



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID : 1OAO  
Title : NIZN[FE4S4] AND NINI[FE4S4] CLUSTERS IN CLOSED AND OPEN ALPHA SUBUNITS OF ACETYL-COA SYNTHASE/CARBON MONOXIDE DEHYDROGENASE  
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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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

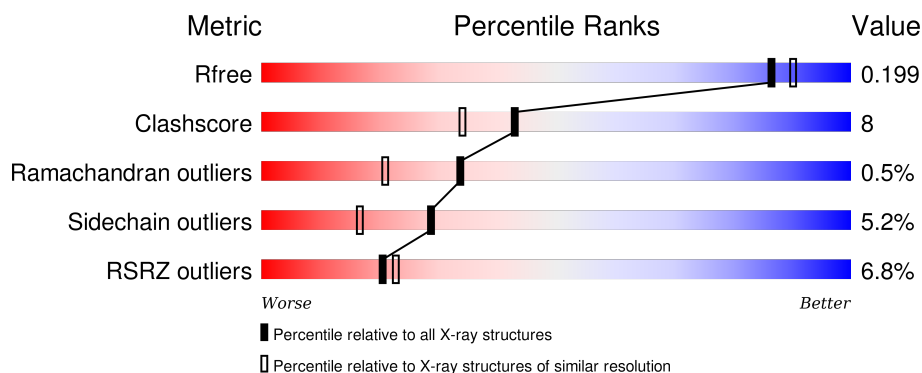
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	674	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	674	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	C	729	<div> <div>9%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
2	D	729	<div> <div>13%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>

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
12	SX	C	1733	-	-	-	X
13	ACT	D	1733	-	-	-	X
4	XCC	A	1677	-	-	X	-
4	XCC	B	1677	-	-	X	-
5	FOR	A	1678	-	-	-	X
5	FOR	B	1678	-	-	-	X
6	SO4	A	1689	-	-	-	X
6	SO4	B	1679	-	-	-	X
6	SO4	D	1738	-	-	-	X
7	GOL	A	1687	-	-	-	X
7	GOL	B	1689	-	-	X	X
7	GOL	B	1690	-	-	-	X
7	GOL	C	1743	-	-	X	-
7	GOL	D	1736	-	-	-	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.

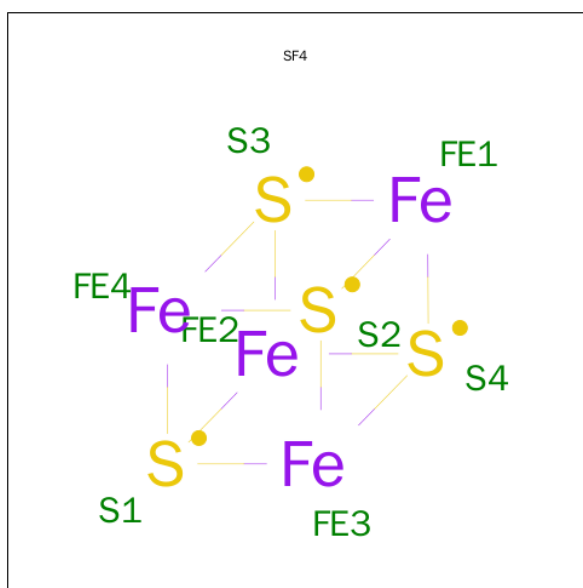
- Molecule 1 is a protein called CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA.

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.

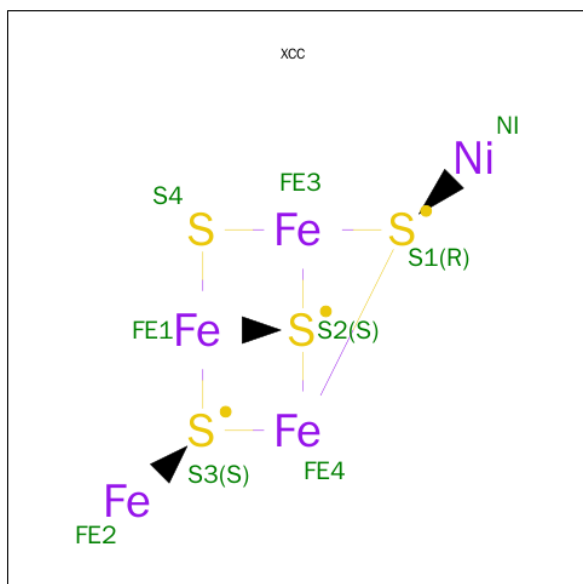
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	729	Total	C	N	O	S	0	11	0
			5788	3712	963	1076	37			
2	D	728	Total	C	N	O	S	0	2	0
			5745	3684	956	1070	35			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



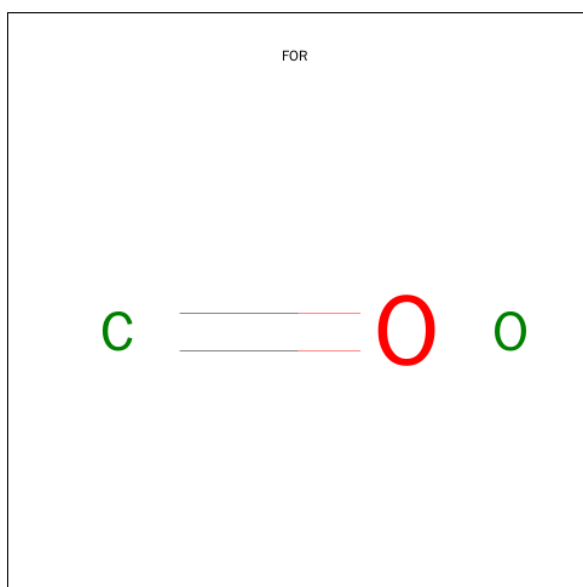
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula:  $\text{Fe}_4\text{NiS}_4$ ).



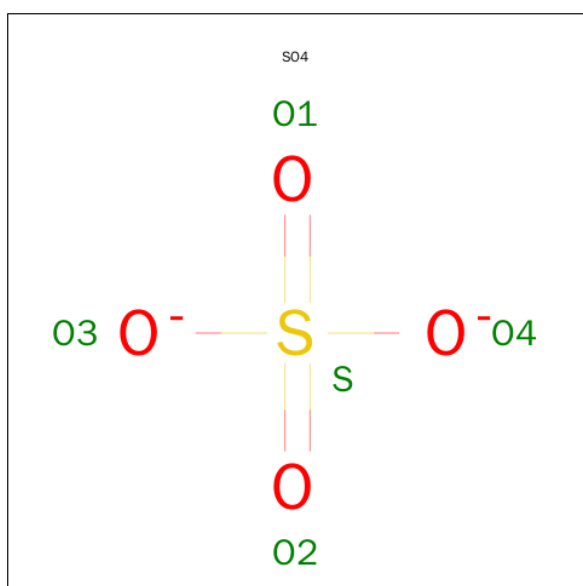
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is FORMYL GROUP (three-letter code: FOR) (formula:  $\text{CH}_2\text{O}$ ).



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 (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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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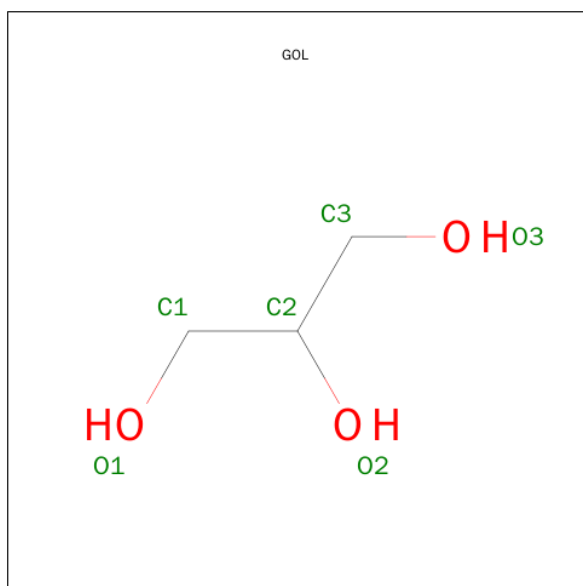
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	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 (three-letter code: 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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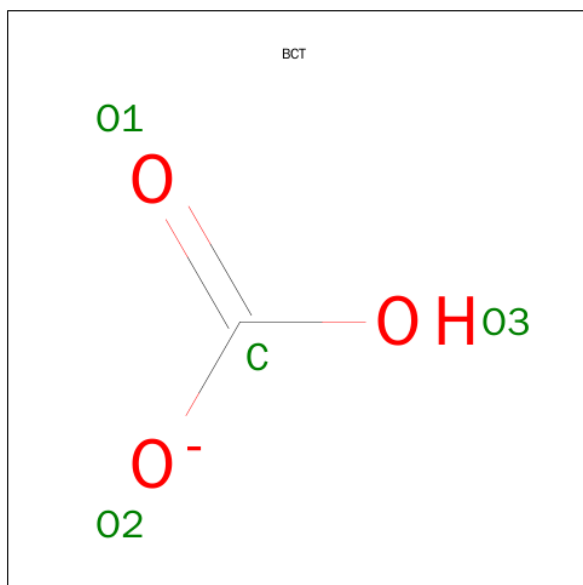
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 9 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

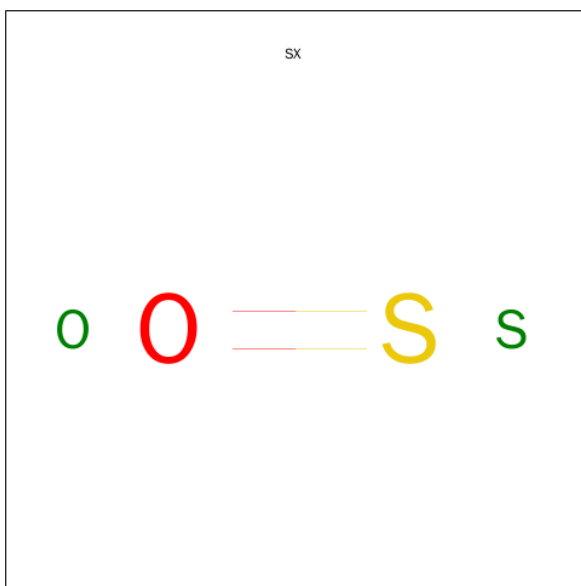
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

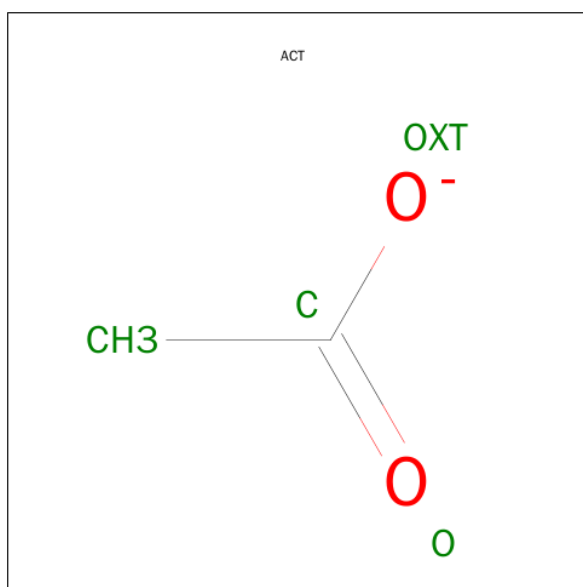
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Ni	0	1
			3	3		
11	C	1	Total	Ni	0	0
			1	1		

- Molecule 12 is SULFUR OXIDE (three-letter code: 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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

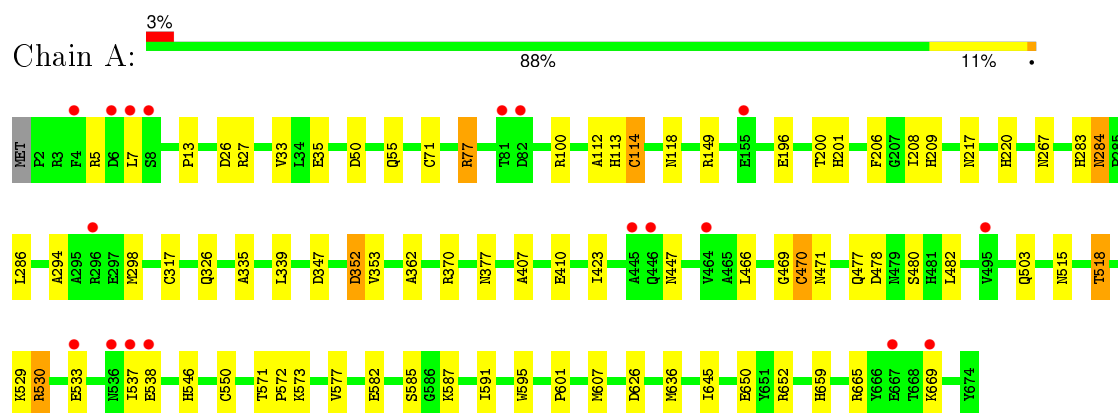
- Molecule 14 is water.

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		

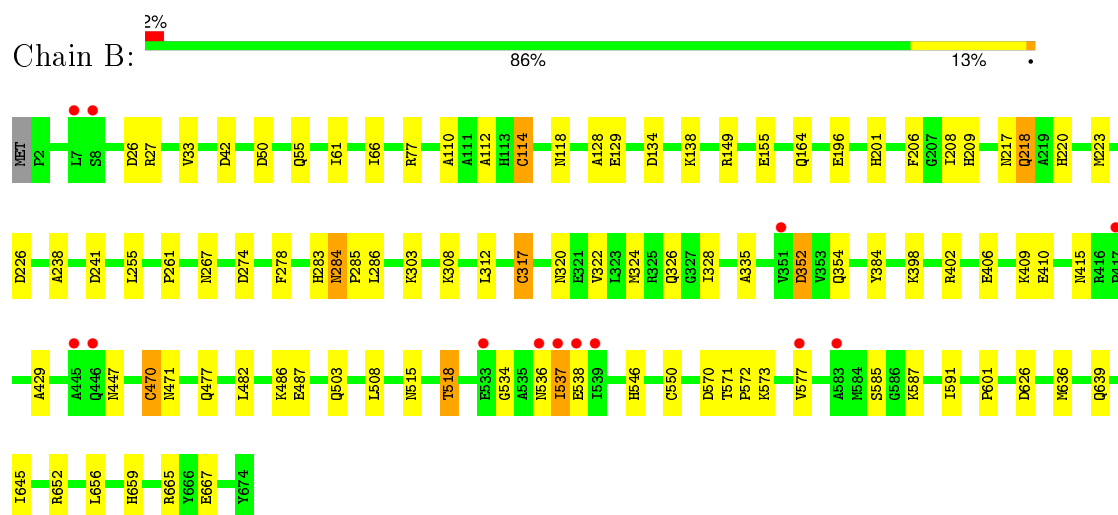
### 3 Residue-property plots [i](#)

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

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

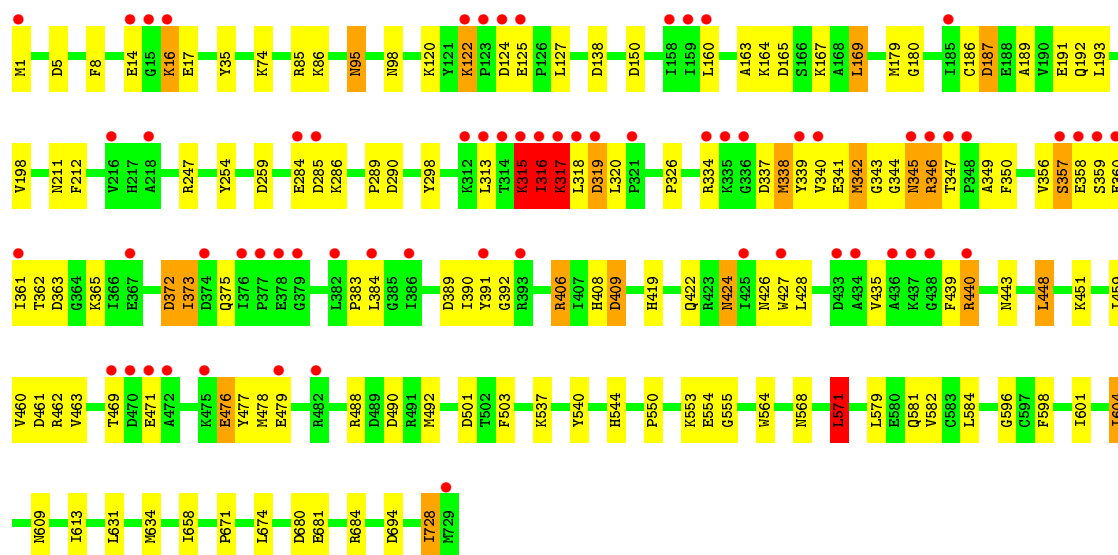


#### • Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

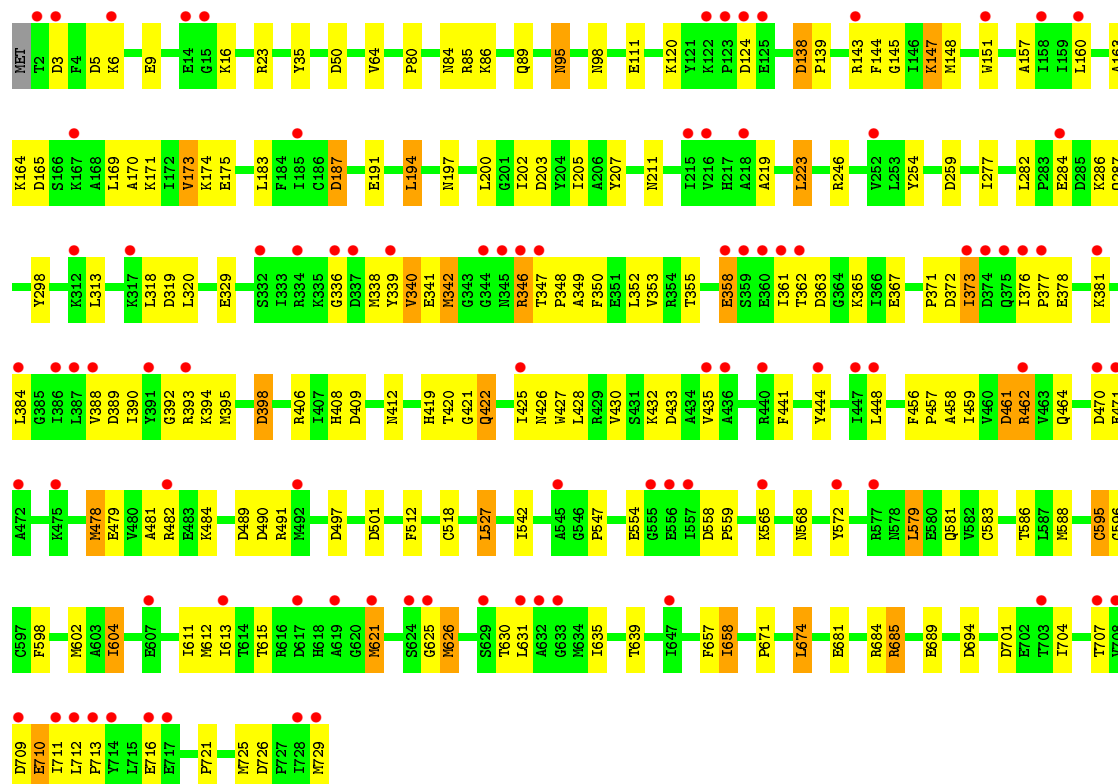
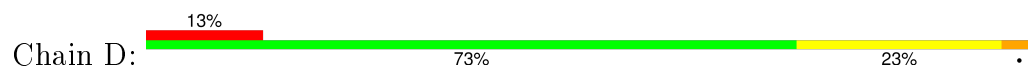


#### • Molecule 2: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA





● 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, $\alpha$ , $\beta$ , $\gamma$	244.57Å 81.89Å 167.22Å 90.00° 96.19° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 29.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (25.00-1.90) 97.8 (29.17-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	12688 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 252670 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	0/5275	0.78	12/7148 (0.2%)
1	B	0.65	0/5278	0.79	12/7152 (0.2%)
2	C	0.60	1/5973 (0.0%)	0.79	18/8087 (0.2%)
2	D	0.47	1/5888 (0.0%)	0.74	21/7974 (0.3%)
All	All	0.59	2/22414 (0.0%)	0.78	63/30361 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	357	SER	C-O	6.54	1.35	1.23
2	D	710	GLU	CD-OE2	6.19	1.32	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	85	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	114[A]	CYS	CA-CB-SG	-8.33	99.01	114.00
1	B	114[B]	CYS	CA-CB-SG	-8.33	99.01	114.00
1	A	339	LEU	CA-CB-CG	-6.73	99.82	115.30
1	A	352	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	42	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	134	ASP	CB-CG-OD2	6.66	124.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	352	ASP	CB-CG-OD2	6.26	123.93	118.30
2	D	489	ASP	CB-CG-OD2	6.25	123.92	118.30
2	D	3	ASP	CB-CG-OD2	6.23	123.91	118.30
2	D	203	ASP	CB-CG-OD2	6.22	123.89	118.30
2	D	138	ASP	CB-CG-OD2	6.20	123.88	118.30
2	C	259	ASP	CB-CG-OD2	6.16	123.84	118.30
2	D	124	ASP	CB-CG-OD2	6.14	123.83	118.30
2	D	5	ASP	CB-CG-OD2	6.11	123.80	118.30
2	C	138	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	26	ASP	CB-CG-OD2	5.93	123.63	118.30
2	C	409	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	50	ASP	CB-CG-OD2	5.87	123.58	118.30
2	C	285	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	226	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	26	ASP	CB-CG-OD2	5.66	123.39	118.30
2	C	372	ASP	CB-CG-OD2	5.57	123.31	118.30
2	C	247	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	C	165	ASP	CB-CG-OD2	5.53	123.27	118.30
2	C	85	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	C	461	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	114[A]	CYS	CB-CA-C	5.45	121.29	110.40
1	A	114[B]	CYS	CB-CA-C	5.45	121.29	110.40
2	C	319	ASP	CB-CG-OD2	5.45	123.20	118.30
2	D	372	ASP	CB-CG-OD2	5.44	123.19	118.30
2	C	680	ASP	CB-CG-OD2	5.42	123.18	118.30
2	D	709	ASP	CB-CG-OD2	5.40	123.16	118.30
2	C	571	LEU	CA-CB-CG	5.39	127.69	115.30
1	B	274	ASP	CB-CG-OD2	5.39	123.15	118.30
2	C	337	ASP	CB-CG-OD2	5.38	123.14	118.30
2	D	319	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	478	ASP	CB-CG-OD2	5.37	123.13	118.30
2	D	461	ASP	CB-CG-OD2	5.33	123.10	118.30
2	D	694	ASP	CB-CG-OD2	5.31	123.08	118.30
2	C	389	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	50	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	165	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	50	ASP	CB-CG-OD2	5.25	123.02	118.30
2	D	259	ASP	CB-CG-OD2	5.24	123.02	118.30
2	D	389	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	626	ASP	CB-CG-OD2	5.21	122.99	118.30
2	D	470	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	490	ASP	CB-CG-OD2	5.21	122.99	118.30
2	C	694	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	100	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	317	CYS	CA-CB-SG	-5.14	104.75	114.00
2	D	701	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	149	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	D	497	ASP	CB-CG-OD2	5.07	122.86	118.30
2	C	150	ASP	CB-CG-OD2	5.05	122.85	118.30
2	D	726	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	570	ASP	CB-CG-OD2	5.04	122.83	118.30
2	D	398	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	114[A]	CYS	CA-CB-SG	-5.00	104.99	114.00
1	A	114[B]	CYS	CA-CB-SG	-5.00	104.99	114.00
2	D	490	ASP	CB-CG-OD2	5.00	122.81	118.30

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	69	0
1	B	5131	0	5123	81	1
2	C	5788	0	5763	102	0
2	D	5745	0	5704	128	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	361	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 (361) 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:D:394:LYS:HD2	2:D:458:ALA:HB1	1.60	0.84
2:D:362:THR:H	2:D:464:GLN:HE21	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:ALA:H	2:C:192:GLN:HE22	1.24	0.83
1:B:482:LEU:HD12	7:B:1689:GOL:C1	2.08	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
2:C:681[A]:GLU:CD	2:C:684:ARG:HH21	1.84	0.80
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:611:ILE:HD12	2:D:613:ILE:HD11	1.65	0.78
2:C:315:LYS:O	2:C:316:ILE:HG23	1.83	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
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
2:D:284:GLU:CD	2:D:284:GLU:H	1.89	0.74
2:D:707:THR:HG1	2:D:710:GLU:HG3	1.50	0.74
1:A:77:ARG:H	1:B:55:GLN:HE22	1.32	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:H	2:C:424:ASN:HD22	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
1:B:384[B]:TYR:HD2	2:D:84:ASN:HB3	1.55	0.72
2:D:342:MET:HG3	2:D:384:LEU:HD22	1.70	0.72
1:A:196[A]:GLU:OE2	2:D:120:LYS:HE2	1.89	0.72
1:B:573:LYS:HZ3	1:B:659:HIS:HD2	1.35	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CG2	2.63	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
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
2:C:169:LEU:HD13	2:C:193:LEU:HG	1.78	0.65
2:D:339:TYR:CD1	2:D:378:GLU:HG3	2.31	0.65
1:B:573:LYS:NZ	1:B:659:HIS:HD2	1.94	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:537:LYS:HZ2	7:C:1743:GOL:H31	1.59	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:CD2	2.16	0.63
1:B:284:ASN:HD22	1:B:284:ASN:C	2.02	0.62
2:C:315:LYS:C	2:C:316:ILE:HG22	2.20	0.62
2:D:340:VAL:CG2	2:D:373:ILE:HD11	2.29	0.62
2:C:316:ILE:CG1	2:C:317:LYS:N	2.62	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:D:371:PRO:CB	2:D:376:ILE:HD11	2.29	0.62
2:C:284:GLU:OE2	2:C:284:GLU:HA	1.99	0.62
1:A:77:ARG:HD3	14:A:2066:HOH:O	1.99	0.61
1:A:335:ALA:H	1:A:471:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:388:VAL:HG12	2:D:390:ILE:CD1	2.31	0.60
2:C:95:ASN:ND2	2:C:98:ASN:H	1.98	0.60
1:A:550[C]:CYS:SG	1:A:591:ILE:CD1	2.89	0.60
2:D:408:HIS:HD2	2:D:419:HIS:ND1	2.00	0.60
1:A:201:HIS:HE1	2:D:35:TYR:OH	1.85	0.60
1:B:486:LYS:HZ2	7:B:1689:GOL:H31	1.64	0.60
1:A:573:LYS:HZ3	1:A:659:HIS:HD2	1.50	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:621:MET:HE1	2:D:625:GLY:HA2	1.83	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:456:PHE:HD2	2:D:542:ILE:HD11	1.68	0.59
1:B:482:LEU:HD11	1:B:508:LEU:HD13	1.84	0.59
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:HG2	2:C:338:MET:O	2.02	0.58
1:B:196:GLU:OE2	2:C:120:LYS:HE2	2.04	0.58
2:D:611:ILE:CD1	2:D:613:ILE:HD11	2.33	0.58
1:A:515:ASN:HD22	1:A:518:THR:HG21	1.68	0.58
2:C:343:GLY:HA2	2:C:347:THR:O	2.03	0.58
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
2:D:568:ASN:ND2	2:D:581:GLN:HE21	2.00	0.56
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
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:D:613:ILE:O	2:D:671:PRO:HD3	2.06	0.56
2:C:342:MET:HB3	2:C:384:LEU:HB2	1.88	0.56
2:D:457:PRO:O	2:D:458:ALA:HB3	2.06	0.56
1:A:284:ASN:ND2	1:A:286:LEU:H	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLU:OE2	1:B:164[B]:GLN:NE2	2.39	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
1:B:335:ALA:H	1:B:471:ASN:HD22	1.55	0.55
2:C:439:PHE:CE1	2:C:443:ASN:HB2	2.42	0.55
2:C:361:ILE:HD11	2:C:391:TYR:HB3	1.89	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
2:C:555:GLY:H	7:C:1737:GOL:H31	1.72	0.54
2:C:392:GLY:HA3	2:C:459:ILE:O	2.07	0.54
2:D:421:GLY:C	2:D:422:GLN:HG3	2.26	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
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
1:A:515:ASN:HA	1:A:518:THR:HG23	1.88	0.53
1:A:515:ASN:HD22	1:A:518:THR:CG2	2.22	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
2:D:685:ARG:O	2:D:689:GLU:HG3	2.10	0.52
1:A:35:GLU:OE2	1:A:423:ILE:HD11	2.09	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
2:D:365:LYS:HE2	2:D:367:GLU:OE2	2.09	0.52
1:A:530:ARG:CG	1:A:530:ARG:HH11	2.22	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
2:C:372:ASP:OD2	2:C:440:ARG:HG2	2.10	0.51
2:C:187:ASP:HA	2:C:211:ASN:ND2	2.25	0.51
1:A:577[A]:VAL:HG21	1:A:645:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:ASN:HD22	2:D:98:ASN:H	1.57	0.51
2:D:205:ILE:O	2:D:205:ILE:HG13	2.11	0.51
1:A:149:ARG:HD2	14:A:2106:HOH:O	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:657:PHE:O	2:D:658:ILE:C	2.49	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
2:D:621:MET:HE2	2:D:625:GLY:O	2.10	0.50
2:D:588:MET:SD	2:D:604:ILE:HD13	2.50	0.50
1:A:571:THR:N	1:A:572:PRO:CD	2.74	0.50
1:A:577[B]:VAL:HG11	1:A:645:ILE:HG23	1.93	0.50
2:C:316:ILE:HG13	2:C:317:LYS:N	2.26	0.50
1:A:201:HIS:CE1	2:D:35:TYR:OH	2.63	0.50
2:C:289:PRO:O	2:C:290:ASP:HB2	2.12	0.50
1:B:482:LEU:HD11	1:B:508:LEU:CD1	2.41	0.50
2:D:284:GLU:N	2:D:284:GLU:CD	2.64	0.50
2:D:340:VAL:HG21	2:D:373:ILE:CD1	2.41	0.50
2:C:339:TYR:CG	2:C:435:VAL:HG21	2.46	0.50
1:B:201:HIS:HE1	2:C:35:TYR:OH	1.95	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:A:284:ASN:C	1:A:284:ASN:HD22	2.15	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
2:D:339:TYR:CD2	2:D:435:VAL:HG21	2.48	0.49
1:B:261:PRO:HA	1:B:429:ALA:O	2.13	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:D:339:TYR:CE1	2:D:378:GLU:HG3	2.48	0.48
1:A:113:HIS:NE2	1:A:550[A]:CYS:SG	2.86	0.48
2:C:408:HIS:HD2	2:C:419:HIS:ND1	2.11	0.48
1:A:283:HIS:CE1	1:A:587:LYS:HZ1	2.31	0.48
1:B:515:ASN:HA	1:B:518:THR:HG23	1.94	0.48
2:D:362:THR:HB	2:D:365:LYS:HB2	1.94	0.48
1:B:577[B]:VAL:HG11	1:B:645:ILE:HG23	1.96	0.48
1:B:534:GLY:HA3	14:B:2241:HOH:O	2.13	0.48
1:B:659:HIS:HE1	2:C:191:GLU:OE1	1.97	0.48
1:A:362:ALA:HB3	7:A:1687:GOL:H32	1.96	0.48
2:D:611:ILE:HD12	2:D:613:ILE:CD1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:383:PRO:O	2:C:469:THR:HA	2.14	0.48
1:A:573:LYS:HZ3	1:A:659:HIS:CD2	2.29	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
1:A:530:ARG:HG3	1:A:530:ARG:NH1	2.24	0.47
2:D:393:ARG:HG3	2:D:461:ASP:OD2	2.14	0.47
1:A:529:LYS:O	1:A:533:GLU:HG3	2.15	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
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:D:376:ILE:CG2	2:D:377:PRO:HD2	2.44	0.46
1:A:200:THR:OG1	1:A:201:HIS:HD2	1.98	0.46
1:A:13:PRO:HG3	1:A:607:MET:HE1	1.97	0.46
2:C:164:LYS:HG2	2:C:298:TYR:CZ	2.51	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: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
2:C:537:LYS:HZ1	7:C:1743:GOL:H31	1.78	0.46
1:B:573:LYS:NZ	1:B:659:HIS:CD2	2.78	0.46
2:D:187:ASP:HA	2:D:211:ASN:ND2	2.30	0.45
1:A:353:VAL:HB	1:B:223:MET:SD	2.56	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
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:B:322:VAL:HG23	1:B:328:ILE:HB	1.97	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
2:D:362:THR:N	2:D:464:GLN:HE21	2.05	0.45
2:C:318:LEU:HD11	2:C:320:LEU:HD21	1.98	0.45
7:A:1687:GOL:H12	14:A:2327:HOH:O	2.16	0.45
2:D:583:CYS:CB	2:D:586:THR:HG22	2.46	0.45
1:B:114[B]:CYS:HB2	1:B:208:ILE:HG21	1.98	0.45
1:A:480:SER:HB2	1:A:582:GLU:HG2	1.98	0.45
2:C:342:MET:CB	2:C:384:LEU:HB2	2.47	0.45
1:B:536:ASN:O	1:B:537:ILE:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:503:PHE:CZ	2:C:553:LYS:HD3	2.52	0.45
2:C:540:TYR:O	2:C:544:HIS:HD2	1.99	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: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:362:THR:HG1	2:C:365:LYS:HD3	1.83	0.44
2:C:613:ILE:O	2:C:671:PRO:HD3	2.18	0.44
2:C:179:MET:HG2	2:C:313:LEU:CD1	2.47	0.44
2:C:451:LYS:HA	2:C:451:LYS:HD2	1.76	0.44
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.82	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:631:LEU:O	2:D:635:ILE:HG12	2.17	0.44
2:D:558:ASP:HA	2:D:559:PRO:HD2	1.84	0.44
2:D:583:CYS:HB3	2:D:586:THR:HG22	1.99	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
2:C:16:LYS:HZ2	2:C:284:GLU:CG	2.30	0.44
1:A:33:VAL:HG21	1:A:477:GLN:HE22	1.83	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:D:681[A]:GLU:OE2	2:D:684:ARG:NH1	2.51	0.43
2:C:95:ASN:HD22	2:C:95:ASN:C	2.21	0.43
2:C:74:LYS:HE3	14:C:2068:HOH:O	2.17	0.43
2:D:170:ALA:O	2:D:174:LYS:HG3	2.18	0.43
2:C:356:VAL:HG21	2:C:361:ILE:HG23	2.00	0.43
1:A:466:LEU:HD22	1:A:595:TRP:HZ2	1.83	0.43
2:D:420:THR:HG22	2:D:427:TRP:HB3	2.01	0.43
2:C:180:GLY:HA2	2:C:326:PRO:HG2	1.99	0.43
1:A:370:ARG:NH2	1:A:410:GLU:OE1	2.32	0.43
2:D:572:TYR:HA	2:D:579:LEU:O	2.18	0.43
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.49	0.43
1:A:114[A]:CYS:SG	1:A:208:ILE:CG2	3.06	0.43
2:D:376:ILE:HG22	2:D:377:PRO:HD2	2.01	0.43
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.48	0.43
2:D:441:PHE:O	2:D:444:TYR:HB2	2.18	0.43
2:D:163:ALA:CB	2:D:169:LEU:HB2	2.49	0.43
2:C:476:GLU:CG	2:C:477:TYR:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:VAL:HG13	2:D:111:GLU:OE2	2.17	0.43
1:A:530:ARG:CG	1:A:530:ARG:NH1	2.82	0.43
2:D:95:ASN:HD22	2:D:95:ASN:C	2.22	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:B:284:ASN:HD21	1:B:286:LEU:HG	1.84	0.42
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.34	0.42
2:C:334:ARG:HD2	2:C:334:ARG:HA	1.75	0.42
2:D:147:LYS:HA	2:D:147:LYS:HD2	1.79	0.42
2:D:157:ALA:HB3	2:D:183:LEU:HD23	1.97	0.42
1:A:480:SER:HB2	1:A:582:GLU:CG	2.49	0.42
2:D:329:GLU:HG3	2:D:412:ASN:HB3	2.02	0.42
2:C:373:ILE:HD13	2:C:373:ILE:HA	1.72	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:427:TRP:C	2:C:428:LEU:HD12	2.40	0.42
2:C:340:VAL:CG1	2:C:373:ILE:HD11	2.49	0.42
1:B:577[A]:VAL:HG21	1:B:645:ILE:CG2	2.47	0.41
1:B:201:HIS:CE1	2:C:35:TYR:OH	2.71	0.41
2:D:355:THR:HG23	2:D:395:MET:HG3	2.02	0.41
2:D:388:VAL:CG1	2:D:390:ILE:HD11	2.50	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:C:540:TYR:CD1	2:C:550:PRO:HD3	2.55	0.41
1:B:398:LYS:O	1:B:402:ARG:HG3	2.21	0.41
2:D:219:ALA:O	2:D:223:LEU:HB2	2.20	0.41
2:D:350:PHE:HD2	2:D:478:MET:HG2	1.83	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: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
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:564:TRP:CZ3	2:C:584:LEU:HD12	2.55	0.41
1:B:320:ASN:O	1:B:324:MET:HG2	2.20	0.41
2:D:145:GLY:O	2:D:148:MET:HB2	2.21	0.41
1:B:278:PHE:HB3	1:B:312:LEU:HD23	2.02	0.41
2:D:164:LYS:HE3	2:D:298:TYR:CD2	2.55	0.41
2:D:85:ARG:O	2:D:89:GLN:HG3	2.21	0.41
2:C:406[B]:ARG:NH1	2:C:409:ASP:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:LYS:HD2	2:C:86:LYS:HA	1.87	0.41
2:C:448:LEU:HA	2:C:448:LEU:HD12	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: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
2:C:16:LYS:HZ3	2:C:284:GLU:HG3	1.83	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
1:A:5:ARG:NH1	1:A:650:GLU:OE2	2.54	0.40
2:D:86:LYS:HD2	2:D:86:LYS:HA	1.91	0.40
2:C:424:ASN:N	2:C:424:ASN:HD22	2.06	0.40
2:D:223:LEU:HD12	2:D:223:LEU:HA	1.94	0.40
2:D:277:ILE:N	2:D:277:ILE:HD12	2.36	0.40
1:B:410:GLU:HG3	14:B:2222:HOH:O	2.22	0.40
2:D:143:ARG:HD2	2:D:144:PHE:CE1	2.56	0.40
2:C:122:LYS:HD2	2:C:125:GLU:OE1	2.22	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%)	56	46
1	B	683/674 (101%)	659 (96%)	21 (3%)	3 (0%)	39	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	738/729 (101%)	710 (96%)	22 (3%)	6 (1%)	24	11
2	D	728/729 (100%)	705 (97%)	20 (3%)	3 (0%)	39	27
All	All	2832/2806 (101%)	2738 (97%)	81 (3%)	13 (0%)	34	21

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%)	535 (97%)	19 (3%)	44	33
1	B	554/543 (102%)	534 (96%)	20 (4%)	42	30
2	C	622/611 (102%)	582 (94%)	40 (6%)	22	10
2	D	612/611 (100%)	570 (93%)	42 (7%)	19	8
All	All	2342/2308 (102%)	2221 (95%)	121 (5%)	29	17

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	71	CYS
1	A	77	ARG
1	A	118	ASN
1	A	206	PHE
1	A	284	ASN
1	A	326	GLN
1	A	352	ASP
1	A	447	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	546	HIS
1	A	636	MET
1	A	665	ARG
1	A	669	LYS
1	B	27	ARG
1	B	66	ILE
1	B	118	ASN
1	B	206	PHE
1	B	218	GLN
1	B	284	ASN
1	B	308	LYS
1	B	326	GLN
1	B	352	ASP
1	B	406	GLU
1	B	415	ASN
1	B	447	ASN
1	B	470	CYS
1	B	518	THR
1	B	538	GLU
1	B	546	HIS
1	B	636	MET
1	B	639	GLN
1	B	656	LEU
1	B	665	ARG
2	C	16	LYS
2	C	17[A]	GLU
2	C	17[B]	GLU
2	C	95	ASN

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Mol	Chain	Res	Type
2	C	122	LYS
2	C	124	ASP
2	C	127	LEU
2	C	169	LEU
2	C	198	VAL
2	C	254	TYR
2	C	286	LYS
2	C	315	LYS
2	C	316	ILE
2	C	317	LYS
2	C	319	ASP
2	C	338	MET
2	C	341	GLU
2	C	342	MET
2	C	345	ASN
2	C	346	ARG
2	C	359	SER
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	476	GLU
2	C	479	GLU
2	C	571	LEU
2	C	598	PHE
2	C	604	ILE
2	C	634	MET
2	C	674	LEU
2	C	728	ILE
2	D	16	LYS
2	D	95	ASN
2	D	147	LYS
2	D	160	LEU
2	D	173	VAL
2	D	194	LEU

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Mol	Chain	Res	Type
2	D	197	ASN
2	D	223	LEU
2	D	246	ARG
2	D	254	TYR
2	D	286	LYS
2	D	313	LEU
2	D	340	VAL
2	D	342	MET
2	D	346	ARG
2	D	358	GLU
2	D	373	ILE
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	595	CYS
2	D	598	PHE
2	D	604	ILE
2	D	621	MET
2	D	626	MET
2	D	639	THR
2	D	674	LEU
2	D	685	ARG
2	D	711	ILE
2	D	729	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	56	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	284	ASN
1	A	326	GLN
1	A	447	ASN
1	A	454	GLN
1	A	471	ASN
1	A	477	GLN
1	A	503	GLN
1	A	515	ASN
1	A	622	GLN
1	A	659	HIS
1	B	55	GLN
1	B	56	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	415	ASN
1	B	447	ASN
1	B	454	GLN
1	B	471	ASN
1	B	477	GLN
1	B	503	GLN
1	B	515	ASN
1	B	622	GLN
1	B	659	HIS
2	C	95	ASN
2	C	192	GLN
2	C	211	ASN
2	C	396	GLN
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	544	HIS
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	396	GLN
2	D	408	HIS
2	D	426	ASN
2	D	464	GLN
2	D	510	GLN
2	D	544	HIS
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 carbohydrates 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	A	1676	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	A	1677	1,8,5	0,11,11	0.00	-	0,19,19	0.00	-
5	FOR	A	1678	4	0,1,1	0.00	-	0,0,0	0.00	-
6	SO4	A	1679	-	4,4,4	0.45	0	6,6,6	0.41	0
6	SO4	A	1680	-	4,4,4	0.44	0	6,6,6	0.40	0
6	SO4	A	1681	-	4,4,4	0.14	0	6,6,6	0.18	0
6	SO4	A	1682	-	4,4,4	0.39	0	6,6,6	0.33	0
6	SO4	A	1683	-	4,4,4	0.20	0	6,6,6	0.17	0
6	SO4	A	1684	-	4,4,4	0.30	0	6,6,6	0.68	0
6	SO4	A	1685	-	4,4,4	0.12	0	6,6,6	0.22	0
6	SO4	A	1686	-	4,4,4	0.16	0	6,6,6	0.11	0
7	GOL	A	1687	-	5,5,5	0.48	0	5,5,5	0.97	0
6	SO4	A	1688	-	4,4,4	0.18	0	6,6,6	0.21	0
6	SO4	A	1689	-	4,4,4	0.12	0	6,6,6	0.23	0
6	SO4	A	1690	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SF4	B	1675	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	1676	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	B	1677	1,8,5	0,11,11	0.00	-	0,19,19	0.00	-
5	FOR	B	1678	4	0,1,1	0.00	-	0,0,0	0.00	-
6	SO4	B	1679	-	4,4,4	0.69	0	6,6,6	0.23	0
6	SO4	B	1680	-	4,4,4	0.14	0	6,6,6	0.46	0
6	SO4	B	1681	-	4,4,4	0.24	0	6,6,6	0.14	0
6	SO4	B	1682	-	4,4,4	0.12	0	6,6,6	0.24	0
6	SO4	B	1683	-	4,4,4	0.28	0	6,6,6	0.36	0
6	SO4	B	1684	-	4,4,4	0.20	0	6,6,6	0.23	0
6	SO4	B	1685	-	4,4,4	0.27	0	6,6,6	0.32	0
6	SO4	B	1686	-	4,4,4	0.15	0	6,6,6	0.20	0
6	SO4	B	1687	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	B	1688	-	4,4,4	0.31	0	6,6,6	0.10	0
7	GOL	B	1689	-	5,5,5	0.37	0	5,5,5	0.20	0
7	GOL	B	1690	-	5,5,5	0.43	0	5,5,5	0.27	0
9	BCT	B	1691	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SF4	C	1730	2	0,12,12	0.00	-	0,24,24	0.00	-
12	SX	C	1733	10	0,1,1	0.00	-	0,0,0	0.00	-
6	SO4	C	1734	-	4,4,4	0.22	0	6,6,6	0.35	0
6	SO4	C	1735	-	4,4,4	0.20	0	6,6,6	0.91	0
6	SO4	C	1736	-	4,4,4	0.17	0	6,6,6	0.25	0
7	GOL	C	1737	-	5,5,5	0.27	0	5,5,5	0.30	0
6	SO4	C	1738	-	4,4,4	0.86	0	6,6,6	0.26	0
7	GOL	C	1739	-	5,5,5	0.32	0	5,5,5	0.40	0
6	SO4	C	1740	-	4,4,4	0.35	0	6,6,6	0.33	0
7	GOL	C	1741	-	5,5,5	0.33	0	5,5,5	0.51	0
6	SO4	C	1742	-	4,4,4	0.22	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	C	1743	-	5,5,5	0.51	0	5,5,5	0.68	0
3	SF4	D	1730	11,2	0,12,12	0.00	-	0,24,24	0.00	-
13	ACT	D	1733	-	1,3,3	0.89	0	0,3,3	0.00	-
6	SO4	D	1734	-	4,4,4	0.14	0	6,6,6	0.20	0
6	SO4	D	1735	-	4,4,4	0.32	0	6,6,6	0.16	0
7	GOL	D	1736	-	5,5,5	0.48	0	5,5,5	0.61	0
6	SO4	D	1737	-	4,4,4	0.21	0	6,6,6	0.10	0
6	SO4	D	1738	-	4,4,4	0.23	0	6,6,6	0.22	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	A	1676	1	-	0/0/48/48	0/6/5/5
4	XCC	A	1677	1,8,5	-	0/0/32/32	0/0/3/3
5	FOR	A	1678	4	-	0/0/0/0	0/0/0/0
6	SO4	A	1679	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1680	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1681	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1682	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1683	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1684	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1685	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1686	-	-	0/0/0/0	0/0/0/0
7	GOL	A	1687	-	-	0/4/4/4	0/0/0/0
6	SO4	A	1688	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1689	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1690	-	-	0/0/0/0	0/0/0/0
3	SF4	B	1675	1	-	0/0/48/48	0/6/5/5
3	SF4	B	1676	1	-	0/0/48/48	0/6/5/5
4	XCC	B	1677	1,8,5	-	0/0/32/32	0/0/3/3
5	FOR	B	1678	4	-	0/0/0/0	0/0/0/0
6	SO4	B	1679	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1680	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1681	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1682	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1683	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1684	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1685	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1686	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1687	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	1688	-	-	0/0/0/0	0/0/0/0
7	GOL	B	1689	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1690	-	-	0/4/4/4	0/0/0/0
9	BCT	B	1691	-	-	0/0/0/0	0/0/0/0
3	SF4	C	1730	2	-	0/0/48/48	0/6/5/5
12	SX	C	1733	10	-	0/0/0/0	0/0/0/0
6	SO4	C	1734	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1735	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1736	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1737	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1738	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1739	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1740	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1741	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1742	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1743	-	-	0/4/4/4	0/0/0/0
3	SF4	D	1730	11,2	-	0/0/48/48	0/6/5/5
13	ACT	D	1733	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1734	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1735	-	-	0/0/0/0	0/0/0/0
7	GOL	D	1736	-	-	0/4/4/4	0/0/0/0
6	SO4	D	1737	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1738	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1737	GOL	2	0
7	C	1741	GOL	1	0
7	C	1743	GOL	4	0
7	D	1736	GOL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	673/674 (99%)	-0.00	18 (2%) 58 61	5, 10, 20, 32	15 (2%)
1	B	673/674 (99%)	-0.04	13 (1%) 70 73	5, 10, 19, 39	18 (2%)
2	C	729/729 (100%)	0.34	66 (9%) 11 13	3, 11, 22, 35	7 (0%)
2	D	728/729 (99%)	0.60	93 (12%) 5 5	4, 11, 21, 39	7 (0%)
All	All	2803/2806 (99%)	0.23	190 (6%) 20 23	3, 10, 21, 39	47 (1%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	345	ASN	8.0
1	B	536	ASN	7.7
2	C	317	LYS	7.6
1	B	537	ILE	6.5
2	C	472	ALA	6.2
2	C	314	THR	6.0
2	D	15	GLY	5.9
2	C	315	LYS	5.9
2	C	359	SER	5.8
2	D	713	PRO	5.7
1	A	538	GLU	5.5
2	C	345	ASN	5.5
2	D	717	GLU	5.5
2	C	348	PRO	5.2
2	D	359	SER	5.1
2	C	319	ASP	5.0
2	C	1	MET	4.9
2	D	334	ARG	4.6
1	A	8	SER	4.6
2	C	316	ILE	4.6
2	D	617	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	4.5
1	B	539	ILE	4.4
2	D	124	ASP	4.3
2	D	393	ARG	4.2
2	C	377	PRO	4.2
2	D	14	GLU	4.2
1	A	536	ASN	4.1
2	C	336	GLY	4.1
2	C	358	GLU	4.0
2	D	358	GLU	4.0
2	D	216	VAL	3.9
1	A	446	GLN	3.9
2	D	714	TYR	3.9
2	D	377	PRO	3.9
2	C	313	LEU	3.9
1	A	537	ILE	3.9
2	D	619	ALA	3.9
2	D	374	ASP	3.9
2	C	15	GLY	3.9
2	D	336	GLY	3.8
2	C	427	TRP	3.8
2	D	448	LEU	3.8
2	D	436	ALA	3.8
2	D	346	ARG	3.8
1	B	8	SER	3.7
2	C	321	PRO	3.7
2	C	318	LEU	3.6
2	D	125	GLU	3.6
2	D	215	ILE	3.6
2	D	362	THR	3.6
2	C	346	ARG	3.6
2	D	344	GLY	3.5
2	C	440	ARG	3.5
2	C	357	SER	3.5
2	C	374	ASP	3.5
2	C	379	GLY	3.5
1	B	446	GLN	3.5
2	C	124	ASP	3.5
2	D	577	ARG	3.5
2	C	312	LYS	3.4
2	C	361	ILE	3.4
1	A	81[A]	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	3.4
2	D	557	ILE	3.4
2	C	125	GLU	3.4
2	C	470	ASP	3.4
2	C	339	TYR	3.3
2	D	729	MET	3.3
2	D	361	ILE	3.3
1	A	445	ALA	3.3
1	B	538	GLU	3.2
2	C	123	PRO	3.2
2	C	393	ARG	3.2
2	D	3	ASP	3.2
2	D	376	ILE	3.2
2	D	631	LEU	3.1
2	D	332	SER	3.1
2	D	447	ILE	3.1
2	D	375	GLN	3.0
2	C	284	GLU	3.0
2	C	475	LYS	3.0
2	D	360	GLU	3.0
2	D	151	TRP	3.0
1	B	7	LEU	3.0
2	D	716	GLU	2.9
2	D	143	ARG	2.9
2	D	444	TYR	2.9
2	D	709	ASP	2.9
2	D	284	GLU	2.8
2	D	471	GLU	2.8
2	D	711	ILE	2.8
2	D	252	VAL	2.8
2	D	391	TYR	2.8
2	C	14	GLU	2.7
2	D	425	ILE	2.7
2	D	123	PRO	2.7
2	D	624	SER	2.7
2	C	436	ALA	2.7
2	C	382	LEU	2.7
2	D	572	TYR	2.7
2	D	160	LEU	2.7
2	C	471	GLU	2.7
2	D	712	LEU	2.7
2	D	158	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	445	ALA	2.6
2	C	360	GLU	2.6
2	D	122	LYS	2.6
2	D	545	ALA	2.6
2	D	2	THR	2.6
2	C	158	ILE	2.6
2	D	386	ILE	2.6
2	D	728	ILE	2.6
2	C	391	TYR	2.6
2	D	462	ARG	2.6
2	C	16	LYS	2.6
2	D	6	LYS	2.6
1	A	669	LYS	2.5
2	D	387	LEU	2.5
1	A	82	ASP	2.5
2	C	367	GLU	2.5
2	D	317	LYS	2.5
2	D	381	LYS	2.5
2	D	470	ASP	2.5
2	C	216	VAL	2.5
2	D	629	SER	2.5
1	B	577[A]	VAL	2.4
1	A	296	ARG	2.4
1	B	417	PRO	2.4
2	D	339	TYR	2.4
1	B	583	ALA	2.4
2	C	386	ILE	2.4
1	A	667	GLU	2.4
2	D	167	LYS	2.4
2	D	633	GLY	2.4
2	D	472	ALA	2.4
2	C	185	ILE	2.4
2	D	607	GLU	2.4
2	C	433	ASP	2.4
2	C	340	VAL	2.4
2	C	729	MET	2.4
2	C	438	GLY	2.3
2	C	437	LYS	2.3
2	D	703	THR	2.3
2	D	613	ILE	2.3
2	C	347	THR	2.3
2	C	159	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	707	THR	2.3
1	A	155	GLU	2.3
1	B	533	GLU	2.3
2	D	440	ARG	2.3
2	D	625	GLY	2.3
2	D	312	LYS	2.3
1	A	464	VAL	2.3
2	C	469	THR	2.3
2	D	555	GLY	2.3
2	D	384	LEU	2.2
2	D	708	VAL	2.2
2	D	475	LYS	2.2
2	D	565	LYS	2.2
1	A	4	PHE	2.2
2	D	337	ASP	2.2
2	C	384	LEU	2.2
2	D	632	ALA	2.2
2	D	435	VAL	2.2
2	D	492	MET	2.2
2	D	373	ILE	2.2
2	C	285	ASP	2.2
2	C	335	LYS	2.2
2	C	378	GLU	2.1
2	C	425	ILE	2.1
2	C	482	ARG	2.1
2	C	218	ALA	2.1
2	C	376	ILE	2.1
2	C	434	ALA	2.1
2	D	388	VAL	2.1
2	C	334	ARG	2.1
2	D	347	THR	2.1
2	D	556	GLU	2.1
2	D	647	ILE	2.1
2	C	479	GLU	2.0
2	D	482	ARG	2.0
2	C	160[A]	LEU	2.0
1	B	351	VAL	2.0
2	D	621	MET	2.0
2	C	122	LYS	2.0
1	A	495	VAL	2.0
1	A	533	GLU	2.0
2	D	218	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	185	ILE	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	FOR	B	1678	2/2	0.91	0.45	17.83	23,23,23,24	2
6	SO4	A	1689	5/5	0.83	0.26	14.01	48,49,50,50	5
7	GOL	A	1687	6/6	0.81	0.23	9.67	29,31,33,34	0
5	FOR	A	1678	2/2	0.96	0.23	6.17	23,23,23,23	2
7	GOL	B	1689	6/6	0.93	0.20	6.00	54,55,56,57	0
13	ACT	D	1733	4/4	0.74	0.26	5.04	18,18,19,19	4
6	SO4	B	1679	5/5	0.99	0.12	4.87	24,24,26,28	0
12	SX	C	1733	2/2	0.99	0.15	3.89	15,15,15,18	0
7	GOL	D	1736	6/6	0.85	0.20	3.35	41,45,47,48	0
6	SO4	D	1738	5/5	0.93	0.22	2.34	58,59,59,60	0
7	GOL	B	1690	6/6	0.74	0.21	2.20	58,60,61,61	0
7	GOL	C	1743	6/6	0.91	0.15	2.00	50,52,53,53	0
6	SO4	B	1688	5/5	0.96	0.16	1.23	42,45,46,46	5
6	SO4	C	1740	5/5	0.88	0.15	1.23	19,25,26,27	5
6	SO4	A	1680	5/5	0.98	0.10	1.03	23,23,24,26	0
6	SO4	A	1679	5/5	0.97	0.11	0.78	18,18,21,25	0
7	GOL	C	1741	6/6	0.91	0.20	0.72	21,30,33,38	0
6	SO4	C	1742	5/5	0.92	0.23	0.71	31,31,31,32	0
6	SO4	B	1685	5/5	0.96	0.12	0.65	59,59,60,60	0
11	NI	D	1731[A]	1/1	0.98	0.12	0.38	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	1683	5/5	0.90	0.14	0.34	33,33,35,36	5
6	SO4	A	1683	5/5	0.97	0.17	0.14	33,33,34,35	0
7	GOL	C	1739	6/6	0.96	0.09	-0.02	10,16,17,19	0
9	BCT	B	1691	4/4	0.93	0.12	-0.08	36,37,37,38	0
6	SO4	D	1737	5/5	0.93	0.13	-0.27	61,61,61,62	5
6	SO4	C	1738	5/5	0.99	0.09	-0.27	21,23,25,27	0
6	SO4	D	1735	5/5	0.98	0.10	-0.43	33,33,35,35	0
11	NI	C	1732	1/1	1.00	0.08	-0.84	9,9,9,9	0
3	SF4	B	1675	8/8	0.99	0.07	-0.99	9,11,11,12	0
8	FE2	A	1700	1/1	0.97	0.10	-1.09	22,22,22,22	1
6	SO4	A	1690	5/5	0.98	0.07	-1.37	49,50,51,52	0
3	SF4	C	1730	8/8	1.00	0.07	-1.39	5,7,8,8	0
11	NI	D	1732	1/1	1.00	0.07	-1.51	9,9,9,9	0
10	ZN	C	1731	1/1	0.99	0.06	-1.63	12,12,12,12	0
3	SF4	D	1730	8/8	0.99	0.06	-1.65	9,9,10,11	0
4	XCC	A	1677	9/9	0.96	0.09	-1.68	17,17,23,24	9
4	XCC	B	1677	9/9	0.97	0.08	-2.39	17,17,22,23	9
8	FE2	B	1700	1/1	0.99	0.06	-2.84	20,20,20,20	1
3	SF4	A	1676	8/8	0.99	0.04	-3.33	7,8,8,9	0
3	SF4	B	1676	8/8	0.99	0.04	-4.20	7,8,8,9	0
6	SO4	D	1734	5/5	0.92	0.17	-	30,30,30,31	5
6	SO4	B	1682	5/5	0.98	0.21	-	29,31,31,31	0
6	SO4	A	1684	5/5	0.98	0.14	-	38,38,39,39	0
6	SO4	B	1680	5/5	0.97	0.13	-	29,31,32,33	0
11	NI	D	1731[B]	1/1	0.98	0.12	-	16,16,16,16	1
6	SO4	B	1686	5/5	0.94	0.26	-	58,58,59,60	0
6	SO4	B	1681	5/5	0.97	0.18	-	31,34,35,36	0
6	SO4	C	1734	5/5	0.94	0.17	-	15,16,23,23	5
6	SO4	A	1681	5/5	0.97	0.18	-	33,34,36,36	0
7	GOL	C	1737	6/6	0.86	0.19	-	36,37,38,38	0
6	SO4	A	1685	5/5	0.98	0.17	-	28,30,32,32	0
6	SO4	A	1682	5/5	0.98	0.14	-	26,28,28,29	0
6	SO4	C	1736	5/5	0.96	0.21	-	27,30,31,31	0
6	SO4	A	1686	5/5	0.92	0.17	-	36,36,37,39	5
6	SO4	B	1684	5/5	0.93	0.28	-	59,59,61,61	0
6	SO4	A	1688	5/5	0.92	0.24	-	59,60,60,61	0
6	SO4	B	1687	5/5	0.83	0.16	-	51,51,51,52	5
6	SO4	C	1735	5/5	0.96	0.17	-	33,35,35,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.