Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:02 PM GMT

PDB ID	:	1N60
Title	:	Crystal Structure of the Cu,Mo-CO Dehydrogenase (CODH); Cyanide-inactivated Form
Authors	:	Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on	:	2002-11-08
Resolution	:	1.19 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:

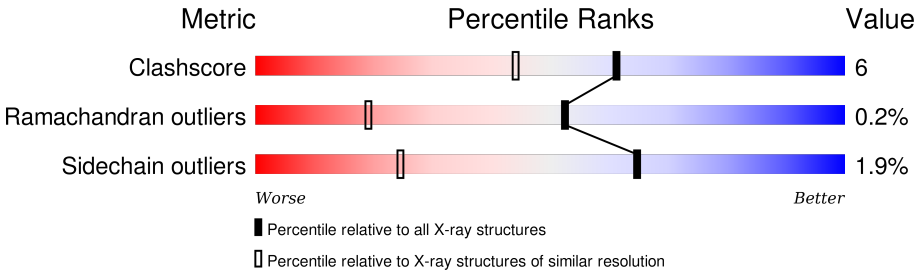
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.19 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	1607 (1.26-1.14)
Ramachandran outliers	100387	1540 (1.26-1.14)
Sidechain outliers	100360	1538 (1.26-1.14)

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	87% 10% • •
1	D	166	84% 11% • 5%
2	B	809	87% 11% ••
2	E	809	87% 10% • •
3	C	288	86% 12% •••
3	F	288	92% 6% • •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22712 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	161	Total	C	N	O	S	9	7	0
			1230	762	219	231	18			
1	D	158	Total	C	N	O	S	7	6	0
			1200	743	216	223	18			

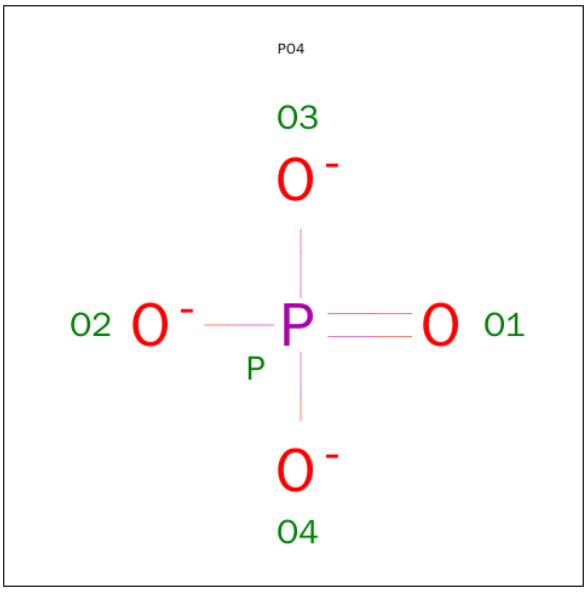
- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	803	Total	C	N	O	S	75	17	0
			6257	3976	1068	1165	48			
2	E	796	Total	C	N	O	S	66	16	0
			6201	3947	1058	1149	47			

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

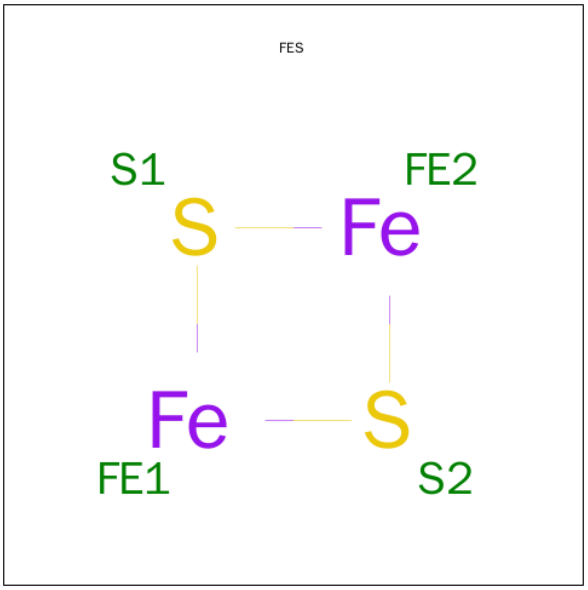
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	33	9	0
			2134	1348	374	400	12			
3	F	286	Total	C	N	O	S	35	7	0
			2123	1341	370	400	12			

- 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
4	E	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

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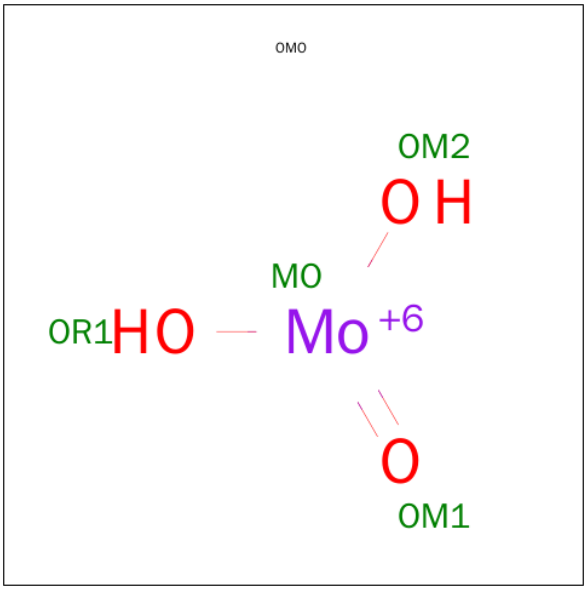
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Fe S 4 2 2	0	0
5	D	1	Total Fe S 4 2 2	0	0

- Molecule 6 is MO(VI)(=O)(OH)2 CLUSTER (three-letter code: OMO) (formula: H_2MoO_3).

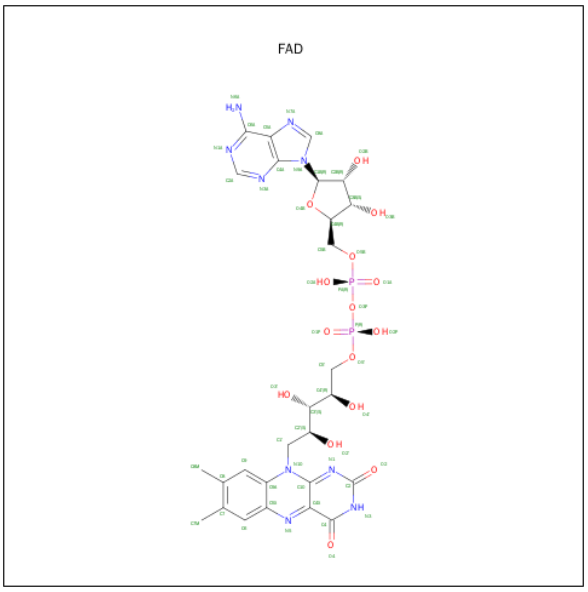


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mo O 4 1 3	0	0
6	E	1	Total Mo O 4 1 3	0	0

- 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	229	Total	O	0	0
			229	229		
9	B	1085	Total	O	0	0
			1085	1085		
9	C	420	Total	O	0	0
			420	420		
9	D	226	Total	O	0	0
			226	226		
9	E	1000	Total	O	0	0
			1000	1000		
9	F	379	Total	O	0	0
			379	379		

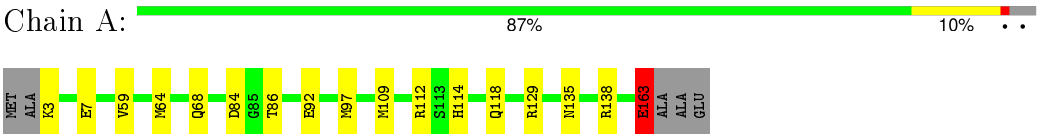
3 Residue-property plots (i)

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.

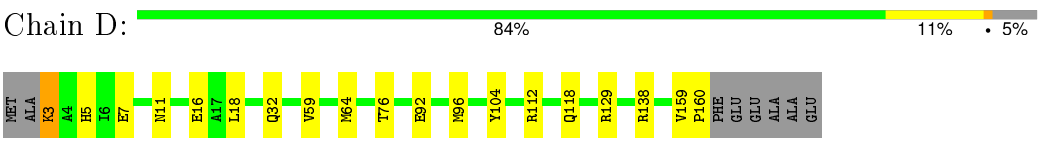
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A:



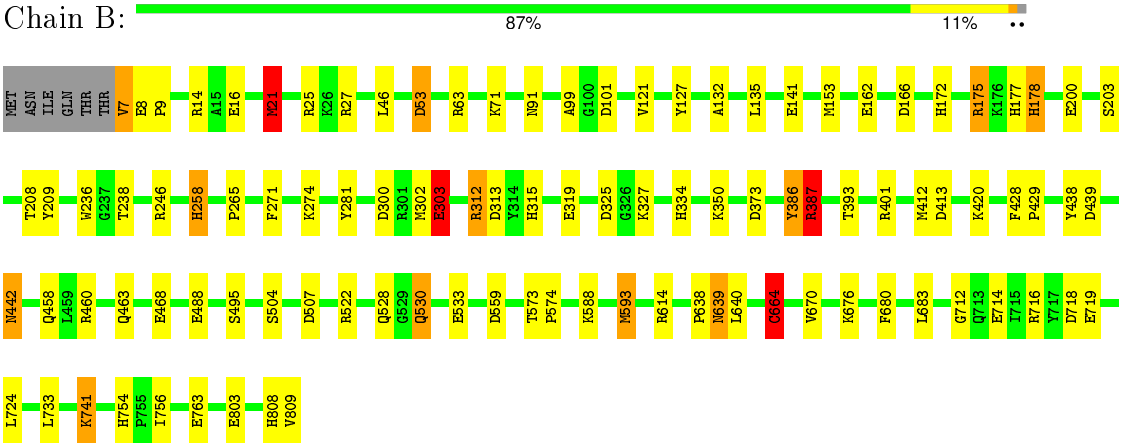
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:



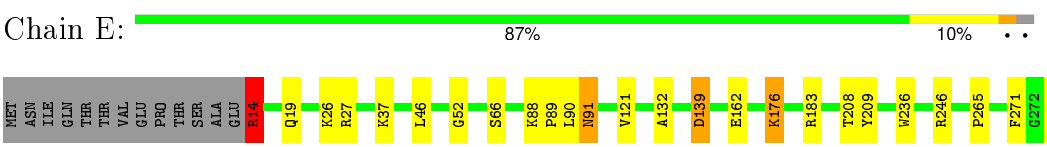
- Molecule 2: Carbon monoxide dehydrogenase large chain

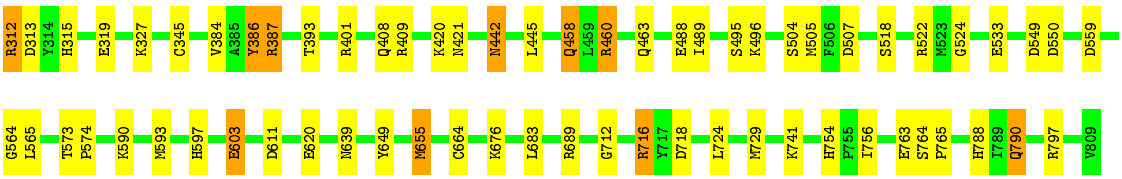
Chain B:



- Molecule 2: Carbon monoxide dehydrogenase large chain

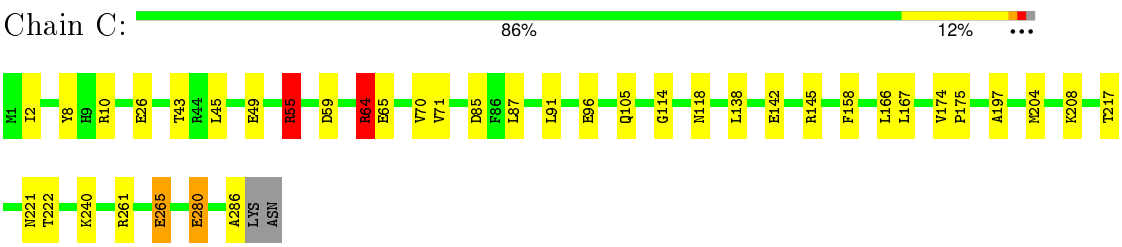
Chain E:





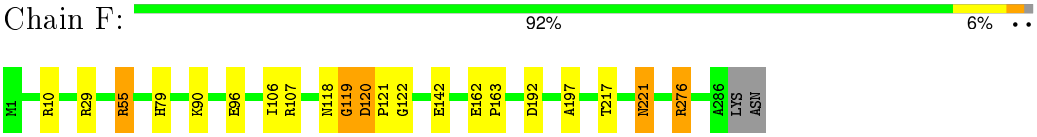
• Molecule 3: Carbon monoxide dehydrogenase medium chain

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	118.57Å 130.64Å 158.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.80 – 1.19	Depositor
% Data completeness (in resolution range)	(Not available) (17.80-1.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.171	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22712	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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, OMO, FES, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.39	7/1281 (0.5%)	1.16	11/1729 (0.6%)
1	D	1.13	4/1245 (0.3%)	0.95	3/1680 (0.2%)
2	B	1.34	23/6483 (0.4%)	1.11	41/8792 (0.5%)
2	E	1.09	16/6423 (0.2%)	1.05	29/8705 (0.3%)
3	C	1.42	8/2207 (0.4%)	1.10	16/2996 (0.5%)
3	F	0.97	4/2188 (0.2%)	0.98	4/2969 (0.1%)
All	All	1.23	62/19827 (0.3%)	1.07	104/26871 (0.4%)

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	3
1	D	0	1
2	B	0	5
2	E	0	4
3	C	0	1
All	All	0	14

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	141	GLU	CD-OE1	44.88	1.75	1.25
3	C	265	GLU	CD-OE2	40.81	1.70	1.25
2	B	200	GLU	CG-CD	30.30	1.97	1.51
1	A	163	GLU	CG-CD	23.00	1.86	1.51
2	B	200	GLU	CD-OE2	22.87	1.50	1.25
2	B	639	ASN	CG-ND2	-20.80	0.80	1.32
2	E	620	GLU	CG-CD	19.52	1.81	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3	LYS	CE-NZ	18.14	1.94	1.49
1	A	92	GLU	CD-OE2	-17.69	1.06	1.25
3	C	65	GLU	CD-OE2	-17.46	1.06	1.25
1	A	92	GLU	CD-OE1	16.99	1.44	1.25
3	C	49	GLU	CD-OE2	-15.85	1.08	1.25
2	B	741	LYS	CD-CE	13.95	1.86	1.51
2	B	141	GLU	CG-CD	-13.68	1.31	1.51
2	E	37	LYS	CE-NZ	13.62	1.83	1.49
2	E	176	LYS	CE-NZ	-13.39	1.15	1.49
2	E	664	CYS	CB-SG	-12.20	1.61	1.82
2	B	809	VAL	CB-CG2	-11.96	1.27	1.52
2	E	14	ARG	CD-NE	11.15	1.65	1.46
2	B	162	GLU	CD-OE2	-10.11	1.14	1.25
2	B	458	GLN	CG-CD	10.09	1.74	1.51
2	E	91	ASN	CB-CG	8.82	1.71	1.51
3	C	142	GLU	CG-CD	8.63	1.64	1.51
2	E	533	GLU	CD-OE2	8.41	1.34	1.25
1	A	163	GLU	CA-CB	8.24	1.72	1.53
1	D	16	GLU	CG-CD	-8.09	1.39	1.51
2	E	664	CYS	CA-CB	8.08	1.71	1.53
2	E	91	ASN	CG-ND2	7.70	1.52	1.32
3	F	55	ARG	CG-CD	7.36	1.70	1.51
2	B	303	GLU	CD-OE2	7.20	1.33	1.25
2	B	533	GLU	CD-OE2	7.17	1.33	1.25
2	B	16	GLU	CG-CD	7.12	1.62	1.51
1	A	163	GLU	CD-OE2	6.95	1.33	1.25
3	C	158	PHE	CD2-CE2	6.87	1.52	1.39
2	E	319	GLU	CD-OE1	-6.86	1.18	1.25
2	E	676	LYS	CE-NZ	6.71	1.65	1.49
3	C	280	GLU	CG-CD	-6.70	1.41	1.51
2	B	664[A]	CYS	CB-SG	6.69	1.93	1.82
2	B	664[B]	CYS	CB-SG	6.69	1.93	1.82
1	D	7	GLU	CD-OE2	-6.50	1.18	1.25
2	B	676	LYS	CE-NZ	6.50	1.65	1.49
2	E	66	SER	CB-OG	-6.33	1.34	1.42
2	E	729[A]	MET	SD-CE	-6.18	1.43	1.77
2	E	729[B]	MET	SD-CE	-6.18	1.43	1.77
2	B	8	GLU	CG-CD	-6.17	1.42	1.51
2	E	420	LYS	CD-CE	6.14	1.66	1.51
1	A	97	MET	SD-CE	-5.90	1.44	1.77
2	B	719	GLU	CB-CG	-5.80	1.41	1.52
3	C	158	PHE	CG-CD2	5.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	104	TYR	CE2-CZ	-5.60	1.31	1.38
3	C	96	GLU	CD-OE2	-5.58	1.19	1.25
2	B	468	GLU	CD-OE1	-5.58	1.19	1.25
2	B	63[A]	ARG	CB-CG	-5.45	1.37	1.52
2	B	63[B]	ARG	CB-CG	-5.45	1.37	1.52
1	A	7	GLU	CD-OE1	5.28	1.31	1.25
2	B	638	PRO	CA-CB	-5.27	1.43	1.53
3	F	96	GLU	CD-OE2	-5.20	1.20	1.25
2	E	603	GLU	CD-OE2	5.19	1.31	1.25
3	F	119	GLY	C-O	-5.19	1.15	1.23
2	B	593	MET	SD-CE	-5.12	1.49	1.77
2	B	8	GLU	CB-CG	5.10	1.61	1.52
3	F	276	ARG	CB-CG	-5.02	1.39	1.52

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	303	GLU	OE1-CD-OE2	-18.14	101.53	123.30
2	B	63[A]	ARG	NE-CZ-NH1	-16.02	112.29	120.30
2	B	63[B]	ARG	NE-CZ-NH1	-16.02	112.29	120.30
1	A	163	GLU	CB-CA-C	-15.35	79.70	110.40
1	A	109[A]	MET	CG-SD-CE	13.20	121.32	100.20
1	A	109[B]	MET	CG-SD-CE	13.20	121.32	100.20
3	C	49	GLU	OE1-CD-OE2	-11.60	109.38	123.30
3	C	265	GLU	CG-CD-OE2	-11.53	95.25	118.30
2	B	175	ARG	NE-CZ-NH2	-11.25	114.68	120.30
2	E	689	ARG	NE-CZ-NH2	-10.98	114.81	120.30
2	E	716	ARG	NE-CZ-NH2	10.86	125.73	120.30
2	B	63[A]	ARG	NE-CZ-NH2	10.72	125.66	120.30
2	B	63[B]	ARG	NE-CZ-NH2	10.72	125.66	120.30
2	E	401	ARG	NE-CZ-NH1	9.98	125.29	120.30
2	E	620	GLU	CG-CD-OE2	-9.95	98.40	118.30
3	C	158	PHE	CB-CG-CD1	9.84	127.69	120.80
2	B	175	ARG	NE-CZ-NH1	9.74	125.17	120.30
2	E	716	ARG	NE-CZ-NH1	-9.64	115.48	120.30
2	E	620	GLU	CG-CD-OE1	9.54	137.37	118.30
1	A	163	GLU	OE1-CD-OE2	-9.51	111.89	123.30
2	E	14	ARG	NE-CZ-NH1	-9.01	115.79	120.30
3	F	29	ARG	NE-CZ-NH2	-8.91	115.85	120.30
2	B	14	ARG	NE-CZ-NH2	-8.90	115.85	120.30
2	B	664[A]	CYS	CA-CB-SG	8.87	129.96	114.00
2	B	664[B]	CYS	CA-CB-SG	8.87	129.96	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	176	LYS	CD-CE-NZ	8.73	131.79	111.70
2	E	620	GLU	CB-CG-CD	-8.66	90.83	114.20
2	B	200	GLU	OE1-CD-OE2	8.60	133.62	123.30
1	D	3	LYS	CD-CE-NZ	-8.59	91.95	111.70
2	B	200	GLU	CB-CG-CD	-8.53	91.17	114.20
2	B	8	GLU	CB-CG-CD	8.52	137.19	114.20
2	B	8	GLU	OE1-CD-OE2	-8.11	113.56	123.30
1	A	163	GLU	CA-CB-CG	8.00	130.99	113.40
2	B	141	GLU	CG-CD-OE2	7.79	133.89	118.30
3	F	107	ARG	NE-CZ-NH1	7.53	124.07	120.30
2	E	611	ASP	CB-CG-OD2	7.51	125.06	118.30
2	B	141	GLU	CG-CD-OE1	-7.30	103.70	118.30
3	C	55	ARG	NE-CZ-NH1	-7.23	116.69	120.30
3	C	145	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	B	63[A]	ARG	CD-NE-CZ	7.19	133.66	123.60
2	B	63[B]	ARG	CD-NE-CZ	7.19	133.66	123.60
3	C	64[A]	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	C	64[B]	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	E	91	ASN	CB-CG-ND2	7.11	133.75	116.70
2	B	614	ARG	NE-CZ-NH1	6.80	123.70	120.30
3	C	158	PHE	CB-CG-CD2	-6.74	116.08	120.80
1	A	163	GLU	N-CA-CB	6.64	122.55	110.60
2	B	246	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	B	387	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	D	129	ARG	NE-CZ-NH1	6.55	123.57	120.30
3	C	64[A]	ARG	NE-CZ-NH2	-6.51	117.05	120.30
3	C	64[B]	ARG	NE-CZ-NH2	-6.51	117.05	120.30
2	E	716	ARG	CD-NE-CZ	6.47	132.66	123.60
2	B	559	ASP	CB-CG-OD1	6.45	124.10	118.30
2	B	281	TYR	CB-CG-CD1	6.38	124.83	121.00
2	B	53	ASP	CB-CG-OD1	6.37	124.04	118.30
2	B	386	TYR	CB-CG-CD1	6.32	124.79	121.00
2	E	386	TYR	CB-CG-CD1	6.32	124.79	121.00
2	B	413	ASP	CB-CG-OD2	6.31	123.98	118.30
2	E	797	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	E	14	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	129	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	E	460	ARG	NE-CZ-NH2	-6.18	117.21	120.30
3	C	166	LEU	CB-CG-CD1	-6.15	100.54	111.00
2	E	401	ARG	NE-CZ-NH2	-6.15	117.22	120.30
2	B	303	GLU	CG-CD-OE2	6.04	130.38	118.30
2	E	559	ASP	CB-CG-OD1	5.98	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	246	ARG	NE-CZ-NH1	5.95	123.28	120.30
2	B	166	ASP	CB-CG-OD2	5.93	123.64	118.30
2	B	101	ASP	CB-CG-OD1	5.91	123.62	118.30
2	E	91	ASN	CA-CB-CG	-5.83	100.57	113.40
2	E	409	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	112	ARG	NE-CZ-NH1	5.77	123.19	120.30
2	B	401	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	E	649	TYR	CB-CG-CD1	5.65	124.39	121.00
2	B	63[A]	ARG	CG-CD-NE	5.62	123.61	111.80
2	B	63[B]	ARG	CG-CD-NE	5.62	123.61	111.80
3	C	261	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	387	ARG	NE-CZ-NH2	-5.62	117.49	120.30
3	C	59	ASP	CB-CG-OD1	5.61	123.35	118.30
2	B	281	TYR	CB-CG-CD2	-5.58	117.66	121.00
2	E	139	ASP	CB-CG-OD2	5.52	123.27	118.30
3	F	120	ASP	CB-CG-OD1	5.51	123.26	118.30
2	E	550	ASP	CB-CG-OD1	5.49	123.24	118.30
3	C	55	ARG	NH1-CZ-NH2	5.49	125.44	119.40
2	B	438	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	92	GLU	CG-CD-OE1	-5.40	107.49	118.30
2	E	37	LYS	CD-CE-NZ	-5.37	99.35	111.70
2	E	14	ARG	N-CA-CB	-5.34	100.98	110.60
3	F	29	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	B	162	GLU	OE1-CD-OE2	5.28	129.64	123.30
2	E	689	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	25	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	97	MET	CG-SD-CE	-5.20	91.88	100.20
1	A	112	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	B	21[A]	MET	CG-SD-CE	-5.15	91.97	100.20
2	B	21[B]	MET	CG-SD-CE	-5.15	91.97	100.20
1	D	112	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	E	246	ARG	NE-CZ-NH2	-5.11	117.75	120.30
3	C	59	ASP	CB-CA-C	-5.09	100.23	110.40
3	C	142	GLU	CB-CG-CD	-5.08	100.48	114.20
2	B	439	ASP	CB-CG-OD1	5.07	122.87	118.30
2	E	655[A]	MET	CG-SD-CE	-5.03	92.16	100.20
2	E	655[B]	MET	CG-SD-CE	-5.03	92.16	100.20

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	HIS	Sidechain
1	A	138	ARG	Sidechain
1	A	163	GLU	Sidechain
2	B	178	HIS	Sidechain
2	B	27	ARG	Sidechain
2	B	303	GLU	Sidechain
2	B	312	ARG	Sidechain
2	B	387	ARG	Sidechain
3	C	265	GLU	Sidechain
1	D	138	ARG	Sidechain
2	E	14	ARG	Sidechain
2	E	27	ARG	Sidechain
2	E	312	ARG	Sidechain
2	E	387	ARG	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	1230	0	1208	16	1
1	D	1200	0	1190	18	0
2	B	6257	0	6135	66	0
2	E	6201	0	6101	64	0
3	C	2134	0	2187	26	0
3	F	2123	0	2171	25	0
4	A	5	0	0	0	0
4	E	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	4	0	0	1	0
6	E	4	0	0	1	0
7	B	44	0	17	1	0
7	E	44	0	17	1	0
8	C	53	0	31	1	0
8	F	53	0	31	3	0
9	A	229	0	0	5	0
9	B	1085	0	0	18	3
9	C	420	0	0	6	1
9	D	226	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	1000	0	0	23	3
9	F	379	0	0	13	0
All	All	22712	0	19088	210	4

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 6.

All (210) 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)
2:E:593[B]:MET:HG2	2:E:603:GLU:OE2	1.18	1.28
2:E:593[A]:MET:HG2	2:E:603:GLU:OE2	1.15	1.26
2:B:236[B]:TRP:CZ2	9:B:6002:HOH:O	1.63	1.25
2:B:236[B]:TRP:CH2	9:B:6002:HOH:O	1.73	1.21
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	1.80	1.12
1:A:59:VAL:HG11	1:A:64[A]:MET:HE1	1.33	1.09
3:F:120:ASP:OD2	3:F:121:PRO:HD2	1.55	1.04
1:D:59:VAL:HG11	1:D:64[A]:MET:CE	1.89	1.02
1:D:118[A]:GLN:OE1	9:D:6025:HOH:O	1.77	1.02
1:D:32:GLN:HG3	9:D:6114:HOH:O	1.60	0.99
1:D:92:GLU:HG3	9:D:6061:HOH:O	1.61	0.99
1:D:59:VAL:HG11	1:D:64[A]:MET:HE1	1.47	0.95
1:D:92:GLU:HG3	9:D:6125:HOH:O	1.66	0.95
2:E:593[A]:MET:CG	2:E:603:GLU:OE2	2.12	0.95
1:D:118[A]:GLN:NE2	9:D:5974:HOH:O	1.97	0.95
1:A:163:GLU:C	9:A:5137:HOH:O	2.06	0.94
2:E:327[B]:LYS:NZ	9:E:6499:HOH:O	2.03	0.91
1:D:11:ASN:HD21	1:D:76:THR:H	1.19	0.90
3:F:118:ASN:O	9:F:6309:HOH:O	1.90	0.88
2:E:639:ASN:OD1	9:E:6750:HOH:O	1.91	0.88
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.22	0.88
1:A:3:LYS:N	9:A:5002:HOH:O	2.06	0.87
1:D:3:LYS:N	9:D:6112:HOH:O	2.06	0.87
2:B:528:GLN:H	2:B:530:GLN:HE22	1.21	0.87
2:E:408:GLN:NE2	9:E:6880:HOH:O	2.08	0.85
2:E:208:THR:H	2:E:790:GLN:HE22	1.19	0.85
3:F:120:ASP:OD2	3:F:121:PRO:CD	2.24	0.85
3:C:64[A]:ARG:HD2	3:C:71:VAL:O	1.78	0.84
3:F:119:GLY:HA3	9:F:6309:HOH:O	1.79	0.83
2:E:593[B]:MET:CG	2:E:603:GLU:OE2	2.14	0.81
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:ASP:HB2	2:B:303:GLU:OE1	1.82	0.80
2:B:716:ARG:NH1	9:B:5328:HOH:O	2.11	0.80
1:A:59:VAL:CG1	1:A:64[A]:MET:CE	2.59	0.79
2:E:716:ARG:CZ	9:E:6749:HOH:O	2.30	0.78
1:D:59:VAL:HG11	1:D:64[A]:MET:HE3	1.64	0.77
2:E:716:ARG:NH1	9:E:6749:HOH:O	2.19	0.75
3:C:55:ARG:HD3	9:C:5133:HOH:O	1.86	0.74
2:E:716:ARG:NE	9:E:6749:HOH:O	2.21	0.74
2:E:327[B]:LYS:HD3	9:E:6247:HOH:O	1.87	0.73
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.36	0.73
1:A:59:VAL:HG11	1:A:64[A]:MET:HE3	1.67	0.73
2:B:46:LEU:HD11	2:B:236[B]:TRP:CZ3	2.23	0.72
1:A:68:GLN:HE21	3:C:55:ARG:HH22	1.39	0.70
3:C:85:ASP:OD1	9:C:5329:HOH:O	2.07	0.70
2:B:528:GLN:H	2:B:530:GLN:NE2	1.89	0.69
2:E:754:HIS:HD2	2:E:756:ILE:H	1.41	0.69
2:E:88:LYS:HB2	2:E:89:PRO:HD3	1.75	0.69
1:D:59:VAL:CG1	1:D:64[A]:MET:CE	2.69	0.69
2:B:588:LYS:HD2	9:B:5252:HOH:O	1.92	0.68
3:F:221:ASN:ND2	9:F:6097:HOH:O	2.26	0.68
2:B:716:ARG:NH1	9:B:5280:HOH:O	2.27	0.68
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.78	0.67
2:B:71:LYS:HE3	2:B:135:LEU:O	1.94	0.66
2:B:327:LYS:HG2	2:B:420:LYS:HE3	1.76	0.66
2:E:458:GLN:HE21	2:E:458:GLN:H	1.45	0.63
2:B:530:GLN:HE21	2:B:530:GLN:H	1.46	0.63
2:E:495:SER:CB	2:E:504[A]:SER:OG	2.47	0.62
1:A:59:VAL:CG1	1:A:64[A]:MET:HE1	2.21	0.62
2:B:754:HIS:HD2	2:B:756:ILE:H	1.47	0.62
1:D:159:VAL:HB	1:D:160:PRO:HD3	1.80	0.62
6:B:4921:OMO:MO	6:B:4921:OMO:OM1	1.70	0.61
2:B:7:VAL:HG13	2:B:9:PRO:HD3	1.83	0.61
1:A:84:ASP:OD1	1:A:86:THR:HG23	2.00	0.61
3:C:280:GLU:HG3	9:C:5089:HOH:O	2.00	0.61
1:D:59:VAL:CG1	1:D:64[A]:MET:HE3	2.28	0.61
2:B:522:ARG:NH1	9:B:6001:HOH:O	2.30	0.60
1:A:118[A]:GLN:NE2	9:A:5128:HOH:O	2.34	0.60
2:E:46:LEU:HD11	2:E:236[B]:TRP:CZ3	2.37	0.60
2:B:236[B]:TRP:HZ2	9:B:6002:HOH:O	1.29	0.60
2:B:670:VAL:O	2:B:808:HIS:HE1	1.84	0.60
3:F:120:ASP:CG	3:F:122:GLY:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:5921:OMO:MO	6:E:5921:OMO:OM1	1.72	0.59
2:E:489:ILE:HG12	2:E:655[A]:MET:HE2	1.83	0.59
2:B:716:ARG:NH2	9:B:5328:HOH:O	2.35	0.58
2:E:593[B]:MET:HG2	2:E:603:GLU:CD	2.18	0.58
2:B:236[B]:TRP:HH2	9:B:6002:HOH:O	1.45	0.57
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.51	0.57
1:A:59:VAL:CG1	1:A:64[A]:MET:HE3	2.30	0.57
1:D:92:GLU:CG	9:D:6125:HOH:O	2.37	0.57
2:E:754:HIS:CD2	2:E:756:ILE:H	2.22	0.57
2:E:327[B]:LYS:HG2	9:E:6761:HOH:O	2.05	0.56
1:A:135:ASN:ND2	3:C:105:GLN:HE22	2.03	0.56
2:B:334:HIS:HE1	2:B:373:ASP:OD2	1.87	0.56
2:B:639:ASN:CA	2:B:639:ASN:ND2	2.69	0.56
3:F:120:ASP:OD2	3:F:121:PRO:N	2.40	0.55
1:A:163:GLU:CA	9:A:5137:HOH:O	2.50	0.55
2:B:172:HIS:HD2	9:B:5633:HOH:O	1.88	0.55
2:E:327[B]:LYS:CD	9:E:6761:HOH:O	2.54	0.55
2:B:716:ARG:CZ	9:B:5328:HOH:O	2.52	0.55
2:E:741:LYS:CE	9:E:6574:HOH:O	2.55	0.55
2:E:741:LYS:NZ	9:E:6574:HOH:O	2.22	0.54
2:E:327[B]:LYS:HD3	9:E:6761:HOH:O	2.07	0.54
3:C:10:ARG:CZ	3:C:55:ARG:HD2	2.38	0.54
3:C:64[A]:ARG:NH1	9:C:5146:HOH:O	2.40	0.54
1:A:68:GLN:HE21	3:C:55:ARG:NH2	2.04	0.53
2:B:754:HIS:CD2	2:B:756:ILE:H	2.26	0.53
2:E:208:THR:OG1	2:E:315:HIS:HD2	1.90	0.53
3:F:10:ARG:CZ	9:F:6047:HOH:O	2.57	0.52
2:E:327[B]:LYS:HE2	2:E:421:ASN:OD1	2.10	0.52
2:B:302:MET:HB3	9:B:5769:HOH:O	2.10	0.52
2:E:593[A]:MET:HG2	2:E:603:GLU:CD	2.21	0.51
2:E:788:HIS:HE2	2:E:790:GLN:NE2	2.08	0.51
2:B:442:ASN:C	2:B:442:ASN:HD22	2.13	0.51
3:F:192:ASP:OD2	9:F:6121:HOH:O	2.19	0.51
3:F:10:ARG:NH1	9:F:6260:HOH:O	2.26	0.50
2:B:593:MET:HE2	2:B:640:LEU:HD21	1.92	0.50
2:B:350:LYS:HE3	9:B:5658:HOH:O	2.11	0.50
3:C:118:ASN:HD22	8:C:4932:FAD:H4B	1.75	0.49
3:F:90:LYS:HE2	9:F:6184:HOH:O	2.12	0.49
3:C:138:LEU:HD23	3:C:167:LEU:HA	1.95	0.49
2:B:460:ARG:NH1	2:B:463:GLN:HE22	2.01	0.49
2:E:327[B]:LYS:CG	9:E:6761:HOH:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:HIS:HD2	9:F:6199:HOH:O	1.95	0.49
2:B:175:ARG:NH2	2:B:178:HIS:O	2.45	0.49
3:F:221:ASN:N	3:F:221:ASN:HD22	2.11	0.49
3:C:114:GLY:O	3:C:118:ASN:HB2	2.13	0.48
2:E:445:LEU:HD22	9:E:6244:HOH:O	2.13	0.48
2:B:530:GLN:NE2	2:B:530:GLN:H	2.11	0.48
2:E:315:HIS:HE1	9:E:6042:HOH:O	1.97	0.48
2:B:208:THR:OG1	2:B:315:HIS:HD2	1.95	0.48
2:E:495:SER:HB3	2:E:504[A]:SER:OG	2.13	0.48
3:C:10:ARG:NH2	3:C:55:ARG:HD2	2.29	0.48
2:B:593:MET:CE	2:B:640:LEU:HD21	2.44	0.47
2:E:19:GLN:NE2	9:E:6303:HOH:O	2.47	0.47
2:B:495:SER:CB	2:B:504[A]:SER:OG	2.62	0.47
3:F:120:ASP:CG	9:F:6282:HOH:O	2.52	0.47
2:B:127:TYR:HA	3:C:2:ILE:HG21	1.97	0.47
2:E:183:ARG:HD2	9:E:6379:HOH:O	2.13	0.47
3:C:43:THR:HG21	9:C:5088:HOH:O	2.14	0.47
2:B:639:ASN:CA	2:B:639:ASN:HD22	2.28	0.47
2:B:387:ARG:HA	2:B:763:GLU:HG2	1.96	0.47
2:E:14:ARG:N	9:E:6916:HOH:O	2.48	0.47
3:F:197:ALA:HB3	3:F:217:THR:HB	1.96	0.47
2:B:46:LEU:HD11	2:B:236[B]:TRP:CH2	2.50	0.46
2:B:53:ASP:OD2	9:B:5865:HOH:O	2.20	0.46
2:E:590:LYS:HA	2:E:593[A]:MET:HE2	1.98	0.46
2:E:208:THR:H	2:E:790:GLN:NE2	1.99	0.46
3:C:8:TYR:OH	3:C:10:ARG:HD3	2.15	0.46
2:E:442:ASN:C	2:E:442:ASN:HD22	2.18	0.46
2:E:597:HIS:HD2	9:E:6565:HOH:O	1.99	0.46
2:B:258:HIS:HE1	2:E:549:ASP:O	1.98	0.46
3:F:118:ASN:HD22	8:F:5931:FAD:H4B	1.80	0.46
2:B:714:GLU:OE2	2:B:716:ARG:NH1	2.48	0.46
2:B:334:HIS:HD2	9:B:5195:HOH:O	1.99	0.46
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.64	0.46
3:F:120:ASP:CB	9:F:6282:HOH:O	2.64	0.45
2:B:21[A]:MET:HE2	2:B:21[A]:MET:HB3	1.89	0.45
2:B:153:MET:HA	2:B:177:HIS:CE1	2.52	0.45
2:E:52:GLY:HA2	2:E:121:VAL:O	2.16	0.45
2:B:99:ALA:O	2:B:172:HIS:HE1	2.00	0.45
3:C:204[A]:MET:HG3	3:C:286:ALA:CB	2.47	0.44
2:E:593[A]:MET:HE1	9:E:6586:HOH:O	2.16	0.44
2:E:522:ARG:NH1	9:E:6666:HOH:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:ASP:O	2:B:420:LYS:HE2	2.17	0.44
3:F:162:GLU:HB3	3:F:163:PRO:HD2	1.99	0.44
2:E:573:THR:O	2:E:754:HIS:HE1	1.99	0.44
2:B:258:HIS:CD2	2:E:518:SER:HB2	2.52	0.44
2:B:573:THR:HB	2:B:574:PRO:HD3	2.00	0.44
3:F:118:ASN:C	9:F:6309:HOH:O	2.44	0.44
3:F:221:ASN:HD22	3:F:221:ASN:H	1.66	0.44
2:E:26[A]:LYS:NZ	9:E:6672:HOH:O	2.51	0.44
2:E:445:LEU:C	2:E:445:LEU:HD13	2.38	0.44
2:B:238:THR:HB	2:B:274:LYS:HD3	2.00	0.44
1:A:64[A]:MET:HB2	1:A:64[A]:MET:HE2	1.84	0.43
9:A:5132:HOH:O	2:B:741:LYS:HD3	2.18	0.43
2:B:203:SER:O	2:B:319:GLU:HA	2.19	0.43
3:F:276:ARG:NH2	9:F:6142:HOH:O	2.49	0.43
2:B:428:PHE:HA	2:B:429:PRO:C	2.39	0.43
2:B:7:VAL:HA	9:B:5455:HOH:O	2.18	0.43
2:B:315:HIS:HE1	9:B:5008:HOH:O	2.01	0.43
3:C:286:ALA:C	9:C:5229:HOH:O	2.57	0.43
2:E:524:GLY:HA3	2:E:564:GLY:HA3	2.01	0.43
2:E:345:CYS:SG	2:E:384:VAL:HG23	2.59	0.43
2:B:733:LEU:HA	2:B:733:LEU:HD23	1.83	0.43
2:E:683:LEU:HD23	2:E:683:LEU:C	2.39	0.43
3:C:70:VAL:HG23	3:C:174:VAL:HG22	2.00	0.42
2:E:573:THR:HB	2:E:574:PRO:HD3	2.01	0.42
2:E:505:MET:HA	2:E:565:LEU:HG	2.00	0.42
1:D:5:HIS:HA	1:D:18:LEU:HD23	2.01	0.42
3:C:91:LEU:HD21	3:C:175:PRO:HD3	2.00	0.42
3:C:197:ALA:HB3	3:C:217:THR:HB	2.02	0.42
2:E:764:SER:N	2:E:765:PRO:HD2	2.33	0.42
1:D:92:GLU:CD	9:D:6120:HOH:O	2.58	0.42
2:E:489:ILE:HD11	2:E:655[A]:MET:HG3	2.01	0.42
2:E:271:PHE:HA	7:E:5920:MCN:S7'	2.60	0.42
2:E:162:GLU:OE2	9:E:6442:HOH:O	2.21	0.42
2:E:718:ASP:HB3	2:E:724:LEU:HD11	2.02	0.42
2:B:714:GLU:OE1	2:B:716:ARG:HD3	2.19	0.42
3:F:10:ARG:NE	9:F:6047:HOH:O	2.52	0.42
2:B:412[B]:MET:HE2	9:B:5930:HOH:O	2.20	0.41
2:B:271:PHE:HA	7:B:4920:MCN:S7'	2.60	0.41
3:F:106:ILE:HD13	8:F:5931:FAD:C7	2.50	0.41
3:F:106:ILE:HD13	8:F:5931:FAD:C8	2.49	0.41
3:C:55:ARG:HD3	3:C:55:ARG:HH11	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:LEU:HA	1:D:18:LEU:HD23	1.92	0.41
2:B:664[A]:CYS:HB2	2:B:680:PHE:CD2	2.54	0.41
2:B:495:SER:HB3	2:B:504[A]:SER:OG	2.21	0.41
2:E:327[B]:LYS:HA	2:E:327[B]:LYS:CE	2.50	0.41
2:B:683:LEU:HD23	2:B:683:LEU:C	2.41	0.41
2:E:387:ARG:HA	2:E:763:GLU:HG2	2.02	0.41
2:E:121:VAL:HG11	2:E:132:ALA:HB3	2.03	0.41
3:C:221[A]:ASN:OD1	3:C:222:THR:HG23	2.21	0.40
3:F:120:ASP:C	3:F:120:ASP:OD2	2.60	0.40
3:C:204[A]:MET:HG3	3:C:286:ALA:HB1	2.04	0.40
2:B:121:VAL:HG11	2:B:132:ALA:HB3	2.04	0.40
2:B:718:ASP:HB3	2:B:724:LEU:HD11	2.03	0.40

All (4) 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)
9:B:5459:HOH:O	9:E:6649:HOH:O[4_477]	1.91	0.29
9:B:5809:HOH:O	9:E:6654:HOH:O[4_477]	2.03	0.17
9:B:6005:HOH:O	9:C:5179:HOH:O[2_675]	2.03	0.17
1:A:163:GLU:CG	9:E:6562:HOH:O[4_477]	2.19	0.01

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	166/166 (100%)	162 (98%)	4 (2%)	0	100	100
1	D	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
2	B	818/809 (101%)	791 (97%)	24 (3%)	3 (0%)	39	11
2	E	809/809 (100%)	784 (97%)	22 (3%)	3 (0%)	39	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	293/288 (102%)	290 (99%)	3 (1%)	0	100 100
3	F	290/288 (101%)	287 (99%)	3 (1%)	0	100 100
All	All	2538/2526 (100%)	2473 (97%)	59 (2%)	6 (0%)	52 19

All (6) Ramachandran outliers are listed below:

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

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	136/131 (104%)	135 (99%)	1 (1%)	88 66
1	D	132/131 (101%)	132 (100%)	0	100 100
2	B	664/653 (102%)	649 (98%)	15 (2%)	58 17
2	E	657/653 (101%)	642 (98%)	15 (2%)	58 17
3	C	219/212 (103%)	212 (97%)	7 (3%)	46 8
3	F	216/212 (102%)	213 (99%)	3 (1%)	74 38
All	All	2024/1992 (102%)	1983 (98%)	41 (2%)	65 21

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

Mol	Chain	Res	Type
1	A	163	GLU
2	B	7	VAL
2	B	21[A]	MET
2	B	21[B]	MET

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	209	TYR
2	B	258	HIS
2	B	313	ASP
2	B	386	TYR
2	B	393	THR
2	B	442	ASN
2	B	488	GLU
2	B	507	ASP
2	B	530	GLN
2	B	664[A]	CYS
2	B	664[B]	CYS
3	C	26	GLU
3	C	45	LEU
3	C	55	ARG
3	C	64[A]	ARG
3	C	64[B]	ARG
3	C	208	LYS
3	C	240	LYS
2	E	14	ARG
2	E	90	LEU
2	E	91	ASN
2	E	139	ASP
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	458	GLN
2	E	488	GLU
2	E	496	LYS
2	E	507	ASP
2	E	790	GLN
3	F	55	ARG
3	F	142	GLU
3	F	221	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS

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Mol	Chain	Res	Type
1	A	34	ASN
1	A	135	ASN
2	B	91	ASN
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	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	19	GLN
2	E	59	HIS
2	E	91	ASN
2	E	115	ASN
2	E	273	ASN
2	E	315	HIS
2	E	442	ASN
2	E	458	GLN
2	E	463	GLN
2	E	597	HIS
2	E	698	GLN
2	E	754	HIS
2	E	790	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 (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)

12 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	4001	-	4,4,4	0.35	0	6,6,6	0.33	0
5	FES	A	4907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	A	4908	1	0,4,4	0.00	-	0,4,4	0.00	-
7	MCN	B	4920	6	32,48,48	2.39	4 (12%)	39,74,74	1.49	6 (15%)
6	OMO	B	4921	7	0,3,3	0.00	-	0,3,3	0.00	-
8	FAD	C	4932	-	48,58,58	1.36	4 (8%)	54,89,89	1.92	6 (11%)
5	FES	D	5907	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FES	D	5908	1	0,4,4	0.00	-	0,4,4	0.00	-
4	PO4	E	5002	-	4,4,4	0.87	0	6,6,6	0.40	0
7	MCN	E	5920	6	32,48,48	2.65	4 (12%)	39,74,74	1.39	4 (10%)
6	OMO	E	5921	7	0,3,3	0.00	-	0,3,3	0.00	-
8	FAD	F	5931	-	48,58,58	1.47	8 (16%)	54,89,89	1.86	9 (16%)

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	4001	-	-	0/0/0/0	0/0/0/0
5	FES	A	4907	1	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FES	A	4908	1	-	0/0/4/4	0/1/1/1
7	MCN	B	4920	6	-	0/18/54/54	0/5/5/5
6	OMO	B	4921	7	-	0/0/0/0	0/0/0/0
8	FAD	C	4932	-	-	0/30/50/50	0/6/6/6
5	FES	D	5907	1	-	0/0/4/4	0/1/1/1
5	FES	D	5908	1	-	0/0/4/4	0/1/1/1
4	PO4	E	5002	-	-	0/0/0/0	0/0/0/0
7	MCN	E	5920	6	-	0/18/54/54	0/5/5/5
6	OMO	E	5921	7	-	0/0/0/0	0/0/0/0
8	FAD	F	5931	-	-	0/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4920	MCN	O4D-C1'	-5.52	1.34	1.41
7	E	5920	MCN	O9'-C9'	-3.96	1.38	1.44
8	C	4932	FAD	C10-N10	-3.42	1.35	1.39
8	F	5931	FAD	C6-C5X	-2.97	1.37	1.41
8	F	5931	FAD	C10-N10	-2.95	1.35	1.39
8	F	5931	FAD	O4B-C4B	-2.92	1.38	1.45
8	C	4932	FAD	C4A-N3A	-2.82	1.31	1.35
8	C	4932	FAD	O4B-C4B	-2.67	1.38	1.45
8	F	5931	FAD	C8A-N7A	-2.59	1.29	1.34
8	F	5931	FAD	C4X-C10	-2.17	1.37	1.41
8	F	5931	FAD	O4B-C1B	2.93	1.44	1.41
8	F	5931	FAD	C5X-N5	3.09	1.40	1.35
8	F	5931	FAD	C4X-N5	3.94	1.39	1.33
7	B	4920	MCN	C7-N8'	3.96	1.41	1.30
7	B	4920	MCN	O9'-C7	4.29	1.42	1.36
8	C	4932	FAD	C4X-N5	4.52	1.40	1.33
7	E	5920	MCN	C7-N8'	4.66	1.43	1.30
7	E	5920	MCN	O9'-C7	5.19	1.44	1.36
7	B	4920	MCN	C6'-N5'	9.98	1.45	1.32
7	E	5920	MCN	C6'-N5'	11.89	1.47	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	4932	FAD	N3A-C2A-N1A	-5.36	124.79	128.89
8	F	5931	FAD	C4-C4X-C10	-4.94	116.78	119.94
7	B	4920	MCN	N1'-C2'-N3'	-4.90	119.98	127.44
8	C	4932	FAD	C4-C4X-C10	-4.04	117.36	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	4932	FAD	C4X-C4-N3	-3.95	118.19	123.59
7	E	5920	MCN	N1'-C2'-N3'	-3.07	122.76	127.44
8	F	5931	FAD	C9A-C5X-N5	-2.42	118.78	122.36
8	F	5931	FAD	C4X-C4-N3	-2.34	120.39	123.59
8	C	4932	FAD	O4B-C1B-N9A	-2.25	103.38	108.10
8	F	5931	FAD	O3'-C3'-C2'	-2.12	103.41	108.75
8	F	5931	FAD	O3B-C3B-C2B	-2.09	105.03	111.83
7	B	4920	MCN	C4A-C4B-N8'	-2.07	118.76	122.11
7	B	4920	MCN	N2'-C2'-N3'	2.17	120.80	117.20
7	B	4920	MCN	C7-N8'-C4B	2.24	118.85	116.63
7	B	4920	MCN	C2-N3-C4	2.36	118.93	115.61
8	F	5931	FAD	O4B-C4B-C5B	2.37	117.81	109.32
7	E	5920	MCN	O4'-C4'-N3'	2.44	123.62	116.98
8	F	5931	FAD	C2B-C1B-N9A	2.63	118.30	114.29
8	C	4932	FAD	C5X-C9A-N10	2.82	119.77	117.62
7	E	5920	MCN	C2'-N3'-C4'	3.39	124.95	116.50
7	B	4920	MCN	C2'-N3'-C4'	3.72	125.77	116.50
7	E	5920	MCN	C7-N8'-C4B	4.25	120.84	116.63
8	F	5931	FAD	C5X-C9A-N10	4.80	121.27	117.62
8	F	5931	FAD	C4-N3-C2	7.68	121.89	115.25
8	C	4932	FAD	C4-N3-C2	9.22	123.22	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4920	MCN	1	0
6	B	4921	OMO	1	0
8	C	4932	FAD	1	0
7	E	5920	MCN	1	0
6	E	5921	OMO	1	0
8	F	5931	FAD	3	0

5.7 Other polymers (i)

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.