-C1B	2.10	1.44	1.41
2	A	1498	FAD	C2A-N1A	2.11	1.37	1.33
3	A	1499	MHF	C17-C12	2.14	1.42	1.39
3	B	1502	MHF	C13-C12	2.23	1.43	1.39
2	A	1498	FAD	C2A-N3A	2.23	1.35	1.32
2	B	1501	FAD	C5X-N5	2.28	1.38	1.35
3	A	1499	MHF	C4-N3	2.30	1.37	1.33
2	B	1501	FAD	O4B-C1B	2.30	1.44	1.41
3	A	1499	MHF	C6-N5	2.32	1.50	1.47
3	A	1499	MHF	C13-C12	2.37	1.43	1.39
3	A	1499	MHF	C15-N10	2.42	1.45	1.38
2	B	1501	FAD	C2A-N1A	2.43	1.38	1.33
3	B	1502	MHF	C6-N5	2.49	1.51	1.47
3	B	1502	MHF	C15-N10	2.56	1.45	1.38
3	A	1499	MHF	C8A-N1	2.56	1.38	1.34
2	B	1501	FAD	C2A-N3A	2.58	1.36	1.32
3	B	1502	MHF	C8A-N1	2.75	1.39	1.34
3	B	1502	MHF	C17-C12	2.91	1.44	1.39
2	B	1501	FAD	C4-N3	3.00	1.38	1.33
2	B	1501	FAD	C10-N1	3.01	1.37	1.33
3	A	1499	MHF	C16-C15	3.07	1.45	1.39
2	A	1498	FAD	C5X-N5	3.13	1.40	1.35
3	B	1502	MHF	C16-C15	3.25	1.45	1.39
2	A	1498	FAD	C9A-N10	3.33	1.43	1.38
2	A	1498	FAD	C4-N3	3.70	1.39	1.33
2	A	1498	FAD	C10-N1	3.89	1.38	1.33
2	B	1501	FAD	C9A-N10	4.01	1.44	1.38
2	B	1501	FAD	C4X-N5	4.95	1.40	1.33
2	A	1498	FAD	C4X-N5	5.20	1.40	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	MHF	C9-N10-C15	-8.41	113.60	122.84
3	A	1499	MHF	C9-N10-C15	-7.40	114.71	122.84
2	B	1501	FAD	C4X-C4-N3	-4.49	117.09	123.48
2	A	1498	FAD	C4X-C4-N3	-4.30	117.36	123.48
2	B	1501	FAD	N3A-C2A-N1A	-3.93	125.43	128.86
2	A	1498	FAD	N3A-C2A-N1A	-3.90	125.46	128.86
3	A	1499	MHF	C11-N10-C15	-3.67	110.40	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	MHF	C11-N10-C15	-3.60	110.60	120.86
3	A	1499	MHF	C4A-C4-N3	-2.79	118.99	123.37
3	B	1502	MHF	C4A-C4-N3	-2.65	119.21	123.37
3	B	1502	MHF	N3-C2-N1	-2.54	121.33	125.45
3	B	1502	MHF	CB-CA-CT	-2.48	108.68	112.28
3	A	1499	MHF	N3-C2-N1	-2.48	121.43	125.45
2	B	1501	FAD	C4-C4X-C10	-2.46	117.97	119.96
3	B	1502	MHF	C14-C15-N10	-2.33	118.12	121.39
2	A	1498	FAD	C4X-C10-N10	-2.23	118.97	120.52
2	A	1498	FAD	C4-C4X-C10	-2.19	118.19	119.96
3	A	1499	MHF	CB-CA-CT	-2.07	109.28	112.28
2	B	1501	FAD	C1'-N10-C9A	2.22	120.38	118.35
3	A	1499	MHF	C12-C-N	2.33	121.27	116.97
2	A	1498	FAD	C4-C4X-N5	2.39	121.30	118.68
3	A	1499	MHF	C9-C6-N5	2.44	106.19	101.86
3	B	1502	MHF	C12-C-N	2.44	121.47	116.97
2	B	1501	FAD	C4-C4X-N5	2.58	121.50	118.68
3	B	1502	MHF	C9-C6-N5	2.58	106.45	101.86
3	B	1502	MHF	C2-N1-C8A	2.59	120.35	114.51
3	A	1499	MHF	C2-N1-C8A	2.59	120.35	114.51
3	A	1499	MHF	C11-N5-C4A	3.02	132.46	122.61
3	B	1502	MHF	C11-N5-C4A	3.07	132.62	122.61
3	A	1499	MHF	C4-N3-C2	3.63	121.29	116.06
3	B	1502	MHF	C4-N3-C2	3.83	121.57	116.06
2	A	1498	FAD	C4X-N5-C5X	3.87	120.85	116.76
2	B	1501	FAD	C4X-N5-C5X	4.10	121.09	116.76
3	B	1502	MHF	C4-C4A-C8A	5.62	118.91	114.43
3	A	1499	MHF	C4-C4A-C8A	5.99	119.20	114.43
2	A	1498	FAD	C4-N3-C2	10.13	124.02	115.16
2	B	1501	FAD	C4-N3-C2	10.71	124.53	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1498	FAD	1	0
2	B	1501	FAD	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	496/525 (94%)	0.15	22 (4%) 35 38	15, 26, 54, 69	0
1	B	499/525 (95%)	0.56	50 (10%) 8 9	18, 34, 66, 90	1 (0%)
All	All	995/1050 (94%)	0.35	72 (7%) 16 18	15, 30, 62, 90	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	SER	9.1
1	B	500	PRO	8.2
1	B	497	GLY	7.4
1	B	165	ASN	7.2
1	B	499	GLY	6.8
1	B	166	SER	6.6
1	B	34	VAL	6.5
1	A	353	GLN	6.3
1	A	497	GLY	6.1
1	B	31	SER	6.0
1	B	354	GLY	5.9
1	B	30	SER	5.9
1	A	166	SER	5.8
1	A	165	ASN	5.6
1	B	498	ASN	5.6
1	B	37	LYS	5.4
1	B	38	GLY	5.4
1	B	2	ASP	5.2
1	B	33	SER	5.1
1	B	443	ARG	4.9
1	B	473	ARG	4.7
1	B	355	LYS	4.6
1	B	484	ARG	4.6
1	A	355	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	356	TRP	4.5
1	A	481	TRP	4.4
1	B	469	GLN	4.3
1	B	485	LEU	4.3
1	A	33	SER	4.2
1	B	35	LYS	4.1
1	B	352	VAL	3.9
1	A	32	SER	3.7
1	A	354	GLY	3.7
1	B	477	GLU	3.6
1	B	164	GLY	3.6
1	B	496	HIS	3.5
1	B	480	HIS	3.4
1	A	34	VAL	3.4
1	B	486	MET	3.4
1	B	224	ASP	3.4
1	A	477	GLU	3.4
1	B	361	LYS	3.3
1	B	472	ARG	3.3
1	B	481	TRP	3.3
1	A	476	LYS	3.0
1	A	443	ARG	3.0
1	B	3	HIS	3.0
1	A	3	HIS	2.9
1	B	478	LYS	2.9
1	B	375	LEU	2.9
1	B	353	GLN	2.8
1	A	2	ASP	2.8
1	A	356	TRP	2.7
1	A	496	HIS	2.7
1	A	37	LYS	2.7
1	B	445	ASP	2.7
1	B	475	PRO	2.7
1	B	86	ASN	2.6
1	A	44	LEU	2.6
1	A	164	GLY	2.5
1	B	13	GLU	2.5
1	B	238	GLU	2.5
1	B	84	PHE	2.5
1	A	35	LYS	2.5
1	B	483	GLY	2.3
1	B	489	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLY	2.2
1	B	234	LYS	2.2
1	B	233	GLU	2.1
1	B	373	TYR	2.1
1	B	36	ARG	2.0
1	A	31	SER	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( $\text{\AA}^2$ )	Q<0.9
3	MHF	A	1499	33/33	0.91	0.12	1.28	16,21,38,47	0
3	MHF	B	1502	33/33	0.90	0.13	0.42	24,27,45,49	0
2	FAD	B	1501	53/53	0.98	0.08	-0.91	18,22,24,25	0
2	FAD	A	1498	53/53	0.98	0.07	-1.35	15,18,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.