



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:33 AM EDT

PDB ID : 2PLS / pdb_00002pls
Title : Structural Genomics, the crystal structure of the CorC/HlyC transporter associated domain of a CBS domain protein from *Chlorobium tepidum* TLS
Authors : Tan, K.; Volkart, L.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-04-20
Resolution : 2.15 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:

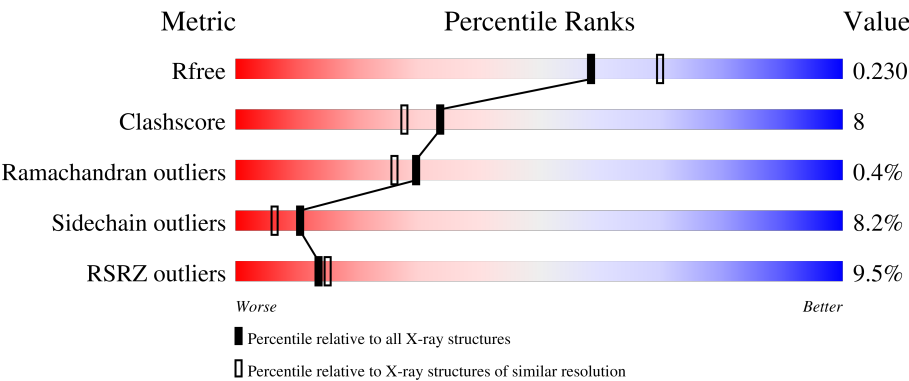
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	86	44% 81% 17% .
1	B	86	7% 87% 9% .
1	C	86	2% 87% 10% .
1	D	86	6% 90% 6% ..
1	E	86	2% 81% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	86	
1	G	86	
1	H	86	
1	I	86	
1	J	86	
1	K	86	
1	L	86	

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
4	FMT	I	805	-	-	X	-
4	FMT	L	806	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8932 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 CBS domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	Se	0	2	0
			699	446	117	133	3			
1	B	86	Total	C	N	O	Se	0	0	0
			688	439	116	130	3			
1	C	86	Total	C	N	O	Se	0	1	0
			693	442	116	132	3			
1	D	85	Total	C	N	O	Se	0	1	0
			686	439	115	129	3			
1	E	85	Total	C	N	O	Se	0	2	0
			696	445	121	127	3			
1	F	85	Total	C	N	O	Se	0	2	0
			693	443	119	128	3			
1	G	85	Total	C	N	O	Se	0	0	0
			680	435	115	127	3			
1	H	85	Total	C	N	O	Se	0	1	0
			687	439	115	130	3			
1	I	86	Total	C	N	O	Se	0	0	0
			688	439	116	130	3			
1	J	86	Total	C	N	O	Se	0	0	0
			688	439	116	130	3			
1	K	86	Total	C	N	O	Se	0	0	0
			688	439	116	130	3			
1	L	86	Total	C	N	O	Se	0	1	0
			695	444	118	130	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	SER	-	cloning artifact	UNP Q8KEZ1
A	344	ASN	-	cloning artifact	UNP Q8KEZ1
A	345	ALA	-	cloning artifact	UNP Q8KEZ1
A	387	MSE	MET	modified residue	UNP Q8KEZ1
A	389	MSE	MET	modified residue	UNP Q8KEZ1

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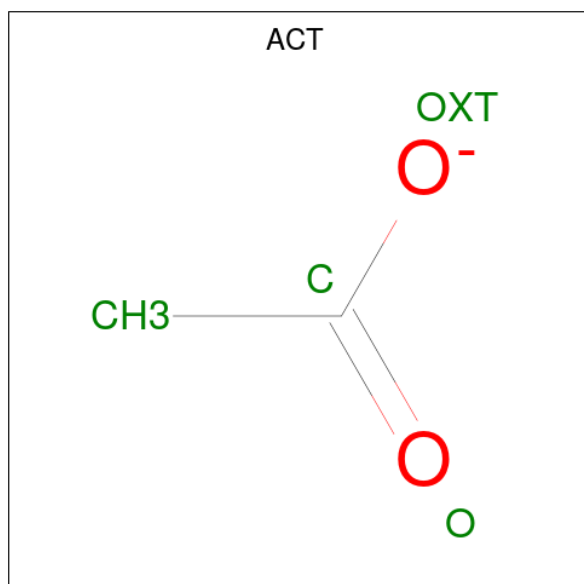
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	MSE	MET	modified residue	UNP Q8KEZ1
B	343	SER	-	cloning artifact	UNP Q8KEZ1
B	344	ASN	-	cloning artifact	UNP Q8KEZ1
B	345	ALA	-	cloning artifact	UNP Q8KEZ1
B	387	MSE	MET	modified residue	UNP Q8KEZ1
B	389	MSE	MET	modified residue	UNP Q8KEZ1
B	414	MSE	MET	modified residue	UNP Q8KEZ1
C	343	SER	-	cloning artifact	UNP Q8KEZ1
C	344	ASN	-	cloning artifact	UNP Q8KEZ1
C	345	ALA	-	cloning artifact	UNP Q8KEZ1
C	387	MSE	MET	modified residue	UNP Q8KEZ1
C	389	MSE	MET	modified residue	UNP Q8KEZ1
C	414	MSE	MET	modified residue	UNP Q8KEZ1
D	343	SER	-	cloning artifact	UNP Q8KEZ1
D	344	ASN	-	cloning artifact	UNP Q8KEZ1
D	345	ALA	-	cloning artifact	UNP Q8KEZ1
D	387	MSE	MET	modified residue	UNP Q8KEZ1
D	389	MSE	MET	modified residue	UNP Q8KEZ1
D	414	MSE	MET	modified residue	UNP Q8KEZ1
E	343	SER	-	cloning artifact	UNP Q8KEZ1
E	344	ASN	-	cloning artifact	UNP Q8KEZ1
E	345	ALA	-	cloning artifact	UNP Q8KEZ1
E	387	MSE	MET	modified residue	UNP Q8KEZ1
E	389	MSE	MET	modified residue	UNP Q8KEZ1
E	414	MSE	MET	modified residue	UNP Q8KEZ1
F	343	SER	-	cloning artifact	UNP Q8KEZ1
F	344	ASN	-	cloning artifact	UNP Q8KEZ1
F	345	ALA	-	cloning artifact	UNP Q8KEZ1
F	387	MSE	MET	modified residue	UNP Q8KEZ1
F	389	MSE	MET	modified residue	UNP Q8KEZ1
F	414	MSE	MET	modified residue	UNP Q8KEZ1
G	343	SER	-	cloning artifact	UNP Q8KEZ1
G	344	ASN	-	cloning artifact	UNP Q8KEZ1
G	345	ALA	-	cloning artifact	UNP Q8KEZ1
G	387	MSE	MET	modified residue	UNP Q8KEZ1
G	389	MSE	MET	modified residue	UNP Q8KEZ1
G	414	MSE	MET	modified residue	UNP Q8KEZ1
H	343	SER	-	cloning artifact	UNP Q8KEZ1
H	344	ASN	-	cloning artifact	UNP Q8KEZ1
H	345	ALA	-	cloning artifact	UNP Q8KEZ1
H	387	MSE	MET	modified residue	UNP Q8KEZ1
H	389	MSE	MET	modified residue	UNP Q8KEZ1

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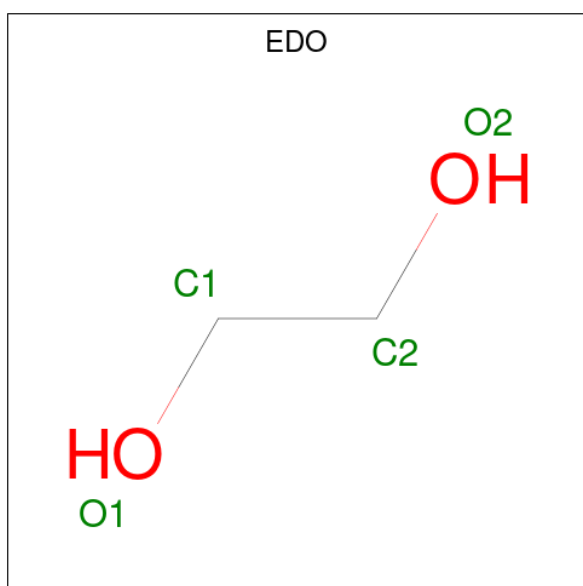
Chain	Residue	Modelled	Actual	Comment	Reference
H	414	MSE	MET	modified residue	UNP Q8KEZ1
I	343	SER	-	cloning artifact	UNP Q8KEZ1
I	344	ASN	-	cloning artifact	UNP Q8KEZ1
I	345	ALA	-	cloning artifact	UNP Q8KEZ1
I	387	MSE	MET	modified residue	UNP Q8KEZ1
I	389	MSE	MET	modified residue	UNP Q8KEZ1
I	414	MSE	MET	modified residue	UNP Q8KEZ1
J	343	SER	-	cloning artifact	UNP Q8KEZ1
J	344	ASN	-	cloning artifact	UNP Q8KEZ1
J	345	ALA	-	cloning artifact	UNP Q8KEZ1
J	387	MSE	MET	modified residue	UNP Q8KEZ1
J	389	MSE	MET	modified residue	UNP Q8KEZ1
J	414	MSE	MET	modified residue	UNP Q8KEZ1
K	343	SER	-	cloning artifact	UNP Q8KEZ1
K	344	ASN	-	cloning artifact	UNP Q8KEZ1
K	345	ALA	-	cloning artifact	UNP Q8KEZ1
K	387	MSE	MET	modified residue	UNP Q8KEZ1
K	389	MSE	MET	modified residue	UNP Q8KEZ1
K	414	MSE	MET	modified residue	UNP Q8KEZ1
L	343	SER	-	cloning artifact	UNP Q8KEZ1
L	344	ASN	-	cloning artifact	UNP Q8KEZ1
L	345	ALA	-	cloning artifact	UNP Q8KEZ1
L	387	MSE	MET	modified residue	UNP Q8KEZ1
L	389	MSE	MET	modified residue	UNP Q8KEZ1
L	414	MSE	MET	modified residue	UNP Q8KEZ1

- 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 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



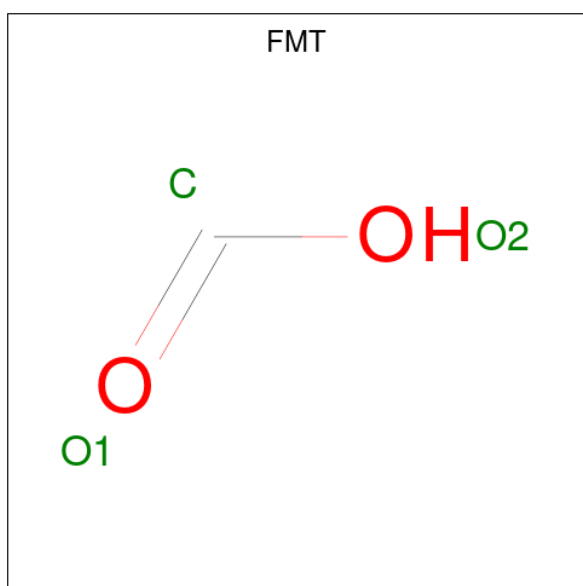
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	I	1	Total	C	O	0	0
			3	1	2		
4	I	1	Total	C	O	0	0
			3	1	2		
4	L	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Mg 1	0	0
5	H	2	Total 2	Mg 2	0	0
5	I	2	Total 2	Mg 2	0	0
5	J	1	Total 1	Mg 1	0	0

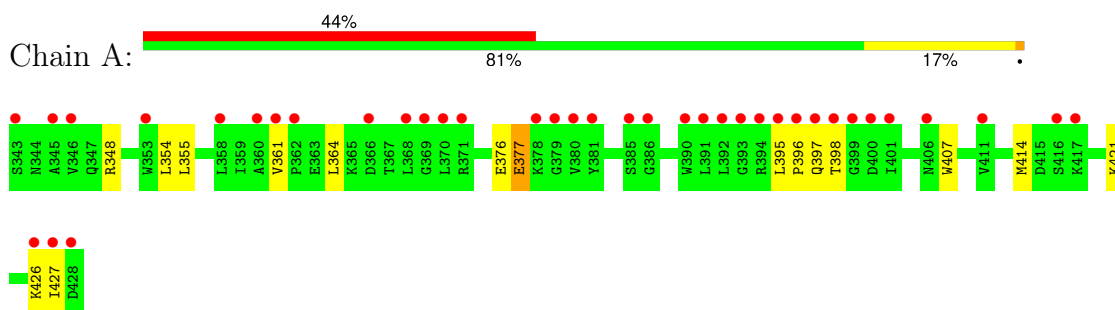
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total 39	O 39	0	0
6	B	54	Total 54	O 54	0	0
6	C	73	Total 73	O 73	0	0
6	D	38	Total 38	O 38	0	0
6	E	50	Total 50	O 50	0	0
6	F	71	Total 71	O 71	0	0
6	G	51	Total 51	O 51	0	0
6	H	21	Total 21	O 21	0	0
6	I	39	Total 39	O 39	0	0
6	J	56	Total 56	O 56	0	0
6	K	46	Total 46	O 46	0	0
6	L	21	Total 21	O 21	0	0

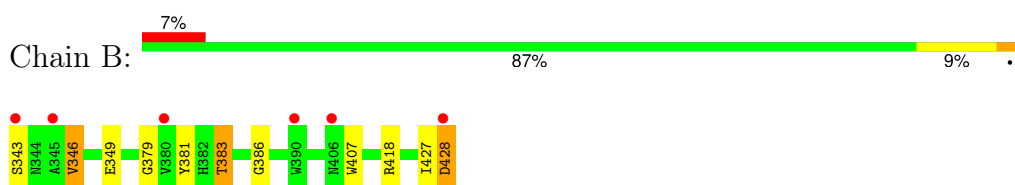
3 Residue-property plots [i](#)

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.

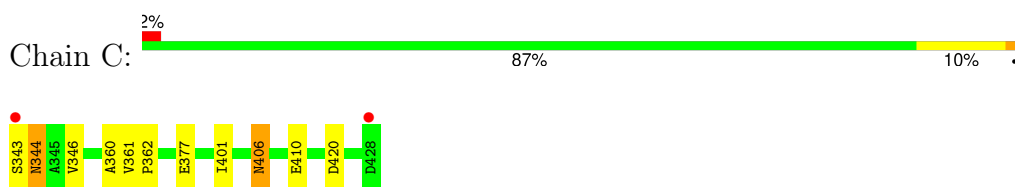
- Molecule 1: CBS domain protein



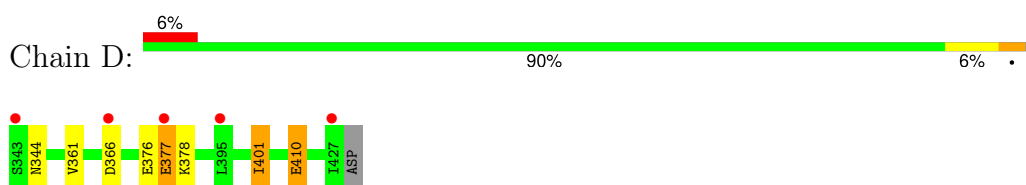
- Molecule 1: CBS domain protein



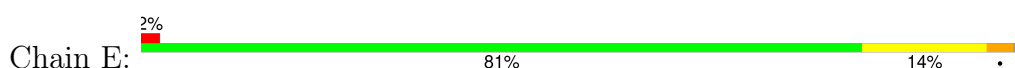
- Molecule 1: CBS domain protein



- Molecule 1: CBS domain protein

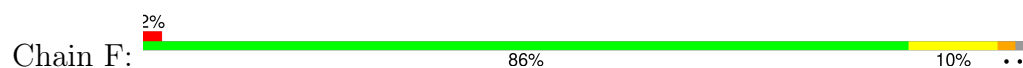


- Molecule 1: CBS domain protein

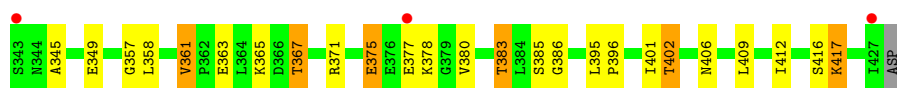




- Molecule 1: CBS domain protein



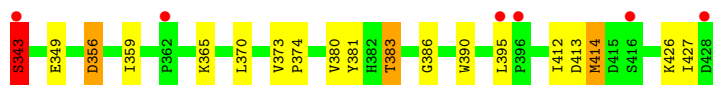
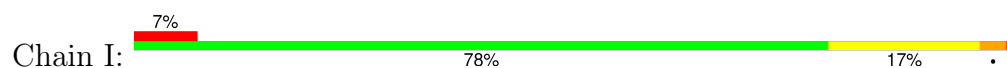
- Molecule 1: CBS domain protein



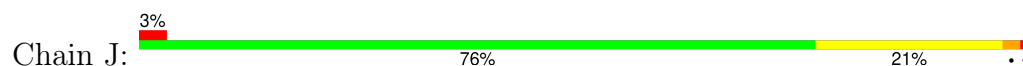
- Molecule 1: CBS domain protein



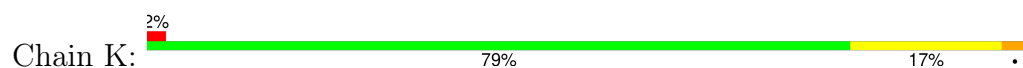
- Molecule 1: CBS domain protein



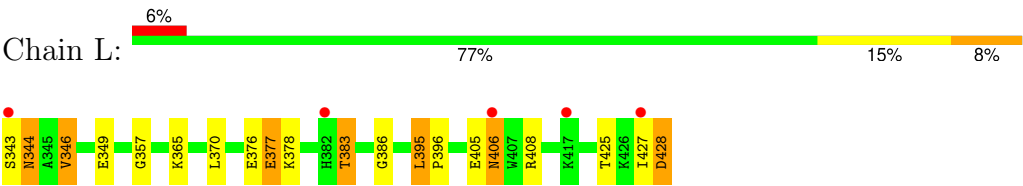
- Molecule 1: CBS domain protein



- Molecule 1: CBS domain protein



● Molecule 1: CBS domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.24Å 108.49Å 106.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.15 48.51 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.51-2.15) 99.1 (48.51-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.232 0.176 , 0.230	Depositor DCC
R_{free} test set	3453 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l 0.017 for -h,-l,-k 0.015 for l,-k,h 0.006 for k,l,h 0.006 for l,h,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8932	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.15% 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: FMT, MG, ACT, 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	1.03	2/715 (0.3%)	0.99	1/964 (0.1%)
1	B	0.91	1/698 (0.1%)	0.98	1/941 (0.1%)
1	C	1.06	1/706 (0.1%)	1.02	1/952 (0.1%)
1	D	1.05	1/699 (0.1%)	1.06	2/942 (0.2%)
1	E	0.95	1/712 (0.1%)	1.00	1/958 (0.1%)
1	F	1.03	1/709 (0.1%)	0.97	0/955
1	G	0.93	1/690 (0.1%)	0.99	0/930
1	H	0.97	4/700 (0.6%)	1.05	1/944 (0.1%)
1	I	0.97	1/698 (0.1%)	1.05	2/941 (0.2%)
1	J	1.02	1/698 (0.1%)	1.04	2/941 (0.2%)
1	K	0.97	0/698	1.04	2/941 (0.2%)
1	L	0.80	1/709 (0.1%)	0.99	1/956 (0.1%)
All	All	0.98	15/8432 (0.2%)	1.02	14/11365 (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	1
1	C	0	1
1	D	0	1
1	I	0	1
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	361	VAL	CA-CB	11.51	1.59	1.54
1	F	361	VAL	CA-CB	9.04	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	361	VAL	CA-CB	8.95	1.58	1.54
1	H	382	HIS	CE1-NE2	8.59	1.41	1.32
1	E	361	VAL	CA-CB	7.03	1.57	1.54
1	H	346	VAL	CA-CB	6.65	1.62	1.54
1	I	414	MSE	CA-C	-5.68	1.45	1.52
1	H	382	HIS	CG-CD2	5.48	1.41	1.35
1	A	361	VAL	CA-CB	5.35	1.57	1.54
1	A	364	LEU	C-N	5.34	1.40	1.33
1	H	382	HIS	CG-ND1	5.30	1.44	1.38
1	G	361	VAL	CA-CB	5.28	1.57	1.54
1	L	346	VAL	CA-CB	5.19	1.60	1.54
1	J	361	VAL	CA-CB	5.09	1.57	1.54
1	B	346	VAL	CA-CB	5.01	1.60	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	378	LYS	N-CA-C	-9.59	101.13	112.92
1	C	344	ASN	N-CA-C	9.50	123.63	109.95
1	J	344	ASN	N-CA-C	8.57	118.35	108.49
1	D	344	ASN	N-CA-C	7.69	118.68	108.07
1	K	405	GLU	CA-C-N	-6.27	113.83	123.17
1	K	405	GLU	C-N-CA	-6.27	113.83	123.17
1	A	407	TRP	N-CA-C	5.83	118.90	109.40
1	I	373	VAL	CA-C-N	-5.75	114.01	119.76
1	I	373	VAL	C-N-CA	-5.75	114.01	119.76
1	L	344	ASN	N-CA-C	5.45	115.22	108.19
1	H	418	ARG	N-CA-C	5.42	117.04	108.96
1	E	344	ASN	N-CA-C	5.41	117.06	110.41
1	J	376	GLU	N-CA-C	5.21	117.36	111.11
1	B	407	TRP	N-CA-C	5.04	117.66	109.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	343	SER	Peptide
1	C	343	SER	Peptide
1	D	376	GLU	Peptide
1	I	343	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	699	0	704	8	0
1	B	688	0	692	6	0
1	C	693	0	696	9	0
1	D	686	0	694	1	0
1	E	696	0	714	13	0
1	F	693	0	707	8	0
1	G	680	0	688	18	0
1	H	687	0	691	17	0
1	I	688	0	692	15	0
1	J	688	0	692	15	0
1	K	688	0	692	10	0
1	L	695	0	699	13	0
2	A	4	0	3	1	0
2	D	4	0	3	1	0
2	E	4	0	3	0	0
2	K	4	0	3	0	0
3	A	8	0	12	1	0
3	B	4	0	6	2	0
3	C	12	0	18	3	0
3	E	8	0	12	2	0
3	F	12	0	18	1	0
3	I	4	0	6	0	0
3	J	4	0	6	2	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
4	I	6	0	2	4	0
4	L	3	0	1	2	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
6	A	39	0	0	1	0
6	B	54	0	0	0	0
6	C	73	0	0	2	0
6	D	38	0	0	0	0
6	E	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	71	0	0	2	0
6	G	51	0	0	0	0
6	H	21	0	0	1	0
6	I	39	0	0	0	0
6	J	56	0	0	6	0
6	K	46	0	0	1	0
6	L	21	0	0	0	0
All	All	8932	0	8457	130	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 8.

All (130) 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:377[A]:GLU:OE1	6:A:924:HOH:O	1.64	1.12
1:I:426:LYS:HZ3	4:I:805:FMT:H	1.10	1.09
1:G:417:LYS:HE3	1:G:417:LYS:HA	1.36	1.08
1:C:360:ALA:HB3	3:C:714:EDO:H11	1.28	1.07
1:I:426:LYS:NZ	4:I:805:FMT:H	1.70	1.06
1:G:417:LYS:HA	1:G:417:LYS:CE	1.93	0.98
1:J:406:ASN:HB2	6:J:751:HOH:O	1.63	0.96
1:H:405:GLU:O	1:H:406:ASN:ND2	2.03	0.92
1:G:383:THR:HG22	1:G:386:GLY:H	1.37	0.90
1:A:376:GLU:O	1:A:377[A]:GLU:HG2	1.73	0.87
1:B:383:THR:HG22	1:B:386:GLY:H	1.41	0.85
1:F:401:ILE:HD12	1:F:410:GLU:HG2	1.58	0.85
1:I:383:THR:HG22	1:I:386:GLY:H	1.41	0.84
1:C:362:PRO:HD2	3:C:714:EDO:H12	1.61	0.82
3:F:713:EDO:H21	6:F:767:HOH:O	1.77	0.82
1:L:425:THR:HG23	4:L:806:FMT:H	1.60	0.81
1:C:360:ALA:HB3	3:C:714:EDO:C1	2.10	0.80
1:G:416:SER:O	1:G:417:LYS:HE3	1.84	0.78
1:C:401:ILE:HD12	1:C:410:GLU:HG2	1.68	0.75
1:B:427:ILE:O	1:B:428:ASP:HB2	1.87	0.75
1:K:383:THR:HG22	1:K:386:GLY:H	1.54	0.72
1:J:357:GLY:O	1:J:383:THR:HG23	1.89	0.71
1:C:406:ASN:HD22	1:C:406:ASN:H	1.37	0.70
1:E:359:ILE:CG1	1:E:363:GLU:HG2	2.23	0.69
1:G:375:GLU:HG3	1:G:378:LYS:HD2	1.74	0.68
1:C:420:ASP:OD2	6:C:873:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:417:LYS:HE3	1:G:417:LYS:CA	2.22	0.66
1:K:359:ILE:HD11	1:K:363:GLU:HG2	1.77	0.66
1:I:426:LYS:HZ3	4:I:805:FMT:C	1.99	0.65
1:L:357:GLY:O	1:L:383:THR:HG23	1.95	0.65
1:E:359:ILE:HD11	1:E:363:GLU:HG2	1.79	0.64
1:F:401:ILE:CD1	1:F:410:GLU:HG2	2.30	0.61
1:D:401:ILE:HD13	1:D:410[B]:GLU:HG2	1.82	0.61
2:D:902:ACT:H3	6:F:769:HOH:O	2.00	0.61
1:I:343:SER:N	1:I:356:ASP:CG	2.59	0.60
1:H:357:GLY:O	1:H:383:THR:HG23	2.02	0.60
1:H:395:LEU:HD22	1:H:396:PRO:HD2	1.81	0.60
1:H:356[B]:ASP:OD1	6:H:617:HOH:O	2.16	0.60
1:A:376:GLU:C	1:A:377[A]:GLU:HG2	2.28	0.58
1:G:363:GLU:O	1:G:367:THR:HG23	2.04	0.58
1:L:427:ILE:O	1:L:428:ASP:HB2	2.04	0.57
1:B:381:TYR:O	3:B:702:EDO:H12	2.05	0.57
1:J:383:THR:HG22	1:J:386:GLY:H	1.68	0.57
1:G:363:GLU:O	1:G:367:THR:CG2	2.53	0.57
1:E:365:LYS:HD3	1:E:373:VAL:HG13	1.87	0.57
1:G:417:LYS:HA	1:G:417:LYS:HE2	1.83	0.57
1:J:425:THR:HG23	3:J:711:EDO:H21	1.88	0.56
1:K:427:ILE:O	1:K:428:ASP:OD1	2.21	0.56
1:B:379:GLY:H	3:B:702:EDO:H22	1.71	0.56
1:E:359:ILE:CD1	1:E:363:GLU:HG2	2.36	0.55
1:F:373:VAL:CG2	1:F:376:GLU:HG2	2.36	0.55
1:K:427:ILE:O	1:K:428:ASP:HB2	2.07	0.55
1:I:412:ILE:HD12	1:J:412:ILE:HD12	1.90	0.54
1:E:353:TRP:HB3	1:E:355:LEU:HD13	1.90	0.54
1:K:427:ILE:O	1:K:428:ASP:CB	2.55	0.53
1:L:383:THR:HG22	1:L:386:GLY:H	1.71	0.53
1:H:380:VAL:HG11	1:H:390:TRP:CD1	2.44	0.52
1:J:427:ILE:O	1:J:428:ASP:O	2.27	0.52
1:G:402:THR:HG22	1:G:409:LEU:HB2	1.91	0.52
1:G:395:LEU:HD12	1:G:396:PRO:HD2	1.90	0.52
1:C:401:ILE:CD1	1:C:410:GLU:HG2	2.39	0.52
1:H:383:THR:HG22	1:H:386:GLY:H	1.75	0.52
1:H:417:LYS:O	1:H:417:LYS:HG2	2.10	0.52
1:J:427:ILE:O	1:J:428:ASP:C	2.55	0.50
1:E:359:ILE:HD11	1:E:363:GLU:CG	2.42	0.50
1:F:343:SER:HA	1:F:359:ILE:HA	1.92	0.50
1:I:380:VAL:HG23	1:I:381:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:412:ILE:HD12	1:H:412:ILE:HD12	1.94	0.49
1:I:426:LYS:HZ1	4:I:805:FMT:H	1.70	0.48
1:J:406:ASN:CB	6:J:751:HOH:O	2.38	0.48
1:K:357:GLY:O	1:K:383:THR:HG23	2.14	0.48
1:E:410:GLU:HG2	1:E:412:ILE:HD12	1.94	0.47
1:L:376:GLU:O	1:L:377:GLU:HB2	2.14	0.47
1:B:427:ILE:O	1:B:428:ASP:CB	2.58	0.47
1:L:425:THR:CG2	4:L:806:FMT:H	2.37	0.47
1:G:357:GLY:O	1:G:383:THR:HG23	2.14	0.47
1:F:373:VAL:HG22	1:F:376:GLU:HG2	1.96	0.47
1:H:353:TRP:HB3	1:H:355:LEU:HD13	1.96	0.47
1:H:361:VAL:HG13	1:H:373:VAL:HG11	1.95	0.47
1:K:344:ASN:HB2	6:K:928:HOH:O	2.15	0.47
1:L:365:LYS:HA	1:L:370:LEU:HB2	1.97	0.47
1:F:359:ILE:HD11	1:F:363:GLU:HG2	1.95	0.46
1:B:418:ARG:NH1	1:H:401:ILE:O	2.47	0.46
1:J:426:LYS:H	3:J:711:EDO:C2	2.27	0.46
1:E:401:ILE:O	3:E:704:EDO:H11	2.14	0.46
1:F:373:VAL:HG23	1:F:376:GLU:HG2	1.97	0.46
1:I:365:LYS:HG2	1:I:370:LEU:HB2	1.98	0.46
1:C:406:ASN:HD22	1:C:406:ASN:N	2.10	0.45
1:J:406:ASN:CA	6:J:751:HOH:O	2.64	0.45
1:E:408[B]:ARG:HH11	1:E:408[B]:ARG:HB3	1.81	0.45
1:L:408:ARG:HB2	1:L:427:ILE:HD11	1.98	0.45
1:H:403:PHE:CE1	1:H:427:ILE:HD11	2.52	0.45
1:J:374:PRO:HB2	1:J:390:TRP:CZ3	2.51	0.45
1:G:361:VAL:O	1:G:365:LYS:HG3	2.17	0.45
1:H:406:ASN:ND2	1:H:407:TRP:CD1	2.85	0.45
1:L:376:GLU:O	1:L:377:GLU:CB	2.65	0.45
1:L:405:GLU:O	1:L:406:ASN:OD1	2.35	0.44
1:A:398:THR:OG1	1:A:414:MSE:HG2	2.16	0.44
1:E:376:GLU:O	1:E:377:GLU:HB2	2.18	0.43
1:G:383:THR:HG23	1:G:385:SER:H	1.84	0.43
1:G:406:ASN:O	1:G:406:ASN:CG	2.61	0.43
1:G:412:ILE:O	1:H:421:LYS:HE3	2.19	0.43
1:L:376:GLU:O	1:L:378:LYS:NZ	2.52	0.43
2:A:904:ACT:H3	6:C:842:HOH:O	2.18	0.43
1:A:397:GLN:HB3	3:A:712:EDO:H11	2.01	0.42
1:I:413:ASP:OD2	1:J:421:LYS:HE2	2.18	0.42
1:K:407:TRP:CH2	1:K:426:LYS:HG3	2.54	0.42
1:L:405:GLU:O	1:L:405:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:374:PRO:HB2	1:I:390:TRP:CZ3	2.55	0.42
1:A:395:LEU:HA	1:A:396:PRO:HD3	1.95	0.42
1:E:371[B]:ARG:HD3	1:G:345:ALA:HB3	2.01	0.42
1:J:426:LYS:HE3	6:J:751:HOH:O	2.20	0.42
1:H:373:VAL:HG22	1:H:376:GLU:HG3	2.01	0.42
1:L:395:LEU:HA	1:L:396:PRO:HD3	1.94	0.42
1:E:401:ILE:H	3:E:704:EDO:C1	2.33	0.41
1:E:359:ILE:HG12	1:E:363:GLU:HG2	2.01	0.41
1:I:380:VAL:HG23	1:I:381:TYR:HD2	1.84	0.41
1:I:356:ASP:O	1:I:359:ILE:HG22	2.20	0.41
1:I:343:SER:N	1:I:356:ASP:OD1	2.53	0.41
1:H:414:MSE:HG2	1:H:419:ILE:HA	2.02	0.41
1:J:344:ASN:HB2	6:J:752:HOH:O	2.20	0.41
1:F:408:ARG:HB2	1:F:427:ILE:HD11	2.03	0.41
1:J:406:ASN:N	6:J:751:HOH:O	2.53	0.41
1:C:406:ASN:H	1:C:406:ASN:ND2	2.13	0.41
1:K:365:LYS:HE3	1:K:365:LYS:HB3	1.84	0.41
1:H:395:LEU:HD21	1:H:417:LYS:HG2	2.03	0.40
1:I:414:MSE:HE3	1:I:414:MSE:HB3	1.92	0.40
1:K:421:LYS:HD3	1:K:421:LYS:HA	1.99	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	86/86 (100%)	81 (94%)	5 (6%)	0	100	100
1	B	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	10	5
1	C	85/86 (99%)	83 (98%)	2 (2%)	0	100	100
1	D	84/86 (98%)	80 (95%)	3 (4%)	1 (1%)	10	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	85/86 (99%)	80 (94%)	5 (6%)	0	100	100
1	F	85/86 (99%)	82 (96%)	3 (4%)	0	100	100
1	G	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
1	H	84/86 (98%)	78 (93%)	4 (5%)	2 (2%)	4	1
1	I	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
1	J	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
1	K	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
1	L	85/86 (99%)	82 (96%)	3 (4%)	0	100	100
All	All	1013/1032 (98%)	969 (96%)	40 (4%)	4 (0%)	30	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	377	GLU
1	H	405	GLU
1	B	349	GLU
1	H	349	GLU

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	77/72 (107%)	69 (90%)	8 (10%)	7	3
1	B	75/72 (104%)	72 (96%)	3 (4%)	28	27
1	C	76/72 (106%)	72 (95%)	4 (5%)	20	17
1	D	75/72 (104%)	70 (93%)	5 (7%)	15	10
1	E	76/72 (106%)	73 (96%)	3 (4%)	28	28
1	F	76/72 (106%)	73 (96%)	3 (4%)	28	28
1	G	74/72 (103%)	63 (85%)	11 (15%)	3	1
1	H	75/72 (104%)	69 (92%)	6 (8%)	11	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	75/72 (104%)	69 (92%)	6 (8%)	11	7
1	J	75/72 (104%)	66 (88%)	9 (12%)	5	2
1	K	75/72 (104%)	67 (89%)	8 (11%)	6	3
1	L	76/72 (106%)	67 (88%)	9 (12%)	5	2
All	All	905/864 (105%)	830 (92%)	75 (8%)	10	6

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	ARG
1	A	354	LEU
1	A	355	LEU
1	A	377[A]	GLU
1	A	377[B]	GLU
1	A	421	LYS
1	A	426	LYS
1	A	427	ILE
1	B	346	VAL
1	B	383	THR
1	B	428	ASP
1	C	344	ASN
1	C	346	VAL
1	C	377	GLU
1	C	406	ASN
1	D	366	ASP
1	D	377	GLU
1	D	401	ILE
1	D	410[A]	GLU
1	D	410[B]	GLU
1	E	344	ASN
1	E	355	LEU
1	E	363	GLU
1	F	346	VAL
1	F	376	GLU
1	F	427	ILE
1	G	349	GLU
1	G	358	LEU
1	G	367	THR
1	G	371	ARG
1	G	375	GLU
1	G	377	GLU

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Mol	Chain	Res	Type
1	G	380	VAL
1	G	383	THR
1	G	401	ILE
1	G	402	THR
1	G	417	LYS
1	H	346	VAL
1	H	355	LEU
1	H	383	THR
1	H	395	LEU
1	H	402	THR
1	H	406	ASN
1	I	343	SER
1	I	349	GLU
1	I	356	ASP
1	I	383	THR
1	I	395	LEU
1	I	427	ILE
1	J	343	SER
1	J	344	ASN
1	J	346	VAL
1	J	358	LEU
1	J	363	GLU
1	J	366	ASP
1	J	383	THR
1	J	395	LEU
1	J	428	ASP
1	K	343	SER
1	K	344	ASN
1	K	346	VAL
1	K	358	LEU
1	K	383	THR
1	K	395	LEU
1	K	412	ILE
1	K	428	ASP
1	L	343	SER
1	L	344	ASN
1	L	346	VAL
1	L	349	GLU
1	L	377	GLU
1	L	383	THR
1	L	395	LEU
1	L	406	ASN

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Mol	Chain	Res	Type
1	L	428	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	C	344	ASN
1	C	406	ASN
1	J	344	ASN
1	L	344	ASN
1	L	347	GLN
1	L	406	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](#)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 for Mogul analysis.

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	$\# Z > 2$
4	FMT	C	802	-	2,2,2	0.74	0	1,1,1	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	I	708	-	3,3,3	0.61	0	2,2,2	0.27	0
3	EDO	A	712	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	F	701	-	3,3,3	0.86	0	2,2,2	0.30	0
3	EDO	C	709	-	3,3,3	0.57	0	2,2,2	0.62	0
3	EDO	E	704	-	3,3,3	0.36	0	2,2,2	0.70	0
3	EDO	E	705	-	3,3,3	0.56	0	2,2,2	0.38	0
3	EDO	A	706	-	3,3,3	0.53	0	2,2,2	0.46	0
4	FMT	B	804	-	2,2,2	0.62	0	1,1,1	0.19	0
2	ACT	K	901	-	3,3,3	0.84	0	3,3,3	1.20	0
4	FMT	L	806	-	2,2,2	0.64	0	1,1,1	0.16	0
3	EDO	C	703	-	3,3,3	0.61	0	2,2,2	0.33	0
4	FMT	I	805	-	2,2,2	0.62	0	1,1,1	0.23	0
2	ACT	D	902	-	3,3,3	1.05	0	3,3,3	0.91	0
3	EDO	B	702	-	3,3,3	0.62	0	2,2,2	0.28	0
4	FMT	D	803	-	2,2,2	0.66	0	1,1,1	0.13	0
3	EDO	C	714	-	3,3,3	0.42	0	2,2,2	0.41	0
2	ACT	E	903	-	3,3,3	0.98	0	3,3,3	1.03	0
3	EDO	F	713	-	3,3,3	0.79	0	2,2,2	0.16	0
2	ACT	A	904	-	3,3,3	1.10	0	3,3,3	1.15	0
3	EDO	F	710	-	3,3,3	0.37	0	2,2,2	0.54	0
4	FMT	I	801	-	2,2,2	0.65	0	1,1,1	0.17	0
3	EDO	J	711	-	3,3,3	0.59	0	2,2,2	0.49	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
3	EDO	I	708	-	-	0/1/1/1	-
3	EDO	A	712	-	-	1/1/1/1	-
3	EDO	F	713	-	-	1/1/1/1	-
3	EDO	F	701	-	-	0/1/1/1	-
3	EDO	B	702	-	-	1/1/1/1	-
3	EDO	F	710	-	-	1/1/1/1	-
3	EDO	C	703	-	-	1/1/1/1	-
3	EDO	J	711	-	-	0/1/1/1	-
3	EDO	C	714	-	-	1/1/1/1	-
3	EDO	C	709	-	-	1/1/1/1	-
3	EDO	E	704	-	-	0/1/1/1	-
3	EDO	E	705	-	-	0/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	EDO	O1-C1-C2-O2
3	C	709	EDO	O1-C1-C2-O2
3	F	713	EDO	O1-C1-C2-O2
3	C	714	EDO	O1-C1-C2-O2
3	A	712	EDO	O1-C1-C2-O2
3	C	703	EDO	O1-C1-C2-O2
3	F	710	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	712	EDO	1	0
3	E	704	EDO	2	0
4	L	806	FMT	2	0
4	I	805	FMT	4	0
2	D	902	ACT	1	0
3	B	702	EDO	2	0
3	C	714	EDO	3	0
3	F	713	EDO	1	0
2	A	904	ACT	1	0
3	J	711	EDO	2	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	83/86 (96%)	1.95	38 (45%) 0 1	26, 42, 57, 68	2 (2%)
1	B	83/86 (96%)	0.93	6 (7%) 21 25	32, 36, 50, 59	0
1	C	83/86 (96%)	0.09	2 (2%) 59 63	20, 29, 43, 53	1 (1%)
1	D	82/86 (95%)	0.30	5 (6%) 27 31	18, 31, 43, 53	1 (1%)
1	E	82/86 (95%)	0.40	2 (2%) 59 63	19, 34, 46, 55	2 (2%)
1	F	82/86 (95%)	0.17	2 (2%) 59 63	18, 32, 40, 53	2 (2%)
1	G	82/86 (95%)	0.60	3 (3%) 45 49	31, 39, 53, 57	0
1	H	82/86 (95%)	1.58	20 (24%) 2 2	26, 45, 53, 58	1 (1%)
1	I	83/86 (96%)	0.97	6 (7%) 21 25	28, 36, 47, 54	0
1	J	83/86 (96%)	0.44	3 (3%) 46 50	26, 33, 47, 53	0
1	K	83/86 (96%)	0.53	2 (2%) 59 63	30, 37, 48, 51	0
1	L	83/86 (96%)	1.04	5 (6%) 27 31	27, 46, 53, 59	1 (1%)
All	All	991/1032 (96%)	0.75	94 (9%) 14 15	18, 37, 52, 68	10 (1%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	LEU	4.6
1	J	343	SER	4.4
1	A	343	SER	4.3
1	C	343	SER	4.1
1	A	380	VAL	4.0
1	H	358	LEU	3.9
1	A	381	TYR	3.8
1	A	428	ASP	3.7
1	A	397	GLN	3.6
1	C	428	ASP	3.6
1	A	401	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	343	SER	3.6
1	K	343	SER	3.5
1	A	393	GLY	3.4
1	F	343	SER	3.4
1	A	417	LYS	3.4
1	D	377	GLU	3.4
1	L	343	SER	3.3
1	D	343	SER	3.3
1	E	427	ILE	3.2
1	A	392	LEU	3.1
1	B	380	VAL	3.1
1	A	391	LEU	3.1
1	H	395	LEU	3.1
1	A	368	LEU	3.0
1	H	419	ILE	3.0
1	H	371	ARG	3.0
1	K	377	GLU	3.0
1	A	394	ARG	3.0
1	I	416	SER	2.9
1	A	370	LEU	2.9
1	A	390	TRP	2.9
1	H	399	GLY	2.8
1	G	377	GLU	2.8
1	A	416	SER	2.8
1	B	343	SER	2.8
1	B	390	TRP	2.8
1	B	428	ASP	2.7
1	A	396	PRO	2.7
1	G	343	SER	2.7
1	I	428	ASP	2.7
1	L	382[A]	HIS	2.7
1	A	360	ALA	2.6
1	B	345	ALA	2.6
1	H	402	THR	2.6
1	A	386	GLY	2.6
1	A	353	TRP	2.6
1	A	427	ILE	2.5
1	H	417	LYS	2.5
1	A	358	LEU	2.5
1	H	370	LEU	2.5
1	A	399	GLY	2.5
1	H	390	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	400	ASP	2.4
1	E	343	SER	2.4
1	A	346	VAL	2.4
1	H	401	ILE	2.4
1	H	344	ASN	2.4
1	D	366	ASP	2.4
1	H	346	VAL	2.4
1	A	378	LYS	2.4
1	H	359	ILE	2.3
1	A	345	ALA	2.3
1	A	379	GLY	2.3
1	H	386	GLY	2.3
1	H	416	SER	2.2
1	A	371	ARG	2.2
1	I	395	LEU	2.2
1	J	377	GLU	2.2
1	I	362	PRO	2.2
1	L	427	ILE	2.2
1	A	362	PRO	2.2
1	H	353	TRP	2.2
1	A	366	ASP	2.2
1	D	427	ILE	2.1
1	D	395	LEU	2.1
1	A	361	VAL	2.1
1	H	408	ARG	2.1
1	A	385	SER	2.1
1	H	368	LEU	2.1
1	A	406[A]	ASN	2.1
1	A	411	VAL	2.1
1	H	380	VAL	2.1
1	L	406	ASN	2.1
1	H	381	TYR	2.1
1	G	427	ILE	2.1
1	B	406	ASN	2.0
1	I	396	PRO	2.0
1	A	426	LYS	2.0
1	F	427	ILE	2.0
1	J	427	ILE	2.0
1	L	417	LYS	2.0
1	A	398	THR	2.0
1	A	369	GLY	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
2	ACT	E	903	4/4	0.71	0.20	52,52,52,53	0
4	FMT	I	801	3/3	0.71	0.19	64,64,64,64	0
2	ACT	A	904	4/4	0.75	0.20	42,44,45,45	0
4	FMT	C	802	3/3	0.76	0.19	44,44,46,46	0
3	EDO	A	706	4/4	0.76	0.17	47,48,48,50	0
4	FMT	I	805	3/3	0.76	0.25	52,52,53,53	0
4	FMT	B	804	3/3	0.77	0.15	60,60,61,61	0
2	ACT	K	901	4/4	0.78	0.17	67,67,67,67	0
4	FMT	D	803	3/3	0.78	0.15	62,62,63,63	0
3	EDO	F	710	4/4	0.80	0.26	41,47,47,50	0
3	EDO	F	701	4/4	0.81	0.15	31,36,38,39	0
3	EDO	E	705	4/4	0.84	0.18	29,36,36,40	0
3	EDO	C	703	4/4	0.85	0.13	37,42,42,44	0
2	ACT	D	902	4/4	0.86	0.16	41,41,42,42	0
3	EDO	C	714	4/4	0.86	0.24	38,39,40,41	0
3	EDO	A	712	4/4	0.88	0.21	36,41,42,46	0
3	EDO	C	709	4/4	0.89	0.20	30,39,41,44	0
3	EDO	B	702	4/4	0.89	0.15	27,35,36,37	0
4	FMT	L	806	3/3	0.89	0.27	46,46,46,46	0
3	EDO	I	708	4/4	0.90	0.17	44,46,46,47	0
3	EDO	F	713	4/4	0.91	0.26	23,37,37,43	0
3	EDO	E	704	4/4	0.91	0.29	25,25,27,28	0
5	MG	J	604	1/1	0.92	0.18	32,32,32,32	0
3	EDO	J	711	4/4	0.93	0.17	33,39,45,48	0
5	MG	G	603	1/1	0.95	0.07	51,51,51,51	0
5	MG	H	602	1/1	0.96	0.19	38,38,38,38	0
5	MG	I	606	1/1	0.98	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	H	601	1/1	0.98	0.11	47,47,47,47	0
5	MG	I	605	1/1	0.99	0.17	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.