



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 AM UTC

PDB ID : 1OAO / pdb_00001oao
Title : NiZn[Fe4S4] and NiNi[Fe4S4] clusters in closed and open alpha subunits of acetyl-CoA synthase/carbon monoxide dehydrogenase
Authors : Darnault, C.; Volbeda, A.; Kim, E.J.; Legrand, P.; Vernede, X.; Lindahl, P.A.; Fontecilla-Camps, J.C.
Deposited on : 2003-01-20
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

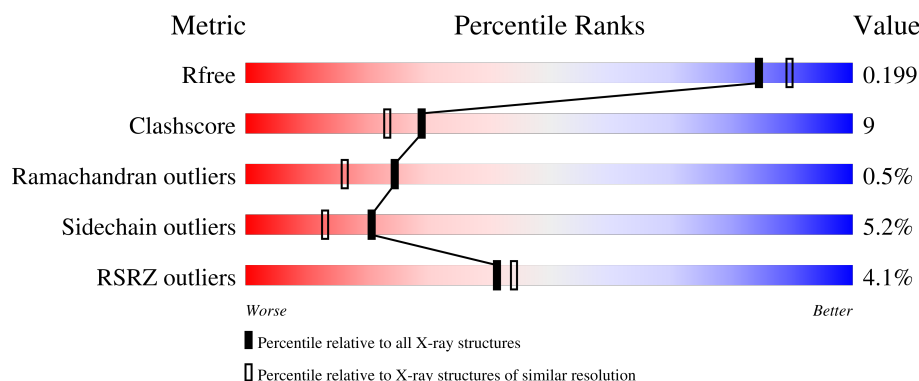
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	674	% 89% 10%
1	B	674	% 87% 12%
2	C	729	6% 80% 16%
2	D	729	8% 74% 22%

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
4	XCC	A	1677	-	-	X	-
4	XCC	B	1677	-	-	X	-
7	GOL	B	1689	-	-	X	-
7	GOL	C	1743	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 23346 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.

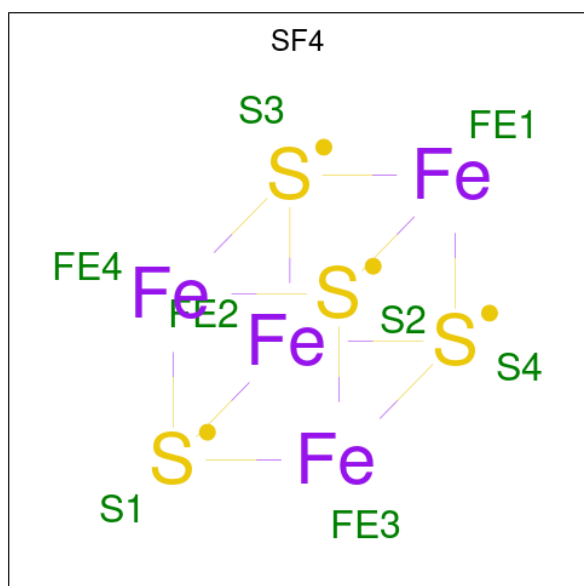
- Molecule 1 is a protein called CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	11	0
			5129	3221	894	968	46			
1	B	673	Total	C	N	O	S	0	11	0
			5131	3224	893	968	46			

- Molecule 2 is a protein called CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA.

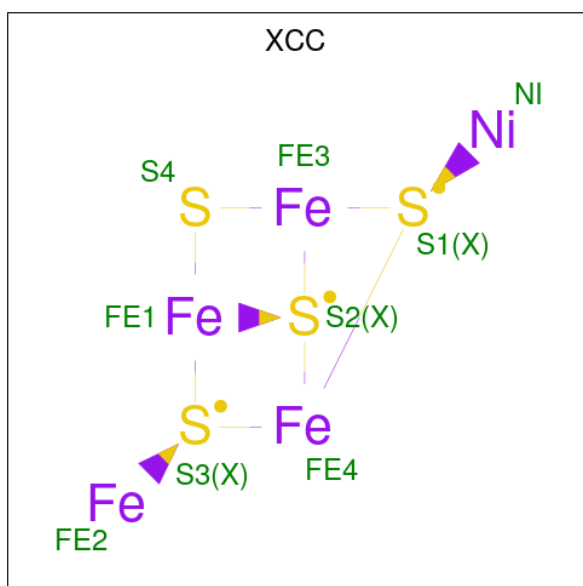
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	729	Total	C	N	O	S	0	11	0
			5788	3712	963	1076	37			
2	D	728	Total	C	N	O	S	0	2	0
			5745	3684	956	1070	35			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



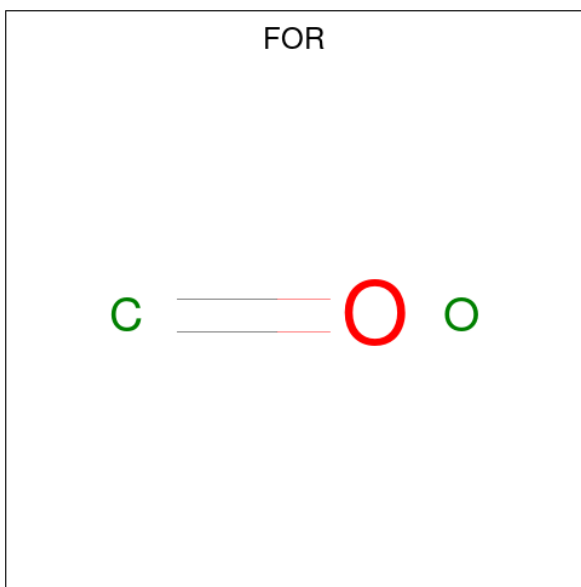
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is FORMYL GROUP (CCD ID: FOR) (formula: CH_2O).



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

- Molecule 6 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

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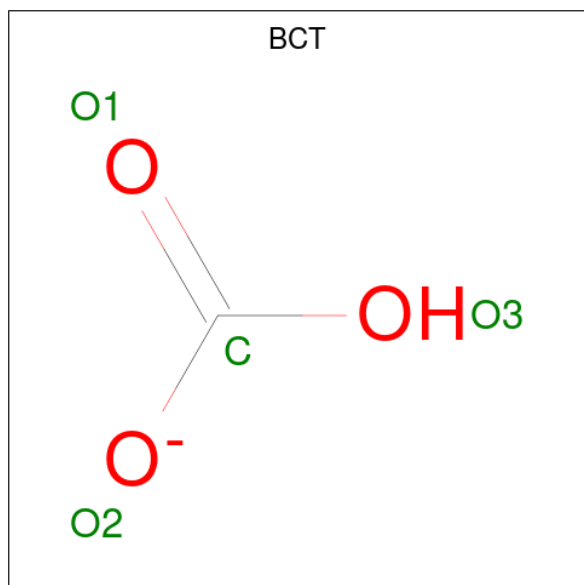
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 9 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	1	3		

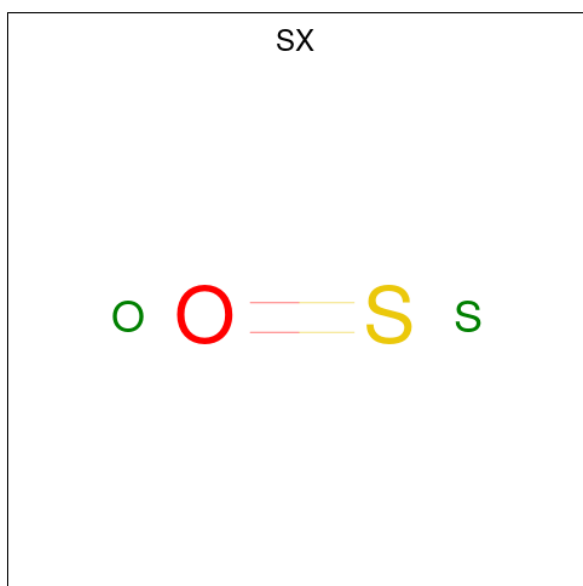
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	Zn	0	0
			1	1		

- Molecule 11 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

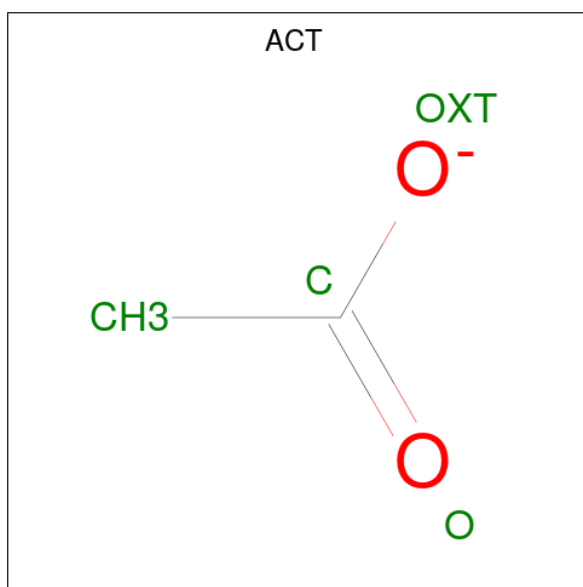
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	Ni	0	0
			1	1		
11	D	2	Total	Ni	0	1
			3	3		

- Molecule 12 is SULFUR OXIDE (CCD ID: SX) (formula: OS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	O	S	0	0
			2	1	1		

- Molecule 13 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	C	O	0	0
			4	2	2		

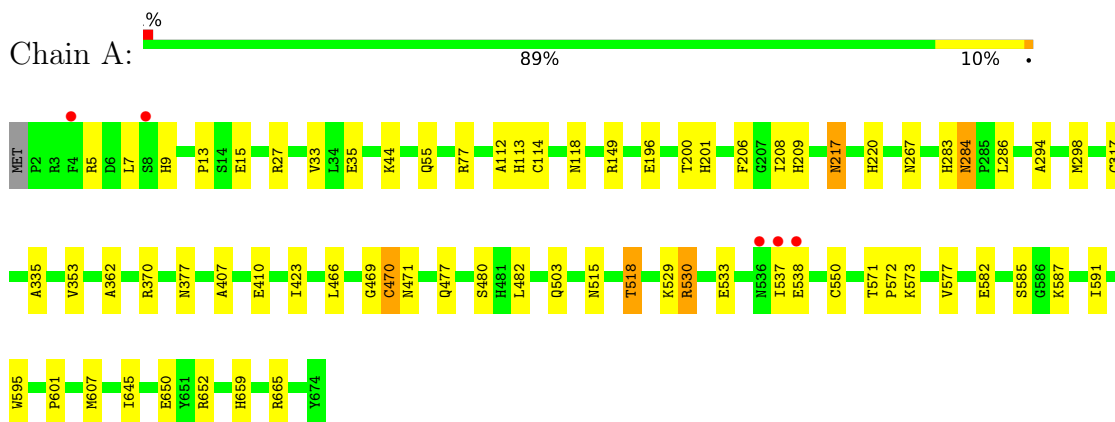
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	331	Total	O	0	0
			331	331		
14	B	357	Total	O	0	0
			357	357		
14	C	341	Total	O	0	0
			341	341		
14	D	242	Total	O	0	0
			242	242		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

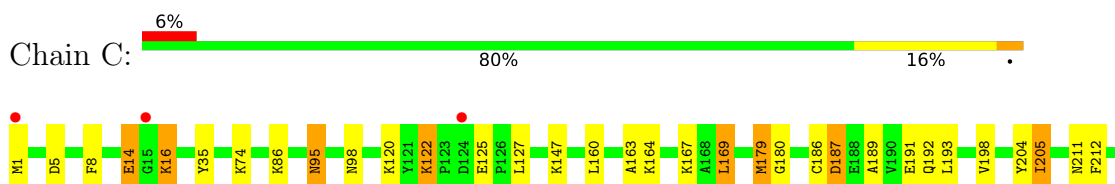
- Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

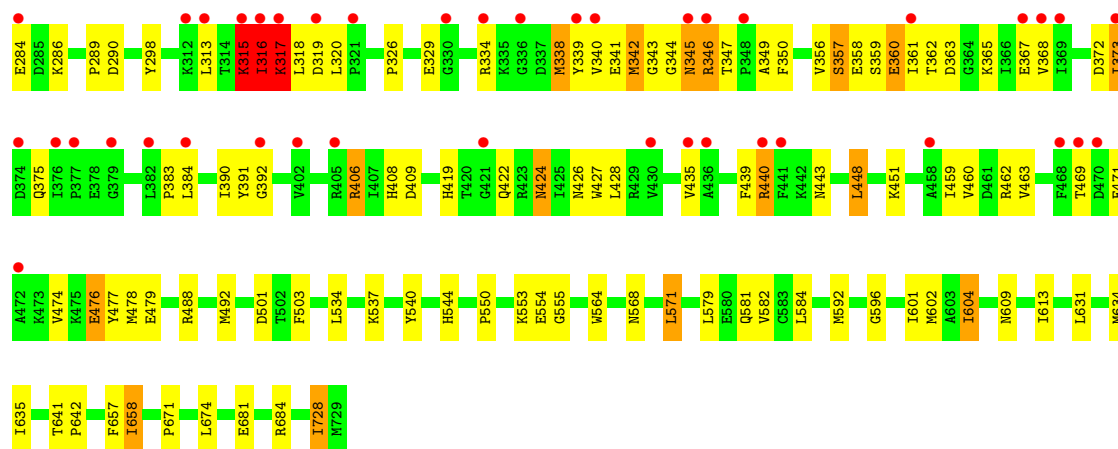


- Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

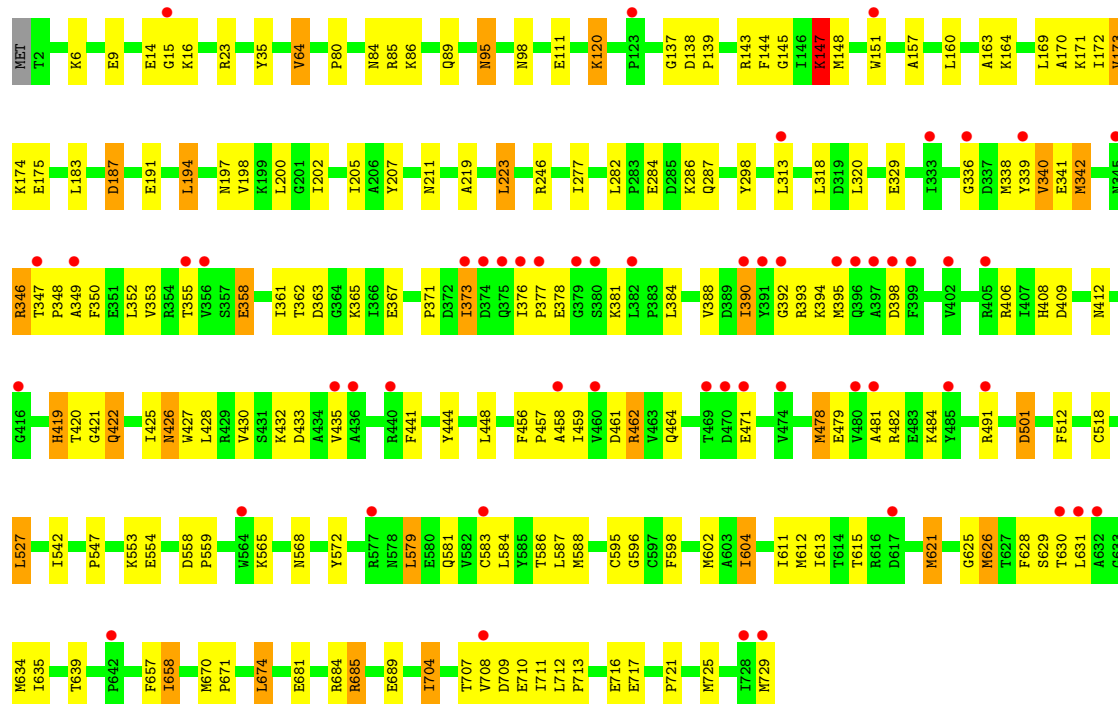
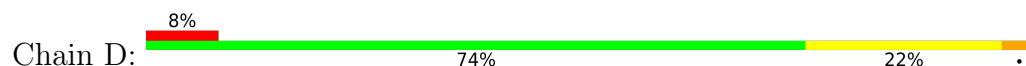


- Molecule 2: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA





● Molecule 2: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	244.57Å 81.89Å 167.22Å 90.00° 96.19° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 25.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (25.00-1.90) 91.6 (25.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.147 , 0.179 0.172 , 0.199	Depositor DCC
R_{free} test set	12689 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23346	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, ZN, ACT, FE2, GOL, SO4, SX, SF4, XCC, BCT, FOR

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	0.74	0/5275	0.91	0/7148
1	B	0.77	0/5278	0.91	0/7152
2	C	0.71	2/5973 (0.0%)	0.89	2/8087 (0.0%)
2	D	0.57	2/5888 (0.0%)	0.86	3/7974 (0.0%)
All	All	0.70	4/22414 (0.0%)	0.89	5/30361 (0.0%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	357	SER	C-O	9.69	1.35	1.23
2	C	179	MET	SD-CE	-6.71	1.62	1.79
2	D	709	ASP	C-N	5.54	1.41	1.33
2	D	709	ASP	C-O	5.32	1.30	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	635	ILE	CA-C-N	-7.90	113.86	122.55
2	C	635	ILE	C-N-CA	-7.90	113.86	122.55
2	D	14	GLU	CB-CA-C	-6.61	108.94	116.54
2	D	15	GLY	N-CA-C	-5.21	106.73	115.80
2	D	147	LYS	N-CA-C	-5.13	105.81	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5129	0	5124	70	0
1	B	5131	0	5123	84	1
2	C	5788	0	5763	108	0
2	D	5745	0	5704	140	0
3	A	8	0	0	0	0
3	B	16	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	55	0	0	0	0
6	B	50	0	0	3	0
6	C	30	0	0	0	0
6	D	20	0	0	0	0
7	A	6	0	8	2	0
7	B	12	0	16	10	0
7	C	24	0	32	7	0
7	D	6	0	8	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	4	0	0	1	0
10	C	1	0	0	0	0
11	C	1	0	0	0	0
11	D	3	0	0	0	0
12	C	2	0	0	0	0
13	D	4	0	3	0	0
14	A	331	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	357	0	0	9	0
14	C	341	0	0	3	0
14	D	242	0	0	3	0
All	All	23346	0	21781	383	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 9.

All (383) 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:C:571:LEU:HD11	2:C:582[A]:VAL:HG23	1.34	1.05
2:D:362:THR:H	2:D:464:GLN:NE2	1.62	0.98
2:D:707:THR:OG1	2:D:710:GLU:HG3	1.65	0.97
6:B:1688:SO4:O2	14:B:2354:HOH:O	1.85	0.92
1:B:550[C]:CYS:SG	1:B:591:ILE:HD11	2.13	0.89
2:C:440:ARG:HH11	2:C:440:ARG:HG3	1.37	0.89
2:D:371:PRO:HB2	2:D:376:ILE:HD11	1.56	0.88
1:A:294:ALA:O	1:A:298:MET:HG3	1.73	0.88
2:C:681[A]:GLU:OE1	2:C:684:ARG:NH2	2.05	0.88
1:B:470:CYS:HB3	4:B:1677:XCC:S2	2.15	0.86
6:B:1679:SO4:O1	14:B:2342:HOH:O	1.95	0.85
2:C:681[A]:GLU:CD	2:C:684:ARG:HH21	1.84	0.85
2:D:394:LYS:HD2	2:D:458:ALA:HB1	1.60	0.84
1:B:482:LEU:HD12	7:B:1689:GOL:C1	2.08	0.83
2:C:163:ALA:H	2:C:192:GLN:HE22	1.24	0.83
2:D:362:THR:H	2:D:464:GLN:HE21	1.25	0.83
1:B:482:LEU:CB	7:B:1689:GOL:H11	2.10	0.82
2:D:358:GLU:OE1	2:D:462:ARG:NH1	2.09	0.82
2:D:612:MET:O	2:D:613:ILE:HD13	1.81	0.81
1:B:155:GLU:HG3	9:B:1691:BCT:O1	1.82	0.80
2:D:568:ASN:HD21	2:D:581:GLN:HE21	1.30	0.80
1:A:55:GLN:HE22	1:B:77:ARG:H	1.30	0.80
2:D:284:GLU:CD	2:D:284:GLU:H	1.89	0.79
2:C:315:LYS:O	2:C:316:ILE:HG23	1.83	0.78
2:D:611:ILE:HD12	2:D:613:ILE:HD11	1.65	0.78
2:D:151:TRP:CZ2	2:D:547:PRO:HD3	2.20	0.77
1:A:530:ARG:HG3	1:A:530:ARG:HH11	1.49	0.77
2:C:571:LEU:CD1	2:C:582[A]:VAL:HG23	2.13	0.77
2:D:95:ASN:ND2	2:D:98:ASN:H	1.82	0.77
1:A:114[B]:CYS:SG	1:A:209:HIS:CE1	2.78	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:338:MET:SD	2:D:341:GLU:HB2	2.26	0.76
2:C:440:ARG:HG3	2:C:440:ARG:NH1	1.95	0.75
2:C:537:LYS:NZ	7:C:1743:GOL:H31	2.02	0.75
1:A:77:ARG:H	1:B:55:GLN:HE22	1.32	0.74
2:D:707:THR:HG1	2:D:710:GLU:HG3	1.50	0.74
2:C:571:LEU:HD11	2:C:582[A]:VAL:CG2	2.13	0.74
2:D:157:ALA:HB3	2:D:183:LEU:CD2	2.18	0.74
1:B:482:LEU:HB3	7:B:1689:GOL:H11	1.68	0.73
2:C:424:ASN:HD22	2:C:424:ASN:H	1.34	0.73
2:D:340:VAL:HG21	2:D:373:ILE:HD11	1.70	0.73
2:D:342:MET:HG2	2:D:428:LEU:HB2	1.69	0.73
2:D:621:MET:HE1	2:D:625:GLY:HA2	1.70	0.73
1:B:384[B]:TYR:HD2	2:D:84:ASN:HB3	1.55	0.72
1:A:196[A]:GLU:OE2	2:D:120:LYS:HE2	1.89	0.72
2:D:342:MET:HG3	2:D:384:LEU:HD22	1.70	0.72
2:C:315:LYS:C	2:C:316:ILE:CG2	2.63	0.71
1:A:470:CYS:HB3	4:A:1677:XCC:S3	2.30	0.71
2:C:609:ASN:HA	2:C:728:ILE:HD11	1.73	0.71
1:B:550[C]:CYS:SG	1:B:591:ILE:CD1	2.78	0.71
1:B:409:LYS:HE2	14:B:2220:HOH:O	1.90	0.71
2:C:316:ILE:O	2:C:317:LYS:HB2	1.91	0.70
1:A:550[C]:CYS:SG	1:A:591:ILE:HD11	2.31	0.70
2:C:16:LYS:NZ	2:C:284:GLU:HG3	2.06	0.70
2:C:488:ARG:O	2:C:492:MET:HG2	1.92	0.70
2:C:187:ASP:HA	2:C:211:ASN:HD22	1.55	0.70
1:B:128:ALA:HB1	1:B:164[A]:GLN:HG3	1.74	0.69
2:D:602:MET:HG2	2:D:613:ILE:HD12	1.74	0.69
1:B:487[A]:GLU:HG2	14:B:2266:HOH:O	1.92	0.69
2:C:604:ILE:HD11	2:C:728:ILE:HD13	1.74	0.69
2:D:478:MET:O	2:D:482:ARG:HG3	1.92	0.69
2:C:14:GLU:HG2	14:C:2009:HOH:O	1.92	0.68
2:D:187:ASP:HA	2:D:211:ASN:HD22	1.57	0.68
1:B:284:ASN:C	1:B:284:ASN:HD22	2.02	0.68
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.29	0.68
1:B:515:ASN:HD22	1:B:518:THR:CG2	2.06	0.68
1:A:573:LYS:NZ	1:A:659:HIS:HD2	1.92	0.67
2:C:315:LYS:C	2:C:316:ILE:HG22	2.20	0.67
7:B:1689:GOL:O1	14:B:2356:HOH:O	2.11	0.67
1:B:482:LEU:HD12	7:B:1689:GOL:H12	1.77	0.66
1:B:114[B]:CYS:SG	1:B:209:HIS:CE1	2.89	0.66
2:C:315:LYS:O	2:C:316:ILE:CG2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:681[A]:GLU:HG2	14:D:2224:HOH:O	1.95	0.66
2:D:23:ARG:NH2	14:D:2011:HOH:O	2.29	0.66
1:B:573:LYS:NZ	1:B:659:HIS:HD2	1.94	0.65
2:C:169:LEU:HD13	2:C:193:LEU:HG	1.78	0.65
2:C:537:LYS:HZ2	7:C:1743:GOL:H31	1.58	0.65
2:D:339:TYR:CD1	2:D:378:GLU:HG3	2.31	0.65
2:C:440:ARG:HH11	2:C:440:ARG:CG	2.10	0.64
2:C:554:GLU:HA	7:C:1737:GOL:H31	1.79	0.64
2:D:363:ASP:HB2	2:D:462:ARG:HG2	1.79	0.64
2:C:362:THR:OG1	2:C:365:LYS:HD3	1.97	0.64
2:D:346:ARG:HB3	2:D:381:LYS:HD3	1.78	0.64
1:B:486:LYS:NZ	7:B:1689:GOL:H31	2.13	0.64
1:A:284:ASN:HD22	1:A:286:LEU:H	1.46	0.64
1:A:587:LYS:HE3	4:A:1677:XCC:S2	2.38	0.63
2:C:568:ASN:HD21	2:C:581:GLN:HE21	1.46	0.63
1:B:573:LYS:HZ3	1:B:659:HIS:HD2	1.47	0.62
2:D:340:VAL:CG2	2:D:373:ILE:HD11	2.29	0.62
2:D:350:PHE:CD2	2:D:478:MET:HG2	2.34	0.62
1:B:550[A]:CYS:SG	14:B:2281:HOH:O	2.56	0.62
2:C:284:GLU:OE2	2:C:284:GLU:HA	1.99	0.62
2:D:371:PRO:CB	2:D:376:ILE:HD11	2.29	0.62
1:A:77:ARG:HD3	14:A:2066:HOH:O	1.99	0.61
2:C:316:ILE:CG1	2:C:317:LYS:N	2.62	0.61
1:A:335:ALA:H	1:A:471:ASN:HD22	1.48	0.61
1:A:55:GLN:NE2	1:B:77:ARG:H	1.97	0.61
2:D:712:LEU:HB3	2:D:713:PRO:HD3	1.83	0.61
1:A:283:HIS:NE2	1:A:587:LYS:NZ	2.49	0.60
2:C:95:ASN:ND2	2:C:98:ASN:H	1.98	0.60
2:D:388:VAL:HG12	2:D:390:ILE:CD1	2.31	0.60
1:A:550[C]:CYS:SG	1:A:591:ILE:CD1	2.89	0.60
1:A:201:HIS:HE1	2:D:35:TYR:OH	1.85	0.60
2:D:408:HIS:HD2	2:D:419:HIS:ND1	2.00	0.60
1:B:486:LYS:HZ2	7:B:1689:GOL:H31	1.64	0.60
2:D:421:GLY:C	2:D:422:GLN:HG3	2.26	0.60
1:A:283:HIS:CE1	1:A:587:LYS:NZ	2.70	0.59
1:B:515:ASN:HD22	1:B:518:THR:HG21	1.67	0.59
2:D:456:PHE:HD2	2:D:542:ILE:HD11	1.68	0.59
2:D:482:ARG:HD2	14:D:2174:HOH:O	2.01	0.59
2:D:721:PRO:O	2:D:725:MET:HG3	2.01	0.59
2:D:587:LEU:HD13	2:D:602:MET:HE2	1.84	0.59
1:B:482:LEU:HD11	1:B:508:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:CD1	7:B:1689:GOL:C1	2.80	0.58
1:B:384[B]:TYR:CD2	2:D:84:ASN:HB3	2.37	0.58
1:B:577[A]:VAL:HG21	1:B:645:ILE:HG23	1.85	0.58
1:A:659:HIS:HE1	2:D:191:GLU:OE1	1.85	0.58
2:C:338:MET:O	2:C:338:MET:HG2	2.02	0.58
1:A:573:LYS:HZ1	1:A:659:HIS:HD2	1.49	0.58
1:B:196:GLU:OE2	2:C:120:LYS:HE2	2.04	0.58
1:A:515:ASN:HD22	1:A:518:THR:HG21	1.68	0.58
2:D:611:ILE:CD1	2:D:613:ILE:HD11	2.33	0.58
2:C:343:GLY:HA2	2:C:347:THR:O	2.03	0.58
2:C:492:MET:HE1	2:C:534:LEU:HD11	1.85	0.58
2:D:602:MET:HE1	2:D:658:ILE:HG21	1.85	0.57
1:B:482:LEU:HB2	7:B:1689:GOL:H11	1.86	0.57
2:C:8:PHE:HB2	7:C:1741:GOL:H31	1.86	0.57
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.40	0.57
2:D:358:GLU:HB2	2:D:462:ARG:NH1	2.20	0.57
1:A:77:ARG:H	1:B:55:GLN:NE2	2.00	0.57
1:B:284:ASN:ND2	1:B:286:LEU:H	2.02	0.56
2:D:406:ARG:NH1	2:D:409:ASP:OD2	2.38	0.56
2:D:568:ASN:ND2	2:D:581:GLN:HE21	2.00	0.56
1:B:284:ASN:HD22	1:B:286:LEU:H	1.52	0.56
2:D:602:MET:HG2	2:D:613:ILE:CD1	2.35	0.56
2:D:361:ILE:HG13	2:D:464:GLN:HB2	1.88	0.56
2:C:342:MET:HB3	2:C:384:LEU:HB2	1.88	0.56
2:D:613:ILE:O	2:D:671:PRO:HD3	2.06	0.56
1:A:284:ASN:ND2	1:A:286:LEU:H	2.04	0.56
2:D:457:PRO:O	2:D:458:ALA:HB3	2.06	0.56
1:B:129:GLU:OE2	1:B:164[B]:GLN:NE2	2.39	0.55
1:B:335:ALA:H	1:B:471:ASN:HD22	1.55	0.55
2:D:157:ALA:HB3	2:D:183:LEU:HD22	1.88	0.55
2:D:353:VAL:HG13	2:D:390:ILE:HD13	1.88	0.55
2:D:657:PHE:O	2:D:658:ILE:C	2.49	0.55
2:C:361:ILE:HD11	2:C:391:TYR:HB3	1.89	0.55
2:C:439:PHE:CE1	2:C:443:ASN:HB2	2.42	0.55
1:A:573:LYS:NZ	1:A:659:HIS:CD2	2.74	0.55
2:D:388:VAL:HG12	2:D:390:ILE:HD11	1.88	0.55
2:D:138:ASP:N	2:D:139:PRO:CD	2.70	0.55
2:D:459:ILE:HD12	2:D:542:ILE:HD11	1.89	0.54
2:D:512:PHE:CE2	2:D:595:CYS:HB2	2.42	0.54
1:A:284:ASN:HD22	1:A:284:ASN:C	2.15	0.54
2:C:555:GLY:H	7:C:1737:GOL:H31	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:392:GLY:HA3	2:C:459:ILE:O	2.07	0.54
2:D:284:GLU:CD	2:D:284:GLU:N	2.64	0.54
2:D:352:LEU:HD22	2:D:481:ALA:HA	1.89	0.54
1:B:114[A]:CYS:SG	1:B:208:ILE:HG21	2.48	0.54
1:B:587:LYS:HE3	4:B:1677:XCC:S4	2.48	0.54
2:C:344:GLY:O	2:C:345:ASN:HB2	2.06	0.53
1:A:515:ASN:HD22	1:A:518:THR:CG2	2.22	0.53
1:A:515:ASN:HA	1:A:518:THR:HG23	1.88	0.53
2:D:340:VAL:HG23	2:D:430:VAL:HB	1.88	0.53
2:D:712:LEU:O	2:D:716:GLU:HG3	2.07	0.53
2:C:163:ALA:HB2	2:C:169:LEU:HG	1.90	0.53
2:C:501:ASP:OD1	7:C:1743:GOL:O2	2.26	0.53
1:A:196[A]:GLU:OE2	2:D:120:LYS:CE	2.57	0.53
2:C:340:VAL:HG11	2:C:373:ILE:HD11	1.90	0.53
2:C:189:ALA:HA	2:C:192:GLN:HE21	1.72	0.53
2:D:398:ASP:OD1	2:D:491:ARG:NH1	2.40	0.53
1:A:585:SER:HB2	1:B:220:HIS:CE1	2.44	0.52
1:B:573:LYS:HZ3	1:B:659:HIS:CD2	2.26	0.52
1:A:35:GLU:OE2	1:A:423:ILE:HD11	2.09	0.52
2:D:685:ARG:O	2:D:689:GLU:HG3	2.10	0.52
2:C:349:ALA:HA	2:C:384:LEU:O	2.09	0.52
2:D:171:LYS:O	2:D:175:GLU:HG3	2.10	0.52
1:A:573:LYS:HZ1	1:A:659:HIS:CD2	2.26	0.52
1:A:530:ARG:HH11	1:A:530:ARG:CG	2.22	0.52
2:D:365:LYS:HE2	2:D:367:GLU:OE2	2.09	0.52
2:D:392:GLY:HA3	2:D:459:ILE:O	2.09	0.52
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.75	0.51
6:B:1683:SO4:O1	14:B:2348:HOH:O	2.18	0.51
1:A:577[A]:VAL:HG21	1:A:645:ILE:HG23	1.91	0.51
2:C:187:ASP:HA	2:C:211:ASN:ND2	2.25	0.51
2:C:372:ASP:OD2	2:C:440:ARG:HG2	2.10	0.51
2:D:95:ASN:HD22	2:D:98:ASN:H	1.57	0.51
1:A:149:ARG:HD2	14:A:2106:HOH:O	2.11	0.51
2:D:205:ILE:O	2:D:205:ILE:HG13	2.11	0.51
2:C:16:LYS:NZ	2:C:284:GLU:CG	2.74	0.51
2:C:363:ASP:HB2	2:C:462:ARG:HD3	1.93	0.51
2:D:194:LEU:HD13	2:D:200:LEU:HD12	1.93	0.51
1:A:466:LEU:HD22	1:A:595:TRP:CZ2	2.46	0.50
1:A:571:THR:N	1:A:572:PRO:CD	2.74	0.50
2:D:588:MET:SD	2:D:604:ILE:HD13	2.50	0.50
1:A:577[B]:VAL:HG11	1:A:645:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:HIS:CE1	2:D:35:TYR:OH	2.63	0.50
2:C:316:ILE:HG13	2:C:317:LYS:N	2.26	0.50
1:B:201:HIS:HE1	2:C:35:TYR:OH	1.95	0.50
1:B:482:LEU:HD11	1:B:508:LEU:CD1	2.41	0.50
2:C:339:TYR:CG	2:C:435:VAL:HG21	2.46	0.50
2:D:340:VAL:HG21	2:D:373:ILE:CD1	2.41	0.50
1:A:114[A]:CYS:SG	1:A:208:ILE:HG21	2.51	0.50
2:C:160[B]:LEU:HD23	2:C:186:CYS:HB3	1.94	0.50
1:B:536:ASN:O	1:B:537:ILE:C	2.55	0.49
2:C:357:SER:O	2:C:360:GLU:N	2.35	0.49
2:C:316:ILE:O	2:C:317:LYS:CB	2.57	0.49
1:B:128:ALA:CB	1:B:164[A]:GLN:HG3	2.42	0.49
1:B:261:PRO:HA	1:B:429:ALA:O	2.13	0.49
2:D:339:TYR:CD2	2:D:435:VAL:HG21	2.48	0.49
2:D:349:ALA:HA	2:D:384:LEU:O	2.13	0.49
2:D:347:THR:HB	2:D:348:PRO:HD2	1.95	0.49
2:C:408:HIS:HD2	2:C:419:HIS:ND1	2.11	0.48
2:D:339:TYR:CE1	2:D:378:GLU:HG3	2.48	0.48
2:C:289:PRO:O	2:C:290:ASP:HB2	2.12	0.48
2:C:95:ASN:HD22	2:C:95:ASN:C	2.21	0.48
1:B:515:ASN:HA	1:B:518:THR:HG23	1.94	0.48
1:B:534:GLY:HA3	14:B:2241:HOH:O	2.13	0.48
1:B:577[B]:VAL:HG11	1:B:645:ILE:HG23	1.96	0.48
2:D:362:THR:HB	2:D:365:LYS:HB2	1.94	0.48
2:D:626:MET:HE3	2:D:631:LEU:HD21	1.94	0.48
1:A:362:ALA:HB3	7:A:1687:GOL:H32	1.96	0.48
1:B:659:HIS:HE1	2:C:191:GLU:OE1	1.97	0.48
2:C:383:PRO:O	2:C:469:THR:HA	2.14	0.48
2:C:592[B]:MET:HB2	2:C:592[B]:MET:HE2	1.69	0.48
2:D:611:ILE:HD12	2:D:613:ILE:CD1	2.39	0.48
2:D:626:MET:HG3	2:D:631:LEU:HG	1.95	0.48
1:B:537:ILE:HD13	1:B:537:ILE:H	1.79	0.47
2:D:95:ASN:HD22	2:D:95:ASN:C	2.22	0.47
2:D:478:MET:HE3	2:D:478:MET:HB3	1.77	0.47
1:A:530:ARG:HG3	1:A:530:ARG:NH1	2.24	0.47
2:D:626:MET:HE3	2:D:631:LEU:CD2	2.44	0.47
1:A:529:LYS:O	1:A:533:GLU:HG3	2.15	0.47
2:D:393:ARG:HG3	2:D:461:ASP:OD2	2.14	0.47
1:B:573:LYS:NZ	1:B:659:HIS:CD2	2.78	0.47
2:D:95:ASN:HD21	2:D:98:ASN:H	1.61	0.47
2:D:388:VAL:HG12	2:D:390:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:ALA:N	2:C:192:GLN:HE22	2.04	0.47
1:A:13:PRO:HG3	1:A:607:MET:CE	2.44	0.47
2:C:427:TRP:C	2:C:428:LEU:HD12	2.40	0.47
1:A:200:THR:OG1	1:A:201:HIS:HD2	1.98	0.46
2:C:164:LYS:HG2	2:C:298:TYR:CZ	2.51	0.46
2:D:376:ILE:CG2	2:D:377:PRO:HD2	2.44	0.46
1:A:220:HIS:CE1	1:B:585:SER:HB2	2.50	0.46
2:D:173:VAL:HB	2:D:183:LEU:HD11	1.97	0.46
2:D:704:ILE:HD13	2:D:704:ILE:N	2.30	0.46
1:B:284:ASN:HD22	1:B:285:PRO:N	2.13	0.46
1:B:571:THR:N	1:B:572:PRO:CD	2.79	0.46
2:C:602:MET:HE1	2:C:658:ILE:HG21	1.97	0.46
2:C:460:VAL:CG1	2:C:463:VAL:CG2	2.94	0.46
2:D:318:LEU:HD21	2:D:320:LEU:HD11	1.96	0.46
1:A:353:VAL:HB	1:B:223:MET:SD	2.56	0.45
2:D:187:ASP:HA	2:D:211:ASN:ND2	2.30	0.45
1:B:33:VAL:HG21	1:B:477:GLN:HE22	1.80	0.45
2:C:424:ASN:HB2	2:C:478:MET:SD	2.56	0.45
1:B:322:VAL:HG23	1:B:328:ILE:HB	1.97	0.45
2:C:383:PRO:HG2	2:C:469:THR:O	2.16	0.45
2:C:601:ILE:HG21	2:C:631:LEU:HG	1.98	0.45
1:A:284:ASN:HD21	1:A:286:LEU:HG	1.81	0.45
2:D:518:CYS:SG	2:D:527:LEU:HD13	2.57	0.45
7:A:1687:GOL:H12	14:A:2327:HOH:O	2.16	0.45
2:C:318:LEU:HD11	2:C:320:LEU:HD21	1.98	0.45
2:C:537:LYS:HZ1	7:C:1743:GOL:H31	1.79	0.45
2:D:362:THR:N	2:D:464:GLN:HE21	2.05	0.45
2:D:583:CYS:CB	2:D:586:THR:HG22	2.46	0.45
1:A:480:SER:HB2	1:A:582:GLU:HG2	1.98	0.45
1:B:114[B]:CYS:HB2	1:B:208:ILE:HG21	1.98	0.45
2:C:342:MET:CB	2:C:384:LEU:HB2	2.47	0.45
2:C:503:PHE:CZ	2:C:553:LYS:HD3	2.52	0.45
2:C:406[B]:ARG:NH1	2:C:409:ASP:CG	2.74	0.45
2:C:540:TYR:O	2:C:544:HIS:HD2	1.99	0.45
2:D:419:HIS:ND1	2:D:419:HIS:C	2.75	0.45
2:C:350:PHE:HA	2:C:424:ASN:HA	1.99	0.44
2:D:336:GLY:O	2:D:432:LYS:HE3	2.17	0.44
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.82	0.44
1:B:61:ILE:HD13	1:B:77:ARG:HD2	1.99	0.44
1:B:114[A]:CYS:SG	1:B:208:ILE:CG2	3.05	0.44
2:C:179:MET:HG2	2:C:313:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:362:THR:HG1	2:C:365:LYS:HD3	1.83	0.44
2:C:451:LYS:HA	2:C:451:LYS:HD2	1.76	0.44
2:C:613:ILE:O	2:C:671:PRO:HD3	2.18	0.44
1:B:110:ALA:O	1:B:114[B]:CYS:HB3	2.17	0.44
2:D:626:MET:HB2	2:D:630:THR:HB	1.99	0.44
2:C:571:LEU:HD13	2:C:579:LEU:HB3	1.99	0.44
2:D:558:ASP:HA	2:D:559:PRO:HD2	1.84	0.44
2:D:631:LEU:O	2:D:635:ILE:HG12	2.17	0.44
1:A:118:ASN:C	1:A:118:ASN:HD22	2.26	0.44
2:D:583:CYS:HB3	2:D:586:THR:HG22	1.99	0.44
1:A:33:VAL:HG21	1:A:477:GLN:HE22	1.83	0.44
1:A:55:GLN:NE2	14:A:2049:HOH:O	2.50	0.44
2:D:151:TRP:CH2	2:D:547:PRO:HD3	2.53	0.44
1:A:377:ASN:HB2	1:B:218:GLN:HG3	1.99	0.44
1:B:283:HIS:CE1	4:B:1677:XCC:S3	3.11	0.44
1:B:515:ASN:HD22	1:B:518:THR:HG23	1.81	0.43
2:C:16:LYS:HZ3	2:C:284:GLU:HG3	1.81	0.43
2:C:74:LYS:HE3	14:C:2068:HOH:O	2.17	0.43
2:D:602:MET:HE3	2:D:611:ILE:HD13	1.99	0.43
2:D:681[A]:GLU:OE2	2:D:684:ARG:NH1	2.51	0.43
1:A:9:HIS:C	1:A:9:HIS:CD2	2.95	0.43
2:D:170:ALA:O	2:D:174:LYS:HG3	2.18	0.43
1:B:606:THR:C	1:B:636:MET:HE2	2.43	0.43
2:C:657:PHE:O	2:C:658:ILE:C	2.61	0.43
1:A:370:ARG:NH2	1:A:410:GLU:OE1	2.32	0.43
1:A:466:LEU:HD22	1:A:595:TRP:HZ2	1.83	0.43
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.49	0.43
1:B:615:LEU:HD23	1:B:615:LEU:C	2.44	0.43
2:C:180:GLY:HA2	2:C:326:PRO:HG2	1.99	0.43
2:C:356:VAL:HG21	2:C:361:ILE:HG23	2.00	0.43
2:D:420:THR:HG22	2:D:427:TRP:HB3	2.01	0.43
2:D:572:TYR:HA	2:D:579:LEU:O	2.18	0.43
1:A:114[A]:CYS:SG	1:A:208:ILE:CG2	3.06	0.43
2:D:628:PHE:O	2:D:629:SER:C	2.61	0.43
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.48	0.43
1:B:20:MET:O	1:B:21:GLU:C	2.61	0.43
2:C:476:GLU:CG	2:C:477:TYR:N	2.82	0.43
2:D:64:VAL:HG13	2:D:111:GLU:OE2	2.17	0.43
2:D:163:ALA:CB	2:D:169:LEU:HB2	2.49	0.43
2:D:376:ILE:HG22	2:D:377:PRO:HD2	2.01	0.43
2:D:441:PHE:O	2:D:444:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ARG:CG	1:A:530:ARG:NH1	2.82	0.43
1:B:515:ASN:ND2	1:B:518:THR:HG21	2.32	0.43
1:B:486:LYS:NZ	7:B:1689:GOL:C3	2.82	0.43
2:C:568:ASN:ND2	2:C:581:GLN:HE21	2.14	0.43
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.34	0.42
1:B:284:ASN:HD21	1:B:286:LEU:HG	1.84	0.42
2:C:334:ARG:HA	2:C:334:ARG:HD2	1.75	0.42
2:D:147:LYS:HA	2:D:147:LYS:HD2	1.79	0.42
1:A:13:PRO:HG3	1:A:607:MET:HE1	2.01	0.42
1:A:480:SER:HB2	1:A:582:GLU:CG	2.49	0.42
2:D:157:ALA:HB3	2:D:183:LEU:HD23	1.97	0.42
2:D:329:GLU:HG3	2:D:412:ASN:HB3	2.02	0.42
1:A:577[A]:VAL:HG21	1:A:645:ILE:CG2	2.50	0.42
1:B:626:ASP:HB3	2:C:212:PHE:CG	2.54	0.42
2:C:373:ILE:HD13	2:C:373:ILE:HA	1.72	0.42
2:D:621:MET:SD	2:D:625:GLY:C	3.03	0.42
2:C:340:VAL:CG1	2:C:373:ILE:HD11	2.49	0.42
2:D:426:ASN:C	2:D:426:ASN:HD22	2.27	0.42
1:B:201:HIS:CE1	2:C:35:TYR:OH	2.71	0.41
1:B:577[A]:VAL:HG21	1:B:645:ILE:CG2	2.47	0.41
2:C:147:LYS:NZ	2:C:329:GLU:OE1	2.46	0.41
2:D:355:THR:HG23	2:D:395:MET:HG3	2.02	0.41
1:B:138:LYS:HG3	1:B:255:LEU:O	2.20	0.41
2:D:202:ILE:HD13	2:D:207:TYR:HD1	1.84	0.41
2:D:388:VAL:CG1	2:D:390:ILE:HD11	2.50	0.41
1:B:398:LYS:O	1:B:402:ARG:HG3	2.21	0.41
2:C:540:TYR:CD1	2:C:550:PRO:HD3	2.55	0.41
2:D:219:ALA:O	2:D:223:LEU:HB2	2.20	0.41
2:C:1:MET:HG3	2:C:5:ASP:HB2	2.02	0.41
2:D:6:LYS:HA	2:D:9:GLU:HG3	2.02	0.41
2:D:137:GLY:C	2:D:139:PRO:HD2	2.45	0.41
2:D:350:PHE:HD2	2:D:478:MET:HG2	1.83	0.41
1:A:370:ARG:HG2	1:A:407:ALA:HB2	2.03	0.41
1:B:238:ALA:O	1:B:241:ASP:HB3	2.20	0.41
2:C:316:ILE:HD11	2:C:318:LEU:HB3	2.01	0.41
2:D:339:TYR:HD2	2:D:340:VAL:HG22	1.86	0.41
2:D:501:ASP:C	2:D:553:LYS:HG3	2.45	0.41
1:B:320:ASN:O	1:B:324:MET:HG2	2.20	0.41
2:C:564:TRP:CZ3	2:C:584:LEU:HD12	2.55	0.41
1:B:278:PHE:HB3	1:B:312:LEU:HD23	2.02	0.41
2:C:204:TYR:C	2:C:205:ILE:HG13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:ARG:O	2:D:89:GLN:HG3	2.21	0.41
2:D:145:GLY:O	2:D:148:MET:HB2	2.21	0.41
2:D:164:LYS:HE3	2:D:298:TYR:CD2	2.55	0.41
1:A:113:HIS:NE2	1:A:550[A]:CYS:SG	2.86	0.41
2:C:86:LYS:HA	2:C:86:LYS:HD2	1.87	0.41
2:C:448:LEU:HD12	2:C:448:LEU:HA	1.70	0.41
2:D:615:THR:HG21	2:D:674:LEU:HG	2.03	0.41
2:C:343:GLY:O	2:C:346:ARG:HG2	2.20	0.40
2:C:641:THR:O	2:C:642:PRO:C	2.64	0.40
2:D:282:LEU:CD1	2:D:287:GLN:HG2	2.50	0.40
1:A:7:LEU:HD11	2:D:164:LYS:HB2	2.03	0.40
2:C:167:LYS:HG3	14:C:2125:HOH:O	2.20	0.40
1:A:5:ARG:NH1	1:A:650:GLU:OE2	2.54	0.40
2:C:358:GLU:OE2	2:C:462:ARG:NH2	2.54	0.40
2:D:80:PRO:HB2	7:D:1736:GOL:H2	2.03	0.40
2:D:86:LYS:HA	2:D:86:LYS:HD2	1.91	0.40
1:B:410:GLU:HG3	14:B:2222:HOH:O	2.22	0.40
2:C:424:ASN:HD22	2:C:424:ASN:N	2.06	0.40
2:D:223:LEU:HD12	2:D:223:LEU:HA	1.94	0.40
2:D:277:ILE:HD12	2:D:277:ILE:N	2.36	0.40
2:D:621:MET:HE1	2:D:625:GLY:CA	2.45	0.40
2:C:122:LYS:HD2	2:C:125:GLU:OE1	2.22	0.40
2:D:143:ARG:HD2	2:D:144:PHE:CE1	2.56	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)
1:B:303:LYS:NZ	1:B:667:GLU:OE2[4_656]	2.17	0.03

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	683/674 (101%)	664 (97%)	18 (3%)	1 (0%)	48	40
1	B	683/674 (101%)	659 (96%)	21 (3%)	3 (0%)	30	22
2	C	738/729 (101%)	710 (96%)	22 (3%)	6 (1%)	16	8
2	D	728/729 (100%)	705 (97%)	20 (3%)	3 (0%)	30	22
All	All	2832/2806 (101%)	2738 (97%)	81 (3%)	13 (0%)	24	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	537	ILE
2	C	316	ILE
2	C	317	LYS
2	D	658	ILE
1	A	267	ASN
1	B	267	ASN
2	C	596	GLY
2	D	596	GLY
2	C	315	LYS
2	D	187	ASP
1	B	354	GLN
2	C	187	ASP
2	C	658	ILE

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	554/543 (102%)	541 (98%)	13 (2%)	44	40
1	B	554/543 (102%)	538 (97%)	16 (3%)	37	31
2	C	622/611 (102%)	581 (93%)	41 (7%)	15	8
2	D	612/611 (100%)	560 (92%)	52 (8%)	10	4
All	All	2342/2308 (102%)	2220 (95%)	122 (5%)	21	13

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	27	ARG
1	A	44	LYS
1	A	206	PHE
1	A	217	ASN
1	A	284	ASN
1	A	470	CYS
1	A	482	LEU
1	A	518	THR
1	A	530	ARG
1	A	537	ILE
1	A	538	GLU
1	A	665	ARG
1	B	27	ARG
1	B	66	ILE
1	B	206	PHE
1	B	217	ASN
1	B	218	GLN
1	B	284	ASN
1	B	308	LYS
1	B	326	GLN
1	B	406	GLU
1	B	415	ASN
1	B	466	LEU
1	B	470	CYS
1	B	518	THR
1	B	538	GLU
1	B	639	GLN
1	B	656	LEU
2	C	14	GLU
2	C	16	LYS
2	C	95	ASN
2	C	122	LYS
2	C	127	LEU
2	C	169	LEU
2	C	198	VAL
2	C	205	ILE
2	C	286	LYS
2	C	315	LYS
2	C	316	ILE
2	C	317	LYS
2	C	319	ASP
2	C	338	MET

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Mol	Chain	Res	Type
2	C	341	GLU
2	C	342	MET
2	C	345	ASN
2	C	346	ARG
2	C	359	SER
2	C	360	GLU
2	C	367	GLU
2	C	368	VAL
2	C	373	ILE
2	C	375	GLN
2	C	390	ILE
2	C	406[A]	ARG
2	C	406[B]	ARG
2	C	422	GLN
2	C	424	ASN
2	C	426	ASN
2	C	440	ARG
2	C	448	LEU
2	C	471	GLU
2	C	474	VAL
2	C	476	GLU
2	C	479	GLU
2	C	571	LEU
2	C	604	ILE
2	C	634	MET
2	C	674	LEU
2	C	728	ILE
2	D	16	LYS
2	D	64	VAL
2	D	95	ASN
2	D	120	LYS
2	D	147	LYS
2	D	160	LEU
2	D	172	ILE
2	D	173	VAL
2	D	194	LEU
2	D	197	ASN
2	D	198	VAL
2	D	223	LEU
2	D	246	ARG
2	D	286	LYS
2	D	313	LEU

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Mol	Chain	Res	Type
2	D	340	VAL
2	D	342	MET
2	D	346	ARG
2	D	358	GLU
2	D	373	ILE
2	D	390	ILE
2	D	419	HIS
2	D	422	GLN
2	D	425	ILE
2	D	426	ASN
2	D	433	ASP
2	D	448	LEU
2	D	462	ARG
2	D	471	GLU
2	D	478	MET
2	D	479	GLU
2	D	484	LYS
2	D	501	ASP
2	D	527	LEU
2	D	554	GLU
2	D	565	LYS
2	D	579	LEU
2	D	584	LEU
2	D	598	PHE
2	D	604	ILE
2	D	621	MET
2	D	626	MET
2	D	634	MET
2	D	639	THR
2	D	670	MET
2	D	674	LEU
2	D	685	ARG
2	D	704	ILE
2	D	708	VAL
2	D	711	ILE
2	D	717	GLU
2	D	729	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN

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Mol	Chain	Res	Type
1	A	58	GLN
1	A	164	GLN
1	A	201	HIS
1	A	217	ASN
1	A	218	GLN
1	A	275	GLN
1	A	284	ASN
1	A	326	GLN
1	A	368	HIS
1	A	443	GLN
1	A	447	ASN
1	A	471	ASN
1	A	477	GLN
1	A	503	GLN
1	A	515	ASN
1	A	659	HIS
1	B	55	GLN
1	B	58	GLN
1	B	122	HIS
1	B	201	HIS
1	B	217	ASN
1	B	218	GLN
1	B	284	ASN
1	B	326	GLN
1	B	368	HIS
1	B	415	ASN
1	B	425	ASN
1	B	447	ASN
1	B	471	ASN
1	B	477	GLN
1	B	479	ASN
1	B	503	GLN
1	B	515	ASN
1	B	659	HIS
2	C	95	ASN
2	C	192	GLN
2	C	211	ASN
2	C	408	HIS
2	C	422	GLN
2	C	424	ASN
2	C	426	ASN
2	C	510	GLN

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Mol	Chain	Res	Type
2	C	515	ASN
2	C	544	HIS
2	C	576	ASN
2	C	581	GLN
2	C	590	ASN
2	C	640	GLN
2	D	95	ASN
2	D	211	ASN
2	D	244	GLN
2	D	345	ASN
2	D	396	GLN
2	D	408	HIS
2	D	422	GLN
2	D	426	ASN
2	D	464	GLN
2	D	510	GLN
2	D	581	GLN
2	D	590	ASN
2	D	640	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 7 are monoatomic - leaving 51 for Mogul analysis.

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	$\# Z > 2$
3	SF4	C	1730	2	0,12,12	-	-	-		
6	SO4	B	1684	-	4,4,4	0.25	0	6,6,6	0.15	0
6	SO4	B	1685	-	4,4,4	0.19	0	6,6,6	0.24	0
6	SO4	B	1687	-	4,4,4	0.23	0	6,6,6	0.18	0
7	GOL	A	1687	-	5,5,5	0.46	0	5,5,5	1.08	0
7	GOL	C	1737	-	5,5,5	0.30	0	5,5,5	0.37	0
6	SO4	A	1682	-	4,4,4	0.23	0	6,6,6	0.26	0
6	SO4	B	1682	-	4,4,4	0.33	0	6,6,6	0.38	0
6	SO4	A	1681	-	4,4,4	0.22	0	6,6,6	0.22	0
6	SO4	B	1681	-	4,4,4	0.33	0	6,6,6	0.24	0
6	SO4	C	1736	-	4,4,4	0.28	0	6,6,6	0.42	0
7	GOL	C	1739	-	5,5,5	0.34	0	5,5,5	0.49	0
6	SO4	C	1734	-	4,4,4	0.29	0	6,6,6	0.42	0
3	SF4	B	1676	1	0,12,12	-	-	-		
4	XCC	A	1677	1	0,11,11	-	-	-		
5	FOR	A	1678	-	0,1,1	-	-	-		
5	FOR	B	1678	-	0,1,1	-	-	-		
6	SO4	D	1734	-	4,4,4	0.24	0	6,6,6	0.18	0
7	GOL	D	1736	-	5,5,5	0.52	0	5,5,5	0.68	0
13	ACT	D	1733	11	3,3,3	0.74	0	3,3,3	1.51	0
3	SF4	B	1675	1	0,12,12	-	-	-		
6	SO4	A	1688	-	4,4,4	0.31	0	6,6,6	0.26	0
6	SO4	B	1683	-	4,4,4	0.27	0	6,6,6	0.47	0
6	SO4	D	1735	-	4,4,4	0.18	0	6,6,6	0.19	0
6	SO4	C	1738	-	4,4,4	0.27	0	6,6,6	0.27	0
6	SO4	A	1683	-	4,4,4	0.24	0	6,6,6	0.28	0
6	SO4	A	1684	-	4,4,4	0.28	0	6,6,6	0.52	0
6	SO4	A	1689	-	4,4,4	0.29	0	6,6,6	0.17	0
6	SO4	A	1679	-	4,4,4	0.43	0	6,6,6	0.37	0
6	SO4	C	1740	-	4,4,4	0.45	0	6,6,6	0.46	0
12	SX	C	1733	10	0,1,1	-	-	-		
4	XCC	B	1677	1	0,11,11	-	-	-		
3	SF4	A	1676	1	0,12,12	-	-	-		
6	SO4	C	1735	-	4,4,4	0.27	0	6,6,6	0.64	0
6	SO4	D	1738	-	4,4,4	0.30	0	6,6,6	0.16	0
7	GOL	B	1690	-	5,5,5	0.47	0	5,5,5	0.21	0
6	SO4	B	1688	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	A	1680	-	4,4,4	0.29	0	6,6,6	0.38	0
6	SO4	A	1690	-	4,4,4	0.21	0	6,6,6	0.31	0
6	SO4	B	1679	-	4,4,4	0.24	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCT	B	1691	-	3,3,3	0.82	0	2,3,3	0.52	0
6	SO4	A	1685	-	4,4,4	0.31	0	6,6,6	0.21	0
3	SF4	D	1730	2	0,12,12	-	-	-		
6	SO4	A	1686	-	4,4,4	0.24	0	6,6,6	0.14	0
6	SO4	B	1680	-	4,4,4	0.25	0	6,6,6	0.42	0
6	SO4	B	1686	-	4,4,4	0.29	0	6,6,6	0.26	0
6	SO4	C	1742	-	4,4,4	0.24	0	6,6,6	0.12	0
7	GOL	B	1689	-	5,5,5	0.39	0	5,5,5	0.26	0
6	SO4	D	1737	-	4,4,4	0.25	0	6,6,6	0.11	0
7	GOL	C	1741	-	5,5,5	0.35	0	5,5,5	0.56	0
7	GOL	C	1743	-	5,5,5	0.52	0	5,5,5	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	C	1730	2	-	-	0/6/5/5
7	GOL	A	1687	-	-	4/4/4/4	-
7	GOL	C	1737	-	-	4/4/4/4	-
3	SF4	B	1675	1	-	-	0/6/5/5
3	SF4	D	1730	2	-	-	0/6/5/5
7	GOL	C	1739	-	-	0/4/4/4	-
7	GOL	B	1690	-	-	1/4/4/4	-
3	SF4	A	1676	1	-	-	0/6/5/5
3	SF4	B	1676	1	-	-	0/6/5/5
4	XCC	B	1677	1	-	-	0/3/3/3
4	XCC	A	1677	1	-	-	0/3/3/3
7	GOL	B	1689	-	-	1/4/4/4	-
7	GOL	C	1741	-	-	2/4/4/4	-
7	GOL	C	1743	-	-	2/4/4/4	-
7	GOL	D	1736	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1687	GOL	O1-C1-C2-O2
7	A	1687	GOL	O1-C1-C2-C3
7	A	1687	GOL	C1-C2-C3-O3
7	C	1737	GOL	O1-C1-C2-C3
7	C	1741	GOL	O1-C1-C2-C3
7	C	1743	GOL	O1-C1-C2-C3
7	D	1736	GOL	O1-C1-C2-O2
7	D	1736	GOL	O1-C1-C2-C3
7	D	1736	GOL	C1-C2-C3-O3
7	D	1736	GOL	O2-C2-C3-O3
7	B	1690	GOL	C1-C2-C3-O3
7	C	1737	GOL	C1-C2-C3-O3
7	A	1687	GOL	O2-C2-C3-O3
7	C	1737	GOL	O1-C1-C2-O2
7	C	1737	GOL	O2-C2-C3-O3
7	C	1741	GOL	O1-C1-C2-O2
7	B	1689	GOL	O2-C2-C3-O3
7	C	1743	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1687	GOL	2	0
7	C	1737	GOL	2	0
4	A	1677	XCC	2	0
7	D	1736	GOL	1	0
6	B	1683	SO4	1	0
4	B	1677	XCC	3	0
6	B	1688	SO4	1	0
6	B	1679	SO4	1	0
9	B	1691	BCT	1	0
7	B	1689	GOL	10	0
7	C	1741	GOL	1	0
7	C	1743	GOL	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	673/674 (99%)	-0.24	5 (0%) 84 86	5, 10, 19, 32	26 (3%)
1	B	673/674 (99%)	-0.23	10 (1%) 72 75	5, 10, 19, 39	29 (4%)
2	C	729/729 (100%)	-0.02	44 (6%) 27 29	3, 10, 22, 35	18 (2%)
2	D	728/729 (99%)	0.33	55 (7%) 20 21	4, 11, 20, 39	9 (1%)
All	All	2803/2806 (99%)	-0.03	114 (4%) 41 44	3, 10, 21, 39	82 (2%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	536	ASN	5.9
2	C	348	PRO	5.1
1	B	537	ILE	4.8
2	D	480	VAL	4.8
2	C	1	MET	4.6
2	D	481	ALA	4.6
2	D	313	LEU	4.4
2	C	367	GLU	4.3
1	B	539	ILE	4.3
2	C	316	ILE	4.2
2	D	485	TYR	4.1
2	D	399	PHE	4.1
2	C	313	LEU	4.1
2	D	336	GLY	3.9
2	D	345	ASN	3.9
1	A	538	GLU	3.6
2	C	382	LEU	3.6
1	B	538	GLU	3.6
2	D	402	VAL	3.5
2	C	317	LYS	3.5
2	D	632	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	8	SER	3.5
2	D	469	THR	3.5
2	D	392	GLY	3.4
2	D	151	TRP	3.3
2	C	402	VAL	3.3
2	C	15	GLY	3.3
2	C	319	ASP	3.3
2	D	631	LEU	3.2
2	C	468	PHE	3.2
2	C	440	ARG	3.2
2	D	377	PRO	3.2
2	C	377	PRO	3.1
2	D	708	VAL	3.1
2	C	472	ALA	3.1
2	C	339	TYR	3.1
2	D	123	PRO	3.1
2	C	376	ILE	3.0
2	C	470	ASP	3.0
2	C	469	THR	3.0
2	D	15	GLY	3.0
2	D	470	ASP	2.9
2	C	330	GLY	2.9
2	D	396	GLN	2.9
2	D	458	ALA	2.9
2	C	336	GLY	2.9
2	D	339	TYR	2.8
2	C	392	GLY	2.8
1	B	368	HIS	2.8
1	A	536	ASN	2.8
2	D	435	VAL	2.8
2	C	374	ASP	2.8
1	A	8	SER	2.8
2	C	458	ALA	2.8
2	D	397	ALA	2.7
2	D	405	ARG	2.7
2	D	382	LEU	2.7
2	D	471	GLU	2.7
2	D	398	ASP	2.6
2	C	312	LYS	2.6
2	D	380	SER	2.6
1	B	388	TYR	2.6
2	D	395	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	2.5
2	D	436	ALA	2.5
2	D	617	ASP	2.5
2	D	356	VAL	2.5
2	D	374	ASP	2.5
2	D	491	ARG	2.4
1	B	417	PRO	2.4
2	C	379	GLY	2.4
2	C	384	LEU	2.4
2	D	577	ARG	2.4
2	C	405	ARG	2.4
2	D	630	THR	2.3
2	C	436	ALA	2.3
2	D	373	ILE	2.3
1	B	533	GLU	2.3
2	D	391	TYR	2.3
2	D	349	ALA	2.3
2	C	124	ASP	2.3
2	D	390	ILE	2.3
1	B	419	TYR	2.2
2	C	441	PHE	2.2
1	A	537	ILE	2.2
2	D	728	ILE	2.2
2	C	421	GLY	2.2
2	D	642	PRO	2.2
2	D	376	ILE	2.2
2	D	564	TRP	2.2
2	C	315	LYS	2.2
2	C	361	ILE	2.1
2	D	375	GLN	2.1
2	D	347	THR	2.1
2	D	474	VAL	2.1
2	D	729	MET	2.1
2	C	430	VAL	2.1
2	D	440	ARG	2.1
2	D	583	CYS	2.1
2	D	333	ILE	2.1
2	D	416	GLY	2.1
2	C	340	VAL	2.1
2	C	345	ASN	2.1
2	C	435	VAL	2.1
2	C	284	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	355	THR	2.0
2	D	379	GLY	2.0
2	C	368	VAL	2.0
2	D	460	VAL	2.0
2	C	334	ARG	2.0
2	C	369	ILE	2.0
2	C	373	ILE	2.0
2	C	321	PRO	2.0
2	C	346	ARG	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
13	ACT	D	1733	4/4	0.42	0.34	18,18,19,19	4
5	FOR	B	1678	2/2	0.73	0.21	23,23,23,24	2
7	GOL	D	1736	6/6	0.78	0.15	41,45,47,48	0
7	GOL	C	1737	6/6	0.79	0.13	36,37,38,38	0
6	SO4	C	1740	5/5	0.80	0.14	19,25,26,27	5
6	SO4	A	1689	5/5	0.81	0.19	48,49,50,50	5
6	SO4	B	1683	5/5	0.82	0.18	33,33,35,36	5
7	GOL	A	1687	6/6	0.83	0.13	29,31,33,34	0
6	SO4	A	1688	5/5	0.84	0.11	59,60,60,61	0
5	FOR	A	1678	2/2	0.84	0.19	23,23,23,23	2
6	SO4	B	1686	5/5	0.85	0.09	58,58,59,60	0
6	SO4	D	1738	5/5	0.85	0.11	58,59,59,60	0
7	GOL	B	1690	6/6	0.86	0.15	58,60,61,61	0
6	SO4	D	1734	5/5	0.86	0.15	30,30,30,31	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	C	1743	6/6	0.86	0.14	50,52,53,53	0
6	SO4	B	1687	5/5	0.86	0.18	51,51,51,52	5
6	SO4	A	1686	5/5	0.86	0.12	36,36,37,39	5
7	GOL	B	1689	6/6	0.88	0.15	54,55,56,57	0
6	SO4	C	1734	5/5	0.88	0.12	15,16,23,23	5
6	SO4	C	1735	5/5	0.88	0.13	33,35,35,36	0
6	SO4	A	1684	5/5	0.90	0.08	38,38,39,39	0
6	SO4	C	1742	5/5	0.90	0.08	31,31,31,32	0
6	SO4	B	1684	5/5	0.90	0.09	59,59,61,61	0
11	NI	D	1731[A]	1/1	0.90	0.10	17,17,17,17	1
11	NI	D	1731[B]	1/1	0.90	0.10	16,16,16,16	1
6	SO4	D	1737	5/5	0.90	0.11	61,61,61,62	5
7	GOL	C	1741	6/6	0.91	0.12	21,30,33,38	0
6	SO4	B	1685	5/5	0.91	0.11	59,59,60,60	0
6	SO4	C	1736	5/5	0.92	0.12	27,30,31,31	0
6	SO4	A	1683	5/5	0.92	0.10	33,33,34,35	0
6	SO4	B	1680	5/5	0.93	0.11	29,31,32,33	0
6	SO4	A	1682	5/5	0.93	0.09	26,28,28,29	0
6	SO4	A	1690	5/5	0.94	0.08	49,50,51,52	0
6	SO4	A	1679	5/5	0.94	0.12	18,18,21,25	0
9	BCT	B	1691	4/4	0.94	0.10	36,37,37,38	0
4	XCC	A	1677	9/9	0.95	0.12	17,17,23,24	9
8	FE2	A	1700	1/1	0.95	0.10	22,22,22,22	1
6	SO4	D	1735	5/5	0.95	0.08	33,33,35,35	0
6	SO4	B	1681	5/5	0.95	0.10	31,34,35,36	0
6	SO4	B	1688	5/5	0.95	0.09	42,45,46,46	5
6	SO4	B	1682	5/5	0.95	0.14	29,31,31,31	0
4	XCC	B	1677	9/9	0.96	0.11	17,17,22,23	9
6	SO4	B	1679	5/5	0.96	0.08	24,24,26,28	0
6	SO4	A	1680	5/5	0.96	0.09	23,23,24,26	0
6	SO4	A	1681	5/5	0.96	0.09	33,34,36,36	0
6	SO4	A	1685	5/5	0.97	0.11	28,30,32,32	0
7	GOL	C	1739	6/6	0.97	0.05	10,16,17,19	0
6	SO4	C	1738	5/5	0.98	0.06	21,23,25,27	0
8	FE2	B	1700	1/1	0.98	0.08	20,20,20,20	1
3	SF4	D	1730	8/8	0.99	0.06	9,9,10,11	0
3	SF4	A	1676	8/8	0.99	0.08	7,8,8,9	0
3	SF4	B	1675	8/8	0.99	0.10	9,11,11,12	0
3	SF4	B	1676	8/8	0.99	0.07	7,8,8,9	0
11	NI	D	1732	1/1	0.99	0.06	9,9,9,9	0
12	SX	C	1733	2/2	0.99	0.10	15,15,15,18	0
3	SF4	C	1730	8/8	0.99	0.03	5,7,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NI	C	1732	1/1	1.00	0.03	9,9,9,9	0
10	ZN	C	1731	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.