



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:50 PM GMT

PDB ID : 1O95
Title : Ternary complex between trimethylamine dehydrogenase and electron transferring flavoprotein
Authors : Leys, D.; Basran, J.; Talfournier, F.; Sutcliffe, M.J.; Scrutton, N.S.
Deposited on : 2002-12-11
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

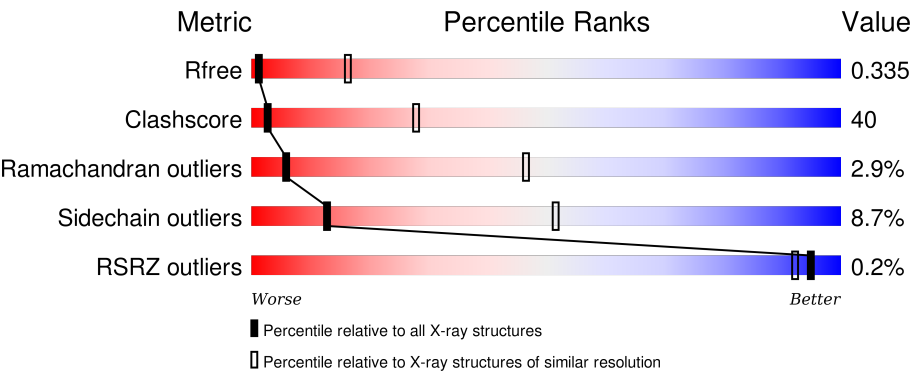
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 <=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	729	<div><div>36%</div><div>48%</div><div>14%</div><div>•</div></div>
1	B	729	<div><div>33%</div><div>53%</div><div>11%</div><div>•</div></div>
2	C	264	<div><div>42%</div><div>34%</div><div>11%</div><div>•</div><div>12%</div></div>
2	E	264	<div><div>39%</div><div>35%</div><div>14%</div><div>•</div><div>11%</div></div>
3	D	320	<div><div>27%</div><div>23%</div><div>7%</div><div>•</div><div>41%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	320	<div><div><div><div>%</div><div></div></div><div><div></div><div>22%</div></div><div><div></div><div>27%</div></div><div><div></div><div>9%</div></div><div><div></div><div>•</div></div><div><div></div><div>41%</div></div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17776 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 TRIMETHYLAMINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5692	3589	996	1079	28			
1	B	729	Total	C	N	O	S	0	0	0
			5676	3583	994	1071	28			

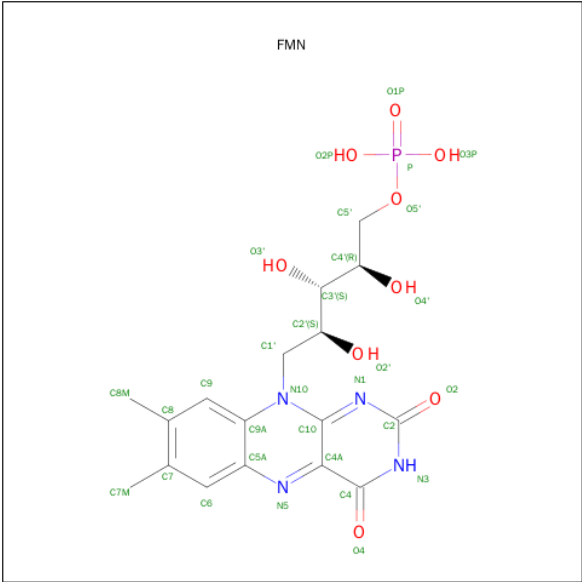
- Molecule 2 is a protein called ELECTRON TRANSFER FLAVOPROTEIN BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	233	Total	C	N	O	S	0	0	0
			1749	1097	301	341	10			
2	E	236	Total	C	N	O	S	0	0	0
			1751	1102	299	340	10			

- Molecule 3 is a protein called ELECTRON TRANSFER FLAVOPROTEIN ALPHA-SUBUNIT.

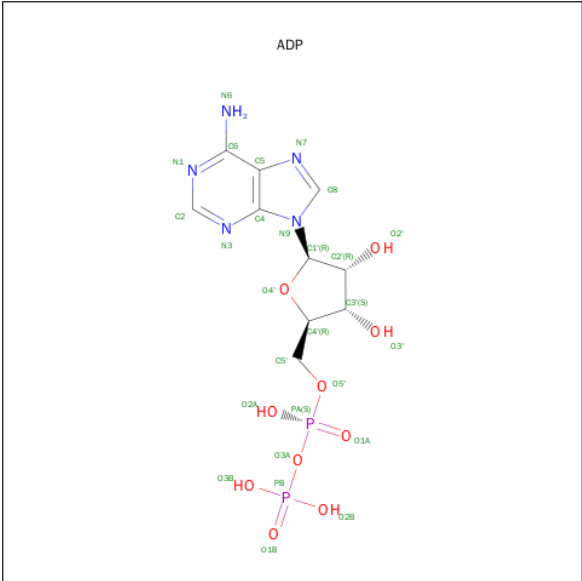
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	189	Total	C	N	O	0	0	0
			1354	857	230	267			
3	F	189	Total	C	N	O	0	0	0
			1376	870	232	274			

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



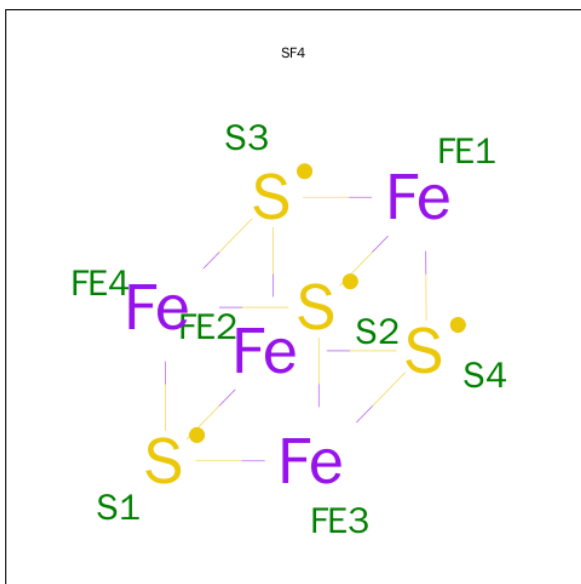
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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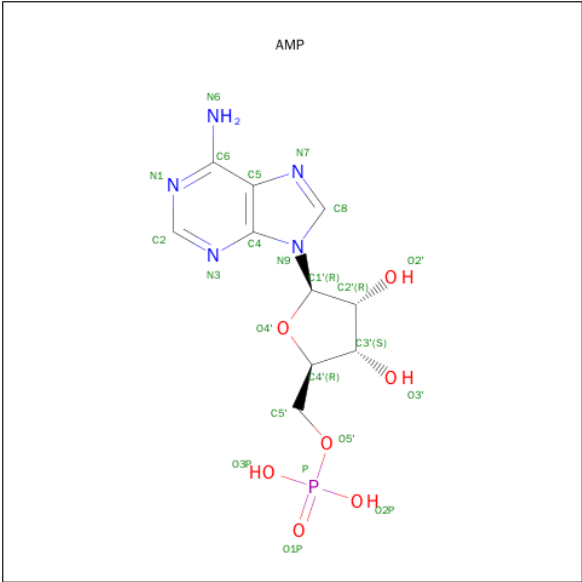
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).

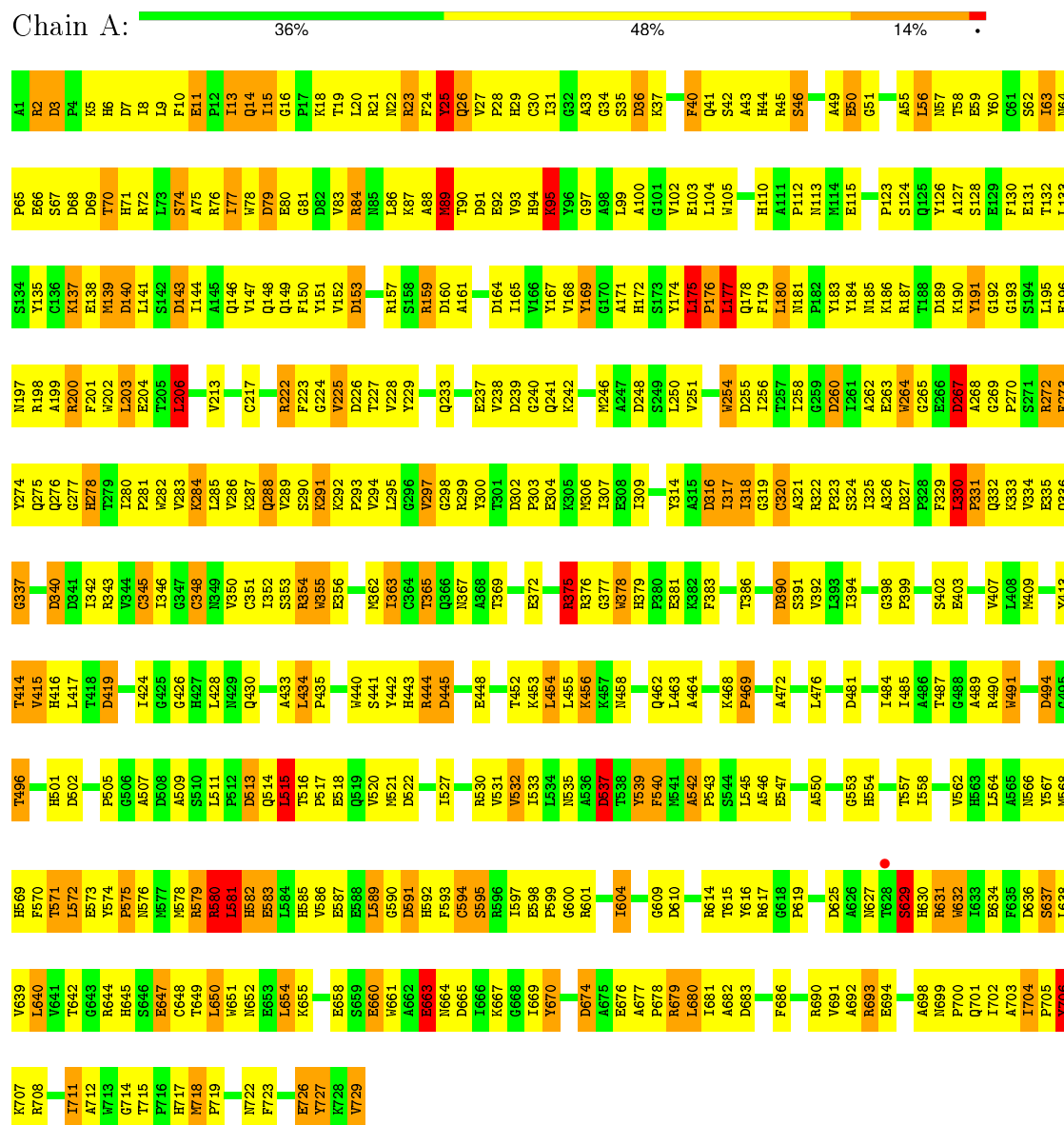


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

3 Residue-property plots

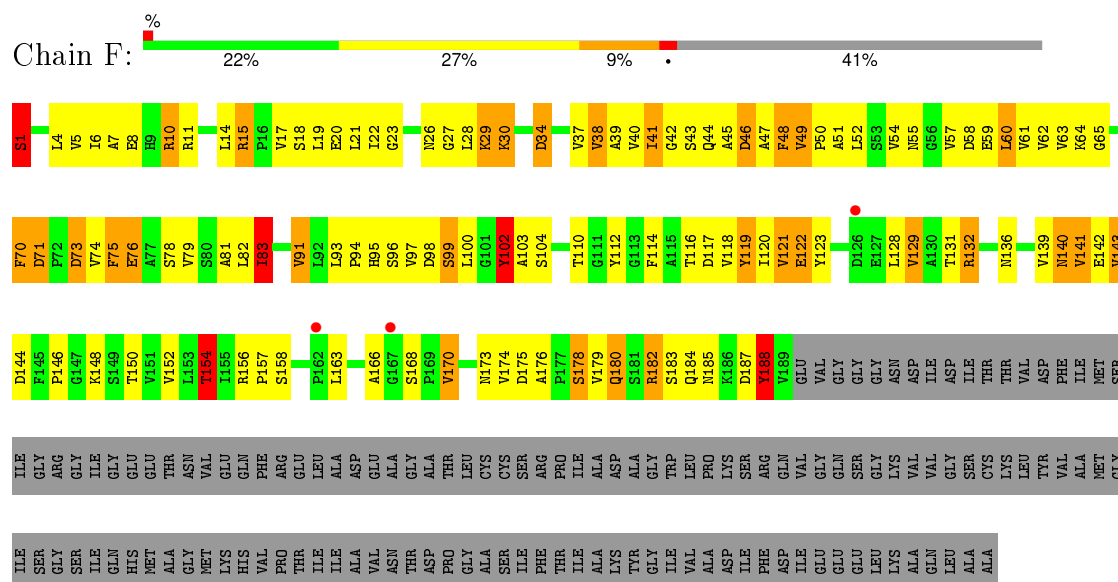
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: TRIMETHYLAMINE DEHYDROGENASE



• Molecule 1: TRIMETHYLAMINE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.50Å 116.51Å 138.71Å 90.00° 95.35° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 19.98 – 3.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.70) 96.9 (19.98-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.252 , 0.353 0.237 , 0.335	Depositor DCC
R_{free} test set	1679 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.862	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 33620 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17776	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2278e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, AMP, SF4, ADP

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	1.61	53/5834 (0.9%)	1.66	102/7918 (1.3%)
1	B	1.63	49/5818 (0.8%)	1.66	97/7902 (1.2%)
2	C	1.60	22/1771 (1.2%)	1.54	24/2399 (1.0%)
2	E	1.70	22/1775 (1.2%)	1.65	34/2408 (1.4%)
3	D	1.61	13/1378 (0.9%)	1.59	21/1884 (1.1%)
3	F	2.01	34/1400 (2.4%)	1.77	26/1913 (1.4%)
All	All	1.66	193/17976 (1.1%)	1.65	304/24424 (1.2%)

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	A	0	4
1	B	0	3
2	E	0	1
3	D	0	3
3	F	0	3
All	All	0	14

The worst 5 of 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	MET	SD-CE	12.45	2.47	1.77
3	F	188	TYR	CE1-CZ	9.02	1.50	1.38
1	B	254	TRP	CB-CG	-8.99	1.34	1.50
2	E	232	MET	C-O	8.98	1.40	1.23
3	D	180	GLN	CB-CG	8.94	1.76	1.52

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	ASP	CB-CG-OD2	13.04	130.03	118.30
1	B	272	ARG	NE-CZ-NH1	-12.16	114.22	120.30
3	F	15	ARG	NE-CZ-NH2	11.80	126.20	120.30
1	A	302	ASP	CB-CG-OD2	11.78	128.90	118.30
1	A	665	ASP	CB-CG-OD2	11.31	128.48	118.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	MET	Peptide
1	A	320	CYS	Peptide
1	A	539	TYR	Peptide
1	A	66	GLU	Peptide
1	B	139	MET	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5692	0	5445	505	0
1	B	5676	0	5424	519	0
2	C	1749	0	1722	121	0
2	E	1751	0	1716	129	0
3	D	1354	0	1311	85	0
3	F	1376	0	1358	129	0
4	A	31	0	18	5	0
4	B	31	0	18	6	0
5	A	27	0	12	6	0
5	B	27	0	12	2	0
6	A	8	0	0	1	0
6	B	8	0	0	0	0
7	C	23	0	11	6	0
7	E	23	0	12	4	0
All	All	17776	0	17059	1402	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 40.

The worst 5 of 1402 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:346:ILE:CD1	1:B:346:ILE:CG1	1.75	1.63
1:B:500:THR:CA	1:B:500:THR:CB	1.75	1.57
3:D:180:GLN:CB	3:D:180:GLN:CG	1.76	1.56
3:D:16:PRO:CB	3:D:16:PRO:CG	1.74	1.48
1:A:718:MET:SD	1:A:718:MET:CE	2.04	1.46

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	727/729 (100%)	624 (86%)	83 (11%)	20 (3%)	6	47
1	B	727/729 (100%)	614 (84%)	98 (14%)	15 (2%)	9	53
2	C	227/264 (86%)	202 (89%)	21 (9%)	4 (2%)	11	56
2	E	234/264 (89%)	210 (90%)	14 (6%)	10 (4%)	3	35
3	D	187/320 (58%)	153 (82%)	24 (13%)	10 (5%)	2	29
3	F	187/320 (58%)	162 (87%)	18 (10%)	7 (4%)	4	40
All	All	2289/2626 (87%)	1965 (86%)	258 (11%)	66 (3%)	6	46

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	GLY
1	A	680	LEU
1	B	264	TRP
1	B	680	LEU
3	D	27	GLY

5.3.2 Protein sidechains [i](#)

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	584/602 (97%)	537 (92%)	47 (8%)	15	55
1	B	578/602 (96%)	527 (91%)	51 (9%)	12	51
2	C	180/216 (83%)	167 (93%)	13 (7%)	18	59
2	E	177/216 (82%)	161 (91%)	16 (9%)	12	50
3	D	143/258 (55%)	123 (86%)	20 (14%)	4	29
3	F	150/258 (58%)	139 (93%)	11 (7%)	17	59
All	All	1812/2152 (84%)	1654 (91%)	158 (9%)	13	51

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	414	THR
1	B	619	PRO
2	E	226	MET
1	B	444	ARG
1	B	539	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	652	ASN
2	C	170	GLN
3	F	26	ASN
2	C	125	GLN
2	C	175	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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$
4	FMN	A	1730	1	32,33,33	2.01	9 (28%)	34,50,50	3.16	15 (44%)
5	ADP	A	1731	-	24,29,29	1.73	6 (25%)	23,45,45	2.89	8 (34%)
6	SF4	A	1732	1	0,12,12	0.00	-	0,24,24	0.00	-
4	FMN	B	1730	1	32,33,33	1.81	7 (21%)	34,50,50	3.12	18 (52%)
5	ADP	B	1731	-	24,29,29	1.49	4 (16%)	23,45,45	3.67	10 (43%)
6	SF4	B	1732	1	0,12,12	0.00	-	0,24,24	0.00	-
7	AMP	C	1236	-	22,25,25	1.93	7 (31%)	22,38,38	4.29	10 (45%)
7	AMP	E	1237	-	22,25,25	2.20	6 (27%)	22,38,38	4.43	10 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	A	1730	1	-	0/18/18/18	0/3/3/3
5	ADP	A	1731	-	-	0/12/32/32	0/3/3/3
6	SF4	A	1732	1	-	0/0/48/48	0/6/5/5
4	FMN	B	1730	1	-	0/18/18/18	0/3/3/3
5	ADP	B	1731	-	-	0/12/32/32	0/3/3/3
6	SF4	B	1732	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AMP	C	1236	-	-	0/6/26/26	0/3/3/3
7	AMP	E	1237	-	-	0/6/26/26	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1237	AMP	C2'-C1'	-4.74	1.46	1.53
5	A	1731	ADP	C2'-C1'	-4.07	1.47	1.53
5	B	1731	ADP	O4'-C4'	-3.98	1.35	1.45
7	C	1236	AMP	O4'-C4'	-3.51	1.37	1.45
5	B	1731	ADP	C2'-C1'	-3.13	1.48	1.53

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	1237	AMP	N3-C2-N1	-15.90	116.38	128.87
5	B	1731	ADP	N3-C2-N1	-14.19	117.73	128.87
7	C	1236	AMP	N3-C2-N1	-12.17	119.31	128.87
7	E	1237	AMP	C1'-N9-C4	-8.44	117.38	126.81
5	A	1731	ADP	O2'-C2'-C1'	-7.76	87.33	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1730	FMN	5	0
5	A	1731	ADP	6	0
6	A	1732	SF4	1	0
4	B	1730	FMN	6	0
5	B	1731	ADP	2	0
7	C	1236	AMP	6	0
7	E	1237	AMP	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	729/729 (100%)	-0.60	1 (0%) 95 94	39, 57, 67, 73	0
1	B	729/729 (100%)	-0.62	0 100 100	38, 57, 67, 73	0
2	C	233/264 (88%)	-0.63	0 100 100	49, 58, 65, 71	0
2	E	236/264 (89%)	-0.56	0 100 100	50, 59, 65, 70	0
3	D	189/320 (59%)	-0.56	0 100 100	55, 61, 69, 75	0
3	F	189/320 (59%)	-0.10	3 (1%) 74 60	56, 62, 71, 76	0
All	All	2305/2626 (87%)	-0.56	4 (0%) 95 92	38, 59, 67, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	126	ASP	3.9
1	A	628	THR	2.9
3	F	162	PRO	2.3
3	F	167	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	FMN	B	1730	31/31	0.95	0.19	0.87	23,39,46,52	0
5	ADP	A	1731	27/27	0.94	0.18	0.30	40,47,52,53	0
5	ADP	B	1731	27/27	0.95	0.17	0.27	45,52,59,61	0
7	AMP	E	1237	23/23	0.93	0.22	0.22	33,52,63,66	0
7	AMP	C	1236	23/23	0.95	0.17	-0.35	34,50,56,60	0
4	FMN	A	1730	31/31	0.95	0.16	-0.39	35,47,60,61	0
6	SF4	A	1732	8/8	1.00	0.12	-1.15	31,36,40,41	0
6	SF4	B	1732	8/8	1.00	0.13	-1.72	33,34,42,44	0

6.5 Other polymers

There are no such residues in this entry.