



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 09:04 PM EDT

PDB ID : 1PIX  
Title : Crystal structure of the carboxyltransferase subunit of the bacterial ion pump  
glutaconyl-coenzyme A decarboxylase  
Authors : Wendt, K.S.; Schall, I.; Huber, R.; Buckel, W.; Jacob, U.  
Deposited on : 2003-05-30  
Resolution : 2.20 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

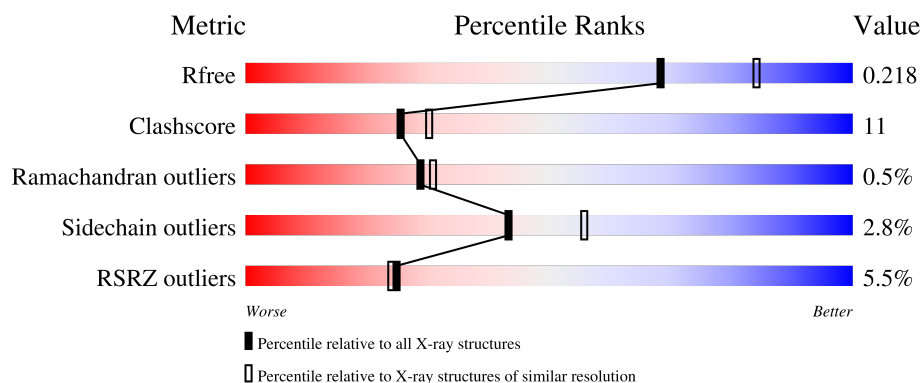
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	587	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	587	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>20%</div> <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
3	FMT	A	2006	-	X	-	-
3	FMT	A	2007	-	X	-	-
3	FMT	A	2008	-	X	-	-
3	FMT	B	2005	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9717 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 Glutaconyl-CoA decarboxylase A subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4502	2855	778	848	21			
1	B	586	Total	C	N	O	S	0	0	0
			4517	2865	780	849	23			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

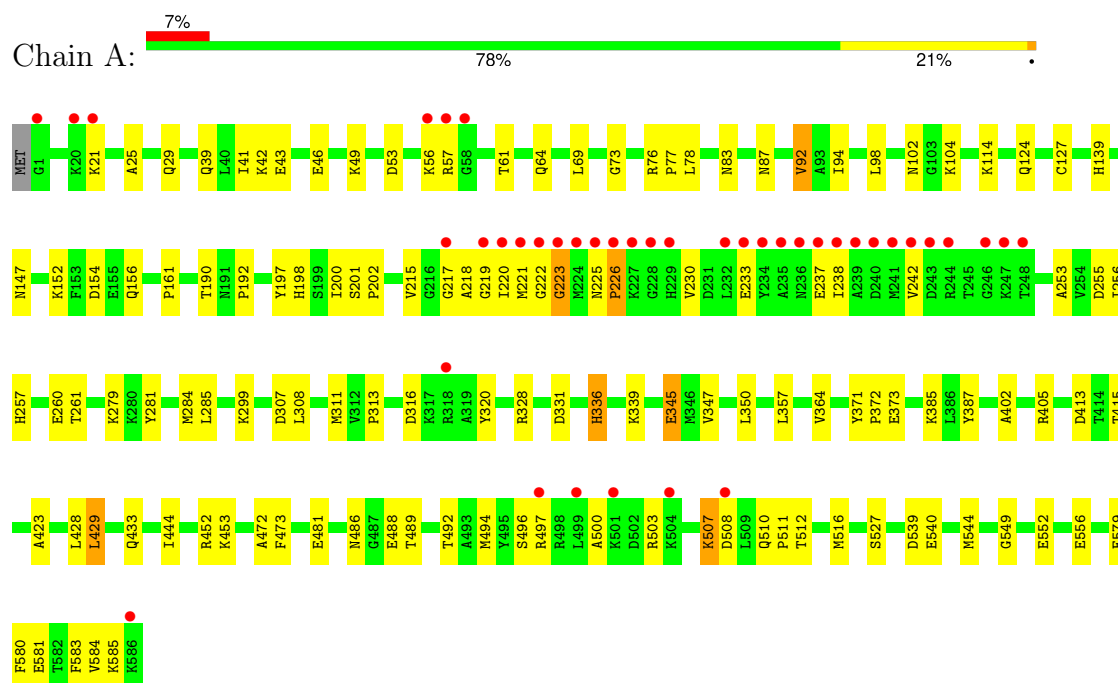
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	316	Total	O	0	0
			316	316		
4	B	345	Total	O	0	0
			345	345		

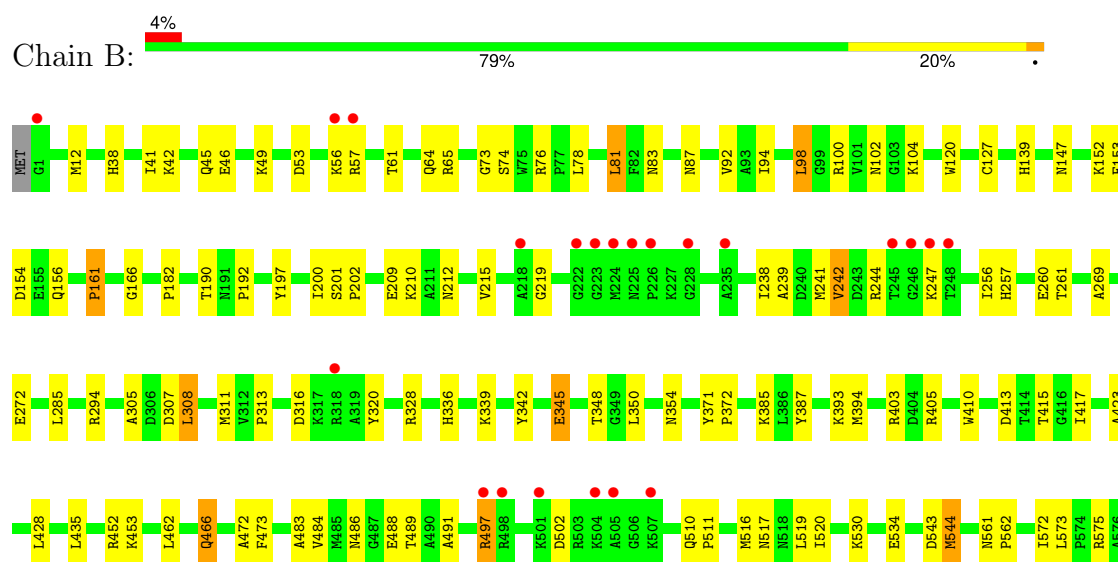
### 3 Residue-property plots

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: Glutaconyl-CoA decarboxylase A subunit



#### • Molecule 1: Glutaconyl-CoA decarboxylase A subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.87Å 151.87Å 163.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.97 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.20) 98.3 (19.97-2.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.201 , 0.227 0.192 , 0.218	Depositor DCC
$R_{free}$ test set	5023 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: SO4, FMT

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	0.32	0/4594	0.63	1/6218 (0.0%)
1	B	0.31	0/4610	0.61	0/6237
All	All	0.32	0/9204	0.62	1/12455 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	PRO	N-CA-CB	5.78	110.24	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	4502	0	4485	106	0
1	B	4517	0	4520	104	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
3	A	9	0	6	0	0
3	B	3	0	2	0	0
4	A	316	0	0	10	0
4	B	345	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9717	0	9013	192	0

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 11.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:HD21	1:B:87:ASN:H	1.10	1.00
1:A:230:VAL:H	1:B:517:ASN:HD21	1.10	0.94
1:B:308:LEU:HB3	1:B:544:MET:HG3	1.54	0.90
1:A:500:ALA:HB2	1:B:242:VAL:HG11	1.50	0.90
1:B:345:GLU:HG2	1:B:387:TYR:HD1	1.34	0.90
1:B:394:MET:HE3	1:B:410:TRP:HZ3	1.37	0.89
1:A:83:ASN:HD21	1:A:87:ASN:H	1.15	0.88
1:A:42:LYS:O	1:A:46:GLU:HG2	1.75	0.86
1:A:316:ASP:HA	1:A:452:ARG:NH2	1.92	0.85
1:A:345:GLU:HG2	1:A:387:TYR:HD1	1.39	0.85
1:B:65:ARG:HH12	1:B:147:ASN:HD22	1.22	0.84
1:B:394:MET:HE1	1:B:435:LEU:HD21	1.61	0.82
1:B:413:ASP:OD2	1:B:452:ARG:HD3	1.79	0.82
1:A:413:ASP:OD2	1:A:452:ARG:HD3	1.81	0.81
1:A:190:THR:HG22	1:A:192:PRO:HD3	1.64	0.80
1:B:190:THR:HG22	1:B:192:PRO:HD3	1.64	0.79
1:A:345:GLU:HG2	1:A:387:TYR:CD1	2.18	0.78
1:B:345:GLU:HG2	1:B:387:TYR:CD1	2.18	0.78
1:A:94:ILE:HD11	1:A:127:CYS:SG	2.23	0.78
1:B:316:ASP:HA	1:B:452:ARG:NH2	2.01	0.75
1:B:530:LYS:O	1:B:534:GLU:HG3	1.87	0.74
1:A:540:GLU:OE1	4:A:1167:HOH:O	2.07	0.73
1:B:466:GLN:NE2	1:B:466:GLN:H	1.88	0.72
1:A:507:LYS:HE3	1:A:507:LYS:HA	1.72	0.70
1:B:394:MET:CE	1:B:410:TRP:HZ3	2.06	0.69
1:B:53:ASP:O	1:B:56:LYS:HG2	1.93	0.68
1:B:403:ARG:CZ	1:B:572:ILE:HD13	2.25	0.67
1:B:385:LYS:HD2	1:B:415:THR:OG1	1.95	0.67
1:B:83:ASN:ND2	1:B:87:ASN:H	1.88	0.66
1:B:316:ASP:HB2	1:B:453:LYS:HE3	1.78	0.66
1:A:238:ILE:O	1:A:242:VAL:HG23	1.97	0.65
1:A:385:LYS:HD2	1:A:415:THR:OG1	1.95	0.65
1:A:539:ASP:O	1:A:540:GLU:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:ND2	1:A:87:ASN:H	1.93	0.64
1:A:152:LYS:HE2	1:A:154:ASP:HB3	1.79	0.64
1:A:494:MET:HE1	1:B:153:PHE:HB2	1.79	0.63
1:A:139:HIS:HD2	4:A:1066:HOH:O	1.81	0.63
1:A:500:ALA:HB2	1:B:242:VAL:CG1	2.26	0.63
1:B:74:SER:HB2	1:B:100:ARG:HG3	1.80	0.63
1:B:104:LYS:HE2	1:B:285:LEU:O	1.98	0.62
1:A:156:GLN:HG3	1:B:484:VAL:HG12	1.81	0.62
1:A:78:LEU:HA	1:A:540:GLU:CG	2.29	0.62
1:B:94:ILE:HD11	1:B:127:CYS:SG	2.39	0.61
1:A:77:PRO:O	1:A:540:GLU:HG3	2.00	0.61
1:B:92:VAL:HG23	1:B:94:ILE:HG12	1.82	0.61
1:B:342:TYR:O	1:B:393:LYS:HE2	2.00	0.61
1:B:516:MET:O	1:B:520:ILE:HG13	2.01	0.61
1:A:429:LEU:HD22	1:B:200:ILE:HG21	1.83	0.61
1:B:394:MET:HE1	1:B:435:LEU:CD2	2.30	0.60
1:A:429:LEU:HA	1:B:215:VAL:HG12	1.83	0.60
1:A:41:ILE:HD11	4:A:1167:HOH:O	2.02	0.60
1:A:503:ARG:HA	4:A:1654:HOH:O	2.00	0.60
1:A:336:HIS:HE1	1:A:581:GLU:OE1	1.85	0.60
1:B:41:ILE:HG12	1:B:81:LEU:HD13	1.83	0.60
1:B:394:MET:CE	1:B:435:LEU:HD21	2.31	0.59
1:A:230:VAL:N	1:B:517:ASN:HD21	1.93	0.59
1:A:156:GLN:NE2	4:A:1003:HOH:O	2.35	0.58
1:B:497:ARG:N	1:B:497:ARG:HD2	2.18	0.58
1:B:247:LYS:HG3	1:B:247:LYS:O	2.04	0.58
1:A:320:TYR:HE2	1:A:452:ARG:HH11	1.52	0.58
1:A:217:GLY:O	1:A:218:ALA:HB3	2.05	0.57
1:A:371:TYR:CD1	1:A:372:PRO:HA	2.39	0.57
1:A:497:ARG:HB3	4:A:1016:HOH:O	2.04	0.57
1:B:348:THR:OG1	1:B:393:LYS:HD2	2.05	0.57
1:A:78:LEU:HA	1:A:540:GLU:HG3	1.86	0.56
1:A:219:GLY:C	1:A:220:ILE:HD12	2.26	0.56
1:B:209:GLU:HG2	1:B:269:ALA:HA	1.88	0.56
1:B:49:LYS:NZ	1:B:57:ARG:NH2	2.53	0.55
1:A:307:ASP:HB2	1:A:328:ARG:HE	1.70	0.55
1:B:61:THR:H	1:B:64:GLN:NE2	2.05	0.55
1:B:56:LYS:HG3	1:B:57:ARG:N	2.22	0.55
1:B:491:ALA:HA	1:B:519:LEU:HD23	1.89	0.55
1:A:156:GLN:HE22	1:B:483:ALA:HA	1.72	0.54
1:B:12:MET:HE2	1:B:336:HIS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:O	1:B:46:GLU:HG3	2.07	0.54
1:B:78:LEU:HD11	1:B:98:LEU:HD13	1.90	0.54
1:A:429:LEU:CA	1:B:215:VAL:HG12	2.38	0.53
1:B:497:ARG:HD3	4:B:1114:HOH:O	2.08	0.53
1:A:371:TYR:CG	1:A:372:PRO:HA	2.43	0.53
1:A:39:GLN:O	1:A:43:GLU:HG2	2.08	0.52
1:A:307:ASP:HB2	1:A:328:ARG:NE	2.24	0.52
1:B:371:TYR:CD1	1:B:372:PRO:HA	2.44	0.52
1:B:577:ILE:O	1:B:581:GLU:HG2	2.09	0.52
1:A:46:GLU:HA	1:A:114:LYS:HE2	1.91	0.52
1:B:320:TYR:HE2	1:B:452:ARG:HH11	1.57	0.52
1:B:73:GLY:O	1:B:76:ARG:NH2	2.43	0.52
1:B:350:LEU:HD21	1:B:573:LEU:HD23	1.92	0.52
1:A:139:HIS:CD2	4:A:1066:HOH:O	2.60	0.52
1:A:104:LYS:HE2	1:A:285:LEU:O	2.10	0.51
1:A:311:MET:O	1:A:313:PRO:HD3	2.10	0.51
1:A:21:LYS:O	1:A:21:LYS:HG3	2.10	0.51
1:B:239:ALA:O	1:B:242:VAL:HG13	2.10	0.51
1:B:38:HIS:HE1	1:B:543:ASP:OD2	1.94	0.51
1:A:230:VAL:H	1:B:517:ASN:ND2	1.92	0.51
1:A:156:GLN:NE2	1:B:483:ALA:HA	2.26	0.50
1:B:209:GLU:OE2	1:B:210:LYS:HE2	2.12	0.50
1:A:486:ASN:ND2	1:A:488:GLU:H	2.09	0.50
1:A:510:GLN:HB3	1:A:511:PRO:HD3	1.93	0.50
1:A:508:ASP:HB3	4:A:1100:HOH:O	2.10	0.50
1:A:512:THR:O	1:A:516:MET:HG3	2.11	0.50
1:B:83:ASN:HD21	1:B:87:ASN:N	1.93	0.50
1:A:61:THR:H	1:A:64:GLN:NE2	2.10	0.49
1:B:371:TYR:CG	1:B:372:PRO:HA	2.48	0.49
1:A:156:GLN:NE2	1:B:484:VAL:H	2.10	0.49
1:B:152:LYS:HG2	1:B:154:ASP:OD1	2.12	0.49
1:B:311:MET:O	1:B:313:PRO:HD3	2.13	0.49
1:A:53:ASP:O	1:A:56:LYS:HG2	2.13	0.49
1:B:238:ILE:O	1:B:242:VAL:HG12	2.13	0.49
1:B:294:ARG:HD3	1:B:354:ASN:O	2.12	0.49
1:B:305:ALA:O	1:B:308:LEU:HB2	2.12	0.49
1:B:94:ILE:HD11	1:B:127:CYS:HB3	1.94	0.48
1:B:120:TRP:CZ3	1:B:166:GLY:HA3	2.48	0.48
1:A:49:LYS:NZ	1:A:57:ARG:NH1	2.61	0.48
1:B:78:LEU:CD1	1:B:98:LEU:HD13	2.43	0.48
1:A:253:ALA:HB3	1:A:255:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASN:HB3	1:A:489:THR:OG1	2.14	0.48
1:A:494:MET:HE3	1:B:153:PHE:HD1	1.79	0.48
1:B:403:ARG:NH2	1:B:572:ILE:HD13	2.28	0.47
1:A:583:PHE:HE2	1:A:585:LYS:HG2	1.79	0.47
1:A:73:GLY:O	1:A:76:ARG:NH2	2.46	0.47
1:B:12:MET:CE	1:B:336:HIS:HB2	2.45	0.47
1:A:152:LYS:HE2	1:A:154:ASP:CB	2.46	0.46
1:A:215:VAL:HG11	1:B:417:ILE:HB	1.97	0.46
1:A:198:HIS:HD2	4:A:1142:HOH:O	1.98	0.45
1:A:413:ASP:OD1	1:A:452:ARG:HB2	2.16	0.45
1:A:92:VAL:HG22	1:A:124:GLN:HA	1.99	0.45
1:B:339:LYS:HA	1:B:580:PHE:CD2	2.50	0.45
1:B:394:MET:HE3	1:B:410:TRP:CZ3	2.30	0.45
1:B:197:TYR:HA	1:B:200:ILE:HG22	1.99	0.45
1:B:272:GLU:H	1:B:272:GLU:CD	2.20	0.45
1:A:78:LEU:HA	1:A:540:GLU:HG2	1.98	0.45
1:A:507:LYS:HE3	1:A:507:LYS:CA	2.43	0.45
1:B:241:MET:HA	1:B:244:ARG:NH1	2.31	0.45
1:A:49:LYS:HZ1	1:A:57:ARG:NH1	2.15	0.45
1:A:308:LEU:CB	1:A:544:MET:HG3	2.47	0.45
1:B:257:HIS:HA	1:B:261:THR:OG1	2.17	0.45
1:A:92:VAL:HG22	1:A:124:GLN:CA	2.46	0.45
1:A:350:LEU:HG	1:A:357:LEU:HD11	1.99	0.45
1:A:49:LYS:NZ	1:A:57:ARG:CZ	2.80	0.44
1:B:256:ILE:O	1:B:260:GLU:HB2	2.18	0.44
1:A:423:ALA:HB1	1:A:428:LEU:HD12	2.00	0.44
1:A:549:GLY:HA3	4:A:1283:HOH:O	2.16	0.44
1:A:197:TYR:HA	1:A:200:ILE:HG22	2.00	0.44
1:B:74:SER:CB	1:B:100:ARG:HG3	2.48	0.44
1:A:308:LEU:HB3	1:A:544:MET:HG3	2.00	0.43
1:A:481:GLU:HA	1:A:527:SER:O	2.18	0.43
1:A:494:MET:CE	1:B:153:PHE:HB2	2.47	0.43
1:B:12:MET:HE2	1:B:12:MET:HB3	1.78	0.43
1:B:472:ALA:O	1:B:473:PHE:HB3	2.18	0.43
1:A:92:VAL:CG1	1:A:94:ILE:HG12	2.48	0.43
1:A:78:LEU:HD11	1:A:98:LEU:HD13	1.99	0.43
1:A:552:GLU:O	1:A:556:GLU:HG3	2.18	0.43
1:A:61:THR:H	1:A:64:GLN:HE21	1.67	0.43
1:A:256:ILE:O	1:A:260:GLU:HB2	2.19	0.43
1:B:201:SER:N	1:B:202:PRO:CD	2.81	0.43
1:A:472:ALA:O	1:A:473:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:HIS:CE1	1:B:543:ASP:OD2	2.71	0.43
1:B:486:ASN:ND2	1:B:489:THR:H	2.16	0.43
1:B:394:MET:HB3	1:B:394:MET:HE2	1.84	0.42
1:B:190:THR:HG23	1:B:212:ASN:OD1	2.19	0.42
1:B:510:GLN:HB3	1:B:511:PRO:HD3	2.02	0.42
1:A:281:TYR:CD2	1:A:284:MET:CE	3.02	0.42
1:A:220:ILE:HD12	1:A:220:ILE:N	2.35	0.42
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.90	0.42
1:A:281:TYR:CD2	1:A:284:MET:HE2	2.54	0.42
1:B:41:ILE:O	1:B:45:GLN:HG3	2.20	0.42
1:A:316:ASP:HB2	1:A:453:LYS:HE3	2.01	0.42
1:A:402:ALA:HA	1:A:444:ILE:HD13	2.02	0.42
1:A:492:THR:O	1:A:496:SER:HB3	2.19	0.42
1:B:307:ASP:HB2	1:B:328:ARG:NE	2.35	0.42
1:B:423:ALA:HB1	1:B:428:LEU:HD12	2.02	0.42
1:A:222:GLY:O	1:A:223:GLY:C	2.58	0.42
1:B:38:HIS:HD2	4:B:1011:HOH:O	2.02	0.42
1:B:94:ILE:HD11	1:B:127:CYS:CB	2.50	0.41
1:A:25:ALA:O	1:A:29:GLN:HG3	2.20	0.41
1:A:201:SER:N	1:A:202:PRO:CD	2.83	0.41
1:A:433:GLN:HG2	1:B:201:SER:HA	2.03	0.41
1:A:92:VAL:HG22	1:A:124:GLN:N	2.35	0.41
1:A:339:LYS:HA	1:A:580:PHE:CD2	2.56	0.41
1:A:584:VAL:HG23	1:A:584:VAL:O	2.19	0.41
1:A:347:VAL:HG23	1:A:364:VAL:HG22	2.03	0.41
1:B:182:PRO:HG2	1:B:285:LEU:HD22	2.01	0.41
1:B:394:MET:CE	1:B:410:TRP:CZ3	2.96	0.41
1:A:104:LYS:HE2	1:A:285:LEU:C	2.41	0.41
1:A:233:GLU:O	1:A:237:GLU:HG3	2.21	0.41
1:A:257:HIS:HA	1:A:261:THR:OG1	2.21	0.41
1:B:394:MET:CE	1:B:462:LEU:HD23	2.51	0.41
1:A:69:LEU:O	1:A:279:LYS:HE2	2.21	0.41
1:B:488:GLU:HG2	1:B:520:ILE:HD13	2.03	0.41
1:B:561:ASN:N	1:B:562:PRO:HD3	2.36	0.41
1:A:494:MET:HE3	1:B:153:PHE:CD1	2.56	0.40
1:A:299:LYS:O	1:A:331:ASP:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	584/587 (100%)	546 (94%)	34 (6%)	4 (1%)	22	22
1	B	584/587 (100%)	552 (94%)	30 (5%)	2 (0%)	41	46
All	All	1168/1174 (100%)	1098 (94%)	64 (6%)	6 (0%)	29	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	226	PRO
1	A	223	GLY
1	A	221	MET
1	B	219	GLY
1	B	161	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/474 (99%)	457 (98%)	11 (2%)	49	62
1	B	473/474 (100%)	458 (97%)	15 (3%)	39	50
All	All	941/948 (99%)	915 (97%)	26 (3%)	43	56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	102	ASN
1	A	147	ASN
1	A	161	PRO
1	A	336	HIS
1	A	345	GLU
1	A	373	GLU
1	A	405	ARG
1	A	429	LEU
1	A	507	LYS
1	A	579	GLU
1	B	81	LEU
1	B	98	LEU
1	B	102	ASN
1	B	139	HIS
1	B	156	GLN
1	B	161	PRO
1	B	242	VAL
1	B	308	LEU
1	B	345	GLU
1	B	405	ARG
1	B	466	GLN
1	B	497	ARG
1	B	502	ASP
1	B	544	MET
1	B	575	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	64	GLN
1	A	83	ASN
1	A	102	ASN
1	A	156	GLN
1	A	177	ASN
1	A	198	HIS
1	A	336	HIS
1	A	354	ASN
1	A	486	ASN
1	A	561	ASN
1	B	38	HIS
1	B	55	ASN

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Mol	Chain	Res	Type
1	B	64	GLN
1	B	83	ASN
1	B	102	ASN
1	B	147	ASN
1	B	156	GLN
1	B	177	ASN
1	B	198	HIS
1	B	354	ASN
1	B	370	ASN
1	B	466	GLN
1	B	517	ASN
1	B	518	ASN
1	B	561	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	B	2003	-	4,4,4	0.36	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	2002	-	4,4,4	0.35	0	6,6,6	0.07	0
3	FMT	B	2005	-	2,2,2	5.37	2 (100%)	1,1,1	1.33	0
2	SO4	B	2004	-	4,4,4	0.39	0	6,6,6	0.12	0
3	FMT	A	2006	-	2,2,2	5.38	2 (100%)	1,1,1	1.31	0
3	FMT	A	2007	-	2,2,2	5.43	2 (100%)	1,1,1	1.29	0
2	SO4	A	2001	-	4,4,4	0.39	0	6,6,6	0.10	0
3	FMT	A	2008	-	2,2,2	5.39	2 (100%)	1,1,1	1.30	0
2	SO4	B	2000	-	4,4,4	0.31	0	6,6,6	0.09	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2007	FMT	O1-C	5.52	1.52	1.22
3	A	2006	FMT	O1-C	5.51	1.52	1.22
3	A	2008	FMT	O1-C	5.46	1.52	1.22
3	B	2005	FMT	O1-C	5.44	1.52	1.22
3	A	2007	FMT	O2-C	5.35	1.56	1.28
3	A	2008	FMT	O2-C	5.32	1.55	1.28
3	B	2005	FMT	O2-C	5.30	1.55	1.28
3	A	2006	FMT	O2-C	5.23	1.55	1.28

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	586/587 (99%)	-0.18	41 (6%)	16 15	21, 32, 62, 86	18 (3%)
1	B	586/587 (99%)	-0.38	23 (3%)	39 37	22, 32, 63, 87	0
All	All	1172/1174 (99%)	-0.28	64 (5%)	25 24	21, 32, 62, 87	18 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	ALA	12.1
1	A	224	MET	11.7
1	A	226	PRO	9.1
1	A	239	ALA	7.5
1	A	238	ILE	7.4
1	A	222	GLY	7.1
1	A	227	LYS	7.1
1	A	247	LYS	7.0
1	A	223	GLY	6.8
1	A	244	ARG	6.5
1	A	221	MET	6.5
1	A	246	GLY	6.2
1	A	219	GLY	6.0
1	A	234	TYR	5.9
1	A	225	ASN	5.7
1	A	228	GLY	5.4
1	B	247	LYS	5.4
1	A	586	LYS	5.2
1	A	220	ILE	5.2
1	B	245	THR	5.1
1	A	241	MET	5.0
1	B	586	LYS	5.0
1	B	497	ARG	4.9
1	A	248	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	57	ARG	4.3
1	A	21	LYS	4.3
1	A	229	HIS	4.2
1	B	57	ARG	4.1
1	A	232	LEU	4.0
1	B	246	GLY	3.9
1	A	233	GLU	3.9
1	A	217	GLY	3.7
1	B	223	GLY	3.7
1	A	236	ASN	3.6
1	A	242	VAL	3.6
1	B	226	PRO	3.6
1	B	225	ASN	3.5
1	A	240	ASP	3.5
1	B	504	LYS	3.5
1	B	224	MET	3.4
1	A	237	GLU	3.4
1	B	248	THR	3.3
1	B	507	LYS	3.1
1	B	56	LYS	3.1
1	B	501	LYS	2.9
1	B	222	GLY	2.9
1	A	56	LYS	2.9
1	A	58	GLY	2.8
1	A	20	LYS	2.7
1	A	504	LYS	2.6
1	A	1	GLY	2.6
1	A	497	ARG	2.6
1	B	228	GLY	2.6
1	B	218	ALA	2.5
1	B	505	ALA	2.4
1	B	235	ALA	2.4
1	A	501	LYS	2.4
1	B	318	ARG	2.3
1	A	499	LEU	2.2
1	A	508	ASP	2.2
1	A	318	ARG	2.2
1	A	243	ASP	2.1
1	B	1	GLY	2.0
1	B	498	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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( $\text{\AA}^2$ )	Q<0.9
3	FMT	A	2008	3/3	0.87	0.11	54,54,55,55	0
3	FMT	A	2007	3/3	0.89	0.12	44,44,46,47	0
3	FMT	B	2005	3/3	0.94	0.10	41,41,41,42	0
3	FMT	A	2006	3/3	0.95	0.15	42,42,43,44	0
2	SO4	A	2002	5/5	0.95	0.25	76,77,77,77	0
2	SO4	A	2001	5/5	0.96	0.17	43,43,46,48	0
2	SO4	B	2004	5/5	0.96	0.15	47,47,49,49	0
2	SO4	B	2003	5/5	0.97	0.23	80,80,81,81	0
2	SO4	B	2000	5/5	1.00	0.05	35,36,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.