



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:46 PM UTC

PDB ID : 8OXS / pdb_00008oxs
Title : Cholera holotoxin variant (chimera with E. coli heat-labile enterotoxin, 4 C-terminal substitutions)
Authors : Kersten, F.; Heim, J.B.; Cordara, G.; Krenzel, U.
Deposited on : 2023-05-02
Resolution : 1.60 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

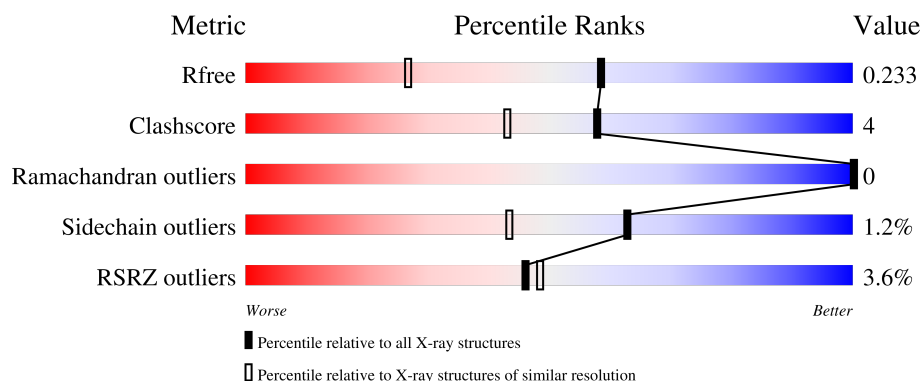
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	240	9% 80% 16% .
1	B	240	10% 84% 11% ..
2	C	103	93% 7%
2	D	103	% 93% 7%
2	E	103	% 90% 10%

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Mol	Chain	Length	Quality of chain
2	F	103	% 91% 9%
2	G	103	2% 95% . .
2	H	103	% 94% 6%
2	I	103	% 91% 8% .
2	J	103	% 97% . .
2	K	103	% 96% .
2	L	103	93% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13700 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 Cholera enterotoxin subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	34	0
			2140	1337	389	407	7			
1	B	231	Total	C	N	O	S	0	17	0
			2007	1250	370	380	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	GLU	ASP	engineered mutation	UNP P01555
A	230	VAL	ILE	engineered mutation	UNP P01555
A	232	ILE	THR	engineered mutation	UNP P01555
A	233	TYR	HIS	engineered mutation	UNP P01555
B	229	GLU	ASP	engineered mutation	UNP P01555
B	230	VAL	ILE	engineered mutation	UNP P01555
B	232	ILE	THR	engineered mutation	UNP P01555
B	233	TYR	HIS	engineered mutation	UNP P01555

- Molecule 2 is a protein called Cholera enterotoxin subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	103	Total	C	N	O	S	0	6	0
			858	537	150	164	7			
2	E	103	Total	C	N	O	S	0	5	0
			855	536	149	164	6			
2	F	103	Total	C	N	O	S	0	7	0
			877	551	155	165	6			
2	G	103	Total	C	N	O	S	0	3	0
			835	523	146	160	6			
2	H	103	Total	C	N	O	S	0	4	0
			846	531	148	160	7			
2	C	103	Total	C	N	O	S	0	4	0
			843	529	147	160	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	103	Total	C	N	O	S	0	6	0
			867	543	154	164	6			
2	J	103	Total	C	N	O	S	0	2	0
			828	518	145	159	6			
2	K	103	Total	C	N	O	S	0	4	0
			844	529	147	161	7			
2	L	103	Total	C	N	O	S	0	7	0
			870	547	151	165	7			

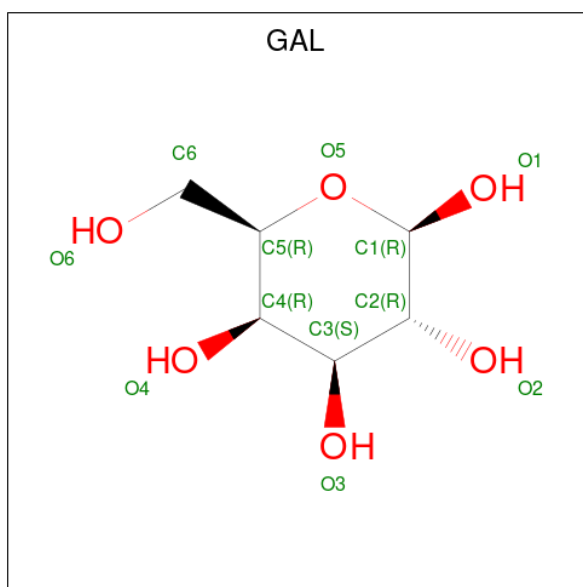
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	18	HIS	TYR	engineered mutation	UNP P01556
D	47	THR	ILE	engineered mutation	UNP P01556
E	18	HIS	TYR	engineered mutation	UNP P01556
E	47	THR	ILE	engineered mutation	UNP P01556
F	18	HIS	TYR	engineered mutation	UNP P01556
F	47	THR	ILE	engineered mutation	UNP P01556
G	18	HIS	TYR	engineered mutation	UNP P01556
G	47	THR	ILE	engineered mutation	UNP P01556
H	18	HIS	TYR	engineered mutation	UNP P01556
H	47	THR	ILE	engineered mutation	UNP P01556
C	18	HIS	TYR	engineered mutation	UNP P01556
C	47	THR	ILE	engineered mutation	UNP P01556
I	18	HIS	TYR	engineered mutation	UNP P01556
I	47	THR	ILE	engineered mutation	UNP P01556
J	18	HIS	TYR	engineered mutation	UNP P01556
J	47	THR	ILE	engineered mutation	UNP P01556
K	18	HIS	TYR	engineered mutation	UNP P01556
K	47	THR	ILE	engineered mutation	UNP P01556
L	18	HIS	TYR	engineered mutation	UNP P01556
L	47	THR	ILE	engineered mutation	UNP P01556

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

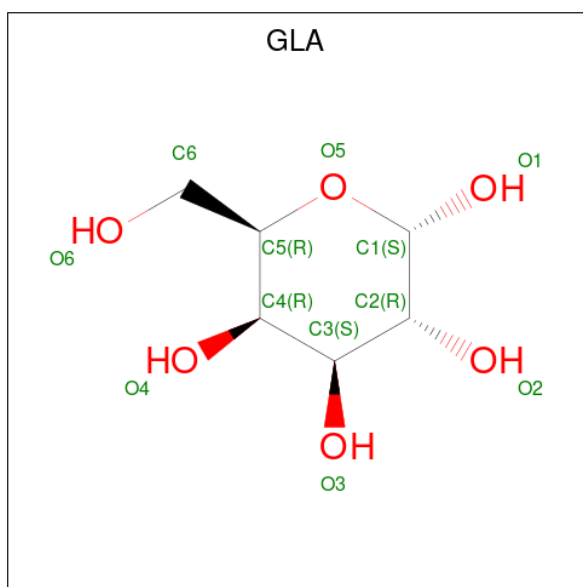
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



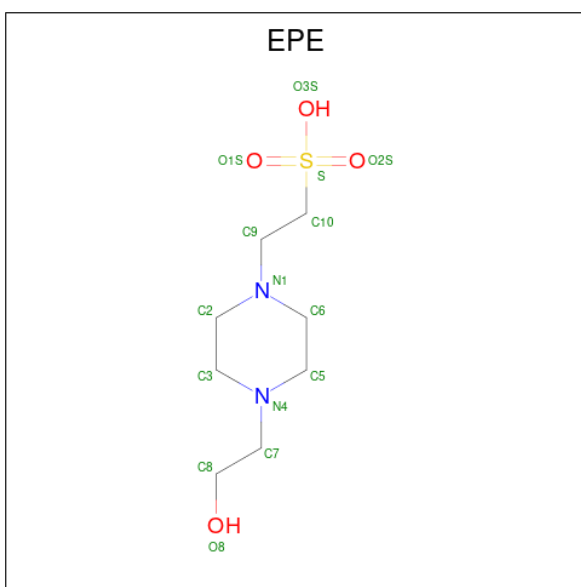
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		
4	E	1	Total	C	O	0	0
			12	6	6		
4	F	1	Total	C	O	0	0
			12	6	6		
4	G	1	Total	C	O	0	0
			12	6	6		
4	H	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	I	1	Total	C	O	0	0
			12	6	6		
4	K	1	Total	C	O	0	0
			12	6	6		
4	L	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is alpha-D-galactopyranose (CCD ID: GLA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			12	6	6		
5	E	1	Total	C	O	0	0
			12	6	6		
5	G	1	Total	C	O	0	0
			12	6	6		
5	H	1	Total	C	O	0	0
			12	6	6		
5	C	1	Total	C	O	0	0
			12	6	6		
5	K	1	Total	C	O	0	0
			12	6	6		
5	L	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	95	Total	O	0	0
			95	95		
7	D	62	Total	O	0	0
			62	62		
7	E	70	Total	O	0	0
			70	70		
7	F	64	Total	O	0	0
			64	64		
7	G	57	Total	O	0	0
			57	57		
7	H	51	Total	O	0	0
			51	51		
7	B	80	Total	O	0	0
			80	80		
7	C	61	Total	O	0	0
			61	61		

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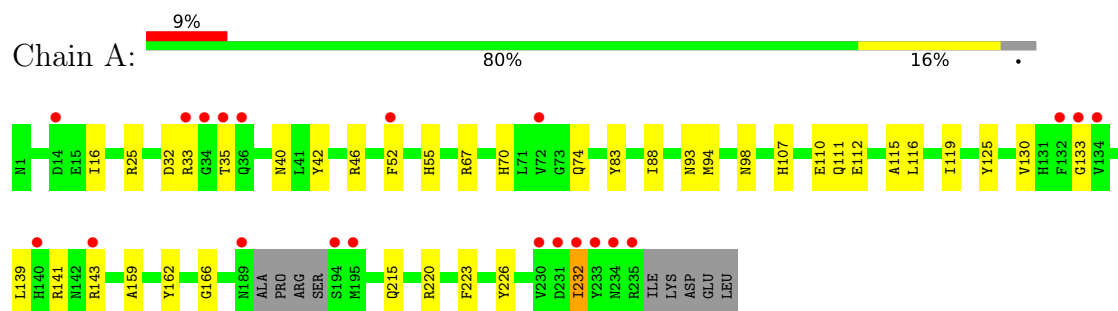
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	61	Total 61	O 61	0	0
7	J	53	Total 53	O 53	0	0
7	K	55	Total 55	O 55	0	0
7	L	55	Total 55	O 55	0	0

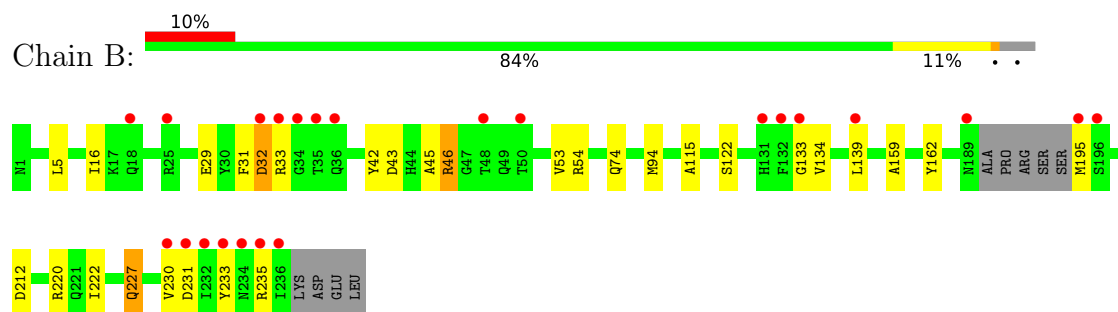
3 Residue-property plots [i](#)

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.

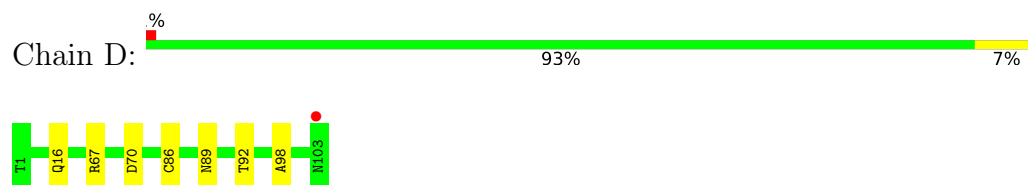
- Molecule 1: Cholera enterotoxin subunit A



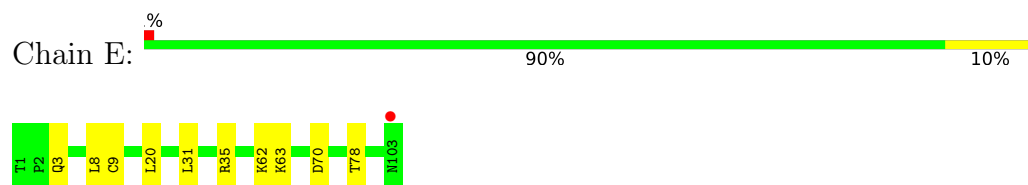
- Molecule 1: Cholera enterotoxin subunit A



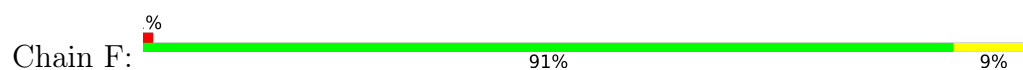
- Molecule 2: Cholera enterotoxin subunit B



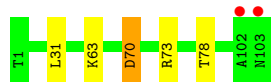
- Molecule 2: Cholera enterotoxin subunit B



- Molecule 2: Cholera enterotoxin subunit B



- Molecule 2: Cholera enterotoxin subunit B



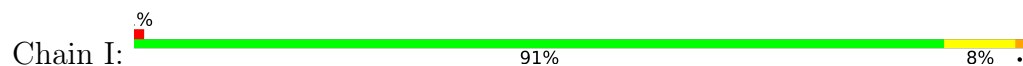
- Molecule 2: Cholera enterotoxin subunit B



- Molecule 2: Cholera enterotoxin subunit B



- Molecule 2: Cholera enterotoxin subunit B



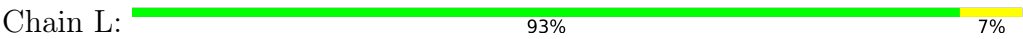
- Molecule 2: Cholera enterotoxin subunit B



- Molecule 2: Cholera enterotoxin subunit B



- Molecule 2: Cholera enterotoxin subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.30Å 89.61Å 141.09Å 90.00° 98.19° 90.00°	Depositor
Resolution (Å)	48.90 – 1.60 48.90 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.90-1.60) 99.9 (48.90-1.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.193 , 0.224 0.203 , 0.233	Depositor DCC
R_{free} test set	2055 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.114	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13700	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0190e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EPE, NA, GAL, GLA

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	0/2200	0.87	0/2980
1	B	0.58	0/2062	0.92	1/2791 (0.0%)
2	C	0.64	0/857	0.92	0/1156
2	D	0.60	0/873	0.84	0/1179
2	E	0.61	0/869	0.90	1/1172 (0.1%)
2	F	0.62	0/893	0.89	0/1204
2	G	0.62	0/849	0.91	1/1145 (0.1%)
2	H	0.57	0/860	0.93	1/1158 (0.1%)
2	I	0.63	1/881 (0.1%)	0.89	1/1185 (0.1%)
2	J	0.63	0/842	0.91	1/1137 (0.1%)
2	K	0.60	0/858	0.89	0/1158
2	L	0.55	0/884	0.88	1/1191 (0.1%)
All	All	0.59	1/12928 (0.0%)	0.89	7/17456 (0.0%)

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	A	0	1
1	B	0	1
2	D	0	1
2	G	0	1
2	I	0	1
2	J	0	1
2	K	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	66	GLU	CD-OE2	6.01	1.36	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	70	ASP	CA-CB-CG	6.69	119.29	112.60
2	I	70	ASP	CA-CB-CG	6.59	119.19	112.60
2	H	70	ASP	CA-CB-CG	6.14	118.74	112.60
2	L	70	ASP	CA-CB-CG	5.60	118.20	112.60
2	J	70	ASP	CA-CB-CG	5.20	117.80	112.60
2	G	70	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	231	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67[A]	ARG	Sidechain
1	B	46[A]	ARG	Sidechain
2	D	67	ARG	Sidechain
2	G	73	ARG	Sidechain
2	I	67[A]	ARG	Sidechain
2	J	49	GLN	Peptide
2	K	73	ARG	Sidechain

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	2140	0	1974	44	0
1	B	2007	0	1860	22	0
2	C	843	0	848	5	0
2	D	858	0	858	4	0
2	E	855	0	856	17	0
2	F	877	0	874	9	0
2	G	835	0	837	6	0
2	H	846	0	853	7	0
2	I	867	0	874	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	828	0	826	2	0
2	K	844	0	848	1	0
2	L	870	0	877	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	12	0	0
4	C	12	0	4	2	0
4	D	12	0	4	0	0
4	E	12	0	4	0	0
4	F	12	0	12	0	0
4	G	12	0	2	0	0
4	H	12	0	4	2	0
4	I	12	0	11	0	0
4	K	12	0	4	0	0
4	L	12	0	5	3	0
5	C	12	0	5	0	0
5	D	12	0	3	0	0
5	E	12	0	6	0	0
5	G	12	0	4	0	0
5	H	12	0	3	0	0
5	K	12	0	4	0	0
5	L	12	0	3	1	0
6	B	15	0	17	0	0
6	E	15	0	17	0	0
6	H	15	0	17	0	0
6	I	15	0	18	0	0
7	A	95	0	0	2	0
7	B	80	0	0	3	0
7	C	61	0	0	0	0
7	D	62	0	0	0	0
7	E	70	0	0	2	0
7	F	64	0	0	2	0
7	G	57	0	0	2	0
7	H	51	0	0	2	0
7	I	61	0	0	0	0
7	J	53	0	0	0	0
7	K	55	0	0	0	0
7	L	55	0	0	0	0
All	All	13700	0	12544	115	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 4.

All (115) 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)
2:E:8[B]:LEU:C	2:E:8[B]:LEU:HD13	1.77	1.08
2:E:8[B]:LEU:HD13	2:E:8[B]:LEU:O	1.57	1.01
2:E:8[B]:LEU:C	2:E:8[B]:LEU:CD1	2.33	1.01
1:B:31[A]:PHE:O	1:B:33[A]:ARG:HG2	1.70	0.91
1:A:112[B]:GLU:OE1	7:A:401:HOH:O	1.89	0.90
1:A:226[B]:TYR:CE1	2:H:78:THR:HG21	2.09	0.87
1:B:42:TYR:O	1:B:45[A]:ALA:O	1.99	0.80
1:B:45[A]:ALA:O	1:B:46[A]:ARG:HB2	1.89	0.72
1:A:32[A]:ASP:O	1:A:33[A]:ARG:HD2	1.91	0.70
2:E:62:LYS:HE3	7:E:364:HOH:O	1.92	0.70
1:B:45[A]:ALA:O	1:B:46[A]:ARG:CB	2.41	0.68
2:E:63[B]:LYS:HA	2:E:63[B]:LYS:HE2	1.76	0.68
2:D:16[B]:GLN:OE1	2:D:89:ASN:ND2	2.21	0.68
1:A:94[A]:MET:SD	1:A:115:ALA:HB2	2.35	0.66
7:B:421:HOH:O	2:L:74[B]:ILE:HG12	1.96	0.66
1:A:32[A]:ASP:C	1:A:33[A]:ARG:HD2	2.22	0.64
1:B:227[A]:GLN:O	7:B:401:HOH:O	2.12	0.64
2:F:24[A]:ILE:HD12	7:F:311:HOH:O	1.97	0.63
1:A:223[B]:PHE:CD1	1:A:226[B]:TYR:CE2	2.87	0.62
2:E:63[B]:LYS:CA	2:E:63[B]:LYS:CE	2.77	0.62
1:A:223[B]:PHE:CE1	1:A:226[B]:TYR:HE2	2.17	0.61
1:A:223[B]:PHE:CD1	1:A:226[B]:TYR:CD2	2.89	0.61
1:A:110[A]:GLU:O	1:A:111[A]:GLN:C	2.44	0.61
2:F:67[B]:ARG:NH2	2:G:70:ASP:OD1	2.34	0.61
1:A:226[B]:TYR:CD1	2:H:78:THR:HG21	2.37	0.59
1:A:223[B]:PHE:HD1	1:A:226[B]:TYR:CD2	2.21	0.58
2:E:3[B]:GLN:HG2	2:F:47:THR:HG21	1.86	0.58
2:E:8[B]:LEU:C	2:E:8[B]:LEU:HD12	2.28	0.56
1:A:74:GLN:HE22	1:A:133:GLY:HA2	1.70	0.56
1:A:143[B]:ARG:NH2	2:G:78:THR:O	2.39	0.55
1:A:42:TYR:CZ	1:A:46[B]:ARG:HD2	2.42	0.55
1:B:94[B]:MET:SD	1:B:115:ALA:HB2	2.47	0.55
1:A:33[A]:ARG:HD3	1:A:215:GLN:OE1	2.07	0.55
2:C:8[A]:LEU:C	2:C:8[A]:LEU:HD23	2.32	0.54
1:A:232:ILE:HD11	2:F:66:GLU:HB3	1.88	0.54
2:I:67[B]:ARG:NH1	2:J:70:ASP:OD1	2.40	0.54
2:G:63[A]:LYS:HE2	7:G:308:HOH:O	2.06	0.54
2:C:70:ASP:OD1	2:L:67:ARG:NH1	2.38	0.53
1:A:232:ILE:HB	2:E:63[B]:LYS:HG3	1.90	0.53
1:A:32[A]:ASP:OD2	1:A:35[A]:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223[B]:PHE:CE1	1:A:226[B]:TYR:CE2	2.97	0.52
2:L:88:TRP:CE2	4:L:202:GAL:H5	2.44	0.52
2:H:88:TRP:CE2	4:H:202:GAL:H5	2.44	0.52
2:D:70:ASP:OD1	2:H:67:ARG:NH1	2.34	0.52
1:A:74:GLN:HE21	1:A:74:GLN:HA	1.75	0.51
2:L:56:GLN:HG3	5:L:201:GLA:O4	2.11	0.51
1:A:223[B]:PHE:HA	1:A:226[B]:TYR:HD2	1.76	0.51
2:C:56:GLN:HG3	4:C:202:GAL:O4	2.12	0.50
2:E:63[B]:LYS:HE3	2:E:63[B]:LYS:N	2.27	0.49
1:A:42:TYR:CE1	1:A:46[B]:ARG:HD2	2.48	0.49
2:F:24[A]:ILE:CD1	7:F:311:HOH:O	2.56	0.48
2:I:81[B]:LYS:HE3	2:I:103:ASN:HB2	1.95	0.48
1:B:230:VAL:HG12	1:B:235:ARG:HD3	1.95	0.47
1:B:45[A]:ALA:O	1:B:46[A]:ARG:HG3	2.13	0.47
1:A:125:TYR:HE2	1:A:139:LEU:HD21	1.79	0.47
1:A:223[B]:PHE:HD1	1:A:226[B]:TYR:HD2	1.63	0.47
1:B:5:LEU:HD12	1:B:94[A]:MET:SD	2.54	0.47
2:L:88:TRP:CD1	4:L:202:GAL:H3	2.50	0.47
1:A:223[B]:PHE:CD1	1:A:226[B]:TYR:HE2	2.31	0.47
2:C:91:LYS:NZ	4:C:202:GAL:O3	2.42	0.47
2:D:92[B]:THR:HG22	7:H:332:HOH:O	2.14	0.46
2:E:8[B]:LEU:HD12	2:E:9[B]:CYS:N	2.30	0.46
1:B:29:GLU:O	1:B:32[A]:ASP:HB3	2.16	0.46
1:A:74:GLN:HE22	1:A:133:GLY:CA	2.29	0.46
1:B:220:ARG:HA	2:I:78:THR:HB	1.97	0.46
2:E:63[B]:LYS:CA	2:E:63[B]:LYS:HE3	2.45	0.46
2:F:67[B]:ARG:HH21	2:G:70:ASP:N	2.14	0.46
2:H:67:ARG:NH1	7:H:301:HOH:O	2.33	0.45
1:A:40:ASN:CG	1:A:166[B]:GLY:HA3	2.41	0.45
2:H:91:LYS:NZ	4:H:202:GAL:O3	2.50	0.45
1:B:29:GLU:HB2	1:B:32[A]:ASP:HB3	1.98	0.45
1:A:93[B]:ASN:OD1	1:A:94[B]:MET:HG3	2.17	0.45
1:B:43:ASP:OD1	1:B:46[A]:ARG:NH2	2.48	0.45
1:A:226[B]:TYR:CE1	2:H:78:THR:CG2	2.91	0.44
1:A:107:HIS:HB3	1:A:110[B]:GLU:HG2	1.99	0.44
1:B:29:GLU:HB2	1:B:32[B]:ASP:HB3	2.00	0.44
2:F:31:LEU:C	2:F:31:LEU:HD12	2.43	0.43
1:A:223[B]:PHE:CD1	1:A:226[B]:TYR:HD2	2.33	0.43
1:A:220:ARG:HA	2:E:78:THR:HB	2.01	0.43
1:A:33[A]:ARG:NH1	1:A:215:GLN:OE1	2.52	0.43
2:L:31:LEU:C	2:L:31:LEU:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CD1	1:A:55[A]:HIS:CE1	3.07	0.42
1:A:116:LEU:C	1:A:116:LEU:HD23	2.44	0.42
7:B:421:HOH:O	2:L:74[B]:ILE:CG1	2.63	0.42
2:L:88:TRP:CH2	4:L:202:GAL:H62	2.54	0.42
2:D:86[B]:CYS:HB3	2:D:98:ALA:HB3	2.01	0.42
2:E:63[B]:LYS:HE2	2:E:63[B]:LYS:CA	2.42	0.42
1:B:74[B]:GLN:HE22	1:B:133:GLY:HA3	1.84	0.42
2:F:18:HIS:HE1	2:F:94:HIS:ND1	2.18	0.42
2:J:31:LEU:C	2:J:31:LEU:HD12	2.45	0.42
2:E:8[B]:LEU:O	2:E:9[B]:CYS:C	2.61	0.42
2:E:35:ARG:NH1	7:E:303:HOH:O	2.45	0.42
1:A:70:HIS:O	1:A:74:GLN:HG2	2.20	0.41
1:A:88:ILE:HD13	1:A:119:ILE:HD13	2.02	0.41
1:B:159:ALA:HA	1:B:162:TYR:CD2	2.54	0.41
1:A:223[B]:PHE:HD1	1:A:226[B]:TYR:CE2	2.35	0.41
1:A:223[B]:PHE:HE1	1:A:226[B]:TYR:HE2	1.65	0.41
1:A:83:TYR:CZ	1:A:130:VAL:HG11	2.55	0.41
2:G:63[A]:LYS:CE	7:G:308:HOH:O	2.66	0.41
1:B:33[A]:ARG:NH2	1:B:212:ASP:OD1	2.54	0.41
1:B:45[A]:ALA:O	1:B:46[A]:ARG:CG	2.67	0.41
1:B:233:TYR:HA	2:I:63[B]:LYS:HE3	2.02	0.41
1:A:159:ALA:HA	1:A:162:TYR:CD2	2.56	0.41
2:K:75:ALA:HB2	2:K:101[B]:MET:HE1	2.03	0.41
1:A:25:ARG:HB2	1:A:55[B]:HIS:CE1	2.56	0.40
1:A:141:ARG:NH1	7:A:404:HOH:O	2.49	0.40
1:B:122:SER:CB	1:B:222:ILE:HD11	2.51	0.40
2:C:15:THR:HA	2:C:87:VAL:O	2.21	0.40
1:A:98:ASN:HD22	1:A:111[A]:GLN:NE2	2.20	0.40
2:E:63[B]:LYS:HA	2:E:63[B]:LYS:CE	2.38	0.40
2:F:15:THR:HA	2:F:87:VAL:O	2.20	0.40
1:B:195:MET:HE3	1:B:195:MET:HB3	2.00	0.40
1:B:53:VAL:O	1:B:54:ARG:C	2.63	0.40
2:I:81[B]:LYS:CE	2:I:103:ASN:HB2	2.52	0.40
2:G:31:LEU:C	2:G:31:LEU:HD12	2.47	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	261/240 (109%)	252 (97%)	9 (3%)	0	100	100
1	B	244/240 (102%)	236 (97%)	8 (3%)	0	100	100
2	C	105/103 (102%)	104 (99%)	1 (1%)	0	100	100
2	D	107/103 (104%)	106 (99%)	1 (1%)	0	100	100
2	E	106/103 (103%)	105 (99%)	1 (1%)	0	100	100
2	F	108/103 (105%)	106 (98%)	2 (2%)	0	100	100
2	G	104/103 (101%)	103 (99%)	1 (1%)	0	100	100
2	H	105/103 (102%)	104 (99%)	1 (1%)	0	100	100
2	I	107/103 (104%)	106 (99%)	1 (1%)	0	100	100
2	J	103/103 (100%)	102 (99%)	1 (1%)	0	100	100
2	K	105/103 (102%)	104 (99%)	1 (1%)	0	100	100
2	L	108/103 (105%)	106 (98%)	2 (2%)	0	100	100
All	All	1563/1510 (104%)	1534 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	226/204 (111%)	224 (99%)	2 (1%)	70	55
1	B	211/204 (103%)	204 (97%)	7 (3%)	33	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	93/89 (104%)	91 (98%)	2 (2%)	45	22
2	D	95/89 (107%)	95 (100%)	0	100	100
2	E	94/89 (106%)	92 (98%)	2 (2%)	47	23
2	F	96/89 (108%)	96 (100%)	0	100	100
2	G	92/89 (103%)	92 (100%)	0	100	100
2	H	93/89 (104%)	91 (98%)	2 (2%)	45	22
2	I	95/89 (107%)	93 (98%)	2 (2%)	47	23
2	J	91/89 (102%)	91 (100%)	0	100	100
2	K	93/89 (104%)	92 (99%)	1 (1%)	65	46
2	L	96/89 (108%)	95 (99%)	1 (1%)	68	50
All	All	1375/1298 (106%)	1356 (99%)	19 (1%)	63	38

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	232	ILE
2	E	20	LEU
2	E	31	LEU
2	H	9[A]	CYS
2	H	9[B]	CYS
1	B	16	ILE
1	B	32[A]	ASP
1	B	32[B]	ASP
1	B	134	VAL
1	B	139	LEU
1	B	227[A]	GLN
1	B	227[B]	GLN
2	C	81[A]	LYS
2	C	81[B]	LYS
2	I	20	LEU
2	I	31	LEU
2	K	20	LEU
2	L	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	36	GLN
1	A	38	ASN
1	A	74	GLN
1	A	138	GLN
1	A	182	HIS
1	A	189	ASN
1	A	234	ASN
2	D	49	GLN
2	E	49	GLN
2	F	18	HIS
2	F	49	GLN
2	G	49	GLN
1	B	152	ASN
1	B	182	HIS
1	B	189	ASN
2	C	49	GLN
2	I	49	GLN
2	J	21	ASN
2	J	49	GLN
2	K	49	GLN
2	L	49	GLN

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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\# Z > 2$
5	GLA	K	201	4	12,12,12	0.43	0	17,17,17	0.89	0
4	GAL	A	302	-	12,12,12	0.53	0	17,17,17	0.64	0
4	GAL	H	202	5	12,12,12	0.33	0	17,17,17	0.80	0
4	GAL	K	202	5	12,12,12	0.33	0	17,17,17	0.88	1 (5%)
5	GLA	D	201	4	12,12,12	0.48	0	17,17,17	0.63	0
4	GAL	D	202	5	12,12,12	0.50	0	17,17,17	0.56	0
5	GLA	L	201	4	12,12,12	0.29	0	17,17,17	0.58	0
4	GAL	G	201	5	12,12,12	0.20	0	17,17,17	0.62	0
4	GAL	C	202	5	12,12,12	0.52	0	17,17,17	0.64	0
5	GLA	C	201	4	12,12,12	0.51	0	17,17,17	0.57	0
6	EPE	B	302	-	15,15,15	0.96	1 (6%)	19,20,20	1.15	3 (15%)
6	EPE	H	201	-	15,15,15	0.97	1 (6%)	19,20,20	0.96	1 (5%)
4	GAL	E	203	5	12,12,12	0.61	0	17,17,17	1.10	1 (5%)
5	GLA	E	202	4	12,12,12	0.53	0	17,17,17	0.83	0
6	EPE	E	201	-	15,15,15	1.07	1 (6%)	19,20,20	1.12	1 (5%)
6	EPE	I	201	-	15,15,15	0.58	0	19,20,20	0.72	0
5	GLA	H	203	4	12,12,12	0.42	0	17,17,17	0.95	1 (5%)
4	GAL	I	202	-	12,12,12	0.60	0	17,17,17	0.69	1 (5%)
5	GLA	G	202	4	12,12,12	0.39	0	17,17,17	0.70	0
4	GAL	L	202	5	12,12,12	0.45	0	17,17,17	0.85	0
4	GAL	F	201	-	12,12,12	0.56	0	17,17,17	0.76	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
5	GLA	K	201	4	-	2/2/22/22	0/1/1/1
4	GAL	A	302	-	-	0/2/22/22	0/1/1/1
4	GAL	H	202	5	-	0/2/22/22	0/1/1/1
4	GAL	K	202	5	-	0/2/22/22	0/1/1/1
5	GLA	D	201	4	-	0/2/22/22	0/1/1/1
4	GAL	D	202	5	-	0/2/22/22	0/1/1/1
5	GLA	L	201	4	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	G	201	5	-	1/2/22/22	0/1/1/1
4	GAL	C	202	5	-	0/2/22/22	0/1/1/1
5	GLA	C	201	4	-	0/2/22/22	0/1/1/1
6	EPE	B	302	-	-	5/9/19/19	0/1/1/1
6	EPE	H	201	-	-	0/9/19/19	0/1/1/1
4	GAL	E	203	5	-	0/2/22/22	0/1/1/1
5	GLA	E	202	4	-	0/2/22/22	0/1/1/1
6	EPE	E	201	-	-	2/9/19/19	0/1/1/1
6	EPE	I	201	-	-	5/9/19/19	0/1/1/1
5	GLA	H	203	4	-	0/2/22/22	0/1/1/1
4	GAL	I	202	-	-	0/2/22/22	0/1/1/1
5	GLA	G	202	4	-	0/2/22/22	0/1/1/1
4	GAL	L	202	5	-	2/2/22/22	0/1/1/1
4	GAL	F	201	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	201	EPE	O1S-S	3.86	1.56	1.45
6	H	201	EPE	O2S-S	3.42	1.54	1.45
6	B	302	EPE	O1S-S	3.33	1.54	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	201	EPE	O1S-S-C10	-3.12	102.01	106.73
6	B	302	EPE	O1S-S-C10	3.09	111.39	106.73
6	H	201	EPE	O3S-S-O1S	2.95	118.78	111.40
4	E	203	GAL	O1-C1-C2	-2.76	100.97	108.98
6	B	302	EPE	O3S-S-O2S	2.65	118.03	111.40
5	H	203	GLA	O2-C2-C3	2.47	116.20	110.38
6	B	302	EPE	O3S-S-O1S	-2.19	105.93	111.40
4	I	202	GAL	C1-O5-C5	-2.15	109.48	113.65
4	K	202	GAL	C1-C2-C3	2.13	114.70	110.36

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	201	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
6	B	302	EPE	C9-C10-S-O1S
6	E	201	EPE	N4-C7-C8-O8
5	K	201	GLA	C4-C5-C6-O6
5	K	201	GLA	O5-C5-C6-O6
6	I	201	EPE	C9-C10-S-O3S
5	L	201	GLA	C4-C5-C6-O6
4	L	202	GAL	O5-C5-C6-O6
5	L	201	GLA	O5-C5-C6-O6
6	B	302	EPE	C9-C10-S-O3S
6	I	201	EPE	C10-C9-N1-C2
6	I	201	EPE	C10-C9-N1-C6
6	B	302	EPE	C9-C10-S-O2S
6	I	201	EPE	C9-C10-S-O1S
6	I	201	EPE	C9-C10-S-O2S
4	L	202	GAL	C4-C5-C6-O6
4	G	201	GAL	C4-C5-C6-O6
6	B	302	EPE	C8-C7-N4-C3
6	B	302	EPE	C8-C7-N4-C5

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	202	GAL	2	0
5	L	201	GLA	1	0
4	C	202	GAL	2	0
4	L	202	GAL	3	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	231/240 (96%)	0.48	21 (9%) 15 15	8, 25, 53, 69	34 (14%)
1	B	231/240 (96%)	0.50	23 (9%) 12 12	10, 26, 54, 74	17 (7%)
2	C	103/103 (100%)	-0.31	0 100 100	8, 20, 29, 54	4 (3%)
2	D	103/103 (100%)	-0.21	1 (0%) 79 83	9, 21, 30, 50	6 (5%)
2	E	103/103 (100%)	-0.15	1 (0%) 79 83	10, 22, 32, 49	5 (4%)
2	F	103/103 (100%)	-0.06	1 (0%) 79 83	8, 21, 30, 52	7 (6%)
2	G	103/103 (100%)	0.15	2 (1%) 66 70	9, 23, 32, 60	3 (2%)
2	H	103/103 (100%)	0.01	1 (0%) 79 83	10, 23, 33, 52	4 (3%)
2	I	103/103 (100%)	-0.09	1 (0%) 79 83	8, 21, 32, 55	6 (5%)
2	J	103/103 (100%)	-0.05	1 (0%) 79 83	11, 21, 30, 52	2 (1%)
2	K	103/103 (100%)	-0.08	1 (0%) 79 83	10, 20, 30, 53	4 (3%)
2	L	103/103 (100%)	-0.16	0 100 100	9, 22, 31, 45	7 (6%)
All	All	1492/1510 (98%)	0.09	53 (3%) 46 48	8, 22, 41, 74	99 (6%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ILE	7.2
1	A	34[A]	GLY	6.7
1	B	132	PHE	5.8
1	A	233	TYR	5.6
1	B	233	TYR	5.5
1	B	236	ILE	5.3
1	B	232	ILE	4.4
1	A	35[A]	THR	4.3
1	A	33[A]	ARG	4.0
1	B	230	VAL	4.0
1	B	35	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	189	ASN	3.7
1	B	33[A]	ARG	3.4
1	A	230	VAL	3.3
2	H	103	ASN	3.2
1	A	132	PHE	3.1
1	B	195	MET	3.1
2	I	103	ASN	3.0
2	E	103	ASN	2.9
1	B	133	GLY	2.8
1	B	48	THR	2.7
1	A	194	SER	2.6
2	G	102	ALA	2.6
1	B	189	ASN	2.6
2	J	103	ASN	2.6
1	A	134[A]	VAL	2.5
1	B	139	LEU	2.5
1	A	133	GLY	2.5
1	B	131[A]	HIS	2.5
1	A	52	PHE	2.5
1	B	32[A]	ASP	2.5
1	A	140[A]	HIS	2.5
1	B	234	ASN	2.4
2	G	103	ASN	2.4
2	F	103	ASN	2.3
1	A	231	ASP	2.3
1	B	235	ARG	2.3
1	A	36	GLN	2.2
1	B	231	ASP	2.2
1	A	195	MET	2.2
1	B	18[A]	GLN	2.1
1	B	25[A]	ARG	2.1
1	A	234	ASN	2.1
1	A	14	ASP	2.1
1	B	36	GLN	2.1
1	A	143[A]	ARG	2.1
1	B	50	THR	2.1
1	B	34[A]	GLY	2.0
2	K	103	ASN	2.0
1	A	72	VAL	2.0
2	D	103	ASN	2.0
1	A	235	ARG	2.0
1	B	196	SER	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
6	EPE	E	201	15/15	0.68	0.25	38,48,52,55	15
6	EPE	I	201	15/15	0.78	0.19	34,44,53,54	15
6	EPE	B	302	15/15	0.87	0.13	32,35,48,50	15
4	GAL	A	302	12/12	0.89	0.09	25,30,33,34	0
4	GAL	G	201	12/12	0.89	0.08	20,23,26,27	12
5	GLA	G	202	12/12	0.89	0.08	18,20,24,27	12
6	EPE	H	201	15/15	0.90	0.12	30,33,37,40	15
4	GAL	I	202	12/12	0.92	0.09	21,25,29,34	0
5	GLA	K	201	12/12	0.92	0.07	19,21,23,23	12
5	GLA	E	202	12/12	0.92	0.08	16,18,19,22	12
4	GAL	E	203	12/12	0.93	0.07	16,17,18,20	12
4	GAL	H	202	12/12	0.93	0.07	21,23,24,25	12
4	GAL	F	201	12/12	0.93	0.08	22,24,28,32	0
5	GLA	L	201	12/12	0.93	0.07	20,22,23,23	12
4	GAL	K	202	12/12	0.94	0.06	16,18,20,20	12
4	GAL	C	202	12/12	0.95	0.06	13,17,20,21	12
5	GLA	H	203	12/12	0.95	0.06	18,20,22,23	12
5	GLA	D	201	12/12	0.95	0.06	18,20,22,22	12
4	GAL	D	202	12/12	0.95	0.06	13,16,18,18	12
4	GAL	L	202	12/12	0.96	0.06	17,18,19,21	12
5	GLA	C	201	12/12	0.96	0.06	13,14,16,16	12
3	NA	B	301	1/1	0.98	0.04	19,19,19,19	0
3	NA	A	301	1/1	0.98	0.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.