



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:58 am GMT

PDB ID : 4MOL
Title : Pyranose 2-oxidase H167A mutant with 2-fluorinated galactose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 2.00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

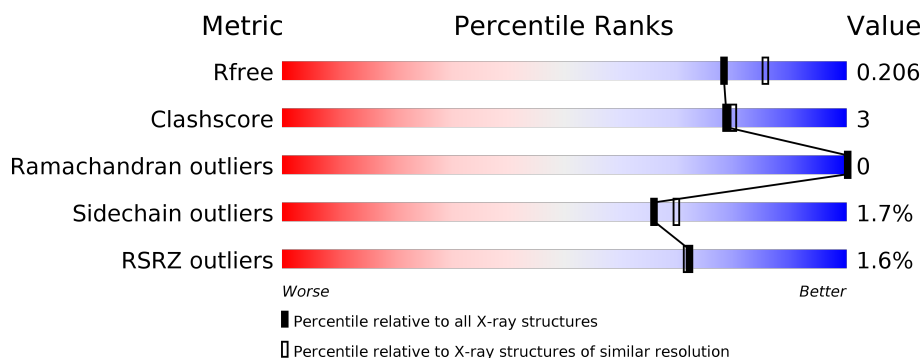
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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 ≥ 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	633	<div> <div>2%</div> <div>81% 9% 9%</div> </div>
1	B	633	<div> <div>2%</div> <div>82% 8% 9%</div> </div>
1	C	633	<div> <div>2%</div> <div>82% 9% 9%</div> </div>
1	D	633	<div> <div>2%</div> <div>82% 8% 9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	12P	A	803	-	-	-	X
4	12P	B	803	-	-	-	X
4	12P	B	804	-	-	-	X
4	12P	D	803	-	-	-	X
5	MES	A	804	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20233 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 Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	3	0
			4535	2863	779	869	24			
1	B	576	Total	C	N	O	S	0	1	0
			4545	2870	778	872	25			
1	C	573	Total	C	N	O	S	0	1	0
			4521	2855	775	867	24			
1	D	573	Total	C	N	O	S	0	1	0
			4521	2855	775	867	24			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
A	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
A	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
A	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
B	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
B	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
B	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
B	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32

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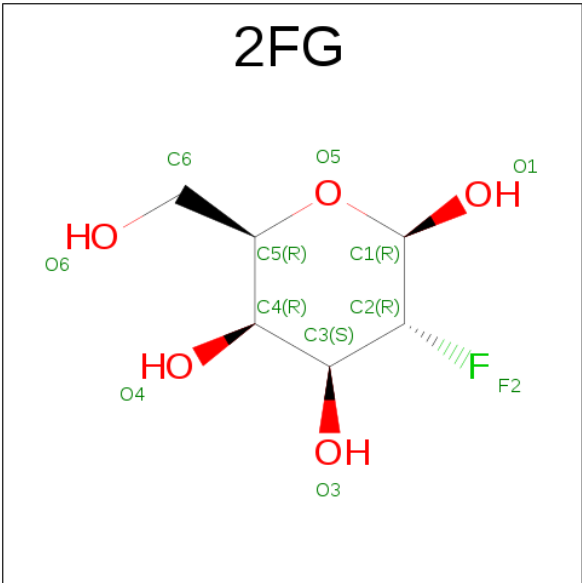
Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
C	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
C	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
C	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
C	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
D	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
D	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
D	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
D	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32

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



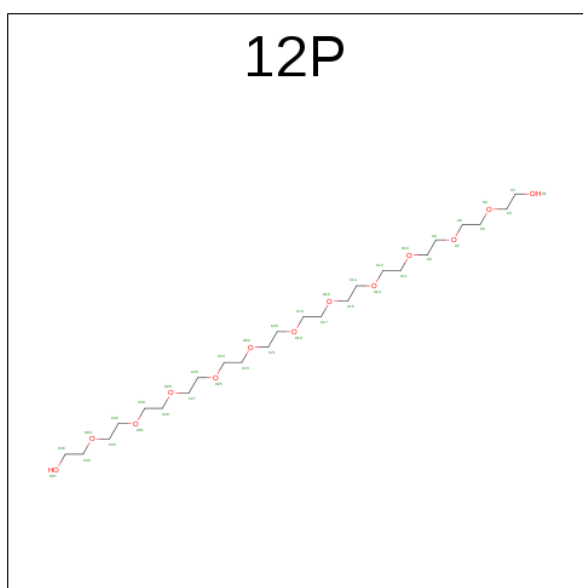
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SUGAR (2-FLUORO-2-DEOXY-BETA-D-GALACTOPYRANOSE) (three-letter code: 2FG) (formula: C₆H₁₁FO₅).



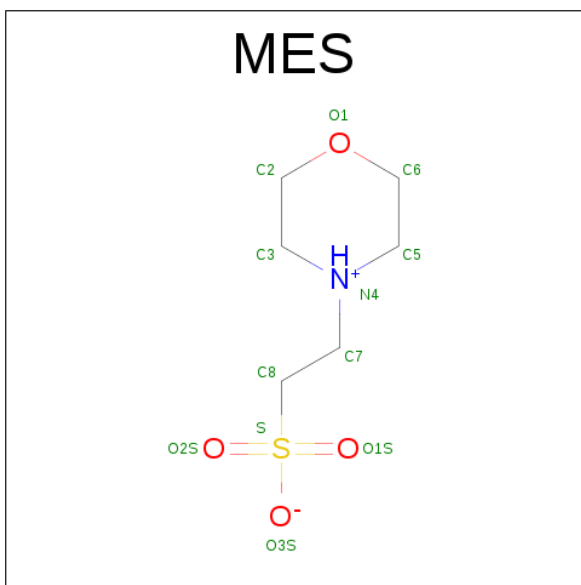
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 4 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

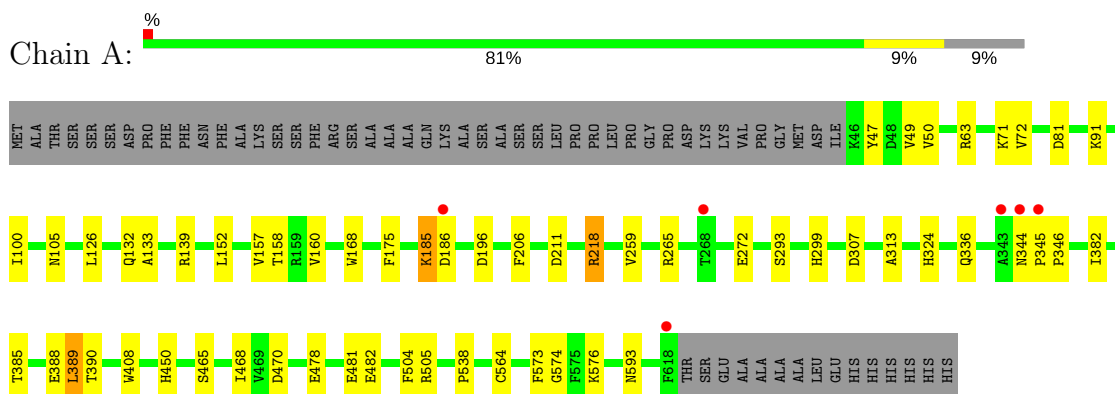
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	516	Total	O	0	0
			516	516		
6	B	518	Total	O	0	0
			518	518		
6	C	409	Total	O	0	0
			409	409		
6	D	323	Total	O	0	0
			323	323		

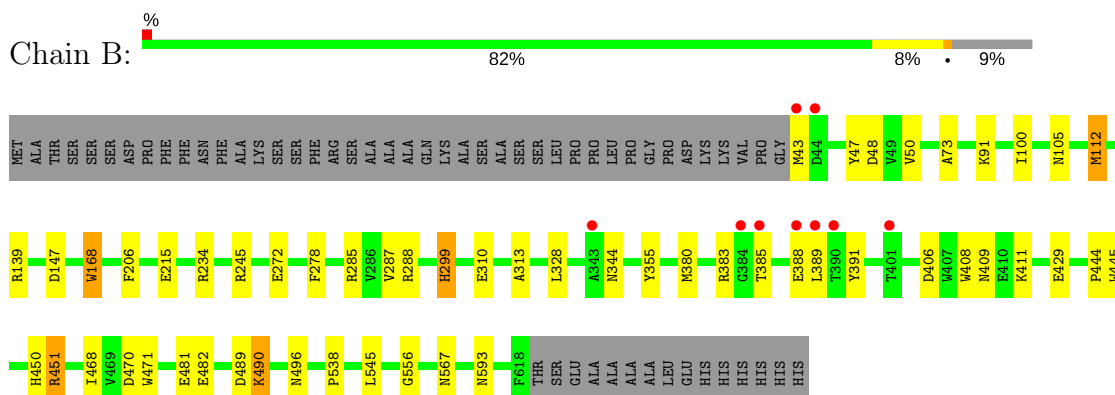
3 Residue-property plots [i](#)

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.

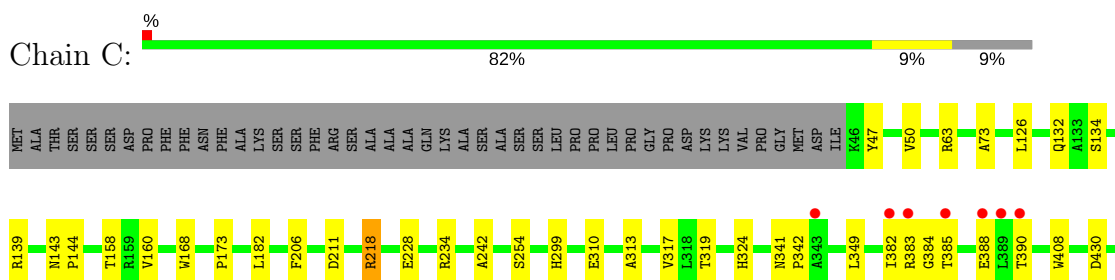
• Molecule 1: Pyranose 2-oxidase



• Molecule 1: Pyranose 2-oxidase

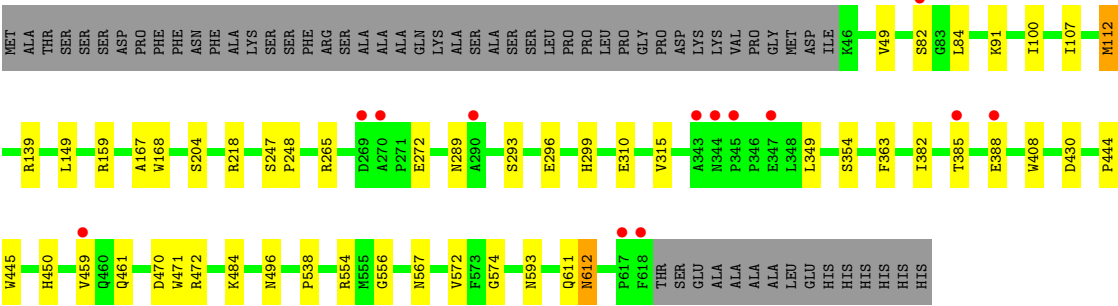
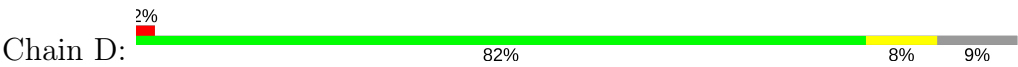


• Molecule 1: Pyranose 2-oxidase





● Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.29Å 102.48Å 137.42Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	48.01 – 2.00 47.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.01-2.00) 98.2 (47.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.222 0.165 , 0.206	Depositor DCC
R_{free} test set	1846 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l 0.014 for k,h,-l 0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20233	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 12P, 2FG, FAD, MES

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	1.05	2/4656 (0.0%)	0.96	14/6329 (0.2%)
1	B	1.01	5/4663 (0.1%)	0.98	14/6339 (0.2%)
1	C	0.93	4/4639 (0.1%)	0.93	11/6307 (0.2%)
1	D	0.84	0/4639	0.86	5/6307 (0.1%)
All	All	0.96	11/18597 (0.1%)	0.93	44/25282 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	478	GLU	CD-OE1	8.47	1.34	1.25
1	A	478	GLU	CD-OE1	7.85	1.34	1.25
1	B	482	GLU	CD-OE1	7.05	1.33	1.25
1	B	299	HIS	CG-CD2	5.98	1.46	1.35
1	A	482	GLU	CD-OE1	5.35	1.31	1.25
1	B	168	TRP	CD2-CE2	5.33	1.47	1.41
1	C	134	SER	CB-OG	-5.20	1.35	1.42
1	B	471	TRP	CD2-CE2	5.20	1.47	1.41
1	C	471	TRP	CD2-CE2	5.17	1.47	1.41
1	C	228	GLU	CD-OE1	5.15	1.31	1.25
1	B	355	TYR	CE1-CZ	-5.02	1.32	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	139	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	139	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	D	139	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	218	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	C	211	ASP	CB-CG-OD1	8.41	125.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	C	218	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	211	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	218	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	C	554	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	C	139	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	265	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	554	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	288	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	470	ASP	CB-CG-OD1	6.55	124.19	118.30
1	D	470	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	245	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	81	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	A	307	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	406	ASP	CB-CG-OD1	6.30	123.97	118.30
1	D	265	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	211	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	B	489	ASP	CB-CG-OD1	6.07	123.77	118.30
1	D	139	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	48	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	218	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	505	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	211	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	470	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	451[A]	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	451[B]	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	112	MET	CG-SD-CE	5.39	108.82	100.20
1	A	389	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	147	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	234	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	234	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	175	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	196	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	505	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	112	MET	CG-SD-CE	5.07	108.32	100.20
1	B	470	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	63	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	71	LYS	CD-CE-NZ	-5.02	100.16	111.70

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	4535	0	4392	31	0
1	B	4545	0	4399	24	0
1	C	4521	0	4375	37	0
1	D	4521	0	4375	31	0
2	A	53	0	29	0	0
2	B	53	0	29	0	0
2	C	53	0	29	0	0
2	D	53	0	29	1	0
3	A	12	0	11	0	0
3	B	12	0	11	0	0
3	C	12	0	11	0	0
3	D	12	0	11	0	0
4	A	16	0	21	0	0
4	B	32	0	42	0	0
4	D	13	0	16	0	0
5	A	12	0	13	3	0
5	C	12	0	13	0	0
6	A	516	0	0	6	0
6	B	518	0	0	4	0
6	C	409	0	0	6	0
6	D	323	0	0	5	0
All	All	20233	0	17806	120	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 3.

All (120) 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:481:GLU:HG2	6:C:1182:HOH:O	1.56	1.03
1:B:299:HIS:HB3	6:B:1206:HOH:O	1.65	0.97
1:C:126:LEU:CD1	1:C:132:GLN:HG3	1.95	0.96
1:D:612:ASN:HD22	1:D:612:ASN:N	1.61	0.91
1:C:126:LEU:HD12	1:C:132:GLN:HG3	1.48	0.90
1:C:126:LEU:CD1	1:C:132:GLN:CG	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:GLN:C	1:D:612:ASN:HD22	1.80	0.83
1:A:126:LEU:HD12	1:A:132:GLN:CG	2.15	0.77
1:B:299:HIS:NE2	1:B:310:GLU:HG3	2.01	0.76
1:C:126:LEU:HD13	1:C:132:GLN:CG	2.18	0.74
1:C:126:LEU:HD13	1:C:132:GLN:HG2	1.69	0.74
1:D:382:ILE:HD13	6:D:1146:HOH:O	1.87	0.73
1:A:126:LEU:HD12	1:A:132:GLN:HG3	1.69	0.73
1:D:612:ASN:N	1:D:612:ASN:ND2	2.36	0.73
1:D:385:THR:O	1:D:388:GLU:HG2	1.90	0.72
1:C:385:THR:OG1	1:C:388:GLU:HG2	1.94	0.67
1:A:382:ILE:HD12	6:A:1127:HOH:O	1.97	0.65
1:C:545:LEU:HD12	6:C:1157:HOH:O	1.97	0.65
1:D:49:VAL:HG22	1:D:315:VAL:HB	1.78	0.64
1:C:384:GLY:HA3	1:C:390:THR:HG22	1.80	0.63
1:A:132:GLN:HE22	5:A:804:MES:HN4	1.47	0.62
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.82	0.62
1:A:388:GLU:HB2	1:A:390:THR:HG22	1.82	0.62
1:B:91:LYS:HD2	1:B:100:ILE:HD11	1.81	0.62
1:B:299:HIS:CD2	1:B:310:GLU:HG3	2.34	0.62
1:C:385:THR:OG1	1:C:388:GLU:CG	2.49	0.61
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.81	0.61
1:B:481:GLU:HG2	6:B:1190:HOH:O	1.99	0.60
1:C:299:HIS:NE2	1:C:310:GLU:HG2	2.17	0.60
1:A:299:HIS:HB3	6:A:1312:HOH:O	2.02	0.58
1:A:126:LEU:CD1	1:A:132:GLN:CG	2.81	0.58
1:A:481:GLU:HG2	6:A:1316:HOH:O	2.03	0.58
1:C:465:SER:HA	1:C:468:ILE:HD12	1.85	0.58
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.04	0.58
1:A:63:ARG:HD2	1:A:259:VAL:O	2.04	0.58
1:D:450:HIS:HD2	6:D:1034:HOH:O	1.87	0.57
6:C:1180:HOH:O	1:D:84:LEU:HD23	2.04	0.57
1:D:299:HIS:NE2	1:D:310:GLU:CG	2.68	0.57
1:B:299:HIS:NE2	1:B:310:GLU:CG	2.68	0.56
1:B:545:LEU:HD12	6:B:1341:HOH:O	2.05	0.56
1:D:299:HIS:HB3	6:D:1148:HOH:O	2.05	0.56
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.41	0.56
1:B:490:LYS:HD3	6:B:1232:HOH:O	2.06	0.55
1:D:450:HIS:CE1	1:D:472:ARG:HH11	2.24	0.55
1:A:388:GLU:CB	1:A:390:THR:HG22	2.36	0.55
1:C:450:HIS:HD2	6:C:852:HOH:O	1.89	0.55
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:NE2	1:D:310:GLU:HG2	2.22	0.54
1:B:383:ARG:O	1:B:391:TYR:HA	2.08	0.54
1:A:133:ALA:HB3	5:A:804:MES:H71	1.90	0.53
1:D:107:ILE:HG12	1:D:167:ALA:HB1	1.90	0.52
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.92	0.52
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.92	0.51
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.93	0.51
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.93	0.50
1:B:43:MET:HG3	1:B:278:PHE:CE1	2.47	0.49
1:B:215:GLU:O	1:B:411:LYS:NZ	2.46	0.49
5:A:804:MES:H22	1:D:149:LEU:HD22	1.95	0.48
1:B:451[A]:ARG:HD3	1:B:468:ILE:O	2.14	0.48
1:A:49:VAL:HB	1:A:72:VAL:HG22	1.95	0.48
1:C:299:HIS:NE2	1:C:310:GLU:CG	2.75	0.48
1:D:459:VAL:CG1	1:D:461:GLN:HE21	2.26	0.48
1:B:556:GLY:O	1:B:567:ASN:HA	2.13	0.48
1:C:382:ILE:HD13	6:C:1177:HOH:O	2.14	0.48
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.14	0.47
1:C:390:THR:HG22	1:C:390:THR:O	2.13	0.47
1:C:537:LEU:HB3	1:C:538:PRO:HD2	1.96	0.47
1:A:47:TYR:O	1:A:313:ALA:HA	2.15	0.46
1:A:564:CYS:HG	1:A:573:PHE:HE2	1.64	0.46
1:C:324:HIS:HD2	6:C:859:HOH:O	1.98	0.46
1:A:336:GLN:NE2	1:A:344:ASN:O	2.49	0.46
1:B:389:LEU:HD12	1:B:389:LEU:HA	1.68	0.46
1:B:47:TYR:CE2	1:B:73:ALA:HB2	2.51	0.45
1:D:611:GLN:C	1:D:612:ASN:ND2	2.59	0.45
1:D:218:ARG:HD2	6:D:916:HOH:O	2.16	0.45
1:B:285:ARG:NH2	1:B:287:VAL:HG22	2.32	0.45
1:C:349:LEU:HD22	1:C:565:CYS:HA	1.99	0.45
1:A:158:THR:CG2	1:A:160:VAL:HG22	2.47	0.44
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.17	0.44
1:D:247:SER:HB2	1:D:248:PRO:CD	2.48	0.43
1:D:289:ASN:HB3	1:D:296:GLU:OE2	2.19	0.43
1:A:345:PRO:HA	1:A:346:PRO:HD3	1.94	0.43
1:C:242:ALA:HB1	1:C:254:SER:HB2	2.01	0.43
1:D:82:SER:N	6:D:1039:HOH:O	2.50	0.43
1:A:389:LEU:HG	6:A:1292:HOH:O	2.18	0.43
1:A:185:LYS:O	1:A:186:ASP:HB2	2.19	0.43
1:C:383:ARG:NH1	1:C:390:THR:HG23	2.34	0.43
1:D:293:SER:HA	1:D:574:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HD2	6:A:1009:HOH:O	2.19	0.42
1:C:384:GLY:HA3	1:C:390:THR:CG2	2.48	0.42
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.84	0.42
1:B:385:THR:O	1:B:388:GLU:HB2	2.18	0.42
1:C:182:LEU:HA	1:C:182:LEU:HD23	1.74	0.42
1:D:91:LYS:HD2	1:D:100:ILE:HD11	2.01	0.42
1:B:328:LEU:C	1:B:328:LEU:HD23	2.40	0.42
1:D:459:VAL:HG13	1:D:461:GLN:HE21	1.84	0.42
1:A:152:LEU:HD21	1:A:504:PHE:CD1	2.55	0.42
1:B:50:VAL:HG13	1:B:313:ALA:HB2	2.00	0.42
1:C:385:THR:OG1	1:C:388:GLU:HG3	2.19	0.42
1:D:363:PHE:HA	1:D:471:TRP:O	2.20	0.42
1:D:354:SER:OG	1:D:484:LYS:NZ	2.51	0.42
1:D:556:GLY:O	1:D:567:ASN:HA	2.20	0.41
1:B:380:MET:HE1	1:B:409:ASN:HB3	2.03	0.41
1:C:143:ASN:HA	1:C:144:PRO:HD2	1.95	0.41
1:D:349:LEU:HD11	1:D:572:VAL:HG13	2.03	0.41
1:C:384:GLY:CA	1:C:390:THR:CG2	2.99	0.41
1:B:328:LEU:O	1:B:328:LEU:HD23	2.21	0.41
1:C:341:ASN:HA	1:C:342:PRO:HD2	1.95	0.41
1:C:384:GLY:HA2	1:C:390:THR:HG21	2.03	0.41
1:A:465[B]:SER:HA	1:A:468:ILE:HD12	2.03	0.41
1:B:444:PRO:HD2	1:B:445:TRP:CZ3	2.55	0.41
1:A:388:GLU:HB2	1:A:390:THR:CG2	2.49	0.41
1:A:105:ASN:HB3	1:B:105:ASN:O	2.21	0.41
1:A:576:LYS:HG3	6:A:1362:HOH:O	2.21	0.41
1:C:317:VAL:HG12	1:C:319:THR:HG23	2.03	0.41
1:A:293:SER:HA	1:A:574:GLY:O	2.21	0.41
1:C:384:GLY:CA	1:C:390:THR:HG22	2.49	0.41
1:C:173:PRO:HG2	1:C:592:ALA:HB1	2.02	0.41
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.56	0.40
1:C:471:TRP:CH2	1:C:526:SER:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/633 (91%)	557 (97%)	17 (3%)	0	100	100
1	B	575/633 (91%)	559 (97%)	16 (3%)	0	100	100
1	C	572/633 (90%)	553 (97%)	19 (3%)	0	100	100
1	D	572/633 (90%)	554 (97%)	18 (3%)	0	100	100
All	All	2293/2532 (91%)	2223 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	503/547 (92%)	495 (98%)	8 (2%)	68	72
1	B	504/547 (92%)	493 (98%)	11 (2%)	57	60
1	C	501/547 (92%)	495 (99%)	6 (1%)	75	80
1	D	501/547 (92%)	492 (98%)	9 (2%)	64	68
All	All	2009/2188 (92%)	1975 (98%)	34 (2%)	66	70

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	272	GLU
1	A	385	THR
1	A	408	TRP
1	A	450	HIS
1	A	593	ASN

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Mol	Chain	Res	Type
1	B	112	MET
1	B	168	TRP
1	B	206	PHE
1	B	272	GLU
1	B	344	ASN
1	B	408	TRP
1	B	429	GLU
1	B	450	HIS
1	B	490	LYS
1	B	496	ASN
1	B	593	ASN
1	C	168	TRP
1	C	206	PHE
1	C	408	TRP
1	C	459	VAL
1	C	462	SER
1	C	593	ASN
1	D	112	MET
1	D	168	TRP
1	D	204	SER
1	D	272	GLU
1	D	408	TRP
1	D	496	ASN
1	D	554	ARG
1	D	593	ASN
1	D	612	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	C	132	GLN
1	C	324	HIS
1	C	450	HIS
1	C	461	GLN
1	D	450	HIS
1	D	461	GLN
1	D	612	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 ⓘ

14 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	801	-	51,58,58	1.56	10 (19%)	54,89,89	3.76	16 (29%)
3	2FG	A	802	-	11,12,12	0.82	0	14,17,17	1.59	4 (28%)
4	12P	A	803	-	15,15,36	0.67	0	14,14,35	0.52	0
5	MES	A	804	-	12,12,12	1.95	1 (8%)	14,16,16	4.38	4 (28%)
2	FAD	B	801	-	51,58,58	1.64	12 (23%)	54,89,89	3.39	17 (31%)
3	2FG	B	802	-	11,12,12	0.77	0	14,17,17	1.40	3 (21%)
4	12P	B	803	-	15,15,36	0.62	0	14,14,35	0.39	0
4	12P	B	804	-	15,15,36	0.53	0	14,14,35	0.58	0
5	MES	C	701	-	12,12,12	1.75	1 (8%)	14,16,16	2.88	4 (28%)
2	FAD	C	702	-	51,58,58	1.39	9 (17%)	54,89,89	4.30	16 (29%)
3	2FG	C	703	-	11,12,12	0.98	1 (9%)	14,17,17	1.74	1 (7%)
2	FAD	D	801	-	51,58,58	1.42	11 (21%)	54,89,89	3.23	23 (42%)
3	2FG	D	802	-	11,12,12	1.43	2 (18%)	14,17,17	2.47	3 (21%)
4	12P	D	803	-	12,12,36	0.67	0	11,11,35	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	801	-	-	0/28/50/50	0/6/6/6
3	2FG	A	802	-	-	0/2/22/22	0/1/1/1
4	12P	A	803	-	-	0/13/13/34	0/0/0/0
5	MES	A	804	-	-	0/6/14/14	0/1/1/1
2	FAD	B	801	-	-	0/28/50/50	0/6/6/6
3	2FG	B	802	-	-	0/2/22/22	0/1/1/1
4	12P	B	803	-	-	0/13/13/34	0/0/0/0
4	12P	B	804	-	-	0/13/13/34	0/0/0/0
5	MES	C	701	-	-	0/6/14/14	0/1/1/1
2	FAD	C	702	-	-	0/28/50/50	0/6/6/6
3	2FG	C	703	-	-	0/2/22/22	0/1/1/1
2	FAD	D	801	-	-	0/28/50/50	0/6/6/6
3	2FG	D	802	-	-	0/2/22/22	0/1/1/1
4	12P	D	803	-	-	0/10/10/34	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	MES	C8-S	-5.58	1.69	1.77
5	C	701	MES	C8-S	-4.64	1.70	1.77
2	C	702	FAD	C2B-C1B	-4.00	1.47	1.53
2	D	801	FAD	O4B-C4B	-3.80	1.36	1.45
2	B	801	FAD	C2B-C3B	-3.78	1.43	1.53
2	B	801	FAD	O3B-C3B	-3.58	1.34	1.43
2	B	801	FAD	C4A-N3A	-3.15	1.30	1.35
2	A	801	FAD	C2B-C3B	-3.14	1.45	1.53
2	A	801	FAD	C2-N1	-3.05	1.32	1.38
2	A	801	FAD	O4B-C4B	-2.94	1.38	1.45
2	A	801	FAD	O3B-C3B	-2.94	1.36	1.43
2	B	801	FAD	C2-N1	-2.91	1.32	1.38
2	A	801	FAD	C2B-C1B	-2.78	1.49	1.53
2	C	702	FAD	C4A-N3A	-2.77	1.31	1.35
2	D	801	FAD	O2B-C2B	-2.40	1.37	1.43
2	A	801	FAD	O2B-C2B	-2.34	1.37	1.43
2	C	702	FAD	C3B-C4B	-2.32	1.46	1.53
2	D	801	FAD	C2B-C3B	-2.24	1.47	1.53
2	C	702	FAD	O4B-C4B	-2.20	1.40	1.45
2	D	801	FAD	C2B-C1B	-2.16	1.50	1.53
2	D	801	FAD	C2-N3	-2.08	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	702	FAD	O2B-C2B	-2.08	1.38	1.43
2	C	702	FAD	O3B-C3B	-2.05	1.38	1.43
2	D	801	FAD	C9A-C5X	-2.05	1.38	1.42
2	B	801	FAD	C2B-C1B	-2.04	1.50	1.53
2	D	801	FAD	O3B-C3B	-2.03	1.38	1.43
3	C	703	2FG	F2-C2	-2.03	1.35	1.40
2	D	801	FAD	C1'-N10	2.07	1.50	1.48
2	C	702	FAD	C8M-C8	2.29	1.55	1.51
2	B	801	FAD	C7M-C7	2.32	1.55	1.51
2	B	801	FAD	C4-N3	2.37	1.37	1.33
2	A	801	FAD	C2A-N1A	2.37	1.38	1.33
3	D	802	2FG	C4-C5	2.64	1.58	1.53
2	C	702	FAD	C4-C4X	2.68	1.46	1.41
2	B	801	FAD	C6-C5X	2.69	1.45	1.41
2	D	801	FAD	C4-C4X	2.70	1.46	1.41
2	C	702	FAD	C2A-N3A	2.77	1.36	1.32
2	A	801	FAD	C10-N1	2.93	1.37	1.33
2	B	801	FAD	C9A-N10	2.93	1.42	1.38
2	B	801	FAD	C10-N1	2.93	1.37	1.33
2	D	801	FAD	C2A-N3A	3.08	1.37	1.32
2	D	801	FAD	C10-N1	3.13	1.37	1.33
3	D	802	2FG	C2-C3	3.14	1.54	1.52
2	B	801	FAD	C4-C4X	3.17	1.47	1.41
2	A	801	FAD	C4-C4X	3.36	1.47	1.41
2	B	801	FAD	C2A-N3A	3.52	1.38	1.32
2	A	801	FAD	C1'-N10	3.94	1.52	1.48

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	FAD	C4X-C4-N3	-13.16	104.74	123.48
2	A	801	FAD	N3A-C2A-N1A	-10.00	120.14	128.86
2	B	801	FAD	C4X-C4-N3	-9.88	109.42	123.48
2	B	801	FAD	N3A-C2A-N1A	-9.56	120.53	128.86
2	C	702	FAD	N3A-C2A-N1A	-9.55	120.54	128.86
2	A	801	FAD	C4X-C4-N3	-9.25	110.31	123.48
2	D	801	FAD	C4-C4X-C10	-8.44	113.13	119.96
2	D	801	FAD	N3A-C2A-N1A	-7.65	122.20	128.86
3	C	703	2FG	F2-C2-C3	-5.63	104.37	108.49
2	D	801	FAD	C4X-C10-N10	-5.16	116.94	120.52
2	B	801	FAD	C4X-C10-N10	-4.87	117.14	120.52
2	D	801	FAD	C4B-O4B-C1B	-4.87	104.59	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	C4B-O4B-C1B	-4.03	105.48	109.77
2	B	801	FAD	C4-C4X-C10	-4.00	116.73	119.96
5	A	804	MES	O2S-S-O1S	-3.85	100.53	113.86
2	D	801	FAD	C4X-C4-N3	-3.78	118.10	123.48
2	C	702	FAD	C4-C4X-N5	-3.55	114.79	118.68
2	C	702	FAD	C4A-C5A-N7A	-3.27	106.25	109.41
5	C	701	MES	O3S-S-O1S	-2.89	104.74	111.37
2	D	801	FAD	C1'-N10-C10	-2.69	115.74	118.50
3	A	802	2FG	O4-C4-C3	-2.51	104.91	110.36
5	A	804	MES	O3S-S-C8	-2.43	103.06	106.06
2	B	801	FAD	C9A-C5X-N5	-2.38	118.70	122.24
3	D	802	2FG	O6-C6-C5	-2.29	103.62	111.34
2	A	801	FAD	C9A-C5X-N5	-2.28	118.84	122.24
3	D	802	2FG	O3-C3-C2	-2.20	104.94	109.15
2	A	801	FAD	C8M-C8-C7	-2.18	116.14	120.72
2	C	702	FAD	C1'-N10-C10	-2.16	116.29	118.50
2	D	801	FAD	C5A-C6A-N1A	-2.15	113.19	119.70
2	C	702	FAD	C8M-C8-C7	-2.08	116.35	120.72
2	D	801	FAD	C4A-C5A-N7A	-2.08	107.40	109.41
2	B	801	FAD	C4'-C3'-C2'	-2.07	108.95	113.41
3	B	802	2FG	O4-C4-C3	-2.05	105.90	110.36
2	A	801	FAD	C2A-N1A-C6A	2.06	122.37	118.77
2	D	801	FAD	O4'-C4'-C5'	2.09	114.65	110.00
2	D	801	FAD	C1B-N9A-C4A	2.10	130.27	126.64
2	D	801	FAD	O2B-C2B-C3B	2.14	118.69	111.83
2	C	702	FAD	O4B-C4B-C5B	2.20	116.82	109.40
2	C	702	FAD	C1B-N9A-C4A	2.20	130.43	126.64
2	A	801	FAD	C5B-C4B-C3B	2.20	123.69	115.29
2	B	801	FAD	O2'-C2'-C3'	2.25	114.66	109.09
3	B	802	2FG	O1-C1-O5	2.26	116.88	110.20
2	C	702	FAD	O2B-C2B-C1B	2.32	118.87	111.61
2	A	801	FAD	O2B-C2B-C1B	2.33	118.90	111.61
3	A	802	2FG	O1-C1-O5	2.33	117.09	110.20
2	B	801	FAD	O4'-C4'-C3'	2.35	114.93	109.09
3	A	802	2FG	O3-C3-C4	2.44	115.67	110.36
2	B	801	FAD	C2A-N1A-C6A	2.55	123.23	118.77
2	B	801	FAD	O3B-C3B-C4B	2.58	118.62	111.09
2	B	801	FAD	O2P-P-O1P	2.59	125.67	112.28
2	D	801	FAD	O4B-C4B-C5B	2.62	118.26	109.40
3	B	802	2FG	O5-C5-C6	2.64	112.73	106.41
2	C	702	FAD	C4-C4X-C10	2.75	122.19	119.96
2	B	801	FAD	C5X-C9A-N10	2.76	119.71	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	FAD	C5B-C4B-C3B	2.80	125.95	115.29
2	B	801	FAD	O2B-C2B-C1B	2.82	120.44	111.61
2	D	801	FAD	C4X-N5-C5X	2.84	119.76	116.76
2	A	801	FAD	O2B-C2B-C3B	2.86	121.00	111.83
2	D	801	FAD	O4B-C4B-C3B	2.95	111.04	105.17
2	D	801	FAD	C2A-N1A-C6A	2.97	123.97	118.77
2	A	801	FAD	O4B-C4B-C5B	3.08	119.79	109.40
3	A	802	2FG	F2-C2-C3	3.10	110.76	108.49
2	D	801	FAD	C5B-C4B-C3B	3.10	127.09	115.29
2	D	801	FAD	O2A-PA-O1A	3.11	128.37	112.28
5	C	701	MES	O2S-S-C8	3.16	109.50	106.79
2	D	801	FAD	O3B-C3B-C4B	3.18	120.37	111.09
2	A	801	FAD	C1'-N10-C10	3.22	121.80	118.50
2	A	801	FAD	O4B-C4B-C3B	3.23	111.59	105.17
2	A	801	FAD	C5A-C6A-N6A	3.25	127.10	120.47
2	D	801	FAD	C5A-C6A-N6A	3.28	127.16	120.47
2	A	801	FAD	C4X-N5-C5X	3.32	120.26	116.76
2	C	702	FAD	C5A-C6A-N6A	3.39	127.39	120.47
2	A	801	FAD	C5X-C9A-N10	3.53	120.28	117.66
2	B	801	FAD	C4X-N5-C5X	3.71	120.68	116.76
2	C	702	FAD	O2B-C2B-C3B	3.87	124.22	111.83
2	B	801	FAD	C1'-N10-C9A	3.89	121.91	118.35
2	D	801	FAD	O2B-C2B-C1B	3.89	123.78	111.61
2	B	801	FAD	O4B-C4B-C5B	4.04	123.05	109.40
5	C	701	MES	O1S-S-C8	4.39	110.56	106.79
2	C	702	FAD	O3B-C3B-C4B	4.63	124.62	111.09
2	D	801	FAD	C1'-N10-C9A	5.22	123.13	118.35
2	D	801	FAD	C4-C4X-N5	6.20	125.47	118.68
2	C	702	FAD	C1'-N10-C9A	6.50	124.30	118.35
5	A	804	MES	O1S-S-C8	6.96	112.77	106.79
3	D	802	2FG	F2-C2-C3	7.86	114.25	108.49
5	C	701	MES	O3S-S-C8	8.07	115.98	106.06
2	D	801	FAD	C4-N3-C2	12.72	126.28	115.16
5	A	804	MES	O2S-S-C8	13.96	118.79	106.79
2	B	801	FAD	C4-N3-C2	15.54	128.75	115.16
2	A	801	FAD	C4-N3-C2	20.59	133.16	115.16
2	C	702	FAD	C4-N3-C2	23.16	135.42	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	MES	3	0
2	D	801	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, 95th 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 ²)	Q<0.9
1	A	573/633 (90%)	-0.36	6 (1%) 82 82	20, 27, 45, 70	0
1	B	576/633 (90%)	-0.33	9 (1%) 72 71	21, 27, 51, 76	0
1	C	573/633 (90%)	-0.27	8 (1%) 75 75	23, 33, 55, 84	0
1	D	573/633 (90%)	-0.14	13 (2%) 61 60	24, 39, 61, 84	0
All	All	2295/2532 (90%)	-0.28	36 (1%) 72 71	20, 32, 56, 84	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	618	PHE	4.9
1	C	389	LEU	4.8
1	D	343	ALA	4.4
1	C	385	THR	4.4
1	D	345	PRO	3.9
1	C	390	THR	3.8
1	C	388	GLU	3.7
1	A	343	ALA	3.6
1	C	343	ALA	3.6
1	B	388	GLU	3.5
1	D	385	THR	3.4
1	C	383	ARG	3.4
1	B	343	ALA	3.4
1	B	385	THR	3.2
1	B	44	ASP	3.1
1	B	384	GLY	3.0
1	D	344	ASN	3.0
1	A	344	ASN	3.0
1	A	186	ASP	2.9
1	B	43	MET	2.7
1	B	401	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	345	PRO	2.6
1	A	268	THR	2.6
1	C	382	ILE	2.6
1	B	390	THR	2.5
1	D	347	GLU	2.3
1	D	290	ALA	2.3
1	D	388	GLU	2.3
1	D	270	ALA	2.3
1	D	617	PRO	2.3
1	D	269	ASP	2.2
1	A	618	PHE	2.2
1	B	389	LEU	2.1
1	D	82	SER	2.1
1	C	618	PHE	2.0
1	D	459	VAL	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, 95th 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 ²)	Q<0.9
4	12P	A	803	16/37	0.83	0.21	11.53	45,56,63,65	0
5	MES	A	804	12/12	0.93	0.30	7.77	42,62,67,67	0
4	12P	B	803	16/37	0.84	0.18	5.96	45,53,70,70	0
4	12P	D	803	13/37	0.87	0.23	4.45	52,60,63,64	0
4	12P	B	804	16/37	0.90	0.19	3.72	47,56,81,96	0
5	MES	C	701	12/12	0.95	0.16	1.38	45,50,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	2FG	D	802	12/12	0.93	0.12	0.58	38,40,42,45	0
3	2FG	C	703	12/12	0.96	0.11	-0.00	36,39,44,49	0
2	FAD	D	801	53/53	0.97	0.10	-0.32	27,32,36,38	0
2	FAD	C	702	53/53	0.98	0.09	-0.90	22,26,32,34	0
2	FAD	B	801	53/53	0.98	0.10	-1.01	18,22,26,27	0
3	2FG	A	802	12/12	0.97	0.10	-1.22	29,33,35,44	0
2	FAD	A	801	53/53	0.98	0.09	-1.27	18,20,24,26	0
3	2FG	B	802	12/12	0.97	0.08	-1.74	32,34,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.