



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:30 PM UTC

PDB ID : 4QHS / pdb_00004qhs
Title : Crystal structure of AAA+sigma 54 activator domain of the flagellar regulatory protein FlrC of *Vibrio cholerae* in nucleotide free state
Authors : Dey, S.; Biswas, M.; Sen, U.; Dasgupta, J.
Deposited on : 2014-05-29
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

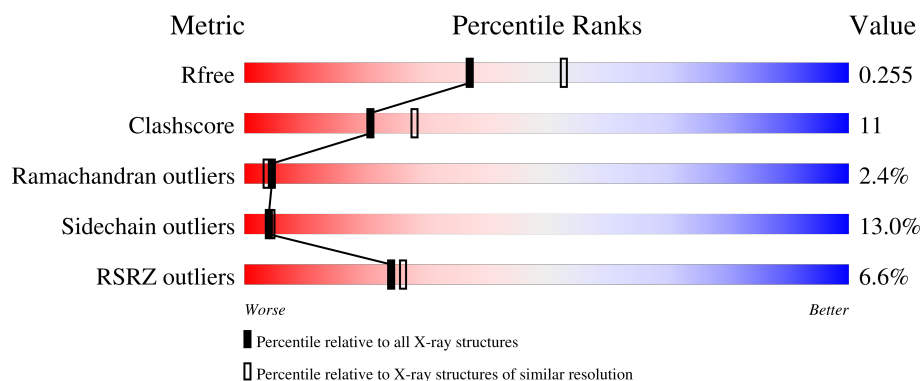
1 Overall quality at a glance

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	267	7% 65% 21% • 9%
1	B	267	8% 65% 19% 5% • 9%
1	C	267	5% 68% 20% • 9%
1	D	267	6% 64% 19% 7% • 9%
1	E	267	4% 67% 19% • • 9%

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Mol	Chain	Length	Quality of chain
1	F	267	6% 67% 19% • 9%
1	G	267	5% 69% 16% • • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14054 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 Flagellar regulatory protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1898	1202	338	350	8			
1	C	243	Total	C	N	O	S	0	1	0
			1901	1204	340	349	8			
1	B	243	Total	C	N	O	S	0	0	0
			1893	1199	337	349	8			
1	F	242	Total	C	N	O	S	0	0	0
			1888	1196	336	348	8			
1	G	243	Total	C	N	O	S	0	0	0
			1893	1199	337	349	8			
1	E	244	Total	C	N	O	S	0	0	0
			1898	1202	338	350	8			
1	D	244	Total	C	N	O	S	0	0	0
			1898	1202	338	350	8			

There are 119 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	HIS	-	expression tag	UNP A5F6D4
A	116	HIS	-	expression tag	UNP A5F6D4
A	117	HIS	-	expression tag	UNP A5F6D4
A	118	HIS	-	expression tag	UNP A5F6D4
A	119	HIS	-	expression tag	UNP A5F6D4
A	120	HIS	-	expression tag	UNP A5F6D4
A	121	SER	-	expression tag	UNP A5F6D4
A	122	SER	-	expression tag	UNP A5F6D4
A	123	GLY	-	expression tag	UNP A5F6D4
A	124	LEU	-	expression tag	UNP A5F6D4
A	125	VAL	-	expression tag	UNP A5F6D4
A	126	PRO	-	expression tag	UNP A5F6D4
A	127	ARG	-	expression tag	UNP A5F6D4
A	128	GLY	-	expression tag	UNP A5F6D4
A	129	SER	-	expression tag	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	130	HIS	-	expression tag	UNP A5F6D4
A	131	MET	-	expression tag	UNP A5F6D4
C	115	HIS	-	expression tag	UNP A5F6D4
C	116	HIS	-	expression tag	UNP A5F6D4
C	117	HIS	-	expression tag	UNP A5F6D4
C	118	HIS	-	expression tag	UNP A5F6D4
C	119	HIS	-	expression tag	UNP A5F6D4
C	120	HIS	-	expression tag	UNP A5F6D4
C	121	SER	-	expression tag	UNP A5F6D4
C	122	SER	-	expression tag	UNP A5F6D4
C	123	GLY	-	expression tag	UNP A5F6D4
C	124	LEU	-	expression tag	UNP A5F6D4
C	125	VAL	-	expression tag	UNP A5F6D4
C	126	PRO	-	expression tag	UNP A5F6D4
C	127	ARG	-	expression tag	UNP A5F6D4
C	128	GLY	-	expression tag	UNP A5F6D4
C	129	SER	-	expression tag	UNP A5F6D4
C	130	HIS	-	expression tag	UNP A5F6D4
C	131	MET	-	expression tag	UNP A5F6D4
B	115	HIS	-	expression tag	UNP A5F6D4
B	116	HIS	-	expression tag	UNP A5F6D4
B	117	HIS	-	expression tag	UNP A5F6D4
B	118	HIS	-	expression tag	UNP A5F6D4
B	119	HIS	-	expression tag	UNP A5F6D4
B	120	HIS	-	expression tag	UNP A5F6D4
B	121	SER	-	expression tag	UNP A5F6D4
B	122	SER	-	expression tag	UNP A5F6D4
B	123	GLY	-	expression tag	UNP A5F6D4
B	124	LEU	-	expression tag	UNP A5F6D4
B	125	VAL	-	expression tag	UNP A5F6D4
B	126	PRO	-	expression tag	UNP A5F6D4
B	127	ARG	-	expression tag	UNP A5F6D4
B	128	GLY	-	expression tag	UNP A5F6D4
B	129	SER	-	expression tag	UNP A5F6D4
B	130	HIS	-	expression tag	UNP A5F6D4
B	131	MET	-	expression tag	UNP A5F6D4
F	115	HIS	-	expression tag	UNP A5F6D4
F	116	HIS	-	expression tag	UNP A5F6D4
F	117	HIS	-	expression tag	UNP A5F6D4
F	118	HIS	-	expression tag	UNP A5F6D4
F	119	HIS	-	expression tag	UNP A5F6D4
F	120	HIS	-	expression tag	UNP A5F6D4

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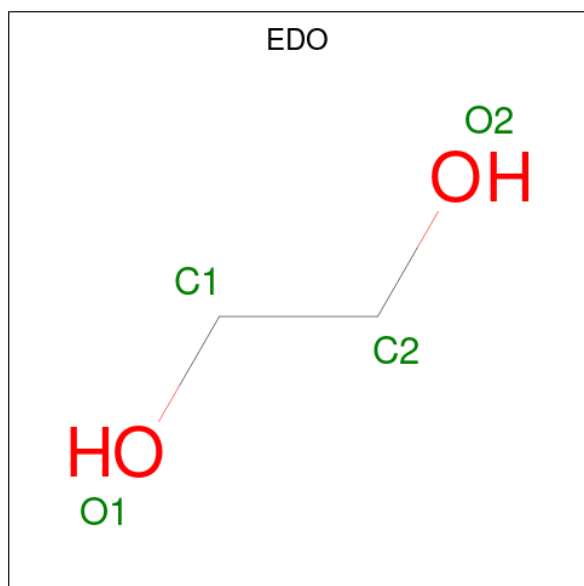
Chain	Residue	Modelled	Actual	Comment	Reference
F	121	SER	-	expression tag	UNP A5F6D4
F	122	SER	-	expression tag	UNP A5F6D4
F	123	GLY	-	expression tag	UNP A5F6D4
F	124	LEU	-	expression tag	UNP A5F6D4
F	125	VAL	-	expression tag	UNP A5F6D4
F	126	PRO	-	expression tag	UNP A5F6D4
F	127	ARG	-	expression tag	UNP A5F6D4
F	128	GLY	-	expression tag	UNP A5F6D4
F	129	SER	-	expression tag	UNP A5F6D4
F	130	HIS	-	expression tag	UNP A5F6D4
F	131	MET	-	expression tag	UNP A5F6D4
G	115	HIS	-	expression tag	UNP A5F6D4
G	116	HIS	-	expression tag	UNP A5F6D4
G	117	HIS	-	expression tag	UNP A5F6D4
G	118	HIS	-	expression tag	UNP A5F6D4
G	119	HIS	-	expression tag	UNP A5F6D4
G	120	HIS	-	expression tag	UNP A5F6D4
G	121	SER	-	expression tag	UNP A5F6D4
G	122	SER	-	expression tag	UNP A5F6D4
G	123	GLY	-	expression tag	UNP A5F6D4
G	124	LEU	-	expression tag	UNP A5F6D4
G	125	VAL	-	expression tag	UNP A5F6D4
G	126	PRO	-	expression tag	UNP A5F6D4
G	127	ARG	-	expression tag	UNP A5F6D4
G	128	GLY	-	expression tag	UNP A5F6D4
G	129	SER	-	expression tag	UNP A5F6D4
G	130	HIS	-	expression tag	UNP A5F6D4
G	131	MET	-	expression tag	UNP A5F6D4
E	115	HIS	-	expression tag	UNP A5F6D4
E	116	HIS	-	expression tag	UNP A5F6D4
E	117	HIS	-	expression tag	UNP A5F6D4
E	118	HIS	-	expression tag	UNP A5F6D4
E	119	HIS	-	expression tag	UNP A5F6D4
E	120	HIS	-	expression tag	UNP A5F6D4
E	121	SER	-	expression tag	UNP A5F6D4
E	122	SER	-	expression tag	UNP A5F6D4
E	123	GLY	-	expression tag	UNP A5F6D4
E	124	LEU	-	expression tag	UNP A5F6D4
E	125	VAL	-	expression tag	UNP A5F6D4
E	126	PRO	-	expression tag	UNP A5F6D4
E	127	ARG	-	expression tag	UNP A5F6D4
E	128	GLY	-	expression tag	UNP A5F6D4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	SER	-	expression tag	UNP A5F6D4
E	130	HIS	-	expression tag	UNP A5F6D4
E	131	MET	-	expression tag	UNP A5F6D4
D	115	HIS	-	expression tag	UNP A5F6D4
D	116	HIS	-	expression tag	UNP A5F6D4
D	117	HIS	-	expression tag	UNP A5F6D4
D	118	HIS	-	expression tag	UNP A5F6D4
D	119	HIS	-	expression tag	UNP A5F6D4
D	120	HIS	-	expression tag	UNP A5F6D4
D	121	SER	-	expression tag	UNP A5F6D4
D	122	SER	-	expression tag	UNP A5F6D4
D	123	GLY	-	expression tag	UNP A5F6D4
D	124	LEU	-	expression tag	UNP A5F6D4
D	125	VAL	-	expression tag	UNP A5F6D4
D	126	PRO	-	expression tag	UNP A5F6D4
D	127	ARG	-	expression tag	UNP A5F6D4
D	128	GLY	-	expression tag	UNP A5F6D4
D	129	SER	-	expression tag	UNP A5F6D4
D	130	HIS	-	expression tag	UNP A5F6D4
D	131	MET	-	expression tag	UNP A5F6D4

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

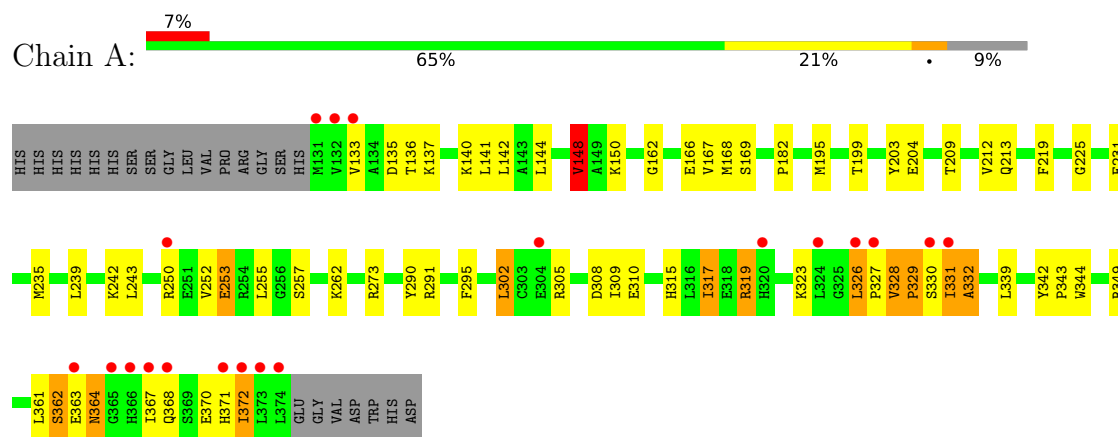
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 95 95	0	0
3	C	109	Total O 109 109	0	0
3	B	108	Total O 108 108	0	0
3	F	107	Total O 107 107	0	0
3	G	134	Total O 134 134	0	0
3	E	105	Total O 105 105	0	0
3	D	99	Total O 99 99	0	0

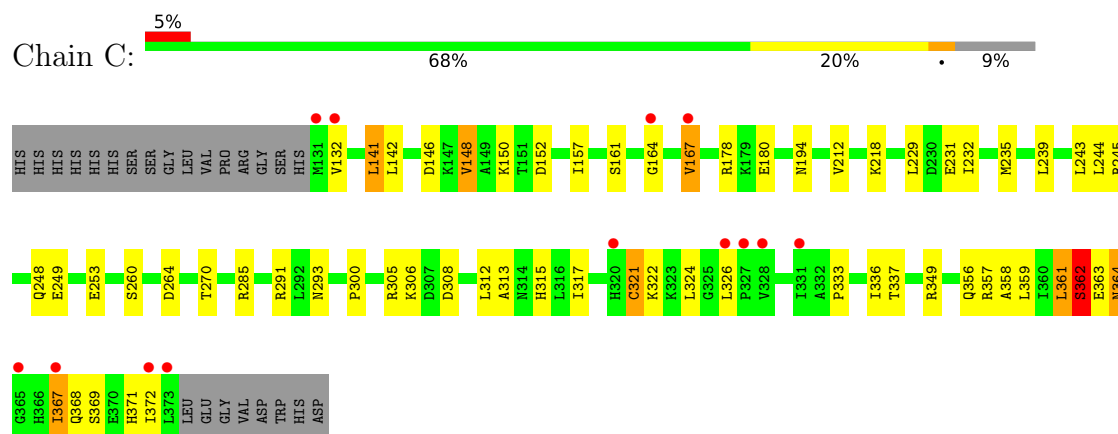
3 Residue-property plots [i](#)

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.

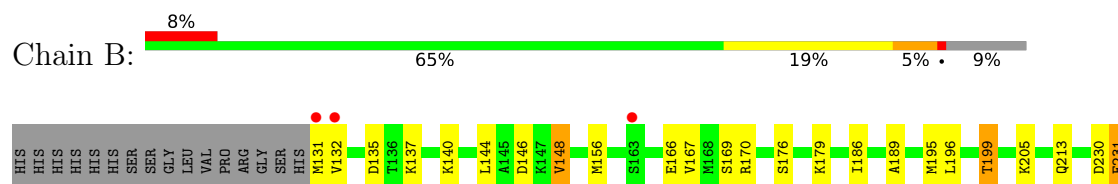
• Molecule 1: Flagellar regulatory protein C

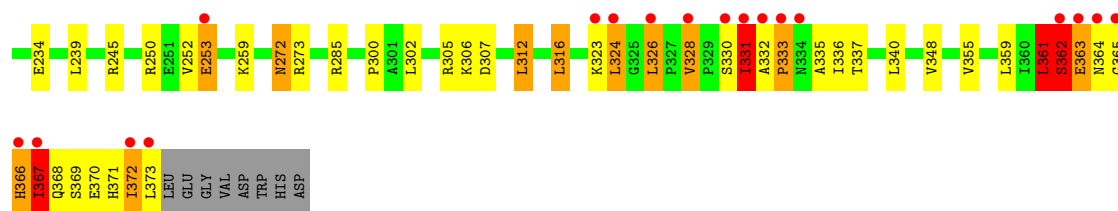


• Molecule 1: Flagellar regulatory protein C

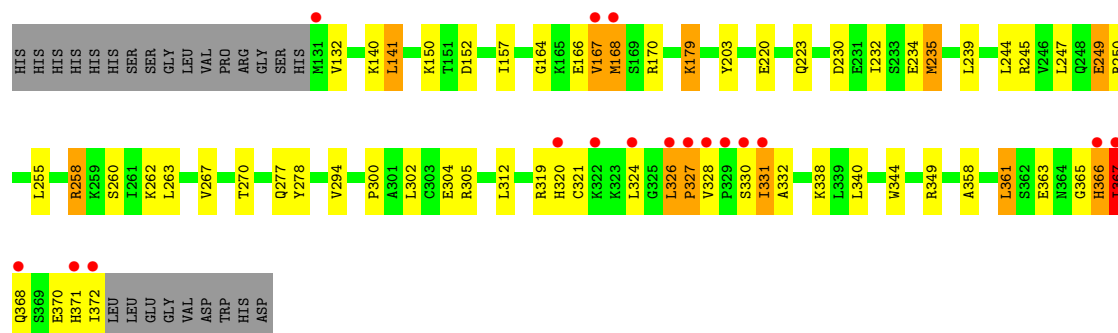


• Molecule 1: Flagellar regulatory protein C

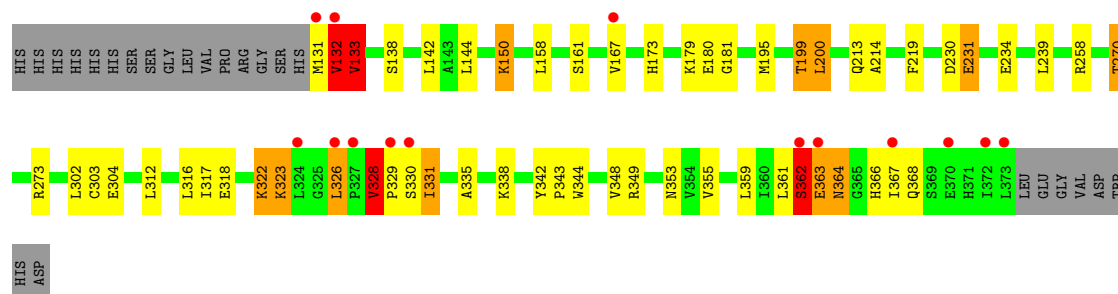




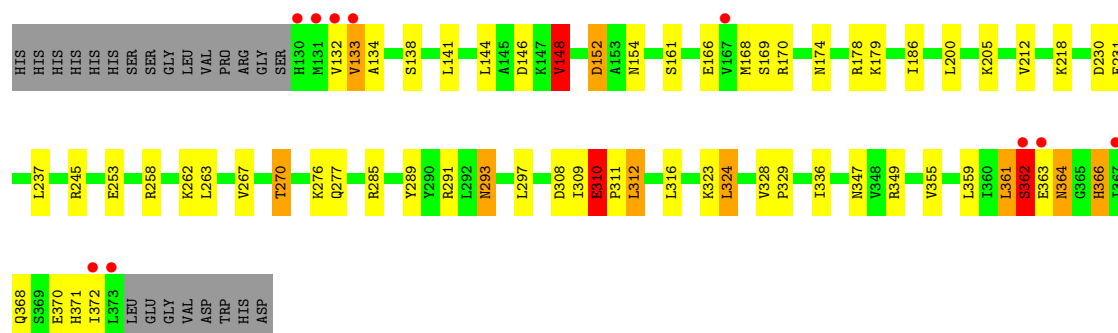
• Molecule 1: Flagellar regulatory protein C



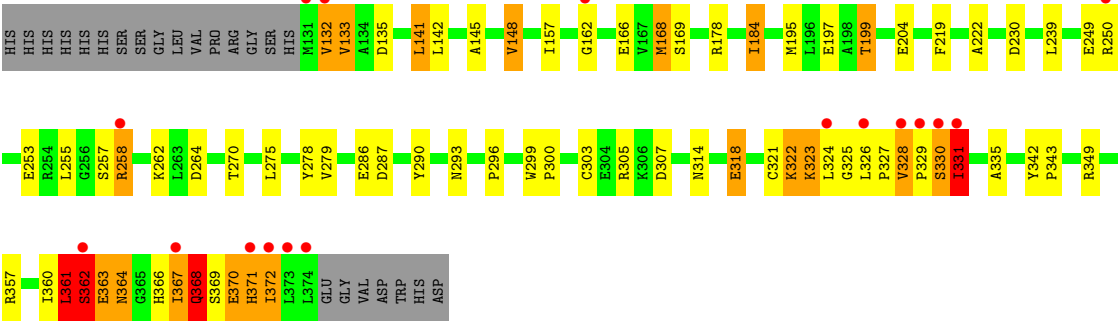
• Molecule 1: Flagellar regulatory protein C



• Molecule 1: Flagellar regulatory protein C



• Molecule 1: Flagellar regulatory protein C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.29Å 153.28Å 193.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.30 49.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.0 (49.39-2.30) 85.4 (49.39-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.192 , 0.255 0.204 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14054	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.26	2/1932 (0.1%)	0.91	2/2616 (0.1%)
1	B	0.85	0/1927	0.89	1/2609 (0.0%)
1	C	0.62	0/1938	0.87	2/2623 (0.1%)
1	D	0.79	0/1932	0.92	2/2616 (0.1%)
1	E	0.79	0/1932	0.87	5/2616 (0.2%)
1	F	1.01	1/1922 (0.1%)	0.90	1/2602 (0.0%)
1	G	0.90	0/1927	0.89	2/2609 (0.1%)
All	All	0.91	3/13510 (0.0%)	0.89	15/18291 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	TRP	C-O	-9.54	1.19	1.23
1	F	344	TRP	C-O	-8.16	1.20	1.23
1	A	310	GLU	C-O	-5.29	1.19	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	SER	N-CA-C	7.82	118.56	108.24
1	F	366	HIS	N-CA-C	7.39	116.99	108.49
1	A	148	VAL	CB-CA-C	-6.75	103.03	112.14
1	D	148	VAL	CB-CA-C	-6.73	103.05	112.14
1	D	363	GLU	N-CA-C	6.73	120.62	108.17
1	G	328	VAL	CA-C-N	6.41	126.42	119.89
1	G	328	VAL	C-N-CA	6.41	126.42	119.89
1	E	347	ASN	CB-CA-C	-6.19	109.42	116.54
1	B	148	VAL	CB-CA-C	-5.89	104.09	112.22
1	A	309	ILE	N-CA-C	5.38	115.82	110.23
1	E	366	HIS	N-CA-C	5.29	116.78	109.54
1	E	148	VAL	CB-CA-C	-5.14	103.94	112.26
1	C	148	VAL	CB-CA-C	-5.11	104.24	112.16
1	E	310	GLU	CA-C-N	-5.11	113.38	119.05
1	E	310	GLU	C-N-CA	-5.11	113.38	119.05

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	LEU	Peptide
1	B	362	SER	Peptide
1	C	361	LEU	Peptide
1	D	361	LEU	Peptide
1	D	362	SER	Peptide
1	D	368	GLN	Peptide
1	E	361	LEU	Peptide
1	F	370	GLU	Peptide
1	G	361	LEU	Peptide
1	G	362	SER	Peptide

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	1898	0	1933	43	0
1	B	1893	0	1931	40	0
1	C	1901	0	1944	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1898	0	1933	67	0
1	E	1898	0	1933	36	0
1	F	1888	0	1929	32	0
1	G	1893	0	1931	42	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	C	4	0	6	1	0
2	D	4	0	6	0	0
2	E	4	0	6	1	0
2	F	4	0	6	0	0
2	G	4	0	6	0	0
3	A	95	0	0	8	0
3	B	108	0	0	8	0
3	C	109	0	0	11	0
3	D	99	0	0	14	0
3	E	105	0	0	8	0
3	F	107	0	0	2	0
3	G	134	0	0	5	0
All	All	14054	0	13576	298	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 (298) 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:273:ARG:NH1	3:A:567:HOH:O	1.77	1.17
1:D:364:ASN:ND2	3:D:501:HOH:O	1.81	1.11
1:D:286:GLU:O	3:D:567:HOH:O	1.76	1.03
1:D:371:HIS:O	1:D:372:ILE:HG23	1.60	0.99
1:F:167:VAL:HG22	1:F:168:MET:N	1.83	0.94
1:G:231:GLU:H	1:G:270:THR:HG22	1.31	0.92
1:E:133:VAL:HG23	1:E:308:ASP:OD1	1.71	0.91
1:B:213:GLN:NE2	3:B:572:HOH:O	2.07	0.87
1:D:329:PRO:O	1:D:331:ILE:N	2.08	0.86
1:G:181:GLY:O	3:G:589:HOH:O	1.95	0.84
1:D:290:TYR:N	3:D:567:HOH:O	1.91	0.84
1:G:364:ASN:OD1	3:G:566:HOH:O	1.96	0.83
1:G:131:MET:O	1:G:132:VAL:HG23	1.79	0.83
1:A:363:GLU:OE1	3:A:593:HOH:O	1.97	0.81
1:F:167:VAL:CG2	1:F:168:MET:N	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:HIS:O	1:D:372:ILE:CG2	2.29	0.80
1:D:371:HIS:O	1:D:372:ILE:CG1	2.30	0.80
1:B:272:ASN:C	1:B:272:ASN:HD22	1.86	0.79
1:C:368:GLN:NE2	3:C:581:HOH:O	2.14	0.77
1:D:363:GLU:O	1:D:364:ASN:HB2	1.85	0.76
1:D:371:HIS:C	1:D:372:ILE:HG13	2.09	0.76
1:B:365:GLY:O	1:B:366:HIS:ND1	2.19	0.76
1:B:306:LYS:NZ	3:B:521:HOH:O	2.20	0.74
1:A:135:ASP:O	1:A:137:LYS:N	2.20	0.74
1:D:371:HIS:O	1:D:372:ILE:HG13	1.87	0.74
1:C:368:GLN:O	3:C:525:HOH:O	2.06	0.73
1:G:131:MET:C	1:G:132:VAL:HG23	2.14	0.73
1:B:300:PRO:HG2	1:B:305:ARG:HD3	1.68	0.73
1:A:213:GLN:OE1	3:A:552:HOH:O	2.06	0.73
1:C:291:ARG:HD2	3:C:516:HOH:O	1.88	0.72
1:D:368:GLN:C	1:D:368:GLN:NE2	2.48	0.72
1:G:326:LEU:HD13	1:G:326:LEU:H	1.55	0.72
1:E:170:ARG:NH1	1:E:174:ASN:OD1	2.23	0.71
1:D:329:PRO:O	3:D:536:HOH:O	2.09	0.71
1:C:357:ARG:NH1	3:C:559:HOH:O	2.07	0.70
1:A:363:GLU:O	1:A:364:ASN:HB3	1.92	0.70
1:F:300:PRO:HG2	1:F:305:ARG:HD3	1.71	0.70
1:B:131:MET:N	3:B:566:HOH:O	2.25	0.69
1:C:300:PRO:HG2	1:C:305:ARG:HD3	1.72	0.69
1:C:358:ALA:HA	1:C:368:GLN:HG2	1.72	0.69
1:F:157:ILE:HB	1:F:270:THR:HG22	1.74	0.69
1:A:328:VAL:HG11	1:A:363:GLU:HG3	1.74	0.69
1:G:131:MET:C	1:G:132:VAL:CG2	2.65	0.69
1:D:321:CYS:O	1:D:323:LYS:N	2.22	0.69
1:D:258:ARG:NH1	3:D:591:HOH:O	2.24	0.68
1:A:231:GLU:OE2	3:A:506:HOH:O	2.11	0.68
1:D:132:VAL:O	3:D:578:HOH:O	2.11	0.67
1:A:362:SER:OG	3:A:559:HOH:O	2.04	0.67
1:G:328:VAL:HG11	1:G:364:ASN:H	1.59	0.67
1:D:363:GLU:O	1:D:364:ASN:CB	2.43	0.67
1:G:335:ALA:HB2	1:G:366:HIS:O	1.94	0.66
1:B:272:ASN:HD22	1:B:273:ARG:N	1.94	0.65
1:D:368:GLN:NE2	1:D:368:GLN:O	2.30	0.65
1:G:329:PRO:O	1:G:331:ILE:N	2.26	0.65
1:G:234:GLU:OE2	1:G:273:ARG:NH1	2.29	0.65
1:G:366:HIS:O	1:G:367:ILE:HD12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:O	1:A:364:ASN:CB	2.46	0.64
1:A:319:ARG:NH2	3:A:588:HOH:O	2.18	0.64
1:G:131:MET:O	1:G:133:VAL:N	2.29	0.64
1:G:173:HIS:NE2	3:G:589:HOH:O	2.10	0.64
1:B:333:PRO:HB3	1:B:337:THR:HG23	1.80	0.64
1:E:291:ARG:NH1	3:E:585:HOH:O	2.29	0.64
1:D:300:PRO:HG2	1:D:305:ARG:HD3	1.80	0.64
1:F:320:HIS:O	1:F:320:HIS:ND1	2.30	0.63
1:B:272:ASN:C	1:B:272:ASN:ND2	2.57	0.62
1:D:329:PRO:HD2	1:D:364:ASN:ND2	2.15	0.62
1:E:133:VAL:HG23	1:E:308:ASP:CG	2.25	0.62
1:E:133:VAL:CG2	1:E:134:ALA:N	2.63	0.61
1:D:371:HIS:O	1:D:372:ILE:CB	2.49	0.61
1:E:205:LYS:NZ	3:E:576:HOH:O	2.32	0.61
1:F:220:GLU:OE2	3:F:563:HOH:O	2.16	0.60
1:E:293:ASN:ND2	3:E:536:HOH:O	2.33	0.60
1:A:329:PRO:C	1:A:331:ILE:N	2.59	0.60
1:C:245[B]:ARG:NH1	1:C:253:GLU:OE1	2.35	0.60
1:B:166:GLU:HG2	1:B:167:VAL:N	2.16	0.60
1:B:137:LYS:HD3	1:B:300:PRO:HG3	1.84	0.59
1:B:205:LYS:NZ	3:B:552:HOH:O	2.29	0.59
1:D:230:ASP:OD1	1:D:270:THR:OG1	2.18	0.59
1:D:372:ILE:HD12	1:D:372:ILE:O	2.02	0.59
1:A:327:PRO:C	1:A:329:PRO:HD2	2.28	0.59
1:F:164:GLY:HA2	1:F:166:GLU:OE2	2.02	0.59
1:E:152:ASP:OD2	1:E:178:ARG:NH1	2.35	0.59
1:A:361:LEU:O	1:A:362:SER:CB	2.51	0.58
1:E:146:ASP:OD2	3:E:579:HOH:O	2.17	0.58
1:D:357:ARG:NH2	3:D:574:HOH:O	2.34	0.58
1:F:167:VAL:HG22	1:F:168:MET:H	1.68	0.58
1:A:329:PRO:C	1:A:331:ILE:H	2.11	0.58
1:D:195:MET:O	1:D:199:THR:HG23	2.03	0.58
1:D:371:HIS:C	1:D:372:ILE:HG23	2.28	0.57
1:C:218:LYS:NZ	3:C:566:HOH:O	2.36	0.57
1:E:231:GLU:H	1:E:270:THR:HG22	1.70	0.56
1:A:331:ILE:O	1:A:332:ALA:C	2.48	0.56
1:D:368:GLN:C	1:D:368:GLN:HE21	2.13	0.56
1:A:305:ARG:HD2	1:A:308:ASP:OD2	2.05	0.56
1:A:315:HIS:O	1:A:319:ARG:HB3	2.05	0.56
1:A:363:GLU:OE2	1:A:363:GLU:N	2.39	0.56
1:E:133:VAL:HG22	1:E:134:ALA:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:HG2	1:B:167:VAL:HG13	1.87	0.55
1:A:326:LEU:HD22	1:A:326:LEU:H	1.72	0.55
1:G:359:LEU:O	1:G:362:SER:HA	2.06	0.55
1:B:366:HIS:O	1:B:367:ILE:HB	2.05	0.55
1:G:331:ILE:HG22	1:G:335:ALA:HB3	1.88	0.55
1:C:146:ASP:O	1:C:150:LYS:NZ	2.38	0.55
1:D:366:HIS:C	1:D:367:ILE:HG13	2.33	0.54
1:B:364:ASN:N	3:B:578:HOH:O	2.40	0.54
1:D:366:HIS:HB3	1:D:367:ILE:HG13	1.89	0.54
1:E:133:VAL:HG21	1:E:138:SER:CB	2.37	0.54
1:C:367:ILE:O	1:C:368:GLN:NE2	2.40	0.54
1:E:323:LYS:HE3	1:E:324:LEU:HD13	1.90	0.53
1:A:252:VAL:HG22	1:A:253:GLU:N	2.23	0.53
1:E:285:ARG:HB3	2:E:401:EDO:H21	1.90	0.53
1:D:329:PRO:C	1:D:331:ILE:H	2.13	0.53
1:E:133:VAL:HG21	1:E:138:SER:HB2	1.91	0.53
1:D:366:HIS:HD2	3:D:558:HOH:O	1.92	0.53
1:G:318:GLU:O	1:G:322:LYS:HG2	2.08	0.52
1:C:308:ASP:O	1:C:312:LEU:HB2	2.10	0.52
1:B:189:ALA:HB2	1:B:234:GLU:HG3	1.91	0.52
1:F:166:GLU:H	1:F:166:GLU:CD	2.18	0.52
1:D:331:ILE:HG23	1:D:335:ALA:HB3	1.91	0.52
1:E:186:ILE:HG21	1:E:200:LEU:HD21	1.92	0.52
1:E:289:TYR:O	1:E:293:ASN:HB2	2.09	0.52
1:E:179:LYS:NZ	3:E:594:HOH:O	2.41	0.52
1:C:244:LEU:O	1:C:248:GLN:HG3	2.11	0.51
1:E:148:VAL:HG13	1:D:360:ILE:HG21	1.92	0.51
1:G:338:LYS:NZ	1:G:367:ILE:HG23	2.26	0.51
1:D:371:HIS:C	1:D:372:ILE:CG1	2.76	0.51
1:A:317:ILE:HG21	1:A:329:PRO:HD3	1.93	0.51
1:B:195:MET:O	1:B:199:THR:HG23	2.11	0.51
1:E:359:LEU:O	1:E:362:SER:HA	2.11	0.50
1:C:161:SER:N	3:C:520:HOH:O	2.36	0.50
1:G:195:MET:O	1:G:199:THR:HG23	2.11	0.50
1:A:342:TYR:CD1	1:A:343:PRO:HD2	2.46	0.50
1:A:329:PRO:O	1:A:331:ILE:N	2.43	0.50
1:F:164:GLY:O	1:F:167:VAL:HG13	2.11	0.50
1:E:166:GLU:HB2	3:E:604:HOH:O	2.11	0.50
1:B:176:SER:O	1:B:179:LYS:HE2	2.12	0.50
1:A:331:ILE:O	1:A:332:ALA:O	2.30	0.49
1:A:195:MET:O	1:A:199:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:ILE:O	1:G:367:ILE:HG22	2.13	0.49
1:B:333:PRO:C	1:B:335:ALA:H	2.19	0.49
1:F:235:MET:HE3	1:F:239:LEU:HG	1.95	0.49
1:D:204:GLU:HG3	1:D:257:SER:HB2	1.94	0.49
1:G:213:GLN:HG2	1:G:214:ALA:O	2.13	0.49
1:D:135:ASP:OD2	1:D:307:ASP:HB2	2.12	0.49
1:D:293:ASN:OD1	1:D:296:PRO:HG3	2.12	0.49
1:D:328:VAL:HG12	1:D:363:GLU:OE2	2.12	0.49
1:B:245:ARG:NH1	3:B:594:HOH:O	2.45	0.48
1:F:371:HIS:O	1:F:371:HIS:ND1	2.46	0.48
1:G:179:LYS:O	3:G:589:HOH:O	2.20	0.48
1:A:148:VAL:HG22	1:A:295:PHE:CE2	2.48	0.48
1:C:367:ILE:O	1:C:367:ILE:HD12	2.14	0.48
1:D:314:ASN:OD1	1:D:330:SER:HA	2.13	0.48
1:C:368:GLN:HB3	3:C:580:HOH:O	2.12	0.48
1:F:330:SER:OG	1:F:331:ILE:N	2.45	0.48
1:C:164:GLY:O	1:C:167:VAL:HG13	2.13	0.48
1:F:365:GLY:O	1:F:366:HIS:CG	2.67	0.48
1:C:364:ASN:OD1	3:C:530:HOH:O	2.20	0.47
1:G:342:TYR:HD2	1:G:344:TRP:CD2	2.32	0.47
1:D:262:LYS:HD2	1:D:262:LYS:N	2.29	0.47
1:D:287:ASP:C	3:D:567:HOH:O	2.56	0.47
1:B:337:THR:HA	1:B:340:LEU:HB2	1.95	0.47
1:E:329:PRO:CB	1:E:364:ASN:H	2.27	0.47
1:D:314:ASN:O	1:D:318:GLU:HG2	2.15	0.47
1:A:203:TYR:HB3	1:A:255:LEU:HB2	1.97	0.47
1:C:245[A]:ARG:NH1	1:C:249:GLU:HG3	2.30	0.46
1:F:247:LEU:HD21	1:F:267:VAL:HG21	1.97	0.46
1:D:361:LEU:O	1:D:362:SER:HB2	2.14	0.46
1:C:285:ARG:HB3	2:C:401:EDO:H12	1.98	0.46
1:C:371:HIS:ND1	1:C:371:HIS:O	2.48	0.46
1:F:300:PRO:HA	3:F:512:HOH:O	2.16	0.46
1:F:365:GLY:O	1:F:366:HIS:ND1	2.49	0.46
1:B:331:ILE:HD13	1:B:331:ILE:HA	1.69	0.46
1:E:308:ASP:O	1:E:312:LEU:HB2	2.16	0.46
1:E:309:ILE:O	1:E:310:GLU:HB3	2.16	0.46
1:D:303:CYS:HB3	1:D:343:PRO:O	2.15	0.46
1:C:212:VAL:HG22	3:D:591:HOH:O	2.16	0.46
1:C:356:GLN:NE2	3:C:550:HOH:O	2.35	0.46
1:D:318:GLU:O	1:D:322:LYS:HG2	2.15	0.46
1:F:141:LEU:HD13	1:F:141:LEU:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:ALA:HB1	1:F:366:HIS:CD2	2.51	0.45
1:E:309:ILE:O	1:E:311:PRO:HD2	2.17	0.45
1:A:291:ARG:NH1	3:A:533:HOH:O	2.50	0.45
1:G:312:LEU:HD21	1:G:348:VAL:HG22	1.98	0.45
1:F:258:ARG:HE	1:F:258:ARG:HB3	1.27	0.45
1:D:157:ILE:HB	1:D:270:THR:HG22	1.98	0.45
1:A:290:TYR:O	1:G:353:ASN:ND2	2.49	0.45
1:A:317:ILE:CG2	1:A:329:PRO:HD3	2.47	0.45
1:E:218:LYS:NZ	3:E:596:HOH:O	2.49	0.45
1:D:323:LYS:HB2	1:D:323:LYS:HE3	1.38	0.45
1:C:157:ILE:HB	1:C:270:THR:HG22	1.98	0.45
1:F:366:HIS:HB3	1:F:367:ILE:H	1.50	0.45
1:D:275:LEU:O	1:D:279:VAL:HG23	2.16	0.45
1:B:166:GLU:HG2	1:B:167:VAL:H	1.80	0.45
1:G:338:LYS:HZ2	1:G:367:ILE:HG23	1.81	0.45
1:C:361:LEU:O	1:C:362:SER:HB2	2.16	0.45
1:E:161:SER:OG	1:E:231:GLU:OE1	2.21	0.45
1:D:370:GLU:O	1:D:372:ILE:N	2.50	0.45
1:A:370:GLU:N	1:A:371:HIS:HA	2.32	0.45
1:G:328:VAL:HG11	1:G:364:ASN:N	2.28	0.45
1:D:141:LEU:HD23	1:D:299:TRP:CE3	2.52	0.45
1:A:219:PHE:HB2	3:A:513:HOH:O	2.17	0.44
1:A:328:VAL:O	1:A:329:PRO:C	2.60	0.44
1:C:363:GLU:O	1:C:364:ASN:HB2	2.16	0.44
1:G:200:LEU:HA	1:G:200:LEU:HD12	1.77	0.44
1:D:162:GLY:HA3	1:D:349:ARG:HG3	1.99	0.44
1:G:328:VAL:HG13	1:G:363:GLU:HG3	1.99	0.44
1:G:161:SER:OG	1:G:231:GLU:OE2	2.35	0.44
1:D:145:ALA:HB2	1:D:168:MET:HE1	1.99	0.44
1:C:178:ARG:NH2	1:C:264:ASP:O	2.51	0.44
1:B:156:MET:HE2	1:B:156:MET:HB2	1.81	0.44
1:G:342:TYR:HA	1:G:343:PRO:HD3	1.73	0.44
1:F:250:ARG:HD3	1:F:250:ARG:HA	1.50	0.44
1:G:326:LEU:HD13	1:G:326:LEU:N	2.26	0.43
1:A:235:MET:HE1	1:A:243:LEU:HD22	2.00	0.43
1:B:135:ASP:OD1	1:B:307:ASP:HB2	2.18	0.43
1:A:162:GLY:HA3	1:A:349:ARG:HG3	2.00	0.43
1:F:203:TYR:HB3	1:F:255:LEU:HB2	2.00	0.43
1:E:133:VAL:CG2	1:E:138:SER:HB2	2.48	0.43
1:D:318:GLU:HG2	1:D:318:GLU:H	1.60	0.43
1:C:132:VAL:HG11	1:C:315:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:THR:N	3:B:562:HOH:O	2.51	0.43
1:A:250:ARG:HA	1:A:250:ARG:HD3	1.51	0.43
1:B:285:ARG:HB3	2:B:401:EDO:H12	2.01	0.43
1:D:369:SER:C	1:D:370:GLU:HG2	2.44	0.43
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.70	0.43
1:B:361:LEU:O	1:B:362:SER:HB2	2.19	0.43
1:G:179:LYS:HB2	1:G:179:LYS:HE3	1.70	0.43
1:B:326:LEU:H	1:B:326:LEU:HG	1.40	0.43
1:G:328:VAL:HA	1:G:329:PRO:HD3	1.89	0.43
1:D:197:GLU:HG2	1:D:255:LEU:HD11	2.01	0.43
1:E:336:ILE:HD13	1:E:336:ILE:HA	1.85	0.43
1:A:372:ILE:HG23	1:A:372:ILE:O	2.19	0.43
1:C:141:LEU:HD13	1:C:141:LEU:HA	1.83	0.42
1:C:235:MET:HE1	1:C:243:LEU:HD22	2.00	0.42
1:C:359:LEU:O	1:C:362:SER:HA	2.19	0.42
1:F:300:PRO:HB2	1:F:304:GLU:HB2	2.00	0.42
1:G:328:VAL:CG1	1:G:363:GLU:HG3	2.49	0.42
1:B:333:PRO:HA	1:B:336:ILE:HB	2.01	0.42
1:A:182:PRO:HD2	1:A:225:GLY:HA3	2.01	0.42
1:B:372:ILE:HB	1:B:373:LEU:H	1.74	0.42
1:D:328:VAL:CG1	1:D:363:GLU:OE2	2.68	0.42
1:B:252:VAL:HG22	1:B:253:GLU:N	2.35	0.42
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.87	0.42
1:E:154:ASN:HA	1:E:267:VAL:O	2.20	0.42
1:D:368:GLN:C	1:D:368:GLN:CD	2.82	0.42
1:B:231:GLU:HG3	3:B:504:HOH:O	2.19	0.42
1:D:342:TYR:HA	1:D:343:PRO:HD3	1.83	0.42
1:C:333:PRO:O	1:C:337:THR:HG23	2.19	0.41
1:B:312:LEU:HD22	1:B:316:LEU:HD22	2.01	0.41
1:D:219:PHE:HB2	3:D:529:HOH:O	2.19	0.41
1:C:291:ARG:NH1	3:C:516:HOH:O	1.95	0.41
1:B:359:LEU:O	1:B:362:SER:HA	2.20	0.41
1:G:326:LEU:H	1:G:326:LEU:CD1	2.21	0.41
1:A:204:GLU:HG3	1:A:257:SER:HB2	2.00	0.41
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.87	0.41
1:G:302:LEU:C	1:G:304:GLU:H	2.28	0.41
1:D:197:GLU:OE2	3:D:557:HOH:O	2.22	0.41
1:A:166:GLU:HG2	1:A:167:VAL:HG13	2.01	0.41
1:C:293:ASN:ND2	3:C:543:HOH:O	2.53	0.41
1:C:317:ILE:O	1:C:321:CYS:HB2	2.20	0.41
1:B:330:SER:HA	1:B:366:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:LEU:HD23	1:F:340:LEU:HA	1.85	0.41
1:D:325:GLY:O	1:D:327:PRO:HD3	2.20	0.41
1:D:364:ASN:HA	3:D:536:HOH:O	2.21	0.41
1:D:178:ARG:NH2	1:D:264:ASP:O	2.54	0.41
1:D:322:LYS:HA	1:D:322:LYS:HD3	1.70	0.41
1:D:372:ILE:HD12	1:D:372:ILE:C	2.46	0.41
1:C:333:PRO:O	1:C:336:ILE:HB	2.20	0.41
1:F:232:ILE:C	1:F:234:GLU:H	2.27	0.41
1:B:362:SER:OG	1:B:363:GLU:N	2.51	0.41
1:F:245:ARG:HG2	1:F:249:GLU:HG3	2.03	0.41
1:G:150:LYS:HE2	1:G:150:LYS:HB2	1.83	0.41
1:E:133:VAL:HG21	1:E:138:SER:HB3	2.02	0.41
1:A:252:VAL:CG2	1:A:253:GLU:N	2.83	0.41
1:A:371:HIS:O	1:A:372:ILE:HG22	2.20	0.41
1:F:361:LEU:HD12	1:F:361:LEU:HA	1.88	0.41
1:D:371:HIS:C	1:D:372:ILE:CG2	2.93	0.41
1:C:322:LYS:HE2	1:C:322:LYS:HB2	1.91	0.41
1:F:324:LEU:C	1:F:326:LEU:H	2.28	0.41
1:G:219:PHE:HB2	3:G:528:HOH:O	2.20	0.41
1:G:303:CYS:HB3	1:G:343:PRO:O	2.21	0.41
1:C:313:ALA:O	1:C:317:ILE:HG13	2.20	0.41
1:C:324:LEU:HB2	1:C:326:LEU:CD2	2.51	0.41
1:B:302:LEU:HD12	1:B:302:LEU:HA	1.95	0.40
1:B:328:VAL:H	1:B:328:VAL:HG13	1.57	0.40
1:F:326:LEU:N	1:F:327:PRO:HD3	2.36	0.40
1:E:237:LEU:HA	1:E:237:LEU:HD23	1.84	0.40
1:E:276:LYS:HA	1:E:276:LYS:HD2	1.75	0.40
1:D:293:ASN:ND2	3:D:504:HOH:O	2.53	0.40
1:B:365:GLY:O	1:B:366:HIS:CG	2.75	0.40
1:F:331:ILE:HD12	1:F:332:ALA:H	1.85	0.40
1:G:317:ILE:HG23	1:G:359:LEU:HD11	2.03	0.40
1:F:223:GLN:NE2	1:F:262:LYS:O	2.49	0.40
1:E:371:HIS:O	1:E:372:ILE:HD13	2.22	0.40
1:G:142:LEU:HD23	1:G:142:LEU:HA	1.90	0.40
1:E:285:ARG:HD2	3:E:503:HOH:O	2.22	0.40
1:E:361:LEU:O	1:E:362:SER:HB2	2.21	0.40
1:D:184:ILE:HD13	1:D:222:ALA:HA	2.03	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	242/267 (91%)	222 (92%)	14 (6%)	6 (2%)	4	3
1	B	241/267 (90%)	220 (91%)	13 (5%)	8 (3%)	3	2
1	C	242/267 (91%)	226 (93%)	14 (6%)	2 (1%)	16	20
1	D	242/267 (91%)	223 (92%)	11 (4%)	8 (3%)	3	2
1	E	242/267 (91%)	228 (94%)	11 (4%)	3 (1%)	10	12
1	F	240/267 (90%)	219 (91%)	14 (6%)	7 (3%)	3	2
1	G	241/267 (90%)	219 (91%)	15 (6%)	7 (3%)	3	2
All	All	1690/1869 (90%)	1557 (92%)	92 (5%)	41 (2%)	4	4

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
1	A	330	SER
1	A	362	SER
1	A	364	ASN
1	C	362	SER
1	C	364	ASN
1	B	323	LYS
1	B	331	ILE
1	B	332	ALA
1	B	362	SER
1	B	367	ILE
1	F	331	ILE
1	F	363	GLU
1	F	367	ILE
1	G	323	LYS
1	G	330	SER
1	G	362	SER
1	E	310	GLU

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Mol	Chain	Res	Type
1	E	362	SER
1	D	322	LYS
1	D	330	SER
1	D	331	ILE
1	D	362	SER
1	D	364	ASN
1	D	372	ILE
1	A	136	THR
1	B	324	LEU
1	F	132	VAL
1	F	321	CYS
1	G	133	VAL
1	G	331	ILE
1	D	371	HIS
1	F	179	LYS
1	G	322	LYS
1	E	364	ASN
1	D	133	VAL
1	A	332	ALA
1	B	333	PRO
1	B	132	VAL
1	G	132	VAL
1	F	327	PRO

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	204/227 (90%)	178 (87%)	26 (13%)	4	5
1	B	204/227 (90%)	171 (84%)	33 (16%)	2	2
1	C	205/227 (90%)	188 (92%)	17 (8%)	10	14
1	D	204/227 (90%)	177 (87%)	27 (13%)	4	4
1	E	204/227 (90%)	174 (85%)	30 (15%)	3	3
1	F	204/227 (90%)	175 (86%)	29 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	204/227 (90%)	180 (88%)	24 (12%)	5	6
All	All	1429/1589 (90%)	1243 (87%)	186 (13%)	4	4

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	VAL
1	A	140	LYS
1	A	141	LEU
1	A	142	LEU
1	A	144	LEU
1	A	148	VAL
1	A	150	LYS
1	A	168	MET
1	A	169	SER
1	A	209	THR
1	A	212	VAL
1	A	239	LEU
1	A	242	LYS
1	A	253	GLU
1	A	262	LYS
1	A	302	LEU
1	A	317	ILE
1	A	319	ARG
1	A	323	LYS
1	A	326	LEU
1	A	328	VAL
1	A	331	ILE
1	A	339	LEU
1	A	367	ILE
1	A	368	GLN
1	A	372	ILE
1	C	141	LEU
1	C	148	VAL
1	C	152	ASP
1	C	167	VAL
1	C	180	GLU
1	C	194	ASN
1	C	229	LEU
1	C	231	GLU
1	C	232	ILE
1	C	239	LEU

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Mol	Chain	Res	Type
1	C	260	SER
1	C	306	LYS
1	C	321	CYS
1	C	349	ARG
1	C	362	SER
1	C	367	ILE
1	C	372	ILE
1	B	140	LYS
1	B	144	LEU
1	B	146	ASP
1	B	148	VAL
1	B	169	SER
1	B	170	ARG
1	B	186	ILE
1	B	196	LEU
1	B	199	THR
1	B	230	ASP
1	B	231	GLU
1	B	239	LEU
1	B	250	ARG
1	B	253	GLU
1	B	259	LYS
1	B	272	ASN
1	B	312	LEU
1	B	316	LEU
1	B	324	LEU
1	B	326	LEU
1	B	328	VAL
1	B	331	ILE
1	B	348	VAL
1	B	355	VAL
1	B	361	LEU
1	B	363	GLU
1	B	366	HIS
1	B	367	ILE
1	B	368	GLN
1	B	369	SER
1	B	370	GLU
1	B	371	HIS
1	B	372	ILE
1	F	140	LYS
1	F	141	LEU

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Mol	Chain	Res	Type
1	F	150	LYS
1	F	152	ASP
1	F	167	VAL
1	F	168	MET
1	F	170	ARG
1	F	179	LYS
1	F	230	ASP
1	F	235	MET
1	F	244	LEU
1	F	249	GLU
1	F	258	ARG
1	F	260	SER
1	F	263	LEU
1	F	277	GLN
1	F	278	TYR
1	F	294	VAL
1	F	302	LEU
1	F	312	LEU
1	F	319	ARG
1	F	326	LEU
1	F	328	VAL
1	F	338	LYS
1	F	349	ARG
1	F	361	LEU
1	F	367	ILE
1	F	368	GLN
1	F	372	ILE
1	G	132	VAL
1	G	133	VAL
1	G	138	SER
1	G	144	LEU
1	G	150	LYS
1	G	158	LEU
1	G	167	VAL
1	G	180	GLU
1	G	199	THR
1	G	200	LEU
1	G	230	ASP
1	G	231	GLU
1	G	239	LEU
1	G	258	ARG
1	G	270	THR

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Mol	Chain	Res	Type
1	G	316	LEU
1	G	323	LYS
1	G	326	LEU
1	G	328	VAL
1	G	349	ARG
1	G	355	VAL
1	G	363	GLU
1	G	364	ASN
1	G	368	GLN
1	E	132	VAL
1	E	133	VAL
1	E	141	LEU
1	E	144	LEU
1	E	148	VAL
1	E	152	ASP
1	E	168	MET
1	E	169	SER
1	E	212	VAL
1	E	230	ASP
1	E	245	ARG
1	E	253	GLU
1	E	258	ARG
1	E	262	LYS
1	E	263	LEU
1	E	270	THR
1	E	277	GLN
1	E	293	ASN
1	E	297	LEU
1	E	312	LEU
1	E	316	LEU
1	E	324	LEU
1	E	328	VAL
1	E	349	ARG
1	E	355	VAL
1	E	362	SER
1	E	363	GLU
1	E	366	HIS
1	E	368	GLN
1	E	370	GLU
1	D	132	VAL
1	D	133	VAL
1	D	141	LEU

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Mol	Chain	Res	Type
1	D	142	LEU
1	D	148	VAL
1	D	166	GLU
1	D	168	MET
1	D	169	SER
1	D	184	ILE
1	D	199	THR
1	D	239	LEU
1	D	249	GLU
1	D	250	ARG
1	D	253	GLU
1	D	258	ARG
1	D	278	TYR
1	D	318	GLU
1	D	323	LYS
1	D	324	LEU
1	D	326	LEU
1	D	328	VAL
1	D	331	ILE
1	D	361	LEU
1	D	362	SER
1	D	367	ILE
1	D	368	GLN
1	D	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	C	315	HIS
1	C	368	GLN
1	B	272	ASN
1	B	364	ASN
1	E	356	GLN
1	D	364	ASN
1	D	368	GLN

5.3.3 RNA ⓘ

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](#)

7 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	EDO	G	401	-	3,3,3	0.49	0	2,2,2	0.15	0
2	EDO	B	401	-	3,3,3	0.50	0	2,2,2	0.01	0
2	EDO	F	401	-	3,3,3	0.59	0	2,2,2	0.19	0
2	EDO	D	401	-	3,3,3	0.52	0	2,2,2	0.04	0
2	EDO	A	401	-	3,3,3	0.58	0	2,2,2	0.12	0
2	EDO	E	401	-	3,3,3	0.49	0	2,2,2	0.32	0
2	EDO	C	401	-	3,3,3	0.58	0	2,2,2	0.13	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	EDO	G	401	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	EDO	1	0
2	E	401	EDO	1	0
2	C	401	EDO	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	244/267 (91%)	0.34	20 (8%)	17	19	30, 52, 100, 136	0
1	B	243/267 (91%)	0.34	21 (8%)	16	17	35, 52, 80, 114	0
1	C	243/267 (91%)	0.32	13 (5%)	32	34	28, 52, 102, 136	1 (0%)
1	D	244/267 (91%)	0.28	17 (6%)	22	24	33, 51, 82, 123	0
1	E	244/267 (91%)	0.17	10 (4%)	41	43	30, 48, 72, 110	0
1	F	242/267 (90%)	0.28	17 (7%)	22	24	31, 52, 101, 136	0
1	G	243/267 (91%)	0.23	14 (5%)	29	31	33, 49, 73, 111	0
All	All	1703/1869 (91%)	0.28	112 (6%)	24	26	28, 51, 88, 136	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	LEU	7.5
1	F	372	ILE	6.0
1	E	367	ILE	5.9
1	C	132	VAL	5.7
1	B	372	ILE	5.6
1	D	329	PRO	5.6
1	E	130	HIS	5.4
1	D	131	MET	5.4
1	B	331	ILE	5.3
1	G	329	PRO	5.3
1	C	131	MET	5.0
1	C	367	ILE	4.8
1	B	131	MET	4.8
1	D	330	SER	4.7
1	G	373	LEU	4.7
1	D	367	ILE	4.7
1	A	373	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	367	ILE	4.5
1	A	367	ILE	4.2
1	B	367	ILE	4.2
1	D	331	ILE	4.2
1	B	364	ASN	4.1
1	E	131	MET	4.1
1	G	367	ILE	4.1
1	G	362	SER	3.9
1	A	131	MET	3.9
1	C	167	VAL	3.9
1	D	326	LEU	3.9
1	G	372	ILE	3.9
1	E	132	VAL	3.8
1	B	324	LEU	3.8
1	D	372	ILE	3.8
1	B	373	LEU	3.8
1	F	328	VAL	3.8
1	B	334	ASN	3.8
1	B	363	GLU	3.7
1	G	324	LEU	3.6
1	B	132	VAL	3.6
1	F	326	LEU	3.6
1	F	131	MET	3.5
1	E	363	GLU	3.5
1	F	330	SER	3.5
1	A	371	HIS	3.5
1	C	372	ILE	3.4
1	E	372	ILE	3.4
1	B	332	ALA	3.4
1	C	373	LEU	3.3
1	A	374	LEU	3.3
1	A	132	VAL	3.3
1	F	327	PRO	3.2
1	B	330	SER	3.2
1	G	132	VAL	3.2
1	B	326	LEU	3.1
1	F	331	ILE	3.1
1	C	320	HIS	3.0
1	D	362	SER	3.0
1	C	328	VAL	3.0
1	D	371	HIS	3.0
1	A	330	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	320	HIS	2.9
1	F	371	HIS	2.9
1	F	167	VAL	2.9
1	A	372	ILE	2.9
1	C	365	GLY	2.8
1	B	333	PRO	2.8
1	E	373	LEU	2.8
1	F	168	MET	2.8
1	A	326	LEU	2.7
1	D	374	LEU	2.7
1	D	162	GLY	2.7
1	B	362	SER	2.7
1	F	320	HIS	2.6
1	C	164	GLY	2.6
1	D	373	LEU	2.5
1	B	366	HIS	2.5
1	B	328	VAL	2.5
1	G	326	LEU	2.5
1	A	366	HIS	2.5
1	A	368	GLN	2.5
1	F	329	PRO	2.5
1	E	362	SER	2.4
1	F	322	LYS	2.4
1	E	167	VAL	2.4
1	F	368	GLN	2.4
1	B	323	LYS	2.3
1	F	324	LEU	2.3
1	G	330	SER	2.3
1	E	133	VAL	2.3
1	A	324	LEU	2.2
1	A	250	ARG	2.2
1	D	258	ARG	2.2
1	B	253	GLU	2.2
1	A	133	VAL	2.2
1	A	363	GLU	2.2
1	G	370	GLU	2.2
1	G	131	MET	2.2
1	B	365	GLY	2.2
1	F	366	HIS	2.2
1	C	326	LEU	2.1
1	G	167	VAL	2.1
1	A	365	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	250	ARG	2.1
1	G	363	GLU	2.1
1	D	328	VAL	2.1
1	A	331	ILE	2.1
1	G	327	PRO	2.1
1	A	304	GLU	2.1
1	C	331	ILE	2.1
1	C	327	PRO	2.1
1	B	163	SER	2.0
1	D	132	VAL	2.0
1	A	327	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(Å ²)	Q<0.9
2	EDO	C	401	4/4	0.87	0.15	51,54,59,61	0
2	EDO	A	401	4/4	0.88	0.15	45,51,58,62	0
2	EDO	E	401	4/4	0.89	0.20	51,55,55,56	0
2	EDO	B	401	4/4	0.90	0.12	43,48,55,57	0
2	EDO	F	401	4/4	0.92	0.12	43,47,49,56	0
2	EDO	D	401	4/4	0.92	0.16	46,51,56,62	0
2	EDO	G	401	4/4	0.94	0.14	44,60,61,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.