



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:42 PM UTC

PDB ID : 4C01 / pdb_00004c01
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

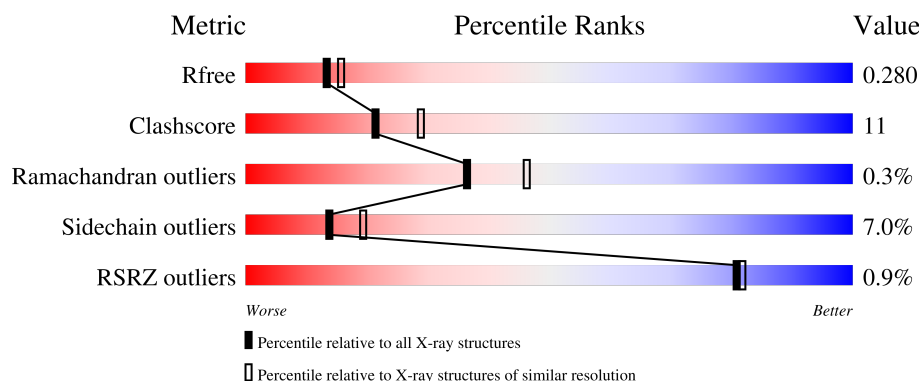
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	282	2% 71% 24% ..
1	B	282	76% 21% ..
1	C	282	77% 19% ..
1	D	282	% 73% 22% ..
1	E	282	75% 21% ..

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Mol	Chain	Length	Quality of chain
1	F	282	% 72% 23% ..

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:

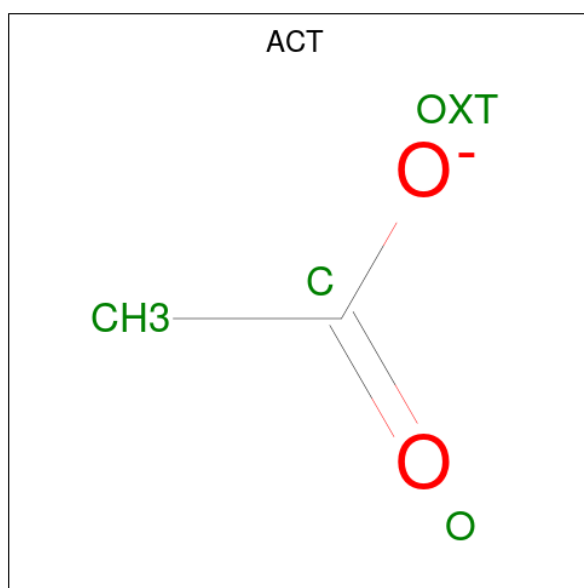
Chain	Residue	Modelled	Actual	Comment	Reference
A	277	HIS	-	expression tag	UNP F9US10
A	278	HIS	-	expression tag	UNP F9US10
A	279	HIS	-	expression tag	UNP F9US10
A	280	HIS	-	expression tag	UNP F9US10
A	281	HIS	-	expression tag	UNP F9US10
A	282	HIS	-	expression tag	UNP F9US10
B	277	HIS	-	expression tag	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 (CCD ID: ACT) (formula: $C_2H_3O_2$).



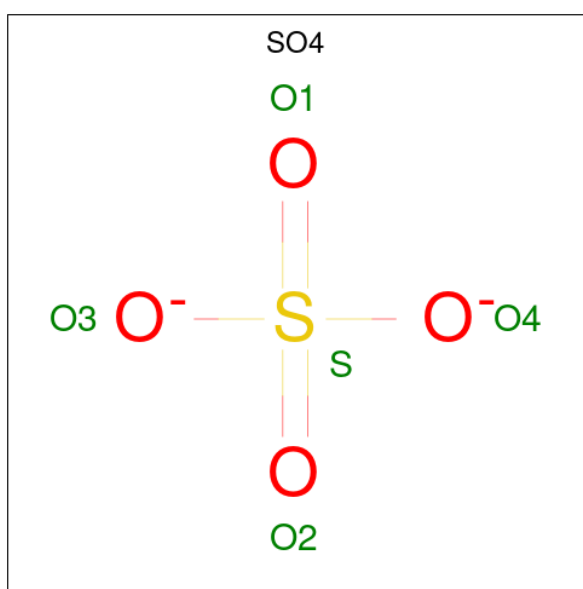
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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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 (CCD ID: SO4) (formula: O₄S).



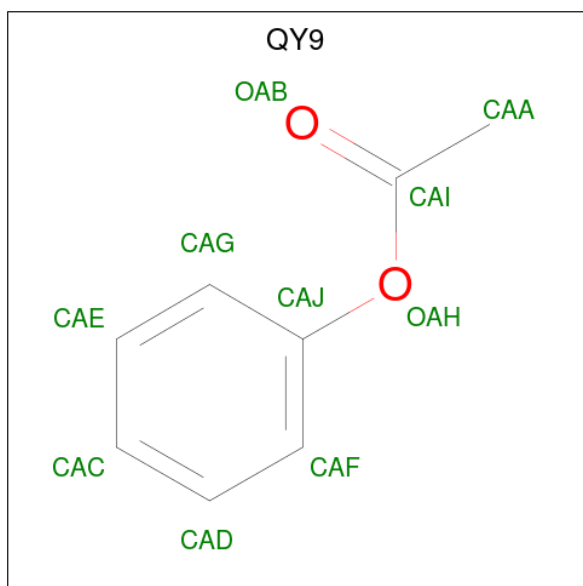
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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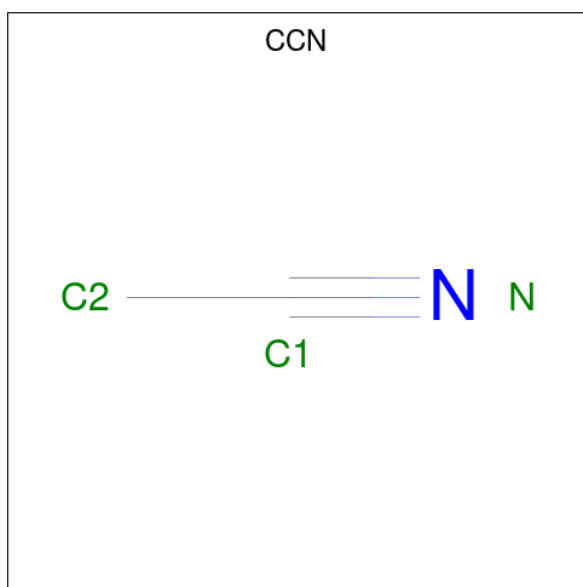
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is phenyl acetate (CCD ID: QY9) (formula: $C_8H_8O_2$).



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 (CCD ID: CCN) (formula: C_2H_3N).



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		

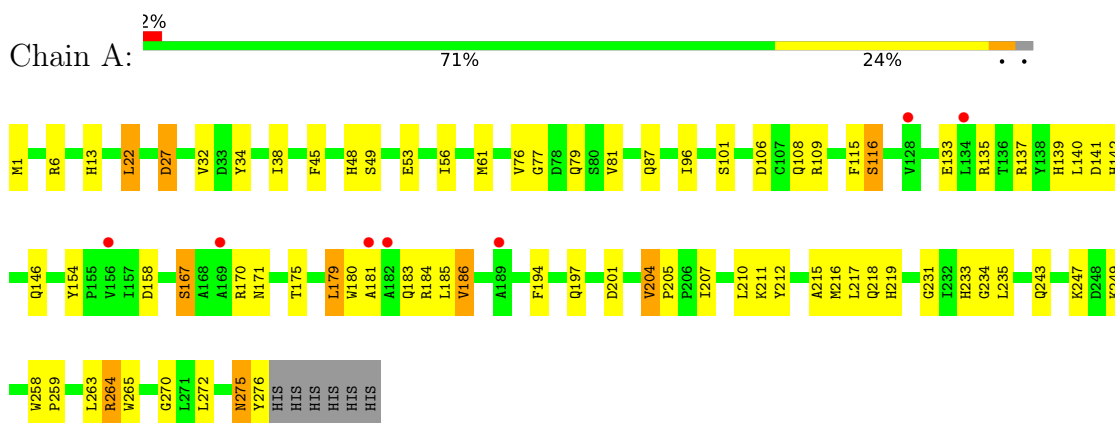
- Molecule 6 is water.

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

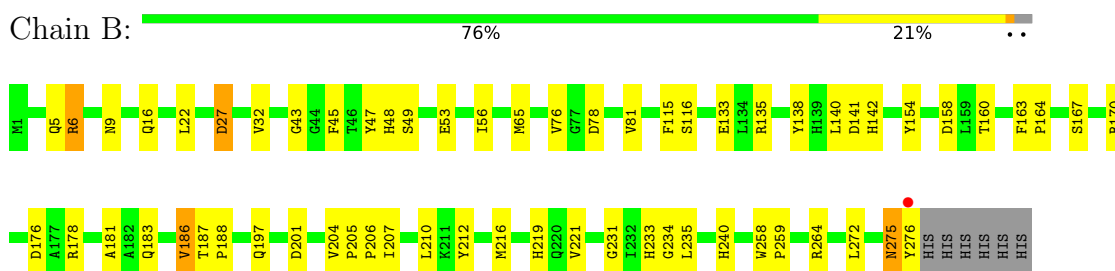
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

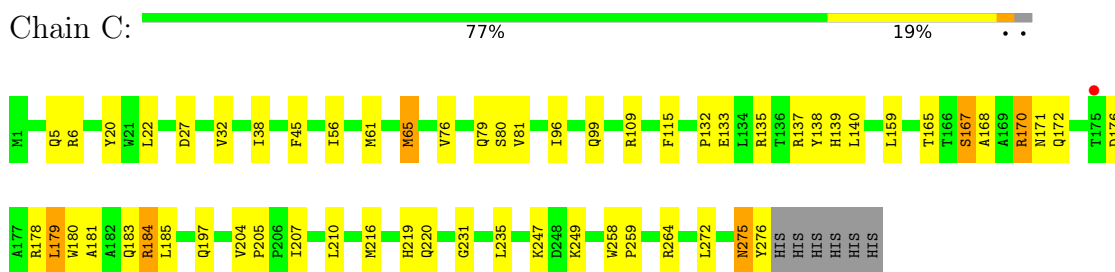
• Molecule 1: CEST-2923



• Molecule 1: CEST-2923

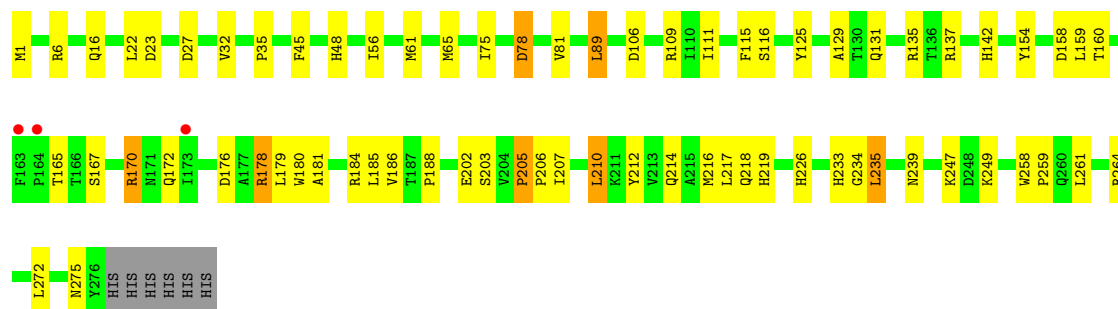


• Molecule 1: CEST-2923

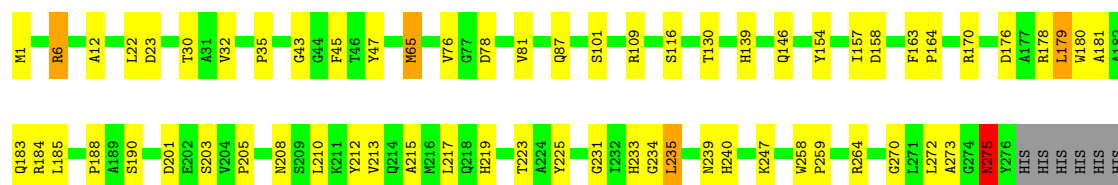
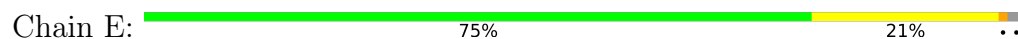


• Molecule 1: CEST-2923

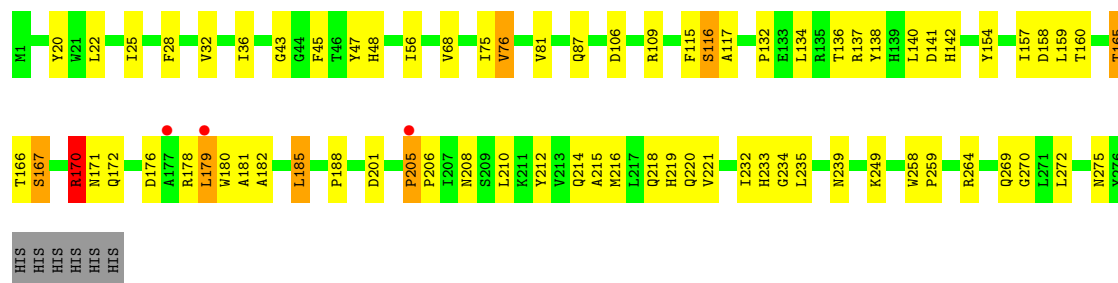




• Molecule 1: CEST-2923



• Molecule 1: CEST-2923



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	42.72 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.225 , 0.279 0.226 , 0.280	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)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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	0.94	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.

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: QY9, ACT, CCN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	1/2214 (0.0%)	0.88	4/3030 (0.1%)
1	B	0.55	1/2203 (0.0%)	0.87	0/3016
1	C	0.54	1/2203 (0.0%)	0.88	3/3016 (0.1%)
1	D	0.55	1/2203 (0.0%)	0.86	2/3016 (0.1%)
1	E	0.55	1/2214 (0.0%)	0.86	2/3030 (0.1%)
1	F	0.55	1/2214 (0.0%)	0.87	4/3030 (0.1%)
All	All	0.55	6/13251 (0.0%)	0.87	15/18138 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ASN	C-N	-6.65	1.24	1.33
1	E	275	ASN	C-N	-6.56	1.24	1.33
1	C	275	ASN	C-N	-6.55	1.24	1.33
1	B	275	ASN	C-N	-6.50	1.24	1.33
1	D	275	ASN	C-N	-6.46	1.24	1.33
1	F	275	ASN	C-N	-6.29	1.24	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	PRO	CA-C-N	6.99	127.57	119.47
1	E	205	PRO	C-N-CA	6.99	127.57	119.47
1	D	205	PRO	CA-C-N	6.00	125.68	119.56
1	D	205	PRO	C-N-CA	6.00	125.68	119.56
1	C	205	PRO	CA-C-N	5.72	126.11	119.47
1	C	205	PRO	C-N-CA	5.72	126.11	119.47
1	F	170	ARG	N-CA-C	-5.70	104.97	111.07
1	A	204	VAL	CA-C-N	5.44	125.98	120.38
1	A	204	VAL	C-N-CA	5.44	125.98	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	VAL	N-CA-C	-5.40	100.43	107.88
1	C	220	GLN	N-CA-C	5.37	118.74	111.17
1	F	205	PRO	CA-C-N	5.23	124.94	119.82
1	F	205	PRO	C-N-CA	5.23	124.94	119.82
1	A	205	PRO	CA-C-N	5.21	126.36	119.84
1	A	205	PRO	C-N-CA	5.21	126.36	119.84

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	52	0
1	B	2144	0	2091	42	0
1	C	2144	0	2091	41	0
1	D	2144	0	2091	45	0
1	E	2155	0	2103	49	0
1	F	2155	0	2103	60	0
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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	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	280	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 (280) 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
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
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:C:20:TYR:HB2	1:C:61:MET:HE1	1.73	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:217:LEU:C	1:A:219:HIS:H	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLN:HG3	1:A:211:LYS:HD2	1.77	0.66
1:A:247:LYS:NZ	3:A:1277:SO4:O3	2.28	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: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:HH11	1:F:170:ARG:HB2	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: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
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:B:275:ASN:HD22	1:E:239:ASN:HB2	1.66	0.59
1:E:247:LYS:NZ	3:E:1278:SO4:S	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:65:MET:HE1	1:D:111:ILE:HD12	1.89	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:56:ILE:HD13	1:D:115:PHE:CZ	2.43	0.54
1:D:109:ARG:NE	6:D:2080:HOH:O	2.33	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:E:1:MET:N	1:E:23:ASP:OD2	2.34	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
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:A:217:LEU:C	1:A:219:HIS:N	2.67	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:249:LYS:NZ	6:C:2175:HOH:O	2.42	0.50
1:A:1:MET:HE3	1:F:20:TYR:CD2	2.46	0.50
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:D:35:PRO:HB2	1:D:65:MET:HE3	1.94	0.50
1:C:20:TYR:CB	1:C:61:MET:HE1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:158:ASP:OD1	1:B:160:THR:OG1	2.29	0.48
6:C:2060:HOH:O	1:D:27:ASP:OD1	2.20	0.48
1:D:249:LYS:NZ	6:D:2126:HOH:O	2.46	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:D:217:LEU:C	1:D:219:HIS:H	2.20	0.48
1:E:65:MET:HE3	1:E:65:MET:HB3	1.72	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
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:27:ASP:OD1	1:B:27:ASP:N	2.46	0.47
1:B:197:GLN:NE2	1:B:204:VAL:O	2.47	0.47
1:E:35:PRO:HB3	1:E:109[A]:ARG:HB3	1.97	0.47
1:E:258:TRP:CG	1:E:259:PRO:HD3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:49:SER:O	1:B:53:GLU:HG3	2.15	0.46
4:B:1278:QY9:CAG	1:C:99:GLN:HE22	2.29	0.46
1:C:275:ASN:OD1	1:D:239:ASN:HB2	2.16	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: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: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:27:ASP:N	1:A:27:ASP:OD1	2.51	0.44
1:A:106:ASP:OD2	1:A:109[A]:ARG:HD2	2.18	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
6:B:2157:HOH:O	1:E:275:ASN:HB2	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1:MET:N	1:D:23:ASP:OD2	2.29	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:36:ILE:HD11	1:F:68:VAL:HG23	1.99	0.43
1:F:220:GLN:N	1:F:220:GLN:OE1	2.51	0.43
1:A:77:GLY:C	1:A:79:GLN:H	2.26	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:B:240:HIS:CD2	1:E:273:ALA:HB3	2.54	0.43
1:C:132:PRO:HA	1:C:135:ARG:HB3	2.01	0.43
6:D:2012:HOH:O	1:E:6:ARG:NH1	2.36	0.43
1:B:181:ALA:HB1	1:B:183:GLN:CD	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ARG:HE	1:F:178:ARG:HB2	1.47	0.42
1:C:27:ASP:OD1	1:C:27:ASP:N	2.53	0.42
1:C:65:MET:HE3	1:C:65:MET:HB3	1.81	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:D:116:SER:OG	1:D:233:HIS:NE2	2.42	0.42
1:D:158:ASP:OD1	1:D:160:THR:OG1	2.25	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:D:131:GLN:O	1:D:135:ARG:N	2.49	0.41
1:D:202:GLU:HB2	5:D:1280:CCN:C1	2.50	0.41
1:E:235:LEU:HD12	1:E:235:LEU:HA	1.83	0.41
1:B:116:SER:OG	1:B:233:HIS:NE2	2.41	0.41
1:B:216:MET:HE3	1:B:221:VAL:HB	2.01	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: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:A:181:ALA:HB1	1:A:183:GLN:CD	2.45	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:154:TYR:CZ	1:E:234:GLY:HA2	2.56	0.41
1:E:219:HIS:HB2	6:E:2122:HOH:O	2.20	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:135:ARG:HG3	1:A:140:LEU:HB2	2.03	0.41
1:A:158:ASP:HA	1:A:180:TRP:O	2.20	0.41
1:A:275:ASN:OD1	1:F:239:ASN:HB2	2.21	0.41
1:B:6:ARG:HG3	6:B:2010:HOH:O	2.20	0.41
1:C:61:MET:HB2	1:C:61:MET:HE3	1.52	0.41
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:C:167:SER:O	1:C:170:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:D:170:ARG:HG3	1.70	0.40
1:A:61:MET:HE3	1:A:61:MET:HB2	1.69	0.40
1:D:89:LEU:HD13	1:D:125:TYR:CG	2.57	0.40
1:A:49:SER:O	1:A:53:GLU:HG3	2.22	0.40
1:A:183:GLN:O	1:A:186:VAL:HG23	2.21	0.40
1:B:178:ARG:HE	1:B:178:ARG:HB2	1.69	0.40
1:C:231:GLY:HA2	6:C:2157:HOH:O	2.21	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%)	30	38
1	B	275/282 (98%)	254 (92%)	21 (8%)	0	100	100
1	C	275/282 (98%)	251 (91%)	23 (8%)	1 (0%)	30	38
1	D	275/282 (98%)	254 (92%)	19 (7%)	2 (1%)	18	23
1	E	276/282 (98%)	256 (93%)	20 (7%)	0	100	100
1	F	276/282 (98%)	255 (92%)	20 (7%)	1 (0%)	30	38
All	All	1653/1692 (98%)	1525 (92%)	123 (7%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLN

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Mol	Chain	Res	Type
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%)	204 (92%)	17 (8%)	12	16
1	B	220/226 (97%)	206 (94%)	14 (6%)	16	23
1	C	220/226 (97%)	204 (93%)	16 (7%)	13	18
1	D	220/226 (97%)	203 (92%)	17 (8%)	12	16
1	E	221/226 (98%)	205 (93%)	16 (7%)	13	18
1	F	221/226 (98%)	208 (94%)	13 (6%)	18	26
All	All	1323/1356 (98%)	1230 (93%)	93 (7%)	14	19

All (93) 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	146	GLN
1	A	167	SER
1	A	179	LEU
1	A	184	ARG
1	A	186	VAL
1	A	207	ILE
1	A	210	LEU

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Mol	Chain	Res	Type
1	A	235	LEU
1	A	264	ARG
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	186	VAL
1	B	187	THR
1	B	207	ILE
1	B	210	LEU
1	B	235	LEU
1	B	264	ARG
1	B	272	LEU
1	C	6	ARG
1	C	22	LEU
1	C	32	VAL
1	C	65	MET
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	61	MET
1	D	78	ASP
1	D	89	LEU
1	D	167	SER
1	D	170	ARG

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Mol	Chain	Res	Type
1	D	178	ARG
1	D	179	LEU
1	D	203	SER
1	D	210	LEU
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	146	GLN
1	E	179	LEU
1	E	184	ARG
1	E	203	SER
1	E	210	LEU
1	E	235	LEU
1	E	264	ARG
1	E	272	LEU
1	E	275	ASN
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	185	LEU
1	F	210	LEU
1	F	221	VAL
1	F	235	LEU
1	F	264	ARG
1	F	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN

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Mol	Chain	Res	Type
1	B	104	HIS
1	B	254	GLN
1	C	99	GLN
1	C	131	GLN
1	D	9	ASN
1	D	131	GLN
1	D	214	GLN
1	E	5	GLN
1	E	131	GLN
1	E	226	HIS
1	E	240	HIS
1	E	269	GLN
1	F	131	GLN
1	F	142	HIS
1	F	275	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	SO4	A	1277	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	C	1278	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	D	1278	-	4,4,4	0.25	0	6,6,6	0.07	0
5	CCN	F	1280	-	2,2,2	0.83	0	1,1,1	0.50	0
4	QY9	A	1278	-	10,10,10	0.67	0	12,12,12	1.51	1 (8%)
5	CCN	B	1280	-	2,2,2	0.71	0	1,1,1	0.60	0
2	ACT	E	1276	-	3,3,3	0.65	0	3,3,3	1.63	1 (33%)
5	CCN	F	1279	-	2,2,2	0.79	0	1,1,1	0.56	0
2	ACT	A	1276	-	3,3,3	0.72	0	3,3,3	1.59	1 (33%)
4	QY9	F	1277	-	10,10,10	0.63	0	12,12,12	1.40	1 (8%)
5	CCN	A	1280	-	2,2,2	0.79	0	1,1,1	0.57	0
3	SO4	D	1277	-	4,4,4	0.19	0	6,6,6	0.13	0
5	CCN	A	1281	-	2,2,2	0.73	0	1,1,1	0.61	0
5	CCN	D	1280	-	2,2,2	0.72	0	1,1,1	0.53	0
5	CCN	D	1279	-	2,2,2	0.73	0	1,1,1	0.60	0
2	ACT	B	1276	-	3,3,3	0.88	0	3,3,3	1.36	0
4	QY9	B	1278	-	10,10,10	0.63	0	12,12,12	1.31	1 (8%)
5	CCN	A	1279	-	2,2,2	0.70	0	1,1,1	0.61	0
2	ACT	F	1276	-	3,3,3	0.91	0	3,3,3	1.24	0
3	SO4	B	1277	-	4,4,4	0.26	0	6,6,6	0.13	0
2	ACT	C	1276	-	3,3,3	0.82	0	3,3,3	1.49	0
5	CCN	F	1278	-	2,2,2	0.67	0	1,1,1	0.56	0
3	SO4	E	1277	-	4,4,4	0.26	0	6,6,6	0.35	0
5	CCN	E	1280	-	2,2,2	0.64	0	1,1,1	0.55	0
4	QY9	E	1279	-	10,10,10	0.66	0	12,12,12	1.33	1 (8%)
5	CCN	B	1279	-	2,2,2	0.67	0	1,1,1	0.59	0
3	SO4	C	1277	-	4,4,4	0.31	0	6,6,6	0.28	0
5	CCN	C	1280	-	2,2,2	0.75	0	1,1,1	0.59	0
2	ACT	D	1276	-	3,3,3	0.84	0	3,3,3	1.41	0
3	SO4	E	1278	-	4,4,4	0.25	0	6,6,6	0.10	0
4	QY9	C	1279	-	10,10,10	0.64	0	12,12,12	1.33	1 (8%)

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	B	1278	-	-	2/4/4/4	0/1/1/1
4	QY9	E	1279	-	-	2/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	QY9	F	1277	-	-	2/4/4/4	0/1/1/1
4	QY9	C	1279	-	-	0/4/4/4	0/1/1/1
4	QY9	A	1278	-	-	4/4/4/4	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1278	QY9	OAH-CAI-CAA	4.42	120.54	110.97
4	F	1277	QY9	OAH-CAI-CAA	4.08	119.81	110.97
4	C	1279	QY9	OAH-CAI-CAA	4.05	119.74	110.97
4	E	1279	QY9	OAH-CAI-CAA	3.75	119.10	110.97
4	B	1278	QY9	OAH-CAI-CAA	3.59	118.74	110.97
2	E	1276	ACT	OXT-C-CH3	2.21	124.34	115.05
2	A	1276	ACT	OXT-C-O	-2.01	114.58	122.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1278	QY9	OAB-CAI-OAH-CAJ
4	B	1278	QY9	CAA-CAI-OAH-CAJ
4	E	1279	QY9	CAA-CAI-OAH-CAJ
4	E	1279	QY9	OAB-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
3	A	1277	SO4	3	0
3	D	1278	SO4	1	0
5	F	1280	CCN	1	0
5	B	1280	CCN	2	0
5	F	1279	CCN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1277	SO4	1	0
5	A	1281	CCN	1	0
5	D	1280	CCN	1	0
5	D	1279	CCN	2	0
4	B	1278	QY9	3	0
2	C	1276	ACT	1	0
3	E	1278	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	276/282 (97%)	-0.31	7 (2%) 58 60	14, 37, 72, 95	2 (0%)
1	B	276/282 (97%)	-0.44	1 (0%) 88 89	13, 37, 74, 104	1 (0%)
1	C	276/282 (97%)	-0.47	1 (0%) 88 89	13, 38, 73, 101	1 (0%)
1	D	276/282 (97%)	-0.47	3 (1%) 78 79	14, 36, 73, 105	1 (0%)
1	E	276/282 (97%)	-0.47	0 100 100	14, 38, 75, 91	2 (0%)
1	F	276/282 (97%)	-0.45	3 (1%) 78 79	15, 37, 71, 87	2 (0%)
All	All	1656/1692 (97%)	-0.43	15 (0%) 81 82	13, 37, 73, 105	9 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	VAL	3.5
1	A	169	ALA	2.8
1	D	164	PRO	2.6
1	A	182	ALA	2.6
1	A	181	ALA	2.5
1	C	175	THR	2.5
1	D	173	ILE	2.3
1	A	134	LEU	2.3
1	A	128	VAL	2.3
1	F	177	ALA	2.3
1	B	276	TYR	2.2
1	A	189	ALA	2.2
1	F	179	LEU	2.2
1	D	163	PHE	2.1
1	F	205	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1277	5/5	0.95	0.10	105,106,107,108	0
3	SO4	B	1277	5/5	0.95	0.10	111,111,112,114	0
3	SO4	D	1278	5/5	0.95	0.11	108,109,110,110	0
3	SO4	E	1278	5/5	0.95	0.10	116,119,120,120	0
2	ACT	B	1276	4/4	0.96	0.08	38,39,45,53	0
5	CCN	A	1280	3/3	0.96	0.08	32,32,36,36	0
5	CCN	F	1280	3/3	0.96	0.08	19,19,30,34	0
4	QY9	C	1279	10/10	0.97	0.11	75,78,87,90	0
4	QY9	F	1277	10/10	0.97	0.12	70,74,81,84	0
5	CCN	A	1279	3/3	0.97	0.07	35,35,37,40	0
3	SO4	C	1278	5/5	0.97	0.11	111,111,113,114	0
5	CCN	B	1279	3/3	0.97	0.07	34,34,35,39	0
5	CCN	C	1280	3/3	0.97	0.07	38,38,39,42	0
5	CCN	E	1280	3/3	0.97	0.08	34,34,34,37	0
3	SO4	D	1277	5/5	0.97	0.09	110,110,112,112	0
5	CCN	A	1281	3/3	0.98	0.07	26,26,27,28	0
4	QY9	E	1279	10/10	0.98	0.08	67,72,73,74	0
5	CCN	B	1280	3/3	0.98	0.05	34,34,34,35	0
4	QY9	A	1278	10/10	0.98	0.09	59,64,71,73	0
5	CCN	D	1279	3/3	0.98	0.08	30,30,33,36	0
5	CCN	D	1280	3/3	0.98	0.07	34,34,37,38	0
4	QY9	B	1278	10/10	0.98	0.10	73,77,85,85	0
5	CCN	F	1278	3/3	0.98	0.06	34,34,36,38	0
5	CCN	F	1279	3/3	0.98	0.06	13,13,26,28	0
2	ACT	E	1276	4/4	0.98	0.08	28,31,37,50	0
2	ACT	D	1276	4/4	0.99	0.05	19,27,33,47	0
3	SO4	C	1277	5/5	0.99	0.06	39,40,46,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	1276	4/4	0.99	0.06	31,32,40,54	0
2	ACT	F	1276	4/4	0.99	0.06	32,35,40,51	0
2	ACT	C	1276	4/4	0.99	0.06	31,39,41,55	0
3	SO4	E	1277	5/5	0.99	0.07	37,44,47,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.