Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2021 – 06:08 PM EDT

PDB ID	:	7N7S
Title	:	Crystal Structure of Hydroxymethylglutaryl-CoA reductase from Elizabethkingia anophelis NUHP1
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2021-06-11
Resolution	:	2.40 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 following versions of software and data (see references (i)) were used in the production of this report:

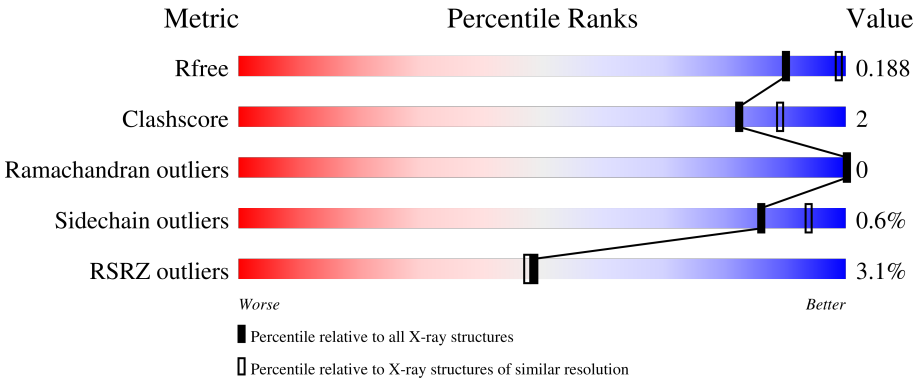
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	450	2% 80% 7% 12%
1	B	450	6% 92% 6%
1	C	450	80% 7% 14%
1	D	450	3% 83% 14%
1	E	450	2% 79% 7% 14%

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Mol	Chain	Length	Quality of chain
1	F	450	2% 80% 6% 14%

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	SO4	A	510	-	-	-	X
3	SO4	C	508	-	-	-	X
3	SO4	E	505	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20350 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 Hydroxymethylglutaryl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	6	0
			3108	1975	522	597	14			
1	B	441	Total	C	N	O	S	0	8	0
			3453	2199	584	655	15			
1	C	389	Total	C	N	O	S	0	6	0
			3071	1952	512	594	13			
1	D	389	Total	C	N	O	S	0	6	0
			3064	1949	513	589	13			
1	E	389	Total	C	N	O	S	0	5	0
			3055	1943	508	591	13			
1	F	389	Total	C	N	O	S	0	6	0
			3070	1950	515	592	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A077EA44
A	-6	ALA	-	expression tag	UNP A0A077EA44
A	-5	HIS	-	expression tag	UNP A0A077EA44
A	-4	HIS	-	expression tag	UNP A0A077EA44
A	-3	HIS	-	expression tag	UNP A0A077EA44
A	-2	HIS	-	expression tag	UNP A0A077EA44
A	-1	HIS	-	expression tag	UNP A0A077EA44
A	0	HIS	-	expression tag	UNP A0A077EA44
B	-7	MET	-	initiating methionine	UNP A0A077EA44
B	-6	ALA	-	expression tag	UNP A0A077EA44
B	-5	HIS	-	expression tag	UNP A0A077EA44
B	-4	HIS	-	expression tag	UNP A0A077EA44
B	-3	HIS	-	expression tag	UNP A0A077EA44
B	-2	HIS	-	expression tag	UNP A0A077EA44
B	-1	HIS	-	expression tag	UNP A0A077EA44
B	0	HIS	-	expression tag	UNP A0A077EA44
C	-7	MET	-	initiating methionine	UNP A0A077EA44

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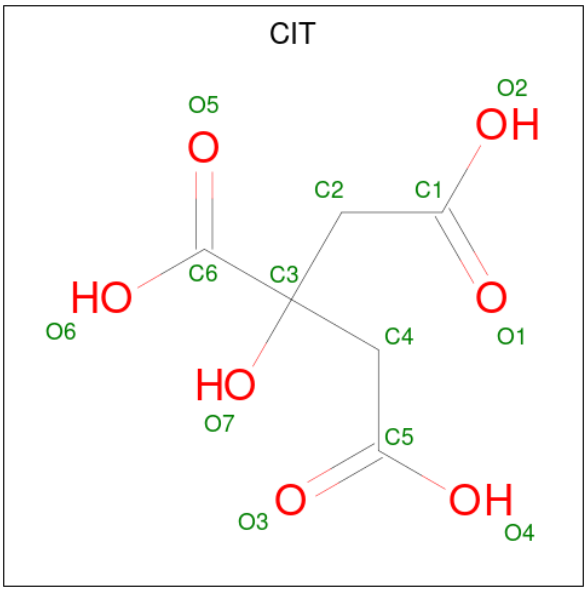
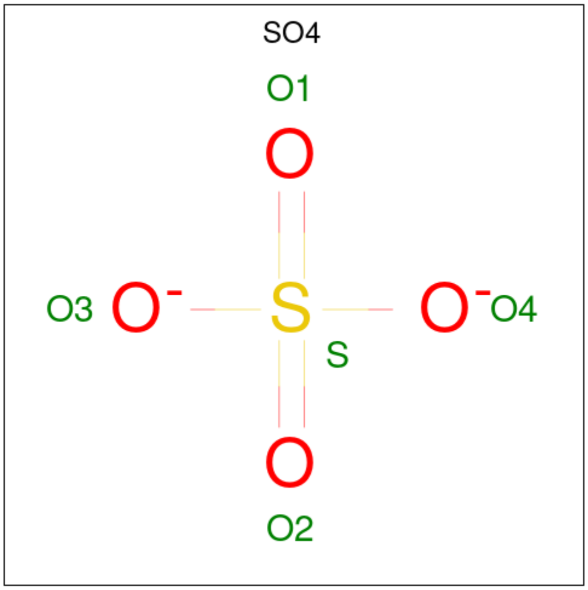
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP A0A077EA44
C	-5	HIS	-	expression tag	UNP A0A077EA44
C	-4	HIS	-	expression tag	UNP A0A077EA44
C	-3	HIS	-	expression tag	UNP A0A077EA44
C	-2	HIS	-	expression tag	UNP A0A077EA44
C	-1	HIS	-	expression tag	UNP A0A077EA44
C	0	HIS	-	expression tag	UNP A0A077EA44
D	-7	MET	-	initiating methionine	UNP A0A077EA44
D	-6	ALA	-	expression tag	UNP A0A077EA44
D	-5	HIS	-	expression tag	UNP A0A077EA44
D	-4	HIS	-	expression tag	UNP A0A077EA44
D	-3	HIS	-	expression tag	UNP A0A077EA44
D	-2	HIS	-	expression tag	UNP A0A077EA44
D	-1	HIS	-	expression tag	UNP A0A077EA44
D	0	HIS	-	expression tag	UNP A0A077EA44
E	-7	MET	-	initiating methionine	UNP A0A077EA44
E	-6	ALA	-	expression tag	UNP A0A077EA44
E	-5	HIS	-	expression tag	UNP A0A077EA44
E	-4	HIS	-	expression tag	UNP A0A077EA44
E	-3	HIS	-	expression tag	UNP A0A077EA44
E	-2	HIS	-	expression tag	UNP A0A077EA44
E	-1	HIS	-	expression tag	UNP A0A077EA44
E	0	HIS	-	expression tag	UNP A0A077EA44
F	-7	MET	-	initiating methionine	UNP A0A077EA44
F	-6	ALA	-	expression tag	UNP A0A077EA44
F	-5	HIS	-	expression tag	UNP A0A077EA44
F	-4	HIS	-	expression tag	UNP A0A077EA44
F	-3	HIS	-	expression tag	UNP A0A077EA44
F	-2	HIS	-	expression tag	UNP A0A077EA44
F	-1	HIS	-	expression tag	UNP A0A077EA44
F	0	HIS	-	expression tag	UNP A0A077EA44

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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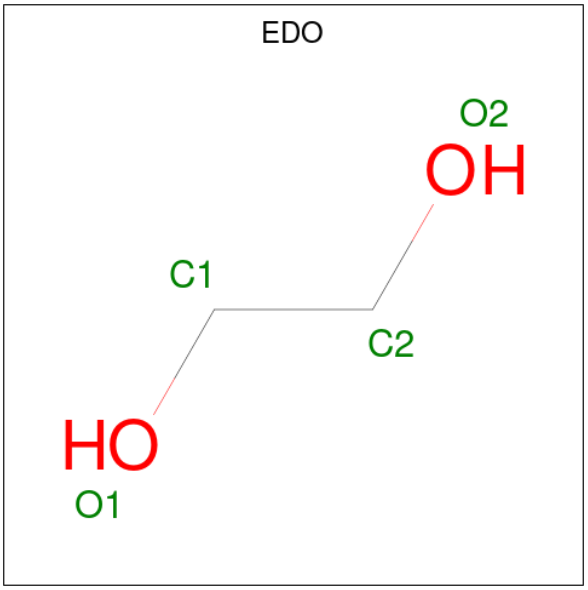
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

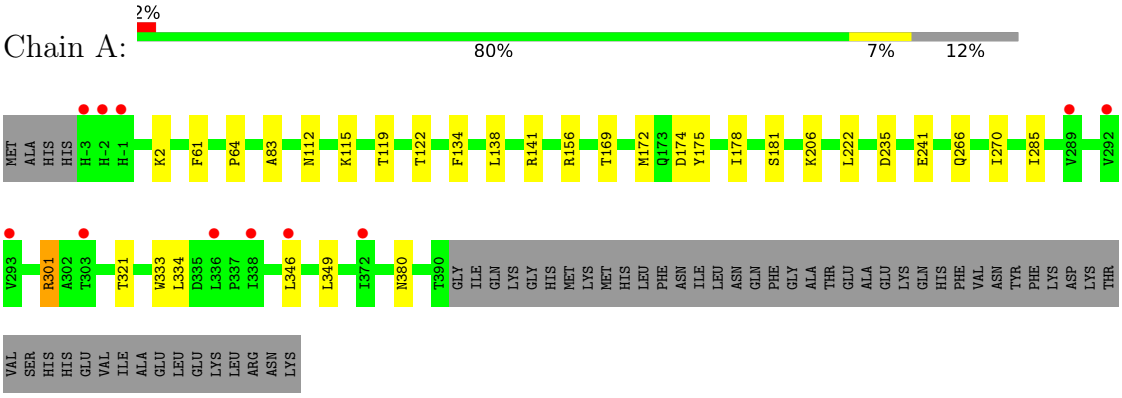
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	262	Total O 262 262	0	0
5	B	229	Total O 230 230	0	1
5	C	202	Total O 202 202	0	0
5	D	195	Total O 196 196	0	1
5	E	182	Total O 184 184	0	2
5	F	152	Total O 153 153	0	1

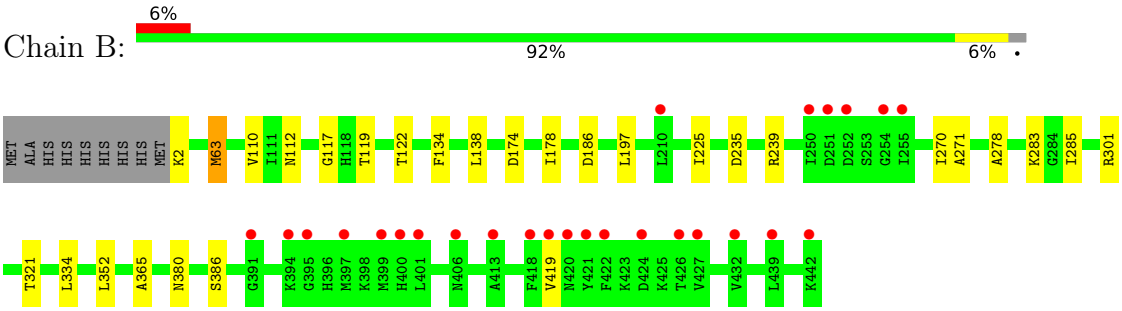
3 Residue-property plots

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.

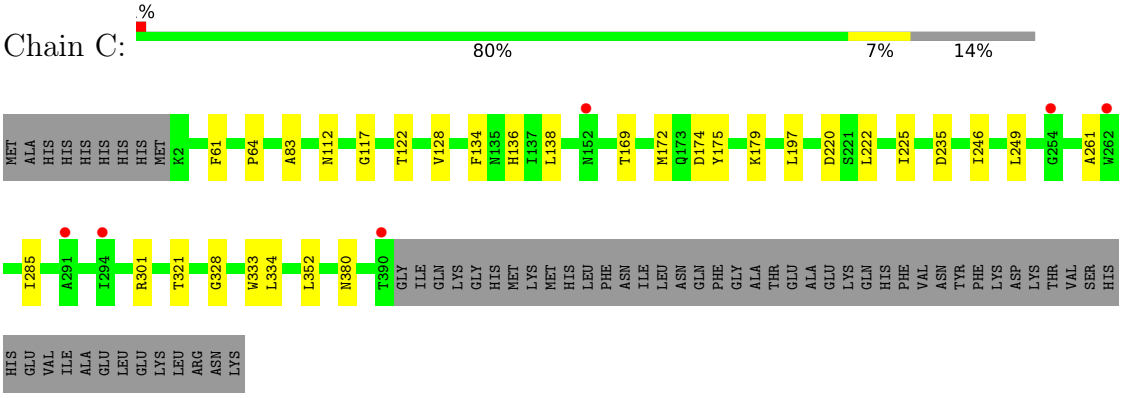
• Molecule 1: Hydroxymethylglutaryl-CoA reductase



• Molecule 1: Hydroxymethylglutaryl-CoA reductase

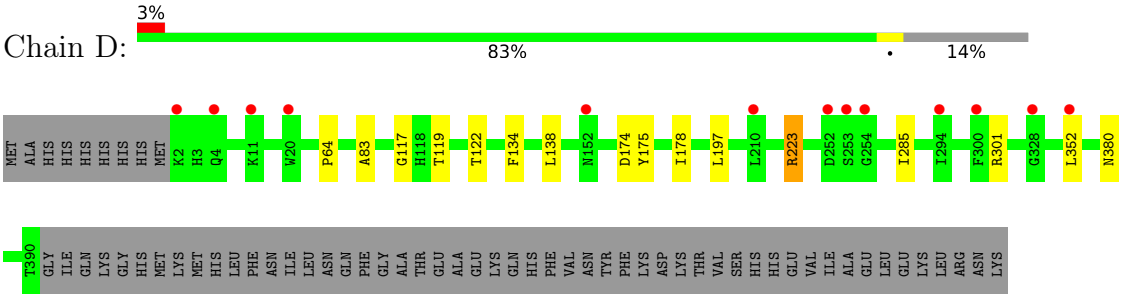


• Molecule 1: Hydroxymethylglutaryl-CoA reductase



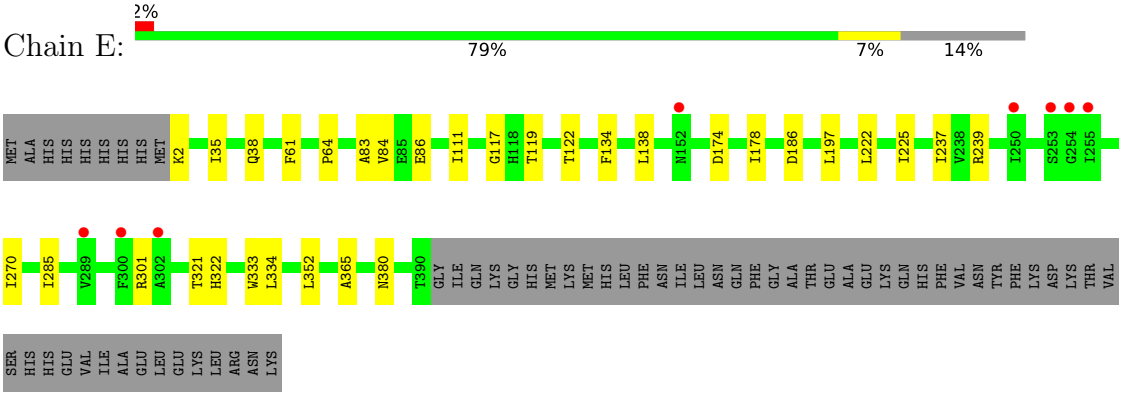
• Molecule 1: Hydroxymethylglutaryl-CoA reductase

Chain D:



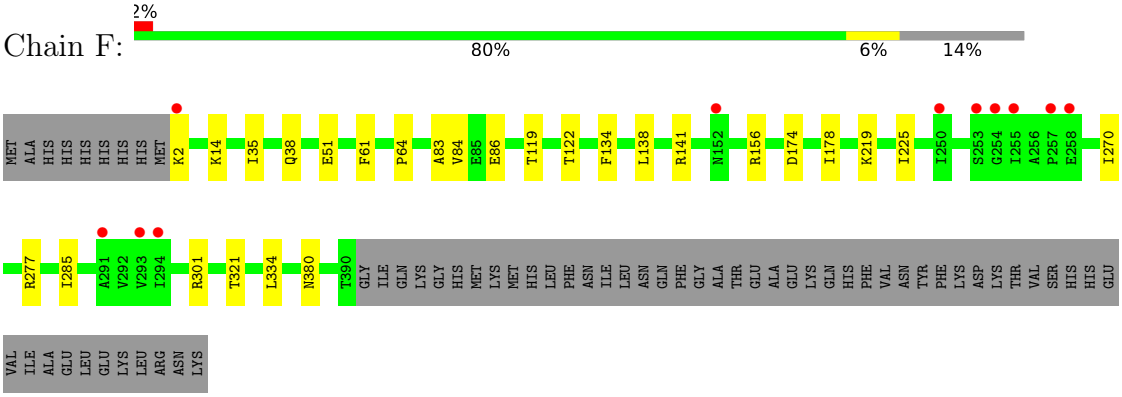
• Molecule 1: Hydroxymethylglutaryl-CoA reductase

Chain E:



• Molecule 1: Hydroxymethylglutaryl-CoA reductase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	183.85Å 206.67Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.40 49.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.26-2.40) 100.0 (49.26-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19 4224	Depositor
R, R_{free}	0.153 , 0.188 0.153 , 0.188	Depositor DCC
R_{free} test set	1956 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20350	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4, CIT

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	0.35	0/3188	0.54	0/4312
1	B	0.34	0/3547	0.51	0/4799
1	C	0.35	0/3150	0.53	0/4262
1	D	0.32	0/3143	0.52	0/4255
1	E	0.32	0/3131	0.50	0/4238
1	F	0.31	0/3149	0.52	0/4262
All	All	0.33	0/19308	0.52	0/26128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3108	0	3051	20	0
1	B	3453	0	3354	20	0
1	C	3071	0	3009	20	0
1	D	3064	0	3004	10	0
1	E	3055	0	2992	19	0
1	F	3070	0	3010	16	0
2	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	50	0	0	1	0
3	B	30	0	0	1	0
3	C	45	0	0	1	0
3	D	35	0	0	0	0
3	E	25	0	0	1	0
3	F	35	0	0	1	0
4	C	4	0	6	1	0
5	A	262	0	0	2	0
5	B	230	0	0	0	0
5	C	202	0	0	2	0
5	D	196	0	0	0	0
5	E	184	0	0	1	0
5	F	153	0	0	2	0
All	All	20350	0	18456	93	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 2.

All (93) 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:C:333:TRP:HE1	4:C:509:EDO:H12	1.54	0.73
1:A:206:LYS:HD2	1:B:419:VAL:HG11	1.72	0.71
1:C:134:PHE:HA	1:C:138:LEU:HB3	1.75	0.68
1:F:156[B]:ARG:NH2	5:F:601:HOH:O	2.31	0.64
1:A:134:PHE:HA	1:A:138:LEU:HB3	1.81	0.63
1:F:219:LYS:NZ	5:F:602:HOH:O	2.31	0.63
1:B:2:LYS:N	3:B:504:SO4:O2	2.33	0.62
1:A:270:ILE:HD11	1:B:225:ILE:HD13	1.83	0.60
1:F:321:THR:HG22	1:F:334:LEU:HB2	1.85	0.58
1:D:285:ILE:HG12	1:D:380:ASN:HB2	1.86	0.57
1:C:321:THR:HG22	1:C:334:LEU:HB2	1.87	0.56
1:A:141[B]:ARG:NH1	5:A:602:HOH:O	2.40	0.55
1:B:134:PHE:HA	1:B:138:LEU:HB3	1.88	0.54
1:D:134:PHE:HA	1:D:138:LEU:HB3	1.89	0.54
3:E:503:SO4:O1	5:E:601:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:PHE:HA	1:F:138:LEU:HB3	1.91	0.52
1:E:119:THR:HB	1:E:178:ILE:HB	1.89	0.52
1:E:134:PHE:HA	1:E:138:LEU:HB3	1.91	0.52
1:C:220:ASP:OD1	5:C:601:HOH:O	2.19	0.52
1:F:84:VAL:HG22	1:F:86:GLU:H	1.76	0.50
1:A:119:THR:HB	1:A:178:ILE:HB	1.93	0.50
1:E:64:PRO:O	1:E:83:ALA:HA	2.12	0.50
1:F:2:LYS:HA	3:F:506:SO4:O4	2.10	0.50
1:B:285:ILE:HG12	1:B:380:ASN:HB2	1.93	0.49
1:A:122:THR:HA	1:A:174:ASP:O	2.12	0.49
1:E:117:GLY:HA3	1:E:197:LEU:HD11	1.94	0.49
1:E:321:THR:HG22	1:E:334:LEU:HB2	1.95	0.49
1:F:122:THR:HA	1:F:174:ASP:O	2.12	0.49
1:C:122:THR:HA	1:C:174:ASP:O	2.12	0.49
1:A:346:LEU:HD12	1:A:349:LEU:HD12	1.95	0.49
1:B:122:THR:HG23	1:B:225:ILE:HD11	1.95	0.49
1:D:122:THR:HA	1:D:174:ASP:O	2.13	0.48
1:A:169:THR:HA	1:A:172:MET:O	2.14	0.47
1:D:352:LEU:HD12	1:F:61:PHE:HA	1.97	0.47
1:A:61:PHE:HA	1:B:352:LEU:HD12	1.97	0.46
1:C:285:ILE:HG12	1:C:380:ASN:HB2	1.97	0.46
1:B:63:MET:HE2	1:B:63:MET:HB2	1.79	0.46
1:C:112:ASN:HB3	1:C:235:ASP:O	2.15	0.46
1:D:119:THR:HB	1:D:178:ILE:HB	1.97	0.46
1:E:352:LEU:HD23	1:E:352:LEU:HA	1.77	0.46
1:C:61:PHE:HA	1:E:352:LEU:HD12	1.99	0.45
1:D:175:TYR:CZ	1:F:270:ILE:HD12	2.52	0.45
1:A:241:GLU:HG3	1:A:333:TRP:HB3	1.99	0.45
1:F:64:PRO:O	1:F:83:ALA:HA	2.17	0.45
1:A:112:ASN:HB3	1:A:235:ASP:O	2.17	0.44
1:B:117:GLY:HA3	1:B:197:LEU:HD11	1.99	0.44
1:C:64:PRO:O	1:C:83:ALA:HA	2.18	0.44
1:B:271:ALA:O	1:B:278:ALA:HB2	2.17	0.44
1:A:64:PRO:O	1:A:83:ALA:HA	2.18	0.44
1:C:122:THR:HG23	1:C:225:ILE:HD11	1.99	0.44
1:E:285:ILE:HG12	1:E:380:ASN:HB2	1.99	0.44
1:B:321:THR:HG22	1:B:334:LEU:HB2	2.00	0.44
3:C:511:SO4:O2	1:E:2:LYS:HA	2.17	0.44
1:E:111:ILE:HB	1:E:237:ILE:HG23	2.00	0.44
1:E:84:VAL:HG22	1:E:86:GLU:H	1.83	0.44
1:A:321:THR:HG22	1:A:334:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:THR:HB	1:B:178:ILE:HB	1.99	0.43
1:F:35:ILE:O	1:F:38:GLN:HG2	2.19	0.43
1:F:285:ILE:HG12	1:F:380:ASN:HB2	2.00	0.43
1:F:14:LYS:NZ	1:F:51:GLU:OE2	2.34	0.43
1:A:175:TYR:CZ	1:B:270:ILE:HD12	2.53	0.43
1:C:249:LEU:HD12	1:C:261:ALA:HB2	2.00	0.43
1:E:122:THR:HA	1:E:174:ASP:O	2.19	0.43
1:F:119:THR:HB	1:F:178:ILE:HB	2.01	0.43
1:B:239:ARG:HD2	1:C:128:VAL:HG21	2.00	0.43
1:A:301:ARG:HB3	1:B:283:LYS:HG2	2.01	0.42
1:B:186:ASP:HA	1:B:365:ALA:HB2	2.01	0.42
1:E:122:THR:HG23	1:E:225:ILE:HD11	2.01	0.42
1:E:35:ILE:O	1:E:38:GLN:HG2	2.19	0.42
1:C:352:LEU:HD23	1:C:352:LEU:HA	1.87	0.42
1:A:115:LYS:O	1:A:181:SER:HA	2.20	0.42
1:F:270:ILE:HG22	1:F:277:ARG:HG2	2.02	0.42
1:A:285:ILE:HG12	1:A:380:ASN:HB2	2.01	0.42
1:E:322:HIS:HB2	1:E:333:TRP:CE2	2.55	0.42
1:C:179:LYS:NZ	5:C:612:HOH:O	2.52	0.42
1:B:122:THR:HA	1:B:174:ASP:O	2.20	0.42
1:D:117:GLY:HA3	1:D:197:LEU:HD11	2.01	0.42
1:C:117:GLY:HA3	1:C:197:LEU:HD11	2.02	0.42
1:D:223:ARG:HB2	1:D:223:ARG:NH1	2.35	0.42
1:D:223:ARG:HB2	1:D:223:ARG:HH11	1.84	0.41
1:D:64:PRO:O	1:D:83:ALA:HA	2.21	0.41
1:C:352:LEU:HD12	1:E:61:PHE:HA	2.02	0.41
1:C:175:TYR:CZ	1:E:270:ILE:HD12	2.56	0.41
1:A:2:LYS:HA	3:A:507:SO4:O4	2.21	0.41
1:A:266:GLN:OE1	1:B:225:ILE:HG12	2.21	0.41
1:B:112:ASN:HB3	1:B:235:ASP:O	2.21	0.40
1:B:110:VAL:O	1:C:136:HIS:HE1	2.04	0.40
1:A:156:ARG:NH1	5:A:605:HOH:O	2.48	0.40
1:E:239:ARG:HA	1:E:334:LEU:O	2.22	0.40
1:C:169:THR:HA	1:C:172:MET:O	2.21	0.40
1:C:246:ILE:HD12	1:C:328:GLY:HA2	2.03	0.40
1:E:186:ASP:HA	1:E:365:ALA:HB2	2.03	0.40
1:F:122:THR:HG23	1:F:225:ILE:HD11	2.04	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	398/450 (88%)	390 (98%)	8 (2%)	0	100	100
1	B	447/450 (99%)	439 (98%)	8 (2%)	0	100	100
1	C	393/450 (87%)	387 (98%)	6 (2%)	0	100	100
1	D	393/450 (87%)	386 (98%)	7 (2%)	0	100	100
1	E	392/450 (87%)	384 (98%)	8 (2%)	0	100	100
1	F	393/450 (87%)	385 (98%)	8 (2%)	0	100	100
All	All	2416/2700 (90%)	2371 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	338/390 (87%)	336 (99%)	2 (1%)	86	94
1	B	367/390 (94%)	364 (99%)	3 (1%)	81	91
1	C	335/390 (86%)	333 (99%)	2 (1%)	86	94
1	D	333/390 (85%)	331 (99%)	2 (1%)	86	94
1	E	333/390 (85%)	331 (99%)	2 (1%)	86	94
1	F	335/390 (86%)	332 (99%)	3 (1%)	78	90
All	All	2041/2340 (87%)	2027 (99%)	14 (1%)	86	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	LEU
1	A	301	ARG
1	B	63	MET
1	B	301	ARG
1	B	386	SER
1	C	222	LEU
1	C	301	ARG
1	D	223	ARG
1	D	301	ARG
1	E	222	LEU
1	E	301	ARG
1	F	141[A]	ARG
1	F	141[B]	ARG
1	F	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	379	GLN
1	B	406	ASN
1	C	124	ASN
1	C	269	ASN
1	C	379	GLN
1	D	379	GLN
1	E	269	ASN
1	E	379	GLN
1	F	379	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)

51 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	$\#\|Z\| > 2$
3	SO4	E	504	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	F	506	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.36	0
3	SO4	B	502	-	4,4,4	0.13	0	6,6,6	0.18	0
3	SO4	D	506	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	D	504	-	4,4,4	0.13	0	6,6,6	0.40	0
3	SO4	D	508	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	F	501	-	4,4,4	0.15	0	6,6,6	0.36	0
3	SO4	E	503	-	4,4,4	0.11	0	6,6,6	0.20	0
3	SO4	A	502	-	4,4,4	0.21	0	6,6,6	0.15	0
2	CIT	D	501	-	3,12,12	1.40	0	3,17,17	1.26	1 (33%)
3	SO4	F	504	-	4,4,4	0.19	0	6,6,6	0.24	0
3	SO4	F	503	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	F	508	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	B	507	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	C	504	-	4,4,4	0.19	0	6,6,6	0.38	0
3	SO4	A	508	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	C	508	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	D	507	-	4,4,4	0.15	0	6,6,6	0.12	0
3	SO4	E	505	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	E	506	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	F	505	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	A	509	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.12	0
2	CIT	B	501	-	3,12,12	1.35	0	3,17,17	1.42	0
3	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	C	510	-	4,4,4	0.16	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	A	510	-	4,4,4	0.12	0	6,6,6	0.09	0
2	CIT	E	501	-	3,12,12	1.70	0	3,17,17	1.20	0
3	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.11	0
2	CIT	C	501	-	3,12,12	1.55	1 (33%)	3,17,17	1.17	0
3	SO4	D	502	-	4,4,4	0.16	0	6,6,6	0.06	0
2	CIT	A	501	-	3,12,12	1.79	1 (33%)	3,17,17	0.95	0
3	SO4	C	511	-	4,4,4	0.12	0	6,6,6	0.20	0
3	SO4	A	507	-	4,4,4	0.17	0	6,6,6	0.32	0
3	SO4	A	511	-	4,4,4	0.12	0	6,6,6	0.13	0
2	CIT	F	502	-	3,12,12	1.49	1 (33%)	3,17,17	1.04	0
3	SO4	A	504	-	4,4,4	0.18	0	6,6,6	0.43	0
3	SO4	C	503	-	4,4,4	0.19	0	6,6,6	0.32	0
4	EDO	C	509	-	3,3,3	0.56	0	2,2,2	0.19	0
3	SO4	D	503	-	4,4,4	0.16	0	6,6,6	0.31	0
3	SO4	A	503	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	F	507	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	E	502	-	4,4,4	0.12	0	6,6,6	0.23	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
2	CIT	D	501	-	-	0/6/16/16	-
2	CIT	F	502	-	-	0/6/16/16	-
4	EDO	C	509	-	-	1/1/1/1	-
2	CIT	E	501	-	-	0/6/16/16	-
2	CIT	C	501	-	-	0/6/16/16	-
2	CIT	B	501	-	-	0/6/16/16	-
2	CIT	A	501	-	-	0/6/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CIT	O7-C3	2.09	1.46	1.43
2	C	501	CIT	O7-C3	2.04	1.46	1.43
2	F	502	CIT	O7-C3	2.00	1.46	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	CIT	C3-C4-C5	-2.08	111.65	114.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	509	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	506	SO4	1	0
3	B	504	SO4	1	0
3	E	503	SO4	1	0
3	C	511	SO4	1	0
3	A	507	SO4	1	0
4	C	509	EDO	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	394/450 (87%)	-0.09	11 (2%)	53	51	26, 37, 61, 104	0
1	B	441/450 (98%)	-0.04	26 (5%)	22	21	25, 39, 94, 130	0
1	C	389/450 (86%)	-0.24	6 (1%)	73	72	31, 40, 66, 106	0
1	D	389/450 (86%)	-0.10	13 (3%)	46	45	32, 41, 68, 111	0
1	E	389/450 (86%)	-0.14	8 (2%)	63	61	32, 44, 68, 100	0
1	F	389/450 (86%)	-0.11	11 (2%)	53	51	32, 46, 70, 105	0
All	All	2391/2700 (88%)	-0.12	75 (3%)	49	47	25, 42, 72, 130	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	HIS	5.5
1	B	421	TYR	5.2
1	B	424	ASP	4.7
1	F	254	GLY	4.5
1	F	253	SER	4.4
1	A	-1	HIS	4.2
1	B	391	GLY	4.1
1	B	210	LEU	4.1
1	B	422	PHE	4.1
1	B	426	THR	3.9
1	B	394	LYS	3.8
1	A	-2	HIS	3.7
1	C	254	GLY	3.6
1	B	254	GLY	3.5
1	E	255	ILE	3.4
1	E	254	GLY	3.3
1	F	255	ILE	3.1
1	B	406	ASN	3.1
1	B	419	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	250	ILE	3.0
1	D	253	SER	2.9
1	D	20	TRP	2.8
1	B	442	LYS	2.8
1	B	252	ASP	2.8
1	B	420	ASN	2.8
1	F	258	GLU	2.8
1	B	395	GLY	2.8
1	A	346	LEU	2.7
1	C	152	ASN	2.7
1	B	427	VAL	2.7
1	B	439	LEU	2.7
1	B	418	PHE	2.6
1	B	251	ASP	2.6
1	D	328	GLY	2.6
1	A	289	VAL	2.6
1	C	291	ALA	2.6
1	E	300	PHE	2.6
1	B	400	HIS	2.6
1	B	401	LEU	2.5
1	B	432	VAL	2.5
1	F	152	ASN	2.5
1	A	293	VAL	2.5
1	D	4	GLN	2.5
1	A	372	ILE	2.4
1	B	397	MET	2.4
1	F	250	ILE	2.4
1	A	338	ILE	2.3
1	D	210	LEU	2.3
1	E	289	VAL	2.3
1	C	390	THR	2.3
1	C	294	ILE	2.3
1	E	302	ALA	2.2
1	D	152	ASN	2.2
1	A	292	VAL	2.2
1	B	250	ILE	2.2
1	E	152	ASN	2.2
1	D	254	GLY	2.2
1	F	257	PRO	2.2
1	F	291	ALA	2.2
1	B	399	MET	2.1
1	D	300	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	2	LYS	2.1
1	D	11	LYS	2.1
1	B	255	ILE	2.1
1	F	294	ILE	2.1
1	B	413	ALA	2.1
1	F	293	VAL	2.1
1	D	294	ILE	2.1
1	A	336	LEU	2.1
1	D	352	LEU	2.1
1	E	253	SER	2.1
1	D	252	ASP	2.0
1	C	262	TRP	2.0
1	A	303	THR	2.0
1	F	2	LYS	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
3	SO4	D	507	5/5	0.51	0.35	58,60,68,76	5
3	SO4	B	505	5/5	0.73	0.36	53,55,72,80	5
3	SO4	A	507	5/5	0.73	0.40	49,61,62,67	5
3	SO4	E	505	5/5	0.73	0.41	68,72,84,84	5
3	SO4	D	506	5/5	0.75	0.39	65,71,76,76	5
3	SO4	C	508	5/5	0.76	0.52	82,83,107,113	5
3	SO4	A	510	5/5	0.76	0.51	66,70,83,84	5
3	SO4	A	508	5/5	0.81	0.50	51,60,65,65	5
3	SO4	B	506	5/5	0.81	0.40	68,71,78,78	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	511	5/5	0.83	0.30	52,65,70,76	5
3	SO4	D	508	5/5	0.85	0.35	65,66,75,78	5
3	SO4	E	504	5/5	0.85	0.30	60,64,65,71	5
3	SO4	C	506	5/5	0.85	0.18	66,74,81,86	5
3	SO4	E	503	5/5	0.87	0.28	47,50,56,58	5
3	SO4	F	507	5/5	0.87	0.33	68,71,78,78	5
3	SO4	A	505	5/5	0.88	0.26	90,96,97,99	5
3	SO4	B	507	5/5	0.88	0.40	69,73,81,83	5
3	SO4	A	509	5/5	0.88	0.50	65,65,70,81	5
4	EDO	C	509	4/4	0.88	0.28	50,51,51,55	0
3	SO4	C	505	5/5	0.89	0.26	58,58,67,71	5
3	SO4	F	508	5/5	0.89	0.28	64,70,79,83	5
3	SO4	C	507	5/5	0.89	0.39	57,59,63,64	5
3	SO4	D	505	5/5	0.91	0.13	61,64,71,71	5
3	SO4	F	505	5/5	0.91	0.19	58,61,66,69	5
3	SO4	F	506	5/5	0.91	0.28	62,68,70,79	5
3	SO4	A	504	5/5	0.93	0.10	44,49,52,60	5
3	SO4	B	503	5/5	0.94	0.14	48,54,67,68	0
3	SO4	C	502	5/5	0.94	0.18	76,77,83,86	0
3	SO4	C	504	5/5	0.94	0.15	47,56,59,64	0
3	SO4	B	504	5/5	0.94	0.17	57,58,62,67	5
3	SO4	D	504	5/5	0.95	0.12	49,50,61,63	0
3	SO4	A	506	5/5	0.95	0.14	50,55,63,68	5
3	SO4	E	506	5/5	0.95	0.15	51,53,64,69	0
3	SO4	F	503	5/5	0.95	0.14	63,71,78,83	0
3	SO4	F	504	5/5	0.95	0.14	58,59,68,70	0
3	SO4	C	503	5/5	0.96	0.09	53,54,64,65	0
3	SO4	D	502	5/5	0.96	0.13	68,69,74,80	0
2	CIT	C	501	13/13	0.97	0.13	34,38,44,44	0
3	SO4	B	502	5/5	0.97	0.12	46,47,57,61	0
3	SO4	C	510	5/5	0.97	0.13	69,69,72,73	0
2	CIT	E	501	13/13	0.97	0.15	35,38,42,42	0
3	SO4	F	501	5/5	0.97	0.11	54,58,62,63	0
2	CIT	F	502	13/13	0.97	0.14	32,38,40,41	0
3	SO4	D	503	5/5	0.98	0.07	42,44,57,59	0
3	SO4	A	503	5/5	0.98	0.17	42,43,49,52	5
3	SO4	E	502	5/5	0.98	0.13	54,56,65,67	0
2	CIT	B	501	13/13	0.98	0.13	29,32,39,40	0
3	SO4	A	502	5/5	0.98	0.11	62,63,67,69	0
3	SO4	A	511	5/5	0.99	0.14	60,60,63,63	0
2	CIT	D	501	13/13	0.99	0.08	35,40,44,46	0
2	CIT	A	501	13/13	0.99	0.14	29,31,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.