



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3FDU
Title : Crystal structure of a putative enoyl-CoA hydratase/isomerase from *Acinetobacter baumannii*
Authors : Bonanno, J.B.; Dickey, M.; Bain, K.T.; Tang, B.K.; Romero, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-11-26
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

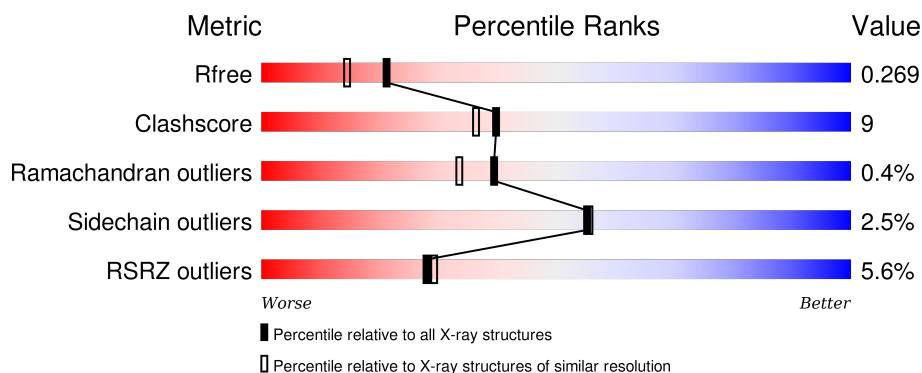
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>2%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	B	266	<div> <div>9%</div> <div>73%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>
1	C	266	<div> <div>3%</div> <div>71%</div> <div>13%</div> <div>•</div> <div>15%</div> </div>
1	D	266	<div> <div>4%</div> <div>73%</div> <div>11%</div> <div>•</div> <div>15%</div> </div>
1	E	266	<div> <div>8%</div> <div>76%</div> <div>11%</div> <div>•</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	266	

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	SO4	A	3	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11085 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 Putative enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	1	0
			1873	1202	317	347	7			
1	B	232	Total	C	N	O	S	0	0	0
			1735	1113	295	321	6			
1	C	227	Total	C	N	O	S	0	0	0
			1710	1096	291	318	5			
1	D	225	Total	C	N	O	S	0	0	0
			1690	1087	289	310	4			
1	E	234	Total	C	N	O	S	0	0	0
			1757	1128	296	327	6			
1	F	215	Total	C	N	O	S	0	0	0
			1611	1034	276	298	3			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP A3M7S1
A	8	SER	-	expression tag	UNP A3M7S1
A	9	LEU	-	expression tag	UNP A3M7S1
A	11	PRO	GLN	engineered	UNP A3M7S1
A	14	ASN	GLN	engineered	UNP A3M7S1
A	59	VAL	ILE	engineered	UNP A3M7S1
A	259	GLN	LYS	engineered	UNP A3M7S1
A	265	GLU	-	expression tag	UNP A3M7S1
A	266	GLY	-	expression tag	UNP A3M7S1
A	267	HIS	-	expression tag	UNP A3M7S1
A	268	HIS	-	expression tag	UNP A3M7S1
A	269	HIS	-	expression tag	UNP A3M7S1
A	270	HIS	-	expression tag	UNP A3M7S1
A	271	HIS	-	expression tag	UNP A3M7S1
A	272	HIS	-	expression tag	UNP A3M7S1
B	7	MET	-	expression tag	UNP A3M7S1
B	8	SER	-	expression tag	UNP A3M7S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	LEU	-	expression tag	UNP A3M7S1
B	11	PRO	GLN	engineered	UNP A3M7S1
B	14	ASN	GLN	engineered	UNP A3M7S1
B	59	VAL	ILE	engineered	UNP A3M7S1
B	259	GLN	LYS	engineered	UNP A3M7S1
B	265	GLU	-	expression tag	UNP A3M7S1
B	266	GLY	-	expression tag	UNP A3M7S1
B	267	HIS	-	expression tag	UNP A3M7S1
B	268	HIS	-	expression tag	UNP A3M7S1
B	269	HIS	-	expression tag	UNP A3M7S1
B	270	HIS	-	expression tag	UNP A3M7S1
B	271	HIS	-	expression tag	UNP A3M7S1
B	272	HIS	-	expression tag	UNP A3M7S1
C	7	MET	-	expression tag	UNP A3M7S1
C	8	SER	-	expression tag	UNP A3M7S1
C	9	LEU	-	expression tag	UNP A3M7S1
C	11	PRO	GLN	engineered	UNP A3M7S1
C	14	ASN	GLN	engineered	UNP A3M7S1
C	59	VAL	ILE	engineered	UNP A3M7S1
C	259	GLN	LYS	engineered	UNP A3M7S1
C	265	GLU	-	expression tag	UNP A3M7S1
C	266	GLY	-	expression tag	UNP A3M7S1
C	267	HIS	-	expression tag	UNP A3M7S1
C	268	HIS	-	expression tag	UNP A3M7S1
C	269	HIS	-	expression tag	UNP A3M7S1
C	270	HIS	-	expression tag	UNP A3M7S1
C	271	HIS	-	expression tag	UNP A3M7S1
C	272	HIS	-	expression tag	UNP A3M7S1
D	7	MET	-	expression tag	UNP A3M7S1
D	8	SER	-	expression tag	UNP A3M7S1
D	9	LEU	-	expression tag	UNP A3M7S1
D	11	PRO	GLN	engineered	UNP A3M7S1
D	14	ASN	GLN	engineered	UNP A3M7S1
D	59	VAL	ILE	engineered	UNP A3M7S1
D	259	GLN	LYS	engineered	UNP A3M7S1
D	265	GLU	-	expression tag	UNP A3M7S1
D	266	GLY	-	expression tag	UNP A3M7S1
D	267	HIS	-	expression tag	UNP A3M7S1
D	268	HIS	-	expression tag	UNP A3M7S1
D	269	HIS	-	expression tag	UNP A3M7S1
D	270	HIS	-	expression tag	UNP A3M7S1
D	271	HIS	-	expression tag	UNP A3M7S1

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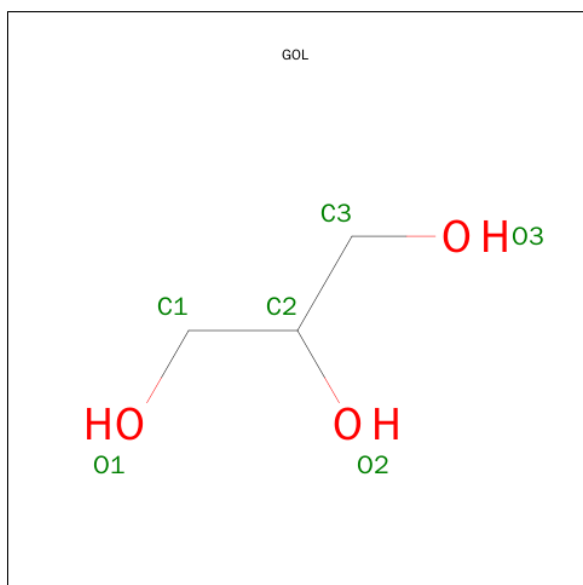
Chain	Residue	Modelled	Actual	Comment	Reference
D	272	HIS	-	expression tag	UNP A3M7S1
E	7	MET	-	expression tag	UNP A3M7S1
E	8	SER	-	expression tag	UNP A3M7S1
E	9	LEU	-	expression tag	UNP A3M7S1
E	11	PRO	GLN	engineered	UNP A3M7S1
E	14	ASN	GLN	engineered	UNP A3M7S1
E	59	VAL	ILE	engineered	UNP A3M7S1
E	259	GLN	LYS	engineered	UNP A3M7S1
E	265	GLU	-	expression tag	UNP A3M7S1
E	266	GLY	-	expression tag	UNP A3M7S1
E	267	HIS	-	expression tag	UNP A3M7S1
E	268	HIS	-	expression tag	UNP A3M7S1
E	269	HIS	-	expression tag	UNP A3M7S1
E	270	HIS	-	expression tag	UNP A3M7S1
E	271	HIS	-	expression tag	UNP A3M7S1
E	272	HIS	-	expression tag	UNP A3M7S1
F	7	MET	-	expression tag	UNP A3M7S1
F	8	SER	-	expression tag	UNP A3M7S1
F	9	LEU	-	expression tag	UNP A3M7S1
F	11	PRO	GLN	engineered	UNP A3M7S1
F	14	ASN	GLN	engineered	UNP A3M7S1
F	59	VAL	ILE	engineered	UNP A3M7S1
F	259	GLN	LYS	engineered	UNP A3M7S1
F	265	GLU	-	expression tag	UNP A3M7S1
F	266	GLY	-	expression tag	UNP A3M7S1
F	267	HIS	-	expression tag	UNP A3M7S1
F	268	HIS	-	expression tag	UNP A3M7S1
F	269	HIS	-	expression tag	UNP A3M7S1
F	270	HIS	-	expression tag	UNP A3M7S1
F	271	HIS	-	expression tag	UNP A3M7S1
F	272	HIS	-	expression tag	UNP A3M7S1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



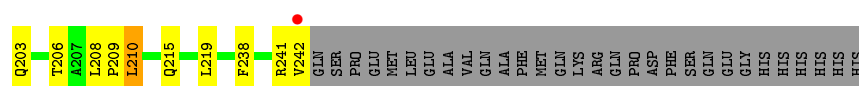
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

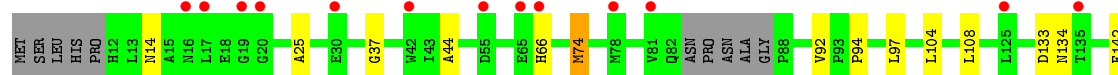
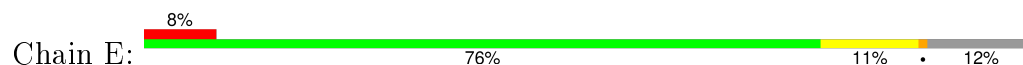
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total	O	0	0
			144	144		
4	B	116	Total	O	0	0
			116	116		
4	C	112	Total	O	0	0
			112	112		
4	D	120	Total	O	0	0
			120	120		
4	E	97	Total	O	0	0
			97	97		
4	F	94	Total	O	0	0
			94	94		

- Molecule 1: Putative enoyl-CoA hydratase/isomerase

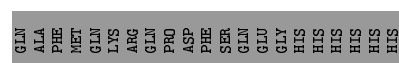
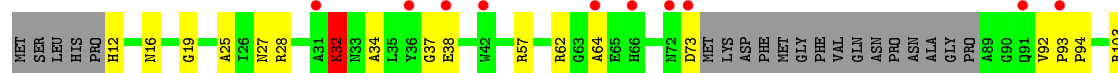




- Molecule 1: Putative enoyl-CoA hydratase/isomerase



- Molecule 1: Putative enoyl-CoA hydratase/isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.58Å 71.73Å 132.88Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 42.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.00) 98.8 (42.55-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.226 , 0.283 0.217 , 0.269	Depositor DCC
R_{free} test set	5416 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.8	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 106782 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11085	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.92	0/1910	0.77	1/2596 (0.0%)
1	B	0.71	0/1765	0.68	0/2400
1	C	0.80	0/1739	0.73	0/2363
1	D	0.69	0/1719	0.69	0/2336
1	E	0.66	0/1786	0.67	0/2425
1	F	0.63	0/1636	0.66	0/2223
All	All	0.75	0/10555	0.70	1/14343 (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	74	MET	CG-SD-CE	7.04	111.46	100.20

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	1873	0	1895	12	0
1	B	1735	0	1747	61	0
1	C	1710	0	1740	38	0
1	D	1690	0	1723	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1757	0	1778	20	2
1	F	1611	0	1644	36	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	E	10	0	0	0	0
3	A	6	0	8	0	0
4	A	144	0	0	1	0
4	B	116	0	0	4	0
4	C	112	0	0	2	1
4	D	120	0	0	3	0
4	E	97	0	0	5	0
4	F	94	0	0	6	1
All	All	11085	0	10535	185	2

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 9.

All (185) 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:77:PHE:HZ	1:B:247:MET:CE	1.34	1.37
1:C:9:LEU:HD23	1:C:10:HIS:N	1.38	1.35
1:B:77:PHE:CZ	1:B:247:MET:CE	2.15	1.27
1:B:239:MET:CE	1:B:239:MET:HA	1.71	1.20
1:B:77:PHE:CZ	1:B:247:MET:HE1	1.80	1.14
1:B:239:MET:HE1	1:B:242:VAL:HG21	1.22	1.13
1:C:92:VAL:HG11	1:C:239:MET:CE	1.77	1.13
1:B:77:PHE:CZ	1:B:247:MET:HE2	1.76	1.11
1:B:16:ASN:HD22	1:B:17:LEU:N	1.52	1.08
1:C:92:VAL:HG11	1:C:239:MET:HE3	1.11	1.08
1:B:77:PHE:HZ	1:B:247:MET:HE2	1.10	1.03
1:C:9:LEU:CD2	1:C:10:HIS:H	1.72	1.02
1:B:239:MET:HE3	1:B:239:MET:HA	1.40	1.00
1:C:92:VAL:CG1	1:C:239:MET:HE3	1.95	0.95
1:B:239:MET:CE	1:B:242:VAL:HG21	1.95	0.95
1:B:16:ASN:C	1:B:16:ASN:HD22	1.69	0.94
1:B:77:PHE:HZ	1:B:247:MET:HE1	1.16	0.94
1:B:239:MET:HA	1:B:239:MET:HE2	1.47	0.94
1:F:113:LYS:HD2	1:F:195:TYR:CZ	2.04	0.93
1:C:9:LEU:CD2	1:C:10:HIS:N	2.29	0.91
1:B:239:MET:HE1	1:B:242:VAL:CG2	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:HB2	4:B:279:HOH:O	1.69	0.90
1:F:203:GLN:HG2	4:F:927:HOH:O	1.72	0.87
1:B:243:GLN:CG	1:B:243:GLN:O	2.23	0.86
1:B:239:MET:CE	1:B:242:VAL:CG2	2.54	0.84
1:F:32:LYS:HE3	4:F:931:HOH:O	1.80	0.81
1:B:65:GLU:HG2	4:B:283:HOH:O	1.81	0.80
1:D:142:PHE:CE2	1:D:150:GLU:HG2	2.16	0.80
1:D:74:MET:HE3	4:D:281:HOH:O	1.80	0.80
1:B:77:PHE:CE2	1:B:247:MET:HE1	2.17	0.79
1:A:41:LEU:O	1:A:45:LYS:HG2	1.83	0.78
1:B:73:ASP:HB3	1:B:76:ASP:HB3	1.67	0.76
1:E:66:HIS:HD2	4:E:304:HOH:O	1.68	0.76
1:B:239:MET:CA	1:B:239:MET:HE3	2.16	0.75
1:B:239:MET:CA	1:B:239:MET:CE	2.60	0.74
1:B:16:ASN:C	1:B:16:ASN:ND2	2.34	0.73
1:B:74:MET:O	1:B:77:PHE:HB3	1.88	0.73
1:B:74:MET:CE	1:B:77:PHE:CD2	2.72	0.71
1:C:95:PHE:HE2	1:C:239:MET:CE	2.03	0.71
1:C:95:PHE:HE2	1:C:239:MET:HE2	1.54	0.71
1:F:225:ASP:O	1:F:229:GLU:HG3	1.91	0.71
1:B:12:HIS:CD2	1:B:28:ARG:HG3	2.27	0.70
1:B:137:LEU:C	1:B:137:LEU:HD13	2.13	0.69
1:B:243:GLN:HG3	1:B:243:GLN:O	1.94	0.68
1:F:57:ARG:HD2	4:F:306:HOH:O	1.93	0.68
1:B:65:GLU:HG3	1:B:66:HIS:N	2.08	0.68
1:B:243:GLN:HG2	1:B:243:GLN:O	1.93	0.67
1:C:92:VAL:CG1	1:C:239:MET:CE	2.63	0.66
1:F:146:GLY:O	1:F:241:ARG:HD3	1.94	0.66
1:B:16:ASN:ND2	1:B:17:LEU:N	2.36	0.64
1:E:229:GLU:HG3	4:E:294:HOH:O	1.98	0.64
1:B:245:PRO:HD3	4:B:290:HOH:O	1.97	0.63
1:B:199:GLN:NE2	1:B:203:GLN:OE1	2.23	0.61
1:B:74:MET:HE2	1:B:77:PHE:CD2	2.35	0.61
1:B:202:ALA:O	1:B:206:THR:HG23	2.01	0.60
1:F:19:GLY:O	4:F:812:HOH:O	2.16	0.60
1:D:147:LEU:HA	1:D:241:ARG:HD3	1.84	0.60
1:B:77:PHE:CE2	1:B:247:MET:CE	2.79	0.59
1:F:148:SER:HB2	1:F:149:PRO:CD	2.32	0.59
1:B:74:MET:HE1	1:B:77:PHE:CD2	2.38	0.58
1:D:133:ASP:OD2	4:D:300:HOH:O	2.17	0.58
1:C:9:LEU:C	1:C:9:LEU:HD23	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:PHE:CZ	1:D:150:GLU:HG2	2.40	0.57
1:A:202:ALA:O	1:A:206:THR:HG23	2.05	0.56
1:F:62:ARG:NH2	1:F:195:TYR:HB3	2.21	0.56
1:F:28:ARG:HG2	1:F:28:ARG:O	2.05	0.55
1:D:74:MET:CE	1:D:74:MET:HA	2.35	0.55
1:E:193:ASP:OD2	1:E:196:ALA:HB2	2.07	0.55
1:C:142:PHE:CE2	1:C:150:GLU:HG2	2.41	0.54
1:B:74:MET:HG3	1:B:77:PHE:HD2	1.73	0.54
1:B:65:GLU:HG3	1:B:66:HIS:H	1.72	0.54
1:D:146:GLY:O	1:D:241:ARG:NH2	2.40	0.54
1:B:9:LEU:HG	1:B:10:HIS:H	1.72	0.54
1:C:214:LYS:HG3	4:C:317:HOH:O	2.08	0.54
1:B:225:ASP:O	1:B:229:GLU:HG3	2.08	0.54
1:C:92:VAL:HG21	1:C:239:MET:CE	2.39	0.53
1:B:246:GLU:HG2	1:C:209:PRO:HB3	1.90	0.53
1:F:62:ARG:HH21	1:F:195:TYR:HB3	1.73	0.53
1:F:113:LYS:HD2	1:F:195:TYR:OH	2.09	0.53
1:E:165:LYS:HE3	4:E:459:HOH:O	2.08	0.53
1:F:92:VAL:HG12	1:F:94:PRO:HD2	1.89	0.53
1:D:119:ILE:O	1:D:119:ILE:HG13	2.09	0.53
1:E:248:LEU:HD12	4:E:645:HOH:O	2.08	0.52
1:C:16:ASN:O	1:C:22:LEU:HD12	2.10	0.52
1:B:74:MET:HA	1:B:74:MET:HE2	1.92	0.52
1:D:74:MET:CE	4:D:281:HOH:O	2.50	0.52
1:D:199:GLN:HE21	1:D:203:GLN:CG	2.23	0.52
1:D:67:ASP:OD1	1:D:115:VAL:HG22	2.10	0.51
1:E:92:VAL:HG12	1:E:94:PRO:HD2	1.93	0.51
1:B:137:LEU:C	1:B:137:LEU:CD1	2.78	0.51
1:E:210:LEU:HG	1:E:214:LYS:HE3	1.92	0.51
1:E:14:ASN:HB2	1:E:25:ALA:HB3	1.93	0.50
1:F:103:ARG:HD2	4:F:963:HOH:O	2.12	0.50
1:A:92:VAL:HG12	1:A:94:PRO:HD2	1.94	0.49
1:C:12:HIS:HD2	1:C:36:TYR:OH	1.94	0.49
1:C:9:LEU:HD23	1:C:10:HIS:H	0.76	0.49
1:D:57:ARG:NH1	1:D:210:LEU:HB2	2.27	0.49
1:B:74:MET:HA	1:B:77:PHE:HB3	1.95	0.49
1:F:114:GLY:O	1:F:136:ALA:HA	2.13	0.49
1:F:34:ALA:HB1	1:F:73:ASP:HA	1.95	0.49
1:E:142:PHE:CZ	1:E:150:GLU:HG2	2.47	0.49
1:D:45:LYS:HE3	1:D:49:GLU:OE2	2.13	0.49
1:D:208:LEU:HB3	1:D:209:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:VAL:HG12	1:C:94:PRO:HD2	1.95	0.48
1:E:134:ASN:OD1	1:E:190:ILE:CG2	2.61	0.48
1:C:145:LEU:HD12	1:C:147:LEU:HD12	1.96	0.48
1:D:219:LEU:HD11	1:F:237:ILE:HD12	1.94	0.48
1:F:113:LYS:HD2	1:F:195:TYR:CE2	2.48	0.48
1:B:73:ASP:O	1:B:77:PHE:N	2.34	0.48
1:E:246:GLU:HG2	1:F:209:PRO:HB3	1.96	0.48
1:F:226:GLN:NE2	1:F:226:GLN:H	2.12	0.48
1:B:12:HIS:CG	1:B:28:ARG:HG3	2.49	0.47
1:F:210:LEU:HG	1:F:210:LEU:O	2.13	0.47
1:E:104:LEU:HD23	1:E:108:LEU:HB2	1.97	0.47
1:F:202:ALA:O	1:F:206:THR:HG23	2.14	0.47
1:A:209:PRO:HB3	1:C:246:GLU:HG2	1.96	0.47
1:C:98:LEU:HD13	1:C:151:GLY:HA2	1.97	0.47
1:D:98:LEU:HD13	1:D:151:GLY:HA2	1.96	0.47
1:D:238:PHE:CE2	1:D:242:VAL:HG21	2.50	0.47
1:F:93:PRO:HB2	1:F:94:PRO:HD3	1.95	0.47
1:B:113:LYS:HE2	4:B:339:HOH:O	2.14	0.47
1:B:74:MET:C	1:B:77:PHE:HB3	2.35	0.47
1:E:193:ASP:OD2	1:E:196:ALA:CB	2.63	0.47
1:C:104:LEU:HD23	1:C:108:LEU:HB2	1.96	0.47
1:F:128:ASP:O	1:F:129:LEU:HD23	2.15	0.47
1:C:95:PHE:HE2	1:C:239:MET:HE1	1.80	0.46
1:F:38:GLU:HG2	4:F:388:HOH:O	2.15	0.46
1:B:199:GLN:HE21	1:B:203:GLN:CD	2.13	0.46
1:B:74:MET:HA	1:B:77:PHE:CB	2.45	0.46
1:C:10:HIS:HA	1:C:11:PRO:HD3	1.81	0.46
1:D:137:LEU:HD11	1:D:175:LYS:HG2	1.96	0.46
1:E:66:HIS:CD2	4:E:304:HOH:O	2.53	0.46
1:E:155:GLN:OE1	1:E:226:GLN:NE2	2.49	0.46
1:D:57:ARG:HB2	1:D:206:THR:HG22	1.98	0.46
1:A:98:LEU:HD13	1:A:151:GLY:HA2	1.99	0.45
1:C:202:ALA:O	1:C:206:THR:HG23	2.16	0.45
1:B:73:ASP:HB3	1:B:76:ASP:CB	2.42	0.45
1:A:237:ILE:HD12	1:B:219:LEU:HD21	1.98	0.45
1:C:146:GLY:O	1:C:241:ARG:HD3	2.16	0.45
1:C:92:VAL:HG21	1:C:239:MET:HE3	1.99	0.45
1:C:242:VAL:O	1:C:242:VAL:CG1	2.65	0.44
1:D:148:SER:HB2	1:D:149:PRO:CD	2.48	0.44
1:C:203:GLN:NE2	4:C:289:HOH:O	2.40	0.44
1:B:172:THR:OG1	1:B:174:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:SER:OG	1:C:146:GLY:HA2	2.18	0.44
1:F:199:GLN:O	1:F:203:GLN:HG3	2.18	0.44
1:A:57:ARG:NH2	4:A:278:HOH:O	2.51	0.44
1:E:133:ASP:OD1	1:E:133:ASP:C	2.56	0.44
1:D:215:GLN:NE2	1:F:237:ILE:HD13	2.33	0.43
1:E:148:SER:HB2	1:E:149:PRO:CD	2.48	0.43
1:E:134:ASN:OD1	1:E:190:ILE:HG21	2.19	0.43
1:B:238:PHE:HD2	1:B:239:MET:HE3	1.83	0.43
1:B:199:GLN:NE2	1:B:203:GLN:HG3	2.33	0.43
1:F:25:ALA:HB1	1:F:64:ALA:HA	1.99	0.43
1:F:133:ASP:OD1	1:F:133:ASP:C	2.56	0.43
1:C:25:ALA:CB	1:C:62:ARG:HD2	2.49	0.43
1:B:239:MET:HE2	1:B:242:VAL:HB	1.99	0.43
1:A:98:LEU:HD13	1:A:151:GLY:CA	2.49	0.43
1:D:210:LEU:HG	1:D:210:LEU:O	2.18	0.42
1:D:199:GLN:O	1:D:203:GLN:HG3	2.19	0.42
1:E:74:MET:HA	1:E:74:MET:HE2	2.02	0.42
1:F:116:ALA:O	1:F:138:PHE:HA	2.19	0.42
1:F:119:ILE:O	1:F:123:ILE:HG22	2.19	0.42
1:A:104:LEU:HD23	1:A:108:LEU:HB2	2.01	0.42
1:D:148:SER:HB2	1:D:149:PRO:HD2	2.01	0.42
1:D:199:GLN:NE2	1:D:203:GLN:CG	2.83	0.41
1:C:232:ASP:O	1:C:236:GLU:HG2	2.21	0.41
1:F:148:SER:HB2	1:F:149:PRO:HD2	2.02	0.41
1:F:28:ARG:CG	1:F:28:ARG:O	2.68	0.41
1:A:148:SER:HB2	1:A:149:PRO:CD	2.50	0.41
1:C:152:GLY:N	1:C:234:GLU:OE1	2.52	0.41
1:F:12:HIS:HA	1:F:27:ASN:O	2.20	0.41
1:C:95:PHE:CE2	1:C:239:MET:CE	2.93	0.41
1:B:148:SER:HB2	1:B:149:PRO:CD	2.51	0.41
1:F:25:ALA:HA	1:F:62:ARG:O	2.20	0.41
1:C:25:ALA:HB2	1:C:62:ARG:HD2	2.03	0.41
1:E:44:ALA:HB2	1:E:97:LEU:HA	2.02	0.41
1:C:74:MET:CE	1:C:74:MET:HA	2.51	0.41
1:B:28:ARG:N	1:B:29:PRO:CD	2.84	0.40
1:B:104:LEU:HD23	1:B:108:LEU:HB2	2.03	0.40
1:C:95:PHE:CE2	1:C:239:MET:HE1	2.56	0.40
1:B:199:GLN:NE2	1:B:203:GLN:CG	2.84	0.40
1:A:189:GLU:HG2	1:A:191:VAL:HG13	2.02	0.40
1:C:92:VAL:CB	1:C:239:MET:HE3	2.51	0.40
1:F:165:LYS:HB2	1:F:165:LYS:HE2	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:GLU:OE2	4:C:295:HOH:O[1_545]	1.97	0.23
1:E:240:GLN:NE2	4:F:275:HOH:O[2_656]	2.12	0.08

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	247/266 (93%)	240 (97%)	7 (3%)	0	100	100
1	B	228/266 (86%)	218 (96%)	9 (4%)	1 (0%)	39	33
1	C	223/266 (84%)	215 (96%)	7 (3%)	1 (0%)	39	33
1	D	221/266 (83%)	213 (96%)	8 (4%)	0	100	100
1	E	230/266 (86%)	224 (97%)	5 (2%)	1 (0%)	39	33
1	F	211/266 (79%)	200 (95%)	9 (4%)	2 (1%)	21	13
All	All	1360/1596 (85%)	1310 (96%)	45 (3%)	5 (0%)	39	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	32	LYS
1	E	37	GLY
1	F	37	GLY
1	B	37	GLY
1	C	37	GLY

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	192/212 (91%)	188 (98%)	4 (2%)	61	63
1	B	176/212 (83%)	170 (97%)	6 (3%)	44	41
1	C	176/212 (83%)	172 (98%)	4 (2%)	58	60
1	D	172/212 (81%)	167 (97%)	5 (3%)	50	49
1	E	179/212 (84%)	176 (98%)	3 (2%)	68	71
1	F	163/212 (77%)	159 (98%)	4 (2%)	55	55
All	All	1058/1272 (83%)	1032 (98%)	26 (2%)	55	55

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

Mol	Chain	Res	Type
1	A	74	MET
1	A	150	GLU
1	A	210	LEU
1	A	241	ARG
1	B	16	ASN
1	B	28	ARG
1	B	74	MET
1	B	78	MET
1	B	239	MET
1	B	243	GLN
1	C	62	ARG
1	C	236	GLU
1	C	241	ARG
1	C	243	GLN
1	D	65	GLU
1	D	75	LYS
1	D	119	ILE
1	D	137	LEU
1	D	210	LEU
1	E	74	MET
1	E	247	MET
1	E	248	LEU
1	F	16	ASN
1	F	32	LYS
1	F	174	LYS
1	F	210	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	226	GLN
1	B	16	ASN
1	B	199	GLN
1	B	203	GLN
1	B	215	GLN
1	C	12	HIS
1	C	14	ASN
1	C	134	ASN
1	C	199	GLN
1	C	203	GLN
1	C	243	GLN
1	D	16	ASN
1	D	199	GLN
1	D	203	GLN
1	D	215	GLN
1	D	226	GLN
1	E	155	GLN
1	E	226	GLN
1	F	12	HIS
1	F	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	GOL	A	1	-	5,5,5	0.18	0	5,5,5	0.65	0
2	SO4	A	3	-	4,4,4	0.22	0	6,6,6	0.45	0
2	SO4	C	4	-	4,4,4	0.15	0	6,6,6	0.29	0
2	SO4	E	1	-	4,4,4	0.34	0	6,6,6	0.30	0
2	SO4	E	2	-	4,4,4	0.36	0	6,6,6	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1	-	-	0/4/4/4	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th 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	248/266 (93%)	0.06	4 (1%) 74 75	16, 22, 33, 42	0
1	B	232/266 (87%)	0.47	24 (10%) 9 9	19, 32, 52, 61	0
1	C	227/266 (85%)	0.31	8 (3%) 48 49	17, 29, 44, 56	0
1	D	225/266 (84%)	0.33	10 (4%) 38 39	23, 33, 44, 59	0
1	E	234/266 (87%)	0.54	20 (8%) 13 14	22, 35, 51, 57	0
1	F	215/266 (80%)	0.51	12 (5%) 28 29	23, 38, 52, 58	0
All	All	1381/1596 (86%)	0.37	78 (5%) 28 29	16, 31, 49, 61	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	LYS	6.4
1	B	9	LEU	5.8
1	B	77	PHE	5.5
1	D	77	PHE	5.2
1	B	42	TRP	5.0
1	E	248	LEU	4.4
1	B	76	ASP	4.3
1	E	19	GLY	4.3
1	D	74	MET	4.1
1	E	42	TRP	4.0
1	B	74	MET	3.9
1	F	38	GLU	3.8
1	E	250	ALA	3.6
1	D	242	VAL	3.6
1	C	245	PRO	3.5
1	B	73	ASP	3.3
1	C	244	SER	3.3
1	B	64	ALA	3.3
1	E	20	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	9	LEU	3.2
1	A	8	SER	3.0
1	A	254	PHE	3.0
1	B	245	PRO	3.0
1	F	42	TRP	3.0
1	B	16	ASN	3.0
1	E	17	LEU	3.0
1	B	246	GLU	2.9
1	B	10	HIS	2.9
1	F	73	ASP	2.9
1	E	249	GLU	2.9
1	E	81	VAL	2.8
1	B	236	GLU	2.8
1	E	206	THR	2.8
1	B	243	GLN	2.8
1	D	31	ALA	2.8
1	E	16	ASN	2.8
1	D	156	LEU	2.8
1	E	55	ASP	2.7
1	C	243	GLN	2.7
1	F	240	GLN	2.7
1	F	36	TYR	2.7
1	B	11	PRO	2.6
1	B	248	LEU	2.6
1	B	247	MET	2.6
1	E	125	LEU	2.5
1	B	19	GLY	2.5
1	F	31	ALA	2.4
1	E	207	ALA	2.4
1	F	93	PRO	2.4
1	E	78	MET	2.4
1	B	31	ALA	2.4
1	D	30	GLU	2.4
1	C	42	TRP	2.4
1	E	240	GLN	2.3
1	C	74	MET	2.3
1	A	253	ALA	2.3
1	E	156	LEU	2.3
1	E	30	GLU	2.3
1	C	184	ALA	2.3
1	F	64	ALA	2.3
1	B	36	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	29	PRO	2.2
1	B	65	GLU	2.2
1	E	66	HIS	2.2
1	B	17	LEU	2.2
1	F	238	PHE	2.2
1	E	135	THR	2.2
1	B	28	ARG	2.2
1	B	244	SER	2.2
1	D	125	LEU	2.2
1	D	87	GLY	2.1
1	A	157	LEU	2.1
1	F	66	HIS	2.1
1	F	72	ASN	2.1
1	D	29	PRO	2.0
1	F	91	GLN	2.0
1	E	65	GLU	2.0
1	C	73	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	3	5/5	0.95	0.25	7.05	58,58,61,61	0
3	GOL	A	1	6/6	0.93	0.14	0.73	36,39,45,51	0
2	SO4	E	1	5/5	0.96	0.10	-0.75	47,49,51,52	0
2	SO4	C	4	5/5	0.92	0.29	-	66,66,67,68	0
2	SO4	E	2	5/5	0.84	0.25	-	53,56,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.