Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1N63
Title	:	Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Carbon monoxide reduced state
Authors	:	Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on	:	2002-11-08
Resolution	:	1.21 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 (i) symbol.

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

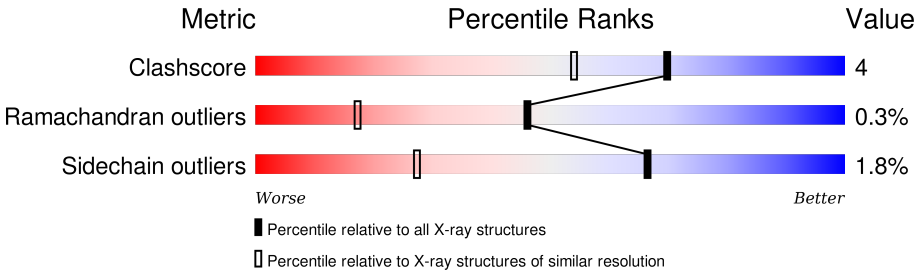
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 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	102246	1295 (1.26-1.18)
Ramachandran outliers	100387	1239 (1.26-1.18)
Sidechain outliers	100360	1237 (1.26-1.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	166	86% 11% •
1	D	166	86% 8% • 5%
2	B	809	85% 12% •
2	E	809	86% 10% ••
3	C	288	90% 9% •
3	F	288	92% 6% ••

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22119 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 Carbon monoxide dehydrogenase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	2	4	0
			1206	748	214	227	17			
1	D	158	Total	C	N	O	S	7	6	0
			1202	745	217	223	17			

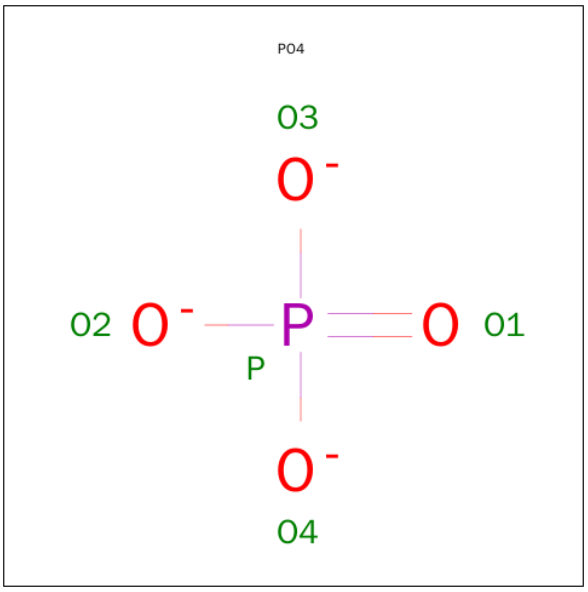
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	805	Total	C	N	O	S	70	23	0
			6292	4003	1070	1170	49			
2	E	795	Total	C	N	O	S	71	15	0
			6187	3936	1052	1152	47			

- Molecule 3 is a protein called Carbon monoxide dehydrogenase medium chain.

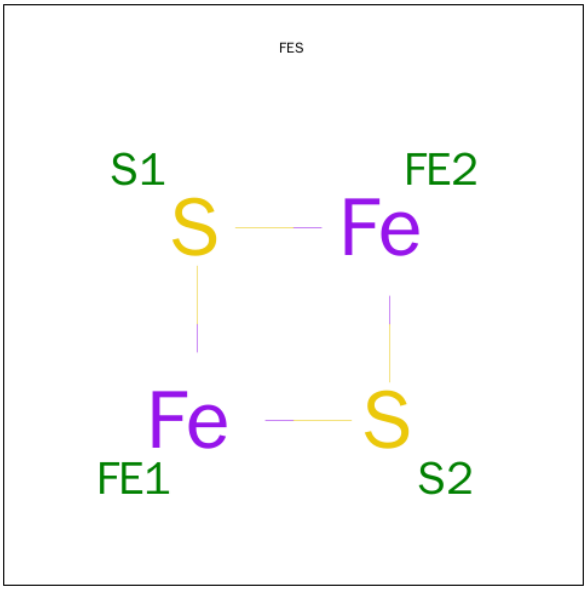
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	38	9	0
			2143	1354	376	401	12			
3	F	286	Total	C	N	O	S	38	7	0
			2123	1341	370	399	13			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 4 2 2	0	0
5	A	1	Total Fe S 4 2 2	0	0
5	D	1	Total Fe S 4 2 2	0	0

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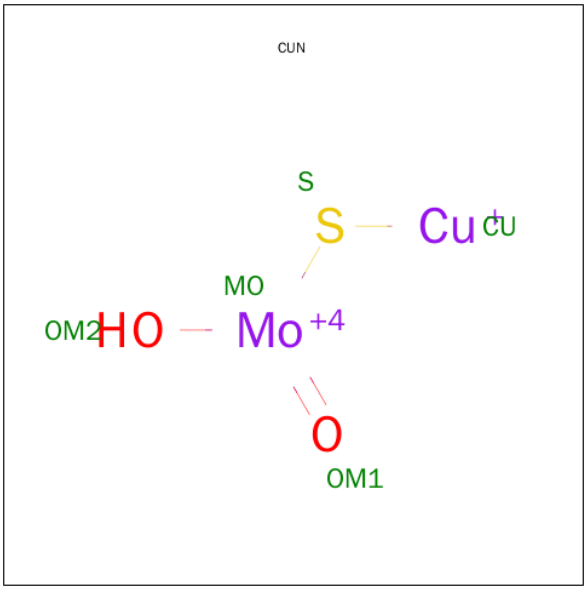
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Fe S 4 2 2	0	0

- Molecule 6 is CU(I)-S-MO(IV)(=O)OH CLUSTER (three-letter code: CUN) (formula: $CuHMoO_2S$).

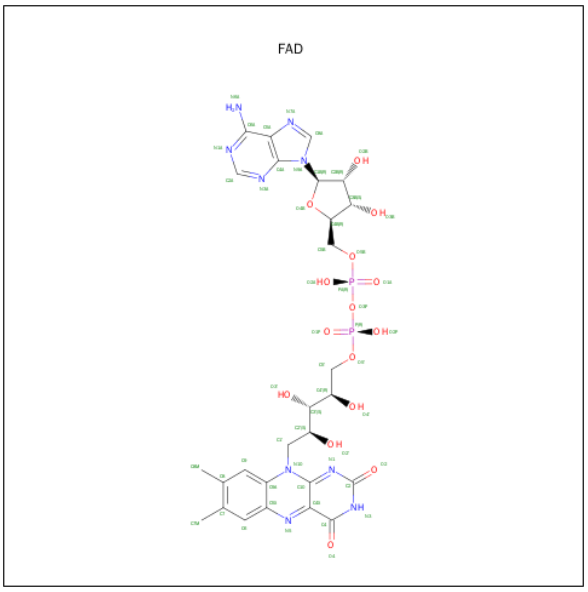


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cu Mo O S 5 1 1 2 1	0	0
6	E	1	Total Cu Mo O S 5 1 1 2 1	0	0

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		
7	E	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	196	Total	O	0	0
			196	196		
9	B	864	Total	O	0	0
			864	864		
9	C	361	Total	O	0	1
			362	362		
9	D	196	Total	O	0	0
			196	196		
9	E	831	Total	O	0	0
			831	831		
9	F	292	Total	O	0	0
			292	292		

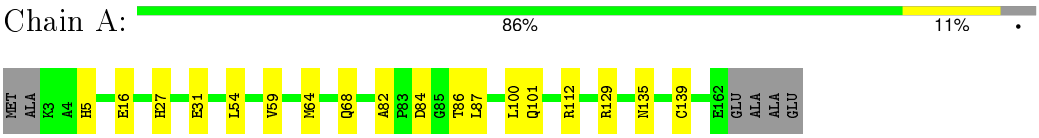
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

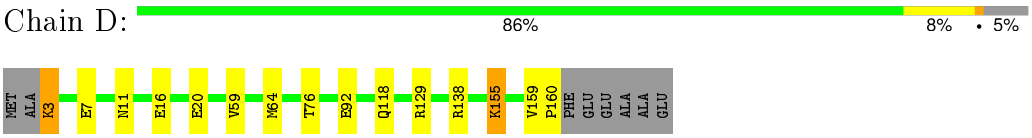
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A:



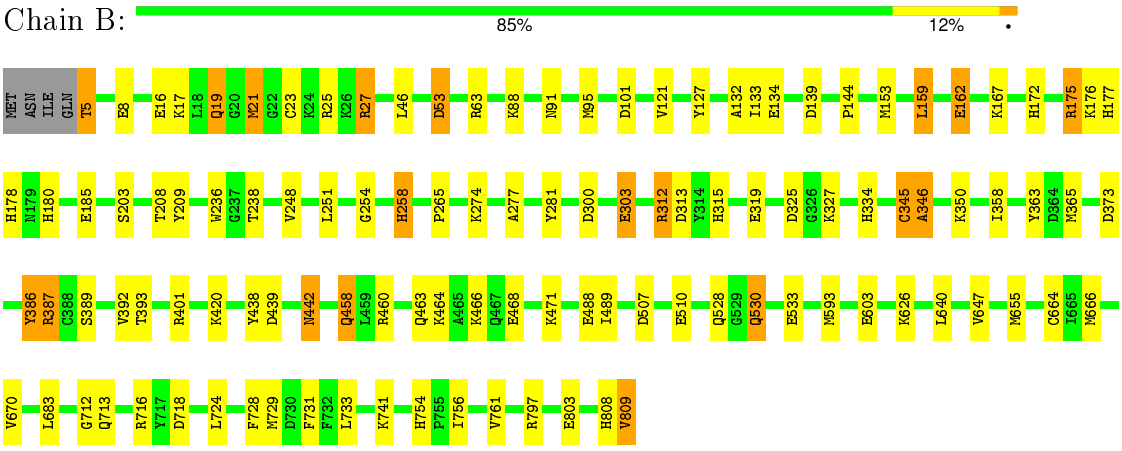
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:



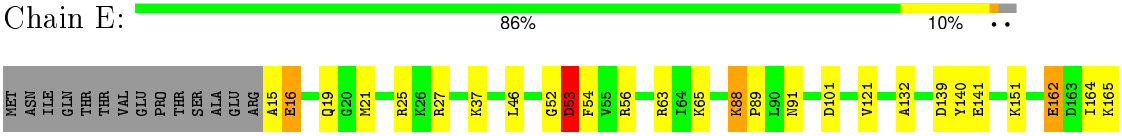
- Molecule 2: Carbon monoxide dehydrogenase large chain

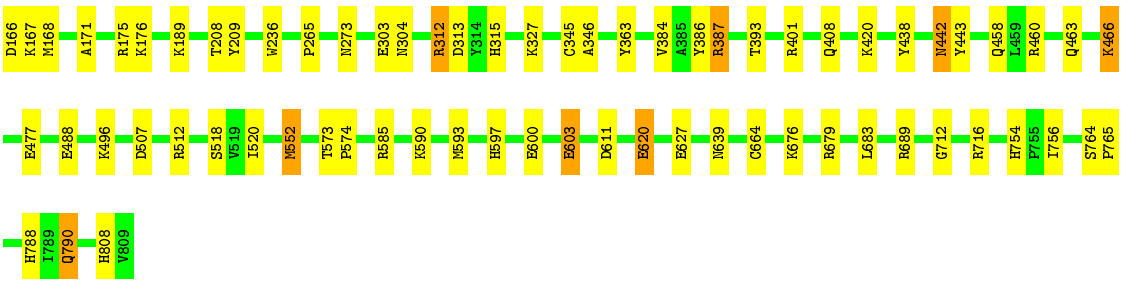
Chain B:



- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain E:





• Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain C:

• Molecule 3: Carbon monoxide dehydrogenase medium chain

Chain F:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.96Å 131.27Å 159.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.21	Depositor
% Data completeness (in resolution range)	(Not available) (17.00-1.21)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.185	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22119	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MCN, PO4, FES, FAD, CUN

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	0.75	0/1244	0.89	2/1681 (0.1%)
1	D	0.89	4/1246 (0.3%)	0.98	4/1681 (0.2%)
2	B	0.96	16/6542 (0.2%)	1.11	29/8875 (0.3%)
2	E	1.40	17/6400 (0.3%)	1.06	34/8678 (0.4%)
3	C	1.01	9/2216 (0.4%)	0.95	11/3007 (0.4%)
3	F	1.51	6/2186 (0.3%)	1.02	12/2966 (0.4%)
All	All	1.18	52/19834 (0.3%)	1.05	92/26888 (0.3%)

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	2
1	D	0	1
2	B	0	14
2	E	0	17
3	C	0	5
3	F	0	5
All	All	0	44

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	303	GLU	CD-OE1	-57.96	0.61	1.25
2	E	303	GLU	CD-OE2	53.93	1.84	1.25
3	F	49	GLU	CD-OE2	53.33	1.84	1.25
2	E	162	GLU	CD-OE1	30.65	1.59	1.25
3	F	23	LYS	CD-CE	-26.46	0.85	1.51
2	B	741	LYS	CE-NZ	24.65	2.10	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	37	LYS	CE-NZ	-20.24	0.98	1.49
2	B	139	ASP	CG-OD1	19.19	1.69	1.25
2	B	809	VAL	CB-CG1	-18.19	1.14	1.52
2	B	139	ASP	CG-OD2	-16.75	0.86	1.25
3	F	49	GLU	CG-CD	-16.62	1.27	1.51
2	E	15	ALA	CA-CB	15.44	1.84	1.52
3	C	265	GLU	CD-OE1	-14.78	1.09	1.25
2	E	189	LYS	CE-NZ	-14.54	1.12	1.49
3	C	142	GLU	CG-CD	14.52	1.73	1.51
3	C	162	GLU	CD-OE2	14.20	1.41	1.25
1	D	16	GLU	CG-CD	13.42	1.72	1.51
2	E	167	LYS	CD-CE	13.41	1.84	1.51
3	C	287	LYS	CB-CG	13.22	1.88	1.52
3	C	240	LYS	CE-NZ	-13.11	1.16	1.49
2	E	88	LYS	CE-NZ	11.88	1.78	1.49
2	B	63	ARG	CD-NE	-9.34	1.30	1.46
1	D	3	LYS	CE-NZ	-9.17	1.26	1.49
2	B	325	ASP	CG-OD1	8.93	1.45	1.25
2	B	664	CYS	CA-CB	8.62	1.73	1.53
2	B	664	CYS	CB-SG	-8.46	1.67	1.82
2	E	496	LYS	CD-CE	8.41	1.72	1.51
3	F	86	PHE	CD2-CE2	-8.30	1.22	1.39
1	D	7	GLU	CD-OE1	-8.10	1.16	1.25
2	B	167	LYS	CB-CG	8.07	1.74	1.52
3	C	287	LYS	C-O	-7.84	1.08	1.23
2	E	664	CYS	CB-SG	-7.81	1.69	1.82
2	B	533	GLU	CG-CD	7.70	1.63	1.51
3	C	265	GLU	CG-CD	7.34	1.62	1.51
2	E	639	ASN	CG-OD1	-7.31	1.07	1.24
2	E	91	ASN	CG-ND2	-7.08	1.15	1.32
3	F	90	LYS	CE-NZ	-6.31	1.33	1.49
2	B	466	LYS	CE-NZ	-6.10	1.33	1.49
1	D	7	GLU	CG-CD	-5.87	1.43	1.51
2	E	466	LYS	CE-NZ	5.83	1.63	1.49
3	C	280	GLU	CG-CD	5.80	1.60	1.51
3	F	240	LYS	CB-CG	5.77	1.68	1.52
2	B	664	CYS	N-CA	5.75	1.57	1.46
2	B	345[A]	CYS	CB-SG	-5.61	1.72	1.81
2	B	345[B]	CYS	CB-SG	-5.61	1.72	1.81
2	E	603	GLU	CD-OE1	5.34	1.31	1.25
2	B	666[A]	MET	CG-SD	-5.33	1.67	1.81
2	B	666[B]	MET	CG-SD	-5.33	1.67	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	676	LYS	CD-CE	5.29	1.64	1.51
3	C	158	PHE	CD1-CE1	5.06	1.49	1.39
2	E	171	ALA	CA-CB	-5.01	1.42	1.52
2	E	664	CYS	CA-CB	5.01	1.65	1.53

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	139	ASP	CB-CG-OD2	31.56	146.71	118.30
2	B	139	ASP	CB-CG-OD1	-21.11	99.31	118.30
2	E	21[A]	MET	CG-SD-CE	-18.47	70.65	100.20
2	E	21[B]	MET	CG-SD-CE	-18.47	70.65	100.20
2	B	5	THR	N-CA-CB	16.70	142.03	110.30
3	F	86	PHE	CB-CG-CD2	14.31	130.81	120.80
2	B	325	ASP	CB-CG-OD1	-14.12	105.59	118.30
2	B	175	ARG	NE-CZ-NH1	-14.00	113.30	120.30
2	E	15	ALA	N-CA-CB	12.65	127.81	110.10
2	E	303	GLU	CG-CD-OE2	-12.55	93.19	118.30
3	F	1[A]	MET	CG-SD-CE	12.08	119.52	100.20
3	F	1[B]	MET	CG-SD-CE	12.08	119.52	100.20
2	E	303	GLU	CG-CD-OE1	11.94	142.18	118.30
2	B	729[A]	MET	CG-SD-CE	-11.82	81.29	100.20
2	B	729[B]	MET	CG-SD-CE	-11.82	81.29	100.20
2	E	189	LYS	CD-CE-NZ	9.60	133.78	111.70
2	B	387	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	D	7	GLU	OE1-CD-OE2	-9.53	111.86	123.30
2	E	162	GLU	CG-CD-OE1	-9.22	99.86	118.30
2	E	16	GLU	CG-CD-OE1	-9.20	99.90	118.30
3	C	287	LYS	CA-C-O	9.18	139.37	120.10
3	F	177	THR	CA-CB-CG2	-8.81	100.06	112.40
2	B	175	ARG	NE-CZ-NH2	8.68	124.64	120.30
3	C	162	GLU	OE1-CD-OE2	8.62	133.64	123.30
2	E	689	ARG	NE-CZ-NH2	-8.58	116.01	120.30
2	B	809	VAL	CG1-CB-CG2	8.45	124.42	110.90
1	D	20	GLU	OE1-CD-OE2	8.26	133.21	123.30
2	B	325	ASP	CB-CG-OD2	8.20	125.68	118.30
2	E	162	GLU	OE1-CD-OE2	-8.09	113.59	123.30
2	B	809	VAL	CA-CB-CG1	7.68	122.42	110.90
2	E	53	ASP	CB-CG-OD1	7.32	124.89	118.30
2	B	626	LYS	CD-CE-NZ	7.31	128.51	111.70
2	E	639	ASN	CB-CG-OD1	7.28	136.16	121.60
2	E	15	ALA	CB-CA-C	-7.28	99.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	177	THR	OG1-CB-CG2	7.22	126.61	110.00
3	C	287	LYS	CA-CB-CG	-7.21	97.53	113.40
2	B	386	TYR	CB-CG-CD1	7.14	125.28	121.00
1	A	129	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	F	86	PHE	CD1-CG-CD2	-7.01	109.18	118.30
2	E	639	ASN	OD1-CG-ND2	-6.99	105.82	121.90
2	B	401	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	E	401	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	B	27	ARG	NE-CZ-NH2	-6.83	116.89	120.30
3	C	158	PHE	CB-CG-CD1	6.70	125.49	120.80
3	F	86	PHE	CG-CD2-CE2	6.68	128.15	120.80
2	E	387	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	E	387	ARG	NE-CZ-NH1	6.39	123.49	120.30
3	F	86	PHE	CZ-CE2-CD2	-6.37	112.45	120.10
3	C	142	GLU	CB-CG-CD	-6.28	97.25	114.20
3	F	49	GLU	CB-CG-CD	6.26	131.10	114.20
2	E	91	ASN	OD1-CG-ND2	-6.25	107.51	121.90
2	B	101	ASP	CB-CG-OD1	6.22	123.90	118.30
2	B	387	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	E	585	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	E	166	ASP	CB-CG-OD2	5.88	123.59	118.30
2	E	139	ASP	CB-CG-OD2	-5.78	113.10	118.30
3	C	240	LYS	CD-CE-NZ	5.71	124.84	111.70
2	E	401	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	112	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	20	GLU	CG-CD-OE1	-5.63	107.03	118.30
2	E	496	LYS	CG-CD-CE	-5.61	95.07	111.90
2	B	439	ASP	CB-CG-OD1	5.58	123.32	118.30
2	E	438	TYR	CB-CG-CD1	5.57	124.34	121.00
2	E	611	ASP	CB-CG-OD2	5.55	123.30	118.30
2	B	365	MET	CG-SD-CE	5.52	109.03	100.20
2	E	16	GLU	CB-CA-C	5.51	121.43	110.40
2	B	728	PHE	CB-CG-CD1	5.47	124.63	120.80
3	C	145	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	B	466	LYS	CD-CE-NZ	5.40	124.12	111.70
2	E	101	ASP	CB-CG-OD1	5.39	123.15	118.30
2	E	679	ARG	NE-CZ-NH2	-5.39	117.61	120.30
3	C	162	GLU	CG-CD-OE2	-5.38	107.55	118.30
2	B	346[A]	ALA	CA-C-O	-5.33	108.92	120.10
2	B	346[B]	ALA	CA-C-O	-5.33	108.92	120.10
3	C	10	ARG	NE-CZ-NH1	-5.29	117.66	120.30
2	B	16	GLU	CG-CD-OE2	5.28	128.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	162	GLU	OE1-CD-OE2	-5.28	116.97	123.30
2	E	438	TYR	CB-CG-CD2	-5.27	117.84	121.00
2	B	797	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	25	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	E	56	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	C	44	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	E	466	LYS	CD-CE-NZ	-5.23	99.67	111.70
2	E	88	LYS	CD-CE-NZ	-5.18	99.79	111.70
2	E	443	TYR	CB-CG-CD1	5.18	124.11	121.00
3	F	59	ASP	CB-CG-OD2	5.18	122.96	118.30
2	E	167	LYS	CD-CE-NZ	-5.13	99.90	111.70
3	C	158	PHE	CD1-CE1-CZ	-5.12	113.96	120.10
2	B	281	TYR	CB-CG-CD2	-5.07	117.96	121.00
2	B	16	GLU	CG-CD-OE1	-5.05	108.21	118.30
1	D	129	ARG	NE-CZ-NH1	5.02	122.81	120.30
3	F	56	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	GLU	Mainchain
1	A	82	ALA	Mainchain
2	B	134	GLU	Sidechain
2	B	162	GLU	Sidechain
2	B	185	GLU	Sidechain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	303	GLU	Sidechain
2	B	312	ARG	Sidechain
2	B	346[A]	ALA	Mainchain
2	B	346[B]	ALA	Mainchain
2	B	363	TYR	Sidechain
2	B	387	ARG	Sidechain
2	B	471	LYS	Mainchain
2	B	53	ASP	Sidechain
2	B	88	LYS	Mainchain
3	C	10	ARG	Sidechain
3	C	286	ALA	Peptide
3	C	29	ARG	Sidechain
3	C	44	ARG	Sidechain,Mainchain
1	D	138	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	140	TYR	Sidechain
2	E	16	GLU	Sidechain
2	E	162	GLU	Sidechain
2	E	168	MET	Mainchain
2	E	175	ARG	Sidechain
2	E	27	ARG	Sidechain
2	E	312	ARG	Sidechain
2	E	346[A]	ALA	Mainchain
2	E	346[B]	ALA	Mainchain
2	E	363	TYR	Sidechain
2	E	387	ARG	Sidechain
2	E	512	ARG	Sidechain
2	E	53	ASP	Mainchain
2	E	600	GLU	Sidechain
2	E	620	GLU	Mainchain
2	E	627	GLU	Sidechain
2	E	808	HIS	Mainchain
3	F	45	LEU	Mainchain
3	F	49	GLU	Sidechain
3	F	69	ASP	Mainchain
3	F	85	ASP	Mainchain
3	F	86	PHE	Sidechain

5.2 Too-close contacts (i)

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	1206	0	1184	17	0
1	D	1202	0	1190	12	0
2	B	6292	0	6169	67	1
2	E	6187	0	6051	39	1
3	C	2143	0	2198	18	0
3	F	2123	0	2168	23	0
4	A	5	0	0	1	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	5	0	0	1	0
6	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	44	0	17	0	0
7	E	44	0	17	0	0
8	C	53	0	31	2	0
8	F	53	0	31	3	0
9	A	196	0	0	1	1
9	B	864	0	0	17	1
9	C	362	0	0	2	0
9	D	196	0	0	2	0
9	E	831	0	0	11	1
9	F	292	0	0	4	0
All	All	22119	0	19056	169	3

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

All (169) 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)
3:F:10:ARG:NH2	3:F:55:ARG:CZ	1.97	1.28
2:E:593:MET:HG2	2:E:603:GLU:OE1	1.19	1.27
3:F:10:ARG:HH21	3:F:55:ARG:NE	1.35	1.24
3:F:10:ARG:HH21	3:F:55:ARG:CZ	1.58	1.11
3:F:10:ARG:NH2	3:F:55:ARG:NE	2.00	1.09
1:D:59:VAL:HG11	1:D:64:MET:HE1	1.34	1.06
1:D:59:VAL:HG11	1:D:64:MET:CE	1.89	1.02
2:B:19:GLN:NE2	2:B:23[A]:CYS:SG	2.43	0.92
2:E:593:MET:CG	2:E:603:GLU:OE1	2.15	0.91
3:F:10:ARG:HD2	3:F:55:ARG:HD3	1.53	0.87
2:B:528:GLN:H	2:B:530:GLN:HE22	1.22	0.84
1:A:68:GLN:HE21	3:C:55[A]:ARG:HH12	1.25	0.84
2:E:208:THR:H	2:E:790:GLN:HE22	1.23	0.84
1:D:11:ASN:HD21	1:D:76:THR:H	1.24	0.83
2:B:464:LYS:NZ	2:B:468:GLU:OE2	2.10	0.83
1:A:59:VAL:HG11	1:A:64[A]:MET:HE3	1.61	0.83
2:E:716:ARG:NE	9:E:5343:HOH:O	2.09	0.83
3:F:10:ARG:CZ	9:F:5072:HOH:O	2.28	0.82
2:B:808:HIS:O	2:B:809:VAL:HB	1.79	0.82
2:B:159:LEU:HD13	2:B:162:GLU:HG2	1.62	0.82
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.28	0.82
9:B:4101:HOH:O	3:C:1[A]:MET:HE1	1.79	0.81
1:D:3:LYS:N	9:D:5042:HOH:O	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:ARG:HH22	3:F:55:ARG:CZ	1.97	0.77
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	2.15	0.77
2:E:408:GLN:NE2	9:E:5704:HOH:O	2.17	0.77
1:D:59:VAL:CG1	1:D:64:MET:CE	2.64	0.75
3:F:10:ARG:CD	3:F:55:ARG:HD3	2.18	0.74
2:B:46:LEU:HD11	2:B:236[C]:TRP:CZ3	2.22	0.73
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.36	0.73
2:B:593:MET:HE2	2:B:640:LEU:HD21	1.69	0.73
2:B:716:ARG:NE	9:B:4266:HOH:O	2.21	0.72
2:B:159:LEU:CD1	2:B:162:GLU:HG2	2.20	0.71
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.36	0.71
2:B:713[A]:GLN:CD	2:B:731:PHE:CZ	2.65	0.69
1:D:159:VAL:HB	1:D:160:PRO:HD3	1.74	0.69
2:E:477:GLU:OE2	9:E:5270:HOH:O	2.11	0.69
3:F:10:ARG:HH21	3:F:55:ARG:CD	2.06	0.68
2:E:46:LEU:HD11	2:E:236[B]:TRP:CZ3	2.28	0.68
2:B:528:GLN:H	2:B:530:GLN:NE2	1.91	0.67
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.77	0.67
1:D:59:VAL:CG1	1:D:64:MET:HE1	2.18	0.66
6:B:3921:CUN:OM1	6:B:3921:CUN:MO	1.66	0.65
3:C:53:ASP:OD2	3:C:55[A]:ARG:HD2	1.97	0.65
1:A:27:HIS:HD2	2:B:127:TYR:OH	1.80	0.65
2:E:754:HIS:HD2	2:E:756:ILE:H	1.45	0.65
1:D:59:VAL:HG11	1:D:64:MET:HE3	1.78	0.64
2:E:716:ARG:CZ	9:E:5343:HOH:O	2.45	0.63
3:C:10:ARG:CZ	3:C:55[B]:ARG:HD3	2.29	0.63
2:B:159:LEU:HD13	2:B:162:GLU:CG	2.28	0.63
2:E:593:MET:HG2	2:E:603:GLU:CD	2.16	0.62
2:B:530:GLN:HE21	2:B:530:GLN:H	1.47	0.62
2:B:248:VAL:HG22	9:B:4721:HOH:O	1.99	0.62
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.46	0.61
2:B:303:GLU:HG2	9:B:4311:HOH:O	2.00	0.61
2:E:458:GLN:HG3	9:E:5132:HOH:O	2.00	0.61
2:B:593:MET:CE	2:B:640:LEU:HD21	2.30	0.60
1:D:118[A]:GLN:NE2	9:D:4977:HOH:O	2.32	0.60
1:A:59:VAL:CG1	1:A:64[A]:MET:HE3	2.31	0.60
3:F:10:ARG:HD2	3:F:55:ARG:CD	2.31	0.58
2:B:300:ASP:HB2	2:B:303:GLU:OE1	2.03	0.58
1:A:5:HIS:HD2	4:A:3001:PO4:O1	1.87	0.58
3:C:118:ASN:HD22	8:C:3932:FAD:H4B	1.69	0.57
2:E:208:THR:H	2:E:790:GLN:NE2	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:LYS:HE3	9:B:4605:HOH:O	2.04	0.56
2:B:670:VAL:O	2:B:808:HIS:HE1	1.89	0.56
1:A:135:ASN:ND2	3:C:105:GLN:HE22	2.04	0.55
2:B:754:HIS:HD2	2:B:756:ILE:H	1.53	0.55
2:B:716:ARG:CZ	9:B:4266:HOH:O	2.54	0.55
1:A:5:HIS:HE1	1:A:16:GLU:OE2	1.89	0.55
3:F:162:GLU:HB3	3:F:163:PRO:HD2	1.89	0.55
3:F:118:ASN:HD22	8:F:4931:FAD:H4B	1.72	0.55
1:A:68:GLN:HE21	3:C:55[A]:ARG:NH1	2.00	0.54
2:E:208:THR:OG1	2:E:315:HIS:HD2	1.90	0.54
2:E:590:LYS:HA	2:E:593:MET:HE2	1.88	0.54
2:B:53:ASP:CG	9:B:4714:HOH:O	2.46	0.54
2:B:21[A]:MET:CE	9:B:4456:HOH:O	2.55	0.54
1:D:59:VAL:CG1	1:D:64:MET:HE3	2.37	0.54
2:B:718:ASP:HB3	2:B:724:LEU:HD11	1.90	0.54
2:B:327:LYS:HG2	2:B:420:LYS:HE3	1.90	0.53
2:E:754:HIS:CD2	2:E:756:ILE:H	2.26	0.53
2:E:466:LYS:HE3	9:E:5712:HOH:O	2.07	0.52
2:B:334:HIS:HE1	2:B:373:ASP:OD2	1.92	0.52
3:C:222:THR:HB	3:C:223:PRO:HD2	1.92	0.52
3:F:106[B]:ILE:HD13	8:F:4931:FAD:C7	2.40	0.51
2:B:442:ASN:C	2:B:442:ASN:HD22	2.12	0.51
2:E:88:LYS:CB	2:E:89:PRO:HD3	2.41	0.51
2:E:597:HIS:HD2	9:E:5552:HOH:O	1.94	0.50
2:B:754:HIS:CD2	2:B:756:ILE:H	2.28	0.50
2:B:172:HIS:HD2	9:B:4586:HOH:O	1.95	0.50
1:A:27:HIS:HE1	9:B:4061:HOH:O	1.94	0.50
2:B:489:ILE:HD11	2:B:655[A]:MET:HG3	1.92	0.50
2:B:8:GLU:HG3	2:B:8:GLU:O	2.10	0.50
2:E:520:ILE:CD1	2:E:552[A]:MET:HG2	2.42	0.49
2:B:53:ASP:HB3	2:B:133:ILE:HD11	1.93	0.49
2:E:788:HIS:HE2	2:E:790:GLN:NE2	2.10	0.49
2:E:327:LYS:HE2	2:E:420:LYS:NZ	2.26	0.49
2:B:593:MET:HG2	2:B:603:GLU:OE2	2.12	0.49
2:E:19[B]:GLN:NE2	9:E:5286:HOH:O	2.16	0.49
2:B:238:THR:HB	2:B:274:LYS:HD3	1.95	0.49
3:C:106:ILE:HD13	8:C:3932:FAD:C7	2.43	0.48
2:B:153:MET:HA	2:B:177:HIS:CE1	2.48	0.48
2:E:442:ASN:HD22	2:E:442:ASN:C	2.16	0.48
2:B:530:GLN:H	2:B:530:GLN:NE2	2.11	0.48
3:C:10:ARG:NH1	3:C:55[B]:ARG:HD3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:221:ASN:ND2	9:F:5098:HOH:O	2.45	0.48
2:B:144:PRO:HD2	9:B:4722:HOH:O	2.14	0.48
2:E:19[A]:GLN:HE21	2:E:25:ARG:HG3	1.78	0.48
2:B:713[B]:GLN:NE2	2:B:733[B]:LEU:HD23	2.30	0.47
2:B:121:VAL:HG11	2:B:132:ALA:HB3	1.95	0.47
3:F:202:LEU:HD12	3:F:202:LEU:C	2.34	0.47
2:B:716:ARG:HD2	9:B:4752:HOH:O	2.13	0.47
3:F:276:ARG:NH1	9:F:5118:HOH:O	2.47	0.47
2:B:510:GLU:HG3	2:B:647[A]:VAL:HG12	1.97	0.47
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.64	0.46
3:C:138:LEU:HD23	3:C:167:LEU:HA	1.97	0.46
3:F:79:HIS:HD2	9:F:5160:HOH:O	1.99	0.46
1:A:27:HIS:CD2	2:B:127:TYR:OH	2.65	0.46
2:B:683:LEU:HD23	2:B:683:LEU:C	2.36	0.45
2:B:208:THR:OG1	2:B:315:HIS:HD2	2.00	0.45
3:F:10:ARG:NH2	3:F:55:ARG:NH1	2.58	0.45
1:A:84:ASP:OD1	1:A:86:THR:HG23	2.17	0.45
1:A:59:VAL:HG11	1:A:64[A]:MET:HE1	1.96	0.44
1:D:64:MET:HB2	1:D:64:MET:HE2	1.72	0.44
2:B:460:ARG:NH1	2:B:463:GLN:HE22	2.06	0.44
3:C:242:ALA:HA	9:C:4201:HOH:O	2.17	0.44
3:F:49:GLU:CG	3:F:49:GLU:OE2	2.64	0.44
2:E:683:LEU:HD23	2:E:683:LEU:C	2.38	0.44
2:B:17:LYS:HG3	9:B:4482:HOH:O	2.17	0.44
2:B:458:GLN:HE21	2:B:458:GLN:H	1.66	0.43
2:B:315:HIS:HE1	9:B:4009:HOH:O	2.01	0.43
2:E:345:CYS:SG	2:E:384:VAL:HG23	2.58	0.43
1:D:92:GLU:OE1	1:D:155[B]:LYS:NZ	2.49	0.43
3:F:10:ARG:HH22	3:F:55:ARG:NH2	2.15	0.43
2:E:63:ARG:HB2	2:E:141:GLU:HB2	2.01	0.43
2:B:95[B]:MET:CE	9:B:4413:HOH:O	2.67	0.43
2:B:358:ILE:HD11	2:B:438:TYR:CE1	2.53	0.43
3:F:10:ARG:HD3	3:F:55:ARG:HH11	1.84	0.43
2:B:258:HIS:H	2:B:258:HIS:CD2	2.37	0.42
2:B:808:HIS:O	2:B:809:VAL:CB	2.57	0.42
1:A:101:GLN:HB2	1:A:139:CYS:HB3	2.01	0.42
2:E:593:MET:HE1	9:E:5566:HOH:O	2.19	0.42
2:B:95[B]:MET:HE1	2:B:277:ALA:HB3	2.01	0.42
3:C:280:GLU:HG3	9:C:4283:HOH:O	2.18	0.42
2:B:176:LYS:HG2	2:B:180:HIS:ND1	2.34	0.42
2:E:121:VAL:HG11	2:E:132:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD12	9:B:4704:HOH:O	2.19	0.42
2:B:258:HIS:CD2	2:E:518:SER:HB2	2.55	0.42
2:B:389:SER:HB2	2:B:392:VAL:HB	2.01	0.42
2:B:713[B]:GLN:HE21	2:B:733[B]:LEU:HD23	1.85	0.42
2:B:175:ARG:NH1	2:B:178:HIS:O	2.53	0.42
2:B:127:TYR:HA	3:C:2:ILE:HG21	2.03	0.41
3:C:10:ARG:CZ	3:C:55[A]:ARG:HD3	2.51	0.41
2:B:303:GLU:HG2	9:B:4394:HOH:O	2.20	0.41
2:E:466:LYS:CE	9:E:5712:HOH:O	2.68	0.41
2:B:203:SER:O	2:B:319:GLU:HA	2.21	0.41
2:E:53:ASP:CG	2:E:54:PHE:H	2.24	0.41
2:E:764:SER:N	2:E:765:PRO:HD2	2.34	0.41
3:F:10:ARG:HD3	3:F:55:ARG:NH1	2.36	0.41
2:B:510:GLU:CG	2:B:647[A]:VAL:HG12	2.51	0.40
2:E:151:LYS:NZ	9:E:5468:HOH:O	2.54	0.40
2:E:52:GLY:HA2	2:E:121:VAL:O	2.19	0.40
2:B:713[A]:GLN:CG	2:B:731:PHE:CE1	3.04	0.40
2:E:573:THR:HB	2:E:574:PRO:HD3	2.04	0.40
2:E:164:ILE:HG13	2:E:165:LYS:HG2	2.04	0.40
9:A:4096:HOH:O	3:C:31:LEU:HD11	2.21	0.40
3:F:106[B]:ILE:HD13	8:F:4931:FAD:C8	2.52	0.40
1:A:54:LEU:C	1:A:54:LEU:HD23	2.42	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	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:CG2	2:B:254:GLY:O[4_477]	1.75	0.45
2:E:458:GLN:OE1	9:B:4741:HOH:O[4_577]	2.01	0.19
9:A:4083:HOH:O	9:E:5155:HOH:O[4_477]	2.12	0.08

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	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
1	D	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
2	B	826/809 (102%)	798 (97%)	24 (3%)	4 (0%)	34	8
2	E	807/809 (100%)	781 (97%)	23 (3%)	3 (0%)	39	12
3	C	293/288 (102%)	289 (99%)	4 (1%)	0	100	100
3	F	289/288 (100%)	285 (99%)	4 (1%)	0	100	100
All	All	2539/2526 (100%)	2471 (97%)	61 (2%)	7 (0%)	46	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	312	ARG
2	E	312	ARG
2	B	265	PRO
2	B	712	GLY
2	E	265	PRO
2	E	712	GLY
2	B	761	VAL

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	132/131 (101%)	131 (99%)	1 (1%)	86	62
1	D	132/131 (101%)	130 (98%)	2 (2%)	72	35
2	B	671/653 (103%)	653 (97%)	18 (3%)	52	12
2	E	654/653 (100%)	641 (98%)	13 (2%)	63	22
3	C	220/212 (104%)	216 (98%)	4 (2%)	66	27
3	F	216/212 (102%)	213 (99%)	3 (1%)	74	38
All	All	2025/1992 (102%)	1984 (98%)	41 (2%)	66	22

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
2	B	21[A]	MET
2	B	21[B]	MET
2	B	91	ASN
2	B	159	LEU
2	B	209	TYR
2	B	251[A]	LEU
2	B	251[B]	LEU
2	B	258	HIS
2	B	313	ASP
2	B	345[A]	CYS
2	B	345[B]	CYS
2	B	386	TYR
2	B	393	THR
2	B	442	ASN
2	B	458	GLN
2	B	488	GLU
2	B	507	ASP
2	B	530	GLN
3	C	26	GLU
3	C	45	LEU
3	C	87[A]	LEU
3	C	87[B]	LEU
1	D	155[A]	LYS
1	D	155[B]	LYS
2	E	65	LYS
2	E	176	LYS
2	E	209	TYR
2	E	313	ASP
2	E	386	TYR
2	E	393	THR
2	E	442	ASN
2	E	488	GLU
2	E	507	ASP
2	E	552[A]	MET
2	E	552[B]	MET
2	E	620	GLU
2	E	790	GLN
3	F	45	LEU
3	F	221	ASN
3	F	240	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	27	HIS
1	A	34	ASN
1	A	68	GLN
1	A	135	ASN
2	B	19	GLN
2	B	115	ASN
2	B	172	HIS
2	B	258	HIS
2	B	273	ASN
2	B	304	ASN
2	B	315	HIS
2	B	334	HIS
2	B	442	ASN
2	B	458	GLN
2	B	463	GLN
2	B	530	GLN
2	B	592	GLN
2	B	639	ASN
2	B	698	GLN
2	B	754	HIS
2	B	808	HIS
3	C	118	ASN
1	D	11	ASN
2	E	59	HIS
2	E	115	ASN
2	E	273	ASN
2	E	315	HIS
2	E	442	ASN
2	E	463	GLN
2	E	597	HIS
2	E	698	GLN
2	E	754	HIS
2	E	790	GLN
2	E	804	GLN
3	F	78	GLN
3	F	79	HIS
3	F	118	ASN
3	F	221	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

11 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	PO4	A	3001	-	4,4,4	1.26	1 (25%)	6,6,6	0.32	0
5	FES	A	3907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	A	3908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	MCN	B	3920	6	32,48,48	3.22	8 (25%)	39,74,74	1.56	5 (12%)
6	CUN	B	3921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	C	3932	-	48,58,58	1.62	8 (16%)	54,89,89	2.39	13 (24%)
5	FES	D	4907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	D	4908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	MCN	E	4920	6	32,48,48	2.92	9 (28%)	39,74,74	2.23	10 (25%)
6	CUN	E	4921	9,2,7	0,4,4	0.00	-	0,4,4	0.00	-
8	FAD	F	4931	-	48,58,58	1.44	9 (18%)	54,89,89	1.62	10 (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
4	PO4	A	3001	-	-	0/0/0/0	0/0/0/0
5	FES	A	3907	1	-	0/0/4/4	0/1/1/1
5	FES	A	3908	1	-	0/0/4/4	0/1/1/1
7	MCN	B	3920	6	-	0/18/54/54	0/5/5/5
6	CUN	B	3921	9,2,7	-	0/0/2/2	0/0/0/0
8	FAD	C	3932	-	-	0/30/50/50	0/6/6/6
5	FES	D	4907	1	-	0/0/4/4	0/1/1/1
5	FES	D	4908	1	-	0/0/4/4	0/1/1/1
7	MCN	E	4920	6	-	0/18/54/54	0/5/5/5
6	CUN	E	4921	9,2,7	-	0/0/2/2	0/0/0/0
8	FAD	F	4931	-	-	0/30/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3920	MCN	C6-C5	-5.13	1.26	1.38
8	F	4931	FAD	C10-N10	-3.48	1.35	1.39
8	F	4931	FAD	C6-C5X	-3.13	1.37	1.41
8	C	3932	FAD	C10-N10	-2.84	1.35	1.39
8	C	3932	FAD	O4B-C4B	-2.75	1.38	1.45
7	E	4920	MCN	O9'-C9'	-2.45	1.40	1.44
4	A	3001	PO4	P-O4	-2.32	1.45	1.53
8	F	4931	FAD	C3B-C4B	-2.08	1.47	1.53
7	B	3920	MCN	PB-O2B	-2.07	1.46	1.54
7	E	4920	MCN	O2'-C2D	-2.00	1.38	1.43
8	F	4931	FAD	O4-C4	2.02	1.29	1.24
8	C	3932	FAD	C2A-N3A	2.07	1.35	1.32
8	C	3932	FAD	C5X-N5	2.12	1.38	1.35
8	C	3932	FAD	C10-N1	2.20	1.39	1.35
8	F	4931	FAD	C4-N3	2.35	1.37	1.33
7	E	4920	MCN	C5-C4	2.45	1.46	1.40
7	E	4920	MCN	C4A-N5'	2.45	1.42	1.37
7	B	3920	MCN	C4'-N3'	2.54	1.43	1.36
8	F	4931	FAD	C5'-C4'	2.55	1.55	1.51
8	C	3932	FAD	O4B-C1B	2.89	1.44	1.41
7	B	3920	MCN	O9'-C9'	2.90	1.48	1.44
8	F	4931	FAD	C4X-N5	3.14	1.38	1.33
8	F	4931	FAD	C2A-N3A	3.31	1.38	1.32
7	E	4920	MCN	C2'-N3'	3.34	1.41	1.35
8	F	4931	FAD	C5X-N5	3.42	1.40	1.35
8	C	3932	FAD	C5'-C4'	3.63	1.57	1.51
7	E	4920	MCN	C6-N1	3.84	1.41	1.35
7	B	3920	MCN	C2'-N3'	4.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4920	MCN	C7-N8'	4.27	1.42	1.30
7	E	4920	MCN	O9'-C7	4.30	1.42	1.36
7	B	3920	MCN	C7-N8'	4.93	1.43	1.30
7	B	3920	MCN	O9'-C7	6.09	1.45	1.36
8	C	3932	FAD	C4X-N5	6.41	1.43	1.33
7	E	4920	MCN	C6'-N5'	12.74	1.48	1.32
7	B	3920	MCN	C6'-N5'	13.38	1.49	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	3932	FAD	N3A-C2A-N1A	-9.55	121.58	128.89
7	E	4920	MCN	N1'-C2'-N3'	-5.77	118.66	127.44
7	E	4920	MCN	C5-C4-N3	-5.48	114.88	121.80
8	C	3932	FAD	C4-C4X-C10	-4.80	116.87	119.94
8	C	3932	FAD	C4X-C4-N3	-3.32	119.05	123.59
8	C	3932	FAD	O4'-C4'-C5'	-3.16	103.30	110.19
7	B	3920	MCN	N1'-C2'-N3'	-2.76	123.23	127.44
8	F	4931	FAD	C4X-C4-N3	-2.65	119.96	123.59
7	E	4920	MCN	O3'-C3'-C2D	-2.57	103.48	111.83
8	F	4931	FAD	C9-C8-C7	-2.40	115.47	120.04
8	C	3932	FAD	C4A-C5A-N7A	-2.20	107.46	109.48
8	F	4931	FAD	O4'-C4'-C5'	-2.16	105.48	110.19
8	F	4931	FAD	N3A-C2A-N1A	-2.08	127.30	128.89
7	B	3920	MCN	O3'-C3'-C2D	-2.08	105.07	111.83
8	C	3932	FAD	C9A-C5X-N5	-2.03	119.35	122.36
8	F	4931	FAD	C4B-O4B-C1B	2.05	111.97	109.72
8	C	3932	FAD	C1'-N10-C9A	2.08	121.19	118.86
8	F	4931	FAD	C4-C4X-N5	2.19	121.38	118.72
8	C	3932	FAD	C6-C5X-C9A	2.22	121.90	118.98
7	B	3920	MCN	N2'-C2'-N1'	2.23	122.08	117.80
7	B	3920	MCN	C2-N3-C4	2.32	118.88	115.61
8	C	3932	FAD	C4B-O4B-C1B	2.42	112.38	109.72
8	C	3932	FAD	C4-C4X-N5	2.48	121.73	118.72
7	E	4920	MCN	C4D-O4D-C1'	2.53	112.50	109.72
7	E	4920	MCN	C2'-N3'-C4'	2.60	122.99	116.50
7	E	4920	MCN	N2'-C2'-N1'	2.83	123.23	117.80
7	E	4920	MCN	C7-N8'-C4B	2.84	119.45	116.63
7	E	4920	MCN	N4-C4-N3	3.27	122.47	116.50
8	F	4931	FAD	C1'-N10-C9A	3.30	122.57	118.86
7	E	4920	MCN	O4'-C4'-C4A	3.40	126.09	119.85
8	F	4931	FAD	C4X-C10-N10	3.46	122.56	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	4931	FAD	C5X-C9A-N10	3.54	120.31	117.62
8	C	3932	FAD	C2A-N1A-C6A	3.56	125.13	118.77
8	C	3932	FAD	C5X-C9A-N10	4.03	120.68	117.62
7	B	3920	MCN	O4'-C4'-C4A	5.38	129.72	119.85
8	F	4931	FAD	C4-N3-C2	5.91	120.35	115.25
7	E	4920	MCN	C2-N3-C4	6.96	125.44	115.61
8	C	3932	FAD	C4-N3-C2	8.92	122.96	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	PO4	1	0
6	B	3921	CUN	1	0
8	C	3932	FAD	2	0
8	F	4931	FAD	3	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.