



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2023 – 07:56 am GMT

PDB ID : 1OAO  
Title : NiZn[Fe<sub>4</sub>S<sub>4</sub>] and NiNi[Fe<sub>4</sub>S<sub>4</sub>] 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](mailto: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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

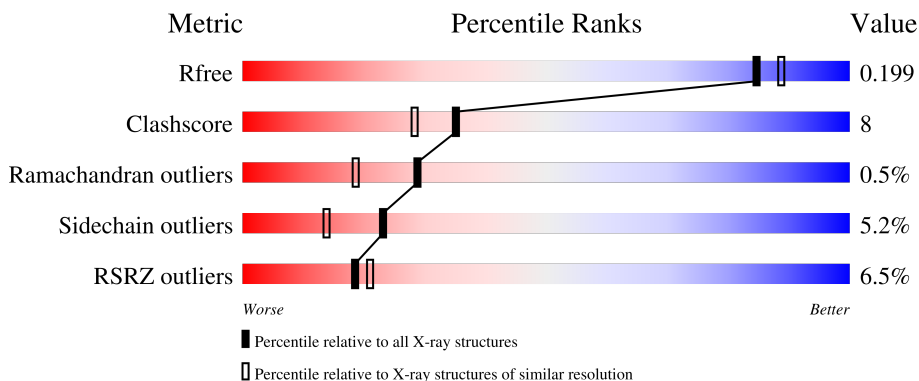
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">3%      88%      11%      .</p>
1	B	674	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">2%      86%      13%      .</p>
2	C	729	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">9%      80%      17%      . .</p>
2	D	729	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <p style="margin-left: 20px;">12%      73%      23%      .</p>

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.

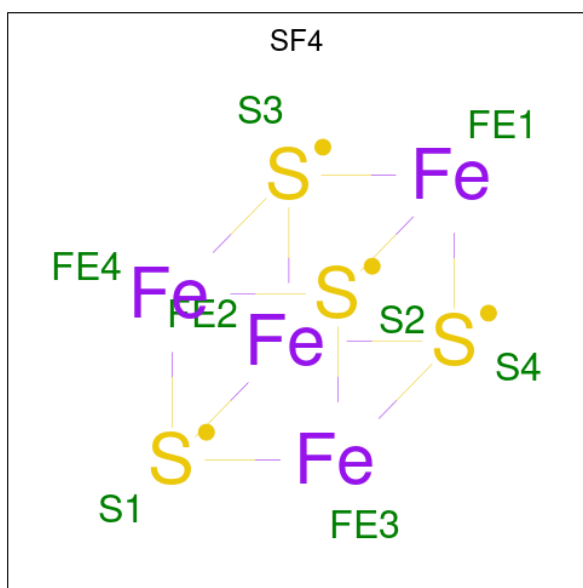
- Molecule 1 is a protein called CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA.

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

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

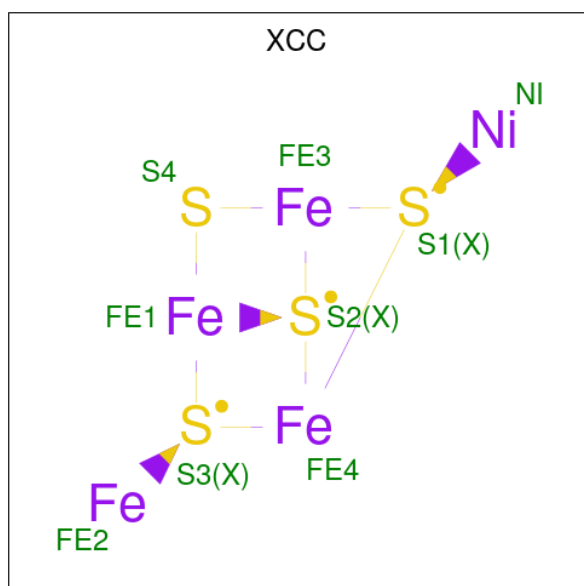
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	729	Total 5788	C 3712	N 963	O 1076	S 37	0	11	0
2	D	728	Total 5745	C 3684	N 956	O 1070	S 35	0	2	0

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



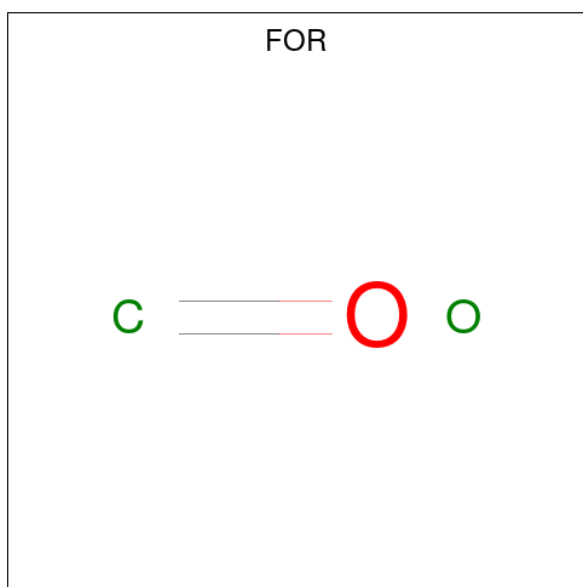
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula: Fe<sub>4</sub>NiS<sub>4</sub>).



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: CH<sub>2</sub>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: SO4) (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		

*Continued on next page...*

*Continued from previous page...*

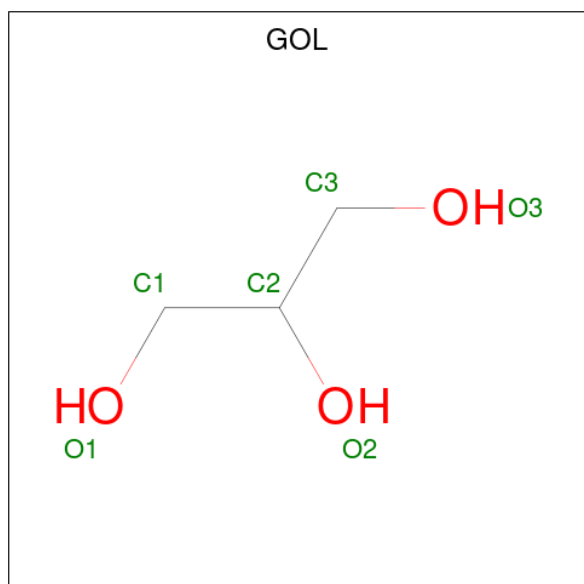
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B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

*Continued on next page...*

Continued from previous page...

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		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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		

Continued on next page...



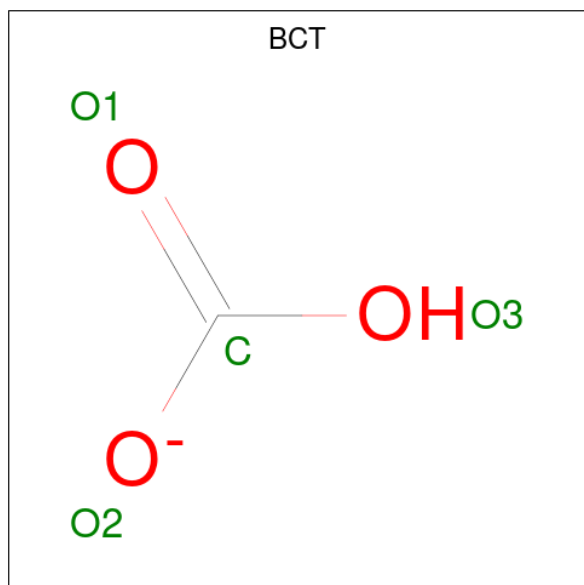
Continued from previous page...

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	A	1	Total	Fe	0	0
			1	1		
8	B	1	Total	Fe	0	0
			1	1		

- Molecule 9 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



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

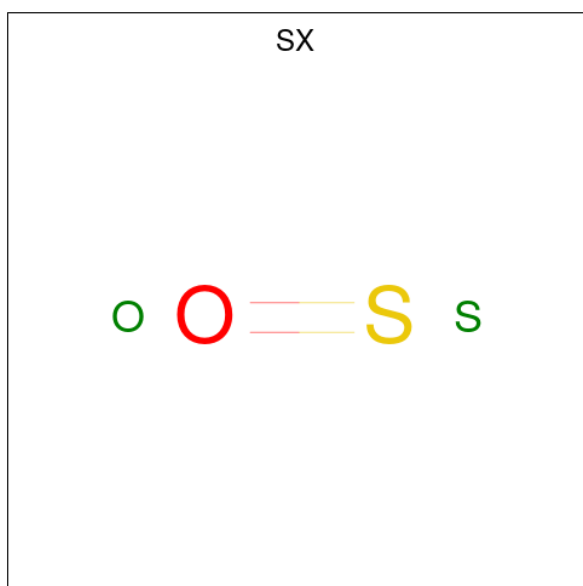
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

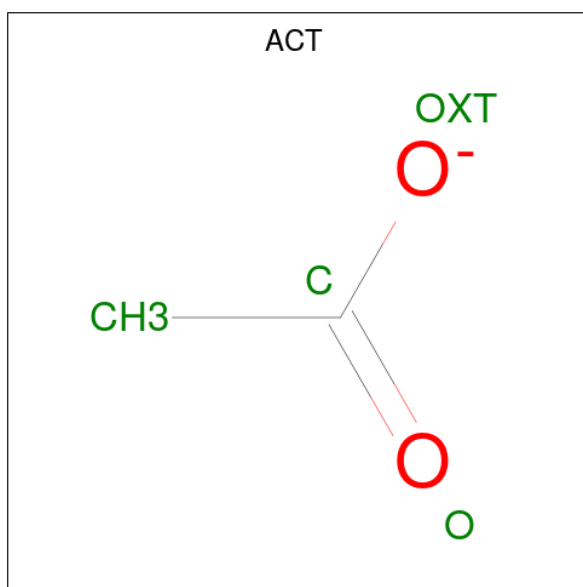
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	Ni	0	0
			1	1		
11	D	2	Total	Ni	0	1
			3	3		

- 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 4 2 2	0	0

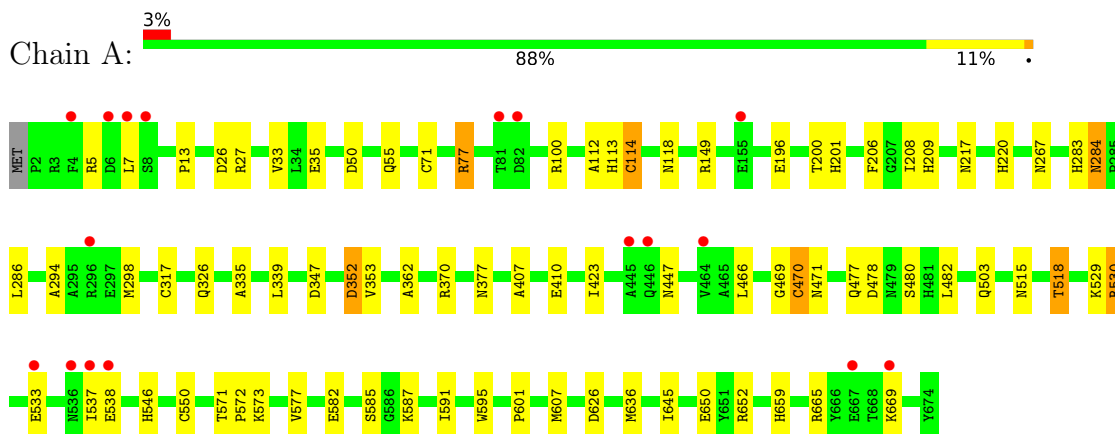
- Molecule 14 is water.

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

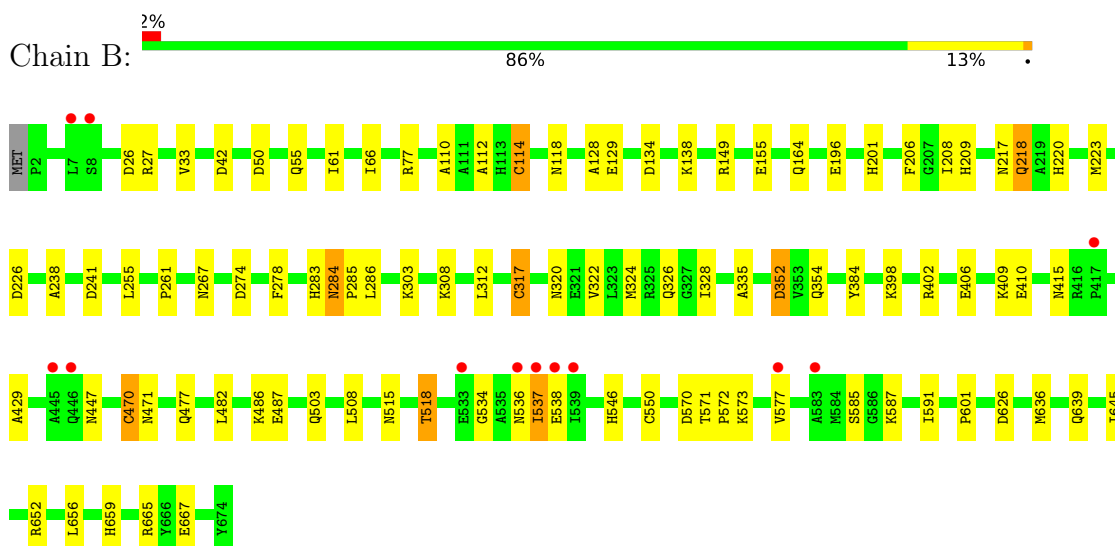
### 3 Residue-property plots [i](#)

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.

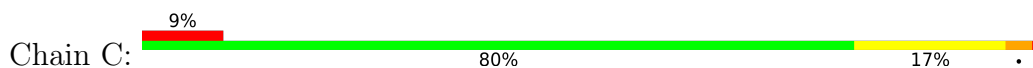
- Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

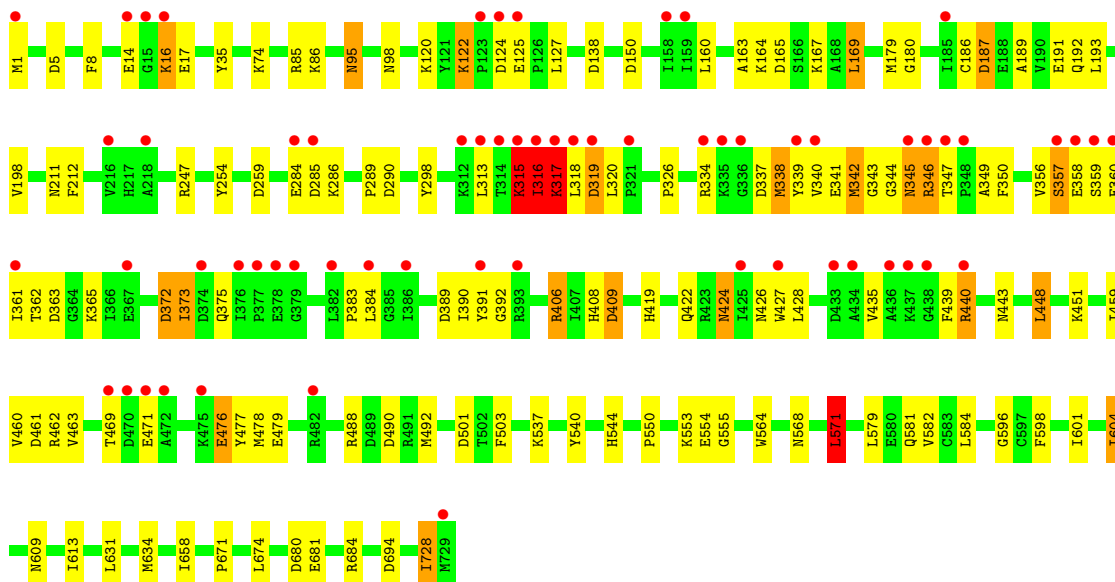


- Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

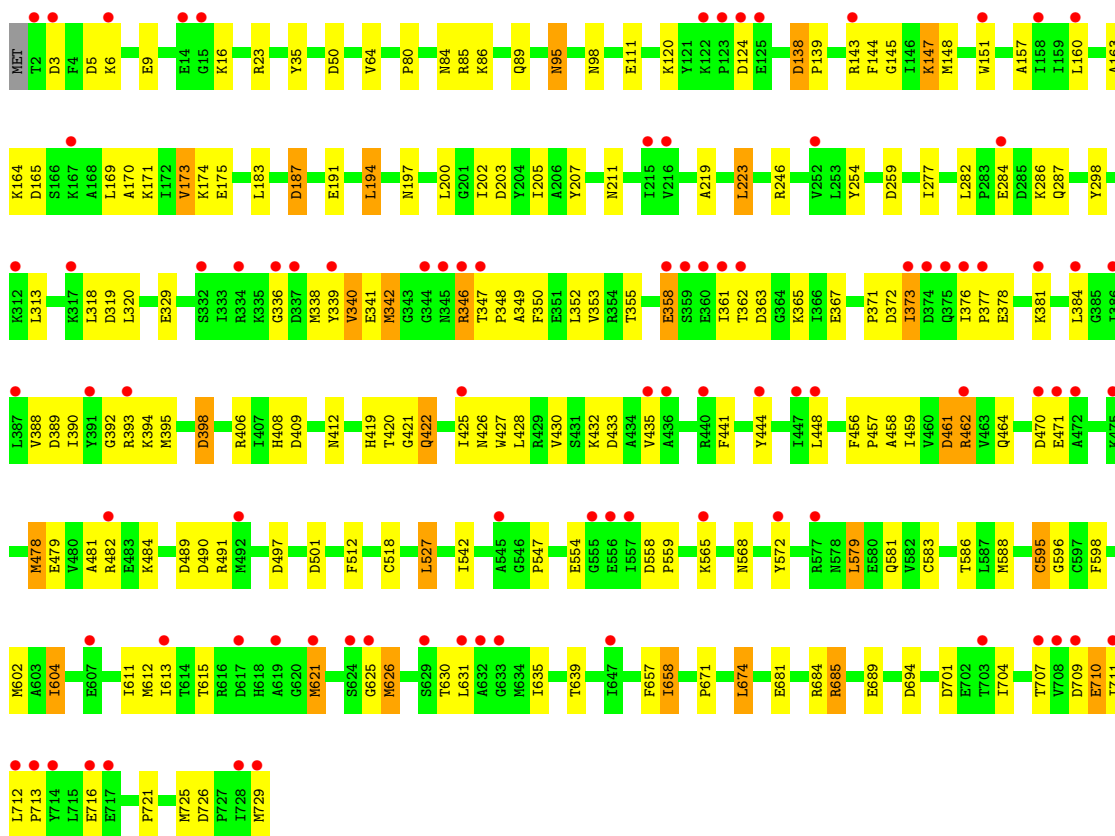
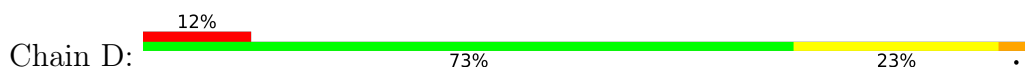


- Molecule 2: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA





● 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, $\alpha$ , $\beta$ , $\gamma$	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)	Xtrriage
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 <sup>2</sup> )	21.8	Xtrriage
Anisotropy	0.375	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



Continued from previous page...

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

Continued on next page...

Continued from previous page...

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
1:B:482:LEU:HD12	7:B:1689:GOL:C1	2.08	0.83

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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
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
1:B:573:LYS:HZ3	1:B:659:HIS:HD2	1.35	0.72
2:D:342:MET:HG3	2:D:384:LEU:HD22	1.70	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

*Continued on next page...*

*Continued from previous page...*

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
1:B:573:LYS:NZ	1:B:659:HIS:HD2	1.94	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:C:537:LYS:HZ2	7:C:1743:GOL:H31	1.59	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:CD2	2.16	0.63
1:B:284:ASN:C	1:B:284:ASN:HD22	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: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
1:A:335:ALA:H	1:A:471:ASN:HD22	1.48	0.61

*Continued on next page...*

*Continued from previous page...*

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: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
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: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
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:O	2:C:338:MET:HG2	2.02	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
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

*Continued on next page...*

*Continued from previous page...*

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
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: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
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
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: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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:657:PHE:O	2:D:658:ILE:C	2.49	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
2:D:621:MET:HE2	2:D:625:GLY:O	2.10	0.50
1:A:577[B]:VAL:HG11	1:A:645:ILE:HG23	1.93	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
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:284:GLU:CD	2:D:284:GLU:N	2.64	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:A:284:ASN:HD22	1:A:284:ASN:C	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
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
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
2:D:339:TYR:CE1	2:D:378:GLU:HG3	2.48	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
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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:611:ILE:HD12	2:D:613:ILE:CD1	2.39	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
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
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
1:A:13:PRO:HG3	1:A:607:MET:HE1	1.97	0.46
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: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:B:573:LYS:NZ	1:B:659:HIS:CD2	2.78	0.46
2:C:537:LYS:HZ1	7:C:1743:GOL:H31	1.78	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: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
1:B:536:ASN:O	1:B:537:ILE:C	2.55	0.45
2:C:342:MET:CB	2:C:384:LEU:HB2	2.47	0.45

*Continued on next page...*



*Continued from previous page...*

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: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
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
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:C:16:LYS:HZ2	2:C:284:GLU:CG	2.30	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:74:LYS:HE3	14:C:2068:HOH:O	2.17	0.43
2:C:95:ASN:HD22	2:C:95:ASN:C	2.21	0.43
2:D:681[A]:GLU:OE2	2:D:684:ARG:NH1	2.51	0.43
2:D:170:ALA:O	2:D:174:LYS:HG3	2.18	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
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
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.48	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:441:PHE:O	2:D:444:TYR:HB2	2.18	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: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: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: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: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: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: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
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:406[B]:ARG:NH1	2:C:409:ASP:CG	2.74	0.41
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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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%)	51 42
1	B	683/674 (101%)	659 (96%)	21 (3%)	3 (0%)	34 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	738/729 (101%)	710 (96%)	22 (3%)	6 (1%)	19	9
2	D	728/729 (100%)	705 (97%)	20 (3%)	3 (0%)	34	24
All	All	2832/2806 (101%)	2738 (97%)	81 (3%)	13 (0%)	29	18

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	554/543 (102%)	535 (97%)	19 (3%)	37	28
1	B	554/543 (102%)	534 (96%)	20 (4%)	35	26
2	C	622/611 (102%)	582 (94%)	40 (6%)	17	8
2	D	612/611 (100%)	570 (93%)	42 (7%)	15	7
All	All	2342/2308 (102%)	2221 (95%)	121 (5%)	23	14

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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

*Continued on next page...*

*Continued from previous page...*

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

Sometimes 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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

*Continued on next page...*



*Continued from previous page...*

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 monosaccharides 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
6	SO4	A	1680	-	4,4,4	0.25	0	6,6,6	0.47	0
6	SO4	C	1734	-	4,4,4	0.20	0	6,6,6	0.42	0
6	SO4	C	1735	-	4,4,4	0.16	0	6,6,6	0.74	0
6	SO4	C	1736	-	4,4,4	0.17	0	6,6,6	0.42	0
7	GOL	B	1690	-	5,5,5	0.46	0	5,5,5	0.21	0
4	XCC	A	1677	1	0,11,11	-	-	-	-	-
6	SO4	A	1689	-	4,4,4	0.18	0	6,6,6	0.13	0
6	SO4	A	1686	-	4,4,4	0.13	0	6,6,6	0.14	0
6	SO4	B	1687	-	4,4,4	0.13	0	6,6,6	0.14	0
6	SO4	B	1681	-	4,4,4	0.24	0	6,6,6	0.24	0
6	SO4	A	1688	-	4,4,4	0.20	0	6,6,6	0.25	0
6	SO4	A	1684	-	4,4,4	0.20	0	6,6,6	0.51	0
6	SO4	B	1686	-	4,4,4	0.18	0	6,6,6	0.25	0
3	SF4	D	1730	2	0,12,12	-	-	-	-	-
6	SO4	D	1738	-	4,4,4	0.20	0	6,6,6	0.18	0
7	GOL	C	1741	-	5,5,5	0.34	0	5,5,5	0.52	0
3	SF4	C	1730	2	0,12,12	-	-	-	-	-
3	SF4	A	1676	1	0,12,12	-	-	-	-	-
6	SO4	A	1681	-	4,4,4	0.11	0	6,6,6	0.21	0
6	SO4	A	1685	-	4,4,4	0.20	0	6,6,6	0.19	0
6	SO4	A	1683	-	4,4,4	0.14	0	6,6,6	0.27	0
6	SO4	D	1734	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SF4	B	1675	1	0,12,12	-	-	-	-	-
4	XCC	B	1677	1	0,11,11	-	-	-	-	-
6	SO4	B	1684	-	4,4,4	0.15	0	6,6,6	0.21	0
6	SO4	B	1688	-	4,4,4	0.15	0	6,6,6	0.17	0
6	SO4	C	1738	-	4,4,4	0.37	0	6,6,6	0.24	0
6	SO4	B	1679	-	4,4,4	0.28	0	6,6,6	0.39	0
6	SO4	D	1735	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SF4	B	1676	1	0,12,12	-	-	-	-	-
5	FOR	B	1678	-	0,1,1	-	-	-	-	-
6	SO4	A	1690	-	4,4,4	0.12	0	6,6,6	0.30	0
7	GOL	D	1736	-	5,5,5	0.50	0	5,5,5	0.64	0
13	ACT	D	1733	11	3,3,3	0.70	0	3,3,3	1.52	0
6	SO4	B	1680	-	4,4,4	0.13	0	6,6,6	0.44	0
6	SO4	A	1679	-	4,4,4	0.34	0	6,6,6	0.39	0
7	GOL	B	1689	-	5,5,5	0.38	0	5,5,5	0.23	0
7	GOL	C	1737	-	5,5,5	0.30	0	5,5,5	0.34	0
6	SO4	A	1682	-	4,4,4	0.18	0	6,6,6	0.27	0
9	BCT	B	1691	-	2,3,3	0.51	0	2,3,3	0.53	0
6	SO4	B	1683	-	4,4,4	0.18	0	6,6,6	0.52	0
6	SO4	D	1737	-	4,4,4	0.15	0	6,6,6	0.09	0
6	SO4	C	1742	-	4,4,4	0.14	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	SX	C	1733	10	0,1,1	-	-	-		
7	GOL	A	1687	-	5,5,5	0.45	0	5,5,5	1.00	0
6	SO4	B	1682	-	4,4,4	0.22	0	6,6,6	0.37	0
5	FOR	A	1678	-	0,1,1	-	-	-		
6	SO4	C	1740	-	4,4,4	0.35	0	6,6,6	0.48	0
7	GOL	C	1739	-	5,5,5	0.33	0	5,5,5	0.45	0
7	GOL	C	1743	-	5,5,5	0.51	0	5,5,5	0.70	0
6	SO4	B	1685	-	4,4,4	0.11	0	6,6,6	0.28	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	B	1676	1	-	-	0/6/5/5
7	GOL	B	1690	-	-	1/4/4/4	-
7	GOL	C	1741	-	-	2/4/4/4	-
7	GOL	D	1736	-	-	4/4/4/4	-
3	SF4	A	1676	1	-	-	0/6/5/5
3	SF4	C	1730	2	-	-	0/6/5/5
4	XCC	A	1677	1	-	-	0/3/3/3
7	GOL	A	1687	-	-	4/4/4/4	-
7	GOL	B	1689	-	-	2/4/4/4	-
7	GOL	C	1737	-	-	4/4/4/4	-
3	SF4	B	1675	1	-	-	0/6/5/5
4	XCC	B	1677	1	-	-	0/3/3/3
7	GOL	C	1739	-	-	0/4/4/4	-
7	GOL	C	1743	-	-	2/4/4/4	-
3	SF4	D	1730	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
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
7	B	1689	GOL	C1-C2-C3-O3

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.04	17 (2%) 57 60	5, 10, 20, 32	15 (2%)
1	B	673/674 (99%)	-0.08	12 (1%) 68 71	5, 10, 19, 39	18 (2%)
2	C	729/729 (100%)	0.30	63 (8%) 10 12	3, 11, 22, 35	7 (0%)
2	D	728/729 (99%)	0.56	90 (12%) 4 4	4, 11, 21, 39	7 (0%)
All	All	2803/2806 (99%)	0.20	182 (6%) 18 21	3, 10, 21, 39	47 (1%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	345	ASN	8.0
1	B	536	ASN	7.6
2	C	317	LYS	7.5
1	B	537	ILE	6.3
2	C	472	ALA	6.1
2	C	314	THR	5.9
2	C	315	LYS	5.9
2	D	15	GLY	5.8
2	D	713	PRO	5.8
2	C	359	SER	5.7
2	C	345	ASN	5.5
2	D	717	GLU	5.4
1	A	538	GLU	5.4
2	C	348	PRO	5.2
2	D	359	SER	5.1
2	C	319	ASP	4.9
2	C	1	MET	4.8
1	A	8	SER	4.6
2	D	334	ARG	4.5
2	D	617	ASP	4.5
2	C	316	ILE	4.5

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	6	ASP	3.3
2	C	361	ILE	3.3
2	C	470	ASP	3.3
2	C	339	TYR	3.3
2	D	729	MET	3.3
2	C	393	ARG	3.2
2	D	557	ILE	3.2
1	A	445	ALA	3.2
2	C	123	PRO	3.2
1	B	538	GLU	3.2
2	D	3	ASP	3.1
2	D	361	ILE	3.1
2	D	376	ILE	3.1
2	D	332	SER	3.1
2	D	375	GLN	3.0
2	D	631	LEU	3.0
2	C	284	GLU	3.0
2	C	475	LYS	3.0
2	D	447	ILE	3.0
2	D	360	GLU	3.0
2	D	709	ASP	2.9
2	D	716	GLU	2.9
2	D	143	ARG	2.9
1	B	7	LEU	2.9
2	D	444	TYR	2.8
2	D	151	TRP	2.8
2	D	284	GLU	2.8
2	D	471	GLU	2.8
2	D	252	VAL	2.7
2	C	14	GLU	2.7
2	D	711	ILE	2.7
2	D	123	PRO	2.7
2	D	391	TYR	2.7
2	D	624	SER	2.7
2	C	471	GLU	2.6
2	C	436	ALA	2.6
2	D	425	ILE	2.6
2	D	122	LYS	2.6
2	C	360	GLU	2.6
2	D	572	TYR	2.6
2	C	382	LEU	2.6
2	D	160	LEU	2.6

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	712	LEU	2.6
1	B	445	ALA	2.6
2	D	2	THR	2.6
2	C	391	TYR	2.6
2	D	158	ILE	2.6
2	D	728	ILE	2.6
2	D	6	LYS	2.5
2	D	545	ALA	2.5
2	D	462	ARG	2.5
1	A	669	LYS	2.5
2	C	16	LYS	2.5
2	C	158	ILE	2.5
2	C	367	GLU	2.5
2	D	386	ILE	2.5
2	D	381	LYS	2.5
2	D	317	LYS	2.4
1	A	82	ASP	2.4
2	D	629	SER	2.4
1	A	296	ARG	2.4
2	D	387	LEU	2.4
2	C	216	VAL	2.4
2	D	339	TYR	2.4
2	D	470	ASP	2.4
2	D	167	LYS	2.4
1	B	417	PRO	2.4
1	A	667	GLU	2.3
2	D	633	GLY	2.3
2	C	729	MET	2.3
2	D	472	ALA	2.3
2	C	437	LYS	2.3
2	D	607	GLU	2.3
1	B	577[A]	VAL	2.3
1	B	583	ALA	2.3
2	C	438	GLY	2.3
2	C	185	ILE	2.3
2	C	433	ASP	2.3
1	A	155	GLU	2.3
1	B	533	GLU	2.3
2	D	312	LYS	2.3
2	C	386	ILE	2.3
2	D	703	THR	2.3
2	D	440	ARG	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	613	ILE	2.2
2	C	347	THR	2.2
2	D	475	LYS	2.2
2	D	565	LYS	2.2
2	D	707	THR	2.2
2	D	625	GLY	2.2
2	C	159	ILE	2.2
2	D	384	LEU	2.2
2	D	337	ASP	2.2
2	D	492	MET	2.2
2	C	340	VAL	2.2
2	D	708	VAL	2.2
2	C	384	LEU	2.2
2	D	632	ALA	2.2
2	C	335	LYS	2.2
1	A	464	VAL	2.2
2	D	555	GLY	2.1
1	A	4	PHE	2.1
2	D	435	VAL	2.1
2	C	285	ASP	2.1
2	C	469	THR	2.1
2	C	482	ARG	2.1
2	C	378	GLU	2.1
2	D	347	THR	2.1
2	C	218	ALA	2.1
2	C	434	ALA	2.1
2	D	556	GLU	2.1
2	C	376	ILE	2.1
2	C	425	ILE	2.1
2	D	373	ILE	2.1
2	C	334	ARG	2.0
2	D	621	MET	2.0
1	A	533	GLU	2.0
2	D	647	ILE	2.0
2	D	482	ARG	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
13	ACT	D	1733	4/4	0.73	0.26	18,18,19,19	4
7	GOL	B	1690	6/6	0.74	0.21	58,60,61,61	0
7	GOL	A	1687	6/6	0.82	0.23	29,31,33,34	0
6	SO4	B	1687	5/5	0.83	0.17	51,51,51,52	5
6	SO4	A	1689	5/5	0.83	0.26	48,49,50,50	5
7	GOL	D	1736	6/6	0.85	0.20	41,45,47,48	0
7	GOL	C	1737	6/6	0.86	0.19	36,37,38,38	0
6	SO4	C	1740	5/5	0.88	0.15	19,25,26,27	5
6	SO4	B	1683	5/5	0.90	0.15	33,33,35,36	5
7	GOL	C	1743	6/6	0.91	0.15	50,52,53,53	0
5	FOR	B	1678	2/2	0.91	0.45	23,23,23,24	2
7	GOL	C	1741	6/6	0.91	0.20	21,30,33,38	0
6	SO4	D	1734	5/5	0.92	0.17	30,30,30,31	5
6	SO4	C	1742	5/5	0.92	0.23	31,31,31,32	0
6	SO4	B	1684	5/5	0.93	0.28	59,59,61,61	0
6	SO4	A	1686	5/5	0.93	0.16	36,36,37,39	5
6	SO4	D	1737	5/5	0.93	0.13	61,61,61,62	5
6	SO4	D	1738	5/5	0.93	0.22	58,59,59,60	0
6	SO4	A	1688	5/5	0.93	0.24	59,60,60,61	0
9	BCT	B	1691	4/4	0.93	0.12	36,37,37,38	0
7	GOL	B	1689	6/6	0.93	0.20	54,55,56,57	0
6	SO4	B	1686	5/5	0.94	0.26	58,58,59,60	0
6	SO4	C	1734	5/5	0.94	0.17	15,16,23,23	5
6	SO4	B	1688	5/5	0.96	0.16	42,45,46,46	5
7	GOL	C	1739	6/6	0.96	0.09	10,16,17,19	0
6	SO4	B	1685	5/5	0.96	0.12	59,59,60,60	0
6	SO4	C	1735	5/5	0.96	0.17	33,35,35,36	0
6	SO4	C	1736	5/5	0.96	0.21	27,30,31,31	0
4	XCC	A	1677	9/9	0.96	0.09	17,17,23,24	9
5	FOR	A	1678	2/2	0.96	0.23	23,23,23,23	2
6	SO4	A	1681	5/5	0.97	0.18	33,34,36,36	0
6	SO4	B	1680	5/5	0.97	0.13	29,31,32,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	1681	5/5	0.97	0.18	31,34,35,36	0
6	SO4	B	1682	5/5	0.97	0.21	29,31,31,31	0
6	SO4	A	1683	5/5	0.97	0.17	33,33,34,35	0
8	FE2	A	1700	1/1	0.97	0.10	22,22,22,22	1
4	XCC	B	1677	9/9	0.97	0.08	17,17,22,23	9
6	SO4	A	1679	5/5	0.97	0.11	18,18,21,25	0
6	SO4	A	1682	5/5	0.98	0.14	26,28,28,29	0
6	SO4	A	1680	5/5	0.98	0.10	23,23,24,26	0
6	SO4	A	1684	5/5	0.98	0.14	38,38,39,39	0
6	SO4	A	1690	5/5	0.98	0.07	49,50,51,52	0
6	SO4	D	1735	5/5	0.98	0.10	33,33,35,35	0
11	NI	D	1731[A]	1/1	0.98	0.12	17,17,17,17	1
11	NI	D	1731[B]	1/1	0.98	0.12	16,16,16,16	1
6	SO4	A	1685	5/5	0.98	0.17	28,30,32,32	0
3	SF4	B	1676	8/8	0.99	0.04	7,8,8,9	0
6	SO4	B	1679	5/5	0.99	0.12	24,24,26,28	0
8	FE2	B	1700	1/1	0.99	0.06	20,20,20,20	1
3	SF4	D	1730	8/8	0.99	0.06	9,9,10,11	0
10	ZN	C	1731	1/1	0.99	0.06	12,12,12,12	0
3	SF4	A	1676	8/8	0.99	0.04	7,8,8,9	0
6	SO4	C	1738	5/5	0.99	0.09	21,23,25,27	0
12	SX	C	1733	2/2	0.99	0.15	15,15,15,18	0
3	SF4	B	1675	8/8	0.99	0.07	9,11,11,12	0
11	NI	D	1732	1/1	1.00	0.07	9,9,9,9	0
3	SF4	C	1730	8/8	1.00	0.07	5,7,8,8	0
11	NI	C	1732	1/1	1.00	0.08	9,9,9,9	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.