Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 08:15 AM EDT

PDB ID	:	3GIT
Title	:	Crystal structure of a truncated acetyl-CoA synthase
Authors	:	Volbeda, A.; Darnault, C.; Fontecilla-Camps, J.C.
Deposited on	:	2009-03-06
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

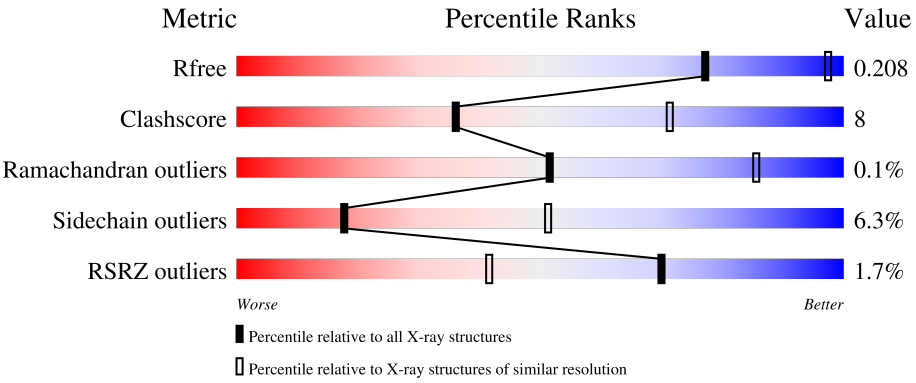
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	427	79% 17%
1	B	427	3% 78% 19%
1	C	427	2% 77% 19%
1	D	427	81% 16%
1	E	427	81% 15%

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Mol	Chain	Length	Quality of chain
1	F	427	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	738	-	-	X	-
5	SO4	B	742	-	-	-	X
5	SO4	F	742	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20147 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 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3297	2084	559	629	25			
1	B	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			
1	C	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			
1	D	422	Total	C	N	O	S	0	0	0
			3297	2084	559	629	25			
1	E	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			
1	F	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	VAL	PHE	conflict	UNP P27988
A	730	ARG	-	expression tag	UNP P27988
A	731	SER	-	expression tag	UNP P27988
A	732	HIS	-	expression tag	UNP P27988
A	733	THR	-	expression tag	UNP P27988
A	734	SER	-	expression tag	UNP P27988
A	735	ARG	-	expression tag	UNP P27988
A	736	GLY	-	expression tag	UNP P27988
A	737	HIS	-	expression tag	UNP P27988
B	682	VAL	PHE	conflict	UNP P27988
B	730	ARG	-	expression tag	UNP P27988
B	731	SER	-	expression tag	UNP P27988
B	732	HIS	-	expression tag	UNP P27988
B	733	THR	-	expression tag	UNP P27988
B	734	SER	-	expression tag	UNP P27988
B	735	ARG	-	expression tag	UNP P27988

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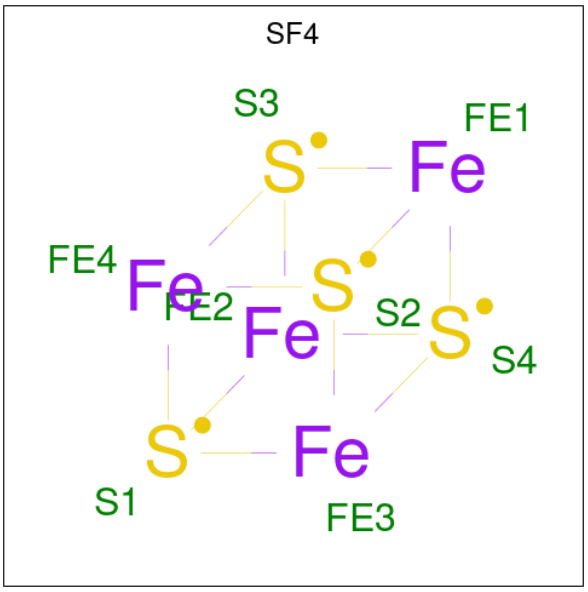
Chain	Residue	Modelled	Actual	Comment	Reference
B	736	GLY	-	expression tag	UNP P27988
B	737	HIS	-	expression tag	UNP P27988
C	682	VAL	PHE	conflict	UNP P27988
C	730	ARG	-	expression tag	UNP P27988
C	731	SER	-	expression tag	UNP P27988
C	732	HIS	-	expression tag	UNP P27988
C	733	THR	-	expression tag	UNP P27988
C	734	SER	-	expression tag	UNP P27988
C	735	ARG	-	expression tag	UNP P27988
C	736	GLY	-	expression tag	UNP P27988
C	737	HIS	-	expression tag	UNP P27988
D	682	VAL	PHE	conflict	UNP P27988
D	730	ARG	-	expression tag	UNP P27988
D	731	SER	-	expression tag	UNP P27988
D	732	HIS	-	expression tag	UNP P27988
D	733	THR	-	expression tag	UNP P27988
D	734	SER	-	expression tag	UNP P27988
D	735	ARG	-	expression tag	UNP P27988
D	736	GLY	-	expression tag	UNP P27988
D	737	HIS	-	expression tag	UNP P27988
E	682	VAL	PHE	conflict	UNP P27988
E	730	ARG	-	expression tag	UNP P27988
E	731	SER	-	expression tag	UNP P27988
E	732	HIS	-	expression tag	UNP P27988
E	733	THR	-	expression tag	UNP P27988
E	734	SER	-	expression tag	UNP P27988
E	735	ARG	-	expression tag	UNP P27988
E	736	GLY	-	expression tag	UNP P27988
E	737	HIS	-	expression tag	UNP P27988
F	682	VAL	PHE	conflict	UNP P27988
F	730	ARG	-	expression tag	UNP P27988
F	731	SER	-	expression tag	UNP P27988
F	732	HIS	-	expression tag	UNP P27988
F	733	THR	-	expression tag	UNP P27988
F	734	SER	-	expression tag	UNP P27988
F	735	ARG	-	expression tag	UNP P27988
F	736	GLY	-	expression tag	UNP P27988
F	737	HIS	-	expression tag	UNP P27988

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

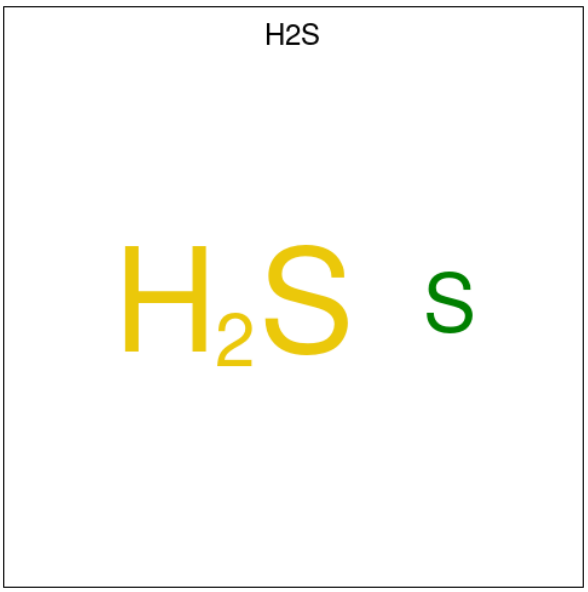


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	E	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

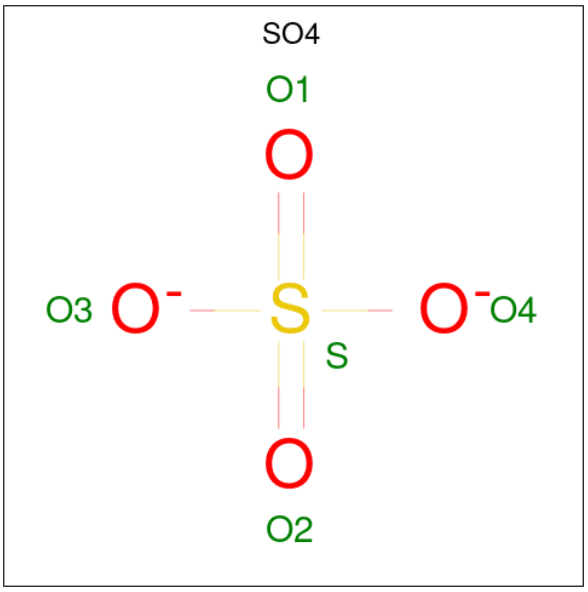
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total S 1 1	0	0
4	B	1	Total S 1 1	0	0
4	C	1	Total S 1 1	0	0
4	D	1	Total S 1 1	0	0
4	E	1	Total S 1 1	0	0
4	F	1	Total S 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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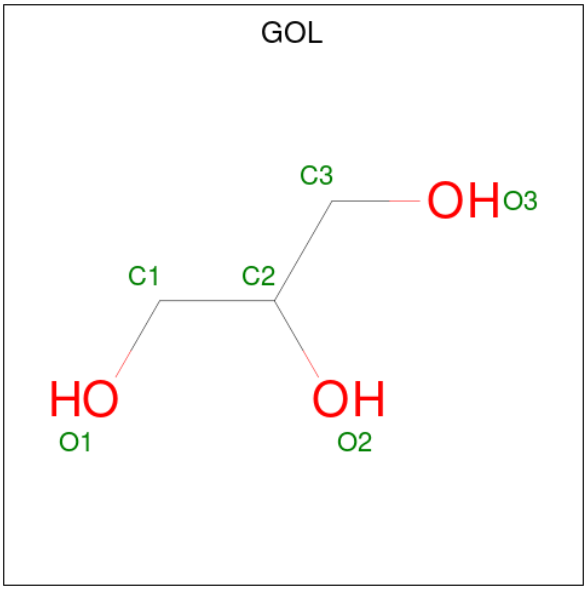
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0
6	F	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

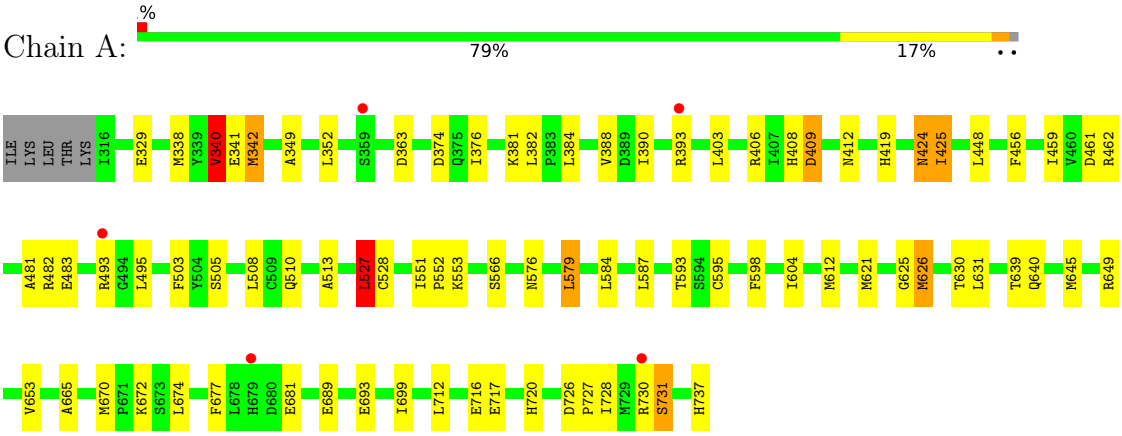
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	33	Total O 33 33	0	0
7	B	27	Total O 27 27	0	0
7	C	25	Total O 25 25	0	0
7	D	37	Total O 37 37	0	0
7	E	37	Total O 37 37	0	0
7	F	30	Total O 30 30	0	0

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.

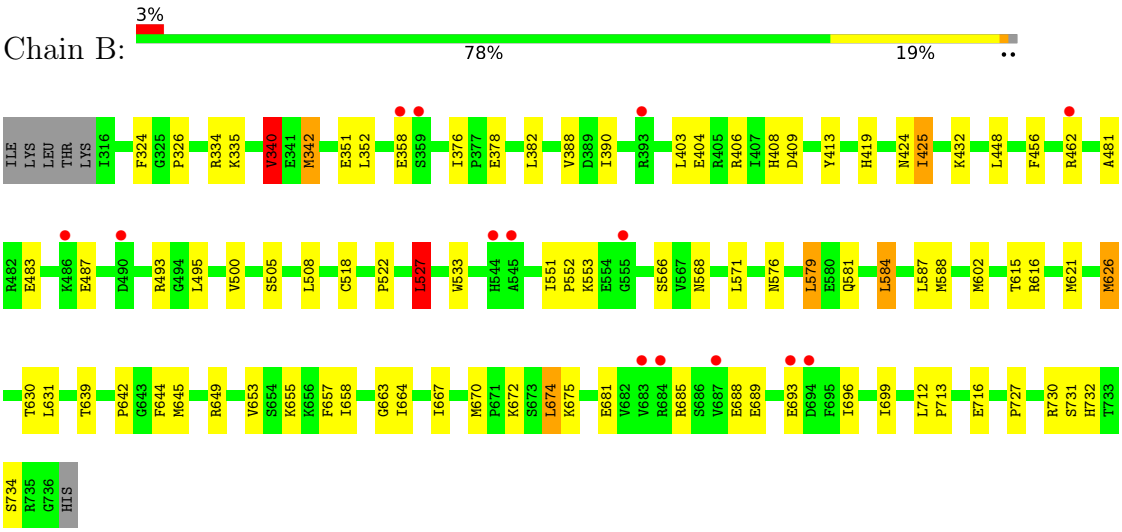
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain A:



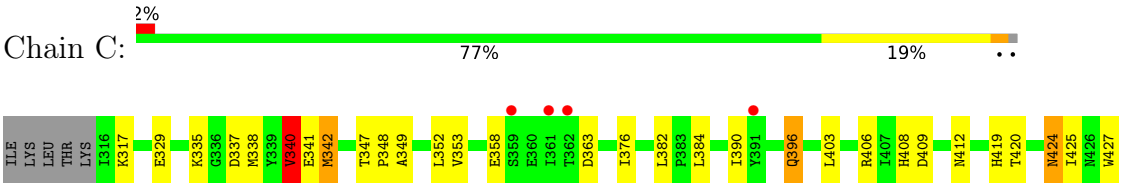
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

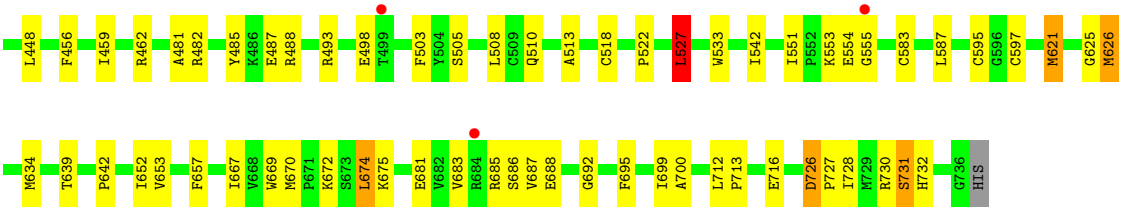
Chain B:



• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

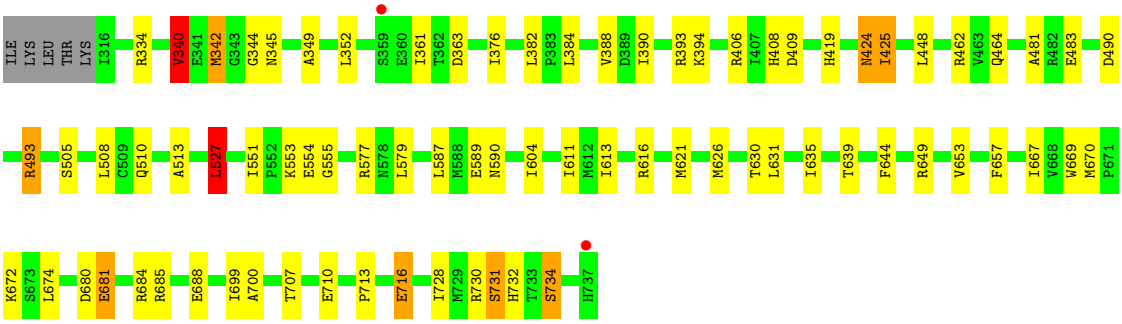
Chain C:





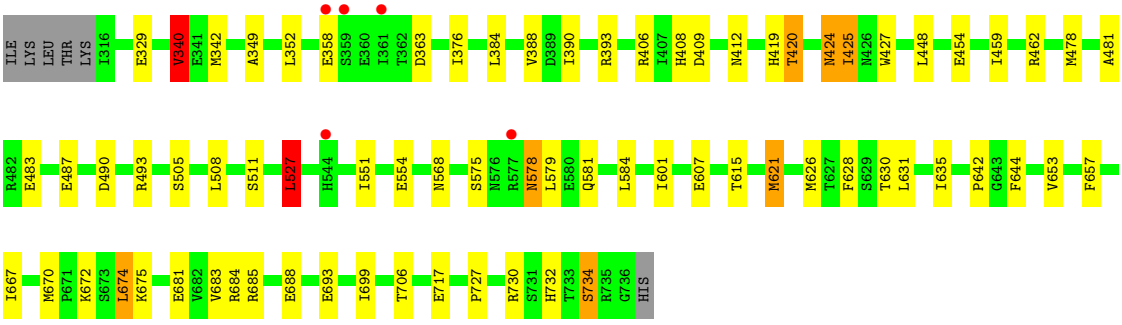
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain D:



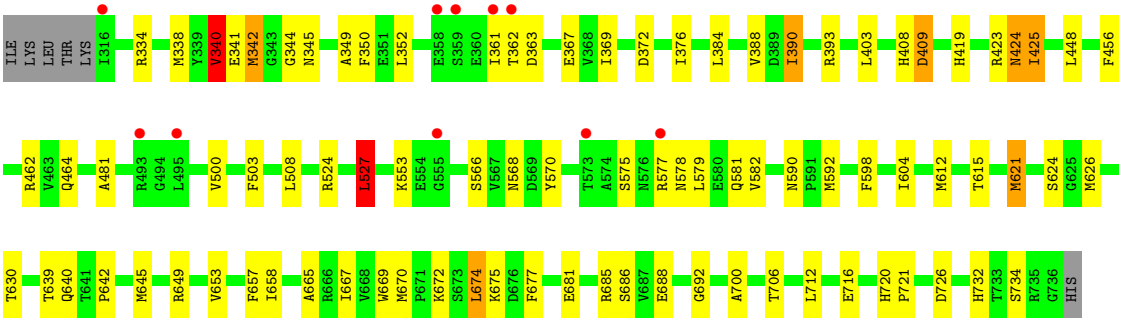
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain E:



• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.40Å 166.40Å 245.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.00 28.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.98-3.00) 99.8 (28.82-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.84 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.208 0.178 , 0.208	Depositor DCC
R_{free} test set	4339 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20147	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: H2S, GOL, SF4, ZN, SO4

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	0.67	0/3366	0.78	4/4549 (0.1%)
1	B	0.63	0/3355	0.75	3/4534 (0.1%)
1	C	0.61	2/3355 (0.1%)	0.73	3/4534 (0.1%)
1	D	0.74	0/3366	0.81	4/4549 (0.1%)
1	E	0.73	1/3355 (0.0%)	0.80	3/4534 (0.1%)
1	F	0.64	0/3355	0.76	4/4534 (0.1%)
All	All	0.67	3/20152 (0.0%)	0.77	21/27234 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	597	CYS	CB-SG	-5.86	1.72	1.81
1	E	734	SER	CB-OG	5.54	1.49	1.42
1	C	583	CYS	CB-SG	-5.18	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	527	LEU	CA-CB-CG	7.63	132.86	115.30
1	F	409	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	E	527	LEU	CA-CB-CG	7.48	132.50	115.30
1	D	527	LEU	CA-CB-CG	7.27	132.02	115.30
1	A	374	ASP	CB-CG-OD1	7.25	124.82	118.30
1	F	340	VAL	CB-CA-C	-7.13	97.85	111.40
1	A	527	LEU	CA-CB-CG	7.03	131.48	115.30
1	F	527	LEU	CA-CB-CG	6.90	131.16	115.30
1	C	527	LEU	CA-CB-CG	6.67	130.65	115.30
1	B	340	VAL	CB-CA-C	-6.33	99.38	111.40
1	D	616	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	D	340	VAL	CB-CA-C	-6.07	99.88	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	340	VAL	CB-CA-C	-5.92	100.16	111.40
1	F	409	ASP	CB-CA-C	-5.81	98.78	110.40
1	E	340	VAL	CB-CA-C	-5.72	100.54	111.40
1	B	616	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	A	340	VAL	CB-CA-C	-5.29	101.35	111.40
1	A	374	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	488	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	734	SER	N-CA-CB	-5.09	102.87	110.50
1	E	734	SER	N-CA-CB	-5.07	102.90	110.50

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	3297	0	3242	50	0
1	B	3287	0	3235	56	0
1	C	3287	0	3235	69	0
1	D	3297	0	3242	47	0
1	E	3287	0	3235	44	0
1	F	3287	0	3235	57	0
2	A	8	0	0	2	0
2	B	8	0	0	1	0
2	C	8	0	0	1	0
2	D	8	0	0	1	0
2	E	8	0	0	1	0
2	F	8	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	25	0	0	0	0
5	B	20	0	0	1	0
5	C	20	0	0	1	0
5	D	20	0	0	2	0
5	E	15	0	0	0	0
5	F	20	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	1	0
6	E	6	0	8	0	0
6	F	6	0	8	0	0
7	A	33	0	0	0	0
7	B	27	0	0	2	0
7	C	25	0	0	2	0
7	D	37	0	0	1	0
7	E	37	0	0	1	0
7	F	30	0	0	1	0
All	All	20147	0	19472	316	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 8.

All (316) 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:E:653:VAL:HG11	1:E:681:GLU:HB2	1.46	0.94
1:F:670:MET:HE3	1:F:675:LYS:HG3	1.49	0.92
1:B:657:PHE:HE2	1:B:667:ILE:HD11	1.36	0.90
1:A:625:GLY:HA3	1:C:634:MET:CE	2.04	0.88
1:C:527:LEU:HD22	2:C:738:SF4:S1	2.13	0.88
1:B:626:MET:HB2	1:B:630:THR:HB	1.57	0.85
1:D:728:ILE:O	1:D:731:SER:HB2	1.77	0.85
1:B:657:PHE:CE2	1:B:667:ILE:HD11	2.11	0.85
1:A:527:LEU:HD22	2:A:738:SF4:S1	2.18	0.83
1:F:657:PHE:HE2	1:F:667:ILE:HD11	1.42	0.82
1:A:363:ASP:HB2	1:A:462:ARG:HG2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLY:HA3	1:C:634:MET:HE2	1.61	0.81
1:D:670:MET:HE2	1:D:699:ILE:HG21	1.61	0.81
1:F:653:VAL:HG11	1:F:681:GLU:HB2	1.63	0.80
1:E:727:PRO:HB2	1:E:730:ARG:HD2	1.65	0.78
1:B:727:PRO:HB2	1:B:730:ARG:HD2	1.67	0.76
1:C:424:ASN:HD22	1:C:424:ASN:H	1.32	0.76
1:C:653:VAL:HG11	1:C:681:GLU:HB2	1.68	0.75
1:F:657:PHE:CE2	1:F:667:ILE:HD11	2.20	0.74
1:E:408:HIS:HD2	1:E:419:HIS:ND1	1.85	0.74
1:A:670:MET:HE2	1:A:699:ILE:HG21	1.69	0.74
1:B:670:MET:HE2	1:B:699:ILE:HG21	1.69	0.73
1:D:657:PHE:CE2	1:D:667:ILE:HD11	2.23	0.72
1:E:527:LEU:HD22	2:E:738:SF4:S1	2.28	0.72
1:B:527:LEU:HD22	2:B:738:SF4:S1	2.28	0.72
1:E:657:PHE:CE2	1:E:667:ILE:HD11	2.25	0.71
1:E:575:SER:O	1:E:578:ASN:HB2	1.91	0.71
1:A:626:MET:HB2	1:A:630:THR:HB	1.73	0.71
1:C:363:ASP:HB2	1:C:462:ARG:HD3	1.72	0.71
1:D:653:VAL:HG11	1:D:681:GLU:HB3	1.71	0.71
1:D:527:LEU:HD22	2:D:738:SF4:S1	2.31	0.70
1:E:670:MET:HE2	1:E:699:ILE:HD13	1.75	0.68
1:B:653:VAL:HG11	1:B:681:GLU:HB2	1.76	0.68
1:D:408:HIS:HD2	1:D:419:HIS:ND1	1.90	0.68
1:A:408:HIS:HD2	1:A:419:HIS:ND1	1.90	0.68
1:E:657:PHE:HE2	1:E:667:ILE:HD11	1.58	0.68
1:F:340:VAL:HG13	1:F:376:ILE:CD1	2.23	0.68
1:F:685:ARG:NH1	1:F:688:GLU:OE1	2.27	0.68
1:B:626:MET:HG3	1:B:631:LEU:HG	1.76	0.67
1:D:342:MET:HB3	1:D:382:LEU:O	1.93	0.67
1:C:340:VAL:HG13	1:C:376:ILE:CD1	2.25	0.67
1:F:670:MET:HE3	1:F:675:LYS:CG	2.25	0.67
1:A:653:VAL:HG11	1:A:681:GLU:HB2	1.77	0.66
1:C:340:VAL:HG13	1:C:376:ILE:HD12	1.78	0.66
1:A:625:GLY:HA3	1:C:634:MET:HE1	1.78	0.65
1:B:642:PRO:HB2	1:B:732:HIS:HE1	1.62	0.65
1:C:408:HIS:HD2	1:C:419:HIS:ND1	1.93	0.65
1:B:342:MET:HB3	1:B:382:LEU:O	1.96	0.65
1:A:579:LEU:HD21	1:A:593:THR:HG21	1.79	0.65
1:D:657:PHE:HE2	1:D:667:ILE:HD11	1.62	0.64
1:F:408:HIS:HD2	1:F:419:HIS:ND1	1.95	0.64
1:B:358:GLU:OE1	1:B:462:ARG:NH1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LEU:HD22	1:D:481:ALA:HA	1.80	0.64
1:B:655:LYS:HA	1:B:685:ARG:NH2	2.12	0.64
1:B:712:LEU:O	1:B:716:GLU:HG2	1.98	0.63
1:E:657:PHE:HE2	1:E:667:ILE:CD1	2.11	0.62
1:C:352:LEU:HD22	1:C:481:ALA:HA	1.80	0.62
1:C:657:PHE:CE2	1:C:667:ILE:HD11	2.34	0.62
1:B:655:LYS:HA	1:B:685:ARG:HH21	1.64	0.62
1:B:408:HIS:HD2	1:B:419:HIS:ND1	1.98	0.62
1:D:657:PHE:HE2	1:D:667:ILE:CD1	2.13	0.61
1:D:340:VAL:HG13	1:D:376:ILE:HD12	1.82	0.61
1:F:626:MET:HB2	1:F:630:THR:HB	1.82	0.61
1:E:626:MET:HB2	1:E:630:THR:HB	1.83	0.61
1:F:424:ASN:HD22	1:F:424:ASN:H	1.48	0.60
1:D:626:MET:HB2	1:D:630:THR:HB	1.83	0.60
1:A:363:ASP:CB	1:A:462:ARG:HG2	2.32	0.60
1:A:625:GLY:CA	1:C:634:MET:HE2	2.33	0.59
1:F:590:ASN:HA	1:F:640:GLN:OE1	2.02	0.59
1:E:642:PRO:HB2	1:E:732:HIS:CE1	2.38	0.59
1:C:670:MET:CE	1:C:675:LYS:HG2	2.33	0.58
1:C:424:ASN:HD22	1:C:424:ASN:N	1.97	0.58
1:F:568:ASN:HD21	1:F:581:GLN:HE21	1.51	0.58
1:F:642:PRO:HB2	1:F:732:HIS:HE1	1.68	0.58
1:B:713:PRO:HA	1:B:716:GLU:HG3	1.86	0.57
1:D:363:ASP:HB2	1:D:462:ARG:HD3	1.84	0.57
1:E:340:VAL:HG13	1:E:376:ILE:HD12	1.87	0.57
1:C:353:VAL:HG13	1:C:390:ILE:HD13	1.86	0.57
1:B:657:PHE:HE2	1:B:667:ILE:CD1	2.13	0.57
1:E:340:VAL:HG13	1:E:376:ILE:CD1	2.35	0.57
1:B:493:ARG:HH11	1:B:493:ARG:HB2	1.69	0.57
1:F:352:LEU:HD22	1:F:481:ALA:HA	1.87	0.57
1:B:642:PRO:HB2	1:B:732:HIS:CE1	2.40	0.56
1:D:406:ARG:NH1	1:D:409:ASP:OD2	2.38	0.56
1:C:621:MET:CE	1:C:625:GLY:O	2.53	0.56
1:F:425:ILE:HG13	1:F:649:ARG:HH11	1.69	0.56
1:F:342:MET:HG3	1:F:384:LEU:HD22	1.86	0.56
1:E:425:ILE:HD13	1:E:425:ILE:N	2.20	0.56
1:C:329:GLU:HA	1:C:412:ASN:O	2.06	0.56
1:A:728:ILE:O	1:A:731:SER:HB2	2.06	0.56
1:C:626:MET:HE1	1:C:634:MET:HE1	1.86	0.56
1:C:657:PHE:HE2	1:C:667:ILE:CD1	2.20	0.55
1:B:334:ARG:HA	5:B:744:SO4:O2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:MET:HE3	1:C:675:LYS:HG2	1.89	0.55
1:A:342:MET:HB3	1:A:382:LEU:O	2.06	0.55
1:C:329:GLU:OE1	7:C:786:HOH:O	2.18	0.55
1:A:408:HIS:CD2	1:A:419:HIS:ND1	2.75	0.54
1:F:372:ASP:OD2	7:F:790:HOH:O	2.19	0.54
1:E:621:MET:HB3	1:E:706:THR:HB	1.89	0.54
1:A:349:ALA:HA	1:A:384:LEU:O	2.08	0.54
1:C:358:GLU:OE1	1:C:462:ARG:NH1	2.40	0.54
1:F:615:THR:HG21	1:F:674:LEU:HG	1.90	0.54
1:F:642:PRO:HB2	1:F:732:HIS:CE1	2.43	0.54
1:D:408:HIS:CD2	1:D:419:HIS:ND1	2.74	0.54
1:B:568:ASN:HD21	1:B:581:GLN:HG3	1.73	0.53
1:C:657:PHE:HE2	1:C:667:ILE:HD11	1.73	0.53
1:A:340:VAL:HG13	1:A:376:ILE:HD12	1.89	0.53
1:D:424:ASN:H	1:D:424:ASN:HD22	1.55	0.53
1:F:566:SER:O	1:F:570:TYR:HD1	1.91	0.53
1:A:670:MET:HE2	1:A:699:ILE:HD13	1.90	0.53
1:F:361:ILE:HG13	1:F:464:GLN:HE21	1.73	0.53
1:C:342:MET:HB3	1:C:382:LEU:O	2.08	0.53
1:F:670:MET:CE	1:F:675:LYS:HG3	2.32	0.53
1:A:505:SER:HB3	1:A:551:ILE:HD11	1.90	0.53
1:C:670:MET:HE3	1:C:675:LYS:CG	2.39	0.53
1:C:518:CYS:SG	1:C:527:LEU:HD13	2.50	0.52
1:E:363:ASP:HB2	1:E:462:ARG:HD3	1.91	0.52
1:A:352:LEU:HD22	1:A:481:ALA:HA	1.91	0.52
1:A:342:MET:HG3	1:A:384:LEU:HD22	1.92	0.52
1:A:403:LEU:HD22	1:A:456:PHE:CD2	2.44	0.52
1:C:424:ASN:H	1:C:424:ASN:ND2	2.06	0.52
1:C:527:LEU:HD21	1:C:595:CYS:SG	2.49	0.52
1:D:587:LEU:HD22	1:D:611:ILE:HD13	1.91	0.52
1:D:657:PHE:CZ	1:D:667:ILE:HD11	2.44	0.52
1:E:642:PRO:HB2	1:E:732:HIS:HE1	1.73	0.52
1:E:408:HIS:CD2	1:E:419:HIS:ND1	2.73	0.52
1:E:683:VAL:HG13	1:E:693:GLU:HB2	1.90	0.52
1:A:425:ILE:N	1:A:425:ILE:HD13	2.26	0.51
1:A:510:GLN:HA	1:A:513:ALA:O	2.09	0.51
1:A:552:PRO:O	1:A:566:SER:OG	2.26	0.51
1:F:575:SER:O	1:F:578:ASN:HB2	2.11	0.51
1:A:424:ASN:HD22	1:A:424:ASN:H	1.57	0.51
1:A:626:MET:HG3	1:A:631:LEU:HG	1.92	0.51
1:B:518:CYS:SG	1:B:527:LEU:HD13	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:VAL:CG1	1:C:376:ILE:CD1	2.89	0.51
1:C:553:LYS:O	1:C:554:GLU:HG3	2.10	0.51
1:C:337:ASP:CG	1:F:334:ARG:HH22	2.14	0.51
1:F:425:ILE:N	1:F:425:ILE:HD13	2.26	0.51
1:C:459:ILE:CD1	1:C:542:ILE:HG23	2.42	0.50
1:B:675:LYS:HE2	1:B:696:ILE:O	2.11	0.50
1:C:459:ILE:HD11	1:C:542:ILE:HG12	1.92	0.50
1:E:340:VAL:CG1	1:E:376:ILE:HD12	2.42	0.50
1:E:615:THR:HG21	1:E:674:LEU:HG	1.93	0.50
1:B:342:MET:CB	1:B:382:LEU:O	2.59	0.50
1:A:587:LEU:HD12	1:A:645:MET:HB2	1.94	0.50
1:B:352:LEU:HD22	1:B:481:ALA:HA	1.93	0.50
1:D:555:GLY:N	5:D:742:SO4:O2	2.45	0.50
1:B:340:VAL:HG13	1:B:376:ILE:CD1	2.41	0.49
1:E:349:ALA:HA	1:E:384:LEU:O	2.12	0.49
1:A:340:VAL:HG13	1:A:376:ILE:CD1	2.42	0.49
1:C:459:ILE:HD11	1:C:542:ILE:HG23	1.93	0.49
1:E:685:ARG:NH1	1:E:688:GLU:OE1	2.35	0.49
1:F:340:VAL:HG13	1:F:376:ILE:HD12	1.91	0.49
1:C:498:GLU:OE1	1:C:498:GLU:N	2.46	0.49
1:C:621:MET:HE3	1:C:625:GLY:O	2.11	0.49
1:B:670:MET:CE	1:B:699:ILE:HG21	2.41	0.49
1:F:670:MET:CE	1:F:675:LYS:CG	2.88	0.49
1:C:408:HIS:CD2	1:C:419:HIS:ND1	2.79	0.48
1:A:406:ARG:NH1	1:A:409:ASP:OD2	2.46	0.48
1:F:388:VAL:HG12	1:F:390:ILE:HD12	1.93	0.48
1:B:493:ARG:HH11	1:B:493:ARG:CB	2.26	0.48
1:C:347:THR:HB	1:C:348:PRO:HD2	1.94	0.48
1:C:505:SER:HB3	1:C:551:ILE:HD11	1.96	0.48
1:C:712:LEU:HB3	1:C:713:PRO:HD3	1.95	0.48
1:C:685:ARG:NH1	1:C:688:GLU:OE1	2.46	0.48
1:D:349:ALA:HA	1:D:384:LEU:O	2.14	0.48
1:B:588:MET:HG3	1:B:731:SER:HB3	1.96	0.48
1:C:727:PRO:HB2	1:C:730:ARG:HG3	1.96	0.48
1:F:712:LEU:O	1:F:716:GLU:HG3	2.14	0.48
1:A:342:MET:CG	1:A:384:LEU:HD22	2.44	0.47
1:A:727:PRO:HB2	1:A:730:ARG:HD2	1.96	0.47
1:F:669:TRP:HA	1:F:700:ALA:O	2.14	0.47
1:D:425:ILE:HD13	1:D:425:ILE:N	2.30	0.47
1:D:681:GLU:OE1	1:D:681:GLU:HA	2.14	0.47
1:E:670:MET:HE2	1:E:699:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:HIS:CD2	1:F:419:HIS:ND1	2.80	0.47
1:C:335:LYS:HE3	7:C:756:HOH:O	2.14	0.47
1:F:403:LEU:HD22	1:F:456:PHE:CD2	2.49	0.47
1:F:720:HIS:ND1	1:F:721:PRO:HD2	2.29	0.47
1:B:388:VAL:HG12	1:B:390:ILE:HD12	1.97	0.47
1:E:388:VAL:HG12	1:E:390:ILE:HD12	1.96	0.47
1:C:403:LEU:HD22	1:C:456:PHE:CD2	2.49	0.47
1:D:635:ILE:CG2	1:D:644:PHE:HB3	2.44	0.47
1:D:680:ASP:HB3	1:D:684:ARG:HH21	1.80	0.46
1:F:367:GLU:OE1	1:F:369:ILE:HD11	2.15	0.46
1:F:503:PHE:CZ	1:F:553:LYS:HD3	2.51	0.46
1:F:527:LEU:HD22	2:F:738:SF4:S1	2.55	0.46
1:F:686:SER:HB3	1:F:692:GLY:O	2.16	0.46
1:B:351:GLU:HG3	7:B:789:HOH:O	2.15	0.46
1:B:493:ARG:CB	1:B:493:ARG:NH1	2.79	0.46
1:D:425:ILE:HG21	1:D:649:ARG:NH1	2.30	0.46
1:D:635:ILE:HG22	1:D:644:PHE:HB3	1.98	0.46
1:E:388:VAL:HG12	1:E:390:ILE:CD1	2.45	0.46
1:B:568:ASN:ND2	1:B:581:GLN:HG3	2.29	0.46
1:C:652:ILE:CD1	1:C:674:LEU:HD11	2.45	0.46
1:D:626:MET:HG3	1:D:631:LEU:HG	1.98	0.46
1:E:352:LEU:HD22	1:E:481:ALA:HA	1.96	0.46
1:B:403:LEU:HD22	1:B:456:PHE:CD2	2.51	0.46
1:B:378:GLU:OE2	1:B:432:LYS:HE2	2.16	0.46
1:B:406:ARG:NH1	1:B:409:ASP:OD2	2.49	0.46
1:D:340:VAL:HG13	1:D:376:ILE:CD1	2.45	0.46
1:B:693:GLU:H	1:B:693:GLU:HG2	1.54	0.46
1:D:361:ILE:HG13	1:D:464:GLN:HE21	1.81	0.46
1:F:425:ILE:HD12	1:F:677:PHE:CE1	2.51	0.45
1:A:403:LEU:HD22	1:A:456:PHE:CE2	2.51	0.45
1:C:396:GLN:HE21	1:C:396:GLN:HB2	1.56	0.45
1:E:358:GLU:OE1	1:E:462:ARG:NH1	2.49	0.45
1:F:349:ALA:HA	1:F:384:LEU:O	2.17	0.45
1:B:615:THR:HG21	1:B:674:LEU:HG	1.99	0.45
1:A:737:HIS:HD2	1:C:716:GLU:OE2	1.99	0.45
1:E:329:GLU:OE1	7:E:799:HOH:O	2.21	0.45
1:C:626:MET:CE	1:C:634:MET:HE1	2.45	0.45
1:A:388:VAL:HG12	1:A:390:ILE:HD12	1.98	0.44
1:D:732:HIS:HE1	1:E:607:GLU:CA	2.29	0.44
1:A:338:MET:SD	1:A:341:GLU:HB2	2.57	0.44
1:A:342:MET:CB	1:A:382:LEU:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LEU:HD21	1:A:595:CYS:SG	2.58	0.44
1:D:604:ILE:HD12	1:D:604:ILE:HA	1.75	0.44
1:B:326:PRO:HG2	1:E:511:SER:HA	2.00	0.44
1:D:553:LYS:O	1:D:554:GLU:HG3	2.17	0.44
1:F:568:ASN:ND2	1:F:581:GLN:HE21	2.14	0.44
1:F:665:ALA:O	1:F:720:HIS:HE1	2.01	0.44
1:A:503:PHE:CZ	1:A:553:LYS:HD3	2.53	0.44
6:D:743:GOL:H2	7:D:758:HOH:O	2.17	0.44
1:C:340:VAL:CG1	1:C:376:ILE:HD12	2.45	0.44
1:C:669:TRP:HA	1:C:700:ALA:O	2.18	0.44
1:D:657:PHE:CE2	1:D:667:ILE:CD1	2.92	0.44
1:B:571:LEU:HD21	1:B:579:LEU:HB3	1.99	0.44
1:C:726:ASP:OD1	1:C:726:ASP:N	2.50	0.44
1:E:670:MET:CE	1:E:699:ILE:HG21	2.48	0.44
1:E:675:LYS:NZ	1:E:699:ILE:O	2.37	0.44
1:F:363:ASP:HB2	1:F:462:ARG:HD3	2.00	0.44
1:A:329:GLU:HA	1:A:412:ASN:O	2.18	0.43
1:A:425:ILE:HG13	1:A:649:ARG:HH11	1.83	0.43
1:C:406:ARG:NH1	1:C:409:ASP:OD2	2.51	0.43
1:C:657:PHE:CZ	1:C:667:ILE:HD11	2.52	0.43
1:A:527:LEU:HG	1:A:598:PHE:HB3	2.01	0.43
1:F:612:MET:SD	1:F:624:SER:HB3	2.58	0.43
1:C:510:GLN:HA	1:C:513:ALA:O	2.17	0.43
1:E:329:GLU:HA	1:E:412:ASN:O	2.19	0.43
1:F:338:MET:SD	1:F:341:GLU:HB2	2.59	0.43
1:B:335:LYS:HE3	7:B:756:HOH:O	2.19	0.43
1:B:340:VAL:HG13	1:B:376:ILE:HD12	2.01	0.43
1:B:587:LEU:HD12	1:B:645:MET:HB2	2.01	0.43
1:B:602:MET:O	1:B:644:PHE:HA	2.18	0.43
1:B:657:PHE:O	1:B:663:GLY:HA2	2.19	0.43
1:C:481:ALA:HB1	1:C:485:TYR:CZ	2.53	0.43
1:B:352:LEU:HA	1:B:404:GLU:OE1	2.19	0.43
1:F:582:VAL:HG21	1:F:592:MET:HG3	2.00	0.43
1:F:350:PHE:HA	1:F:423:ARG:O	2.18	0.43
1:C:522:PRO:HD3	1:C:533:TRP:CD1	2.53	0.43
1:D:669:TRP:HA	1:D:700:ALA:O	2.19	0.42
1:F:604:ILE:HD12	1:F:604:ILE:HA	1.84	0.42
1:A:604:ILE:HD12	1:A:604:ILE:HA	1.82	0.42
1:B:505:SER:HB3	1:B:551:ILE:HD11	2.00	0.42
1:C:728:ILE:O	1:C:731:SER:HB2	2.19	0.42
1:F:621:MET:HB3	1:F:706:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:PRO:O	1:B:566:SER:OG	2.26	0.42
1:C:683:VAL:O	1:C:687:VAL:HG23	2.19	0.42
1:D:685:ARG:NH1	1:D:688:GLU:OE1	2.41	0.42
1:F:577:ARG:HH11	1:F:577:ARG:HG2	1.85	0.42
1:B:403:LEU:HD22	1:B:456:PHE:CE2	2.55	0.42
1:C:503:PHE:CZ	1:C:553:LYS:HD3	2.54	0.42
1:D:713:PRO:HA	1:D:716:GLU:HG3	2.02	0.42
1:C:555:GLY:N	5:C:742:SO4:O2	2.53	0.42
1:C:686:SER:HB3	1:C:692:GLY:O	2.20	0.42
1:D:388:VAL:HG12	1:D:390:ILE:HD12	2.02	0.42
1:D:344:GLY:O	1:D:345:ASN:HB2	2.20	0.42
1:E:424:ASN:HD22	1:E:424:ASN:H	1.67	0.42
1:B:500:VAL:O	1:B:553:LYS:HE2	2.20	0.42
1:D:424:ASN:HD22	1:D:424:ASN:N	2.16	0.41
1:E:626:MET:HG3	1:E:631:LEU:HG	2.02	0.41
1:E:657:PHE:CZ	1:E:667:ILE:HD11	2.54	0.41
1:A:459:ILE:HD13	1:A:459:ILE:HA	1.77	0.41
1:A:528:CYS:HB3	2:A:738:SF4:S1	2.60	0.41
1:F:524:ARG:NH2	1:F:645:MET:SD	2.90	0.41
1:D:510:GLN:HA	1:D:513:ALA:O	2.21	0.41
1:D:589:GLU:O	1:D:590:ASN:C	2.57	0.41
1:A:342:MET:N	1:A:342:MET:SD	2.94	0.41
1:D:505:SER:HB3	1:D:551:ILE:HD11	2.01	0.41
1:D:707:THR:OG1	1:D:710:GLU:HG3	2.20	0.41
1:E:601:ILE:HD12	1:E:628:PHE:CD2	2.55	0.41
1:A:393:ARG:HG3	1:A:461:ASP:OD2	2.21	0.41
1:C:642:PRO:HB2	1:C:732:HIS:CE1	2.56	0.41
1:D:490:ASP:O	1:D:493:ARG:HB2	2.20	0.41
1:D:670:MET:HE3	1:D:670:MET:HB2	1.89	0.41
1:E:490:ASP:O	1:E:493:ARG:HB2	2.20	0.41
1:F:362:THR:H	1:F:464:GLN:NE2	2.18	0.41
1:A:712:LEU:O	1:A:716:GLU:HG2	2.20	0.41
1:B:522:PRO:HD3	1:B:533:TRP:CD1	2.56	0.41
1:C:338:MET:SD	1:C:341:GLU:HB2	2.61	0.41
1:C:424:ASN:N	1:C:424:ASN:ND2	2.66	0.41
1:E:420:THR:HG22	1:E:427:TRP:HB3	2.03	0.41
1:E:635:ILE:HG22	1:E:644:PHE:HB3	2.02	0.41
1:F:376:ILE:O	1:F:376:ILE:HG13	2.19	0.41
1:B:425:ILE:HG13	1:B:649:ARG:HH11	1.86	0.41
1:A:665:ALA:O	1:A:720:HIS:HE1	2.03	0.41
1:B:584:LEU:HD22	1:B:584:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:VAL:CG1	1:E:376:ILE:CD1	2.99	0.41
1:A:425:ILE:HD12	1:A:677:PHE:CE1	2.56	0.41
1:C:420:THR:HG22	1:C:427:TRP:HB3	2.02	0.41
1:E:568:ASN:HD21	1:E:581:GLN:HE21	1.68	0.41
1:F:344:GLY:O	1:F:345:ASN:HB2	2.21	0.41
1:F:640:GLN:HE21	1:F:640:GLN:HB2	1.65	0.41
1:B:388:VAL:HG12	1:B:390:ILE:CD1	2.51	0.40
1:C:695:PHE:CE2	1:C:699:ILE:HD11	2.55	0.40
1:B:664:ILE:HA	1:B:667:ILE:HD12	2.02	0.40
1:C:349:ALA:HA	1:C:384:LEU:O	2.20	0.40
1:C:657:PHE:CE2	1:C:667:ILE:CD1	2.98	0.40
1:F:527:LEU:C	1:F:527:LEU:HD23	2.42	0.40
1:F:527:LEU:HG	1:F:598:PHE:HB3	2.03	0.40
1:B:324:PHE:HA	1:B:413:TYR:O	2.21	0.40
1:D:334:ARG:HA	5:D:744:SO4:O2	2.22	0.40
1:D:553:LYS:O	1:D:554:GLU:CG	2.70	0.40
1:E:505:SER:HB3	1:E:551:ILE:HD11	2.03	0.40
1:F:500:VAL:O	1:F:553:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

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	420/427 (98%)	398 (95%)	22 (5%)	0	100	100
1	B	419/427 (98%)	403 (96%)	15 (4%)	1 (0%)	47	82
1	C	419/427 (98%)	396 (94%)	22 (5%)	1 (0%)	47	82
1	D	420/427 (98%)	402 (96%)	18 (4%)	0	100	100
1	E	419/427 (98%)	405 (97%)	14 (3%)	0	100	100
1	F	419/427 (98%)	403 (96%)	15 (4%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2516/2562 (98%)	2407 (96%)	106 (4%)	3 (0%)	51 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	317	LYS
1	F	658	ILE
1	B	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	357/364 (98%)	329 (92%)	28 (8%)	12 42
1	B	356/364 (98%)	335 (94%)	21 (6%)	19 54
1	C	356/364 (98%)	337 (95%)	19 (5%)	22 58
1	D	357/364 (98%)	334 (94%)	23 (6%)	17 51
1	E	356/364 (98%)	330 (93%)	26 (7%)	14 44
1	F	356/364 (98%)	339 (95%)	17 (5%)	25 62
All	All	2138/2184 (98%)	2004 (94%)	134 (6%)	18 51

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	VAL
1	A	342	MET
1	A	381	LYS
1	A	409	ASP
1	A	424	ASN
1	A	425	ILE
1	A	448	LEU
1	A	482	ARG
1	A	483	GLU

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Mol	Chain	Res	Type
1	A	493	ARG
1	A	495	LEU
1	A	508	LEU
1	A	527	LEU
1	A	576	ASN
1	A	579	LEU
1	A	584	LEU
1	A	612	MET
1	A	621	MET
1	A	626	MET
1	A	639	THR
1	A	640	GLN
1	A	672	LYS
1	A	674	LEU
1	A	689	GLU
1	A	693	GLU
1	A	717	GLU
1	A	726	ASP
1	A	731	SER
1	B	340	VAL
1	B	342	MET
1	B	424	ASN
1	B	425	ILE
1	B	448	LEU
1	B	483	GLU
1	B	487	GLU
1	B	495	LEU
1	B	508	LEU
1	B	527	LEU
1	B	576	ASN
1	B	579	LEU
1	B	584	LEU
1	B	621	MET
1	B	626	MET
1	B	639	THR
1	B	672	LYS
1	B	674	LEU
1	B	688	GLU
1	B	689	GLU
1	B	734	SER
1	C	340	VAL
1	C	342	MET

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Mol	Chain	Res	Type
1	C	396	GLN
1	C	424	ASN
1	C	425	ILE
1	C	448	LEU
1	C	482	ARG
1	C	487	GLU
1	C	493	ARG
1	C	508	LEU
1	C	527	LEU
1	C	587	LEU
1	C	621	MET
1	C	626	MET
1	C	639	THR
1	C	672	LYS
1	C	674	LEU
1	C	726	ASP
1	C	731	SER
1	D	340	VAL
1	D	342	MET
1	D	393	ARG
1	D	394	LYS
1	D	424	ASN
1	D	425	ILE
1	D	448	LEU
1	D	483	GLU
1	D	493	ARG
1	D	508	LEU
1	D	527	LEU
1	D	577	ARG
1	D	579	LEU
1	D	613	ILE
1	D	621	MET
1	D	639	THR
1	D	672	LYS
1	D	674	LEU
1	D	681	GLU
1	D	716	GLU
1	D	730	ARG
1	D	731	SER
1	D	734	SER
1	E	340	VAL
1	E	342	MET

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Mol	Chain	Res	Type
1	E	393	ARG
1	E	406	ARG
1	E	409	ASP
1	E	420	THR
1	E	424	ASN
1	E	425	ILE
1	E	448	LEU
1	E	454	GLU
1	E	459	ILE
1	E	478	MET
1	E	483	GLU
1	E	487	GLU
1	E	508	LEU
1	E	527	LEU
1	E	554	GLU
1	E	578	ASN
1	E	579	LEU
1	E	584	LEU
1	E	621	MET
1	E	672	LYS
1	E	674	LEU
1	E	684	ARG
1	E	717	GLU
1	E	734	SER
1	F	340	VAL
1	F	342	MET
1	F	390	ILE
1	F	393	ARG
1	F	409	ASP
1	F	424	ASN
1	F	425	ILE
1	F	448	LEU
1	F	508	LEU
1	F	527	LEU
1	F	579	LEU
1	F	621	MET
1	F	639	THR
1	F	672	LYS
1	F	674	LEU
1	F	726	ASP
1	F	734	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	GLN
1	A	408	HIS
1	A	424	ASN
1	A	510	GLN
1	A	544	HIS
1	A	581	GLN
1	A	590	ASN
1	A	640	GLN
1	A	737	HIS
1	B	408	HIS
1	B	464	GLN
1	B	510	GLN
1	B	568	ASN
1	B	581	GLN
1	B	590	ASN
1	B	640	GLN
1	B	732	HIS
1	C	396	GLN
1	C	408	HIS
1	C	424	ASN
1	C	464	GLN
1	C	510	GLN
1	C	581	GLN
1	C	590	ASN
1	C	640	GLN
1	D	408	HIS
1	D	424	ASN
1	D	464	GLN
1	D	510	GLN
1	D	544	HIS
1	D	581	GLN
1	D	590	ASN
1	D	640	GLN
1	D	732	HIS
1	E	396	GLN
1	E	408	HIS
1	E	424	ASN
1	E	464	GLN
1	E	510	GLN
1	E	581	GLN
1	E	590	ASN
1	F	396	GLN

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Mol	Chain	Res	Type
1	F	408	HIS
1	F	424	ASN
1	F	464	GLN
1	F	510	GLN
1	F	578	ASN
1	F	581	GLN
1	F	590	ASN
1	F	732	HIS

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 48 ligands modelled in this entry, 6 are monoatomic and 6 are modelled with single atom - leaving 36 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	$\#\|Z\| > 2$
5	SO4	B	742	-	4,4,4	0.73	0	6,6,6	0.27	0
6	GOL	A	743	-	5,5,5	0.31	0	5,5,5	0.53	0
5	SO4	F	745	-	4,4,4	0.26	0	6,6,6	0.30	0
2	SF4	F	738	1	0,12,12	-	-	-		
2	SF4	E	738	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	E	744	-	4,4,4	0.43	0	6,6,6	0.85	0
5	SO4	C	741	-	4,4,4	0.22	0	6,6,6	0.23	0
6	GOL	B	743	-	5,5,5	0.37	0	5,5,5	0.43	0
5	SO4	A	741	-	4,4,4	0.30	0	6,6,6	0.34	0
5	SO4	F	741	-	4,4,4	0.25	0	6,6,6	0.48	0
5	SO4	E	742	-	4,4,4	0.20	0	6,6,6	0.24	0
6	GOL	C	743	-	5,5,5	0.36	0	5,5,5	0.37	0
2	SF4	D	738	1	0,12,12	-	-	-		
5	SO4	A	744	-	4,4,4	0.25	0	6,6,6	0.69	0
5	SO4	A	742	-	4,4,4	0.18	0	6,6,6	0.19	0
5	SO4	B	744	-	4,4,4	0.24	0	6,6,6	0.85	0
5	SO4	D	745	-	4,4,4	0.24	0	6,6,6	0.24	0
6	GOL	E	743	-	5,5,5	0.52	0	5,5,5	0.55	0
5	SO4	F	744	-	4,4,4	0.19	0	6,6,6	0.67	0
5	SO4	C	745	-	4,4,4	0.11	0	6,6,6	0.20	0
2	SF4	C	738	1	0,12,12	-	-	-		
5	SO4	F	742	-	4,4,4	0.21	0	6,6,6	0.27	0
5	SO4	D	742	-	4,4,4	0.17	0	6,6,6	0.47	0
5	SO4	B	745	-	4,4,4	0.18	0	6,6,6	0.29	0
2	SF4	A	738	1	0,12,12	-	-	-		
2	SF4	B	738	1	0,12,12	-	-	-		
5	SO4	E	745	-	4,4,4	0.19	0	6,6,6	0.31	0
5	SO4	D	741	-	4,4,4	0.30	0	6,6,6	0.34	0
5	SO4	A	745	-	4,4,4	0.18	0	6,6,6	0.26	0
5	SO4	D	744	-	4,4,4	0.22	0	6,6,6	0.82	0
6	GOL	F	743	-	5,5,5	0.42	0	5,5,5	0.26	0
5	SO4	A	746	-	4,4,4	0.20	0	6,6,6	0.36	0
5	SO4	C	744	-	4,4,4	0.24	0	6,6,6	0.65	0
5	SO4	C	742	-	4,4,4	0.17	0	6,6,6	0.40	0
5	SO4	B	741	-	4,4,4	0.16	0	6,6,6	0.28	0
6	GOL	D	743	-	5,5,5	0.50	0	5,5,5	0.65	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
6	GOL	C	743	-	-	3/4/4/4	-
2	SF4	D	738	1	-	-	0/6/5/5
6	GOL	A	743	-	-	2/4/4/4	-
6	GOL	F	743	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	738	1	-	-	0/6/5/5
2	SF4	F	738	1	-	-	0/6/5/5
6	GOL	E	743	-	-	3/4/4/4	-
2	SF4	E	738	1	-	-	0/6/5/5
2	SF4	A	738	1	-	-	0/6/5/5
2	SF4	B	738	1	-	-	0/6/5/5
6	GOL	B	743	-	-	3/4/4/4	-
6	GOL	D	743	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	743	GOL	C1-C2-C3-O3
6	B	743	GOL	C1-C2-C3-O3
6	C	743	GOL	C1-C2-C3-O3
6	D	743	GOL	C1-C2-C3-O3
6	E	743	GOL	C1-C2-C3-O3
6	B	743	GOL	O2-C2-C3-O3
6	C	743	GOL	O2-C2-C3-O3
6	D	743	GOL	O2-C2-C3-O3
6	E	743	GOL	O2-C2-C3-O3
6	A	743	GOL	O2-C2-C3-O3
6	D	743	GOL	O1-C1-C2-O2
6	D	743	GOL	O1-C1-C2-C3
6	C	743	GOL	O1-C1-C2-O2
6	E	743	GOL	O1-C1-C2-O2
6	B	743	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	738	SF4	1	0
2	E	738	SF4	1	0
2	D	738	SF4	1	0
5	B	744	SO4	1	0
2	C	738	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	742	SO4	1	0
2	A	738	SF4	2	0
2	B	738	SF4	1	0
5	D	744	SO4	1	0
5	C	742	SO4	1	0
6	D	743	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	422/427 (98%)	-0.18	5 (1%)	79	54	53, 57, 60, 64	11 (2%)
1	B	421/427 (98%)	-0.08	14 (3%)	46	20	53, 57, 60, 65	11 (2%)
1	C	421/427 (98%)	-0.13	7 (1%)	70	41	54, 57, 60, 64	11 (2%)
1	D	422/427 (98%)	-0.24	2 (0%)	91	75	53, 57, 61, 77	12 (2%)
1	E	421/427 (98%)	-0.23	5 (1%)	79	54	53, 57, 61, 67	11 (2%)
1	F	421/427 (98%)	-0.15	10 (2%)	59	30	54, 57, 60, 64	11 (2%)
All	All	2528/2562 (98%)	-0.17	43 (1%)	70	41	53, 57, 60, 77	67 (2%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	358	GLU	4.5
1	B	687	VAL	3.8
1	C	362	THR	3.6
1	A	730	ARG	3.4
1	F	493	ARG	3.3
1	E	359	SER	3.1
1	F	555	GLY	3.0
1	C	361	ILE	2.9
1	B	359	SER	2.8
1	F	577	ARG	2.7
1	B	544	HIS	2.7
1	F	362	THR	2.6
1	F	359	SER	2.6
1	B	393	ARG	2.6
1	F	573	THR	2.6
1	A	393	ARG	2.5
1	B	555	GLY	2.5
1	C	391	TYR	2.4
1	D	737	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	359	SER	2.4
1	F	361	ILE	2.4
1	A	493	ARG	2.3
1	B	684	ARG	2.3
1	C	684	ARG	2.3
1	E	544	HIS	2.2
1	B	693	GLU	2.2
1	E	361	ILE	2.2
1	D	359	SER	2.2
1	F	316	ILE	2.2
1	B	486	LYS	2.2
1	B	358	GLU	2.2
1	C	555	GLY	2.1
1	B	490	ASP	2.1
1	B	462	ARG	2.1
1	B	545	ALA	2.1
1	B	683	VAL	2.1
1	B	694	ASP	2.1
1	E	577	ARG	2.1
1	C	359	SER	2.1
1	F	495	LEU	2.0
1	C	499	THR	2.0
1	E	358	GLU	2.0
1	A	679	HIS	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	742	5/5	0.71	0.55	52,52,53,53	5
5	SO4	F	742	5/5	0.75	0.42	64,65,66,66	5
5	SO4	C	745	5/5	0.78	0.37	62,62,63,63	5
5	SO4	F	741	5/5	0.79	0.23	79,79,81,81	5
5	SO4	A	742	5/5	0.80	0.25	56,57,57,57	5
6	GOL	D	743	6/6	0.80	0.29	79,84,85,87	0
5	SO4	E	745	5/5	0.81	0.25	65,66,67,67	5
5	SO4	B	745	5/5	0.82	0.33	62,62,64,64	5
6	GOL	E	743	6/6	0.82	0.32	84,87,87,87	0
5	SO4	C	742	5/5	0.83	0.41	58,58,59,59	5
5	SO4	F	745	5/5	0.85	0.25	65,66,67,67	5
5	SO4	D	745	5/5	0.86	0.24	70,71,72,72	5
4	H2S	F	740	1/1	0.87	0.23	59,59,59,59	1
5	SO4	A	745	5/5	0.88	0.19	63,63,64,65	5
6	GOL	A	743	6/6	0.88	0.22	80,81,81,82	0
6	GOL	F	743	6/6	0.88	0.34	81,83,83,84	0
5	SO4	B	744	5/5	0.89	0.25	77,79,82,83	5
4	H2S	C	740	1/1	0.89	0.24	58,58,58,58	1
6	GOL	C	743	6/6	0.89	0.29	87,90,91,92	0
6	GOL	B	743	6/6	0.90	0.30	81,83,84,85	0
4	H2S	E	740	1/1	0.90	0.22	59,59,59,59	1
5	SO4	D	741	5/5	0.90	0.32	71,71,73,74	5
5	SO4	A	746	5/5	0.90	0.28	69,70,71,71	5
5	SO4	A	744	5/5	0.90	0.19	72,72,75,76	5
4	H2S	D	740	1/1	0.91	0.22	58,58,58,58	1
5	SO4	E	744	5/5	0.91	0.18	72,75,77,77	5
5	SO4	A	741	5/5	0.91	0.15	78,79,80,81	5
5	SO4	D	742	5/5	0.91	0.26	57,57,58,58	5
5	SO4	E	742	5/5	0.92	0.40	59,59,60,61	5
5	SO4	C	741	5/5	0.92	0.25	68,69,70,70	5
5	SO4	D	744	5/5	0.92	0.18	71,73,75,77	5
5	SO4	B	741	5/5	0.92	0.23	70,71,71,71	5
5	SO4	F	744	5/5	0.93	0.13	65,66,68,70	5
5	SO4	C	744	5/5	0.93	0.20	66,66,67,70	5
4	H2S	A	740	1/1	0.95	0.13	60,60,60,60	1
4	H2S	B	740	1/1	0.95	0.21	57,57,57,57	1
3	ZN	D	739	1/1	0.96	0.11	57,57,57,57	1
3	ZN	C	739	1/1	0.97	0.10	57,57,57,57	1
3	ZN	B	739	1/1	0.97	0.07	57,57,57,57	1
3	ZN	E	739	1/1	0.97	0.11	59,59,59,59	1
3	ZN	F	739	1/1	0.97	0.12	57,57,57,57	1
3	ZN	A	739	1/1	0.98	0.09	57,57,57,57	1
2	SF4	A	738	8/8	0.99	0.10	56,56,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SF4	B	738	8/8	0.99	0.10	54,55,57,57	0
2	SF4	C	738	8/8	0.99	0.09	54,55,57,57	0
2	SF4	D	738	8/8	0.99	0.10	52,54,56,58	0
2	SF4	E	738	8/8	0.99	0.11	54,55,57,57	0
2	SF4	F	738	8/8	0.99	0.11	54,56,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.