



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:32 AM GMT

PDB ID : 1E8G  
Title : STRUCTURE OF THE H61T DOUBLE MUTANT OF VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH FLUORO-CRESOL  
Authors : Fraaije, M.W.; Mattevi, A.  
Deposited on : 2000-09-20  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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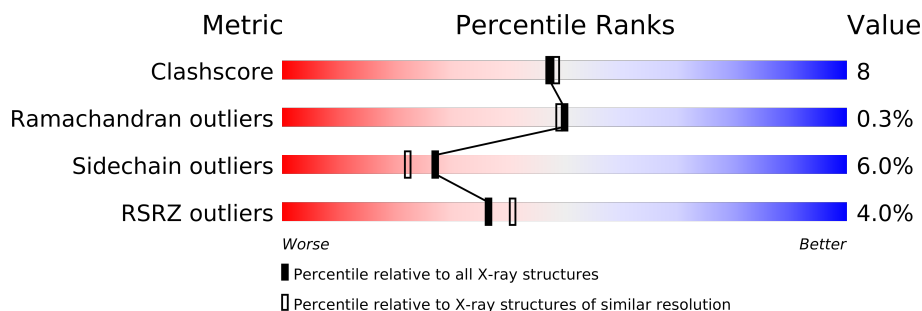
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	FCR	A	601	-	X
3	FCR	B	601	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9209 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

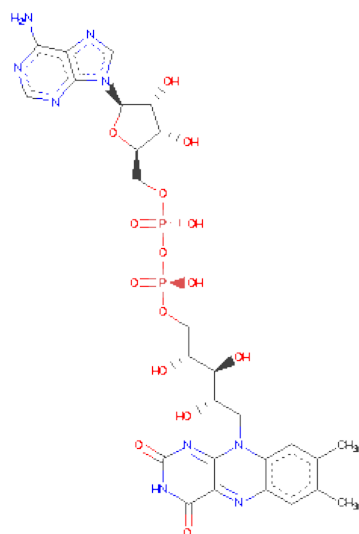
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	110	0	0
			4348	2791	742	791	24			
1	B	550	Total	C	N	O	S	110	0	0
			4348	2791	742	791	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	ENGINEERED	UNP P56216
B	61	THR	HIS	ENGINEERED	UNP P56216

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



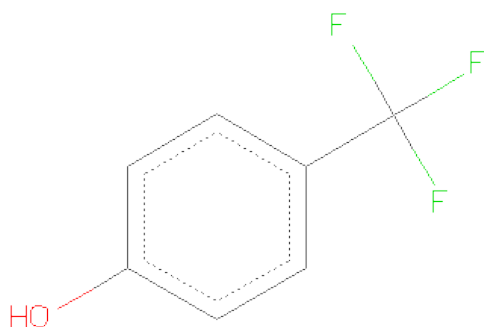
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is ALPHA,ALPHA,ALPHA-TRIFLUORO-P-CRESOL (three-letter code: FCR) (formula: C<sub>7</sub>H<sub>5</sub>F<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			11	7	3	1		
3	B	1	Total	C	F	O	0	0
			11	7	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	204	Total	O	0	0
			204	204		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.29Å 130.29Å 132.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.10) 98.9 (14.91-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.218 , 0.258 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 64.8	EDS
Estimated twinning fraction	0.000 for l,-k,h 0.009 for -l,-k,-h 0.011 for -h,-l,-k 0.000 for -h,l,k 0.023 for -h,k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63487 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCR, 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	1.11	17/4466 (0.4%)	1.56	69/6070 (1.1%)
1	B	1.20	17/4466 (0.4%)	1.54	70/6070 (1.2%)
All	All	1.16	34/8932 (0.4%)	1.55	139/12140 (1.1%)

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	A	3	1
1	B	4	1
All	All	7	2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	ARG	CB-CG	-35.33	0.57	1.52
1	A	161	ARG	CB-CG	-33.56	0.61	1.52
1	B	52	MET	CB-CG	29.09	2.44	1.51
1	A	52	MET	CB-CG	29.09	2.44	1.51
1	B	66	GLN	CA-CB	-27.20	0.94	1.53
1	B	344	LYS	CB-CG	-26.86	0.80	1.52
1	A	344	LYS	CB-CG	-24.55	0.86	1.52
1	B	341	LYS	CB-CG	-22.43	0.92	1.52
1	A	341	LYS	CB-CG	-22.42	0.92	1.52
1	B	65	ASP	CA-CB	-16.89	1.16	1.53
1	B	53	LYS	CB-CG	14.75	1.92	1.52
1	A	53	LYS	CB-CG	14.72	1.92	1.52
1	A	7	PHE	CA-CB	12.00	1.80	1.53
1	B	7	PHE	CA-CB	11.15	1.78	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CB-CG	10.12	1.71	1.52
1	A	26	GLN	CA-CB	-10.00	1.31	1.53
1	A	53	LYS	CA-CB	9.96	1.75	1.53
1	B	221	LYS	CG-CD	-9.09	1.21	1.52
1	B	8	ARG	CA-CB	-8.79	1.34	1.53
1	A	445	LYS	CG-CD	7.87	1.79	1.52
1	B	53	LYS	CA-CB	7.78	1.71	1.53
1	A	30	ARG	CA-CB	-7.37	1.37	1.53
1	B	67	ASP	CA-CB	-6.98	1.38	1.53
1	B	7	PHE	CB-CG	6.88	1.63	1.51
1	A	7	PHE	CB-CG	6.87	1.63	1.51
1	A	67	ASP	CA-CB	-6.67	1.39	1.53
1	B	332	GLU	CA-CB	-6.56	1.39	1.53
1	A	8	ARG	CA-CB	-6.38	1.40	1.53
1	A	65	ASP	CA-CB	-6.16	1.40	1.53
1	A	8	ARG	CB-CG	5.66	1.67	1.52
1	B	8	ARG	CB-CG	5.64	1.67	1.52
1	B	341	LYS	CA-CB	-5.36	1.42	1.53
1	A	221	LYS	CG-CD	-5.28	1.34	1.52
1	B	26	GLN	CA-CB	-5.09	1.42	1.53

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CD-NE-CZ	31.00	166.99	123.60
1	A	211	ARG	CD-NE-CZ	30.17	165.84	123.60
1	B	67	ASP	CB-CA-C	20.24	150.88	110.40
1	A	67	ASP	CB-CA-C	20.22	150.85	110.40
1	A	52	MET	CA-CB-CG	-18.37	82.07	113.30
1	B	52	MET	CA-CB-CG	-17.98	82.73	113.30
1	B	303	MET	CB-CA-C	16.72	143.84	110.40
1	B	162	ASP	CB-CG-OD2	-14.49	105.26	118.30
1	A	37	VAL	CA-C-N	13.82	147.61	117.20
1	A	53	LYS	CB-CG-CD	-13.78	75.77	111.60
1	B	53	LYS	CB-CG-CD	-13.78	75.77	111.60
1	B	330	ARG	N-CA-CB	-13.12	86.98	110.60
1	A	303	MET	CB-CA-C	12.89	136.18	110.40
1	B	65	ASP	CB-CA-C	12.66	135.73	110.40
1	B	221	LYS	CB-CG-CD	12.42	143.90	111.60
1	A	330	ARG	N-CA-CB	-12.36	88.36	110.60
1	B	162	ASP	CB-CG-OD1	11.85	128.96	118.30
1	A	297	ARG	NE-CZ-NH1	11.72	126.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CA-CB-CG	11.63	138.98	113.40
1	A	364	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	162	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	A	364	ARG	CD-NE-CZ	11.30	139.42	123.60
1	B	161	ARG	CA-CB-CG	10.72	137.00	113.40
1	B	303	MET	CA-CB-CG	10.69	131.47	113.30
1	A	7	PHE	N-CA-CB	-10.63	91.46	110.60
1	B	53	LYS	N-CA-CB	10.41	129.34	110.60
1	A	53	LYS	N-CA-CB	10.32	129.18	110.60
1	B	66	GLN	N-CA-CB	10.13	128.83	110.60
1	A	211	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	37	VAL	CA-C-O	-10.10	98.89	120.10
1	B	104	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	A	161	ARG	CA-CB-CG	9.76	134.86	113.40
1	B	7	PHE	N-CA-CB	-9.69	93.16	110.60
1	B	297	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	221	LYS	CB-CG-CD	9.62	136.61	111.60
1	B	303	MET	N-CA-CB	-9.17	94.10	110.60
1	B	177	LEU	CA-CB-CG	9.16	136.37	115.30
1	A	161	ARG	CB-CG-CD	9.12	135.32	111.60
1	B	7	PHE	N-CA-C	8.98	135.25	111.00
1	A	177	LEU	CA-CB-CG	8.89	135.76	115.30
1	A	177	LEU	CB-CG-CD1	8.86	126.06	111.00
1	A	162	ASP	CB-CG-OD1	8.85	126.26	118.30
1	A	297	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	303	MET	CA-CB-CG	8.65	128.00	113.30
1	B	161	ARG	CB-CG-CD	8.56	133.87	111.60
1	A	7	PHE	N-CA-C	8.39	133.66	111.00
1	A	211	ARG	CA-CB-CG	8.39	131.86	113.40
1	B	104	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	297	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	A	364	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	364	ARG	CD-NE-CZ	8.20	135.08	123.60
1	B	128	ASN	CB-CA-C	-8.16	94.09	110.40
1	B	412	LYS	CB-CG-CD	-8.08	90.59	111.60
1	A	128	ASN	CB-CA-C	-8.03	94.34	110.40
1	A	344	LYS	CA-CB-CG	-7.99	95.82	113.40
1	B	221	LYS	CG-CD-CE	7.97	135.80	111.90
1	A	446	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	67	ASP	N-CA-CB	-7.69	96.75	110.60
1	A	128	ASN	N-CA-CB	-7.62	96.89	110.60
1	B	312	ARG	NE-CZ-NH2	-7.57	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	505	THR	N-CA-CB	7.47	124.50	110.30
1	A	211	ARG	CB-CG-CD	7.36	130.74	111.60
1	A	142	VAL	N-CA-CB	-7.29	95.45	111.50
1	B	35	GLU	CB-CG-CD	-7.26	94.59	114.20
1	B	187	TYR	CB-CG-CD1	-7.24	116.65	121.00
1	B	344	LYS	CA-CB-CG	-7.15	97.66	113.40
1	A	200	MET	CA-CB-CG	7.11	125.39	113.30
1	A	221	LYS	CG-CD-CE	7.07	133.09	111.90
1	B	128	ASN	N-CA-CB	-7.04	97.93	110.60
1	B	53	LYS	CB-CA-C	7.01	124.42	110.40
1	A	286	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	344	LYS	CB-CG-CD	-6.93	93.57	111.60
1	A	35	GLU	CB-CG-CD	-6.89	95.58	114.20
1	B	142	VAL	N-CA-CB	-6.88	96.35	111.50
1	A	505	THR	CB-CA-C	-6.88	93.04	111.60
1	A	66	GLN	CB-CA-C	6.87	124.14	110.40
1	B	67	ASP	N-CA-CB	-6.67	98.59	110.60
1	B	560	LEU	CA-C-O	-6.66	106.12	120.10
1	B	504	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	462	MET	CA-CB-CG	-6.62	102.04	113.30
1	B	505	THR	CB-CA-C	-6.61	93.76	111.60
1	B	104	ARG	CD-NE-CZ	6.54	132.75	123.60
1	A	211	ARG	CG-CD-NE	6.51	125.47	111.80
1	B	183	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	457	THR	CB-CA-C	-6.34	94.47	111.60
1	B	177	LEU	CB-CG-CD1	6.29	121.69	111.00
1	B	162	ASP	CA-CB-CG	-6.28	99.58	113.40
1	B	300	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	A	412	LYS	CB-CG-CD	-6.27	95.29	111.60
1	A	30	ARG	N-CA-CB	6.24	121.84	110.60
1	B	482	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	53	LYS	CB-CA-C	6.13	122.66	110.40
1	A	457	THR	CB-CA-C	-6.10	95.13	111.60
1	B	211	ARG	CG-CD-NE	6.09	124.58	111.80
1	A	232	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	306	GLN	CB-CG-CD	5.98	127.16	111.60
1	A	104	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	136	GLU	CA-CB-CG	5.91	126.40	113.40
1	A	190	TYR	CG-CD1-CE1	5.90	126.02	121.30
1	A	419	ASN	CA-CB-CG	-5.90	100.42	113.40
1	A	412	LYS	CA-CB-CG	-5.84	100.54	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	VAL	O-C-N	-5.84	113.36	122.70
1	B	505	THR	N-CA-CB	5.79	121.30	110.30
1	B	244	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	23	GLU	CA-CB-CG	-5.75	100.74	113.40
1	A	482	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	231	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	A	560	LEU	CA-C-O	-5.72	108.09	120.10
1	A	358	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	A	306	GLN	CB-CG-CD	5.71	126.44	111.60
1	B	304	ALA	N-CA-CB	5.64	118.00	110.10
1	A	440	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	440	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	489	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	B	127	MET	C-N-CA	5.50	135.46	121.70
1	B	482	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	128	ASN	N-CA-C	5.46	125.73	111.00
1	A	217	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	196	MET	CG-SD-CE	5.43	108.89	100.20
1	B	244	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	211	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	255	SER	N-CA-CB	5.37	118.56	110.50
1	B	344	LYS	CB-CG-CD	-5.37	97.64	111.60
1	B	364	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	358	TYR	CB-CG-CD1	5.31	124.19	121.00
1	A	332	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	B	332	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	B	446	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	200	MET	CA-CB-CG	5.17	122.10	113.30
1	A	65	ASP	CB-CA-C	-5.16	100.07	110.40
1	B	231	GLU	CB-CG-CD	5.14	128.09	114.20
1	B	128	ASN	N-CA-C	5.14	124.88	111.00
1	A	104	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	463	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	493	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	162	ASP	CA-CB-CG	-5.07	102.24	113.40
1	A	503	TYR	CB-CG-CD2	5.04	124.03	121.00
1	B	398	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	53	LYS	CA

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Mol	Chain	Res	Type	Atom
1	A	67	ASP	CA
1	A	303	MET	CA
1	B	53	LYS	CA
1	B	66	GLN	CA
1	B	67	ASP	CA
1	B	303	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	PHE	Sidechain
1	B	7	PHE	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4348	0	4290	73	3
1	B	4348	0	4290	74	3
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	11	0	4	0	0
3	B	11	0	5	0	0
4	A	181	0	0	6	0
4	B	204	0	0	6	0
All	All	9209	0	8651	135	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:550:PRO:HB2	1:A:552:GLN:HE21	1.33	0.93
1:A:349:GLY:H	1:A:352:ASN:HD21	1.11	0.92
1:B:550:PRO:HB2	1:B:552:GLN:HE21	1.36	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:349:GLY:H	1:B:352:ASN:HD21	1.25	0.82
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.60	0.82
1:A:516:THR:HG21	4:A:2147:HOH:O	1.83	0.78
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.98	0.78
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.68	0.76
1:B:516:THR:HG21	4:B:2164:HOH:O	1.89	0.72
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.73	0.70
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.06	0.69
1:B:341:LYS:O	1:B:345:GLN:HG3	1.96	0.65
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.78	0.65
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.78	0.64
1:A:61:THR:HB	1:A:421:ALA:HB1	1.78	0.64
1:A:188:THR:HB	1:A:189:PRO:HD2	1.79	0.63
1:A:194:TRP:O	1:A:197:HIS:HD2	1.82	0.62
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.81	0.61
1:B:188:THR:HB	1:B:189:PRO:CD	2.31	0.61
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.00	0.61
1:A:152:HIS:HD2	4:A:2127:HOH:O	1.84	0.60
1:B:61:THR:HB	1:B:421:ALA:HB1	1.84	0.60
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.36	0.60
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.38	0.59
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.01	0.59
1:B:290:LYS:HB2	1:B:437:MET:HG3	1.85	0.59
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.84	0.58
1:A:244:TYR:OH	1:B:195:MET:HG2	2.02	0.58
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.18	0.58
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.38	0.57
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.89	0.56
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.85	0.56
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.71	0.56
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.87	0.56
1:A:79:ASN:ND2	1:A:82:ASP:H	2.03	0.56
1:A:253:LEU:CD1	1:B:253:LEU:HD21	2.34	0.56
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.41	0.56
1:A:195:MET:HG2	1:B:244:TYR:OH	2.05	0.56
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.41	0.55
1:B:194:TRP:O	1:B:197:HIS:HD2	1.89	0.55
1:B:365:ARG:HD2	4:B:2130:HOH:O	2.07	0.55
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.89	0.54
1:B:457:THR:HG21	4:B:2126:HOH:O	2.06	0.54
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.42	0.54
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.91	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:ILE:HD11	1:A:74:ILE:HD13	1.89	0.54
1:A:513:ILE:O	1:A:516:THR:HB	2.08	0.54
1:A:188:THR:HB	1:A:189:PRO:CD	2.38	0.54
1:A:123:MET:O	1:A:127:MET:HB2	2.08	0.53
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.38	0.53
1:B:99:PRO:HD2	4:B:2024:HOH:O	2.09	0.53
1:A:457:THR:HG21	4:A:2108:HOH:O	2.07	0.53
1:A:57:THR:HG22	1:A:74:ILE:CD1	2.38	0.53
1:B:513:ILE:O	1:B:516:THR:HB	2.09	0.53
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.88	0.53
1:B:237:LYS:HG3	1:B:238:ILE:HG12	1.90	0.52
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.25	0.52
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.90	0.52
1:A:198:SER:O	1:A:240:HIS:HD2	1.93	0.52
1:A:79:ASN:HD22	1:A:82:ASP:H	1.57	0.51
1:A:290:LYS:HB2	1:A:437:MET:HG3	1.92	0.51
1:A:333:PRO:HB2	1:A:448:GLN:NE2	2.26	0.51
1:A:341:LYS:O	1:A:345:GLN:HG3	2.10	0.51
1:B:188:THR:CB	1:B:189:PRO:CD	2.88	0.51
1:B:333:PRO:HB2	1:B:448:GLN:NE2	2.26	0.51
1:B:79:ASN:ND2	1:B:82:ASP:H	2.08	0.50
1:B:387:GLU:CD	1:B:387:GLU:H	2.15	0.50
1:A:61:THR:CB	1:A:421:ALA:HB1	2.42	0.50
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.94	0.50
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.94	0.49
1:A:253:LEU:HD21	1:B:253:LEU:CD1	2.42	0.49
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.95	0.49
1:B:505:THR:HG23	4:B:2166:HOH:O	2.12	0.49
1:B:79:ASN:HD22	1:B:82:ASP:H	1.61	0.48
1:B:306:GLN:HG3	4:B:2124:HOH:O	2.13	0.48
1:B:24:PHE:HD1	1:B:25:ILE:HD13	1.78	0.48
1:A:149:HIS:HD1	1:A:408:TYR:HH	1.61	0.48
1:B:505:THR:HG21	1:B:509:PHE:HB2	1.96	0.48
1:A:257:SER:HA	4:A:2096:HOH:O	2.13	0.48
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.96	0.47
1:B:324:LYS:HG3	1:B:416:TRP:CZ2	2.49	0.47
1:B:198:SER:O	1:B:240:HIS:HD2	1.97	0.47
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.80	0.47
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.45	0.47
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.44	0.46
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.97	0.46
1:A:189:PRO:HG2	1:A:270:MET:CE	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.97	0.46
1:B:188:THR:HB	1:B:189:PRO:HD2	1.97	0.45
1:B:312:ARG:CG	1:B:457:THR:HG23	2.44	0.45
1:B:427:PRO:HA	1:B:502:GLU:HA	1.98	0.45
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.52	0.45
1:B:40:ILE:HD11	1:B:74:ILE:HD13	1.98	0.45
1:A:324:LYS:HG3	1:A:416:TRP:CZ2	2.52	0.45
1:A:188:THR:CB	1:A:189:PRO:CD	2.93	0.44
1:A:349:GLY:H	1:A:352:ASN:ND2	1.94	0.44
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.99	0.44
1:B:149:HIS:HD1	1:B:408:TYR:HH	1.65	0.44
1:A:280:LEU:HB3	1:A:395:LEU:HD22	2.00	0.44
1:B:555:HIS:CG	1:B:559:LYS:HE3	2.53	0.44
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.82	0.44
1:A:210:LEU:HD23	1:A:211:ARG:N	2.33	0.43
1:A:188:THR:CB	1:A:189:PRO:HD2	2.48	0.43
1:B:51:TYR:CZ	1:B:104:ARG:HD3	2.53	0.43
1:B:61:THR:CB	1:B:421:ALA:HB1	2.47	0.43
1:A:13:PRO:HG3	1:A:95:PHE:CZ	2.53	0.43
1:A:549:TRP:HA	1:A:550:PRO:HD3	1.86	0.43
1:B:210:LEU:HD23	1:B:211:ARG:N	2.34	0.43
1:A:427:PRO:HA	1:A:502:GLU:HA	2.01	0.43
1:A:361:GLU:HB3	1:A:362:PRO:HD3	2.01	0.43
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.54	0.43
1:B:290:LYS:HE3	1:B:294:ASP:OD2	2.19	0.43
1:B:280:LEU:HB3	1:B:395:LEU:HD22	2.01	0.43
1:B:63:VAL:HG12	1:B:473:PHE:CZ	2.53	0.42
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.49	0.42
1:B:310:THR:HG22	1:B:459:THR:HG22	2.01	0.42
1:B:24:PHE:CD1	1:B:25:ILE:HD13	2.55	0.42
1:A:237:LYS:HG3	1:A:238:ILE:HG12	2.00	0.42
1:A:79:ASN:HD22	1:A:79:ASN:C	2.23	0.42
1:A:387:GLU:CD	1:A:387:GLU:H	2.22	0.42
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.50	0.41
1:A:51:TYR:CZ	1:A:104:ARG:HD3	2.54	0.41
1:B:275:GLY:HA3	1:B:359:GLY:O	2.21	0.41
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.56	0.41
1:A:62:HIS:HB2	4:A:2007:HOH:O	2.19	0.41
1:B:365:ARG:O	1:B:369:GLU:HG3	2.20	0.41
1:B:79:ASN:C	1:B:79:ASN:HD22	2.23	0.41
1:B:270:MET:HA	1:B:271:PRO:HD3	1.92	0.41
1:A:505:THR:HG23	4:A:2131:HOH:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:ILE:HG22	1:A:238:ILE:O	2.22	0.40
1:A:51:TYR:O	1:A:54:PRO:HD3	2.22	0.40
1:A:385:PHE:HB3	1:A:386:PRO:HD2	2.02	0.40
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.57	0.40
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.56	0.40
1:A:315:LEU:HA	1:A:318:ALA:HB3	2.04	0.40

All (3) 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	Distance(Å)	Clash(Å)
1:A:53:LYS:CG	1:B:412:LYS:CE[6_655]	1.68	0.52
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	1.80	0.40
1:A:419:ASN:OD1	1:B:329:SER:OG[6_655]	2.09	0.11

## 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	546/560 (98%)	524 (96%)	21 (4%)	1 (0%)	56	57
1	B	546/560 (98%)	527 (96%)	17 (3%)	2 (0%)	43	39
All	All	1092/1120 (98%)	1051 (96%)	38 (4%)	3 (0%)	50	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ASP
1	A	418	PRO
1	B	418	PRO

### 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	470/481 (98%)	443 (94%)	27 (6%)	29	24
1	B	470/481 (98%)	441 (94%)	29 (6%)	26	21
All	All	940/962 (98%)	884 (94%)	56 (6%)	27	22

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ARG
1	A	25	ILE
1	A	62	HIS
1	A	67	ASP
1	A	79	ASN
1	A	95	PHE
1	A	128	ASN
1	A	142	VAL
1	A	149	HIS
1	A	161	ARG
1	A	177	LEU
1	A	211	ARG
1	A	231	GLU
1	A	301	LEU
1	A	303	MET
1	A	306	GLN
1	A	328	SER
1	A	329	SER
1	A	336	ASP
1	A	341	LYS
1	A	391	GLU
1	A	432	SER
1	A	457	THR
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	B	7	PHE
1	B	8	ARG
1	B	25	ILE
1	B	62	HIS
1	B	66	GLN
1	B	67	ASP

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Mol	Chain	Res	Type
1	B	79	ASN
1	B	95	PHE
1	B	128	ASN
1	B	142	VAL
1	B	149	HIS
1	B	177	LEU
1	B	211	ARG
1	B	231	GLU
1	B	251	ASP
1	B	301	LEU
1	B	303	MET
1	B	306	GLN
1	B	328	SER
1	B	329	SER
1	B	336	ASP
1	B	341	LYS
1	B	391	GLU
1	B	432	SER
1	B	457	THR
1	B	462	MET
1	B	503	TYR
1	B	505	THR
1	B	516	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	128	ASN
1	A	158	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	439	GLN
1	A	448	GLN
1	A	467	HIS
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	128	ASN

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Mol	Chain	Res	Type
1	B	158	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	439	GLN
1	B	448	GLN
1	B	467	HIS
1	B	485	GLN
1	B	520	ASN
1	B	552	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	600	-	58,58,58	1.83	15 (25%)	85,89,89	1.82	17 (20%)
3	FCR	A	601	-	11,11,11	0.86	0	16,16,16	1.71	3 (18%)
2	FAD	B	600	-	58,58,58	1.88	13 (22%)	85,89,89	1.84	22 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FCR	B	601	-	11,11,11	0.70	0	16,16,16	1.53	3 (18%)

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	600	-	-	0/34/50/50	0/1/6/6
3	FCR	A	601	-	-	0/6/6/6	0/1/1/1
2	FAD	B	600	-	-	0/34/50/50	0/1/6/6
3	FCR	B	601	-	-	0/6/6/6	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-7.14	1.46	1.59
2	B	600	FAD	P-O3P	-5.72	1.49	1.59
2	B	600	FAD	C1'-C2'	4.70	1.56	1.51
2	B	600	FAD	PA-O2A	-4.47	1.35	1.55
2	A	600	FAD	PA-O2A	-4.08	1.36	1.55
2	A	600	FAD	C1'-C2'	3.80	1.55	1.51
2	B	600	FAD	C5'-C4'	3.74	1.57	1.51
2	B	600	FAD	P-O2P	-3.47	1.39	1.55
2	B	600	FAD	O5'-C5'	3.23	1.58	1.44
2	A	600	FAD	O5'-C5'	3.20	1.58	1.44
2	B	600	FAD	PA-O3P	-3.10	1.54	1.59
2	A	600	FAD	P-O2P	-3.04	1.41	1.55
2	A	600	FAD	C2-N3	2.96	1.43	1.37
2	B	600	FAD	C2B-C1B	-2.91	1.49	1.53
2	A	600	FAD	C5'-C4'	2.86	1.56	1.51
2	B	600	FAD	C2-N3	2.84	1.42	1.37
2	B	600	FAD	C4X-C10	2.67	1.45	1.40
2	A	600	FAD	C4X-C10	2.65	1.45	1.40
2	B	600	FAD	C10-N10	-2.64	1.33	1.38
2	B	600	FAD	O4B-C1B	2.63	1.45	1.41
2	A	600	FAD	C9A-N10	2.36	1.42	1.38
2	A	600	FAD	C4-C4X	2.30	1.45	1.41
2	A	600	FAD	C10-N10	-2.28	1.33	1.38
2	A	600	FAD	PA-O3P	-2.17	1.55	1.59
2	A	600	FAD	O4B-C1B	2.13	1.44	1.41
2	A	600	FAD	C2B-C1B	-2.12	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	O2-C2	-2.08	1.18	1.23
2	A	600	FAD	PA-O5B	-2.05	1.49	1.59

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C2-N1-C10	7.14	122.17	114.98
2	B	600	FAD	C2-N1-C10	6.43	121.46	114.98
2	A	600	FAD	O4B-C1B-N9A	-5.68	103.16	108.44
2	A	600	FAD	N3A-C2A-N1A	-4.87	124.64	128.71
2	A	600	FAD	C4X-C10-N1	-4.81	117.92	122.73
2	B	600	FAD	O4'-C4'-C3'	4.72	120.79	109.05
2	B	600	FAD	O4B-C1B-N9A	-4.47	104.28	108.44
2	B	600	FAD	C4X-C10-N1	-4.30	118.44	122.73
3	A	601	FCR	F1-C7-C1	3.63	121.37	112.97
3	B	601	FCR	F1-C7-C1	3.54	121.16	112.97
2	B	600	FAD	O2P-P-O3P	3.50	121.74	105.14
2	A	600	FAD	P-O3P-PA	3.34	141.49	131.68
2	B	600	FAD	N6A-C6A-N1A	3.32	125.88	119.36
2	B	600	FAD	C4A-C5A-N7A	3.25	112.30	109.52
3	A	601	FCR	F2-C7-C1	-3.13	105.75	112.97
2	B	600	FAD	O5B-PA-O1A	-3.08	97.30	109.37
2	A	600	FAD	N3A-C4A-N9A	3.04	130.92	125.43
2	A	600	FAD	C4A-C5A-N7A	3.02	112.11	109.52
2	B	600	FAD	C5A-C4A-N9A	-2.93	102.94	107.16
2	A	600	FAD	O2P-P-O3P	2.90	118.91	105.14
2	A	600	FAD	C2A-N1A-C6A	2.84	123.90	118.77
2	B	600	FAD	N3A-C4A-N9A	2.81	130.50	125.43
2	B	600	FAD	C2A-N1A-C6A	2.76	123.75	118.77
2	A	600	FAD	C5A-C4A-N9A	-2.67	103.30	107.16
2	A	600	FAD	C1'-N10-C10	2.66	122.94	119.17
2	A	600	FAD	C1'-N10-C9A	-2.65	116.29	118.87
2	B	600	FAD	C4-N3-C2	-2.63	119.99	125.39
2	A	600	FAD	C4-N3-C2	-2.56	120.14	125.39
2	A	600	FAD	N1-C10-N10	2.54	122.64	115.97
3	B	601	FCR	F2-C7-C1	-2.52	107.16	112.97
3	B	601	FCR	F3-C7-C1	-2.50	107.19	112.97
2	B	600	FAD	C5'-C4'-C3'	-2.50	107.34	112.06
2	B	600	FAD	N1-C10-N10	2.35	122.16	115.97
2	B	600	FAD	O2P-P-O5'	-2.30	96.93	108.51
2	B	600	FAD	P-O5'-C5'	2.29	138.49	122.03
2	A	600	FAD	C4-C4X-C10	2.28	120.63	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4X-C10-N10	-2.26	119.38	120.51
2	B	600	FAD	O3'-C3'-C2'	-2.23	103.09	108.74
2	B	600	FAD	O4'-C4'-C5'	-2.23	105.54	110.12
3	A	601	FCR	F3-C7-C1	-2.22	107.84	112.97
2	B	600	FAD	O2P-P-O1P	2.21	124.58	112.21
2	A	600	FAD	C4X-C10-N10	-2.18	119.42	120.51
2	B	600	FAD	C4-C4X-C10	2.13	120.39	116.95
2	B	600	FAD	P-O3P-PA	2.07	137.74	131.68
2	A	600	FAD	O4'-C4'-C3'	2.05	114.15	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	550/560 (98%)	0.02	17 (3%)	47 52	29, 42, 65, 79	24 (4%)
1	B	550/560 (98%)	0.05	27 (4%)	28 31	29, 42, 64, 79	24 (4%)
All	All	1100/1120 (98%)	0.04	44 (4%)	36 41	29, 42, 65, 79	48 (4%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	ARG	5.1
1	B	47	VAL	5.1
1	B	48	ASP	4.6
1	A	61	THR	4.3
1	B	50	SER	4.2
1	B	51	TYR	3.6
1	B	49	GLY	3.5
1	B	66	GLN	3.5
1	A	331	THR	3.4
1	B	67	ASP	3.4
1	B	61	THR	3.4
1	B	52	MET	3.3
1	A	329	SER	3.3
1	A	330	ARG	3.3
1	A	66	GLN	3.2
1	B	329	SER	3.1
1	B	415	ASP	3.1
1	B	331	THR	3.0
1	B	325	ARG	3.0
1	A	7	PHE	2.8
1	A	391	GLU	2.8
1	A	62	HIS	2.8
1	B	62	HIS	2.6
1	A	302	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	60	PRO	2.5
1	A	328	SER	2.4
1	B	159	ASN	2.4
1	B	369	GLU	2.3
1	B	418	PRO	2.3
1	B	157	ALA	2.3
1	B	25	ILE	2.3
1	A	31	ILE	2.2
1	B	391	GLU	2.2
1	B	337	GLU	2.2
1	B	365	ARG	2.1
1	B	7	PHE	2.1
1	A	47	VAL	2.1
1	B	68	TYR	2.1
1	A	51	TYR	2.1
1	B	24	PHE	2.1
1	A	19	SER	2.1
1	A	50	SER	2.1
1	A	285	LYS	2.1
1	B	303	MET	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FCR	B	601	11/11	0.19	4.13	42,44,49,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FCR	A	601	11/11	0.15	3.98	42,45,48,49	0
2	FAD	A	600	53/53	0.09	-0.60	36,39,44,44	0
2	FAD	B	600	53/53	0.09	-0.67	36,39,43,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.