



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:45 am BST

PDB ID : 4HR7
Title : Crystal Structure of Biotin Carboxyl Carrier Protein-Biotin Carboxylase Complex from E.coli
Authors : Broussard, T.C.; Kobe, M.J.; Pakhomova, S.; Neau, D.B.; Price, A.E.; Champion, T.S.; Waldrop, G.L.
Deposited on : 2012-10-26
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

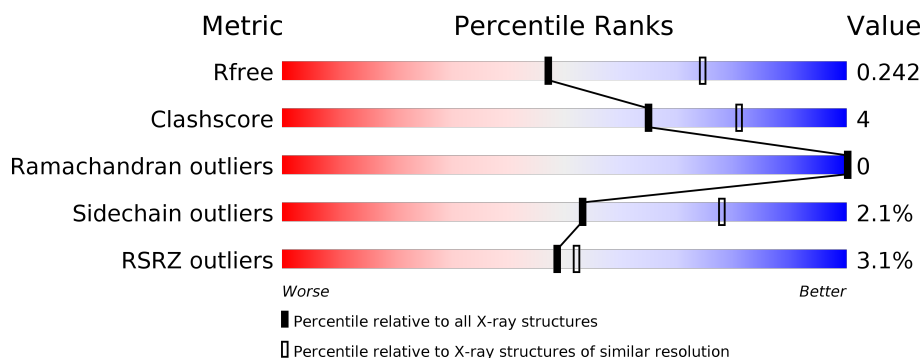
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>••</div> </div>
1	C	449	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>
1	E	449	<div> <div>2%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	F	449	<div> <div>3%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
2	B	176	<div> <div>2%</div> <div>39%</div> <div>6%</div> <div>• 55%</div> </div>
2	D	176	<div> <div>7%</div> <div>37%</div> <div>7%</div> <div>• 56%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	176	<p>2% 38% 6% 56%</p>
2	I	176	<p>41% 1% 56%</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16162 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 Biotin carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3408	2146	609	632	21			
1	C	425	Total	C	N	O	S	0	0	0
			3295	2083	584	608	20			
1	E	423	Total	C	N	O	S	0	3	0
			3297	2086	589	603	19			
1	F	427	Total	C	N	O	S	0	0	0
			3301	2085	586	609	21			

- Molecule 2 is a protein called Biotin carboxyl carrier protein of acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	C	N	O	S	0	0	0
			603	383	98	117	5			
2	D	78	Total	C	N	O	S	0	0	0
			581	367	94	115	5			
2	G	77	Total	C	N	O	S	0	0	0
			575	365	94	111	5			
2	I	77	Total	C	N	O	S	0	0	0
			583	370	95	113	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP P0ABD8
B	-18	GLY	-	EXPRESSION TAG	UNP P0ABD8
B	-17	SER	-	EXPRESSION TAG	UNP P0ABD8
B	-16	SER	-	EXPRESSION TAG	UNP P0ABD8
B	-15	HIS	-	EXPRESSION TAG	UNP P0ABD8
B	-14	HIS	-	EXPRESSION TAG	UNP P0ABD8
B	-13	HIS	-	EXPRESSION TAG	UNP P0ABD8
B	-12	HIS	-	EXPRESSION TAG	UNP P0ABD8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	EXPRESSION TAG	UNP P0ABD8
B	-10	HIS	-	EXPRESSION TAG	UNP P0ABD8
B	-9	SER	-	EXPRESSION TAG	UNP P0ABD8
B	-8	SER	-	EXPRESSION TAG	UNP P0ABD8
B	-7	GLY	-	EXPRESSION TAG	UNP P0ABD8
B	-6	LEU	-	EXPRESSION TAG	UNP P0ABD8
B	-5	VAL	-	EXPRESSION TAG	UNP P0ABD8
B	-4	PRO	-	EXPRESSION TAG	UNP P0ABD8
B	-3	ARG	-	EXPRESSION TAG	UNP P0ABD8
B	-2	GLY	-	EXPRESSION TAG	UNP P0ABD8
B	-1	SER	-	EXPRESSION TAG	UNP P0ABD8
B	0	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-19	MET	-	EXPRESSION TAG	UNP P0ABD8
D	-18	GLY	-	EXPRESSION TAG	UNP P0ABD8
D	-17	SER	-	EXPRESSION TAG	UNP P0ABD8
D	-16	SER	-	EXPRESSION TAG	UNP P0ABD8
D	-15	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-14	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-13	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-12	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-11	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-10	HIS	-	EXPRESSION TAG	UNP P0ABD8
D	-9	SER	-	EXPRESSION TAG	UNP P0ABD8
D	-8	SER	-	EXPRESSION TAG	UNP P0ABD8
D	-7	GLY	-	EXPRESSION TAG	UNP P0ABD8
D	-6	LEU	-	EXPRESSION TAG	UNP P0ABD8
D	-5	VAL	-	EXPRESSION TAG	UNP P0ABD8
D	-4	PRO	-	EXPRESSION TAG	UNP P0ABD8
D	-3	ARG	-	EXPRESSION TAG	UNP P0ABD8
D	-2	GLY	-	EXPRESSION TAG	UNP P0ABD8
D	-1	SER	-	EXPRESSION TAG	UNP P0ABD8
D	0	HIS	-	EXPRESSION TAG	UNP P0ABD8
G	-19	MET	-	EXPRESSION TAG	UNP P0ABD8
G	-18	GLY	-	EXPRESSION TAG	UNP P0ABD8
G	-17	SER	-	EXPRESSION TAG	UNP P0ABD8
G	-16	SER	-	EXPRESSION TAG	UNP P0ABD8
G	-15	HIS	-	EXPRESSION TAG	UNP P0ABD8
G	-14	HIS	-	EXPRESSION TAG	UNP P0ABD8
G	-13	HIS	-	EXPRESSION TAG	UNP P0ABD8
G	-12	HIS	-	EXPRESSION TAG	UNP P0ABD8
G	-11	HIS	-	EXPRESSION TAG	UNP P0ABD8
G	-10	HIS	-	EXPRESSION TAG	UNP P0ABD8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	SER	-	EXPRESSION TAG	UNP P0ABD8
G	-8	SER	-	EXPRESSION TAG	UNP P0ABD8
G	-7	GLY	-	EXPRESSION TAG	UNP P0ABD8
G	-6	LEU	-	EXPRESSION TAG	UNP P0ABD8
G	-5	VAL	-	EXPRESSION TAG	UNP P0ABD8
G	-4	PRO	-	EXPRESSION TAG	UNP P0ABD8
G	-3	ARG	-	EXPRESSION TAG	UNP P0ABD8
G	-2	GLY	-	EXPRESSION TAG	UNP P0ABD8
G	-1	SER	-	EXPRESSION TAG	UNP P0ABD8
G	0	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-19	MET	-	EXPRESSION TAG	UNP P0ABD8
I	-18	GLY	-	EXPRESSION TAG	UNP P0ABD8
I	-17	SER	-	EXPRESSION TAG	UNP P0ABD8
I	-16	SER	-	EXPRESSION TAG	UNP P0ABD8
I	-15	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-14	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-13	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-12	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-11	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-10	HIS	-	EXPRESSION TAG	UNP P0ABD8
I	-9	SER	-	EXPRESSION TAG	UNP P0ABD8
I	-8	SER	-	EXPRESSION TAG	UNP P0ABD8
I	-7	GLY	-	EXPRESSION TAG	UNP P0ABD8
I	-6	LEU	-	EXPRESSION TAG	UNP P0ABD8
I	-5	VAL	-	EXPRESSION TAG	UNP P0ABD8
I	-4	PRO	-	EXPRESSION TAG	UNP P0ABD8
I	-3	ARG	-	EXPRESSION TAG	UNP P0ABD8
I	-2	GLY	-	EXPRESSION TAG	UNP P0ABD8
I	-1	SER	-	EXPRESSION TAG	UNP P0ABD8
I	0	HIS	-	EXPRESSION TAG	UNP P0ABD8

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

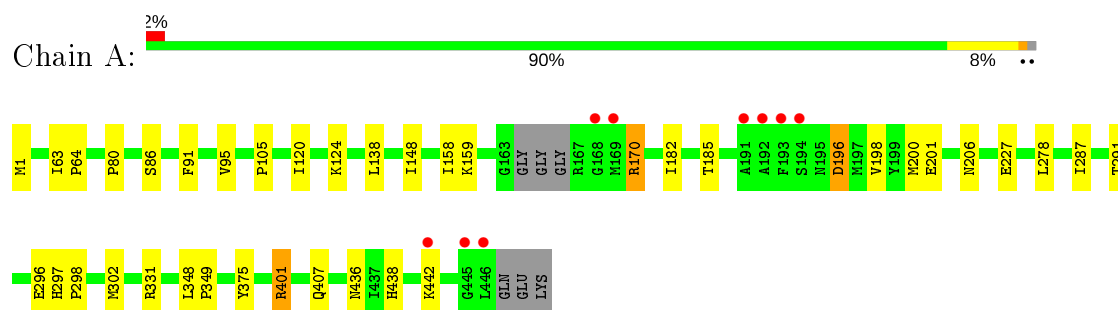
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	22	Total	O	0	0
			22	22		
5	C	96	Total	O	0	0
			96	96		
5	D	6	Total	O	0	0
			6	6		
5	E	116	Total	O	0	0
			116	116		
5	F	77	Total	O	0	0
			77	77		
5	G	8	Total	O	0	0
			8	8		
5	I	9	Total	O	0	0
			9	9		

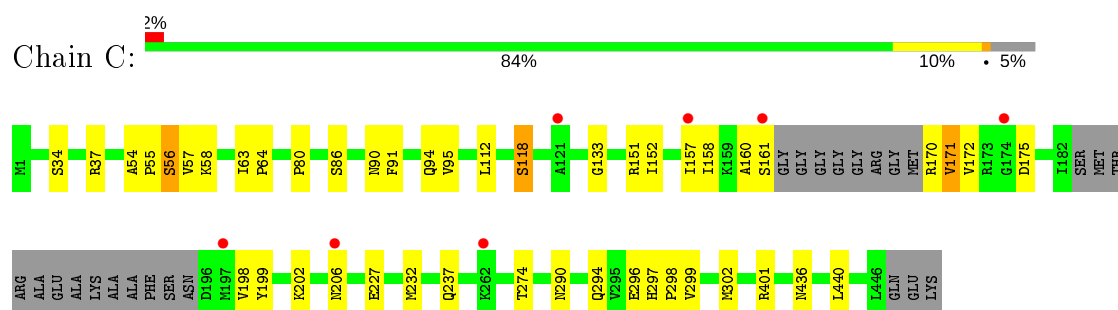
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

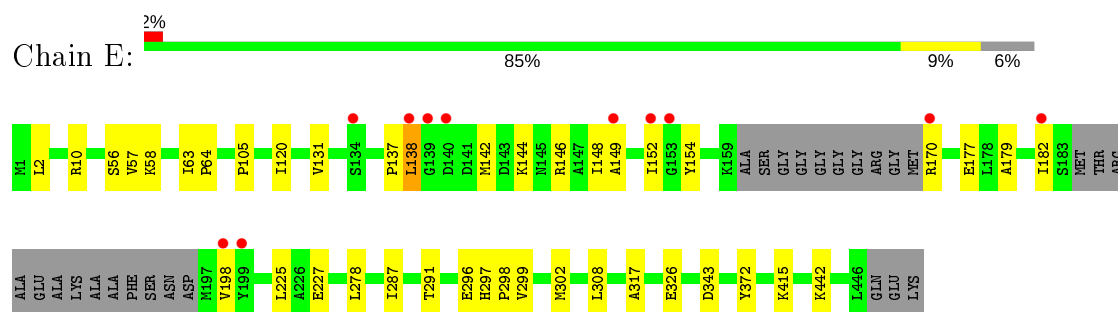
• Molecule 1: Biotin carboxylase



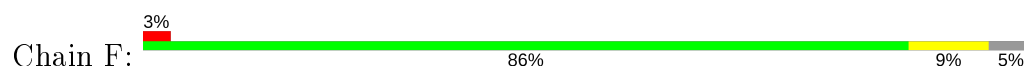
• Molecule 1: Biotin carboxylase

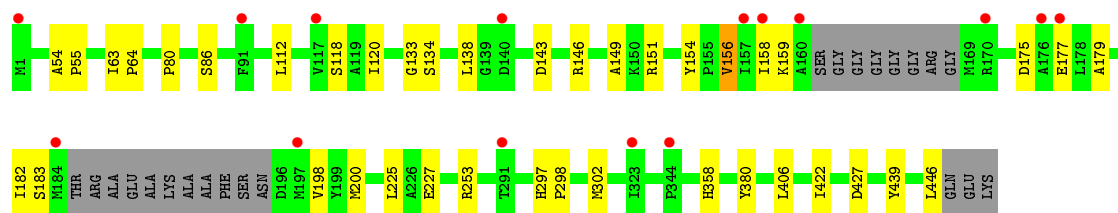


• Molecule 1: Biotin carboxylase

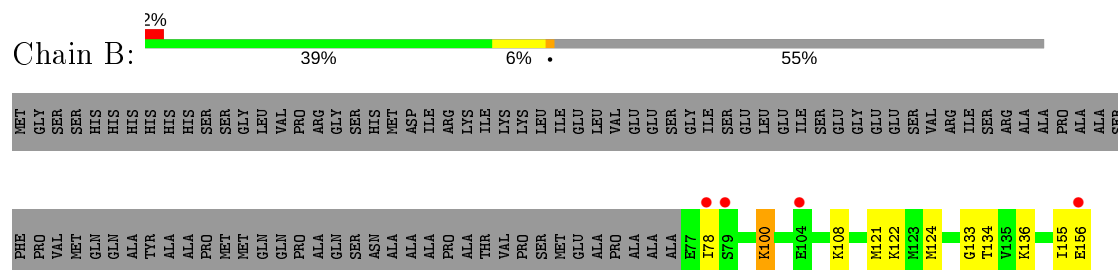


• Molecule 1: Biotin carboxylase

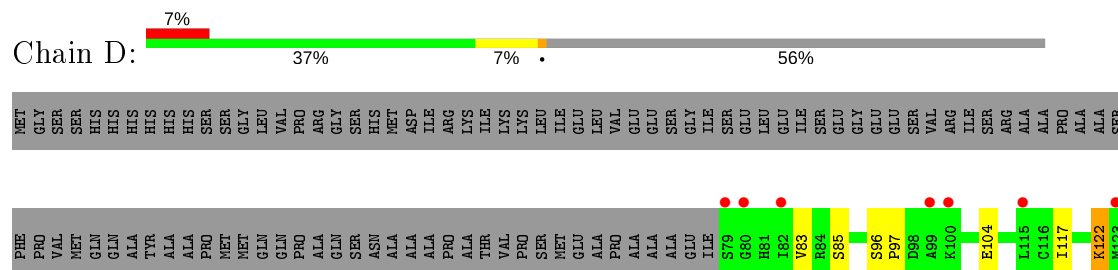




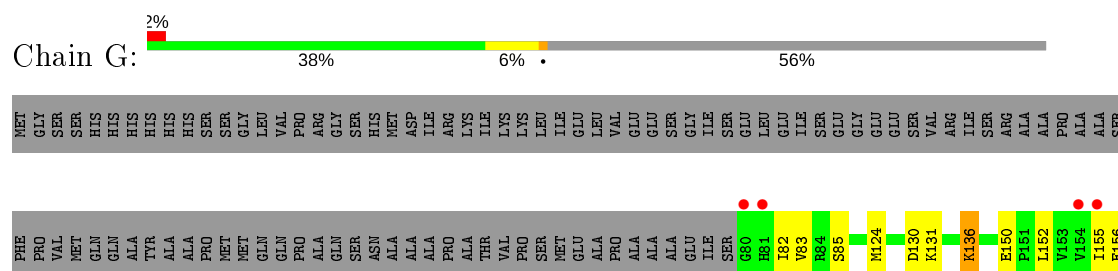
- Molecule 2: Biotin carboxyl carrier protein of acetyl-CoA carboxylase



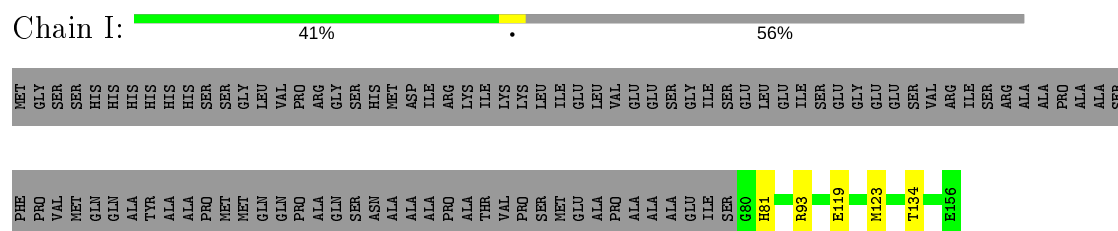
- Molecule 2: Biotin carboxyl carrier protein of acetyl-CoA carboxylase



- Molecule 2: Biotin carboxyl carrier protein of acetyl-CoA carboxylase



- Molecule 2: Biotin carboxyl carrier protein of acetyl-CoA carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.00 Å 96.39 Å 120.57 Å 90.00° 120.15° 90.00°	Depositor
Resolution (Å)	104.26 – 2.50 104.26 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (104.26-2.50) 98.4 (104.26-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.48 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.195 , 0.229 0.213 , 0.242	Depositor DCC
R_{free} test set	3979 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16162	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/3469	0.43	0/4684
1	C	0.23	0/3355	0.42	0/4530
1	E	0.23	0/3363	0.44	0/4540
1	F	0.24	0/3360	0.43	0/4536
2	B	0.23	0/612	0.45	0/827
2	D	0.22	0/590	0.45	0/801
2	G	0.23	0/584	0.45	0/792
2	I	0.22	0/592	0.44	0/801
All	All	0.23	0/15925	0.43	0/21511

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 [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	3408	0	3424	23	0
1	C	3295	0	3324	27	0
1	E	3297	0	3333	28	0
1	F	3301	0	3328	26	0
2	B	603	0	609	4	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	581	0	575	9	0
2	G	575	0	577	11	0
2	I	583	0	592	3	0
3	A	25	0	0	1	0
3	C	10	0	0	1	0
3	E	15	0	0	2	0
3	F	10	0	0	0	0
4	C	4	0	6	0	0
5	A	121	0	0	1	0
5	B	22	0	0	0	0
5	C	96	0	0	0	0
5	D	6	0	0	0	0
5	E	116	0	0	2	0
5	F	77	0	0	0	0
5	G	8	0	0	0	0
5	I	9	0	0	1	0
All	All	16162	0	15768	129	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (129) 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:A:375:TYR:OH	3:A:505:SO4:O1	2.01	0.77
1:F:143:ASP:OD1	1:F:146:ARG:NH2	2.18	0.74
2:I:119:GLU:OE1	5:I:207:HOH:O	2.05	0.74
1:F:227:GLU:OE1	1:F:253:ARG:NH1	2.22	0.73
1:A:401:ARG:NH2	5:A:719:HOH:O	2.27	0.68
1:F:158:ILE:HG23	1:F:198:VAL:HG11	1.76	0.67
1:F:159:LYS:O	1:F:198:VAL:HG13	1.96	0.65
2:B:121:MET:O	2:B:122:LYS:HG2	1.97	0.64
2:G:150:GLU:O	2:G:152:LEU:HD22	1.98	0.63
2:G:85:SER:HB2	2:G:152:LEU:HD21	1.80	0.63
1:E:2:LEU:CD1	1:E:317:ALA:HB2	2.29	0.62
1:E:149:ALA:HB1	1:E:154:TYR:CZ	2.34	0.62
1:C:160:ALA:O	1:C:161:SER:CB	2.49	0.60
1:F:133:GLY:O	1:F:151:ARG:NH2	2.34	0.60
1:C:112:LEU:O	1:C:118:SER:OG	2.21	0.59
2:D:83:VAL:CG1	2:D:153:VAL:HB	2.34	0.57
1:C:133:GLY:O	1:C:151:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:HIS:N	1:C:298:PRO:CD	2.67	0.57
2:G:152:LEU:N	2:G:152:LEU:HD22	2.19	0.57
1:A:297:HIS:N	1:A:298:PRO:CD	2.68	0.57
2:D:117:ILE:HG21	2:D:124:MET:SD	2.44	0.57
1:F:297:HIS:N	1:F:298:PRO:CD	2.68	0.56
1:E:297:HIS:N	1:E:298:PRO:CD	2.69	0.56
2:G:150:GLU:O	2:G:152:LEU:CD2	2.55	0.55
1:C:63:ILE:HB	1:C:64:PRO:HD3	1.88	0.55
2:B:134:THR:O	2:B:156:GLU:N	2.39	0.54
1:A:120:ILE:CG2	1:A:124:LYS:HE3	2.38	0.54
1:E:326:GLU:OE1	1:E:326:GLU:N	2.39	0.54
1:A:438:HIS:O	1:A:442:LYS:HB2	2.06	0.54
1:C:37:ARG:NH2	1:F:380:TYR:OH	2.41	0.54
1:E:142:MET:HG3	1:E:146:ARG:NH1	2.23	0.54
1:F:158:ILE:CG2	1:F:198:VAL:HG11	2.39	0.53
1:A:206:ASN:OD1	1:A:206:ASN:O	2.27	0.53
1:E:138:LEU:HD21	1:E:144:LYS:HB3	1.92	0.52
1:E:179:ALA:O	1:E:182:ILE:HG12	2.10	0.52
1:E:142:MET:CG	1:E:146:ARG:NH1	2.73	0.52
1:E:63:ILE:HB	1:E:64:PRO:HD3	1.91	0.51
1:A:63:ILE:HB	1:A:64:PRO:HD3	1.91	0.51
1:A:138:LEU:HD12	1:A:198:VAL:HG23	1.93	0.50
1:F:179:ALA:O	1:F:182:ILE:HG12	2.11	0.50
1:A:158:ILE:CD1	1:A:182:ILE:HG13	2.41	0.50
1:A:227:GLU:N	1:A:227:GLU:OE1	2.45	0.50
1:C:56:SER:OG	3:C:501:SO4:O4	2.30	0.49
2:D:83:VAL:HG12	2:D:153:VAL:O	2.12	0.49
1:F:134:SER:HB3	1:F:200:MET:HB3	1.94	0.49
1:F:297:HIS:CG	1:F:298:PRO:HD3	2.48	0.49
1:E:148:ILE:CG2	1:E:152:ILE:HD12	2.42	0.49
1:E:225:LEU:HD22	1:E:308:LEU:HD21	1.94	0.49
1:A:348:LEU:HD12	1:A:349:PRO:HD2	1.94	0.49
1:C:157:ILE:HD13	1:C:171:VAL:HG23	1.95	0.49
1:E:278:LEU:HG	1:E:287:ILE:HD11	1.94	0.49
1:E:56:SER:OG	3:E:501:SO4:O4	2.20	0.48
1:E:131:VAL:HG23	5:E:660:HOH:O	2.12	0.48
1:F:158:ILE:HG23	1:F:198:VAL:CG1	2.42	0.48
2:G:85:SER:N	2:G:152:LEU:CD2	2.77	0.48
1:A:159:LYS:NZ	1:A:201:GLU:OE1	2.47	0.48
1:C:227:GLU:N	1:C:227:GLU:OE2	2.47	0.47
2:I:123:MET:HE2	2:I:123:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PRO:HB2	1:F:86:SER:HA	1.97	0.47
1:A:278:LEU:HG	1:A:287:ILE:HD11	1.96	0.47
1:A:206:ASN:OD1	1:A:436:ASN:HB3	2.14	0.46
1:C:57:VAL:HG23	1:C:58:LYS:HG3	1.97	0.46
1:C:296:GLU:O	1:C:299:VAL:HG22	2.14	0.46
1:C:160:ALA:O	1:C:161:SER:HB2	2.16	0.46
1:E:298:PRO:O	1:E:302:MET:HG2	2.15	0.46
1:F:427:ASP:OD1	1:F:439:TYR:OH	2.29	0.46
1:C:297:HIS:CG	1:C:298:PRO:HD3	2.51	0.46
2:D:134:THR:O	2:D:156:GLU:N	2.43	0.46
1:E:177:GLU:O	1:E:177:GLU:HG2	2.15	0.46
1:F:63:ILE:HB	1:F:64:PRO:HD3	1.96	0.46
1:A:206:ASN:C	1:A:206:ASN:OD1	2.54	0.46
1:A:196:ASP:CG	1:A:196:ASP:O	2.53	0.45
1:C:152:ILE:HG23	1:C:202:LYS:HB2	1.98	0.45
1:E:343:ASP:OD2	5:E:680:HOH:O	2.21	0.45
2:D:104:GLU:O	2:D:135:VAL:HG21	2.16	0.45
1:C:34:SER:O	1:C:37:ARG:NH1	2.49	0.45
1:F:406:LEU:HB3	1:F:422:ILE:HD11	1.98	0.45
2:I:81:HIS:CD2	2:I:81:HIS:C	2.89	0.45
1:C:290:ASN:OD1	1:C:294:GLN:NE2	2.50	0.45
1:E:10:ARG:NH2	3:E:503:SO4:O4	2.47	0.45
2:D:96:SER:OG	2:D:97:PRO:HD2	2.17	0.44
1:A:105:PRO:HG3	1:A:291:THR:HB	1.99	0.44
1:E:227:GLU:OE1	1:E:227:GLU:N	2.50	0.44
1:F:179:ALA:O	1:F:182:ILE:CG1	2.66	0.44
1:A:80:PRO:HB2	1:A:86:SER:HA	1.99	0.44
1:A:91:PHE:O	1:A:95:VAL:HG23	2.18	0.43
1:E:297:HIS:CG	1:E:298:PRO:HD3	2.53	0.43
1:F:227:GLU:OE1	1:F:227:GLU:N	2.51	0.43
2:G:83:VAL:HG23	2:G:155:ILE:HD13	2.00	0.43
1:A:170:ARG:HB3	1:A:185:THR:HG21	2.00	0.43
1:A:148:ILE:HG22	1:A:200:MET:CE	2.49	0.43
1:F:154:TYR:CD1	1:F:156:VAL:HG22	2.53	0.43
2:D:85:SER:HB2	2:D:152:LEU:HD11	2.00	0.43
2:D:83:VAL:HG13	2:D:83:VAL:O	2.18	0.43
1:A:298:PRO:O	1:A:302:MET:HG2	2.19	0.43
1:C:206:ASN:CG	1:C:436:ASN:ND2	2.72	0.43
1:E:225:LEU:HD12	1:E:225:LEU:N	2.34	0.43
2:G:130:ASP:OD1	2:G:130:ASP:N	2.52	0.43
1:C:198:VAL:CG1	1:C:199:TYR:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:MET:CE	1:C:440:LEU:HD13	2.49	0.42
2:G:85:SER:N	2:G:152:LEU:HD21	2.35	0.42
1:C:91:PHE:O	1:C:95:VAL:HG23	2.20	0.42
1:C:158:ILE:HD11	1:C:172:VAL:HG21	2.01	0.42
2:G:155:ILE:HG22	2:G:156:GLU:N	2.35	0.42
1:C:158:ILE:HD11	1:C:172:VAL:CG2	2.50	0.41
1:C:54:ALA:HB3	1:C:55:PRO:HD3	2.02	0.41
2:D:122:LYS:C	2:D:122:LYS:HD2	2.41	0.41
1:F:149:ALA:HB1	1:F:154:TYR:CZ	2.56	0.41
1:C:80:PRO:HB2	1:C:86:SER:HA	2.02	0.41
1:A:296:GLU:C	1:A:298:PRO:HD2	2.41	0.41
1:E:372:TYR:HB3	1:F:358:HIS:CE1	2.56	0.41
2:B:155:ILE:O	2:B:156:GLU:OXT	2.39	0.41
1:E:105:PRO:HG3	1:E:291:THR:HB	2.02	0.41
1:E:296:GLU:O	1:E:299:VAL:HG22	2.20	0.41
1:C:90:ASN:OD1	1:C:94:GLN:NE2	2.53	0.41
1:E:137:PRO:HA	1:E:198:VAL:O	2.21	0.41
1:F:298:PRO:O	1:F:302:MET:HG2	2.19	0.41
1:E:57:VAL:HG13	1:E:58:LYS:HG3	2.02	0.40
1:F:112:LEU:HD12	1:F:118:SER:OG	2.21	0.40
1:F:54:ALA:HB3	1:F:55:PRO:HD3	2.03	0.40
1:F:406:LEU:CB	1:F:422:ILE:HD11	2.52	0.40
2:G:136:LYS:HD2	2:G:156:GLU:CB	2.51	0.40
2:B:108:LYS:HD2	2:B:133:GLY:O	2.21	0.40
1:C:298:PRO:O	1:C:302:MET:HG2	2.22	0.40
1:E:148:ILE:HG22	1:E:152:ILE:HD12	2.02	0.40
1:F:182:ILE:HG13	1:F:183:SER:N	2.36	0.40
1:C:274:THR:HG21	1:C:294:GLN:OE1	2.21	0.40
1:E:343:ASP:HB2	1:E:415:LYS:HD3	2.02	0.40
2:G:155:ILE:N	2:G:155:ILE:HD12	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:NZ	2:B:100:LYS:NZ[2_756]	1.80	0.40

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/449 (98%)	422 (96%)	17 (4%)	0	100	100
1	C	419/449 (93%)	404 (96%)	15 (4%)	0	100	100
1	E	420/449 (94%)	405 (96%)	15 (4%)	0	100	100
1	F	421/449 (94%)	407 (97%)	14 (3%)	0	100	100
2	B	78/176 (44%)	77 (99%)	1 (1%)	0	100	100
2	D	76/176 (43%)	75 (99%)	1 (1%)	0	100	100
2	G	75/176 (43%)	74 (99%)	1 (1%)	0	100	100
2	I	75/176 (43%)	74 (99%)	1 (1%)	0	100	100
All	All	2003/2500 (80%)	1938 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/361 (98%)	349 (98%)	6 (2%)	60	82
1	C	347/361 (96%)	340 (98%)	7 (2%)	55	79
1	E	346/361 (96%)	342 (99%)	4 (1%)	71	88
1	F	347/361 (96%)	340 (98%)	7 (2%)	55	79
2	B	67/144 (46%)	63 (94%)	4 (6%)	19	37
2	D	65/144 (45%)	64 (98%)	1 (2%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	64/144 (44%)	60 (94%)	4 (6%)	18	34
2	I	66/144 (46%)	64 (97%)	2 (3%)	41	68
All	All	1657/2020 (82%)	1622 (98%)	35 (2%)	53	78

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	170	ARG
1	A	196	ASP
1	A	331	ARG
1	A	401	ARG
1	A	407	GLN
2	B	78	ILE
2	B	100	LYS
2	B	124	MET
2	B	136	LYS
1	C	56	SER
1	C	118	SER
1	C	170	ARG
1	C	171	VAL
1	C	175	ASP
1	C	237	GLN
1	C	401	ARG
2	D	122	LYS
1	E	120	ILE
1	E	138	LEU
1	E	170	ARG
1	E	442	LYS
1	F	120	ILE
1	F	138	LEU
1	F	156	VAL
1	F	175	ASP
1	F	177	GLU
1	F	225	LEU
1	F	446	LEU
2	G	82	ILE
2	G	124	MET
2	G	131	LYS
2	G	136	LYS
2	I	93	ARG

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Mol	Chain	Res	Type
2	I	134	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	A	504	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	E	502	-	4,4,4	0.13	0	6,6,6	0.09	0
4	EDO	C	503	-	3,3,3	0.45	0	2,2,2	0.32	0
3	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	503	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.09	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
4	EDO	C	503	-	-	0/1/1/1	-

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	SO4	1	0
3	A	505	SO4	1	0
3	E	503	SO4	1	0
3	E	501	SO4	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, 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	443/449 (98%)	-0.02	9 (2%) 65 68	13, 28, 62, 322	0
1	C	425/449 (94%)	0.07	7 (1%) 72 74	15, 35, 68, 105	0
1	E	423/449 (94%)	-0.05	11 (2%) 56 59	12, 27, 72, 118	0
1	F	427/449 (95%)	0.25	15 (3%) 44 47	19, 43, 80, 116	0
2	B	80/176 (45%)	0.12	4 (5%) 28 30	15, 29, 64, 95	0
2	D	78/176 (44%)	1.02	12 (15%) 2 1	40, 62, 107, 144	0
2	G	77/176 (43%)	0.44	4 (5%) 27 29	39, 50, 72, 82	0
2	I	77/176 (43%)	0.08	0 100 100	20, 43, 70, 99	0
All	All	2030/2500 (81%)	0.11	62 (3%) 49 52	12, 35, 73, 322	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	LEU	16.2
1	E	138	LEU	5.1
2	G	80	GLY	4.8
1	A	168	GLY	4.7
1	F	158	ILE	4.5
2	D	156	GLU	4.5
1	A	191	ALA	4.2
2	G	155	ILE	4.0
2	D	115	LEU	3.9
1	C	197	MET	3.8
2	D	79	SER	3.8
1	C	206	ASN	3.8
1	E	139	GLY	3.7
1	E	153	GLY	3.7
2	B	156	GLU	3.7
2	D	124	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	197	MET	3.6
1	C	174	GLY	3.5
1	E	152	ILE	3.5
2	B	78	ILE	3.3
2	D	130	ASP	3.2
1	A	445	GLY	3.2
1	A	169	MET	3.2
1	C	121	ALA	3.1
1	F	160	ALA	3.0
1	E	140	ASP	3.0
2	D	100	LYS	3.0
2	D	123	MET	3.0
1	A	192	ALA	3.0
1	A	193	PHE	2.9
2	D	80	GLY	2.8
1	F	157	ILE	2.8
1	F	177	GLU	2.7
2	B	79	SER	2.7
2	B	104	GLU	2.7
1	E	149	ALA	2.6
1	F	91	PHE	2.6
2	G	81	HIS	2.5
1	A	442	LYS	2.5
1	F	140	ASP	2.5
1	C	161	SER	2.5
2	D	82	ILE	2.5
1	E	134	SER	2.4
1	F	117	VAL	2.4
1	F	170	ARG	2.4
2	G	154	VAL	2.4
2	D	154	VAL	2.3
1	F	184	MET	2.3
1	E	170	ARG	2.3
1	C	262	LYS	2.3
1	F	176	ALA	2.2
2	D	99	ALA	2.2
1	F	323	ILE	2.2
1	F	344	PRO	2.2
1	A	194	SER	2.2
1	E	198	VAL	2.1
1	F	1	MET	2.1
1	C	157	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	155	ILE	2.1
1	E	182	ILE	2.1
1	E	199	TYR	2.0
1	F	291	THR	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. 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	B-factors(\AA^2)	Q<0.9
3	SO4	E	503	5/5	0.88	0.56	34,34,35,35	5
3	SO4	F	502	5/5	0.90	0.21	53,53,54,54	0
4	EDO	C	503	4/4	0.92	0.31	38,39,40,40	0
3	SO4	A	504	5/5	0.93	0.23	62,62,63,63	0
3	SO4	A	502	5/5	0.94	0.23	48,49,50,50	0
3	SO4	F	501	5/5	0.94	0.23	45,46,46,46	0
3	SO4	A	505	5/5	0.95	0.44	32,33,34,35	5
3	SO4	E	502	5/5	0.95	0.14	40,40,41,41	0
3	SO4	A	503	5/5	0.96	0.14	52,53,53,53	0
3	SO4	C	502	5/5	0.97	0.10	39,40,40,41	0
3	SO4	C	501	5/5	0.98	0.12	32,32,33,33	0
3	SO4	A	501	5/5	0.99	0.14	20,20,20,21	0
3	SO4	E	501	5/5	0.99	0.13	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.