



Full wwPDB X-ray Structure Validation Report ⓘ

May 1, 2019 – 09:23 PM EDT

PDB ID : 1W2T
Title : beta-fructosidase from *Thermotoga maritima* in complex with raffinose
Authors : Alberto, F.; Henrissat, B.; Czjzek, M.
Deposited on : 2004-07-08
Resolution : 1.87 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

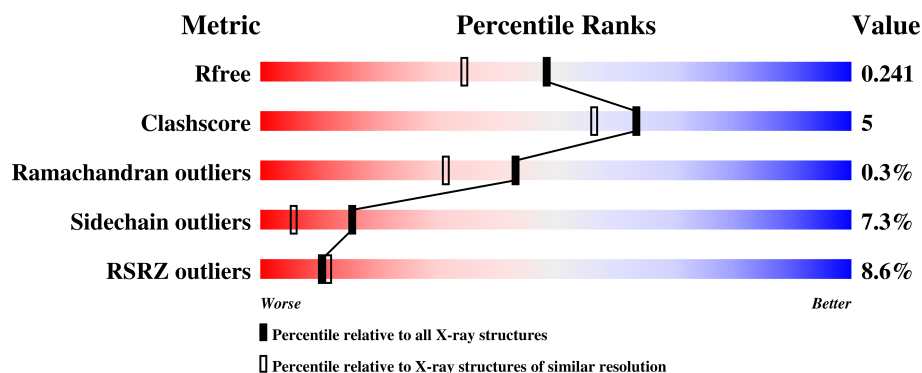
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	111664	8255 (1.90-1.86)
Clashscore	122126	9028 (1.90-1.86)
Ramachandran outliers	120053	8930 (1.90-1.86)
Sidechain outliers	120020	8930 (1.90-1.86)
RSRZ outliers	108989	8087 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	432	<div> <div>5%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	432	<div> <div>11%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	C	432	<div> <div>9%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	432	<div> <div>8%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	432	<div> <div>10%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	432	<div><div></div><div>8%</div><div>87%</div><div>12%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23234 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 BETA FRUCTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3517	2250	589	665	13			
1	B	432	Total	C	N	O	S	0	0	0
			3519	2252	589	665	13			
1	C	432	Total	C	N	O	S	0	0	0
			3519	2252	589	665	13			
1	D	432	Total	C	N	O	S	0	0	0
			3518	2251	589	665	13			
1	E	432	Total	C	N	O	S	0	0	0
			3518	2251	589	665	13			
1	F	432	Total	C	N	O	S	0	0	0
			3518	2252	588	665	13			

There are 18 discrepancies between the modelled and reference sequences:

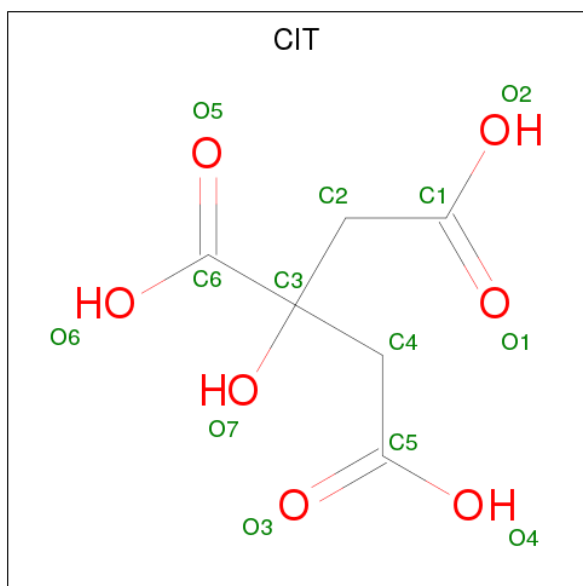
Chain	Residue	Modelled	Actual	Comment	Reference
A	190	ASP	GLU	engineered mutation	UNP O33833
A	108	VAL	ALA	cloning artifact	UNP O33833
A	179	ALA	VAL	cloning artifact	UNP O33833
B	190	ASP	GLU	engineered mutation	UNP O33833
B	108	VAL	ALA	cloning artifact	UNP O33833
B	179	ALA	VAL	cloning artifact	UNP O33833
C	190	ASP	GLU	engineered mutation	UNP O33833
C	108	VAL	ALA	cloning artifact	UNP O33833
C	179	ALA	VAL	cloning artifact	UNP O33833
D	190	ASP	GLU	engineered mutation	UNP O33833
D	108	VAL	ALA	cloning artifact	UNP O33833
D	179	ALA	VAL	cloning artifact	UNP O33833
E	190	ASP	GLU	engineered mutation	UNP O33833
E	108	VAL	ALA	cloning artifact	UNP O33833
E	179	ALA	VAL	cloning artifact	UNP O33833
F	190	ASP	GLU	engineered mutation	UNP O33833
F	108	VAL	ALA	cloning artifact	UNP O33833

Continued on next page...

Continued from previous page...

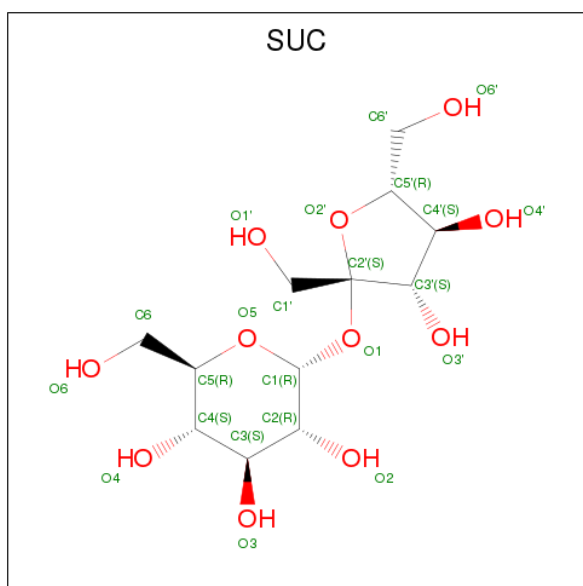
Chain	Residue	Modelled	Actual	Comment	Reference
F	179	ALA	VAL	cloning artifact	UNP O33833

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



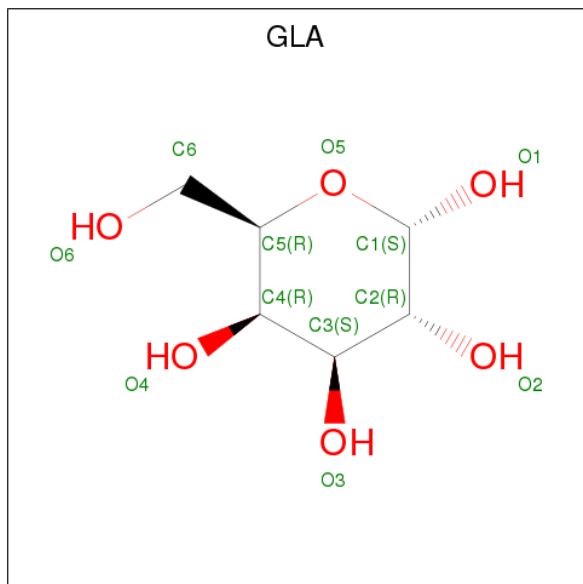
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



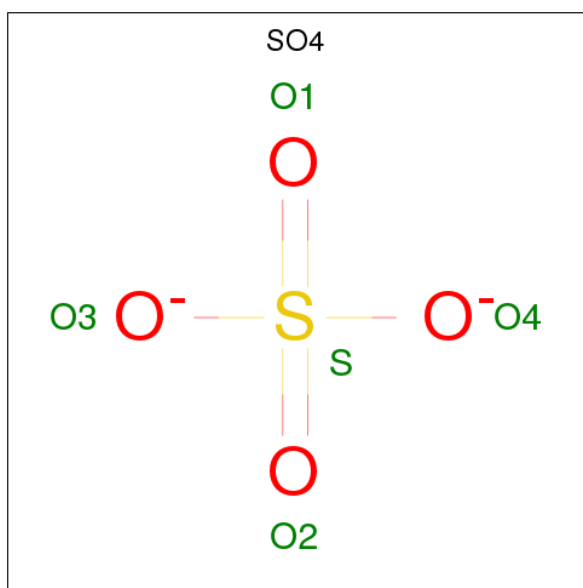
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		
3	E	1	Total	C	O	0	0
			23	12	11		
3	F	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is ALPHA D-GALACTOSE (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

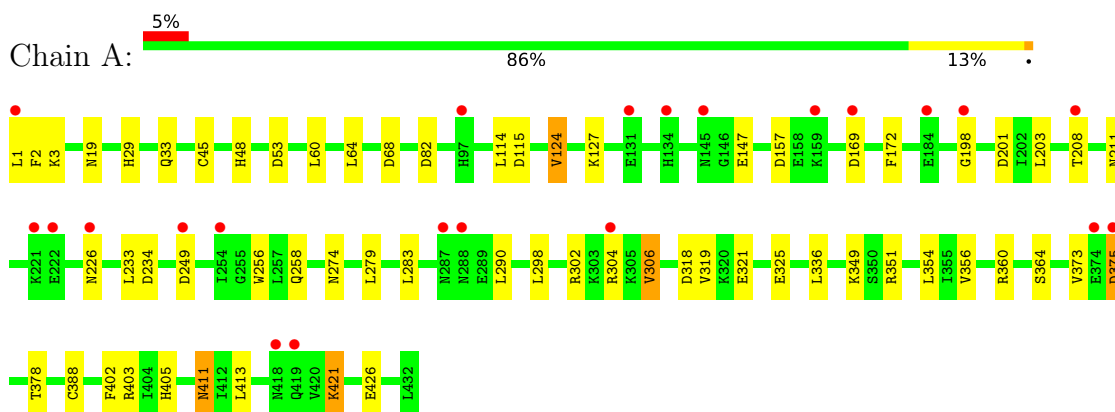
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	259	Total	O	0	0
			259	259		
6	C	316	Total	O	0	0
			316	316		
6	D	364	Total	O	0	0
			364	364		
6	E	296	Total	O	0	0
			296	296		
6	F	314	Total	O	0	0
			314	314		

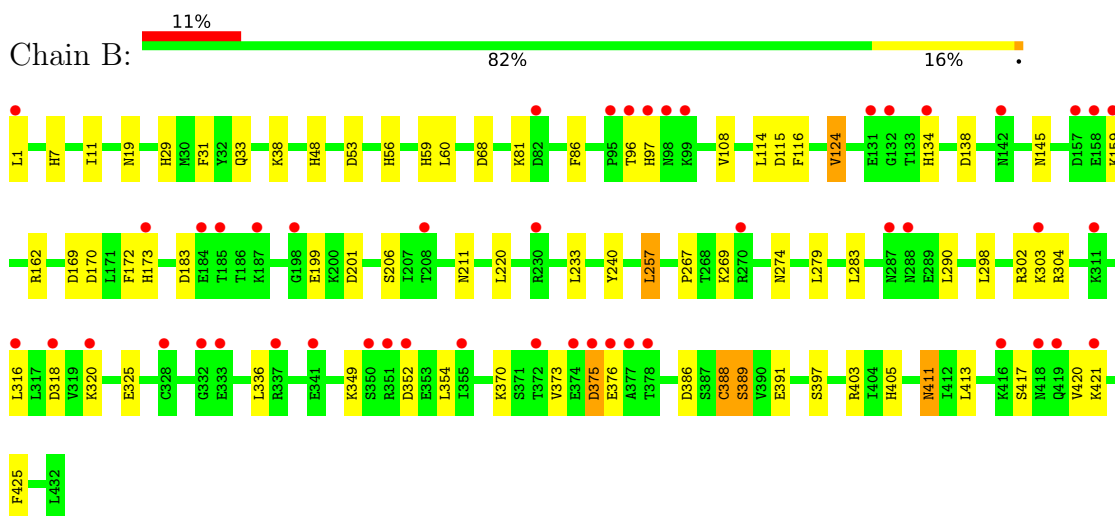
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

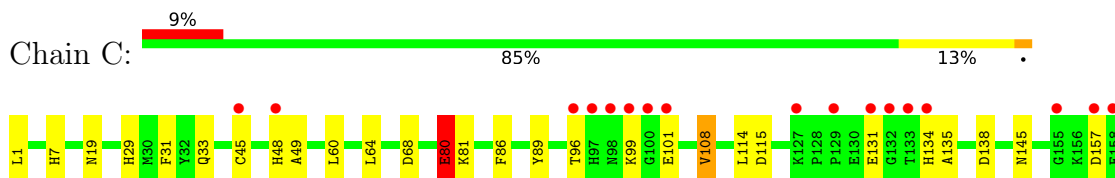
• Molecule 1: BETA FRUCTOSIDASE

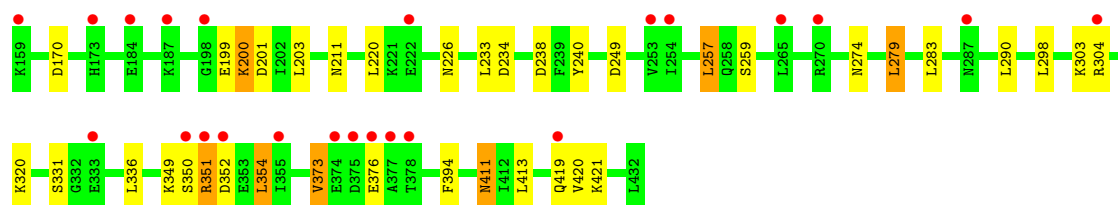


• Molecule 1: BETA FRUCTOSIDASE

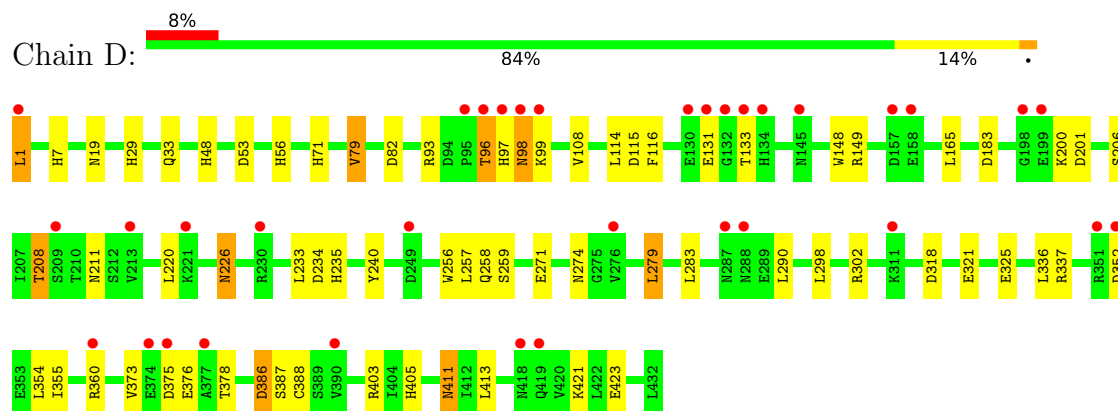


• Molecule 1: BETA FRUCTOSIDASE

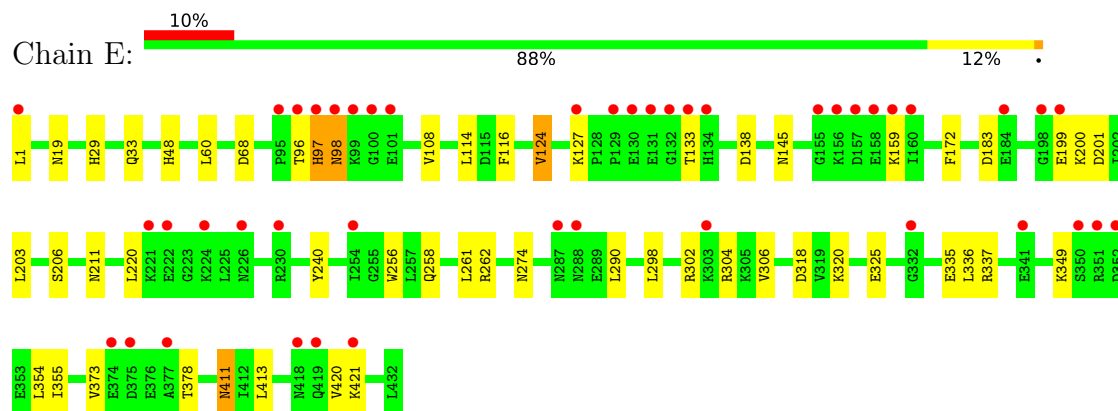




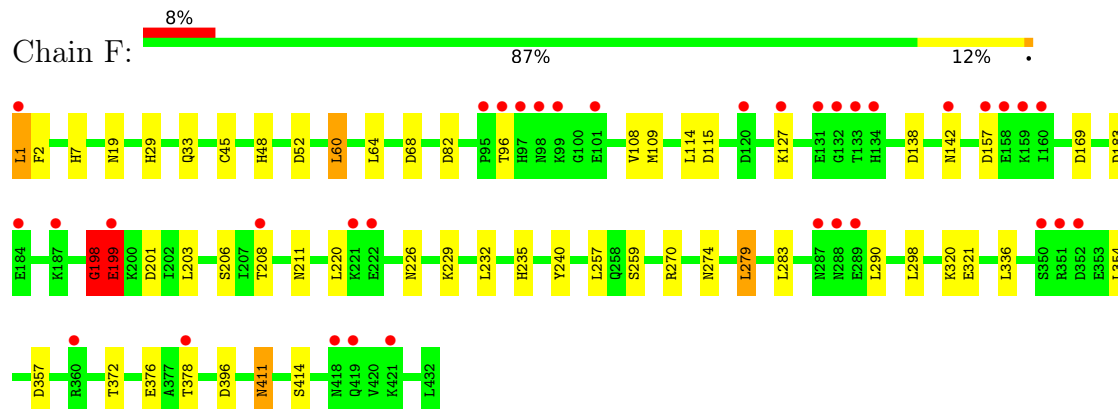
• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.50Å 114.70Å 130.00Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	40.00 – 1.87 32.11 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-1.87) 97.7 (32.11-1.87)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.229 0.213 , 0.241	Depositor DCC
R_{free} test set	11055 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.2	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	0.94	EDS
Total number of atoms	23234	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, SUC, SO4, CIT

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	0.34	1/3607 (0.0%)	0.73	13/4881 (0.3%)
1	B	0.32	0/3610	0.71	8/4885 (0.2%)
1	C	0.39	1/3610 (0.0%)	0.70	9/4885 (0.2%)
1	D	0.32	0/3608	0.70	8/4883 (0.2%)
1	E	0.31	0/3609	0.70	4/4883 (0.1%)
1	F	0.33	0/3609	0.74	14/4884 (0.3%)
All	All	0.34	2/21653 (0.0%)	0.71	56/29301 (0.2%)

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	F	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	80	GLU	C-N	12.95	1.63	1.34
1	A	2	PHE	C-N	-5.36	1.21	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	198	GLY	CA-C-N	8.66	136.25	117.20
1	F	198	GLY	CA-C-O	-8.53	105.24	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	198	GLY	O-C-N	-7.91	110.04	122.70
1	A	2	PHE	O-C-N	-7.81	110.21	122.70
1	A	1	LEU	CB-CA-C	-5.99	98.82	110.20
1	C	68	ASP	CB-CG-OD2	5.92	123.62	118.30
1	B	115	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	201	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	318	ASP	CB-CG-OD2	5.71	123.44	118.30
1	F	199	GLU	N-CA-C	5.71	126.41	111.00
1	D	115	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	318	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	115	ASP	CB-CG-OD2	5.60	123.34	118.30
1	F	357	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	183	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	68	ASP	CB-CG-OD2	5.57	123.31	118.30
1	F	183	ASP	CB-CG-OD2	5.54	123.28	118.30
1	E	183	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	115	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	201	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	169	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	249	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	68	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	82	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	2	PHE	CA-C-N	5.45	129.20	117.20
1	E	138	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	82	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	201	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	138	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	115	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	53	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	318	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	201	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	249	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	68	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	201	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	157	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	375	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	52	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	82	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	68	ASP	CB-CG-OD2	5.20	122.98	118.30
1	F	157	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	170	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	157	ASP	CB-CG-OD2	5.14	122.93	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	375	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	352	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	396	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	234	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	234	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	386	ASP	CB-CG-OD2	5.07	122.87	118.30
1	F	201	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	138	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	234	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	183	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	138	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	388	CYS	Mainchain
1	C	80	GLU	Mainchain
1	F	198	GLY	Mainchain,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	3517	0	3398	31	0
1	B	3519	0	3411	33	0
1	C	3519	0	3411	42	0
1	D	3518	0	3404	35	0
1	E	3518	0	3407	31	0
1	F	3518	0	3406	20	0
2	A	13	0	5	5	0
3	A	23	0	20	0	0
3	B	23	0	20	0	0
3	C	23	0	20	0	0
3	D	23	0	20	0	0
3	E	23	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	23	0	20	0	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
4	C	11	0	10	0	0
4	D	11	0	10	0	0
4	E	11	0	10	0	0
4	F	11	0	10	0	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
5	E	5	0	0	0	0
6	A	339	0	0	16	0
6	B	259	0	0	1	0
6	C	316	0	0	5	0
6	D	364	0	0	4	0
6	E	296	0	0	4	0
6	F	314	0	0	6	0
All	All	23234	0	20622	191	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 5.

All (191) 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:211:ASN:OD1	6:A:2179:HOH:O	1.56	1.20
1:F:270:ARG:CZ	6:F:2203:HOH:O	1.88	1.18
1:B:267:PRO:HD2	1:B:405:HIS:CD2	1.87	1.08
2:A:1433:CIT:O2	6:A:2332:HOH:O	1.75	1.03
1:C:211:ASN:HD21	1:C:259:SER:HA	1.19	1.02
1:E:211:ASN:ND2	1:E:261:LEU:HG	1.89	0.88
1:C:31:PHE:CZ	1:C:48:HIS:CE1	2.65	0.85
1:F:270:ARG:NE	6:F:2203:HOH:O	2.04	0.83
2:A:1433:CIT:O3	6:A:2331:HOH:O	1.95	0.83
2:A:1433:CIT:C6	6:A:2336:HOH:O	2.27	0.82
1:C:211:ASN:HD21	1:C:259:SER:CA	1.93	0.81
2:A:1433:CIT:O5	6:A:2336:HOH:O	1.97	0.81
1:E:97:HIS:O	1:E:98:ASN:HB2	1.79	0.80
1:C:211:ASN:ND2	1:C:259:SER:HA	1.95	0.80
1:C:31:PHE:CE2	1:C:48:HIS:ND1	2.51	0.79
1:C:211:ASN:ND2	1:C:259:SER:CB	2.47	0.77
1:B:11:ILE:HG23	1:B:59:HIS:CE1	2.20	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:HIS:O	1:E:98:ASN:ND2	2.17	0.77
1:E:97:HIS:O	1:E:98:ASN:CB	2.36	0.74
1:C:96:THR:OG1	1:C:99:LYS:HB2	1.87	0.73
1:F:45:CYS:HB2	1:F:64:LEU:O	1.89	0.73
2:A:1433:CIT:O6	6:A:2333:HOH:O	2.06	0.73
1:E:262:ARG:NH2	6:E:2184:HOH:O	2.22	0.71
1:B:267:PRO:CD	1:B:405:HIS:CD2	2.70	0.71
1:F:48:HIS:CE1	1:F:60:LEU:HD23	2.26	0.70
1:A:3:LYS:NZ	6:A:2002:HOH:O	2.04	0.70
1:A:360:ARG:NE	6:A:2281:HOH:O	2.25	0.70
1:D:7:HIS:CE1	1:D:279:LEU:HD13	2.27	0.69
1:E:97:HIS:C	1:E:98:ASN:HD22	1.95	0.69
1:C:211:ASN:CG	6:C:2163:HOH:O	2.31	0.69
1:E:19:ASN:HD21	1:E:33:GLN:HE21	1.39	0.68
1:C:211:ASN:ND2	1:C:259:SER:CA	2.55	0.68
1:B:145:ASN:OD1	1:C:81:LYS:HA	1.94	0.68
1:F:7:HIS:CE1	1:F:279:LEU:HD13	2.29	0.68
1:C:45:CYS:HB2	1:C:64:LEU:O	1.94	0.67
1:D:208:THR:O	1:D:211:ASN:ND2	2.28	0.67
1:E:211:ASN:HD21	1:E:261:LEU:HG	1.58	0.67
1:B:267:PRO:HD2	1:B:405:HIS:HD2	1.60	0.65
1:D:19:ASN:HD21	1:D:33:GLN:HE21	1.45	0.65
1:F:19:ASN:HD21	1:F:33:GLN:HE21	1.45	0.65
1:E:336:LEU:HD11	1:E:413:LEU:HD11	1.77	0.65
1:D:79:VAL:HG11	1:D:148:TRP:CZ3	2.31	0.64
1:A:19:ASN:HD21	1:A:33:GLN:HE21	1.46	0.63
1:D:1:LEU:HD12	1:D:1:LEU:N	2.15	0.62
1:C:211:ASN:ND2	1:C:259:SER:OG	2.32	0.61
1:D:96:THR:OG1	1:D:99:LYS:HB2	2.01	0.60
1:A:360:ARG:CD	6:A:2281:HOH:O	2.48	0.60
1:A:360:ARG:CG	6:A:2280:HOH:O	2.50	0.60
1:F:1:LEU:CD1	1:F:2:PHE:CD1	2.86	0.59
1:C:211:ASN:ND2	6:C:2163:HOH:O	2.35	0.58
1:C:351:ARG:NH2	6:C:2258:HOH:O	2.36	0.58
1:E:335:GLU:OE1	1:E:337:ARG:NE	2.37	0.58
1:B:19:ASN:HD21	1:B:33:GLN:HE21	1.52	0.58
1:D:1:LEU:HD12	1:D:1:LEU:H3	1.67	0.58
1:E:211:ASN:HD21	1:E:261:LEU:H	1.52	0.57
1:C:211:ASN:HD22	1:C:259:SER:CB	2.13	0.57
1:E:302:ARG:HD3	1:E:325:GLU:OE1	2.04	0.57
1:C:411:ASN:HD22	1:C:411:ASN:H	1.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ASN:ND2	1:E:33:GLN:HE21	2.02	0.57
1:B:31:PHE:CE2	1:B:48:HIS:CE1	2.92	0.57
1:B:31:PHE:CZ	1:B:48:HIS:CE1	2.93	0.56
1:D:302:ARG:HD3	1:D:325:GLU:OE1	2.06	0.56
1:B:7:HIS:HD2	1:B:386:ASP:OD2	1.88	0.56
1:A:336:LEU:HD11	1:A:413:LEU:HD11	1.88	0.56
1:D:29:HIS:HD2	1:D:48:HIS:NE2	2.04	0.56
1:E:1:LEU:HD23	6:E:2002:HOH:O	2.06	0.55
1:E:29:HIS:HD2	1:E:48:HIS:NE2	2.04	0.55
1:C:31:PHE:CZ	1:C:48:HIS:HE1	2.20	0.55
1:D:235:HIS:HD2	6:D:2308:HOH:O	1.90	0.55
1:D:19:ASN:ND2	1:D:33:GLN:HE21	2.05	0.55
1:F:411:ASN:HD22	1:F:411:ASN:H	1.54	0.55
1:C:134:HIS:CD2	1:C:135:ALA:H	2.25	0.54
1:C:31:PHE:CE2	1:C:48:HIS:CE1	2.94	0.54
1:B:11:ILE:HG23	1:B:59:HIS:ND1	2.22	0.54
1:C:19:ASN:HD21	1:C:33:GLN:HE21	1.53	0.54
1:C:29:HIS:HD2	1:C:48:HIS:NE2	2.06	0.54
1:A:360:ARG:HD3	6:A:2281:HOH:O	2.05	0.54
1:F:232:LEU:HB2	1:F:235:HIS:CE1	2.42	0.54
1:B:29:HIS:HD2	1:B:48:HIS:NE2	2.06	0.54
1:D:388:CYS:HB2	1:D:405:HIS:CE1	2.43	0.54
1:A:302:ARG:HD3	1:A:325:GLU:OE1	2.08	0.54
1:D:149:ARG:HD2	6:D:2130:HOH:O	2.08	0.54
1:A:360:ARG:HG2	6:A:2280:HOH:O	2.07	0.53
1:F:1:LEU:HD12	1:F:2:PHE:N	2.24	0.53
1:B:7:HIS:HE1	1:B:391:GLU:OE1	1.92	0.53
1:D:97:HIS:O	1:D:98:ASN:CG	2.46	0.53
1:A:208:THR:HG22	6:A:2165:HOH:O	2.08	0.53
1:F:7:HIS:ND1	1:F:279:LEU:HD13	2.25	0.52
1:F:19:ASN:ND2	1:F:33:GLN:HE21	2.07	0.52
1:A:304:ARG:NE	6:A:2319:HOH:O	2.42	0.52
1:B:411:ASN:H	1:B:411:ASN:HD22	1.57	0.52
1:B:145:ASN:HA	1:C:80:GLU:O	2.10	0.51
1:A:351:ARG:NH2	1:C:220:LEU:O	2.42	0.51
1:B:336:LEU:HD11	1:B:413:LEU:HD11	1.92	0.51
1:E:411:ASN:HD22	1:E:411:ASN:H	1.58	0.51
1:B:81:LYS:NZ	1:B:86:PHE:CZ	2.80	0.50
1:D:7:HIS:HD2	1:D:386:ASP:OD2	1.93	0.50
1:E:211:ASN:ND2	1:E:261:LEU:H	2.10	0.50
1:F:270:ARG:NH2	6:F:2203:HOH:O	2.21	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:HH21	1:A:405:HIS:HE1	1.58	0.50
1:F:1:LEU:HD22	6:F:2287:HOH:O	2.11	0.50
1:C:134:HIS:CD2	1:C:135:ALA:N	2.80	0.49
1:C:81:LYS:HB3	1:C:86:PHE:CE1	2.46	0.49
1:A:19:ASN:ND2	1:A:33:GLN:HE21	2.08	0.49
1:B:302:ARG:HD2	1:B:425:PHE:CG	2.47	0.49
1:D:336:LEU:HD11	1:D:413:LEU:HD11	1.94	0.49
1:B:11:ILE:CG2	1:B:59:HIS:CE1	2.95	0.49
1:F:29:HIS:HD2	1:F:48:HIS:NE2	2.11	0.49
1:C:19:ASN:ND2	1:C:33:GLN:HE21	2.12	0.48
1:C:336:LEU:HD11	1:C:413:LEU:HD11	1.94	0.48
1:A:375:ASP:OD2	1:C:200:LYS:NZ	2.46	0.48
1:E:1:LEU:HB3	6:E:2002:HOH:O	2.13	0.48
1:D:337:ARG:O	1:D:413:LEU:HD12	2.14	0.48
1:E:206:SER:HB3	1:E:240:TYR:CE1	2.49	0.48
1:B:108:VAL:HG11	1:B:116:PHE:HB3	1.96	0.48
1:B:29:HIS:HE1	6:B:2015:HOH:O	1.97	0.48
1:D:97:HIS:O	1:D:98:ASN:ND2	2.47	0.48
1:E:108:VAL:HG11	1:E:116:PHE:HB3	1.94	0.48
1:B:124:VAL:HG22	1:B:172:PHE:O	2.13	0.48
1:B:19:ASN:ND2	1:B:33:GLN:HE21	2.11	0.48
1:D:108:VAL:HG11	1:D:116:PHE:HB3	1.96	0.48
1:C:101:GLU:CD	1:C:134:HIS:CE1	2.87	0.47
1:E:211:ASN:ND2	1:E:261:LEU:CG	2.70	0.47
1:A:426:GLU:CD	6:A:2319:HOH:O	2.53	0.47
1:C:7:HIS:NE2	1:C:279:LEU:HD13	2.29	0.47
1:D:7:HIS:CD2	1:D:386:ASP:OD2	2.68	0.47
1:D:53:ASP:OD2	1:D:56:HIS:HD2	1.98	0.47
1:F:1:LEU:HD13	1:F:2:PHE:CD1	2.49	0.47
1:C:29:HIS:HE1	6:C:2020:HOH:O	1.98	0.47
1:E:108:VAL:CG1	1:E:116:PHE:HB3	2.45	0.47
1:A:421:LYS:NZ	1:E:318:ASP:HB3	2.29	0.47
1:A:421:LYS:HG2	1:E:306:VAL:HA	1.97	0.46
1:B:53:ASP:OD2	1:B:56:HIS:HD2	1.98	0.46
1:C:351:ARG:CZ	6:C:2258:HOH:O	2.62	0.46
1:E:19:ASN:HD21	1:E:33:GLN:NE2	2.11	0.46
1:D:411:ASN:H	1:D:411:ASN:HD22	1.63	0.46
1:B:388:CYS:O	1:B:389:SER:HB3	2.15	0.46
1:C:238:ASP:O	1:C:257:LEU:HD23	2.16	0.46
1:D:96:THR:HB	1:D:97:HIS:H	1.58	0.46
1:C:354:LEU:HB2	1:C:373:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:HIS:ND1	1:D:279:LEU:HD13	2.31	0.46
1:F:270:ARG:NH2	6:F:2204:HOH:O	2.49	0.46
1:B:302:ARG:HD3	1:B:325:GLU:OE1	2.16	0.45
1:F:1:LEU:HD12	1:F:2:PHE:H	1.81	0.45
1:B:267:PRO:HD2	1:B:405:HIS:NE2	2.25	0.45
1:A:29:HIS:HD2	1:A:48:HIS:NE2	2.15	0.45
1:C:211:ASN:OD1	1:C:240:TYR:HB2	2.16	0.45
1:A:388:CYS:HB2	1:A:405:HIS:CE1	2.52	0.45
1:D:108:VAL:CG1	1:D:116:PHE:HB3	2.46	0.45
1:D:1:LEU:HD13	1:D:271:GLU:OE1	2.16	0.45
1:C:48:HIS:CD2	1:C:49:ALA:N	2.85	0.44
1:A:306:VAL:HG12	1:A:426:GLU:HG3	2.00	0.44
1:A:45:CYS:HB3	1:A:64:LEU:O	2.18	0.44
1:C:48:HIS:CD2	1:C:60:LEU:HD12	2.53	0.44
1:E:124:VAL:HG22	1:E:172:PHE:O	2.18	0.44
1:E:336:LEU:CD1	1:E:413:LEU:HD11	2.47	0.43
1:D:149:ARG:CG	1:D:165:LEU:HD11	2.48	0.43
1:A:306:VAL:HG21	1:A:319:VAL:HG13	2.00	0.43
1:A:356:VAL:HG11	1:A:402:PHE:CE2	2.54	0.43
1:B:108:VAL:CG1	1:B:116:PHE:HB3	2.48	0.43
1:B:257:LEU:HD23	1:B:403:ARG:HG2	1.99	0.43
1:D:1:LEU:O	1:D:387:SER:HB3	2.18	0.43
1:D:360:ARG:HG2	6:D:2293:HOH:O	2.18	0.43
1:D:226:ASN:HD22	1:D:226:ASN:N	2.17	0.43
1:D:256:TRP:CE2	1:D:258:GLN:HB3	2.53	0.43
1:A:124:VAL:HG22	1:A:172:PHE:O	2.18	0.42
1:C:7:HIS:CD2	1:C:279:LEU:HD13	2.54	0.42
1:F:206:SER:HB3	1:F:240:TYR:CE1	2.53	0.42
1:B:170:ASP:OD2	1:B:173:HIS:HD2	2.01	0.42
1:C:373:VAL:HG11	1:C:394:PHE:CD2	2.55	0.42
1:E:256:TRP:CE2	1:E:258:GLN:HB3	2.54	0.42
1:C:101:GLU:OE2	1:C:134:HIS:CE1	2.72	0.42
1:E:29:HIS:CD2	1:E:48:HIS:NE2	2.87	0.42
1:A:360:ARG:HG3	6:A:2280:HOH:O	2.15	0.42
1:A:411:ASN:HD22	1:A:411:ASN:H	1.66	0.42
1:A:124:VAL:CG2	1:A:172:PHE:HA	2.49	0.42
1:C:350:SER:O	1:C:351:ARG:C	2.58	0.42
1:B:206:SER:HB3	1:B:240:TYR:CE1	2.55	0.42
1:D:206:SER:HB3	1:D:240:TYR:CE1	2.55	0.41
1:B:19:ASN:HD21	1:B:33:GLN:NE2	2.16	0.41
1:B:11:ILE:CG2	1:B:59:HIS:ND1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:SER:HB3	1:B:420:VAL:CG1	2.50	0.41
1:E:145:ASN:ND2	6:E:2128:HOH:O	2.48	0.41
1:E:97:HIS:C	1:E:98:ASN:ND2	2.67	0.41
1:A:364:SER:OG	1:A:405:HIS:HD2	2.04	0.41
1:C:89:TYR:HE1	1:C:108:VAL:HG22	1.85	0.41
1:D:29:HIS:HE1	6:D:2018:HOH:O	2.04	0.41
1:F:320:LYS:NZ	6:F:2244:HOH:O	2.37	0.40
1:D:403:ARG:HH21	1:D:405:HIS:HE1	1.68	0.40
1:A:256:TRP:CE2	1:A:258:GLN:HB3	2.56	0.40
1:D:71:HIS:ND1	1:D:93:ARG:HA	2.37	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	430/432 (100%)	411 (96%)	18 (4%)	1 (0%)	49	38
1	B	430/432 (100%)	412 (96%)	17 (4%)	1 (0%)	49	38
1	C	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	49	38
1	D	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	49	38
1	E	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	49	38
1	F	430/432 (100%)	412 (96%)	16 (4%)	2 (0%)	31	18
All	All	2580/2592 (100%)	2477 (96%)	96 (4%)	7 (0%)	43	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	ARG
1	F	199	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	98	ASN
1	E	98	ASN
1	B	389	SER
1	A	198	GLY
1	F	198	GLY

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	385/387 (100%)	363 (94%)	22 (6%)	23	11
1	B	387/387 (100%)	352 (91%)	35 (9%)	10	3
1	C	387/387 (100%)	359 (93%)	28 (7%)	16	6
1	D	386/387 (100%)	358 (93%)	28 (7%)	15	5
1	E	387/387 (100%)	362 (94%)	25 (6%)	19	8
1	F	386/387 (100%)	355 (92%)	31 (8%)	13	4
All	All	2318/2322 (100%)	2149 (93%)	169 (7%)	15	5

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	114	LEU
1	A	124	VAL
1	A	127	LYS
1	A	147	GLU
1	A	203	LEU
1	A	226	ASN
1	A	233	LEU
1	A	274	ASN
1	A	279	LEU
1	A	283	LEU
1	A	290	LEU
1	A	298	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	306	VAL
1	A	321	GLU
1	A	349	LYS
1	A	354	LEU
1	A	373	VAL
1	A	375	ASP
1	A	378	THR
1	A	411	ASN
1	A	421	LYS
1	B	1	LEU
1	B	38	LYS
1	B	60	LEU
1	B	96	THR
1	B	97	HIS
1	B	114	LEU
1	B	124	VAL
1	B	134	HIS
1	B	159	LYS
1	B	162	ARG
1	B	199	GLU
1	B	211	ASN
1	B	220	LEU
1	B	233	LEU
1	B	257	LEU
1	B	269	LYS
1	B	274	ASN
1	B	279	LEU
1	B	283	LEU
1	B	290	LEU
1	B	298	LEU
1	B	303	LYS
1	B	304	ARG
1	B	316	LEU
1	B	320	LYS
1	B	349	LYS
1	B	352	ASP
1	B	354	LEU
1	B	370	LYS
1	B	373	VAL
1	B	375	ASP
1	B	376	GLU
1	B	397	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	411	ASN
1	B	421	LYS
1	C	1	LEU
1	C	108	VAL
1	C	114	LEU
1	C	131	GLU
1	C	145	ASN
1	C	199	GLU
1	C	200	LYS
1	C	203	LEU
1	C	226	ASN
1	C	233	LEU
1	C	257	LEU
1	C	274	ASN
1	C	279	LEU
1	C	283	LEU
1	C	290	LEU
1	C	298	LEU
1	C	303	LYS
1	C	304	ARG
1	C	320	LYS
1	C	331	SER
1	C	349	LYS
1	C	354	LEU
1	C	373	VAL
1	C	376	GLU
1	C	411	ASN
1	C	419	GLN
1	C	420	VAL
1	C	421	LYS
1	D	1	LEU
1	D	79	VAL
1	D	96	THR
1	D	114	LEU
1	D	131	GLU
1	D	133	THR
1	D	200	LYS
1	D	208	THR
1	D	220	LEU
1	D	226	ASN
1	D	233	LEU
1	D	257	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	259	SER
1	D	274	ASN
1	D	279	LEU
1	D	283	LEU
1	D	290	LEU
1	D	298	LEU
1	D	321	GLU
1	D	352	ASP
1	D	354	LEU
1	D	355	ILE
1	D	373	VAL
1	D	376	GLU
1	D	378	THR
1	D	411	ASN
1	D	421	LYS
1	D	423	GLU
1	E	60	LEU
1	E	96	THR
1	E	97	HIS
1	E	114	LEU
1	E	124	VAL
1	E	127	LYS
1	E	133	THR
1	E	159	LYS
1	E	199	GLU
1	E	200	LYS
1	E	203	LEU
1	E	220	LEU
1	E	274	ASN
1	E	290	LEU
1	E	298	LEU
1	E	304	ARG
1	E	320	LYS
1	E	349	LYS
1	E	354	LEU
1	E	355	ILE
1	E	373	VAL
1	E	378	THR
1	E	411	ASN
1	E	420	VAL
1	E	421	LYS
1	F	1	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	60	LEU
1	F	96	THR
1	F	108	VAL
1	F	109	MET
1	F	114	LEU
1	F	127	LYS
1	F	142	ASN
1	F	169	ASP
1	F	199	GLU
1	F	203	LEU
1	F	208	THR
1	F	211	ASN
1	F	220	LEU
1	F	226	ASN
1	F	229	LYS
1	F	257	LEU
1	F	259	SER
1	F	274	ASN
1	F	279	LEU
1	F	283	LEU
1	F	290	LEU
1	F	298	LEU
1	F	321	GLU
1	F	336	LEU
1	F	354	LEU
1	F	372	THR
1	F	376	GLU
1	F	378	THR
1	F	411	ASN
1	F	414	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	29	HIS
1	A	98	ASN
1	A	211	ASN
1	A	235	HIS
1	A	243	GLN
1	A	274	ASN
1	A	405	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	411	ASN
1	B	7	HIS
1	B	19	ASN
1	B	29	HIS
1	B	56	HIS
1	B	59	HIS
1	B	211	ASN
1	B	235	HIS
1	B	243	GLN
1	B	274	ASN
1	B	411	ASN
1	C	19	ASN
1	C	29	HIS
1	C	56	HIS
1	C	134	HIS
1	C	211	ASN
1	C	235	HIS
1	C	243	GLN
1	C	274	ASN
1	C	411	ASN
1	D	7	HIS
1	D	19	ASN
1	D	29	HIS
1	D	56	HIS
1	D	59	HIS
1	D	98	ASN
1	D	226	ASN
1	D	235	HIS
1	D	243	GLN
1	D	274	ASN
1	D	405	HIS
1	D	411	ASN
1	E	19	ASN
1	E	29	HIS
1	E	56	HIS
1	E	59	HIS
1	E	98	ASN
1	E	211	ASN
1	E	235	HIS
1	E	243	GLN
1	E	274	ASN
1	E	405	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	411	ASN
1	F	19	ASN
1	F	29	HIS
1	F	56	HIS
1	F	59	HIS
1	F	235	HIS
1	F	243	GLN
1	F	274	ASN
1	F	405	HIS
1	F	411	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

17 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	CIT	A	1433	-	3,12,12	1.47	0	3,17,17	2.03	1 (33%)
3	SUC	A	1434	4	24,24,24	1.42	1 (4%)	36,36,36	1.40	6 (16%)
4	GLA	A	1435	3	11,11,12	0.62	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1433	-	4,4,4	0.18	0	6,6,6	0.17	0
3	SUC	B	1434	4	24,24,24	1.39	1 (4%)	36,36,36	0.68	1 (2%)
4	GLA	B	1435	3	11,11,12	0.54	0	15,15,17	0.74	1 (6%)
5	SO4	C	1433	-	4,4,4	0.21	0	6,6,6	0.34	0
5	SO4	C	1434	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SUC	C	1435	4	24,24,24	1.39	1 (4%)	36,36,36	0.67	1 (2%)
4	GLA	C	1436	3	11,11,12	0.57	0	15,15,17	0.62	0
3	SUC	D	1433	4	24,24,24	1.41	2 (8%)	36,36,36	1.50	8 (22%)
4	GLA	D	1434	3	11,11,12	0.61	0	15,15,17	0.55	0
5	SO4	E	1433	-	4,4,4	0.50	0	6,6,6	0.85	0
3	SUC	E	1434	4	24,24,24	1.44	1 (4%)	36,36,36	1.39	5 (13%)
4	GLA	E	1435	3	11,11,12	0.54	0	15,15,17	0.55	0
3	SUC	F	1433	4	24,24,24	1.38	1 (4%)	36,36,36	0.99	3 (8%)
4	GLA	F	1434	3	11,11,12	0.55	0	15,15,17	0.68	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	CIT	A	1433	-	-	0/6/16/16	0/0/0/0
3	SUC	A	1434	4	-	0/12/51/51	0/2/2/2
4	GLA	A	1435	3	-	0/2/19/22	0/1/1/1
5	SO4	B	1433	-	-	0/0/0/0	0/0/0/0
3	SUC	B	1434	4	-	0/12/51/51	0/2/2/2
4	GLA	B	1435	3	-	0/2/19/22	0/1/1/1
5	SO4	C	1433	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1434	-	-	0/0/0/0	0/0/0/0
3	SUC	C	1435	4	-	0/12/51/51	0/2/2/2
4	GLA	C	1436	3	-	0/2/19/22	0/1/1/1
3	SUC	D	1433	4	-	0/12/51/51	0/2/2/2
4	GLA	D	1434	3	-	0/2/19/22	0/1/1/1
5	SO4	E	1433	-	-	0/0/0/0	0/0/0/0
3	SUC	E	1434	4	-	0/12/51/51	0/2/2/2
4	GLA	E	1435	3	-	0/2/19/22	0/1/1/1
3	SUC	F	1433	4	-	0/12/51/51	0/2/2/2
4	GLA	F	1434	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1434	SUC	O6'-C6'	-6.54	1.14	1.42
3	C	1435	SUC	O6'-C6'	-6.50	1.15	1.42
3	B	1434	SUC	O6'-C6'	-6.43	1.15	1.42
3	A	1434	SUC	O6'-C6'	-6.41	1.15	1.42
3	F	1433	SUC	O6'-C6'	-6.38	1.15	1.42
3	D	1433	SUC	O6'-C6'	-6.26	1.16	1.42
3	D	1433	SUC	C4-C5	2.02	1.57	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1433	SUC	C1-O5-C5	-4.00	105.82	113.70
3	A	1434	SUC	C1-O5-C5	-3.31	107.17	113.70
3	F	1433	SUC	O5-C1-C2	-3.08	103.77	110.35
3	E	1434	SUC	C1-O5-C5	-2.68	108.41	113.70
3	D	1433	SUC	C1-C2-C3	-2.57	104.62	109.98
3	A	1434	SUC	C1-C2-C3	-2.07	105.66	109.98
3	E	1434	SUC	O5-C5-C4	2.01	113.34	109.68
3	C	1435	SUC	O2'-C2'-C1'	2.13	113.21	108.03
3	A	1434	SUC	O1-C1-C2	2.17	114.73	108.28
3	D	1433	SUC	O5-C5-C4	2.17	113.64	109.68
3	F	1433	SUC	O1-C1-C2	2.20	114.83	108.28
3	B	1434	SUC	O2'-C2'-C1'	2.28	113.59	108.03
3	A	1434	SUC	C2'-O1-C1	2.35	123.67	117.33
3	E	1434	SUC	C2'-O1-C1	2.35	123.68	117.33
3	D	1433	SUC	C2'-O1-C1	2.36	123.71	117.33
4	B	1435	GLA	O5-C5-C6	2.44	111.01	107.15
3	D	1433	SUC	O1-C1-C2	2.46	115.60	108.28
3	E	1434	SUC	O2'-C2'-C1'	2.71	114.63	108.03
3	A	1434	SUC	O2'-C2'-C1'	2.77	114.77	108.03
3	F	1433	SUC	O2'-C2'-C1'	2.86	114.98	108.03
3	D	1433	SUC	O5-C1-O1	2.88	118.76	109.73
3	D	1433	SUC	O2'-C2'-C1'	2.88	115.05	108.03
3	D	1433	SUC	O5-C1-C2	3.17	117.11	110.35
2	A	1433	CIT	C4-C3-C2	3.22	117.45	109.60
3	A	1434	SUC	O5-C1-O1	4.28	123.14	109.73
3	E	1434	SUC	O5-C1-O1	4.86	124.94	109.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1433	CIT	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	80:GLU	C	81:LYS	N	1.63

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	432/432 (100%)	0.32	22 (5%) 28 30	7, 16, 28, 33	4 (0%)
1	B	432/432 (100%)	0.63	48 (11%) 5 6	8, 17, 28, 34	6 (1%)
1	C	432/432 (100%)	0.50	40 (9%) 8 9	7, 17, 28, 34	8 (1%)
1	D	432/432 (100%)	0.52	34 (7%) 12 14	8, 16, 28, 34	8 (1%)
1	E	432/432 (100%)	0.50	44 (10%) 7 7	8, 16, 28, 34	9 (2%)
1	F	432/432 (100%)	0.51	35 (8%) 12 13	7, 16, 28, 34	10 (2%)
All	All	2592/2592 (100%)	0.50	223 (8%) 10 11	7, 16, 28, 34	45 (1%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	98	ASN	11.9
1	D	98	ASN	10.9
1	E	97	HIS	10.5
1	B	97	HIS	10.3
1	C	97	HIS	10.2
1	E	96	THR	9.3
1	B	98	ASN	9.2
1	F	97	HIS	8.6
1	E	99	LYS	8.2
1	D	97	HIS	8.1
1	F	96	THR	7.7
1	B	99	LYS	7.5
1	F	98	ASN	6.3
1	B	96	THR	5.9
1	C	132	GLY	5.7
1	B	134	HIS	5.6
1	E	131	GLU	5.6
1	E	198	GLY	5.6
1	B	351	ARG	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	96	THR	5.4
1	D	134	HIS	5.4
1	E	134	HIS	5.3
1	C	134	HIS	5.2
1	B	287	ASN	5.2
1	C	131	GLU	5.2
1	A	418	ASN	5.1
1	F	287	ASN	5.1
1	E	95	PRO	5.0
1	D	418	ASN	5.0
1	F	134	HIS	5.0
1	C	351	ARG	4.9
1	C	270	ARG	4.8
1	B	352	ASP	4.7
1	D	199	GLU	4.7
1	B	131	GLU	4.6
1	E	100	GLY	4.5
1	B	350	SER	4.5
1	B	288	ASN	4.4
1	E	158	GLU	4.3
1	E	159	LYS	4.3
1	F	1	LEU	4.3
1	E	377	ALA	4.3
1	A	159	LYS	4.2
1	B	418	ASN	4.2
1	B	372	THR	4.2
1	B	230	ARG	4.0
1	E	157	ASP	4.0
1	B	1	LEU	3.9
1	F	159	LYS	3.9
1	C	99	LYS	3.9
1	B	332	GLY	3.8
1	A	419	GLN	3.8
1	E	351	ARG	3.8
1	C	377	ALA	3.7
1	F	288	ASN	3.7
1	E	101	GLU	3.7
1	E	352	ASP	3.7
1	F	352	ASP	3.7
1	F	158	GLU	3.7
1	C	352	ASP	3.7
1	D	287	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	159	LYS	3.6
1	D	352	ASP	3.5
1	C	155	GLY	3.4
1	E	155	GLY	3.4
1	B	132	GLY	3.4
1	D	419	GLN	3.4
1	F	208	THR	3.4
1	E	156	LYS	3.4
1	D	131	GLU	3.4
1	F	131	GLU	3.4
1	F	351	ARG	3.3
1	E	1	LEU	3.3
1	F	184	GLU	3.3
1	F	289	GLU	3.3
1	F	99	LYS	3.2
1	F	157	ASP	3.2
1	B	159	LYS	3.2
1	C	378	THR	3.2
1	D	377	ALA	3.2
1	B	341	GLU	3.1
1	B	374	GLU	3.1
1	C	375	ASP	3.1
1	C	96	THR	3.1
1	D	351	ARG	3.1
1	F	222	GLU	3.1
1	D	198	GLY	3.1
1	E	132	GLY	3.1
1	A	134	HIS	3.1
1	C	333	GLU	3.1
1	A	208	THR	3.0
1	E	288	ASN	3.0
1	F	418	ASN	3.0
1	B	375	ASP	3.0
1	D	1	LEU	3.0
1	A	145	ASN	3.0
1	F	187	LYS	3.0
1	C	350	SER	3.0
1	F	419	GLN	3.0
1	A	287	ASN	3.0
1	E	129	PRO	3.0
1	D	145	ASN	3.0
1	F	360	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	198	GLY	2.9
1	E	184	GLU	2.9
1	C	157	ASP	2.9
1	F	199	GLU	2.9
1	D	157	ASP	2.9
1	E	133	THR	2.9
1	F	133	THR	2.9
1	F	95	PRO	2.9
1	D	374	GLU	2.9
1	E	199	GLU	2.9
1	D	95	PRO	2.8
1	C	376	GLU	2.8
1	E	332	GLY	2.8
1	A	222	GLU	2.8
1	E	375	ASP	2.8
1	C	133	THR	2.7
1	E	350	SER	2.7
1	A	184	GLU	2.7
1	A	198	GLY	2.7
1	E	130	GLU	2.7
1	D	360	ARG	2.7
1	D	249	ASP	2.7
1	B	158	GLU	2.7
1	D	99	LYS	2.7
1	B	157	ASP	2.7
1	B	184	GLU	2.7
1	C	100	GLY	2.7
1	B	419	GLN	2.7
1	C	265	LEU	2.7
1	B	82	ASP	2.6
1	B	355	ILE	2.6
1	C	419	GLN	2.6
1	B	376	GLU	2.6
1	F	221	LYS	2.6
1	C	374	GLU	2.6
1	F	421	LYS	2.6
1	C	158	GLU	2.5
1	B	187	LYS	2.5
1	C	127	LYS	2.5
1	E	254	ILE	2.5
1	D	158	GLU	2.5
1	A	374	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	142	ASN	2.5
1	F	350	SER	2.5
1	C	101	GLU	2.5
1	A	249	ASP	2.5
1	E	421	LYS	2.5
1	B	95	PRO	2.4
1	C	222	GLU	2.4
1	A	1	LEU	2.4
1	E	419	GLN	2.4
1	A	131	GLU	2.4
1	C	187	LYS	2.4
1	E	230	ARG	2.4
1	B	328	CYS	2.4
1	B	333	GLU	2.4
1	B	416	LYS	2.4
1	F	101	GLU	2.4
1	E	418	ASN	2.4
1	A	221	LYS	2.4
1	D	311	LYS	2.4
1	E	222	GLU	2.4
1	B	377	ALA	2.4
1	B	421	LYS	2.4
1	E	374	GLU	2.4
1	E	160	ILE	2.4
1	D	209	SER	2.3
1	D	221	LYS	2.3
1	C	254	ILE	2.3
1	C	129	PRO	2.3
1	F	120	ASP	2.3
1	C	355	ILE	2.3
1	F	132	GLY	2.3
1	E	303	LYS	2.3
1	C	184	GLU	2.3
1	A	304	ARG	2.3
1	A	288	ASN	2.3
1	C	287	ASN	2.3
1	B	318	ASP	2.3
1	B	337	ARG	2.3
1	D	132	GLY	2.3
1	B	185	THR	2.2
1	A	254	ILE	2.2
1	A	169	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	98	ASN	2.2
1	B	198	GLY	2.2
1	C	304	ARG	2.2
1	B	311	LYS	2.2
1	D	133	THR	2.2
1	C	173	HIS	2.2
1	D	213	VAL	2.2
1	D	230	ARG	2.2
1	E	221	LYS	2.2
1	B	173	HIS	2.2
1	A	375	ASP	2.2
1	A	97	HIS	2.1
1	B	316	LEU	2.1
1	F	127	LYS	2.1
1	C	253	VAL	2.1
1	A	226	ASN	2.1
1	D	130	GLU	2.1
1	E	226	ASN	2.1
1	D	375	ASP	2.1
1	E	287	ASN	2.1
1	D	390	VAL	2.1
1	F	378	THR	2.1
1	B	208	THR	2.1
1	E	127	LYS	2.1
1	B	142	ASN	2.1
1	D	288	ASN	2.1
1	E	341	GLU	2.1
1	B	320	LYS	2.1
1	B	303	LYS	2.0
1	E	224	LYS	2.0
1	B	270	ARG	2.0
1	F	160	ILE	2.0
1	C	45	CYS	2.0
1	B	378	THR	2.0
1	C	48	HIS	2.0
1	D	276	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
4	GLA	B	1435	11/12	0.68	0.22	41,42,42,43	0
3	SUC	C	1435	23/23	0.68	0.19	24,29,35,37	0
4	GLA	C	1436	11/12	0.72	0.27	43,44,45,45	0
3	SUC	B	1434	23/23	0.74	0.17	25,27,34,36	0
2	CIT	A	1433	13/13	0.75	0.23	50,51,51,52	0
4	GLA	A	1435	11/12	0.80	0.17	29,30,31,31	0
4	GLA	E	1435	11/12	0.81	0.17	35,36,37,38	0
3	SUC	E	1434	23/23	0.82	0.13	21,25,29,30	0
5	SO4	C	1434	5/5	0.82	0.24	44,45,45,46	0
5	SO4	B	1433	5/5	0.85	0.19	43,44,44,45	0
4	GLA	F	1434	11/12	0.85	0.27	33,35,36,36	0
3	SUC	F	1433	23/23	0.86	0.13	18,20,25,26	0
3	SUC	D	1433	23/23	0.88	0.13	16,18,22,24	0
3	SUC	A	1434	23/23	0.89	0.11	17,20,25,27	0
4	GLA	D	1434	11/12	0.89	0.17	29,31,32,32	0
5	SO4	C	1433	5/5	0.89	0.44	2,2,13,14	0
5	SO4	E	1433	5/5	0.94	0.39	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.