



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:23 AM GMT

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 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/ValidationPDFNotes.html>

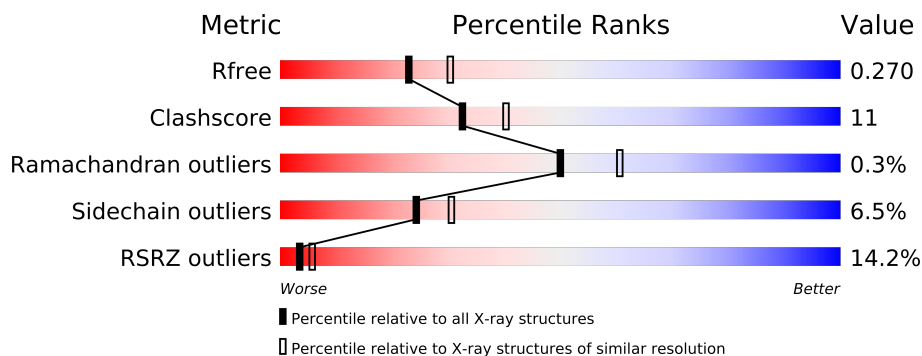
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	
1	E	282	
1	F	282	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	C	1278	-	X
4	QY9	A	1278	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	QY9	B	1278	-	X
4	QY9	C	1279	-	X
4	QY9	E	1279	-	X
4	QY9	F	1277	-	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 hydrogen and 0 are deuterium.

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:

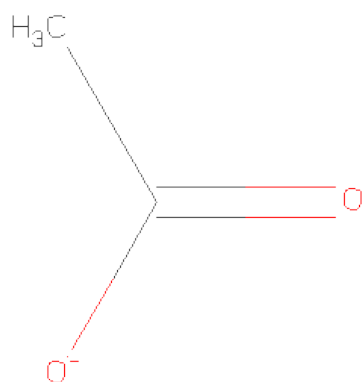
Chain	Residue	Modelled	Actual	Comment	Reference
A	277	HIS	-	EXPRESSION TAG	UNP F9US10
A	278	HIS	-	EXPRESSION TAG	UNP F9US10
A	279	HIS	-	EXPRESSION TAG	UNP F9US10
A	280	HIS	-	EXPRESSION TAG	UNP F9US10
A	281	HIS	-	EXPRESSION TAG	UNP F9US10
A	282	HIS	-	EXPRESSION TAG	UNP F9US10
B	277	HIS	-	EXPRESSION TAG	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

Continued on next page...

Continued from previous page...

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: C₂H₃O₂).



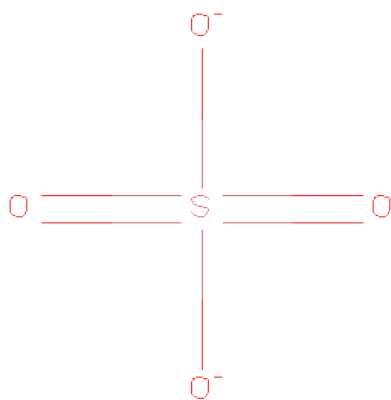
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

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



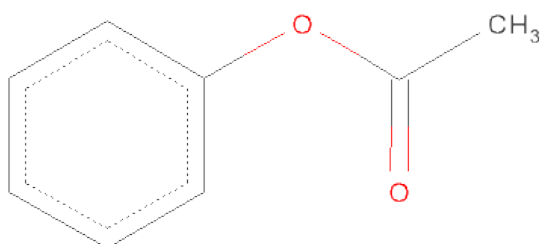
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

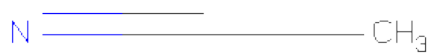
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHENYL ACETATE (three-letter code: QY9) (formula: C₈H₈O₂).



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

- Molecule 5 is ACETONITRILE (three-letter code: CCN) (formula: C₂H₃N).



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

- Molecule 6 is water.

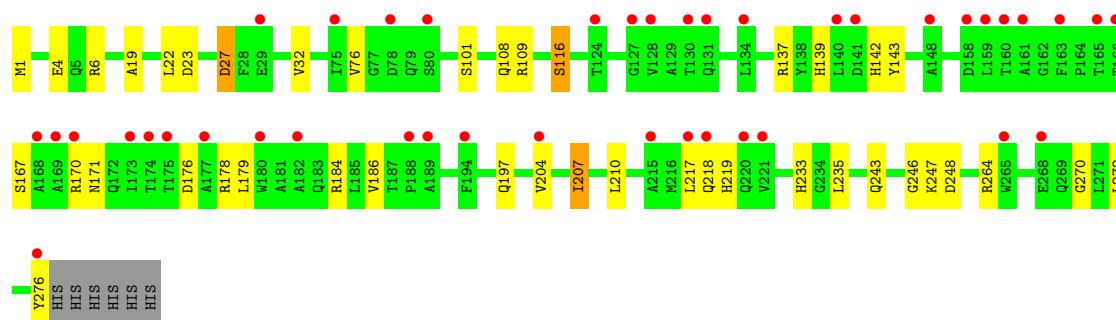
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	193	Total 193	O 193	0	0
6	B	182	Total 182	O 182	0	0
6	C	191	Total 191	O 191	0	0
6	D	137	Total 137	O 137	0	0
6	E	152	Total 152	O 152	0	0
6	F	159	Total 159	O 159	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

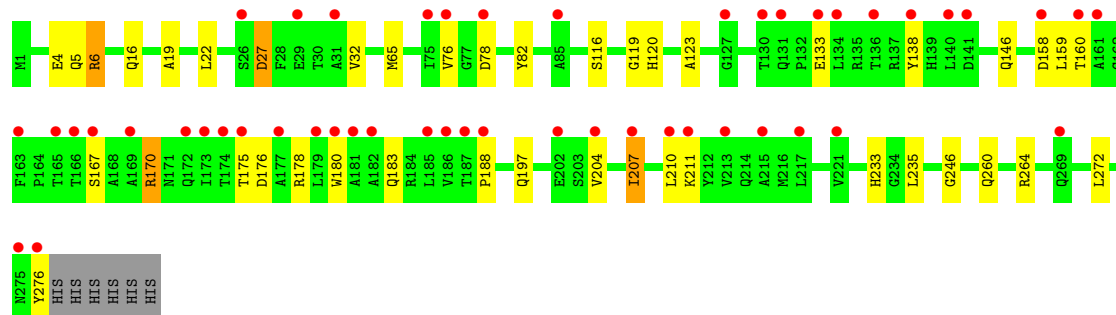
• Molecule 1: CEST-2923

Chain A: 



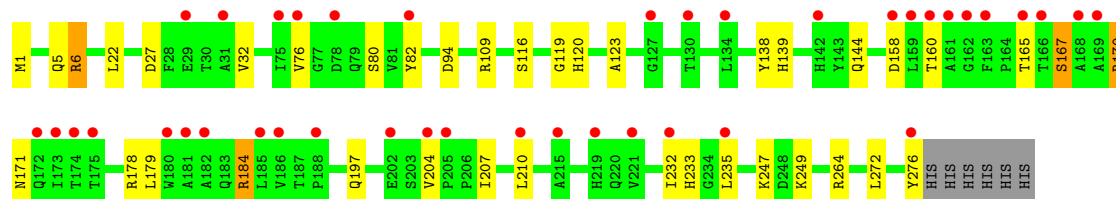
• Molecule 1: CEST-2923

Chain B: 



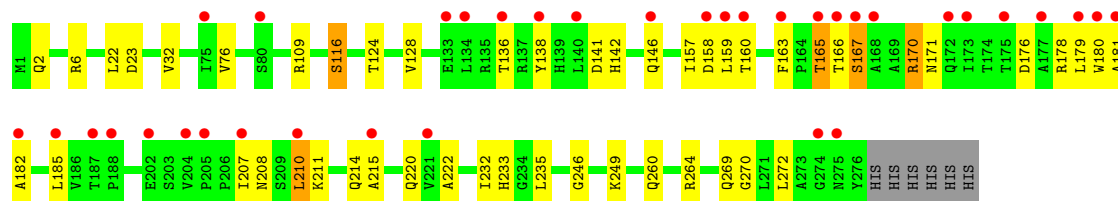
• Molecule 1: CEST-2923

Chain C: 



• Molecule 1: CEST-2923

Chain D: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	43.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.279 0.219 , 0.270	Depositor DCC
R_{free} test set	6010 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
Estimated twinning fraction	0.450 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.439 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 0.448 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 124507 reflections (0.002%)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2155	0	0	23	0
1	B	2144	0	0	25	0
1	C	2144	0	0	21	0
1	D	2144	0	0	19	0
1	E	2155	0	0	25	0
1	F	2155	0	0	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	3	0	0
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	1	0
3	D	10	0	0	3	0
3	E	10	0	0	2	0
4	A	10	0	8	0	0
4	B	10	0	8	1	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	0	0
5	B	6	0	6	0	0
5	C	3	0	3	0	0
5	D	6	0	6	0	0
5	E	3	0	3	0	0
5	F	9	0	9	0	0
6	A	193	0	0	9	0
6	B	182	0	0	12	0
6	C	191	0	0	10	0
6	D	137	0	0	8	0
6	E	152	0	0	11	0
6	F	159	0	0	19	0
All	All	14061	0	94	148	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (148) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:170:ARG:NH1	1:A:171:ASN:OD1	2.03	0.90
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	0.83
1:E:208:ASN:ND2	6:E:2103:HOH:O	2.15	0.80
1:F:176:ASP:O	6:F:2112:HOH:O	1.99	0.78
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:HIS:ND1	1:E:78:ASP:OD2	2.19	0.74
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:222:ALA:N	6:F:2131:HOH:O	2.21	0.72
1:D:78:ASP:OD2	1:E:139:HIS:ND1	2.23	0.72
1:F:178:ARG:O	6:F:2114:HOH:O	2.08	0.71
1:D:184:ARG:NH2	6:D:2106:HOH:O	2.25	0.69
1:F:182:ALA:O	6:F:2084:HOH:O	2.11	0.69
1:D:109:ARG:NH2	3:D:1278:SO4:O1	2.26	0.69
1:E:188:PRO:O	6:E:2116:HOH:O	2.12	0.68
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:C:138:TYR:OH	1:C:178:ARG:NE	2.27	0.66
1:D:1:MET:N	1:D:23:ASP:OD2	2.29	0.66
1:C:247:LYS:NZ	6:C:2167:HOH:O	2.29	0.65
1:F:215:ALA:O	6:F:2125:HOH:O	2.14	0.65
1:E:170:ARG:NH2	6:E:2108:HOH:O	2.30	0.64
1:C:170:ARG:NH1	1:C:171:ASN:OD1	2.30	0.64
1:F:157:ILE:O	1:F:182:ALA:N	2.31	0.63
1:A:276:TYR:N	6:A:2192:HOH:O	2.31	0.63
1:E:207:ILE:N	6:E:2120:HOH:O	2.32	0.63
1:D:247:LYS:NZ	3:D:1277:SO4:O2	2.32	0.63
1:E:158:ASP:N	1:E:208:ASN:OD1	2.33	0.62
1:B:260:GLN:NE2	6:B:2173:HOH:O	2.32	0.61
1:D:109:ARG:NE	6:D:2080:HOH:O	2.33	0.61
1:E:1:MET:N	1:E:23:ASP:OD2	2.34	0.61
1:A:247:LYS:NZ	3:A:1277:SO4:S	2.73	0.61
1:A:247:LYS:NZ	3:A:1277:SO4:O2	2.34	0.60
1:E:176:ASP:OD2	1:E:178:ARG:NH2	2.35	0.60
1:E:215:ALA:O	6:E:2122:HOH:O	2.17	0.60
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:207:ILE:N	6:B:2146:HOH:O	2.35	0.59
1:F:180:TRP:N	6:F:2112:HOH:O	2.36	0.58
6:D:2012:HOH:O	1:E:6:ARG:NH1	2.36	0.58
1:F:109[A]:ARG:NH2	1:F:270:GLY:O	2.35	0.58
1:F:249:LYS:NZ	6:F:2144:HOH:O	2.36	0.58
1:A:207:ILE:N	6:A:2152:HOH:O	2.37	0.57
1:F:246:GLY:N	6:F:2143:HOH:O	2.38	0.57
1:F:167:SER:O	1:F:170:ARG:NH1	2.39	0.56
1:F:170:ARG:NH1	1:F:171:ASN:OD1	2.38	0.56
1:D:247:LYS:NZ	3:D:1277:SO4:S	2.79	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:SER:OG	1:A:233:HIS:NE2	2.40	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:D:207:ILE:N	6:D:2112:HOH:O	2.39	0.55
1:F:146:GLN:N	6:F:2078:HOH:O	2.40	0.55
1:F:158:ASP:N	1:F:208:ASN:OD1	2.40	0.54
1:B:116:SER:OG	1:B:233:HIS:NE2	2.41	0.54
1:D:158:ASP:OD1	1:D:160:THR:OG1	2.25	0.54
2:C:1276:ACT:H3	6:C:2058:HOH:O	2.07	0.53
1:B:246:GLY:N	6:B:2163:HOH:O	2.40	0.53
1:B:5:GLN:NE2	6:B:2015:HOH:O	2.42	0.52
1:A:1:MET:N	1:A:23:ASP:OD2	2.42	0.52
1:F:159:LEU:N	1:F:180:TRP:O	2.43	0.52
1:F:207:ILE:O	1:F:211:LYS:N	2.43	0.52
1:C:247:LYS:NZ	6:C:2172:HOH:O	2.42	0.52
1:B:276:TYR:N	6:B:2181:HOH:O	2.42	0.52
1:E:247:LYS:NZ	3:E:1278:SO4:O3	2.43	0.51
1:F:160:THR:N	6:F:2102:HOH:O	2.44	0.51
1:D:157:ILE:O	1:D:182:ALA:N	2.44	0.51
1:C:249:LYS:NZ	6:C:2175:HOH:O	2.42	0.51
1:F:163:PHE:N	6:F:2101:HOH:O	2.44	0.51
1:D:116:SER:OG	1:D:233:HIS:NE2	2.42	0.51
1:F:116:SER:OG	1:F:233:HIS:NE2	2.44	0.51
1:E:207:ILE:O	1:E:211:LYS:N	2.44	0.50
1:C:197:GLN:NE2	1:C:204:VAL:O	2.44	0.50
1:B:6:ARG:NH1	6:B:2009:HOH:O	2.43	0.50
1:C:109:ARG:NE	6:C:2111:HOH:O	2.44	0.50
1:D:159:LEU:N	6:D:2096:HOH:O	2.45	0.50
1:A:197:GLN:NE2	1:A:204:VAL:O	2.46	0.49
1:B:167:SER:O	1:B:170:ARG:NH1	2.46	0.49
1:B:158:ASP:OD1	1:B:160:THR:OG1	2.29	0.49
6:C:2060:HOH:O	1:D:27:ASP:OD1	2.20	0.48
1:A:176:ASP:OD2	1:A:178:ARG:NH2	2.46	0.48
1:D:249:LYS:NZ	6:D:2126:HOH:O	2.46	0.48
1:D:170:ARG:NH2	6:D:2099:HOH:O	2.46	0.48
1:B:27:ASP:N	1:B:27:ASP:OD1	2.46	0.48
1:D:82:TYR:OH	1:D:120:HIS:ND1	2.46	0.48
1:E:116:SER:OG	1:E:233:HIS:NE2	2.47	0.48
1:A:217:LEU:O	1:A:219:HIS:N	2.46	0.48
1:A:217:LEU:C	1:A:219:HIS:N	2.67	0.48
1:F:136:THR:OG1	1:F:141:ASP:OD2	2.31	0.48
1:C:82:TYR:OH	1:C:120:HIS:ND1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:210:LEU:O	1:F:214:GLN:N	2.47	0.48
1:B:188:PRO:O	6:B:2142:HOH:O	2.20	0.47
1:F:124:THR:O	1:F:128:VAL:N	2.47	0.47
4:B:1278:QY9:HAF	6:B:2030:HOH:O	2.14	0.47
1:A:264:ARG:NH1	6:A:2185:HOH:O	2.48	0.47
1:D:94:ASP:OD2	1:D:144:GLN:N	2.48	0.47
1:B:197:GLN:NE2	1:B:204:VAL:O	2.47	0.47
1:C:116:SER:OG	1:C:233:HIS:NE2	2.48	0.46
1:A:142:HIS:O	6:A:2125:HOH:O	2.21	0.46
1:B:176:ASP:OD2	1:B:178:ARG:NH2	2.49	0.46
1:E:219:HIS:N	6:E:2122:HOH:O	2.48	0.46
1:D:131:GLN:O	1:D:135:ARG:N	2.49	0.46
1:E:187:THR:N	6:E:2085:HOH:O	2.48	0.46
1:A:246:GLY:N	6:A:2173:HOH:O	2.49	0.46
1:C:158:ASP:OD1	1:C:160:THR:OG1	2.33	0.45
1:C:232:ILE:N	6:C:2157:HOH:O	2.49	0.45
1:E:232:ILE:N	6:E:2127:HOH:O	2.49	0.45
1:B:207:ILE:O	1:B:211:LYS:N	2.50	0.45
1:B:133:GLU:OE2	6:B:2118:HOH:O	2.21	0.45
1:B:146:GLN:N	6:B:2104:HOH:O	2.50	0.45
1:A:4:GLU:O	1:A:19:ALA:N	2.50	0.45
1:E:109[A]:ARG:NH2	1:E:270:GLY:O	2.50	0.44
1:C:94:ASP:OD2	1:C:144:GLN:N	2.50	0.44
1:C:109:ARG:NH2	3:C:1278:SO4:O2	2.50	0.44
1:F:165:THR:OG1	1:F:166:THR:N	2.50	0.44
1:E:246:GLY:N	6:E:2133:HOH:O	2.51	0.44
1:A:27:ASP:OD1	1:A:27:ASP:N	2.51	0.44
1:E:13:HIS:ND1	1:E:73:GLN:OE1	2.51	0.44
1:E:269:GLN:NE2	6:E:2148:HOH:O	2.50	0.44
1:B:82:TYR:OH	1:B:120:HIS:ND1	2.51	0.44
1:C:276:TYR:N	6:C:2187:HOH:O	2.50	0.44
1:F:158:ASP:OD1	1:F:160:THR:OG1	2.35	0.44
1:E:94:ASP:OD2	1:E:144:GLN:N	2.51	0.43
1:C:5:GLN:NE2	6:C:2013:HOH:O	2.51	0.43
1:F:220:GLN:N	1:F:220:GLN:OE1	2.51	0.43
1:E:82:TYR:OH	1:E:120:HIS:ND1	2.51	0.43
6:B:2014:HOH:O	1:C:6:ARG:NH1	2.51	0.43
1:D:129:ALA:O	6:D:2085:HOH:O	2.21	0.43
1:F:232:ILE:N	6:F:2135:HOH:O	2.52	0.43
1:C:167:SER:O	1:C:170:ARG:NH1	2.52	0.43
1:B:159:LEU:N	1:B:180:TRP:O	2.52	0.43
1:A:109[A]:ARG:NH2	1:A:270:GLY:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:175:THR:O	1:B:175:THR:OG1	2.36	0.42
1:F:159:LEU:N	6:F:2102:HOH:O	2.52	0.42
1:C:119:GLY:O	1:C:123:ALA:N	2.52	0.42
1:F:260:GLN:NE2	6:F:2149:HOH:O	2.52	0.42
1:C:27:ASP:N	1:C:27:ASP:OD1	2.53	0.42
1:F:2:GLN:NE2	1:F:23:ASP:OD1	2.53	0.42
1:A:137:ARG:NH2	6:A:2123:HOH:O	2.53	0.42
1:B:175:THR:N	6:B:2090:HOH:O	2.53	0.41
1:B:119:GLY:O	1:B:123:ALA:N	2.53	0.41
1:A:143:TYR:N	6:A:2118:HOH:O	2.52	0.41
1:A:108:GLN:NE2	6:A:2107:HOH:O	2.53	0.41
1:F:142:HIS:O	6:F:2094:HOH:O	2.22	0.41
1:B:4:GLU:O	1:B:19:ALA:N	2.55	0.40
1:A:243:GLN:OE1	6:A:2171:HOH:O	2.22	0.40
1:B:158:ASP:OD2	1:B:183:GLN:NE2	2.54	0.40

There are no symmetry-related clashes.

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	276/282 (98%)	255 (92%)	20 (7%)	1 (0%)	43	52
1	B	275/282 (98%)	254 (92%)	21 (8%)	0	100	100
1	C	275/282 (98%)	251 (91%)	23 (8%)	1 (0%)	43	52
1	D	275/282 (98%)	254 (92%)	19 (7%)	2 (1%)	30	34
1	E	276/282 (98%)	256 (93%)	20 (7%)	0	100	100
1	F	276/282 (98%)	255 (92%)	20 (7%)	1 (0%)	43	52
All	All	1653/1692 (98%)	1525 (92%)	123 (7%)	5 (0%)	50	60

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 ⓘ

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%)	21	25
1	B	220/226 (97%)	207 (94%)	13 (6%)	28	35
1	C	220/226 (97%)	204 (93%)	16 (7%)	20	24
1	D	220/226 (97%)	205 (93%)	15 (7%)	22	28
1	E	221/226 (98%)	207 (94%)	14 (6%)	25	32
1	F	221/226 (98%)	209 (95%)	12 (5%)	31	40
All	All	1323/1356 (98%)	1237 (94%)	86 (6%)	24	30

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
2	ACT	A	1276	-	1,3,3	1.10	0	0,3,3	0.00	-
3	SO4	A	1277	-	4,4,4	0.28	0	6,6,6	0.14	0
4	QY9	A	1278	-	10,10,10	0.68	0	12,12,12	1.45	1 (8%)
5	CCN	A	1279	-	2,2,2	0.62	0	1,1,1	0.61	0
5	CCN	A	1280	-	2,2,2	0.69	0	1,1,1	0.58	0
5	CCN	A	1281	-	2,2,2	0.65	0	1,1,1	0.62	0
2	ACT	B	1276	-	1,3,3	1.31	0	0,3,3	0.00	-
3	SO4	B	1277	-	4,4,4	0.27	0	6,6,6	0.10	0
4	QY9	B	1278	-	10,10,10	0.64	0	12,12,12	1.29	1 (8%)
5	CCN	B	1279	-	2,2,2	0.60	0	1,1,1	0.59	0
5	CCN	B	1280	-	2,2,2	0.63	0	1,1,1	0.60	0
2	ACT	C	1276	-	1,3,3	0.68	0	0,3,3	0.00	-
3	SO4	C	1277	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	C	1278	-	4,4,4	0.23	0	6,6,6	0.14	0
4	QY9	C	1279	-	10,10,10	0.65	0	12,12,12	1.30	1 (8%)
5	CCN	C	1280	-	2,2,2	0.67	0	1,1,1	0.59	0
2	ACT	D	1276	-	1,3,3	0.71	0	0,3,3	0.00	-
3	SO4	D	1277	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	D	1278	-	4,4,4	0.21	0	6,6,6	0.12	0
5	CCN	D	1279	-	2,2,2	0.65	0	1,1,1	0.60	0
5	CCN	D	1280	-	2,2,2	0.64	0	1,1,1	0.55	0
2	ACT	E	1276	-	1,3,3	1.16	0	0,3,3	0.00	-
3	SO4	E	1277	-	4,4,4	0.32	0	6,6,6	0.36	0
3	SO4	E	1278	-	4,4,4	0.26	0	6,6,6	0.12	0
4	QY9	E	1279	-	10,10,10	0.68	0	12,12,12	1.26	1 (8%)
5	CCN	E	1280	-	2,2,2	0.58	0	1,1,1	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	F	1276	-	1,3,3	1.10	0	0,3,3	0.00	-
4	QY9	F	1277	-	10,10,10	0.65	0	12,12,12	1.34	1 (8%)
5	CCN	F	1278	-	2,2,2	0.60	0	1,1,1	0.57	0
5	CCN	F	1279	-	2,2,2	0.69	0	1,1,1	0.57	0
5	CCN	F	1280	-	2,2,2	0.73	0	1,1,1	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	1276	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1277	-	-	0/0/0/0	0/0/0/0
4	QY9	A	1278	-	-	0/4/4/4	0/1/1/1
5	CCN	A	1279	-	-	0/0/0/0	0/0/0/0
5	CCN	A	1280	-	-	0/0/0/0	0/0/0/0
5	CCN	A	1281	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1276	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1277	-	-	0/0/0/0	0/0/0/0
4	QY9	B	1278	-	-	0/4/4/4	0/1/1/1
5	CCN	B	1279	-	-	0/0/0/0	0/0/0/0
5	CCN	B	1280	-	-	0/0/0/0	0/0/0/0
2	ACT	C	1276	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1277	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1278	-	-	0/0/0/0	0/0/0/0
4	QY9	C	1279	-	-	0/4/4/4	0/1/1/1
5	CCN	C	1280	-	-	0/0/0/0	0/0/0/0
2	ACT	D	1276	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1277	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1278	-	-	0/0/0/0	0/0/0/0
5	CCN	D	1279	-	-	0/0/0/0	0/0/0/0
5	CCN	D	1280	-	-	0/0/0/0	0/0/0/0
2	ACT	E	1276	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1277	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1278	-	-	0/0/0/0	0/0/0/0
4	QY9	E	1279	-	-	0/4/4/4	0/1/1/1
5	CCN	E	1280	-	-	0/0/0/0	0/0/0/0
2	ACT	F	1276	-	-	0/0/0/0	0/0/0/0
4	QY9	F	1277	-	-	0/4/4/4	0/1/1/1
5	CCN	F	1278	-	-	0/0/0/0	0/0/0/0
5	CCN	F	1279	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CCN	F	1280	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1278	QY9	OAH-CAI-CAA	4.21	120.54	110.91
4	F	1277	QY9	OAH-CAI-CAA	3.89	119.81	110.91
4	C	1279	QY9	OAH-CAI-CAA	3.86	119.74	110.91
4	E	1279	QY9	OAH-CAI-CAA	3.58	119.10	110.91
4	B	1278	QY9	OAH-CAI-CAA	3.42	118.74	110.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	276/282 (97%)	1.07	41 (14%) 3 5	14, 37, 72, 95	0
1	B	276/282 (97%)	1.11	49 (17%) 2 3	13, 37, 74, 104	0
1	C	276/282 (97%)	1.00	40 (14%) 3 5	13, 38, 73, 101	0
1	D	276/282 (97%)	0.95	33 (11%) 5 8	14, 36, 73, 105	0
1	E	276/282 (97%)	1.06	40 (14%) 3 5	14, 38, 75, 91	0
1	F	276/282 (97%)	0.98	36 (13%) 4 7	15, 37, 71, 87	0
All	All	1656/1692 (97%)	1.03	239 (14%) 3 5	13, 37, 73, 105	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	TYR	8.8
1	A	175	THR	6.4
1	B	161	ALA	6.0
1	F	168	ALA	5.7
1	C	159	LEU	5.0
1	E	172	GLN	5.0
1	E	175	THR	4.8
1	B	160	THR	4.8
1	F	159	LEU	4.7
1	B	140	LEU	4.5
1	E	168	ALA	4.4
1	C	31	ALA	4.3
1	A	188	PRO	4.2
1	F	204	VAL	4.2
1	A	204	VAL	4.2
1	F	134	LEU	4.1
1	D	173	ILE	4.0
1	C	180	TRP	3.9
1	C	202	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	161	ALA	3.8
1	C	166	THR	3.8
1	D	161	ALA	3.8
1	F	205	PRO	3.7
1	C	134	LEU	3.7
1	A	80[A]	SER	3.7
1	B	76	VAL	3.7
1	D	175	THR	3.6
1	A	128	VAL	3.6
1	C	210	LEU	3.6
1	E	180	TRP	3.6
1	C	175	THR	3.6
1	A	134	LEU	3.5
1	E	141	ASP	3.5
1	B	136	THR	3.5
1	D	188	PRO	3.5
1	E	169	ALA	3.5
1	E	30	THR	3.4
1	B	29	GLU	3.4
1	A	161	ALA	3.4
1	D	140	LEU	3.4
1	A	189	ALA	3.3
1	F	221	VAL	3.3
1	E	173	ILE	3.3
1	C	168	ALA	3.3
1	E	160	THR	3.3
1	E	204	VAL	3.3
1	F	80[A]	SER	3.3
1	C	161	ALA	3.3
1	B	166	THR	3.3
1	E	163	PHE	3.3
1	D	75	ILE	3.2
1	B	78	ASP	3.2
1	E	78	ASP	3.2
1	C	165	THR	3.2
1	C	204	VAL	3.2
1	A	78	ASP	3.2
1	D	78	ASP	3.2
1	A	168	ALA	3.2
1	D	177	ALA	3.2
1	C	169	ALA	3.2
1	B	175	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	168	ALA	3.2
1	F	138	TYR	3.2
1	B	134	LEU	3.1
1	F	75	ILE	3.1
1	B	180	TRP	3.1
1	C	172	GLN	3.1
1	F	180	TRP	3.1
1	A	160	THR	3.1
1	D	220	GLN	3.1
1	C	186	VAL	3.1
1	D	186	VAL	3.1
1	F	133	GLU	3.1
1	A	75	ILE	3.1
1	E	158	ASP	3.1
1	A	158	ASP	3.0
1	E	166	THR	3.0
1	A	174	THR	3.0
1	B	182	ALA	3.0
1	B	215	ALA	3.0
1	B	221	VAL	3.0
1	D	169	ALA	3.0
1	B	275	ASN	3.0
1	D	170	ARG	3.0
1	C	174	THR	2.9
1	C	173	ILE	2.9
1	B	130	THR	2.9
1	D	136	THR	2.9
1	E	159	LEU	2.9
1	E	130	THR	2.9
1	F	163	PHE	2.9
1	F	172	GLN	2.9
1	D	160	THR	2.9
1	A	169	ALA	2.9
1	D	77	GLY	2.9
1	D	221	VAL	2.9
1	E	75	ILE	2.9
1	F	188	PRO	2.9
1	E	76	VAL	2.8
1	D	276	TYR	2.8
1	F	140	LEU	2.8
1	F	177	ALA	2.8
1	B	131	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	130	THR	2.8
1	E	199	ALA	2.8
1	B	213	VAL	2.8
1	D	203	SER	2.8
1	C	76	VAL	2.7
1	B	165	THR	2.7
1	F	173	ILE	2.7
1	A	177	ALA	2.7
1	A	165	THR	2.7
1	E	174	THR	2.7
1	F	165	THR	2.7
1	F	166	THR	2.7
1	F	187	THR	2.7
1	A	194	PHE	2.7
1	F	185	LEU	2.7
1	A	166	THR	2.7
1	F	175	THR	2.7
1	E	190	SER	2.7
1	C	205	PRO	2.7
1	F	275	ASN	2.7
1	A	221	VAL	2.6
1	B	173	ILE	2.6
1	E	177	ALA	2.6
1	F	182	ALA	2.6
1	C	185	LEU	2.6
1	F	167	SER	2.6
1	A	180	TRP	2.6
1	B	185	LEU	2.6
1	F	202	GLU	2.6
1	C	219	HIS	2.6
1	B	169	ALA	2.6
1	E	185	LEU	2.6
1	D	199	ALA	2.6
1	A	159	LEU	2.6
1	C	162	GLY	2.5
1	A	29	GLU	2.5
1	C	160	THR	2.5
1	E	210	LEU	2.5
1	B	207	ILE	2.5
1	F	207	ILE	2.5
1	B	172	GLN	2.5
1	B	163	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	276	TYR	2.5
1	B	188	PRO	2.5
1	B	202	GLU	2.5
1	A	220	GLN	2.5
1	D	218	GLN	2.5
1	E	77	GLY	2.4
1	B	75	ILE	2.4
1	D	141	ASP	2.4
1	E	214	GLN	2.4
1	A	140	LEU	2.4
1	F	215	ALA	2.4
1	C	78	ASP	2.4
1	A	182	ALA	2.4
1	E	127	GLY	2.4
1	B	217	LEU	2.4
1	B	127	GLY	2.4
1	C	158	ASP	2.4
1	F	181	ALA	2.4
1	B	174	THR	2.3
1	C	130	THR	2.3
1	E	165	THR	2.3
1	E	245	PRO	2.3
1	A	265	TRP	2.3
1	F	210	LEU	2.3
1	A	268	GLU	2.3
1	C	29	GLU	2.3
1	A	170	ARG	2.3
1	B	187	THR	2.3
1	F	136	THR	2.3
1	A	217	LEU	2.3
1	C	142	HIS	2.3
1	A	130	THR	2.3
1	B	138	TYR	2.3
1	F	179	LEU	2.3
1	E	232	ILE	2.3
1	B	26	SER	2.3
1	A	131	GLN	2.3
1	E	220	GLN	2.3
1	C	276	TYR	2.2
1	F	274	GLY	2.2
1	C	232	ILE	2.2
1	F	146	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	178	ARG	2.2
1	C	215	ALA	2.2
1	E	134	LEU	2.2
1	A	141	ASP	2.2
1	E	176	ASP	2.2
1	B	133	GLU	2.2
1	C	188	PRO	2.2
1	A	127	GLY	2.2
1	E	215	ALA	2.2
1	B	186	VAL	2.2
1	D	138	TYR	2.2
1	A	173	ILE	2.2
1	C	163	PHE	2.2
1	B	177	ALA	2.2
1	D	181	ALA	2.2
1	D	134	LEU	2.2
1	B	204	VAL	2.2
1	A	215	ALA	2.2
1	C	235	LEU	2.2
1	E	179	LEU	2.2
1	A	218	GLN	2.1
1	A	163	PHE	2.1
1	F	160	THR	2.1
1	B	85	ALA	2.1
1	C	182	ALA	2.1
1	B	167	SER	2.1
1	B	31	ALA	2.1
1	C	82	TYR	2.1
1	C	75	ILE	2.1
1	A	124	THR	2.1
1	D	166	THR	2.1
1	F	158	ASP	2.1
1	E	216	MET	2.1
1	D	180	TRP	2.1
1	D	202	GLU	2.1
1	B	158	ASP	2.1
1	E	27	ASP	2.1
1	A	148	ALA	2.1
1	C	127	GLY	2.0
1	B	179	LEU	2.0
1	B	210	LEU	2.0
1	E	142	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	167	SER	2.0
1	C	181	ALA	2.0
1	B	141	ASP	2.0
1	D	184	ARG	2.0
1	E	137	ARG	2.0
1	B	181	ALA	2.0
1	C	221	VAL	2.0
1	B	211	LYS	2.0
1	B	269	GLN	2.0
1	D	172	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	QY9	B	1278	10/10	0.35	6.25	73,77,85,85	0
5	CCN	D	1279	3/3	0.26	6.05	30,30,33,36	0
4	QY9	A	1278	10/10	0.32	5.23	59,64,71,73	0
4	QY9	C	1279	10/10	0.33	4.52	75,78,87,90	0
4	QY9	F	1277	10/10	0.28	4.50	70,74,81,84	0
3	SO4	C	1278	5/5	0.26	2.66	111,111,113,114	0
4	QY9	E	1279	10/10	0.28	2.19	67,72,73,74	0
5	CCN	F	1280	3/3	0.21	1.82	19,19,30,34	0
2	ACT	D	1276	4/4	0.26	1.42	19,27,33,47	0
5	CCN	A	1281	3/3	0.19	1.13	26,26,27,28	0
2	ACT	E	1276	4/4	0.20	0.93	28,31,37,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	E	1278	5/5	0.30	0.64	116,119,120,120	0
2	ACT	F	1276	4/4	0.18	0.30	32,35,40,51	0
3	SO4	B	1277	5/5	0.25	0.29	111,111,112,114	0
5	CCN	A	1279	3/3	0.21	0.23	35,35,37,40	0
5	CCN	E	1280	3/3	0.23	0.21	34,34,34,37	0
5	CCN	B	1280	3/3	0.17	0.04	34,34,34,35	0
2	ACT	C	1276	4/4	0.18	-0.02	31,39,41,55	0
5	CCN	F	1278	3/3	0.20	-0.07	34,34,36,38	0
3	SO4	D	1277	5/5	0.20	-0.11	110,110,112,112	0
3	SO4	A	1277	5/5	0.22	-0.20	105,106,107,108	0
3	SO4	D	1278	5/5	0.15	-0.29	108,109,110,110	0
3	SO4	C	1277	5/5	0.16	-0.54	39,40,46,59	0
5	CCN	C	1280	3/3	0.18	-0.65	38,38,39,42	0
5	CCN	B	1279	3/3	0.16	-0.66	34,34,35,39	0
2	ACT	B	1276	4/4	0.15	-0.77	38,39,45,53	0
3	SO4	E	1277	5/5	0.16	-0.85	37,44,47,66	0
2	ACT	A	1276	4/4	0.16	-1.07	31,32,40,54	0
5	CCN	D	1280	3/3	0.14	-1.20	34,34,37,38	0
5	CCN	A	1280	3/3	0.12	-1.87	32,32,36,36	0
5	CCN	F	1279	3/3	0.13	-2.08	13,13,26,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.