Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:35 pm BST

PDB ID	:	4C01
Title	:	Complete crystal structure of carboxylesterase Cest-2923 (lp_2923) from Lactobacillus plantarum WCFS1
Authors	:	Benavente, R.; Esteban-Torres, M.; Acebron, I.; de las Rivas, B.; Munoz, R.; Alvarez, Y.; Mancheno, J.M.
Deposited on	:	2013-07-30
Resolution	:	2.30 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:

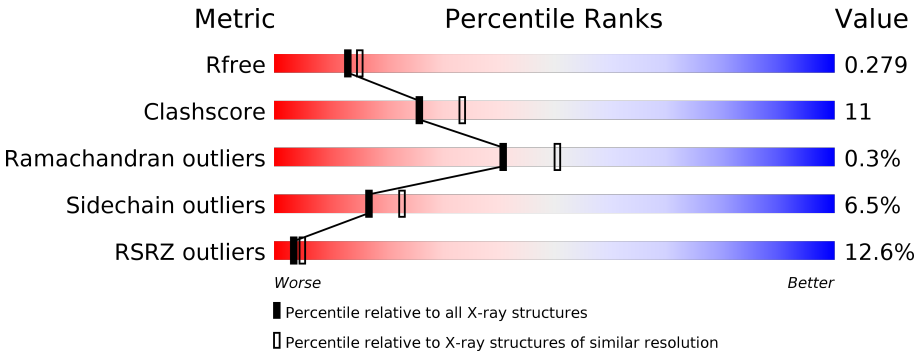
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	282	12% 71% 25%
1	B	282	14% 78% 19%
1	C	282	12% 78% 19%
1	D	282	10% 74% 22%
1	E	282	13% 76% 20%
1	F	282	12% 71% 25%

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	1277	-	-	X	-
5	CCN	B	1280	-	-	X	-
5	CCN	D	1279	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14061 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 CEST-2923.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	2	1
			2155	1373	381	393	8			
1	B	276	Total	C	N	O	S	0	1	1
			2144	1367	377	392	8			
1	C	276	Total	C	N	O	S	0	1	1
			2144	1367	377	392	8			
1	D	276	Total	C	N	O	S	0	1	1
			2144	1367	377	392	8			
1	E	276	Total	C	N	O	S	0	2	1
			2155	1373	381	393	8			
1	F	276	Total	C	N	O	S	0	2	1
			2155	1373	381	393	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	HIS	-	expression tag	UNP F9US10
A	278	HIS	-	expression tag	UNP F9US10
A	279	HIS	-	expression tag	UNP F9US10
A	280	HIS	-	expression tag	UNP F9US10
A	281	HIS	-	expression tag	UNP F9US10
A	282	HIS	-	expression tag	UNP F9US10
B	277	HIS	-	expression tag	UNP F9US10
B	278	HIS	-	expression tag	UNP F9US10
B	279	HIS	-	expression tag	UNP F9US10
B	280	HIS	-	expression tag	UNP F9US10
B	281	HIS	-	expression tag	UNP F9US10
B	282	HIS	-	expression tag	UNP F9US10
C	277	HIS	-	expression tag	UNP F9US10
C	278	HIS	-	expression tag	UNP F9US10
C	279	HIS	-	expression tag	UNP F9US10
C	280	HIS	-	expression tag	UNP F9US10
C	281	HIS	-	expression tag	UNP F9US10

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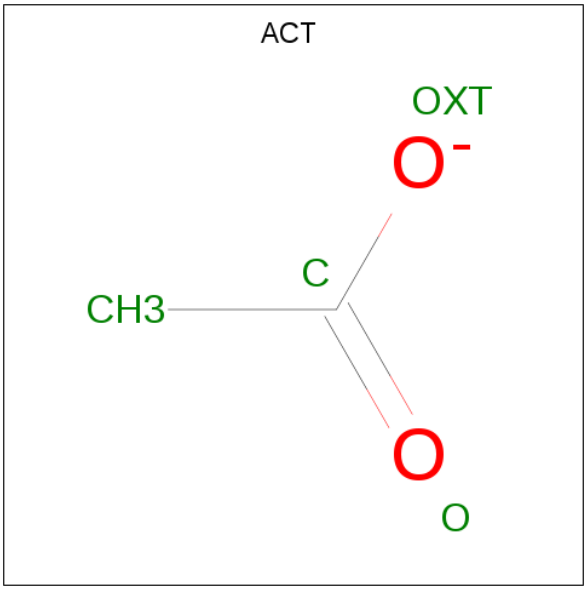
Chain	Residue	Modelled	Actual	Comment	Reference
C	282	HIS	-	expression tag	UNP F9US10
D	277	HIS	-	expression tag	UNP F9US10
D	278	HIS	-	expression tag	UNP F9US10
D	279	HIS	-	expression tag	UNP F9US10
D	280	HIS	-	expression tag	UNP F9US10
D	281	HIS	-	expression tag	UNP F9US10
D	282	HIS	-	expression tag	UNP F9US10
E	277	HIS	-	expression tag	UNP F9US10
E	278	HIS	-	expression tag	UNP F9US10
E	279	HIS	-	expression tag	UNP F9US10
E	280	HIS	-	expression tag	UNP F9US10
E	281	HIS	-	expression tag	UNP F9US10
E	282	HIS	-	expression tag	UNP F9US10
F	277	HIS	-	expression tag	UNP F9US10
F	278	HIS	-	expression tag	UNP F9US10
F	279	HIS	-	expression tag	UNP F9US10
F	280	HIS	-	expression tag	UNP F9US10
F	281	HIS	-	expression tag	UNP F9US10
F	282	HIS	-	expression tag	UNP F9US10

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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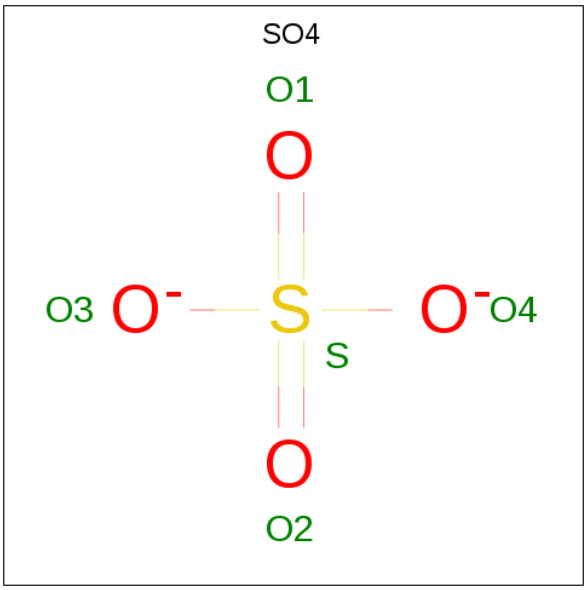
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- 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	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	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

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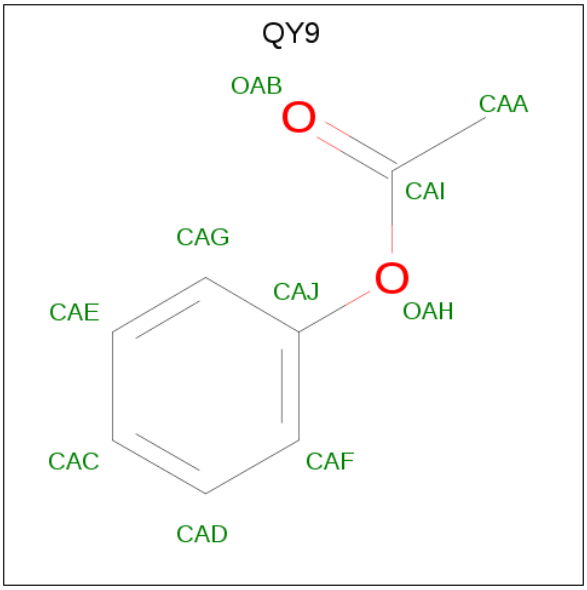
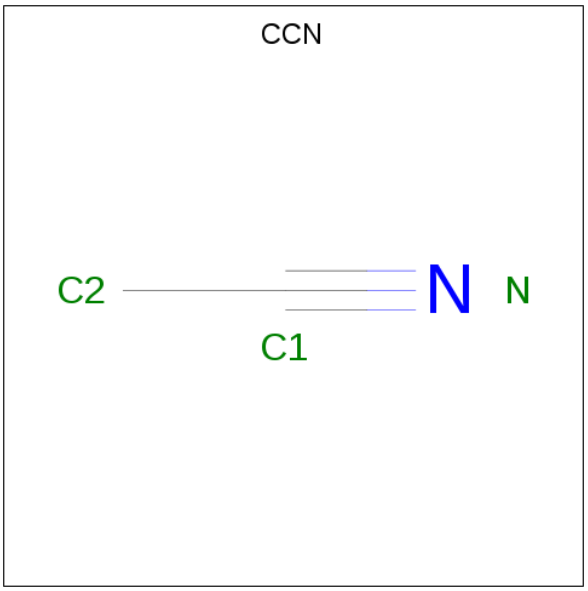
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is phenyl acetate (three-letter code: QY9) (formula: $C_8H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 8 2	0	0
4	B	1	Total C O 10 8 2	0	0
4	C	1	Total C O 10 8 2	0	0
4	E	1	Total C O 10 8 2	0	0
4	F	1	Total C O 10 8 2	0	0

- Molecule 5 is ACETONITRILE (three-letter code: CCN) (formula: C_2H_3N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 3 2 1	0	0
5	A	1	Total C N 3 2 1	0	0
5	A	1	Total C N 3 2 1	0	0
5	B	1	Total C N 3 2 1	0	0
5	B	1	Total C N 3 2 1	0	0
5	C	1	Total C N 3 2 1	0	0
5	D	1	Total C N 3 2 1	0	0
5	D	1	Total C N 3 2 1	0	0
5	E	1	Total C N 3 2 1	0	0
5	F	1	Total C N 3 2 1	0	0
5	F	1	Total C N 3 2 1	0	0
5	F	1	Total C N 3 2 1	0	0

- Molecule 6 is water.

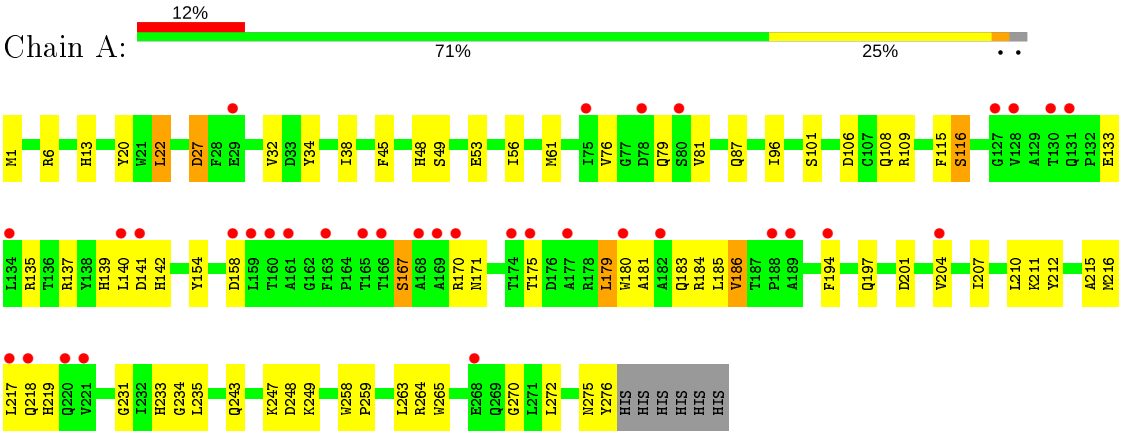
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	193	Total O 193 193	0	0
6	B	182	Total O 182 182	0	0
6	C	191	Total O 191 191	0	0
6	D	137	Total O 137 137	0	0
6	E	152	Total O 152 152	0	0
6	F	159	Total O 159 159	0	0

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.

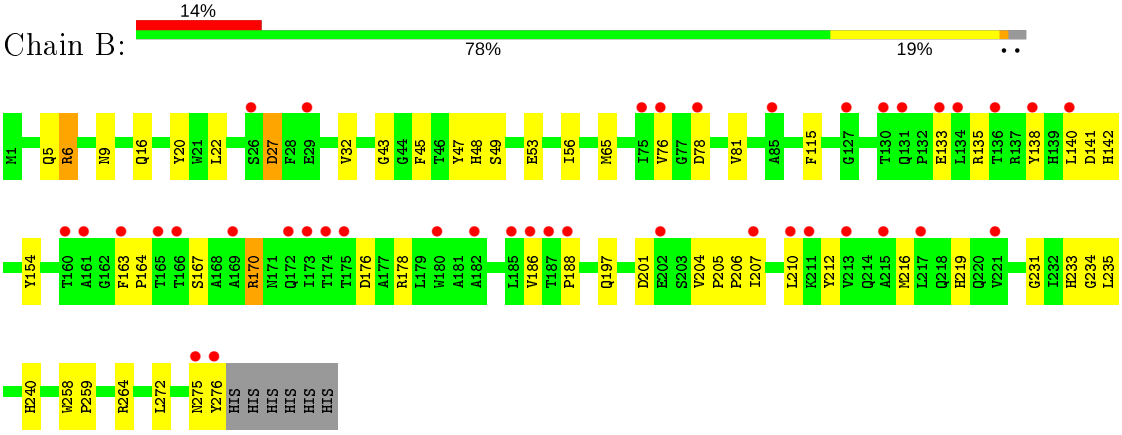
- Molecule 1: CEST-2923

Chain A:



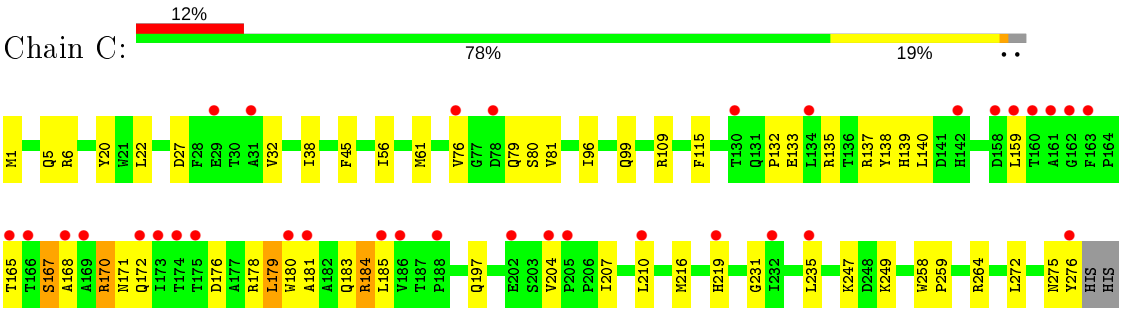
- Molecule 1: CEST-2923

Chain B:

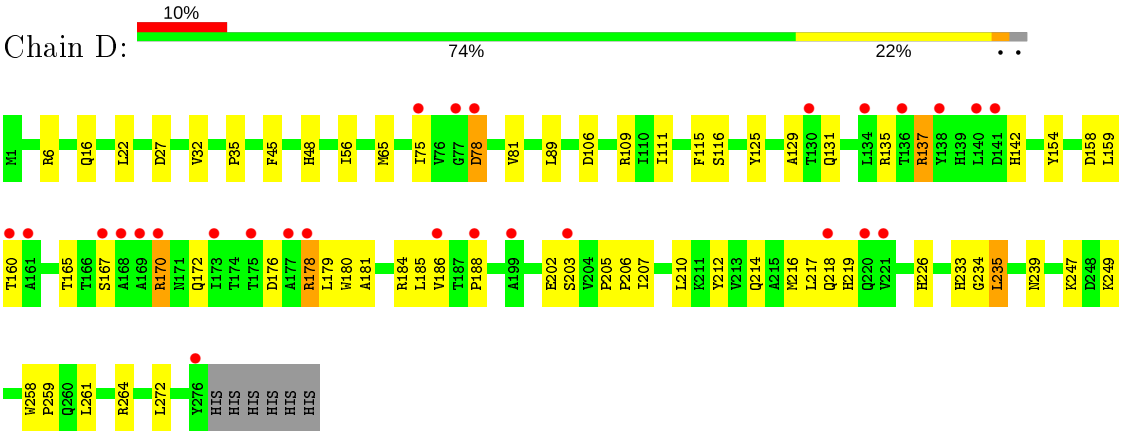


- Molecule 1: CEST-2923

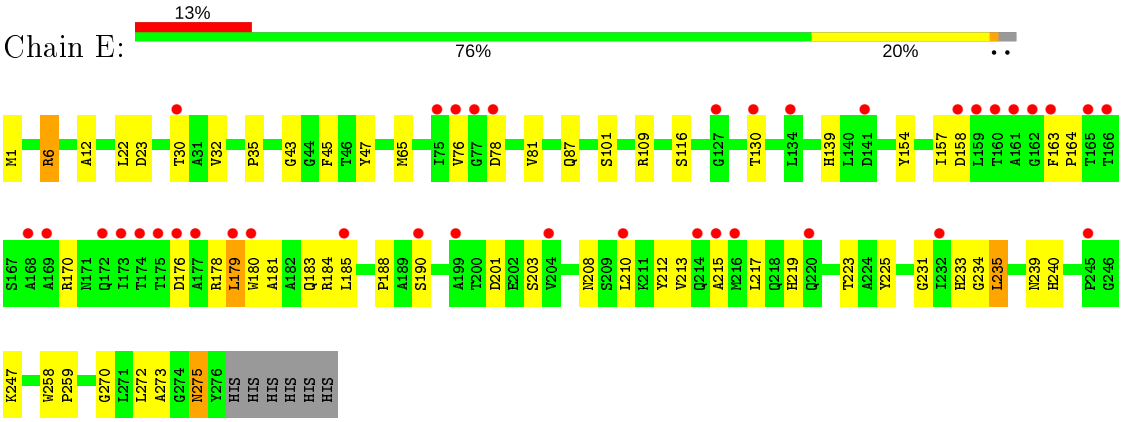
Chain C:



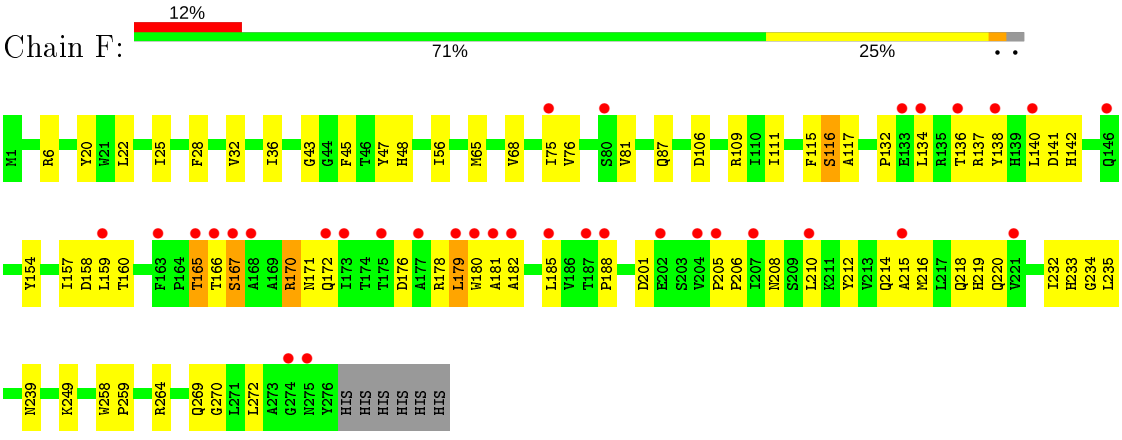
• Molecule 1: CEST-2923



• Molecule 1: CEST-2923



• Molecule 1: CEST-2923



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	244.89Å 141.38Å 82.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.30 49.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.20-2.30) 95.8 (49.20-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	42.72 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.279 0.225 , 0.279	Depositor DCC
R_{free} test set	6266 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.458 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.448 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.449 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.438 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.440 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14061	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: CCN, QY9, SO4, ACT

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	0.43	0/2214	0.59	0/3030
1	B	0.43	0/2203	0.58	0/3016
1	C	0.42	0/2203	0.59	0/3016
1	D	0.43	0/2203	0.57	0/3016
1	E	0.43	0/2214	0.58	0/3030
1	F	0.43	0/2214	0.60	0/3030
All	All	0.43	0/13251	0.59	0/18138

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	2155	0	2103	51	0
1	B	2144	0	2091	39	0
1	C	2144	0	2091	38	0
1	D	2144	0	2091	43	0
1	E	2155	0	2103	49	0
1	F	2155	0	2103	61	0
2	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	3	0	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
3	A	5	0	0	3	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	2	0
3	E	10	0	0	1	0
4	A	10	0	8	0	0
4	B	10	0	8	3	0
4	C	10	0	8	0	0
4	E	10	0	8	0	0
4	F	10	0	8	0	0
5	A	9	0	9	1	0
5	B	6	0	6	2	0
5	C	3	0	3	0	0
5	D	6	0	6	3	0
5	E	3	0	3	0	0
5	F	9	0	9	2	0
6	A	193	0	0	11	0
6	B	182	0	0	10	0
6	C	191	0	0	13	0
6	D	137	0	0	9	0
6	E	152	0	0	11	0
6	F	159	0	0	18	0
All	All	14061	0	12676	271	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (271) 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:170:ARG:NH1	1:A:171:ASN:OD1	2.03	0.90
1:D:178:ARG:HH12	1:D:185:LEU:HD21	1.39	0.88
1:C:167:SER:HA	1:C:170:ARG:HD3	1.57	0.86
1:F:208:ASN:ND2	6:F:2103:HOH:O	2.08	0.85
1:B:78:ASP:OD2	1:C:139:HIS:ND1	2.11	0.81
1:F:167:SER:HA	1:F:170:ARG:HD3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:ASP:O	6:F:2112:HOH:O	1.99	0.78
1:C:20:TYR:HB2	1:C:61:MET:HE1	1.64	0.77
1:F:138:TYR:OH	1:F:178:ARG:NH2	2.18	0.77
1:C:184:ARG:NH1	6:C:2141:HOH:O	2.17	0.75
1:F:181:ALA:O	6:F:2116:HOH:O	2.05	0.74
1:E:213:VAL:O	6:E:2121:HOH:O	2.06	0.73
1:F:178:ARG:O	6:F:2114:HOH:O	2.08	0.71
1:B:9:ASN:H	5:F:1280:CCN:H22	1.55	0.70
1:E:208:ASN:ND2	6:E:2103:HOH:O	2.15	0.70
1:C:247:LYS:HD2	1:C:249:LYS:HE2	1.74	0.69
1:F:182:ALA:O	6:F:2084:HOH:O	2.11	0.69
1:A:247:LYS:HD2	1:A:249:LYS:HE2	1.76	0.68
1:E:188:PRO:O	6:E:2116:HOH:O	2.12	0.68
1:E:179:LEU:HB3	1:E:185:LEU:HD11	1.76	0.67
1:B:138:TYR:OH	1:B:178:ARG:NH2	2.27	0.67
1:A:247:LYS:NZ	3:A:1277:SO4:O3	2.28	0.66
1:A:183:GLN:HG3	1:A:211:LYS:HD2	1.77	0.66
1:B:167:SER:HA	1:B:170:ARG:HD3	1.76	0.66
1:B:186:VAL:HG12	6:B:2141:HOH:O	1.96	0.66
1:C:179:LEU:HB3	1:C:185:LEU:HD11	1.79	0.65
1:C:247:LYS:NZ	6:C:2167:HOH:O	2.29	0.65
1:F:219:HIS:HB2	6:F:2125:HOH:O	1.97	0.65
1:A:217:LEU:C	1:A:219:HIS:H	1.99	0.65
1:F:215:ALA:O	6:F:2125:HOH:O	2.14	0.65
1:C:170:ARG:NH1	1:C:171:ASN:OD1	2.30	0.64
1:A:276:TYR:N	6:A:2192:HOH:O	2.31	0.63
1:F:170:ARG:HB2	1:F:170:ARG:HH11	1.63	0.63
1:D:109:ARG:NH2	3:D:1278:SO4:O1	2.26	0.62
1:B:188:PRO:HD3	1:B:219:HIS:CD2	2.34	0.62
1:E:158:ASP:N	1:E:208:ASN:OD1	2.33	0.62
1:A:215:ALA:O	1:A:219:HIS:HB2	2.00	0.61
1:D:65:MET:HE1	1:D:111:ILE:HD12	1.82	0.61
1:D:188:PRO:HD3	1:D:219:HIS:CD2	2.35	0.61
1:A:247:LYS:NZ	3:A:1277:SO4:S	2.73	0.61
1:A:139:HIS:ND1	1:E:78:ASP:OD2	2.19	0.61
1:A:45:PHE:CD1	1:A:81:VAL:HG21	2.36	0.60
1:B:188:PRO:HD3	1:B:219:HIS:HD2	1.66	0.60
1:F:158:ASP:HA	1:F:181:ALA:HA	1.83	0.60
1:A:48:HIS:H	5:A:1281:CCN:H22	1.66	0.60
1:F:45:PHE:CD1	1:F:81:VAL:HG21	2.37	0.60
1:E:188:PRO:HD3	1:E:219:HIS:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ALA:O	6:E:2122:HOH:O	2.17	0.60
1:A:87:GLN:NE2	1:A:139:HIS:HB2	2.17	0.59
1:E:45:PHE:CD1	1:E:81:VAL:HG21	2.37	0.59
1:F:185:LEU:N	6:F:2116:HOH:O	2.35	0.59
1:E:247:LYS:NZ	3:E:1278:SO4:S	2.75	0.59
1:B:275:ASN:HD22	1:E:239:ASN:HB2	1.66	0.59
1:F:176:ASP:HB3	6:F:2111:HOH:O	2.03	0.59
1:F:109[A]:ARG:NH2	1:F:270:GLY:O	2.35	0.58
1:F:180:TRP:N	6:F:2112:HOH:O	2.36	0.58
1:B:48:HIS:H	5:B:1280:CCN:H21	1.69	0.58
1:B:47:TYR:HB2	5:B:1280:CCN:H21	1.85	0.58
1:A:247:LYS:NZ	3:A:1277:SO4:O2	2.34	0.58
1:C:170:ARG:HB2	1:C:170:ARG:HH11	1.67	0.58
1:C:219:HIS:HB2	6:C:2144:HOH:O	2.04	0.58
1:F:214:GLN:HG2	1:F:218:GLN:OE1	2.05	0.57
1:B:275:ASN:HB3	1:E:240:HIS:H	1.71	0.56
1:D:186:VAL:HG13	6:D:2109:HOH:O	2.04	0.56
1:F:170:ARG:NH1	1:F:171:ASN:OD1	2.38	0.56
1:E:170:ARG:NH2	6:E:2108:HOH:O	2.30	0.56
1:A:186:VAL:HG12	6:A:2146:HOH:O	2.04	0.55
1:E:176:ASP:HB3	6:E:2110:HOH:O	2.06	0.55
1:C:137:ARG:HG2	1:C:138:TYR:CE2	2.41	0.55
1:E:130:THR:HG21	1:E:190:SER:HA	1.89	0.55
1:F:269:GLN:NE2	6:F:2154:HOH:O	2.40	0.55
1:F:176:ASP:OD2	1:F:178:ARG:NH2	2.39	0.55
1:B:45:PHE:CD1	1:B:81:VAL:HG21	2.42	0.55
1:A:116:SER:OG	1:A:233:HIS:NE2	2.40	0.54
1:F:158:ASP:N	1:F:208:ASN:OD1	2.40	0.54
1:D:247:LYS:NZ	3:D:1277:SO4:S	2.79	0.54
1:D:109:ARG:NE	6:D:2080:HOH:O	2.33	0.54
1:D:56:ILE:HD13	1:D:115:PHE:CZ	2.43	0.54
1:D:78:ASP:OD2	1:E:139:HIS:ND1	2.23	0.53
2:C:1276:ACT:H3	6:C:2058:HOH:O	2.07	0.53
6:A:2081:HOH:O	1:D:142:HIS:HB3	2.09	0.53
1:C:45:PHE:CD1	1:C:81:VAL:HG21	2.43	0.53
1:B:5:GLN:NE2	6:B:2015:HOH:O	2.42	0.52
1:F:167:SER:O	1:F:170:ARG:NH1	2.39	0.52
1:C:159:LEU:HD12	1:C:180:TRP:CD1	2.45	0.52
1:B:276:TYR:N	6:B:2181:HOH:O	2.42	0.52
1:A:264:ARG:HD3	6:A:2185:HOH:O	2.10	0.52
1:D:48:HIS:H	5:D:1279:CCN:C2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ASN:ND2	1:E:240:HIS:HD2	2.09	0.51
1:E:43:GLY:HA3	1:E:47:TYR:O	2.10	0.51
1:F:157:ILE:O	1:F:182:ALA:N	2.31	0.51
1:A:167:SER:HB2	1:A:170:ARG:NH2	2.26	0.51
1:D:212:TYR:O	1:D:216:MET:HG2	2.11	0.51
1:C:197:GLN:NE2	1:C:204:VAL:O	2.44	0.50
1:D:176:ASP:HB3	6:D:2101:HOH:O	2.10	0.50
1:C:133:GLU:HG2	6:C:2119:HOH:O	2.12	0.50
1:C:216:MET:HA	6:C:2144:HOH:O	2.11	0.50
1:C:132:PRO:HA	1:C:135:ARG:CB	2.42	0.50
1:C:109:ARG:NE	6:C:2111:HOH:O	2.44	0.50
1:C:176:ASP:OD1	1:C:178:ARG:HB3	2.12	0.50
1:D:159:LEU:N	6:D:2096:HOH:O	2.45	0.50
1:E:12:ALA:H	1:E:87:GLN:NE2	2.09	0.50
1:B:142:HIS:HB3	6:B:2122:HOH:O	2.11	0.49
1:D:45:PHE:CD1	1:D:81:VAL:HG21	2.47	0.49
1:D:75:ILE:HD13	1:D:172:GLN:HB3	1.93	0.49
1:C:20:TYR:CB	1:C:61:MET:HE1	2.39	0.49
1:F:170:ARG:HB2	1:F:170:ARG:NH1	2.27	0.49
1:A:197:GLN:NE2	1:A:204:VAL:O	2.46	0.49
1:E:217:LEU:HG	6:E:2121:HOH:O	2.11	0.49
1:E:188:PRO:HD3	1:E:219:HIS:HD2	1.76	0.49
1:B:56:ILE:HD13	1:B:115:PHE:CZ	2.47	0.49
1:F:56:ILE:HD13	1:F:115:PHE:CZ	2.48	0.49
1:F:48:HIS:H	5:F:1279:CCN:C2	2.25	0.49
1:D:249:LYS:NZ	6:D:2126:HOH:O	2.46	0.48
6:C:2060:HOH:O	1:D:27:ASP:OD1	2.20	0.48
1:A:154:TYR:CE2	1:A:234:GLY:HA2	2.48	0.48
1:F:43:GLY:HA3	1:F:47:TYR:O	2.13	0.48
1:A:217:LEU:O	1:A:219:HIS:N	2.46	0.48
1:E:213:VAL:HG21	1:E:225:TYR:CG	2.49	0.48
1:C:258:TRP:CG	1:C:259:PRO:HD3	2.49	0.48
1:F:136:THR:OG1	1:F:141:ASP:OD2	2.31	0.48
1:F:188:PRO:HD3	1:F:219:HIS:CD2	2.49	0.48
1:B:188:PRO:O	6:B:2142:HOH:O	2.20	0.47
1:E:154:TYR:CE2	1:E:234:GLY:HA2	2.49	0.47
1:D:35:PRO:HB3	1:D:109:ARG:HB3	1.96	0.47
1:F:116:SER:OG	1:F:233:HIS:NE2	2.44	0.47
1:B:275:ASN:ND2	1:E:239:ASN:HB2	2.29	0.47
1:D:205:PRO:HA	1:D:206:PRO:HD3	1.82	0.47
4:B:1278:QY9:HAF	6:B:2030:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:HIS:H	5:D:1279:CCN:H23	1.79	0.47
1:F:75:ILE:HD13	1:F:172:GLN:HB3	1.96	0.47
1:B:197:GLN:NE2	1:B:204:VAL:O	2.47	0.47
1:B:27:ASP:N	1:B:27:ASP:OD1	2.46	0.47
1:E:258:TRP:CG	1:E:259:PRO:HD3	2.50	0.47
1:E:35:PRO:HB3	1:E:109[A]:ARG:HB3	1.97	0.47
1:F:106:ASP:OD2	1:F:109[A]:ARG:HD2	2.15	0.47
1:F:157:ILE:HG23	1:F:182:ALA:HB3	1.96	0.47
1:A:56:ILE:HD13	1:A:115:PHE:CZ	2.49	0.47
1:B:167:SER:O	1:B:170:ARG:NH1	2.46	0.46
1:F:116:SER:HB3	1:F:117:ALA:H	1.57	0.46
1:A:142:HIS:O	6:A:2125:HOH:O	2.21	0.46
1:A:1:MET:HE3	1:F:20:TYR:CD2	2.50	0.46
1:B:49:SER:O	1:B:53:GLU:HG3	2.15	0.46
1:C:275:ASN:OD1	1:D:239:ASN:HB2	2.16	0.46
4:B:1278:QY9:CAG	1:C:99:GLN:HE22	2.29	0.46
1:F:159:LEU:N	1:F:180:TRP:O	2.43	0.46
1:D:258:TRP:CG	1:D:259:PRO:HD3	2.50	0.46
1:B:176:ASP:OD2	1:B:178:ARG:NH2	2.49	0.46
1:C:168:ALA:O	1:C:172:GLN:HG3	2.15	0.46
1:E:1:MET:N	1:E:23:ASP:OD2	2.34	0.46
1:A:217:LEU:C	1:A:219:HIS:N	2.67	0.46
1:D:137:ARG:HH12	1:D:178:ARG:HD2	1.81	0.46
1:A:231:GLY:HA2	6:A:2162:HOH:O	2.16	0.45
1:E:181:ALA:HB1	1:E:183:GLN:OE1	2.17	0.45
1:D:158:ASP:HA	1:D:181:ALA:HA	1.99	0.45
6:C:2085:HOH:O	1:F:142:HIS:HB3	2.15	0.45
1:F:179:LEU:HA	6:F:2115:HOH:O	2.15	0.45
1:A:258:TRP:CG	1:A:259:PRO:HD3	2.51	0.45
1:B:133:GLU:OE2	6:B:2118:HOH:O	2.21	0.45
1:E:163:PHE:HA	1:E:164:PRO:HA	1.79	0.45
1:E:219:HIS:N	6:E:2122:HOH:O	2.48	0.45
1:B:163:PHE:HA	1:B:164:PRO:HA	1.81	0.45
1:D:217:LEU:C	1:D:219:HIS:H	2.20	0.45
1:C:167:SER:O	1:C:170:ARG:HB2	2.17	0.45
1:F:160:THR:N	6:F:2102:HOH:O	2.44	0.45
1:B:43:GLY:HA3	1:B:47:TYR:O	2.16	0.44
1:D:159:LEU:HD12	1:D:180:TRP:CD1	2.52	0.44
1:E:109[A]:ARG:NH2	1:E:270:GLY:O	2.50	0.44
1:F:165:THR:OG1	1:F:166:THR:N	2.50	0.44
1:A:106:ASP:OD2	1:A:109[A]:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:N	1:A:27:ASP:OD1	2.51	0.44
1:B:231:GLY:HA2	6:B:2154:HOH:O	2.16	0.44
1:E:176:ASP:OD2	1:E:178:ARG:NH2	2.35	0.44
1:E:201:ASP:OD1	1:E:233:HIS:HB2	2.17	0.44
1:A:212:TYR:O	1:A:216:MET:HG2	2.18	0.44
1:C:135:ARG:HG3	1:C:140:LEU:HB2	2.00	0.44
1:D:207:ILE:HA	1:D:210:LEU:HB2	2.00	0.44
6:B:2157:HOH:O	1:E:275:ASN:HB2	2.16	0.44
1:E:87:GLN:OE1	1:E:139:HIS:HB2	2.17	0.44
1:F:206:PRO:HD2	6:F:2059:HOH:O	2.16	0.44
1:D:170:ARG:NH2	6:D:2099:HOH:O	2.46	0.44
1:C:276:TYR:N	6:C:2187:HOH:O	2.50	0.44
1:F:212:TYR:O	1:F:216:MET:HG2	2.18	0.44
1:A:194:PHE:HB2	1:A:265:TRP:CE3	2.53	0.44
1:B:201:ASP:OD1	1:B:233:HIS:HB2	2.18	0.44
1:C:79:GLN:HG3	6:C:2084:HOH:O	2.17	0.44
1:E:231:GLY:HA2	6:E:2127:HOH:O	2.17	0.44
1:C:5:GLN:NE2	6:C:2013:HOH:O	2.51	0.43
1:D:226:HIS:CE1	1:D:261:LEU:HD13	2.53	0.43
1:F:134:LEU:O	1:F:138:TYR:HD2	2.01	0.43
1:C:132:PRO:HA	1:C:135:ARG:HB2	2.00	0.43
1:F:220:GLN:N	1:F:220:GLN:OE1	2.51	0.43
1:F:36:ILE:HD11	1:F:68:VAL:HG23	1.99	0.43
1:F:87:GLN:HA	1:F:140:LEU:CD2	2.48	0.43
4:B:1278:QY9:HAG	1:C:99:GLN:HE22	1.82	0.43
1:A:38:ILE:HD11	1:A:96:ILE:HD12	2.01	0.43
1:D:129:ALA:O	6:D:2085:HOH:O	2.21	0.43
1:B:154:TYR:CE1	1:B:234:GLY:HA2	2.53	0.43
1:C:132:PRO:HA	1:C:135:ARG:HB3	2.01	0.43
1:B:240:HIS:CD2	1:E:273:ALA:HB3	2.54	0.43
6:D:2012:HOH:O	1:E:6:ARG:NH1	2.36	0.43
1:E:223:THR:HG21	6:E:2121:HOH:O	2.17	0.43
1:F:154:TYR:CZ	1:F:234:GLY:HA2	2.53	0.43
1:F:132:PRO:HD3	6:F:2086:HOH:O	2.19	0.43
1:A:201:ASP:OD1	1:A:233:HIS:HB2	2.19	0.43
1:A:133:GLU:HG2	6:A:2116:HOH:O	2.18	0.43
1:B:212:TYR:O	1:B:216:MET:HG2	2.19	0.43
1:C:56:ILE:HD13	1:C:115:PHE:CZ	2.54	0.43
1:F:201:ASP:OD1	1:F:233:HIS:HB2	2.19	0.43
1:A:109[A]:ARG:NH2	1:A:270:GLY:O	2.52	0.42
1:B:135:ARG:HG2	1:B:141:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ARG:NH1	1:D:185:LEU:HD21	2.19	0.42
1:A:13:HIS:HE1	1:A:79:GLN:OE1	2.01	0.42
1:E:158:ASP:HA	1:E:180:TRP:O	2.20	0.42
1:F:159:LEU:N	6:F:2102:HOH:O	2.52	0.42
1:A:135:ARG:HG2	1:A:141:ASP:OD1	2.20	0.42
1:C:38:ILE:HD11	1:C:96:ILE:HD12	2.01	0.42
1:F:205:PRO:HA	1:F:206:PRO:HD3	1.75	0.42
1:A:175:THR:HG23	6:A:2086:HOH:O	2.19	0.42
1:D:154:TYR:CE2	1:D:234:GLY:HA2	2.54	0.42
1:F:178:ARG:HB2	1:F:178:ARG:HE	1.47	0.42
1:C:27:ASP:N	1:C:27:ASP:OD1	2.53	0.42
1:E:12:ALA:H	1:E:87:GLN:HE21	1.67	0.42
1:E:158:ASP:HA	1:E:181:ALA:HA	2.02	0.42
1:F:216:MET:HA	6:F:2125:HOH:O	2.19	0.42
1:A:137:ARG:NH2	6:A:2123:HOH:O	2.53	0.42
1:A:20:TYR:CB	1:A:61:MET:HE1	2.49	0.42
1:D:116:SER:OG	1:D:233:HIS:NE2	2.42	0.42
1:A:259:PRO:O	1:A:263:LEU:HG	2.20	0.41
1:F:154:TYR:CE2	1:F:234:GLY:HA2	2.55	0.41
1:B:258:TRP:CG	1:B:259:PRO:HD3	2.55	0.41
1:E:116:SER:OG	1:E:233:HIS:NE2	2.47	0.41
1:E:157:ILE:HG21	1:E:212:TYR:HB2	2.01	0.41
1:A:20:TYR:HB2	1:A:61:MET:HE1	2.02	0.41
1:D:202:GLU:HB2	5:D:1280:CCN:C1	2.50	0.41
1:D:131:GLN:O	1:D:135:ARG:N	2.49	0.41
1:E:235:LEU:HD12	1:E:235:LEU:HA	1.83	0.41
1:F:137:ARG:HD2	1:F:138:TYR:CE2	2.56	0.41
1:B:205:PRO:HA	1:B:206:PRO:HD3	1.88	0.41
1:C:181:ALA:HB1	1:C:183:GLN:OE1	2.20	0.41
1:A:181:ALA:HB1	1:A:183:GLN:OE1	2.20	0.41
1:D:158:ASP:OD1	1:D:160:THR:OG1	2.25	0.41
1:D:188:PRO:HD3	1:D:219:HIS:HD2	1.82	0.41
1:F:258:TRP:CG	1:F:259:PRO:HD3	2.55	0.41
1:A:22:LEU:HD23	1:A:34:TYR:CG	2.56	0.41
1:D:184:ARG:NH2	6:D:2106:HOH:O	2.25	0.41
1:D:235:LEU:HD12	1:D:235:LEU:HA	1.96	0.41
1:E:219:HIS:HB2	6:E:2122:HOH:O	2.20	0.41
1:E:154:TYR:CZ	1:E:234:GLY:HA2	2.56	0.41
1:A:108:GLN:NE2	6:A:2107:HOH:O	2.53	0.41
1:B:135:ARG:HG3	1:B:140:LEU:HB2	2.02	0.41
1:A:158:ASP:HA	1:A:180:TRP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:PRO:HB3	1:E:219:HIS:HB3	2.02	0.41
1:F:142:HIS:O	6:F:2094:HOH:O	2.22	0.41
1:A:135:ARG:HG3	1:A:140:LEU:HB2	2.03	0.41
1:B:6:ARG:HG3	6:B:2010:HOH:O	2.20	0.41
1:A:275:ASN:OD1	1:F:239:ASN:HB2	2.21	0.41
1:C:167:SER:O	1:C:170:ARG:NH1	2.52	0.41
1:F:232:ILE:HD13	1:F:249:LYS:HG3	2.03	0.41
1:F:25:ILE:HD12	1:F:28:PHE:CZ	2.56	0.40
1:A:179:LEU:HB3	1:A:185:LEU:HD11	2.02	0.40
1:A:243:GLN:OE1	6:A:2171:HOH:O	2.22	0.40
1:D:106:ASP:OD2	1:D:109:ARG:HD2	2.21	0.40
1:D:170:ARG:HG3	1:D:170:ARG:H	1.70	0.40
1:B:20:TYR:CD2	1:E:1:MET:HE3	2.56	0.40
1:D:89:LEU:HD13	1:D:125:TYR:CG	2.57	0.40
1:A:183:GLN:O	1:A:186:VAL:HG23	2.21	0.40
1:A:49:SER:O	1:A:53:GLU:HG3	2.22	0.40
1:B:178:ARG:HB2	1:B:178:ARG:HE	1.69	0.40
1:C:231:GLY:HA2	6:C:2157:HOH:O	2.21	0.40
1:F:65:MET:HE1	1:F:111:ILE:HD12	2.03	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	276/282 (98%)	255 (92%)	20 (7%)	1 (0%)	34 42
1	B	275/282 (98%)	254 (92%)	21 (8%)	0	100 100
1	C	275/282 (98%)	251 (91%)	23 (8%)	1 (0%)	34 42
1	D	275/282 (98%)	254 (92%)	19 (7%)	2 (1%)	22 26
1	E	276/282 (98%)	256 (93%)	20 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	276/282 (98%)	255 (92%)	20 (7%)	1 (0%)	34 42
All	All	1653/1692 (98%)	1525 (92%)	123 (7%)	5 (0%)	41 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	D	165	THR
1	C	165	THR
1	D	218	GLN
1	F	165	THR

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	221/226 (98%)	205 (93%)	16 (7%)	14 18
1	B	220/226 (97%)	207 (94%)	13 (6%)	19 27
1	C	220/226 (97%)	204 (93%)	16 (7%)	14 18
1	D	220/226 (97%)	205 (93%)	15 (7%)	16 21
1	E	221/226 (98%)	207 (94%)	14 (6%)	18 24
1	F	221/226 (98%)	209 (95%)	12 (5%)	22 30
All	All	1323/1356 (98%)	1237 (94%)	86 (6%)	17 23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	22	LEU
1	A	27	ASP
1	A	32	VAL
1	A	76	VAL
1	A	101	SER

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Mol	Chain	Res	Type
1	A	116	SER
1	A	167	SER
1	A	179	LEU
1	A	184	ARG
1	A	186	VAL
1	A	207	ILE
1	A	210	LEU
1	A	235	LEU
1	A	248	ASP
1	A	272	LEU
1	B	6	ARG
1	B	16	GLN
1	B	22	LEU
1	B	27	ASP
1	B	32	VAL
1	B	65	MET
1	B	76	VAL
1	B	170	ARG
1	B	207	ILE
1	B	210	LEU
1	B	235	LEU
1	B	264	ARG
1	B	272	LEU
1	C	1	MET
1	C	6	ARG
1	C	22	LEU
1	C	32	VAL
1	C	76	VAL
1	C	80[A]	SER
1	C	80[B]	SER
1	C	167	SER
1	C	170	ARG
1	C	179	LEU
1	C	184	ARG
1	C	207	ILE
1	C	210	LEU
1	C	235	LEU
1	C	264	ARG
1	C	272	LEU
1	D	6	ARG
1	D	16	GLN
1	D	22	LEU

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Mol	Chain	Res	Type
1	D	32	VAL
1	D	78	ASP
1	D	137	ARG
1	D	167	SER
1	D	170	ARG
1	D	178	ARG
1	D	179	LEU
1	D	203	SER
1	D	214	GLN
1	D	235	LEU
1	D	264	ARG
1	D	272	LEU
1	E	6	ARG
1	E	22	LEU
1	E	30	THR
1	E	32	VAL
1	E	65	MET
1	E	76	VAL
1	E	101	SER
1	E	179	LEU
1	E	184	ARG
1	E	203	SER
1	E	210	LEU
1	E	235	LEU
1	E	272	LEU
1	E	275	ASN
1	F	6	ARG
1	F	22	LEU
1	F	32	VAL
1	F	76	VAL
1	F	116	SER
1	F	167	SER
1	F	170	ARG
1	F	179	LEU
1	F	210	LEU
1	F	235	LEU
1	F	264	ARG
1	F	272	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	GLN
1	E	226	HIS
1	E	240	HIS
1	F	275	ASN

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

31 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	$\#\|Z\| > 2$
5	CCN	A	1281	-	2,2,2	0.70	0	1,1,1	0.62	0
2	ACT	F	1276	-	1,3,3	1.31	0	0,3,3	0.00	-
2	ACT	D	1276	-	1,3,3	0.87	0	0,3,3	0.00	-
5	CCN	D	1280	-	2,2,2	0.69	0	1,1,1	0.54	0
5	CCN	D	1279	-	2,2,2	0.69	0	1,1,1	0.60	0
3	SO4	C	1278	-	4,4,4	0.14	0	6,6,6	0.13	0
5	CCN	A	1279	-	2,2,2	0.66	0	1,1,1	0.61	0
5	CCN	F	1279	-	2,2,2	0.75	0	1,1,1	0.57	0
4	QY9	E	1279	-	10,10,10	0.64	0	12,12,12	1.28	1 (8%)
3	SO4	E	1277	-	4,4,4	0.18	0	6,6,6	0.34	0
2	ACT	C	1276	-	1,3,3	0.85	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CCN	B	1279	-	2,2,2	0.64	0	1,1,1	0.60	0
3	SO4	B	1277	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	D	1278	-	4,4,4	0.15	0	6,6,6	0.11	0
4	QY9	A	1278	-	10,10,10	0.65	0	12,12,12	1.46	1 (8%)
2	ACT	A	1276	-	1,3,3	1.30	0	0,3,3	0.00	-
5	CCN	F	1280	-	2,2,2	0.79	0	1,1,1	0.51	0
3	SO4	D	1277	-	4,4,4	0.12	0	6,6,6	0.13	0
2	ACT	B	1276	-	1,3,3	1.54	0	0,3,3	0.00	-
5	CCN	B	1280	-	2,2,2	0.68	0	1,1,1	0.60	0
5	CCN	A	1280	-	2,2,2	0.75	0	1,1,1	0.58	0
4	QY9	B	1278	-	10,10,10	0.61	0	12,12,12	1.26	1 (8%)
5	CCN	E	1280	-	2,2,2	0.62	0	1,1,1	0.55	0
4	QY9	C	1279	-	10,10,10	0.62	0	12,12,12	1.29	1 (8%)
5	CCN	F	1278	-	2,2,2	0.64	0	1,1,1	0.57	0
4	QY9	F	1277	-	10,10,10	0.62	0	12,12,12	1.34	1 (8%)
3	SO4	E	1278	-	4,4,4	0.17	0	6,6,6	0.15	0
2	ACT	E	1276	-	1,3,3	1.37	0	0,3,3	0.00	-
5	CCN	C	1280	-	2,2,2	0.72	0	1,1,1	0.60	0
3	SO4	A	1277	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	C	1277	-	4,4,4	0.21	0	6,6,6	0.29	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	QY9	E	1279	-	-	2/4/4/4	0/1/1/1
4	QY9	C	1279	-	-	0/4/4/4	0/1/1/1
4	QY9	B	1278	-	-	2/4/4/4	0/1/1/1
4	QY9	F	1277	-	-	2/4/4/4	0/1/1/1
4	QY9	A	1278	-	-	4/4/4/4	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1278	QY9	OAH-CAI-CAA	4.31	120.54	110.98
4	F	1277	QY9	OAH-CAI-CAA	3.98	119.81	110.98
4	C	1279	QY9	OAH-CAI-CAA	3.95	119.74	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1279	QY9	OAH-CAI-CAA	3.66	119.10	110.98
4	B	1278	QY9	OAH-CAI-CAA	3.50	118.74	110.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1279	QY9	CAA-CAI-OAH-CAJ
4	E	1279	QY9	OAB-CAI-OAH-CAJ
4	A	1278	QY9	OAB-CAI-OAH-CAJ
4	B	1278	QY9	CAA-CAI-OAH-CAJ
4	F	1277	QY9	CAA-CAI-OAH-CAJ
4	A	1278	QY9	CAA-CAI-OAH-CAJ
4	F	1277	QY9	OAB-CAI-OAH-CAJ
4	B	1278	QY9	OAB-CAI-OAH-CAJ
4	A	1278	QY9	CAF-CAJ-OAH-CAI
4	A	1278	QY9	CAG-CAJ-OAH-CAI

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1281	CCN	1	0
5	D	1280	CCN	1	0
5	D	1279	CCN	2	0
5	F	1279	CCN	1	0
2	C	1276	ACT	1	0
3	D	1278	SO4	1	0
5	F	1280	CCN	1	0
3	D	1277	SO4	1	0
5	B	1280	CCN	2	0
4	B	1278	QY9	3	0
3	E	1278	SO4	1	0
3	A	1277	SO4	3	0

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, 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	276/282 (97%)	0.91	35 (12%) 3 5	14, 37, 72, 95	0
1	B	276/282 (97%)	0.96	40 (14%) 2 3	13, 37, 74, 104	0
1	C	276/282 (97%)	0.85	34 (12%) 4 6	13, 38, 73, 101	0
1	D	276/282 (97%)	0.81	27 (9%) 7 10	14, 36, 73, 105	0
1	E	276/282 (97%)	0.90	38 (13%) 2 4	14, 38, 75, 91	0
1	F	276/282 (97%)	0.83	34 (12%) 4 6	15, 37, 71, 87	0
All	All	1656/1692 (97%)	0.88	208 (12%) 3 5	13, 37, 73, 105	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	TYR	9.4
1	A	175	THR	6.1
1	B	161	ALA	5.7
1	F	168	ALA	5.3
1	E	172	GLN	4.9
1	C	159	LEU	4.9
1	E	175	THR	4.6
1	B	160	THR	4.6
1	B	140	LEU	4.6
1	F	159	LEU	4.5
1	C	31	ALA	4.4
1	A	188	PRO	4.1
1	E	168	ALA	4.1
1	A	204	VAL	4.0
1	F	134	LEU	4.0
1	C	202	GLU	3.9
1	C	180	TRP	3.8
1	F	204	VAL	3.7
1	D	173	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	166	THR	3.6
1	B	76	VAL	3.6
1	C	210	LEU	3.6
1	C	134	LEU	3.6
1	D	161	ALA	3.5
1	B	29	GLU	3.5
1	D	188	PRO	3.5
1	E	161	ALA	3.4
1	F	205	PRO	3.4
1	A	128	VAL	3.4
1	E	180	TRP	3.3
1	A	80[A]	SER	3.3
1	D	175	THR	3.3
1	E	141	ASP	3.3
1	C	175	THR	3.3
1	B	136	THR	3.3
1	D	140	LEU	3.3
1	E	30	THR	3.3
1	A	134	LEU	3.2
1	B	134	LEU	3.2
1	F	80[A]	SER	3.2
1	A	168	ALA	3.2
1	E	169	ALA	3.2
1	A	189	ALA	3.2
1	E	173	ILE	3.1
1	B	78	ASP	3.1
1	C	165	THR	3.1
1	E	78	ASP	3.1
1	E	159	LEU	3.1
1	F	75	ILE	3.1
1	C	204	VAL	3.1
1	D	78	ASP	3.1
1	E	166	THR	3.0
1	D	75	ILE	3.0
1	E	163	PHE	3.0
1	F	133	GLU	3.0
1	F	138	TYR	3.0
1	D	177	ALA	3.0
1	A	160	THR	3.0
1	B	166	THR	3.0
1	C	172	GLN	3.0
1	F	221	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	175	THR	3.0
1	D	170	ARG	3.0
1	D	220	GLN	2.9
1	B	180	TRP	2.9
1	E	160	THR	2.9
1	A	161	ALA	2.9
1	C	168	ALA	2.9
1	D	276	TYR	2.9
1	D	136	THR	2.9
1	B	221	VAL	2.9
1	C	186	VAL	2.9
1	A	75	ILE	2.8
1	E	204	VAL	2.8
1	B	182	ALA	2.8
1	F	180	TRP	2.8
1	C	174	THR	2.8
1	D	186	VAL	2.8
1	D	218	GLN	2.8
1	B	275	ASN	2.8
1	E	158	ASP	2.8
1	E	130	THR	2.8
1	F	163	PHE	2.8
1	D	168	ALA	2.8
1	A	174	THR	2.8
1	E	75	ILE	2.8
1	E	76	VAL	2.7
1	B	130	THR	2.7
1	F	166	THR	2.7
1	D	169	ALA	2.7
1	D	221	VAL	2.7
1	D	160	THR	2.7
1	A	158	ASP	2.7
1	F	177	ALA	2.7
1	B	215	ALA	2.7
1	C	169	ALA	2.7
1	E	174	THR	2.7
1	D	77	GLY	2.7
1	F	188	PRO	2.7
1	A	177	ALA	2.7
1	B	217	LEU	2.7
1	C	76	VAL	2.7
1	F	140	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	162	GLY	2.7
1	D	203	SER	2.7
1	C	173	ILE	2.7
1	A	169	ALA	2.7
1	F	172	GLN	2.7
1	A	29	GLU	2.6
1	B	185	LEU	2.6
1	A	165	THR	2.6
1	C	185	LEU	2.6
1	D	130	THR	2.6
1	A	78	ASP	2.6
1	A	159	LEU	2.6
1	C	205	PRO	2.6
1	D	199	ALA	2.6
1	A	194	PHE	2.6
1	C	161	ALA	2.6
1	F	175	THR	2.5
1	A	166	THR	2.5
1	B	131	GLN	2.5
1	F	185	LEU	2.5
1	F	187	THR	2.5
1	E	190	SER	2.5
1	B	165	THR	2.5
1	F	165	THR	2.5
1	B	213	VAL	2.5
1	F	173	ILE	2.5
1	F	202	GLU	2.5
1	C	158	ASP	2.4
1	F	167	SER	2.4
1	B	188	PRO	2.4
1	C	160	THR	2.4
1	B	75	ILE	2.4
1	E	185	LEU	2.4
1	F	275	ASN	2.4
1	A	180	TRP	2.4
1	B	207	ILE	2.4
1	A	220	GLN	2.4
1	E	177	ALA	2.4
1	F	182	ALA	2.4
1	B	187	THR	2.4
1	C	130	THR	2.4
1	B	172	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	210	LEU	2.4
1	A	221	VAL	2.4
1	F	207	ILE	2.3
1	D	141	ASP	2.3
1	C	219	HIS	2.3
1	E	214	GLN	2.3
1	A	182	ALA	2.3
1	E	199	ALA	2.3
1	B	174	THR	2.3
1	C	142	HIS	2.3
1	C	29	GLU	2.3
1	B	163	PHE	2.3
1	C	78	ASP	2.3
1	B	169	ALA	2.3
1	F	136	THR	2.3
1	B	138	TYR	2.3
1	B	133	GLU	2.3
1	E	245	PRO	2.3
1	B	173	ILE	2.3
1	E	232	ILE	2.3
1	F	215	ALA	2.3
1	A	170	ARG	2.2
1	D	138	TYR	2.2
1	E	220	GLN	2.2
1	E	165	THR	2.2
1	A	140	LEU	2.2
1	F	179	LEU	2.2
1	A	217	LEU	2.2
1	F	146	GLN	2.2
1	F	181	ALA	2.2
1	B	202	GLU	2.2
1	A	130	THR	2.2
1	D	178	ARG	2.2
1	A	141	ASP	2.1
1	D	134	LEU	2.1
1	A	218	GLN	2.1
1	C	188	PRO	2.1
1	F	274	GLY	2.1
1	E	176	ASP	2.1
1	A	268	GLU	2.1
1	C	276	TYR	2.1
1	B	26	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	163	PHE	2.1
1	B	127	GLY	2.1
1	E	127	GLY	2.1
1	B	210	LEU	2.1
1	B	211	LYS	2.1
1	E	134	LEU	2.1
1	E	77	GLY	2.1
1	E	162	GLY	2.1
1	A	131	GLN	2.0
1	C	232	ILE	2.0
1	F	210	LEU	2.0
1	E	215	ALA	2.0
1	D	167	SER	2.0
1	B	186	VAL	2.0
1	A	163	PHE	2.0
1	E	216	MET	2.0
1	A	127	GLY	2.0
1	C	235	LEU	2.0
1	E	179	LEU	2.0
1	B	85	ALA	2.0
1	C	181	ALA	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, 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
4	QY9	A	1278	10/10	0.59	0.33	59,64,71,73	0
3	SO4	C	1278	5/5	0.60	0.27	111,111,113,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	1277	5/5	0.66	0.24	111,111,112,114	0
4	QY9	B	1278	10/10	0.67	0.37	73,77,85,85	0
4	QY9	F	1277	10/10	0.68	0.30	70,74,81,84	0
4	QY9	C	1279	10/10	0.70	0.33	75,78,87,90	0
5	CCN	F	1280	3/3	0.73	0.21	19,19,30,34	0
4	QY9	E	1279	10/10	0.76	0.29	67,72,73,74	0
3	SO4	D	1277	5/5	0.77	0.19	110,110,112,112	0
3	SO4	A	1277	5/5	0.77	0.22	105,106,107,108	0
2	ACT	D	1276	4/4	0.78	0.26	19,27,33,47	0
5	CCN	E	1280	3/3	0.80	0.25	34,34,34,37	0
3	SO4	D	1278	5/5	0.80	0.15	108,109,110,110	0
2	ACT	F	1276	4/4	0.82	0.19	32,35,40,51	0
3	SO4	E	1278	5/5	0.83	0.29	116,119,120,120	0
5	CCN	F	1278	3/3	0.83	0.19	34,34,36,38	0
5	CCN	A	1281	3/3	0.84	0.19	26,26,27,28	0
2	ACT	C	1276	4/4	0.85	0.17	31,39,41,55	0
5	CCN	D	1279	3/3	0.85	0.24	30,30,33,36	0
2	ACT	B	1276	4/4	0.85	0.15	38,39,45,53	0
5	CCN	A	1279	3/3	0.86	0.20	35,35,37,40	0
5	CCN	D	1280	3/3	0.86	0.15	34,34,37,38	0
5	CCN	C	1280	3/3	0.86	0.19	38,38,39,42	0
5	CCN	B	1279	3/3	0.86	0.16	34,34,35,39	0
5	CCN	B	1280	3/3	0.88	0.18	34,34,34,35	0
2	ACT	E	1276	4/4	0.88	0.20	28,31,37,50	0
2	ACT	A	1276	4/4	0.93	0.16	31,32,40,54	0
5	CCN	A	1280	3/3	0.94	0.10	32,32,36,36	0
5	CCN	F	1279	3/3	0.95	0.12	13,13,26,28	0
3	SO4	C	1277	5/5	0.95	0.14	39,40,46,59	0
3	SO4	E	1277	5/5	0.96	0.15	37,44,47,66	0

6.5 Other polymers

There are no such residues in this entry.