



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:41 am GMT

PDB ID : 1ZMC
Title : Crystal Structure of Human dihydrolipoamide dehydrogenase complexed to NAD+
Authors : Brautigam, C.A.; Chuang, J.L.; Tomchick, D.R.; Machius, M.; Chuang, D.T.
Deposited on : 2005-05-10
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

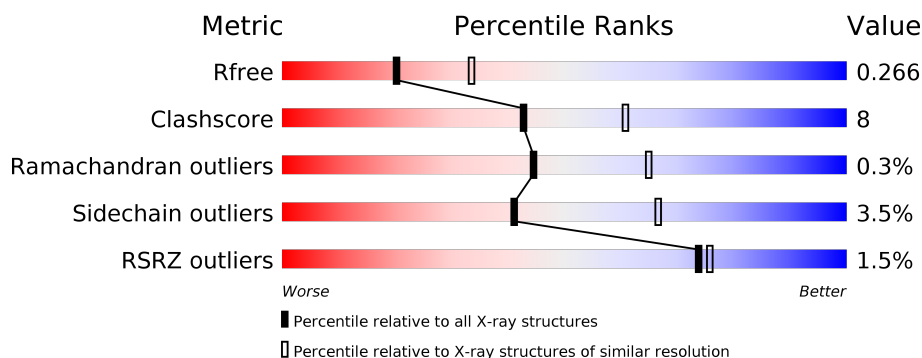
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4636 (2.54-2.50)
Clashscore	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)
RSRZ outliers	101464	4669 (2.54-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	474	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>..</div> </div> </div>
1	C	474	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>22%</div> <div>..</div> </div> </div>
1	D	474	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	E	474	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	F	474	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	474	
1	H	474	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2003	-	-	X	-
2	SO4	B	2005	-	-	-	X
2	SO4	B	2007	-	-	X	-
2	SO4	D	2014	-	-	X	-
2	SO4	D	2016	-	-	X	-
2	SO4	F	2024	-	-	-	X
2	SO4	G	2030	-	-	-	X
2	SO4	H	2033	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30312 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 Dihydrolipoyl dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	1	0
			3515	2214	609	673	19			
1	B	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			
1	C	471	Total	C	N	O	S	6	0	0
			3496	2203	604	670	19			
1	D	474	Total	C	N	O	S	0	1	0
			3528	2221	611	677	19			
1	E	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	F	471	Total	C	N	O	S	4	1	0
			3506	2209	607	671	19			
1	G	472	Total	C	N	O	S	0	1	0
			3515	2214	609	673	19			
1	H	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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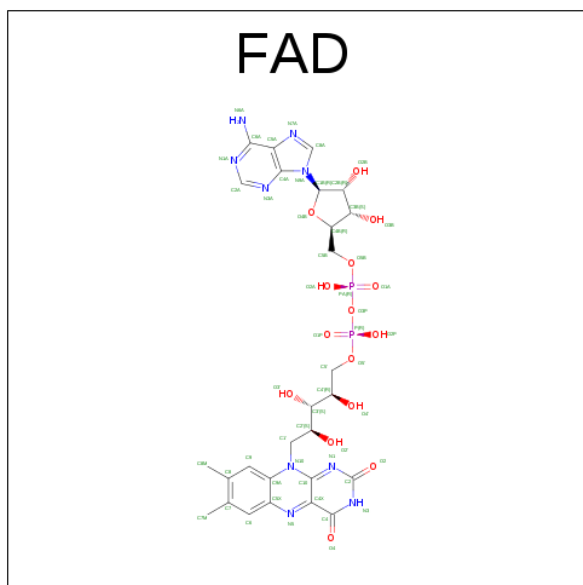
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

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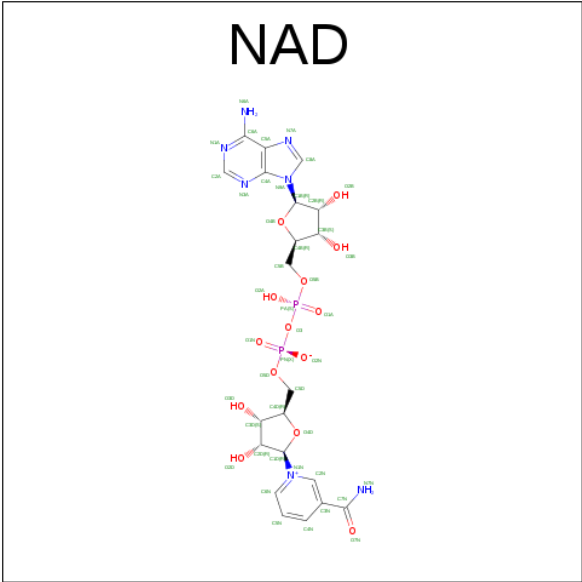
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		
5	B	137	Total	O	0	0
			137	137		
5	C	138	Total	O	0	0
			138	138		
5	D	144	Total	O	0	0
			144	144		

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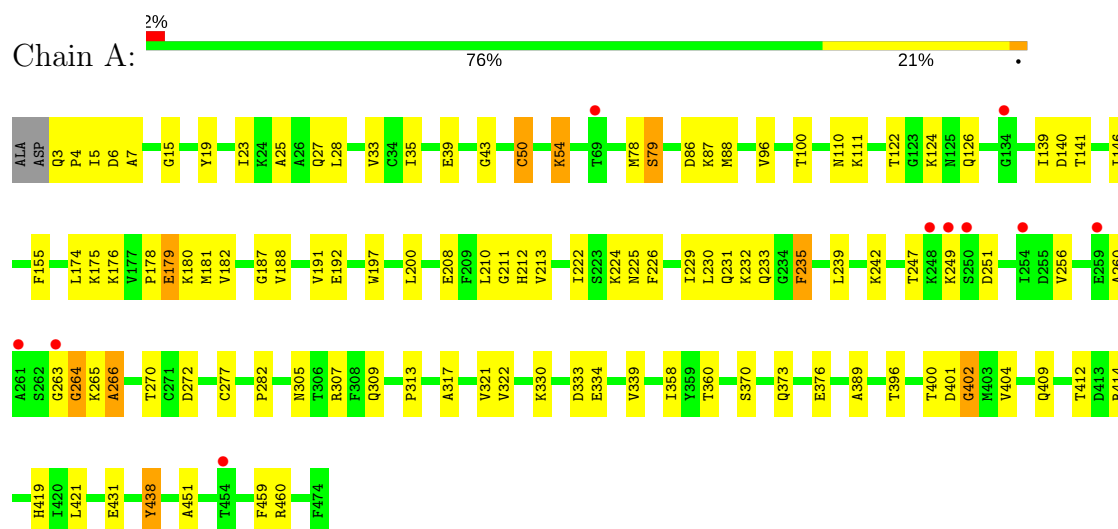
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	175	Total 175	O 175	0	0
5	F	229	Total 229	O 229	0	0
5	G	247	Total 247	O 247	0	0
5	H	173	Total 173	O 173	0	0

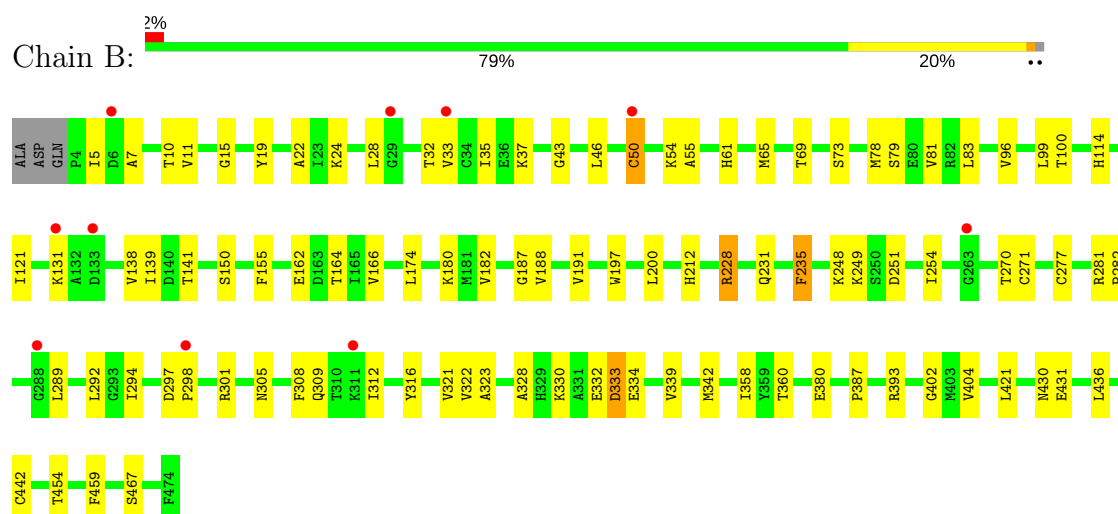
3 Residue-property plots [i](#)

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

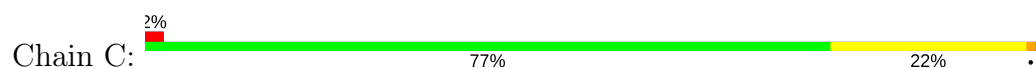
• Molecule 1: Dihydrolipoyl dehydrogenase

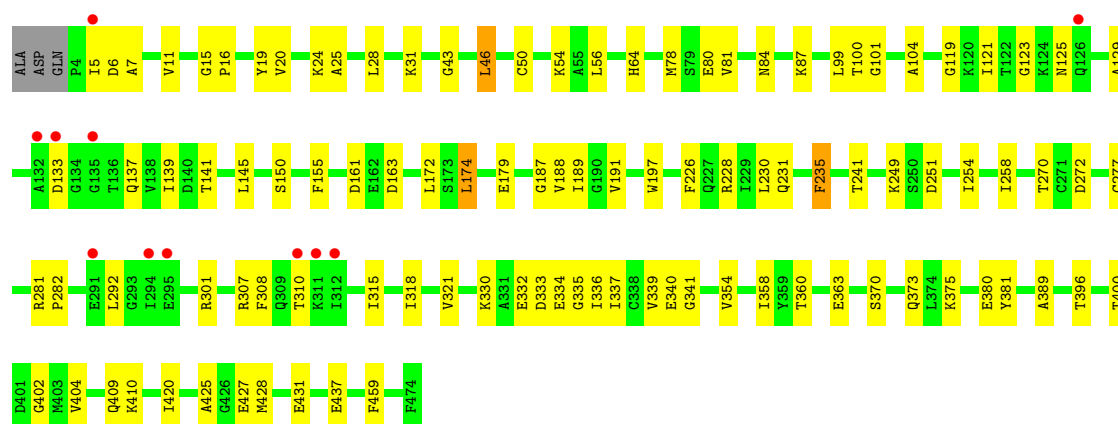


• Molecule 1: Dihydrolipoyl dehydrogenase

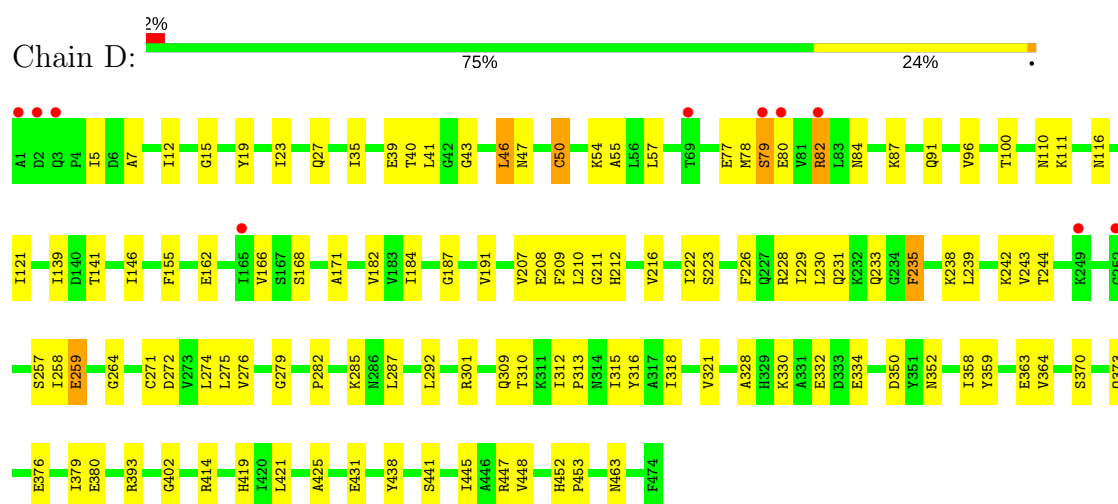


• Molecule 1: Dihydrolipoyl dehydrogenase

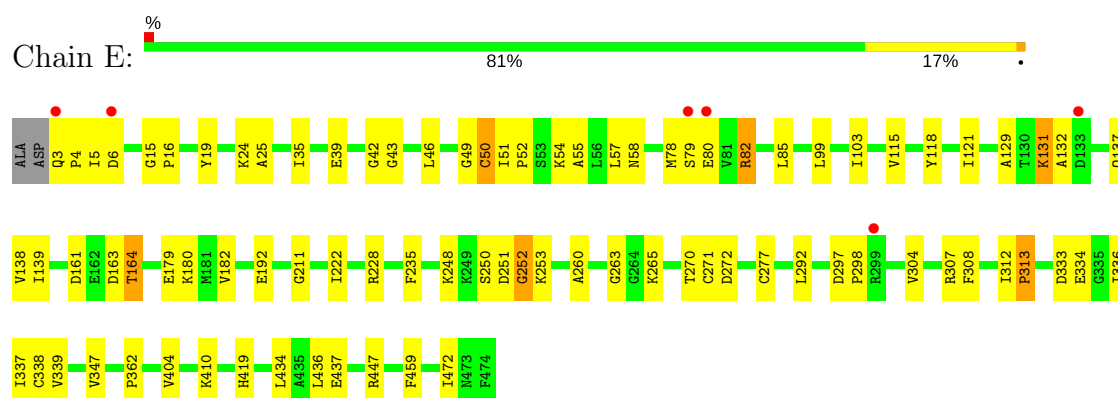




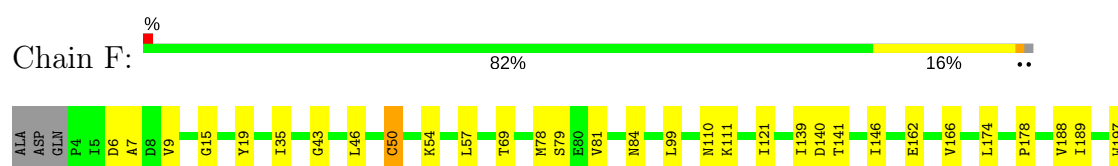
• Molecule 1: Dihydrolipoyl dehydrogenase

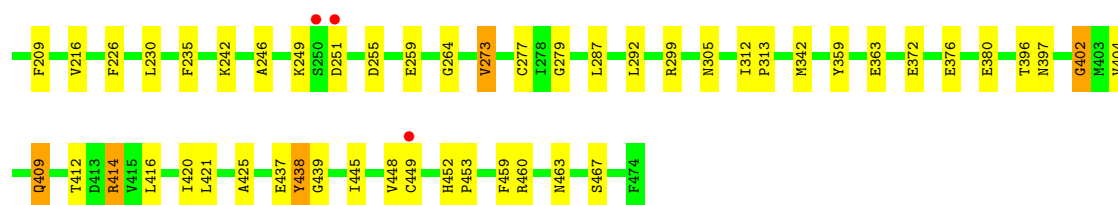


• Molecule 1: Dihydrolipoyl dehydrogenase

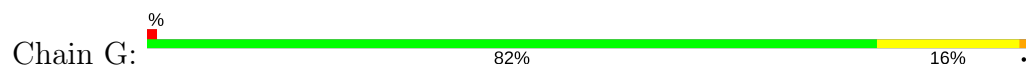


• Molecule 1: Dihydrolipoyl dehydrogenase

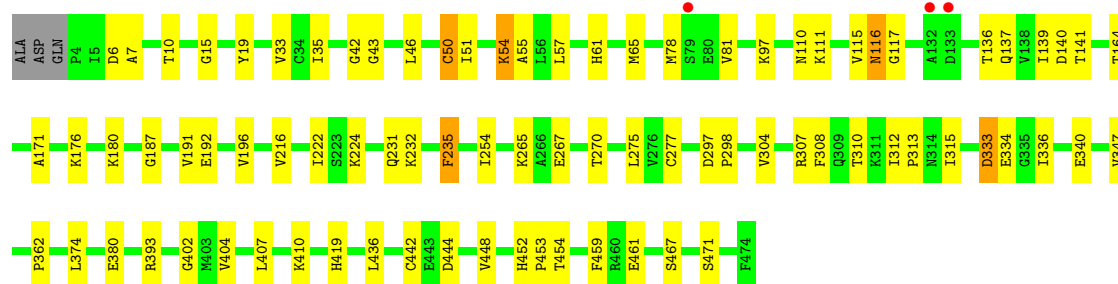
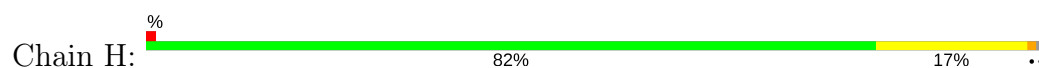




• Molecule 1: Dihydrolipoyl dehydrogenase



• Molecule 1: Dihydrolipoyl dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	176.12Å 210.76Å 126.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.09 – 2.53 43.09 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.09-2.53) 99.4 (43.09-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.267 0.211 , 0.266	Depositor DCC
R_{free} test set	940 reflections (0.60%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30312	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 53.36 % 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 4.2598e-05. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, NAD, 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	0.51	0/3571	0.76	3/4824 (0.1%)
1	B	0.52	0/3551	0.75	1/4796 (0.0%)
1	C	0.51	0/3551	0.73	2/4796 (0.0%)
1	D	0.50	0/3584	0.75	1/4842 (0.0%)
1	E	0.53	0/3560	0.76	2/4809 (0.0%)
1	F	0.57	0/3562	0.79	3/4811 (0.1%)
1	G	0.57	0/3571	0.78	1/4824 (0.0%)
1	H	0.57	1/3551 (0.0%)	0.76	2/4796 (0.0%)
All	All	0.54	1/28501 (0.0%)	0.76	15/38498 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	176	LYS	CD-CE	5.25	1.64	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	CYS	CA-CB-SG	7.18	126.92	114.00
1	C	50	CYS	CA-CB-SG	6.52	125.74	114.00
1	A	264	GLY	N-CA-C	6.15	128.48	113.10
1	A	50	CYS	CA-CB-SG	6.01	124.83	114.00
1	E	50	CYS	CA-CB-SG	5.92	124.65	114.00
1	G	402	GLY	N-CA-C	5.88	127.79	113.10
1	H	50	CYS	CA-CB-SG	5.42	123.75	114.00
1	D	50	CYS	CA-CB-SG	5.38	123.69	114.00
1	A	402	GLY	N-CA-C	5.32	126.41	113.10
1	H	402	GLY	N-CA-C	5.26	126.24	113.10
1	F	50	CYS	CA-CB-SG	5.21	123.38	114.00
1	E	252	GLY	N-CA-C	-5.18	100.16	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	402	GLY	N-CA-C	5.06	125.76	113.10
1	C	402	GLY	N-CA-C	5.01	125.63	113.10
1	F	84	ASN	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3515	0	3562	68	0
1	B	3496	0	3549	60	0
1	C	3496	0	3549	61	0
1	D	3528	0	3574	73	0
1	E	3505	0	3556	56	0
1	F	3506	0	3555	64	0
1	G	3515	0	3562	49	0
1	H	3496	0	3549	53	0
2	A	20	0	0	3	0
2	B	20	0	0	3	0
2	C	20	0	0	1	0
2	D	25	0	0	4	0
2	E	25	0	0	1	0
2	F	20	0	0	1	0
2	G	25	0	0	1	0
2	H	25	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	4	0
3	C	53	0	31	3	0
3	D	53	0	31	3	0
3	E	53	0	31	3	0
3	F	53	0	31	2	0
3	G	53	0	31	3	0
3	H	53	0	31	2	0
4	A	44	0	26	0	0
4	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	27	0	12	0	0
4	D	44	0	26	2	0
4	E	27	0	12	0	0
4	F	27	0	12	2	0
4	G	27	0	12	0	0
4	H	27	0	12	1	0
5	A	158	0	0	3	0
5	B	137	0	0	1	0
5	C	138	0	0	1	0
5	D	144	0	0	2	0
5	E	175	0	0	4	0
5	F	229	0	0	2	0
5	G	247	0	0	4	0
5	H	173	0	0	2	1
All	All	30312	0	28828	449	1

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 8.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLU:HG3	1:D:448:VAL:HG22	1.37	1.05
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.27	0.98
1:C:78:MET:HG2	1:D:78:MET:HG2	1.53	0.88
1:B:228:ARG:HG2	1:B:228:ARG:NH1	1.94	0.79
1:E:297:ASP:HB2	1:E:298:PRO:HD2	1.65	0.79
1:H:180:LYS:HE3	1:H:270:THR:O	1.83	0.79
1:A:79:SER:OG	1:B:79:SER:HB2	1.86	0.75
1:D:207:VAL:HG12	1:D:238:LYS:HB2	1.71	0.73
1:A:28:LEU:HD12	1:A:339:VAL:HG12	1.71	0.72
1:E:437:GLU:HG3	1:F:448:VAL:HG22	1.72	0.72
1:B:228:ARG:CG	1:B:228:ARG:HH11	2.01	0.71
1:C:121:ILE:HG21	1:C:292:LEU:HD11	1.73	0.71
1:B:10:THR:HG23	1:B:33:VAL:HG13	1.75	0.69
1:C:28:LEU:HD12	1:C:339:VAL:HG12	1.75	0.69
1:E:251:ASP:HB3	1:E:253:LYS:H	1.59	0.68
1:B:297:ASP:HB2	1:B:298:PRO:HD2	1.74	0.68
1:G:178:PRO:HG3	1:G:181:MET:HE2	1.74	0.68
1:E:180:LYS:HE3	1:E:270:THR:O	1.94	0.67
1:E:42:GLY:HA3	1:E:46:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:GLU:HB2	1:F:425:ALA:HB3	1.76	0.67
1:G:15:GLY:HA3	3:G:480:FAD:H52A	1.77	0.66
1:G:402:GLY:HA3	1:G:421:LEU:O	1.94	0.66
1:D:379:ILE:HG23	2:D:2014:SO4:O2	1.96	0.66
1:A:212:HIS:ND1	2:A:2003:SO4:O3	2.29	0.65
1:C:43:GLY:HA2	3:C:480:FAD:O3B	1.97	0.65
1:A:232:LYS:O	1:A:232:LYS:HD3	1.96	0.65
1:A:178:PRO:HG3	1:A:181:MET:HE2	1.79	0.64
1:B:289:LEU:HB3	1:B:294:ILE:HB	1.78	0.64
1:B:15:GLY:HA3	3:B:480:FAD:H52A	1.79	0.64
1:D:43:GLY:HA2	3:D:480:FAD:O3B	1.98	0.64
1:D:121:ILE:HG21	1:D:292:LEU:HD11	1.81	0.63
1:F:43:GLY:HA2	3:F:480:FAD:O3B	1.98	0.63
1:G:43:GLY:HA2	3:G:480:FAD:O3B	1.99	0.63
1:H:15:GLY:HA3	3:H:480:FAD:H52A	1.82	0.62
1:G:249:LYS:HD2	1:G:255:ASP:OD1	1.98	0.62
1:D:40:THR:HG22	1:D:41:LEU:O	2.00	0.62
1:E:118:TYR:O	1:E:129:ALA:HA	2.00	0.62
1:A:33:VAL:HG11	1:A:139:ILE:HD13	1.81	0.62
1:E:15:GLY:HA3	3:E:480:FAD:H52A	1.82	0.61
1:B:212:HIS:ND1	2:B:2007:SO4:O1	2.33	0.61
1:A:305:ASN:HB2	1:F:438:TYR:O	2.00	0.61
1:E:57:LEU:HD11	1:E:192:GLU:HB3	1.82	0.61
1:F:9:VAL:HG22	1:F:342:MET:CE	2.30	0.61
1:E:434:LEU:HD12	1:F:448:VAL:HG21	1.82	0.61
1:G:78:MET:HG2	1:H:81:VAL:HG22	1.80	0.61
1:C:307:ARG:O	1:C:308:PHE:HB2	2.01	0.61
1:H:297:ASP:HB2	1:H:298:PRO:HD2	1.80	0.61
1:D:182:VAL:HG23	1:D:271:CYS:HB3	1.82	0.61
1:B:69:THR:HG22	2:B:2004:SO4:O1	2.01	0.61
1:E:43:GLY:HA2	3:E:480:FAD:O3B	2.01	0.61
1:F:9:VAL:HG22	1:F:342:MET:HE1	1.81	0.61
1:A:263:GLY:HA3	1:H:97:LYS:NZ	2.16	0.61
1:A:15:GLY:HA3	3:A:480:FAD:H52A	1.83	0.60
1:D:370:SER:OG	1:D:373:GLN:HG3	2.01	0.60
1:D:110:ASN:O	1:D:111:LYS:HB2	2.02	0.60
1:H:231:GLN:HA	1:H:235:PHE:O	2.02	0.59
1:C:241:THR:HG21	1:C:258:ILE:HD12	1.84	0.59
1:E:362:PRO:HA	5:E:2157:HOH:O	2.03	0.59
1:B:231:GLN:HA	1:B:235:PHE:O	2.03	0.58
1:E:35:ILE:HD12	1:E:115:VAL:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:N	1:A:4:PRO:HD3	2.19	0.58
1:E:49:GLY:O	1:E:52:PRO:HD2	2.04	0.58
1:H:43:GLY:HA2	3:H:480:FAD:O3B	2.02	0.58
1:H:42:GLY:HA3	1:H:46:LEU:HD23	1.85	0.58
1:C:15:GLY:HA3	3:C:480:FAD:H52A	1.86	0.58
1:D:96:VAL:O	1:D:100:THR:HG23	2.04	0.58
1:C:46:LEU:HD21	1:C:99:LEU:HB2	1.86	0.58
1:H:10:THR:HB	1:H:141:THR:HG21	1.86	0.58
1:G:396:THR:CG2	1:H:55:ALA:HB2	2.34	0.57
1:G:249:LYS:HD2	1:G:255:ASP:CG	2.24	0.57
1:B:43:GLY:HA2	3:B:480:FAD:O3B	2.05	0.57
1:D:208:GLU:HG3	1:D:210:LEU:H	1.69	0.57
1:F:279:GLY:HA2	4:F:481:NAD:O1A	2.04	0.57
1:B:96:VAL:O	1:B:100:THR:HG23	2.04	0.56
1:F:110:ASN:O	1:F:111:LYS:HB2	2.04	0.56
1:D:40:THR:HG23	1:D:100:THR:HB	1.87	0.56
1:H:116:ASN:HD22	1:H:117:GLY:N	2.03	0.56
1:D:309:GLN:HG2	1:D:316:TYR:CE2	2.40	0.56
1:E:15:GLY:HA2	1:E:43:GLY:HA3	1.88	0.56
1:G:254:ILE:O	1:G:270:THR:HA	2.05	0.56
1:A:211:GLY:O	1:A:239:LEU:HD13	2.06	0.56
1:B:150:SER:HB2	1:B:281:ARG:O	2.06	0.56
1:D:380:GLU:HB2	2:D:2014:SO4:O4	2.06	0.56
1:G:259:GLU:HB2	1:G:264:GLY:O	2.06	0.56
1:B:212:HIS:CE1	2:B:2007:SO4:O1	2.58	0.55
1:D:244:THR:OG1	1:D:257:SER:HB2	2.05	0.55
1:A:122:THR:OG1	1:A:126:GLN:HG2	2.06	0.55
1:D:229:ILE:O	1:D:233:GLN:HG3	2.06	0.55
1:D:226:PHE:CZ	1:D:230:LEU:HD11	2.41	0.55
1:D:7:ALA:O	1:D:141:THR:HA	2.05	0.55
1:A:414:ARG:HH21	1:F:305:ASN:HA	1.71	0.55
1:A:451:ALA:H	1:B:430:ASN:HD21	1.52	0.55
1:A:78:MET:HG3	1:B:81:VAL:HG22	1.88	0.55
1:G:256:VAL:HB	1:G:269:ILE:HG13	1.89	0.54
1:C:363:GLU:HB2	1:C:425:ALA:HB3	1.88	0.54
1:E:78:MET:HG3	1:F:81:VAL:HG22	1.88	0.54
1:C:187:GLY:O	1:C:191:VAL:HG23	2.06	0.54
1:F:404:VAL:HG22	1:F:420:ILE:HG23	1.90	0.54
1:G:404:VAL:HG11	1:G:459:PHE:HA	1.89	0.54
1:D:5:ILE:HG23	1:D:139:ILE:HG23	1.89	0.54
1:E:79:SER:HB2	1:F:79:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:GLU:HG2	5:D:2035:HOH:O	2.07	0.54
1:D:328:ALA:O	1:D:332:GLU:HG3	2.08	0.54
1:E:137:GLN:HE21	1:E:138:VAL:N	2.05	0.54
1:C:16:PRO:O	1:C:332:GLU:HG2	2.08	0.53
1:A:370:SER:OG	1:A:373:GLN:HG3	2.08	0.53
1:H:336:ILE:O	1:H:340:GLU:HG3	2.08	0.53
1:A:260:ALA:HB3	1:A:263:GLY:O	2.08	0.53
1:B:404:VAL:HG11	1:B:459:PHE:HA	1.90	0.53
1:G:412:THR:O	1:G:413:ASP:HB3	2.09	0.53
1:A:305:ASN:ND2	1:A:309:GLN:HB2	2.23	0.53
1:B:35:ILE:HD11	1:B:139:ILE:HD12	1.91	0.53
1:E:248:LYS:HE2	1:E:252:GLY:O	2.09	0.52
1:E:336:ILE:O	1:E:339:VAL:HG12	2.09	0.52
1:C:150:SER:HB2	1:C:281:ARG:O	2.10	0.52
1:D:182:VAL:O	1:D:274:LEU:HD12	2.08	0.52
1:F:57:LEU:HD13	1:F:359:TYR:HB2	1.92	0.52
1:C:174:LEU:HB2	1:C:197:TRP:CZ2	2.45	0.52
1:D:46:LEU:HD13	1:D:100:THR:HG22	1.90	0.52
1:G:445:ILE:HG21	1:G:463:ASN:ND2	2.25	0.52
1:E:80:GLU:OE1	1:E:82:ARG:HD2	2.10	0.52
1:A:229:ILE:O	1:A:233:GLN:HG3	2.09	0.52
1:H:57:LEU:HD11	1:H:192:GLU:HB3	1.92	0.52
1:B:330:LYS:HE2	1:B:334:GLU:OE2	2.10	0.52
1:B:380:GLU:HG2	5:B:2037:HOH:O	2.10	0.52
1:C:333:ASP:O	1:C:337:ILE:HG12	2.10	0.52
1:C:56:LEU:HD12	1:C:172:LEU:HD23	1.91	0.52
1:E:99:LEU:O	1:E:103:ILE:HG12	2.09	0.52
1:E:307:ARG:HA	1:E:347:VAL:HG11	1.91	0.52
1:B:305:ASN:HD21	1:B:309:GLN:CG	2.24	0.51
1:G:15:GLY:CA	3:G:480:FAD:H52A	2.40	0.51
1:D:258:ILE:O	1:D:259:GLU:HB3	2.11	0.51
1:A:43:GLY:HA2	3:A:480:FAD:O3B	2.10	0.51
1:C:46:LEU:HD13	1:C:100:THR:HG22	1.93	0.51
1:G:330:LYS:O	1:G:334:GLU:HG3	2.10	0.51
1:H:216:VAL:HG22	4:H:481:NAD:O5D	2.10	0.51
1:H:308:PHE:CZ	1:H:334:GLU:HG2	2.45	0.51
1:A:360:THR:HB	5:A:2032:HOH:O	2.11	0.51
1:F:174:LEU:HD12	1:F:197:TRP:CE2	2.46	0.51
1:A:226:PHE:CZ	1:A:230:LEU:HD11	2.45	0.51
1:D:23:ILE:O	1:D:27:GLN:HG3	2.11	0.51
1:E:131:LYS:O	1:E:132:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:HG22	1:B:358:ILE:CD1	2.41	0.51
1:F:178:PRO:HB3	1:F:273:VAL:HG13	1.92	0.51
1:D:40:THR:HG21	1:D:100:THR:HG21	1.93	0.51
1:A:187:GLY:O	1:A:191:VAL:HG23	2.11	0.50
1:E:25:ALA:HB2	1:E:339:VAL:HG21	1.92	0.50
1:C:318:ILE:HD13	1:C:335:GLY:HA2	1.92	0.50
1:B:5:ILE:HG22	1:B:138:VAL:O	2.11	0.50
1:C:310:THR:HG23	1:C:315:ILE:O	2.12	0.50
1:D:363:GLU:HB3	1:D:425:ALA:HB3	1.94	0.50
1:E:222:ILE:HG13	1:E:419:HIS:HB3	1.94	0.50
1:A:110:ASN:O	1:A:111:LYS:HB2	2.11	0.50
1:E:137:GLN:HE21	1:E:138:VAL:H	1.60	0.50
1:D:216:VAL:HG23	4:D:481:NAD:O1N	2.12	0.50
1:A:23:ILE:O	1:A:27:GLN:HG3	2.12	0.49
1:A:409:GLN:HB3	1:A:412:THR:OG1	2.12	0.49
1:A:54:LYS:CA	1:A:54:LYS:HE3	2.42	0.49
1:C:375:LYS:HE3	1:C:381:TYR:OH	2.12	0.49
1:G:96:VAL:O	1:G:100:THR:HG23	2.13	0.49
1:G:409:GLN:OE1	1:G:411:SER:N	2.45	0.49
1:B:339:VAL:O	1:B:342:MET:HB2	2.13	0.49
1:C:5:ILE:HB	1:C:139:ILE:CD1	2.42	0.49
1:E:35:ILE:CD1	1:E:115:VAL:HB	2.42	0.49
1:F:15:GLY:HA3	3:F:480:FAD:H52A	1.94	0.49
1:H:116:ASN:HD22	1:H:117:GLY:H	1.60	0.49
1:E:434:LEU:CD1	1:F:448:VAL:HG21	2.43	0.49
1:F:372:GLU:CD	1:F:372:GLU:H	2.16	0.49
1:A:305:ASN:HD21	1:A:309:GLN:HB2	1.77	0.49
1:A:358:ILE:HG22	1:A:360:THR:HG23	1.93	0.49
1:B:393:ARG:HD2	1:B:454:THR:HA	1.93	0.49
1:E:3:GLN:N	1:E:4:PRO:HD3	2.28	0.49
1:C:5:ILE:HG12	1:C:137:GLN:NE2	2.28	0.49
1:C:28:LEU:HD12	1:C:339:VAL:CG1	2.41	0.49
1:H:57:LEU:HD23	1:H:196:VAL:HG23	1.94	0.49
1:A:174:LEU:HB2	1:A:197:TRP:CZ2	2.48	0.49
1:A:96:VAL:O	1:A:100:THR:HG23	2.12	0.49
1:C:228:ARG:HH11	1:C:228:ARG:HG3	1.78	0.49
1:G:453:PRO:HA	1:G:457:GLU:OE2	2.13	0.49
1:H:232:LYS:NZ	5:H:2106:HOH:O	2.37	0.49
1:A:404:VAL:HG11	1:A:459:PHE:HA	1.95	0.49
1:B:164:THR:HG21	1:B:248:LYS:NZ	2.27	0.49
1:C:24:LYS:O	1:C:28:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASP:O	1:C:31:LYS:HE3	2.13	0.49
1:C:7:ALA:O	1:C:141:THR:HA	2.13	0.49
1:B:322:VAL:CG1	1:B:323:ALA:N	2.76	0.48
1:B:7:ALA:O	1:B:141:THR:HA	2.13	0.48
1:E:131:LYS:NZ	1:E:137:GLN:HB2	2.27	0.48
1:B:294:ILE:HD11	1:B:312:ILE:HD13	1.94	0.48
1:D:310:THR:HG23	1:D:315:ILE:O	2.13	0.48
1:H:362:PRO:HA	5:H:2103:HOH:O	2.13	0.48
1:C:5:ILE:HB	1:C:139:ILE:HD13	1.95	0.48
1:H:110:ASN:O	1:H:111:LYS:HB2	2.12	0.48
1:A:402:GLY:HA3	1:A:421:LEU:O	2.13	0.48
1:E:333:ASP:O	1:E:337:ILE:HG12	2.13	0.48
1:H:35:ILE:HA	1:H:115:VAL:O	2.13	0.48
1:A:224:LYS:HD2	5:A:2053:HOH:O	2.14	0.48
1:C:254:ILE:O	1:C:270:THR:HA	2.13	0.48
1:E:78:MET:HG2	1:F:78:MET:SD	2.54	0.48
1:A:414:ARG:NH2	1:F:305:ASN:HA	2.29	0.48
1:G:225:ASN:O	1:G:229:ILE:HG13	2.13	0.48
1:A:211:GLY:HA3	2:A:2003:SO4:O4	2.13	0.48
1:C:20:VAL:HG12	1:C:336:ILE:HG13	1.94	0.48
1:C:370:SER:OG	1:C:373:GLN:HG3	2.13	0.48
1:D:57:LEU:HD13	1:D:359:TYR:HB2	1.96	0.48
1:F:249:LYS:HD2	1:F:255:ASP:OD1	2.13	0.48
1:G:460:ARG:NH1	5:G:2132:HOH:O	2.46	0.48
1:A:35:ILE:HD11	1:A:139:ILE:HD12	1.95	0.48
1:B:11:VAL:HG11	1:B:22:ALA:HB2	1.96	0.48
1:D:187:GLY:O	1:D:191:VAL:HG23	2.14	0.48
1:D:155:PHE:HZ	1:D:243:VAL:O	1.97	0.48
1:B:328:ALA:O	1:B:332:GLU:HG3	2.13	0.48
1:D:168:SER:HB2	3:D:480:FAD:HM71	1.96	0.48
1:D:208:GLU:HG3	1:D:210:LEU:N	2.28	0.48
1:A:307:ARG:HH12	1:F:437:GLU:HG3	1.79	0.48
1:G:242:LYS:NZ	5:G:2247:HOH:O	2.47	0.48
1:G:61:HIS:HD2	5:G:2083:HOH:O	1.96	0.48
1:A:54:LYS:N	1:A:54:LYS:HE3	2.28	0.47
1:F:414:ARG:HH11	1:F:414:ARG:CG	2.27	0.47
1:D:222:ILE:HG13	1:D:419:HIS:HB3	1.97	0.47
1:F:7:ALA:O	1:F:141:THR:HA	2.14	0.47
1:G:161:ASP:OD1	1:G:163:ASP:HB3	2.14	0.47
1:H:393:ARG:HD2	1:H:454:THR:HA	1.96	0.47
1:E:260:ALA:HB2	1:E:265:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ASP:HA	1:G:140:ASP:O	2.13	0.47
1:F:409:GLN:HB2	1:F:416:LEU:HD11	1.97	0.47
1:E:179:GLU:HB3	1:E:272:ASP:OD2	2.15	0.47
1:E:5:ILE:O	1:E:139:ILE:HA	2.15	0.47
1:E:164:THR:HG21	1:E:248:LYS:NZ	2.29	0.47
1:A:208:GLU:HG3	1:A:210:LEU:H	1.78	0.47
1:F:414:ARG:HD2	1:F:439:GLY:O	2.15	0.47
1:F:121:ILE:HG21	1:F:292:LEU:HD11	1.96	0.47
5:E:2076:HOH:O	1:F:449:CYS:HB3	2.15	0.47
1:C:64:HIS:O	1:C:64:HIS:CD2	2.68	0.46
1:F:299:ARG:NH1	5:F:2186:HOH:O	2.47	0.46
1:D:279:GLY:HA2	4:D:481:NAD:O1A	2.15	0.46
1:H:139:ILE:N	1:H:139:ILE:HD12	2.31	0.46
1:B:61:HIS:O	1:B:65:MET:HG2	2.15	0.46
1:B:37:LYS:HE2	3:B:480:FAD:O2B	2.15	0.46
1:G:162:GLU:HA	1:G:166:VAL:HG12	1.97	0.46
1:F:226:PHE:CZ	1:F:230:LEU:HD11	2.50	0.46
1:F:409:GLN:HG2	5:F:2227:HOH:O	2.15	0.46
1:C:431:GLU:HA	1:D:431:GLU:HG3	1.98	0.46
1:G:220:MET:O	1:G:224:LYS:HG2	2.15	0.46
1:F:249:LYS:HB2	1:F:251:ASP:OD1	2.16	0.46
1:F:69:THR:O	1:F:69:THR:HG22	2.16	0.46
1:H:442:CYS:HB2	1:H:467:SER:HB2	1.98	0.46
1:C:11:VAL:HG22	1:C:145:LEU:HD23	1.98	0.46
1:E:55:ALA:HB2	1:F:396:THR:HG23	1.98	0.46
1:A:188:VAL:O	1:A:192:GLU:HG3	2.16	0.46
1:A:321:VAL:HG23	1:A:322:VAL:HG13	1.98	0.46
1:B:282:PRO:HB3	1:B:321:VAL:HA	1.97	0.46
1:F:162:GLU:HA	1:F:166:VAL:HG12	1.97	0.46
1:G:179:GLU:HG3	5:G:2263:HOH:O	2.15	0.46
1:D:212:HIS:HB2	1:D:223:SER:OG	2.16	0.46
1:D:80:GLU:HG2	1:D:82:ARG:HH11	1.81	0.46
1:H:164:THR:HB	1:H:254:ILE:HD11	1.97	0.46
1:A:5:ILE:HG23	1:A:139:ILE:HG23	1.97	0.45
1:C:389:ALA:HA	1:C:400:THR:HB	1.97	0.45
1:E:312:ILE:HA	1:E:313:PRO:HD2	1.73	0.45
1:C:81:VAL:HG22	1:D:78:MET:HG2	1.97	0.45
1:A:78:MET:HG2	1:B:78:MET:SD	2.55	0.45
1:D:212:HIS:ND1	2:D:2016:SO4:O4	2.49	0.45
1:D:211:GLY:O	1:D:239:LEU:HD13	2.16	0.45
1:E:121:ILE:HG21	1:E:292:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:GLU:HB2	2:F:2024:SO4:O2	2.16	0.45
1:H:116:ASN:ND2	1:H:117:GLY:N	2.65	0.45
1:A:438:TYR:O	1:F:305:ASN:HB2	2.16	0.45
1:B:182:VAL:HG23	1:B:271:CYS:HB3	1.99	0.45
1:H:187:GLY:O	1:H:191:VAL:HG23	2.16	0.45
1:C:84:ASN:ND2	1:D:77:GLU:OE2	2.49	0.45
1:D:80:GLU:HG3	1:D:82:ARG:HD3	1.98	0.45
1:D:414:ARG:HA	1:D:441:SER:HA	1.97	0.45
1:H:452:HIS:HA	1:H:453:PRO:HA	1.71	0.45
1:A:282:PRO:HB3	1:A:321:VAL:HA	1.97	0.45
1:B:162:GLU:HA	1:B:166:VAL:HG12	1.99	0.45
1:D:231:GLN:HA	1:D:235:PHE:O	2.16	0.45
1:E:404:VAL:HG11	1:E:459:PHE:HA	1.98	0.45
1:E:79:SER:HB2	1:F:79:SER:HG	1.82	0.45
5:E:2075:HOH:O	1:F:397:ASN:HB3	2.17	0.45
1:H:61:HIS:O	1:H:65:MET:HG2	2.17	0.45
1:E:447:ARG:HH11	1:E:447:ARG:HG2	1.82	0.45
1:C:404:VAL:HG11	1:C:459:PHE:HA	1.99	0.45
1:C:81:VAL:HG22	1:D:78:MET:CG	2.46	0.45
1:B:174:LEU:HD12	1:B:197:TRP:CE2	2.51	0.44
1:F:246:ALA:HA	1:F:255:ASP:O	2.16	0.44
1:F:414:ARG:NH1	1:F:414:ARG:HG2	2.32	0.44
1:A:175:LYS:O	1:A:176:LYS:HG2	2.18	0.44
1:B:282:PRO:HG3	1:B:301:ARG:HG3	1.99	0.44
1:G:57:LEU:HD13	1:G:359:TYR:HB2	1.99	0.44
1:A:88:MET:HE2	1:A:200:LEU:HD11	1.98	0.44
1:A:389:ALA:HA	1:A:400:THR:HB	1.99	0.44
1:G:460:ARG:HH22	1:H:333:ASP:CG	2.21	0.44
1:E:24:LYS:HB3	1:E:339:VAL:HG11	1.99	0.44
1:G:20:VAL:HG12	1:G:336:ILE:HG13	1.99	0.44
1:C:330:LYS:O	1:C:334:GLU:HG3	2.17	0.44
1:D:350:ASP:OD2	1:D:352:ASN:HB3	2.18	0.44
1:D:452:HIS:HA	1:D:453:PRO:HA	1.76	0.44
1:E:211:GLY:N	2:E:2021:SO4:O1	2.48	0.44
1:H:310:THR:HG23	1:H:315:ILE:O	2.17	0.44
1:B:297:ASP:CB	1:B:298:PRO:HD2	2.46	0.44
1:B:402:GLY:HA3	1:B:421:LEU:O	2.17	0.44
1:F:162:GLU:OE1	1:F:162:GLU:HA	2.18	0.44
1:F:216:VAL:HG22	4:F:481:NAD:O2N	2.18	0.44
1:A:263:GLY:HA3	1:H:97:LYS:CE	2.47	0.44
1:B:164:THR:OG1	1:B:254:ILE:HD11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLY:HA3	3:D:480:FAD:H52A	2.00	0.44
1:H:374:LEU:HD12	1:H:407:LEU:HD13	1.98	0.44
1:B:442:CYS:HB2	1:B:467:SER:HB2	2.00	0.43
1:C:25:ALA:HA	1:C:339:VAL:HG11	2.00	0.43
1:H:461:GLU:OE2	1:H:471:SER:HB2	2.18	0.43
1:C:28:LEU:CD1	1:C:339:VAL:HG12	2.46	0.43
1:H:171:ALA:HB2	1:H:275:LEU:HD13	2.00	0.43
1:A:222:ILE:HG13	1:A:419:HIS:HB3	2.00	0.43
1:H:312:ILE:HA	1:H:313:PRO:HD3	1.83	0.43
1:A:330:LYS:O	1:A:334:GLU:HG3	2.18	0.43
1:E:182:VAL:HG23	1:E:271:CYS:HB3	2.00	0.43
1:F:35:ILE:HD11	1:F:139:ILE:HD13	2.01	0.43
1:D:91:GLN:NE2	5:D:2099:HOH:O	2.50	0.43
1:F:209:PHE:HD1	1:F:242:LYS:HB3	1.83	0.43
1:C:341:GLY:HA3	5:C:2144:HOH:O	2.18	0.43
1:H:307:ARG:HA	1:H:347:VAL:HG11	2.01	0.43
1:B:180:LYS:HD3	1:B:270:THR:O	2.18	0.43
1:C:249:LYS:HB2	1:C:251:ASP:OD1	2.19	0.43
1:G:211:GLY:N	2:G:2030:SO4:O3	2.47	0.43
1:H:404:VAL:HG11	1:H:459:PHE:HA	2.00	0.43
1:A:7:ALA:O	1:A:141:THR:HA	2.17	0.43
1:B:121:ILE:HG21	1:B:292:LEU:HD22	2.01	0.43
1:D:330:LYS:O	1:D:334:GLU:HG3	2.18	0.43
1:D:40:THR:HG21	1:D:100:THR:CG2	2.47	0.43
1:G:209:PHE:CE1	1:G:210:LEU:HG	2.53	0.43
1:D:146:ILE:HG23	1:D:287:LEU:HD21	2.00	0.43
1:D:162:GLU:HA	1:D:166:VAL:HG12	2.00	0.43
1:F:404:VAL:HG11	1:F:459:PHE:HA	2.01	0.43
1:G:208:GLU:O	1:G:239:LEU:HA	2.19	0.43
1:G:372:GLU:CD	1:G:372:GLU:H	2.21	0.43
1:H:304:VAL:HB	1:H:308:PHE:HA	2.01	0.43
1:C:80:GLU:HG2	1:C:81:VAL:N	2.33	0.43
1:D:171:ALA:HB2	1:D:275:LEU:HD13	2.01	0.43
1:H:222:ILE:HG13	1:H:419:HIS:HB3	1.99	0.43
1:A:225:ASN:O	1:A:229:ILE:HG13	2.19	0.42
1:D:445:ILE:HG21	1:D:463:ASN:ND2	2.33	0.42
1:E:46:LEU:O	1:E:46:LEU:HD12	2.19	0.42
1:H:6:ASP:HB2	1:H:140:ASP:O	2.19	0.42
1:H:46:LEU:HA	1:H:51:ILE:CG1	2.49	0.42
1:A:179:GLU:HB2	1:A:272:ASP:OD2	2.18	0.42
1:A:25:ALA:CA	1:A:339:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLY:O	1:B:191:VAL:HG23	2.19	0.42
1:A:431:GLU:HA	1:B:431:GLU:HG3	2.01	0.42
1:D:40:THR:HG21	1:D:47:ASN:OD1	2.19	0.42
1:D:79:SER:O	1:D:80:GLU:HB3	2.19	0.42
1:F:146:ILE:HG23	1:F:287:LEU:HD11	2.02	0.42
1:A:87:LYS:HE2	1:B:73:SER:HA	2.00	0.42
1:B:15:GLY:CA	3:B:480:FAD:H52A	2.47	0.42
1:D:184:ILE:HD12	1:D:276:VAL:HG22	2.01	0.42
1:D:402:GLY:HA3	1:D:421:LEU:O	2.19	0.42
1:E:51:ILE:HB	1:E:52:PRO:HD3	2.01	0.42
1:F:6:ASP:HA	1:F:140:ASP:O	2.19	0.42
1:E:333:ASP:OD1	1:F:460:ARG:NH2	2.49	0.42
1:G:309:GLN:HG2	1:G:316:TYR:CE2	2.54	0.42
1:A:211:GLY:CA	2:A:2003:SO4:O4	2.67	0.42
1:C:380:GLU:HG3	1:C:410:LYS:HD3	2.01	0.42
1:F:35:ILE:HD11	1:F:139:ILE:CD1	2.50	0.42
1:B:46:LEU:HD11	1:B:99:LEU:HB2	2.01	0.42
1:F:46:LEU:O	1:F:46:LEU:HD12	2.19	0.42
1:A:264:GLY:C	1:A:266:ALA:H	2.23	0.42
1:C:101:GLY:O	1:C:104:ALA:HB3	2.19	0.42
1:C:409:GLN:NE2	2:C:2009:SO4:O1	2.52	0.42
1:F:412:THR:OG1	1:F:414:ARG:HB2	2.19	0.42
1:C:119:GLY:HA2	1:C:129:ALA:HA	2.01	0.42
1:E:228:ARG:HG3	1:E:228:ARG:HH11	1.84	0.42
1:G:312:ILE:HA	1:G:313:PRO:HD2	1.89	0.42
1:G:414:ARG:HA	1:G:441:SER:HA	2.01	0.42
1:A:231:GLN:HA	1:A:235:PHE:O	2.20	0.42
1:B:249:LYS:HB2	1:B:251:ASP:OD1	2.20	0.42
1:F:402:GLY:HA3	1:F:421:LEU:O	2.20	0.42
1:H:136:THR:HG22	1:H:137:GLN:N	2.35	0.42
1:C:336:ILE:O	1:C:340:GLU:HG3	2.19	0.41
1:D:282:PRO:HG2	1:D:301:ARG:HG3	2.01	0.41
1:H:54:LYS:HE3	1:H:54:LYS:CA	2.50	0.41
1:G:396:THR:HG22	1:H:55:ALA:HB2	2.02	0.41
1:C:123:GLY:C	1:C:125:ASN:N	2.74	0.41
1:E:308:PHE:CZ	1:E:334:GLU:HG2	2.55	0.41
1:F:259:GLU:HB2	1:F:264:GLY:O	2.19	0.41
1:F:46:LEU:HD11	1:F:99:LEU:HB2	2.01	0.41
1:H:136:THR:CG2	1:H:137:GLN:N	2.83	0.41
1:H:7:ALA:HB2	1:H:33:VAL:HG23	2.01	0.41
1:C:231:GLN:HA	1:C:235:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:ILE:HA	1:F:313:PRO:HD3	1.73	0.41
1:H:265:LYS:O	1:H:267:GLU:HG3	2.19	0.41
1:H:444:ASP:O	1:H:448:VAL:HG23	2.20	0.41
1:H:46:LEU:HA	1:H:51:ILE:HG12	2.02	0.41
1:B:24:LYS:O	1:B:28:LEU:HD13	2.20	0.41
1:A:460:ARG:HH22	1:B:333:ASP:CG	2.23	0.41
1:D:318:ILE:HD12	1:D:318:ILE:C	2.41	0.41
1:A:396:THR:CG2	1:B:55:ALA:HB2	2.51	0.41
1:B:330:LYS:O	1:B:334:GLU:HG3	2.21	0.41
1:D:84:ASN:ND2	1:D:87:LYS:HB2	2.35	0.41
1:E:304:VAL:HB	1:E:308:PHE:HA	2.02	0.41
1:F:452:HIS:HA	1:F:453:PRO:HA	1.80	0.41
1:F:9:VAL:HG22	1:F:342:MET:HE2	2.01	0.41
1:G:412:THR:O	1:G:413:ASP:CB	2.68	0.41
1:C:282:PRO:CG	1:C:301:ARG:HG2	2.50	0.41
1:D:259:GLU:HB2	1:D:264:GLY:O	2.20	0.41
1:D:35:ILE:HD11	1:D:139:ILE:CD1	2.50	0.41
1:C:420:ILE:HD13	1:C:428:MET:HB3	2.02	0.41
1:D:209:PHE:HD1	1:D:242:LYS:HB3	1.86	0.41
1:D:312:ILE:HA	1:D:313:PRO:HD2	1.68	0.41
1:H:410:LYS:HE2	1:H:410:LYS:HB2	1.84	0.41
1:G:146:ILE:O	1:G:317:ALA:HA	2.20	0.41
1:G:20:VAL:CG1	1:G:336:ILE:HG13	2.51	0.41
1:C:189:ILE:HG23	3:C:480:FAD:HM73	2.02	0.41
1:C:226:PHE:CZ	1:C:230:LEU:HD11	2.55	0.41
1:D:12:ILE:HD13	1:D:287:LEU:HD11	2.02	0.41
1:E:85:LEU:HD12	1:E:85:LEU:HA	1.91	0.41
1:F:445:ILE:HG21	1:F:463:ASN:ND2	2.36	0.41
1:A:39:GLU:HG3	5:A:2096:HOH:O	2.20	0.41
1:B:322:VAL:HG12	1:B:323:ALA:N	2.35	0.41
1:C:161:ASP:OD1	1:C:163:ASP:HB3	2.21	0.41
1:D:121:ILE:CG2	1:D:292:LEU:HD11	2.48	0.41
1:E:161:ASP:OD1	1:E:163:ASP:HB3	2.21	0.41
1:G:174:LEU:HD12	1:G:197:TRP:CE2	2.56	0.41
1:B:83:LEU:HD22	1:B:200:LEU:HD22	2.03	0.41
1:D:358:ILE:HD12	1:D:364:VAL:HB	2.03	0.41
1:F:188:VAL:HG23	1:F:189:ILE:N	2.36	0.41
1:G:80:GLU:HB2	1:G:82:ARG:CZ	2.50	0.41
1:E:46:LEU:HD11	1:E:99:LEU:HB2	2.02	0.40
1:E:58:ASN:ND2	5:E:2085:HOH:O	2.55	0.40
1:F:372:GLU:CD	1:F:372:GLU:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282:PRO:HB3	1:G:321:VAL:HA	2.02	0.40
1:A:180:LYS:HD3	1:A:270:THR:O	2.20	0.40
1:A:182:VAL:HG11	1:A:256:VAL:HG21	2.03	0.40
1:B:308:PHE:O	1:B:316:TYR:HB3	2.21	0.40
1:C:188:VAL:HG13	1:C:358:ILE:HG12	2.03	0.40
1:E:16:PRO:HD2	3:E:480:FAD:O5'	2.21	0.40
1:F:414:ARG:NH1	1:F:414:ARG:CG	2.85	0.40
1:A:6:ASP:HA	1:A:140:ASP:O	2.22	0.40
1:B:150:SER:CB	1:B:281:ARG:O	2.70	0.40
1:G:209:PHE:C	1:G:209:PHE:CD1	2.95	0.40
1:G:222:ILE:HG23	1:G:421:LEU:HB2	2.04	0.40
1:G:50:CYS:O	1:G:54:LYS:HD2	2.20	0.40
1:H:297:ASP:C	1:H:297:ASP:OD1	2.59	0.40
1:A:146:ILE:O	1:A:317:ALA:HA	2.22	0.40
1:C:179:GLU:HB3	1:C:272:ASP:OD2	2.21	0.40
1:C:396:THR:HG23	1:D:55:ALA:HB2	2.04	0.40
1:D:210:LEU:HB3	2:D:2016:SO4:O4	2.21	0.40
1:F:409:GLN:HG3	1:F:412:THR:H	1.87	0.40
1:G:216:VAL:O	1:G:216:VAL:HG13	2.21	0.40
1:H:436:LEU:HD12	1:H:436:LEU:HA	1.82	0.40

All (1) 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)
5:H:2166:HOH:O	5:H:2166:HOH:O[2_675]	2.00	0.20

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	471/474 (99%)	447 (95%)	21 (4%)	3 (1%)	28 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	469/474 (99%)	444 (95%)	23 (5%)	2 (0%)	38	58
1	C	469/474 (99%)	441 (94%)	26 (6%)	2 (0%)	38	58
1	D	473/474 (100%)	448 (95%)	24 (5%)	1 (0%)	51	72
1	E	470/474 (99%)	448 (95%)	19 (4%)	3 (1%)	28	47
1	F	470/474 (99%)	453 (96%)	17 (4%)	0	100	100
1	G	471/474 (99%)	451 (96%)	19 (4%)	1 (0%)	51	72
1	H	469/474 (99%)	448 (96%)	21 (4%)	0	100	100
All	All	3762/3792 (99%)	3580 (95%)	170 (4%)	12 (0%)	44	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	G	79	SER
1	A	266	ALA
1	E	131	LYS
1	B	131	LYS
1	B	360	THR
1	C	360	THR
1	C	133	ASP
1	D	259	GLU
1	E	313	PRO
1	E	263	GLY
1	A	313	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/373 (100%)	354 (95%)	19 (5%)	28	48
1	B	371/373 (100%)	359 (97%)	12 (3%)	44	70
1	C	371/373 (100%)	361 (97%)	10 (3%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	374/373 (100%)	357 (96%)	17 (4%)	32	54
1	E	372/373 (100%)	358 (96%)	14 (4%)	38	63
1	F	372/373 (100%)	361 (97%)	11 (3%)	46	72
1	G	373/373 (100%)	362 (97%)	11 (3%)	48	73
1	H	371/373 (100%)	361 (97%)	10 (3%)	50	76
All	All	2977/2984 (100%)	2873 (96%)	104 (4%)	41	66

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	50	CYS
1	A	54	LYS
1	A	86	ASP
1	A	124	LYS
1	A	155	PHE
1	A	179	GLU
1	A	213	VAL
1	A	235	PHE
1	A	242	LYS
1	A	247	THR
1	A	249	LYS
1	A	251	ASP
1	A	265	LYS
1	A	277	CYS
1	A	333	ASP
1	A	376	GLU
1	A	401	ASP
1	A	438	TYR
1	B	19	TYR
1	B	32	THR
1	B	50	CYS
1	B	54	LYS
1	B	114	HIS
1	B	155	PHE
1	B	228	ARG
1	B	235	PHE
1	B	277	CYS
1	B	333	ASP
1	B	387	PRO

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Mol	Chain	Res	Type
1	B	436	LEU
1	C	19	TYR
1	C	46	LEU
1	C	54	LYS
1	C	87	LYS
1	C	155	PHE
1	C	174	LEU
1	C	235	PHE
1	C	277	CYS
1	C	321	VAL
1	C	354	VAL
1	D	19	TYR
1	D	39	GLU
1	D	46	LEU
1	D	50	CYS
1	D	54	LYS
1	D	79	SER
1	D	82	ARG
1	D	116	ASN
1	D	228	ARG
1	D	235	PHE
1	D	272	ASP
1	D	285	LYS
1	D	321	VAL
1	D	376	GLU
1	D	393	ARG
1	D	438	TYR
1	D	447	ARG
1	E	6	ASP
1	E	19	TYR
1	E	39	GLU
1	E	50	CYS
1	E	54	LYS
1	E	82	ARG
1	E	164	THR
1	E	235	PHE
1	E	250	SER
1	E	277	CYS
1	E	338	CYS
1	E	410	LYS
1	E	436	LEU
1	E	472	ILE

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Mol	Chain	Res	Type
1	F	19	TYR
1	F	50	CYS
1	F	54	LYS
1	F	235	PHE
1	F	273	VAL
1	F	277	CYS
1	F	376	GLU
1	F	409	GLN
1	F	414	ARG
1	F	438	TYR
1	F	467	SER
1	G	3	GLN
1	G	19	TYR
1	G	50	CYS
1	G	54	LYS
1	G	80	GLU
1	G	136	THR
1	G	213	VAL
1	G	235	PHE
1	G	277	CYS
1	G	431	GLU
1	G	438	TYR
1	H	19	TYR
1	H	50	CYS
1	H	54	LYS
1	H	78	MET
1	H	116	ASN
1	H	224	LYS
1	H	235	PHE
1	H	277	CYS
1	H	333	ASP
1	H	380	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	B	67	HIS
1	B	409	GLN
1	C	137	GLN
1	D	116	ASN
1	E	58	ASN

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Mol	Chain	Res	Type
1	E	125	ASN
1	E	137	GLN
1	E	225	ASN
1	G	231	GLN
1	G	361	HIS
1	H	114	HIS
1	H	116	ASN
1	H	225	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](#)

52 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	2000	-	4,4,4	0.71	0	6,6,6	0.06	0
2	SO4	A	2001	-	4,4,4	0.71	0	6,6,6	0.06	0
2	SO4	A	2002	-	4,4,4	0.70	0	6,6,6	0.05	0
2	SO4	A	2003	-	4,4,4	0.71	0	6,6,6	0.10	0
3	FAD	A	480	-	51,58,58	1.45	8 (15%)	54,89,89	2.07	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	A	481	-	41,48,48	0.84	2 (4%)	43,73,73	1.90	3 (6%)
2	SO4	B	2004	-	4,4,4	0.69	0	6,6,6	0.07	0
2	SO4	B	2005	-	4,4,4	0.71	0	6,6,6	0.06	0
2	SO4	B	2006	-	4,4,4	0.71	0	6,6,6	0.07	0
2	SO4	B	2007	-	4,4,4	0.71	0	6,6,6	0.10	0
3	FAD	B	480	-	51,58,58	1.70	10 (19%)	54,89,89	2.17	9 (16%)
4	NAD	B	481	-	25,29,48	1.05	1 (4%)	24,45,73	2.32	3 (12%)
2	SO4	C	2008	-	4,4,4	0.70	0	6,6,6	0.05	0
2	SO4	C	2009	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	C	2010	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	C	2011	-	4,4,4	0.70	0	6,6,6	0.09	0
3	FAD	C	480	-	51,58,58	1.83	9 (17%)	54,89,89	2.19	9 (16%)
4	NAD	C	481	-	25,29,48	1.14	3 (12%)	24,45,73	2.18	3 (12%)
2	SO4	D	2012	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	D	2013	-	4,4,4	0.69	0	6,6,6	0.08	0
2	SO4	D	2014	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	D	2015	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	D	2016	-	4,4,4	0.72	0	6,6,6	0.10	0
3	FAD	D	480	-	51,58,58	1.55	9 (17%)	54,89,89	2.01	9 (16%)
4	NAD	D	481	-	41,48,48	0.85	2 (4%)	43,73,73	1.88	3 (6%)
2	SO4	E	2017	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	E	2018	-	4,4,4	0.71	0	6,6,6	0.06	0
2	SO4	E	2019	-	4,4,4	0.70	0	6,6,6	0.08	0
2	SO4	E	2020	-	4,4,4	0.71	0	6,6,6	0.07	0
2	SO4	E	2021	-	4,4,4	0.71	0	6,6,6	0.09	0
3	FAD	E	480	-	51,58,58	1.55	7 (13%)	54,89,89	2.08	9 (16%)
4	NAD	E	481	-	25,29,48	1.06	1 (4%)	24,45,73	2.11	3 (12%)
2	SO4	F	2022	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	F	2023	-	4,4,4	0.71	0	6,6,6	0.06	0
2	SO4	F	2024	-	4,4,4	0.70	0	6,6,6	0.05	0
2	SO4	F	2025	-	4,4,4	0.70	0	6,6,6	0.05	0
3	FAD	F	480	-	51,58,58	1.60	9 (17%)	54,89,89	2.07	9 (16%)
4	NAD	F	481	-	25,29,48	1.13	2 (8%)	24,45,73	2.17	2 (8%)
2	SO4	G	2026	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	G	2027	-	4,4,4	0.71	0	6,6,6	0.07	0
2	SO4	G	2028	-	4,4,4	0.71	0	6,6,6	0.07	0
2	SO4	G	2029	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	G	2030	-	4,4,4	0.71	0	6,6,6	0.09	0
3	FAD	G	480	-	51,58,58	1.58	9 (17%)	54,89,89	2.07	8 (14%)
4	NAD	G	481	-	25,29,48	1.07	1 (4%)	24,45,73	2.10	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	H	2031	-	4,4,4	0.70	0	6,6,6	0.05	0
2	SO4	H	2032	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	H	2033	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	H	2034	-	4,4,4	0.70	0	6,6,6	0.07	0
2	SO4	H	2035	-	4,4,4	0.71	0	6,6,6	0.07	0
3	FAD	H	480	-	51,58,58	1.47	8 (15%)	54,89,89	2.16	9 (16%)
4	NAD	H	481	-	25,29,48	1.06	1 (4%)	24,45,73	2.23	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	2000	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
3	FAD	A	480	-	-	0/28/50/50	0/6/6/6
4	NAD	A	481	-	-	0/22/62/62	0/5/5/5
2	SO4	B	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2005	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2007	-	-	0/0/0/0	0/0/0/0
3	FAD	B	480	-	-	0/28/50/50	0/6/6/6
4	NAD	B	481	-	-	0/12/32/62	0/3/3/5
2	SO4	C	2008	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2009	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2010	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2011	-	-	0/0/0/0	0/0/0/0
3	FAD	C	480	-	-	0/28/50/50	0/6/6/6
4	NAD	C	481	-	-	0/12/32/62	0/3/3/5
2	SO4	D	2012	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2013	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2014	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2015	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2016	-	-	0/0/0/0	0/0/0/0
3	FAD	D	480	-	-	0/28/50/50	0/6/6/6
4	NAD	D	481	-	-	0/22/62/62	0/5/5/5
2	SO4	E	2017	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2018	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2019	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	2020	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2021	-	-	0/0/0/0	0/0/0/0
3	FAD	E	480	-	-	0/28/50/50	0/6/6/6
4	NAD	E	481	-	-	0/12/32/62	0/3/3/5
2	SO4	F	2022	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2023	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2024	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2025	-	-	0/0/0/0	0/0/0/0
3	FAD	F	480	-	-	0/28/50/50	0/6/6/6
4	NAD	F	481	-	-	0/12/32/62	0/3/3/5
2	SO4	G	2026	-	-	0/0/0/0	0/0/0/0
2	SO4	G	2027	-	-	0/0/0/0	0/0/0/0
2	SO4	G	2028	-	-	0/0/0/0	0/0/0/0
2	SO4	G	2029	-	-	0/0/0/0	0/0/0/0
2	SO4	G	2030	-	-	0/0/0/0	0/0/0/0
3	FAD	G	480	-	-	0/28/50/50	0/6/6/6
4	NAD	G	481	-	-	0/12/32/62	0/3/3/5
2	SO4	H	2031	-	-	0/0/0/0	0/0/0/0
2	SO4	H	2032	-	-	0/0/0/0	0/0/0/0
2	SO4	H	2033	-	-	0/0/0/0	0/0/0/0
2	SO4	H	2034	-	-	0/0/0/0	0/0/0/0
2	SO4	H	2035	-	-	0/0/0/0	0/0/0/0
3	FAD	H	480	-	-	0/28/50/50	0/6/6/6
4	NAD	H	481	-	-	0/12/32/62	0/3/3/5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	481	NAD	PN-O5D	-2.07	1.46	1.54
3	F	480	FAD	C2A-N1A	2.01	1.37	1.33
3	H	480	FAD	C5X-N5	2.01	1.38	1.35
3	B	480	FAD	C8-C7	2.01	1.46	1.41
4	D	481	NAD	C6N-N1N	2.03	1.40	1.35
4	A	481	NAD	C6N-N1N	2.04	1.40	1.35
3	A	480	FAD	C2A-N1A	2.04	1.37	1.33
3	D	480	FAD	C2A-N1A	2.05	1.37	1.33
3	C	480	FAD	C9-C8	2.08	1.43	1.37
4	A	481	NAD	C3N-C7N	2.10	1.53	1.50
3	A	480	FAD	C5X-N5	2.12	1.38	1.35
4	F	481	NAD	O4B-C1B	2.14	1.44	1.41
3	G	480	FAD	C6-C7	2.17	1.43	1.37
4	C	481	NAD	O4B-C1B	2.17	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	480	FAD	C4-N3	2.18	1.37	1.33
3	D	480	FAD	C5B-C4B	2.26	1.58	1.51
3	C	480	FAD	C2A-N1A	2.26	1.38	1.33
3	B	480	FAD	C5B-C4B	2.27	1.58	1.51
3	H	480	FAD	C2A-N1A	2.28	1.38	1.33
4	D	481	NAD	O4D-C1D	2.29	1.44	1.41
3	G	480	FAD	C2A-N1A	2.30	1.38	1.33
3	E	480	FAD	C2A-N1A	2.34	1.38	1.33
3	H	480	FAD	C5B-C4B	2.38	1.59	1.51
3	G	480	FAD	O4B-C1B	2.39	1.44	1.41
3	B	480	FAD	C2A-N1A	2.46	1.38	1.33
3	E	480	FAD	C2A-N3A	2.48	1.36	1.32
3	F	480	FAD	C5B-C4B	2.55	1.59	1.51
3	B	480	FAD	C1'-N10	2.55	1.51	1.48
3	G	480	FAD	C2A-N3A	2.60	1.36	1.32
3	A	480	FAD	O4B-C1B	2.63	1.44	1.41
3	D	480	FAD	C1'-N10	2.63	1.51	1.48
3	B	480	FAD	C2A-N3A	2.63	1.36	1.32
3	F	480	FAD	C4-N3	2.67	1.37	1.33
3	H	480	FAD	C4-N3	2.67	1.37	1.33
3	D	480	FAD	C10-N1	2.67	1.37	1.33
3	F	480	FAD	O4B-C1B	2.69	1.45	1.41
3	E	480	FAD	C5X-N5	2.69	1.39	1.35
3	A	480	FAD	C2A-N3A	2.70	1.36	1.32
3	E	480	FAD	C4-N3	2.70	1.37	1.33
3	D	480	FAD	O4B-C1B	2.73	1.45	1.41
3	F	480	FAD	C9A-N10	2.80	1.42	1.38
3	B	480	FAD	C4-N3	2.81	1.38	1.33
3	D	480	FAD	C9A-N10	2.87	1.42	1.38
3	D	480	FAD	C5X-N5	2.88	1.39	1.35
3	C	480	FAD	C2A-N3A	2.89	1.37	1.32
3	H	480	FAD	C10-N1	3.00	1.37	1.33
3	G	480	FAD	C4-N3	3.00	1.38	1.33
3	A	480	FAD	C10-N1	3.02	1.37	1.33
3	G	480	FAD	C5B-C4B	3.03	1.61	1.51
3	C	480	FAD	C1'-N10	3.08	1.51	1.48
3	F	480	FAD	C2A-N3A	3.11	1.37	1.32
4	E	481	NAD	PN-O1N	3.16	1.61	1.50
4	B	481	NAD	PN-O1N	3.17	1.61	1.50
4	H	481	NAD	PN-O1N	3.19	1.61	1.50
4	G	481	NAD	PN-O1N	3.23	1.61	1.50
3	H	480	FAD	C1'-N10	3.27	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	480	FAD	C9A-N10	3.30	1.43	1.38
4	C	481	NAD	PN-O1N	3.31	1.62	1.50
4	F	481	NAD	PN-O1N	3.32	1.62	1.50
3	A	480	FAD	C9A-N10	3.38	1.43	1.38
3	C	480	FAD	C4-N3	3.43	1.39	1.33
3	B	480	FAD	C5X-N5	3.44	1.40	1.35
3	C	480	FAD	C5X-N5	3.54	1.40	1.35
3	F	480	FAD	C1'-N10	3.62	1.52	1.48
3	F	480	FAD	C4X-N5	3.66	1.38	1.33
3	D	480	FAD	C4-N3	3.74	1.39	1.33
3	G	480	FAD	C9A-N10	3.74	1.43	1.38
3	E	480	FAD	C9A-N10	3.83	1.43	1.38
3	B	480	FAD	C9A-N10	3.98	1.44	1.38
3	G	480	FAD	C10-N1	4.24	1.39	1.33
3	E	480	FAD	C10-N1	4.28	1.39	1.33
3	A	480	FAD	C4X-N5	4.29	1.39	1.33
3	G	480	FAD	C4X-N5	4.30	1.39	1.33
3	F	480	FAD	C10-N1	4.43	1.39	1.33
3	E	480	FAD	C4X-N5	4.44	1.39	1.33
3	H	480	FAD	C4X-N5	4.62	1.40	1.33
3	D	480	FAD	C4X-N5	4.63	1.40	1.33
3	B	480	FAD	C10-N1	4.84	1.40	1.33
3	C	480	FAD	C9A-N10	4.88	1.45	1.38
3	C	480	FAD	C10-N1	5.24	1.40	1.33
3	C	480	FAD	C4X-N5	5.31	1.41	1.33
3	B	480	FAD	C4X-N5	5.33	1.41	1.33

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	481	NAD	N3A-C2A-N1A	-9.21	120.84	128.86
4	D	481	NAD	N3A-C2A-N1A	-9.20	120.84	128.86
4	F	481	NAD	N3A-C2A-N1A	-9.06	120.97	128.86
4	G	481	NAD	N3A-C2A-N1A	-8.87	121.14	128.86
4	H	481	NAD	N3A-C2A-N1A	-8.79	121.20	128.86
4	C	481	NAD	N3A-C2A-N1A	-8.78	121.21	128.86
4	B	481	NAD	N3A-C2A-N1A	-8.76	121.23	128.86
4	E	481	NAD	N3A-C2A-N1A	-8.41	121.53	128.86
4	D	481	NAD	C4B-O4B-C1B	-6.24	103.12	109.77
4	A	481	NAD	C4B-O4B-C1B	-6.18	103.19	109.77
4	B	481	NAD	C4B-O4B-C1B	-6.10	103.27	109.77
4	H	481	NAD	C4B-O4B-C1B	-5.13	104.31	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	481	NAD	C4B-O4B-C1B	-4.84	104.61	109.77
3	D	480	FAD	C4X-C4-N3	-4.82	116.62	123.48
3	C	480	FAD	C4X-C4-N3	-4.66	116.84	123.48
4	E	481	NAD	C4B-O4B-C1B	-4.66	104.81	109.77
3	F	480	FAD	N3A-C2A-N1A	-4.64	124.82	128.86
3	H	480	FAD	C4X-C4-N3	-4.57	116.98	123.48
3	A	480	FAD	C4X-C4-N3	-4.48	117.10	123.48
3	H	480	FAD	N3A-C2A-N1A	-4.31	125.11	128.86
3	E	480	FAD	C4X-C4-N3	-4.27	117.41	123.48
3	F	480	FAD	C4X-C4-N3	-4.18	117.53	123.48
3	G	480	FAD	N3A-C2A-N1A	-4.18	125.22	128.86
4	F	481	NAD	C4B-O4B-C1B	-4.16	105.34	109.77
3	G	480	FAD	C4X-C4-N3	-4.06	117.71	123.48
3	B	480	FAD	C4X-C4-N3	-4.05	117.71	123.48
3	B	480	FAD	N3A-C2A-N1A	-3.99	125.38	128.86
3	C	480	FAD	N3A-C2A-N1A	-3.83	125.52	128.86
3	H	480	FAD	C4B-O4B-C1B	-3.77	105.75	109.77
3	A	480	FAD	C4B-O4B-C1B	-3.60	105.94	109.77
3	E	480	FAD	N3A-C2A-N1A	-3.56	125.76	128.86
3	D	480	FAD	N3A-C2A-N1A	-3.55	125.77	128.86
3	A	480	FAD	N3A-C2A-N1A	-3.40	125.89	128.86
4	A	481	NAD	C4D-O4D-C1D	-3.11	106.46	109.77
3	G	480	FAD	C4B-O4B-C1B	-3.11	106.46	109.77
3	B	480	FAD	C4-C4X-C10	-3.08	117.47	119.96
3	D	480	FAD	C4B-O4B-C1B	-3.04	106.54	109.77
4	G	481	NAD	C4B-O4B-C1B	-3.02	106.56	109.77
3	B	480	FAD	C4B-O4B-C1B	-2.80	106.79	109.77
3	H	480	FAD	C4-C4X-C10	-2.76	117.73	119.96
3	E	480	FAD	C4B-O4B-C1B	-2.71	106.88	109.77
3	C	480	FAD	C4B-O4B-C1B	-2.70	106.89	109.77
3	E	480	FAD	C4-C4X-C10	-2.58	117.88	119.96
3	E	480	FAD	C4X-C10-N10	-2.45	118.82	120.52
3	D	480	FAD	C4-C4X-C10	-2.42	118.00	119.96
3	C	480	FAD	C4-C4X-C10	-2.41	118.02	119.96
4	D	481	NAD	C3N-C7N-N7N	-2.31	115.13	117.77
3	F	480	FAD	C4X-C10-N10	-2.26	118.95	120.52
3	F	480	FAD	C4B-O4B-C1B	-2.26	107.36	109.77
3	C	480	FAD	C4X-C10-N10	-2.22	118.97	120.52
3	A	480	FAD	C4-C4X-C10	-2.19	118.19	119.96
3	G	480	FAD	C4X-C10-N10	-2.16	119.02	120.52
3	G	480	FAD	C4-C4X-C10	-2.16	118.22	119.96
3	F	480	FAD	C4-C4X-C10	-2.15	118.22	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	481	NAD	C4A-C5A-N7A	-2.14	107.34	109.41
4	H	481	NAD	C4A-C5A-N7A	-2.12	107.36	109.41
4	E	481	NAD	C4A-C5A-N7A	-2.09	107.39	109.41
4	B	481	NAD	C4A-C5A-N7A	-2.04	107.44	109.41
3	H	480	FAD	O4'-C4'-C3'	2.02	114.11	109.09
3	D	480	FAD	C5X-C9A-N10	2.10	119.22	117.66
3	E	480	FAD	C1'-N10-C9A	2.15	120.32	118.35
3	A	480	FAD	C4-C4X-N5	2.24	121.14	118.68
3	B	480	FAD	C5X-C9A-N10	2.25	119.33	117.66
3	C	480	FAD	C4-C4X-N5	2.50	121.42	118.68
3	F	480	FAD	C5X-C9A-N10	2.53	119.54	117.66
3	E	480	FAD	C4-C4X-N5	2.55	121.48	118.68
3	D	480	FAD	C4-C4X-N5	2.58	121.51	118.68
3	B	480	FAD	C4-C4X-N5	2.60	121.53	118.68
3	H	480	FAD	C4-C4X-N5	2.68	121.61	118.68
3	F	480	FAD	C1'-N10-C9A	2.86	120.97	118.35
3	C	480	FAD	C1'-N10-C9A	3.04	121.13	118.35
3	G	480	FAD	C1'-N10-C9A	3.05	121.15	118.35
3	A	480	FAD	C1'-N10-C9A	3.10	121.18	118.35
3	D	480	FAD	C4X-N5-C5X	3.18	120.12	116.76
3	H	480	FAD	C1'-N10-C9A	3.23	121.31	118.35
3	B	480	FAD	C1'-N10-C9A	3.45	121.51	118.35
3	D	480	FAD	C1'-N10-C9A	3.47	121.53	118.35
3	F	480	FAD	C4X-N5-C5X	3.63	120.59	116.76
3	B	480	FAD	C4X-N5-C5X	3.76	120.73	116.76
3	A	480	FAD	C4X-N5-C5X	3.83	120.81	116.76
3	H	480	FAD	C4X-N5-C5X	4.02	121.00	116.76
3	G	480	FAD	C4X-N5-C5X	4.14	121.14	116.76
3	C	480	FAD	C4X-N5-C5X	4.55	121.57	116.76
3	E	480	FAD	C4X-N5-C5X	4.60	121.62	116.76
3	D	480	FAD	C4-N3-C2	10.03	123.93	115.16
3	G	480	FAD	C4-N3-C2	10.40	124.26	115.16
3	F	480	FAD	C4-N3-C2	10.43	124.28	115.16
3	H	480	FAD	C4-N3-C2	10.54	124.38	115.16
3	E	480	FAD	C4-N3-C2	10.61	124.44	115.16
3	A	480	FAD	C4-N3-C2	10.95	124.74	115.16
3	B	480	FAD	C4-N3-C2	11.28	125.02	115.16
3	C	480	FAD	C4-N3-C2	11.52	125.23	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2003	SO4	3	0
3	A	480	FAD	2	0
2	B	2004	SO4	1	0
2	B	2007	SO4	2	0
3	B	480	FAD	4	0
2	C	2009	SO4	1	0
3	C	480	FAD	3	0
2	D	2014	SO4	2	0
2	D	2016	SO4	2	0
3	D	480	FAD	3	0
4	D	481	NAD	2	0
2	E	2021	SO4	1	0
3	E	480	FAD	3	0
2	F	2024	SO4	1	0
3	F	480	FAD	2	0
4	F	481	NAD	2	0
2	G	2030	SO4	1	0
3	G	480	FAD	3	0
3	H	480	FAD	2	0
4	H	481	NAD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	472/474 (99%)	-0.02	10 (2%) 64 66	22, 37, 60, 82	0
1	B	471/474 (99%)	0.01	10 (2%) 64 66	18, 40, 70, 84	0
1	C	471/474 (99%)	0.03	11 (2%) 61 63	18, 41, 69, 83	1 (0%)
1	D	474/474 (100%)	0.03	10 (2%) 64 66	22, 37, 61, 84	0
1	E	472/474 (99%)	-0.02	6 (1%) 77 79	17, 35, 64, 85	0
1	F	471/474 (99%)	-0.18	3 (0%) 89 90	17, 29, 47, 68	1 (0%)
1	G	472/474 (99%)	-0.18	4 (0%) 86 87	18, 29, 46, 64	0
1	H	471/474 (99%)	-0.10	3 (0%) 89 90	15, 34, 56, 69	0
All	All	3774/3792 (99%)	-0.05	57 (1%) 74 76	15, 35, 62, 85	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	6.6
1	D	3	GLN	5.6
1	G	250	SER	4.7
1	D	249	LYS	4.2
1	F	250	SER	4.1
1	E	79	SER	4.0
1	H	79	SER	4.0
1	A	263	GLY	3.6
1	D	2	ASP	3.3
1	C	132	ALA	3.3
1	G	80	GLU	3.1
1	C	295	GLU	3.1
1	C	133	ASP	3.1
1	H	133	ASP	3.0
1	A	69	THR	2.9
1	B	29	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	5	ILE	2.7
1	C	135	GLY	2.6
1	D	82	ARG	2.6
1	A	261	ALA	2.6
1	B	133	ASP	2.6
1	B	50	CYS	2.5
1	F	251	ASP	2.5
1	A	254	ILE	2.5
1	D	165	ILE	2.4
1	A	248	LYS	2.4
1	B	6	ASP	2.4
1	C	291	GLU	2.4
1	A	259	GLU	2.4
1	E	299	ARG	2.4
1	E	133	ASP	2.4
1	C	312	ILE	2.3
1	A	454	THR	2.3
1	E	3	GLN	2.3
1	B	33	VAL	2.3
1	H	132	ALA	2.3
1	F	449	CYS	2.3
1	B	131	LYS	2.2
1	D	69	THR	2.2
1	E	80	GLU	2.2
1	B	288	GLY	2.2
1	B	298	PRO	2.2
1	G	451	ALA	2.1
1	C	310	THR	2.1
1	C	311	LYS	2.1
1	C	126	GLN	2.1
1	C	294	ILE	2.1
1	G	3	GLN	2.1
1	A	249	LYS	2.1
1	B	311	LYS	2.1
1	D	79	SER	2.1
1	B	263	GLY	2.1
1	D	252	GLY	2.1
1	E	6	ASP	2.0
1	D	80	GLU	2.0
1	A	134	GLY	2.0
1	A	250	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	G	2030	5/5	0.94	0.29	9.10	79,79,80,80	0
2	SO4	F	2024	5/5	0.88	0.35	3.60	121,121,121,121	0
2	SO4	B	2005	5/5	0.91	0.26	3.42	88,88,89,89	0
2	SO4	H	2033	5/5	0.94	0.21	2.28	81,81,82,83	0
2	SO4	C	2009	5/5	0.88	0.18	1.70	91,91,91,91	0
4	NAD	F	481	27/44	0.87	0.20	1.59	50,57,80,81	0
4	NAD	C	481	27/44	0.87	0.20	1.52	70,73,87,87	0
4	NAD	B	481	27/44	0.89	0.20	1.33	63,66,81,82	0
4	NAD	H	481	27/44	0.90	0.19	1.02	51,55,69,69	0
4	NAD	E	481	27/44	0.89	0.20	0.99	58,64,71,72	0
2	SO4	E	2019	5/5	0.95	0.17	0.98	78,79,80,80	0
4	NAD	A	481	44/44	0.86	0.20	0.96	52,64,86,88	0
2	SO4	H	2032	5/5	0.80	0.23	0.93	120,120,121,121	0
2	SO4	E	2018	5/5	0.77	0.30	0.90	120,120,120,120	0
3	FAD	G	480	53/53	0.96	0.17	0.60	18,23,28,31	0
3	FAD	A	480	53/53	0.94	0.17	0.53	22,30,34,36	0
2	SO4	A	2001	5/5	0.91	0.24	0.39	82,83,83,83	0
3	FAD	H	480	53/53	0.94	0.17	0.10	24,31,43,44	0
4	NAD	D	481	44/44	0.94	0.16	0.08	55,59,64,64	0
3	FAD	D	480	53/53	0.96	0.15	0.03	21,29,33,35	0
2	SO4	D	2013	5/5	0.91	0.23	-0.07	87,88,88,88	0
4	NAD	G	481	27/44	0.93	0.15	-0.07	31,37,63,64	0
3	FAD	B	480	53/53	0.94	0.17	-0.09	32,37,45,46	0
3	FAD	E	480	53/53	0.94	0.16	-0.10	26,32,44,44	0
3	FAD	F	480	53/53	0.97	0.14	-0.14	19,22,28,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	F	2023	5/5	0.93	0.17	-0.26	76,76,77,77	0
3	FAD	C	480	53/53	0.94	0.15	-0.35	27,37,51,52	0
2	SO4	G	2027	5/5	0.91	0.17	-0.40	80,80,81,81	0
2	SO4	C	2011	5/5	0.90	0.25	-	82,83,83,84	0
2	SO4	G	2029	5/5	0.72	0.27	-	119,119,119,120	0
2	SO4	H	2034	5/5	0.87	0.16	-	80,80,81,81	0
2	SO4	G	2028	5/5	0.81	0.48	-	127,127,128,128	0
2	SO4	E	2017	5/5	0.97	0.15	-	56,56,57,59	0
2	SO4	A	2003	5/5	0.94	0.46	-	87,87,87,88	0
2	SO4	B	2004	5/5	0.98	0.17	-	64,64,65,66	0
2	SO4	G	2026	5/5	0.95	0.17	-	62,63,64,66	0
2	SO4	B	2006	5/5	0.88	0.16	-	104,104,104,104	0
2	SO4	B	2007	5/5	0.93	0.30	-	78,78,79,79	0
2	SO4	A	2002	5/5	0.76	0.24	-	123,124,124,124	0
2	SO4	H	2031	5/5	0.97	0.15	-	57,58,59,60	0
2	SO4	D	2014	5/5	0.81	0.75	-	148,148,148,148	0
2	SO4	E	2020	5/5	0.93	0.15	-	90,90,91,91	0
2	SO4	A	2000	5/5	0.96	0.14	-	67,68,69,69	0
2	SO4	D	2012	5/5	0.96	0.17	-	71,71,72,72	0
2	SO4	C	2008	5/5	0.99	0.20	-	64,65,66,66	0
2	SO4	C	2010	5/5	0.90	0.17	-	103,103,103,103	0
2	SO4	E	2021	5/5	0.95	0.22	-	79,79,79,80	0
2	SO4	D	2016	5/5	0.90	0.38	-	83,83,84,84	0
2	SO4	H	2035	5/5	0.96	0.31	-	78,78,78,78	0
2	SO4	F	2022	5/5	0.95	0.19	-	62,62,64,66	0
2	SO4	F	2025	5/5	0.58	0.24	-	107,108,109,109	0
2	SO4	D	2015	5/5	0.78	0.25	-	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.