



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:01 PM GMT

PDB ID : 4D47
Title : X-ray structure of the levansucrase from Erwinia amylovora
Authors : Wuerges, J.; Caputi, L.; Cianci, M.; Benini, S.
Deposited on : 2014-10-27
Resolution : 2.77 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

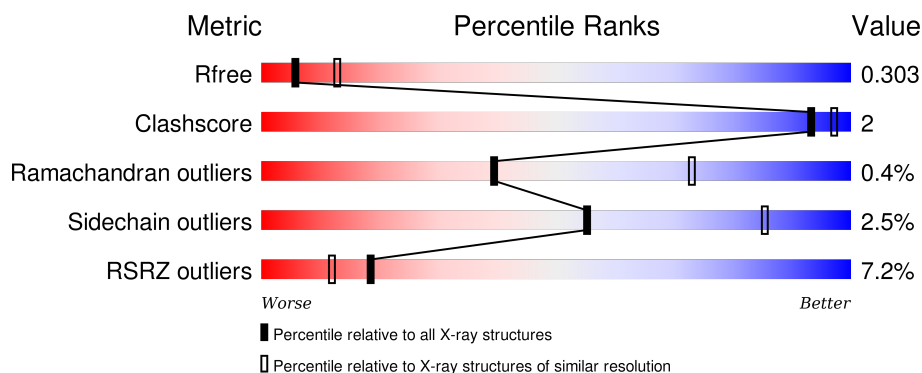
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	415	<div> <div>2%</div> <div>93%</div> <div>6%</div> </div>
1	B	415	<div> <div>4%</div> <div>92%</div> <div>6%</div> </div>
1	C	415	<div> <div>15%</div> <div>93%</div> <div>5%</div> </div>
1	D	415	<div> <div>8%</div> <div>92%</div> <div>6%</div> </div>
1	E	415	<div> <div>12%</div> <div>91%</div> <div>8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	415	
1	G	415	
1	H	415	

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
2	FRU	A	1415	-	-	-	X
2	FRU	H	1415	-	-	-	X
3	GLC	A	1416	-	-	-	X
3	GLC	B	1416	-	-	-	X
3	GLC	C	1416	-	-	-	X
3	GLC	D	1416	-	-	-	X
3	GLC	E	1416	-	-	-	X
3	GLC	G	1416	-	-	-	X
3	GLC	H	1416	-	-	-	X

2 Entry composition

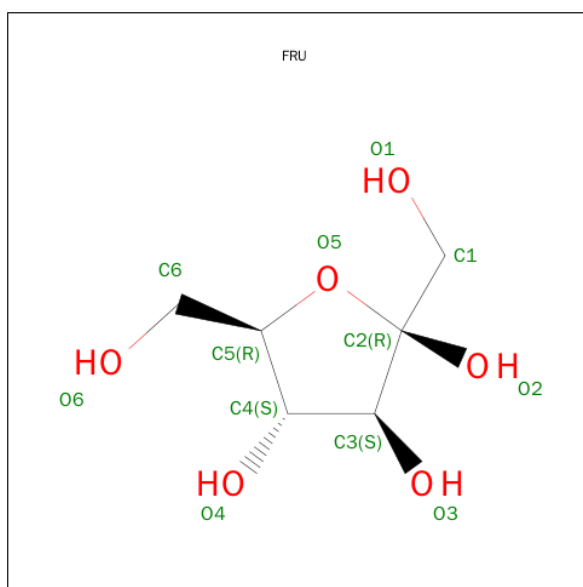
There are 4 unique types of molecules in this entry. The entry contains 26263 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LEVANSUCRASE.

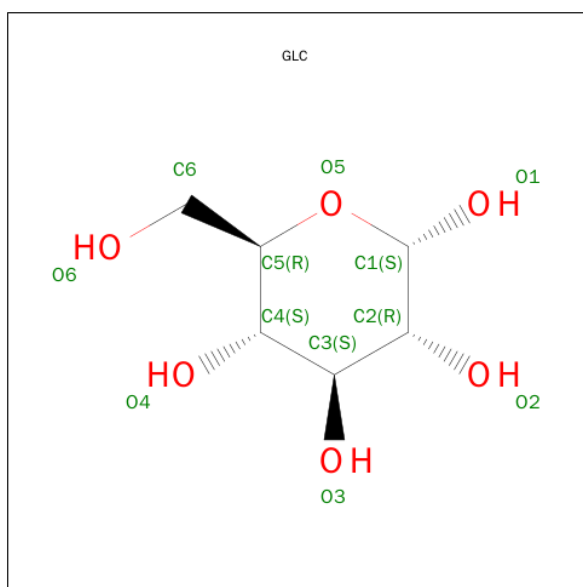
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	B	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	C	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	D	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	E	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	F	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	G	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			
1	H	411	Total	C	N	O	S	0	0	0
			3247	2072	535	628	12			

- Molecule 2 is SUGAR (FRUCTOSE) (three-letter code: FRU) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			12	6	6		
2	G	1	Total	C	O	0	0
			12	6	6		
2	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	4	Total	O	0	0
			4	4		
4	C	11	Total	O	0	0
			11	11		
4	D	8	Total	O	0	0
			8	8		

Continued on next page...

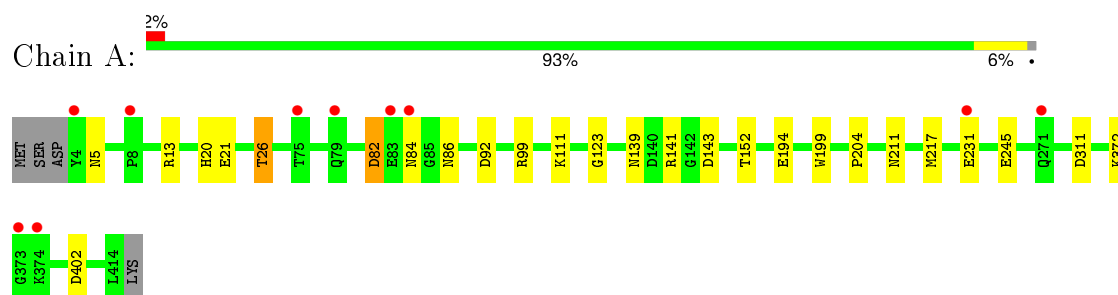
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	12	Total 12	O 12	0	0
4	F	16	Total 16	O 16	0	0
4	G	6	Total 6	O 6	0	0
4	H	13	Total 13	O 13	0	0

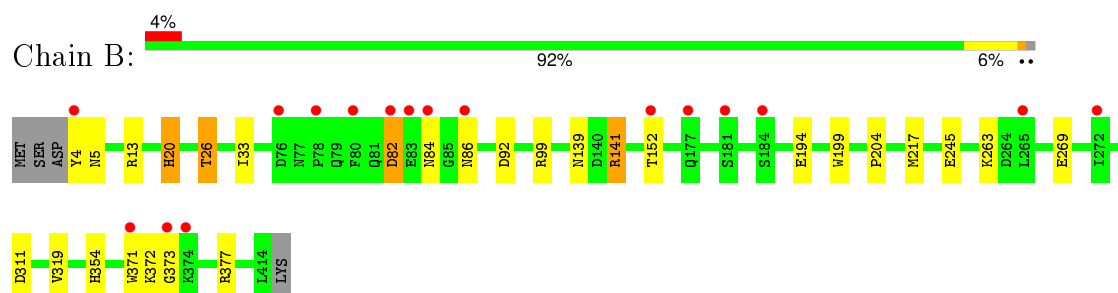
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

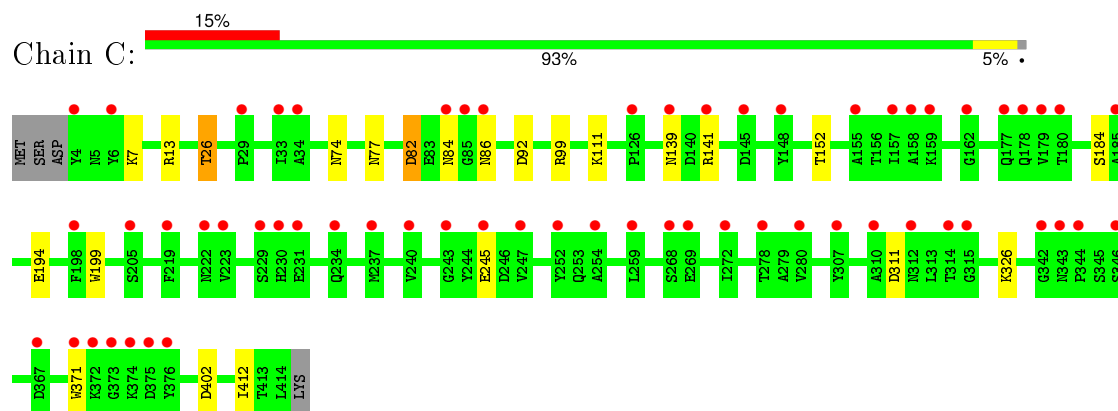
• Molecule 1: LEVANSUCRASE



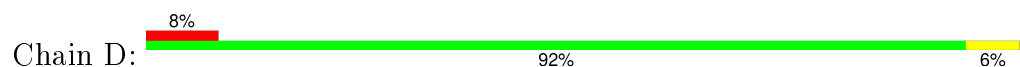
• Molecule 1: LEVANSUCRASE

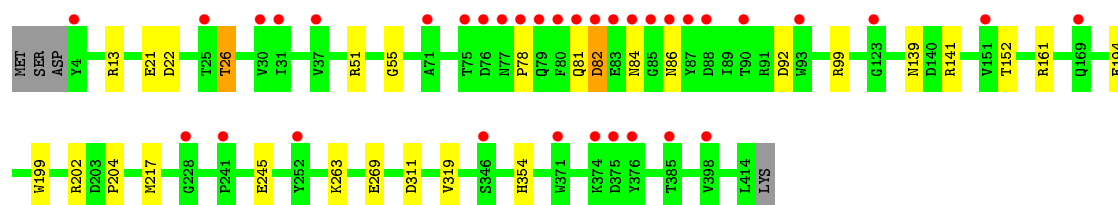


• Molecule 1: LEVANSUCRASE

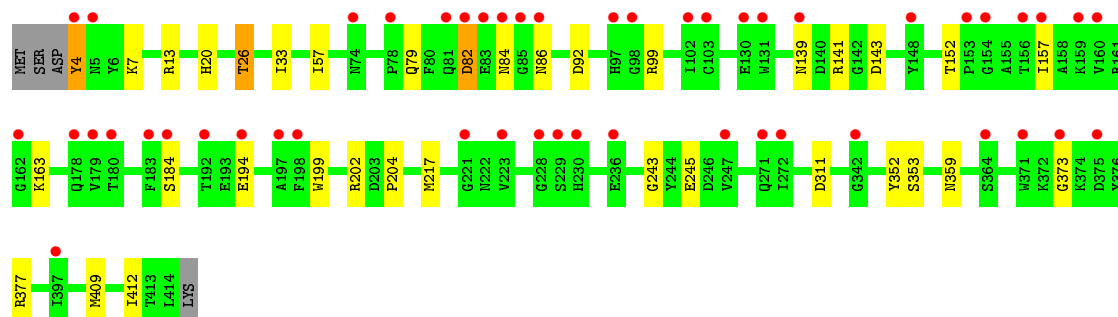
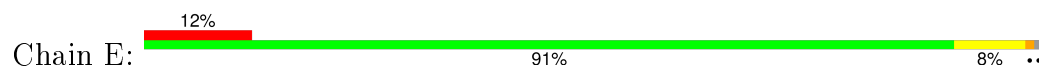


• Molecule 1: LEVANSUCRASE

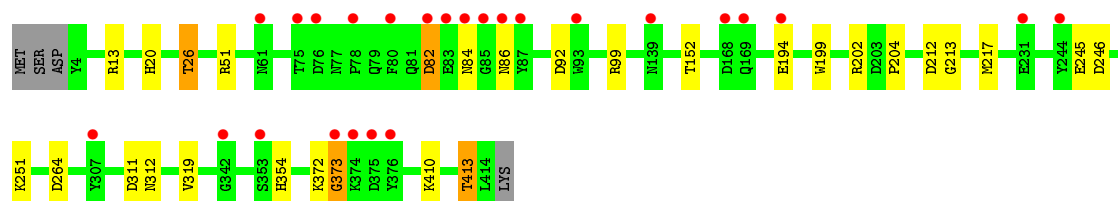
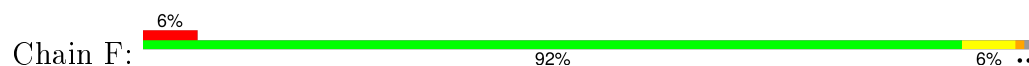




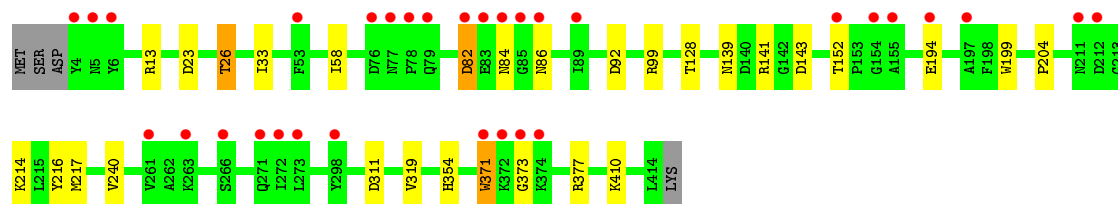
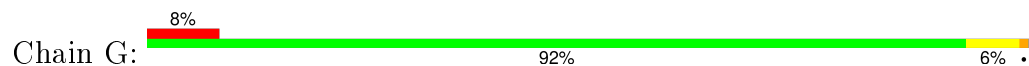
• Molecule 1: LEVANSUCRASE



• Molecule 1: LEVANSUCRASE



• Molecule 1: LEVANSUCRASE



• Molecule 1: LEVANSUCRASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.59Å 178.74Å 158.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.85 – 2.77 94.38 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.85-2.77) 99.8 (94.38-2.77)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.262 , 0.298 0.269 , 0.303	Depositor DCC
R_{free} test set	5632 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	17 of 112730 reflections (0.015%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26263	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.21 % 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 1.0017e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GLC, FRU

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	0.27	0/3340	0.48	0/4555
1	B	0.27	0/3340	0.49	0/4555
1	C	0.26	0/3340	0.48	0/4555
1	D	0.25	0/3340	0.47	0/4555
1	E	0.28	0/3340	0.50	0/4555
1	F	0.27	0/3340	0.49	0/4555
1	G	0.28	0/3340	0.50	0/4555
1	H	0.28	0/3340	0.49	0/4555
All	All	0.27	0/26720	0.49	0/36440

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	5	ASN	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	3247	0	3087	12	0
1	B	3247	0	3087	13	0
1	C	3247	0	3087	8	0
1	D	3247	0	3087	14	0
1	E	3247	0	3087	20	0
1	F	3247	0	3087	16	0
1	G	3247	0	3087	14	0
1	H	3247	0	3087	10	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	1	0
2	E	12	0	12	1	0
2	F	12	0	12	1	0
2	G	12	0	12	0	0
2	H	12	0	12	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
3	E	12	0	12	0	0
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	12	0	12	0	0
4	A	25	0	0	0	0
4	B	4	0	0	0	0
4	C	11	0	0	0	0
4	D	8	0	0	0	0
4	E	12	0	0	0	0
4	F	16	0	0	1	0
4	G	6	0	0	0	0
4	H	13	0	0	0	0
All	All	26263	0	24888	99	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 2.

All (99) 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:G:139:ASN:HB3	1:G:141:ARG:H	1.63	0.63
1:C:92:ASP:OD1	1:C:99:ARG:NH2	2.34	0.60
1:D:141:ARG:NH2	1:F:213:GLY:O	2.32	0.60
1:A:13:ARG:NH2	1:A:311:ASP:O	2.35	0.60
1:F:92:ASP:OD1	1:F:99:ARG:NH2	2.34	0.59
1:D:13:ARG:NH2	1:D:311:ASP:O	2.35	0.59
1:A:92:ASP:OD1	1:A:99:ARG:NH2	2.36	0.59
1:G:33:ILE:HD13	1:G:371:TRP:HB3	1.84	0.59
1:H:13:ARG:NH2	1:H:311:ASP:O	2.36	0.58
1:G:92:ASP:OD1	1:G:99:ARG:NH2	2.36	0.58
1:H:92:ASP:OD1	1:H:99:ARG:NH2	2.37	0.58
1:B:13:ARG:NH2	1:B:311:ASP:O	2.38	0.57
1:E:20:HIS:CD2	1:F:20:HIS:CE1	2.92	0.56
1:E:20:HIS:HB2	1:F:20:HIS:CD2	2.40	0.56
1:G:13:ARG:NH2	1:G:311:ASP:O	2.39	0.55
1:B:92:ASP:OD1	1:B:99:ARG:NH2	2.40	0.55
1:F:202:ARG:NE	2:F:1415:FRU:O1	2.38	0.55
1:A:111:LYS:HE2	1:A:402:ASP:OD2	2.08	0.54
1:E:82:ASP:N	1:E:86:ASN:O	2.30	0.54
1:E:92:ASP:OD1	1:E:99:ARG:NH2	2.41	0.54
1:E:243:GLY:N	1:E:245:GLU:OE2	2.42	0.53
1:C:13:ARG:NH2	1:C:311:ASP:O	2.41	0.53
1:G:82:ASP:N	1:G:86:ASN:O	2.36	0.52
1:E:13:ARG:NH2	1:E:311:ASP:O	2.43	0.52
1:E:57:ILE:HG12	1:E:409:MET:HE3	1.91	0.52
1:F:13:ARG:NH2	1:F:311:ASP:O	2.43	0.51
1:F:204:PRO:HB3	1:F:217:MET:HE1	1.92	0.51
1:A:20:HIS:CD2	1:A:21:GLU:O	2.64	0.51
1:D:263:LYS:HD3	1:D:269:GLU:HB2	1.93	0.50
1:E:359:ASN:H	1:E:409:MET:HE1	1.76	0.50
1:E:139:ASN:ND2	1:E:143:ASP:OD2	2.45	0.50
1:A:20:HIS:HB2	1:B:20:HIS:CD2	2.46	0.50
1:H:139:ASN:HB3	1:H:141:ARG:H	1.76	0.50
1:G:58:ILE:HD12	1:G:410:LYS:HD2	1.93	0.50
1:F:212:ASP:OD1	1:F:213:GLY:N	2.45	0.49
1:B:82:ASP:N	1:B:86:ASN:O	2.31	0.49
1:B:263:LYS:HD3	1:B:269:GLU:HB2	1.94	0.49
1:C:82:ASP:N	1:C:86:ASN:O	2.36	0.49
1:G:58:ILE:CD1	1:G:410:LYS:HD2	2.43	0.49
1:D:92:ASP:OD1	1:D:99:ARG:NH2	2.46	0.48
1:F:51:ARG:NH1	4:F:2009:HOH:O	2.35	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:HB3	1:F:413:THR:HG21	1.95	0.48
1:D:204:PRO:HB3	1:D:217:MET:HE1	1.96	0.48
1:F:372:LYS:HG2	1:F:373:GLY:H	1.78	0.48
1:A:139:ASN:HB3	1:A:141:ARG:H	1.78	0.47
1:B:204:PRO:HB3	1:B:217:MET:HE1	1.95	0.47
1:A:82:ASP:N	1:A:86:ASN:O	2.32	0.46
1:B:26:THR:O	1:B:26:THR:HG23	2.14	0.46
1:C:111:LYS:HE2	1:C:402:ASP:HB3	1.96	0.46
1:F:246:ASP:OD2	1:F:312:ASN:ND2	2.48	0.46
1:E:141:ARG:O	1:E:163:LYS:NZ	2.38	0.46
1:G:26:THR:HG23	1:G:26:THR:O	2.16	0.45
1:H:26:THR:HG23	1:H:26:THR:O	2.17	0.45
1:E:202:ARG:NE	2:E:1415:FRU:O1	2.48	0.45
1:D:161:ARG:NH1	1:F:264:ASP:OD2	2.50	0.45
1:E:26:THR:HG23	1:E:26:THR:O	2.16	0.45
1:D:139:ASN:HB3	1:D:141:ARG:H	1.81	0.45
1:E:4:TYR:C	1:E:4:TYR:HD1	2.20	0.45
1:E:4:TYR:C	1:H:122:GLU:HG3	2.36	0.45
1:G:33:ILE:O	1:G:377:ARG:NH1	2.45	0.45
1:E:4:TYR:C	1:E:4:TYR:CD1	2.90	0.45
1:F:82:ASP:N	1:F:86:ASN:O	2.36	0.44
1:D:78:PRO:HA	1:D:81:GLN:HG3	1.99	0.44
1:A:26:THR:O	1:A:26:THR:HG23	2.16	0.44
1:C:26:THR:HG23	1:C:26:THR:O	2.16	0.44
1:D:319:VAL:HB	1:D:354:HIS:HB2	1.99	0.44
1:B:139:ASN:HB3	1:B:141:ARG:H	1.83	0.44
1:D:26:THR:O	1:D:26:THR:HG23	2.16	0.44
1:B:263:LYS:CD	1:B:269:GLU:HB2	2.47	0.44
1:D:51:ARG:HD2	1:D:55:GLY:HA2	2.00	0.44
1:G:23:ASP:HB3	1:G:26:THR:HG22	2.00	0.44
1:B:319:VAL:HB	1:B:354:HIS:HB2	2.00	0.43
1:F:26:THR:O	1:F:26:THR:HG23	2.19	0.43
1:G:319:VAL:HB	1:G:354:HIS:HB2	2.00	0.43
1:A:139:ASN:ND2	1:A:143:ASP:OD2	2.51	0.43
1:C:139:ASN:HB3	1:C:141:ARG:H	1.84	0.43
1:G:204:PRO:HB3	1:G:217:MET:HE1	2.00	0.43
1:H:82:ASP:N	1:H:86:ASN:O	2.35	0.42
1:C:74:ASN:HB3	1:C:77:ASN:HB3	2.02	0.42
1:H:118:ARG:HH12	1:H:122:GLU:HG2	1.85	0.42
1:B:141:ARG:NH1	1:B:141:ARG:HG3	2.35	0.42
1:D:202:ARG:NE	2:D:1415:FRU:O1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ARG:HH22	1:H:122:GLU:HG2	1.85	0.42
1:E:352:TYR:CG	1:E:353:SER:N	2.88	0.41
1:G:214:LYS:HB2	1:G:216:TYR:CE2	2.55	0.41
1:G:139:ASN:ND2	1:G:143:ASP:OD2	2.51	0.41
1:A:204:PRO:HB3	1:A:217:MET:HE1	2.02	0.41
1:F:319:VAL:HB	1:F:354:HIS:HB2	2.03	0.41
1:D:21:GLU:O	1:D:22:ASP:HB2	2.21	0.41
1:E:204:PRO:HB3	1:E:217:MET:HE1	2.02	0.41
1:E:139:ASN:HB3	1:E:141:ARG:H	1.84	0.41
1:B:33:ILE:O	1:B:377:ARG:NH1	2.48	0.41
1:H:319:VAL:HB	1:H:354:HIS:HB2	2.02	0.41
1:E:33:ILE:O	1:E:377:ARG:NH1	2.48	0.41
1:D:82:ASP:N	1:D:86:ASN:O	2.35	0.41
1:H:115:PHE:CE2	1:H:117:GLY:HA2	2.56	0.41
1:B:371:TRP:CE3	1:B:372:LYS:HB2	2.56	0.41
1:E:157:ILE:HG21	1:E:217:MET:HE1	2.03	0.40
1:A:123:GLY:O	1:C:326:LYS:HD3	2.22	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	409/415 (99%)	388 (95%)	20 (5%)	1 (0%)	52	84
1	B	409/415 (99%)	388 (95%)	19 (5%)	2 (0%)	34	68
1	C	409/415 (99%)	389 (95%)	19 (5%)	1 (0%)	52	84
1	D	409/415 (99%)	388 (95%)	20 (5%)	1 (0%)	52	84
1	E	409/415 (99%)	389 (95%)	18 (4%)	2 (0%)	34	68
1	F	409/415 (99%)	388 (95%)	19 (5%)	2 (0%)	34	68
1	G	409/415 (99%)	388 (95%)	19 (5%)	2 (0%)	34	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	409/415 (99%)	388 (95%)	20 (5%)	1 (0%)	52 84
All	All	3272/3320 (99%)	3106 (95%)	154 (5%)	12 (0%)	39 73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	GLY
1	E	373	GLY
1	F	373	GLY
1	G	373	GLY
1	B	152	THR
1	F	152	THR
1	G	152	THR
1	A	152	THR
1	C	152	THR
1	D	152	THR
1	E	152	THR
1	H	152	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	351/355 (99%)	342 (97%)	9 (3%)	54 85
1	B	351/355 (99%)	342 (97%)	9 (3%)	54 85
1	C	351/355 (99%)	341 (97%)	10 (3%)	51 83
1	D	351/355 (99%)	345 (98%)	6 (2%)	68 91
1	E	351/355 (99%)	341 (97%)	10 (3%)	51 83
1	F	351/355 (99%)	342 (97%)	9 (3%)	54 85
1	G	351/355 (99%)	343 (98%)	8 (2%)	58 87
1	H	351/355 (99%)	343 (98%)	8 (2%)	58 87
All	All	2808/2840 (99%)	2739 (98%)	69 (2%)	55 85

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	26	THR
1	A	82	ASP
1	A	84	ASN
1	A	194	GLU
1	A	199	TRP
1	A	231	GLU
1	A	245	GLU
1	A	372	LYS
1	B	4	TYR
1	B	20	HIS
1	B	26	THR
1	B	82	ASP
1	B	84	ASN
1	B	141	ARG
1	B	194	GLU
1	B	199	TRP
1	B	245	GLU
1	C	7	LYS
1	C	26	THR
1	C	82	ASP
1	C	84	ASN
1	C	184	SER
1	C	194	GLU
1	C	199	TRP
1	C	245	GLU
1	C	371	TRP
1	C	412	ILE
1	D	26	THR
1	D	82	ASP
1	D	84	ASN
1	D	194	GLU
1	D	199	TRP
1	D	245	GLU
1	E	4	TYR
1	E	7	LYS
1	E	26	THR
1	E	79	GLN
1	E	82	ASP
1	E	84	ASN
1	E	184	SER
1	E	194	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	199	TRP
1	E	412	ILE
1	F	26	THR
1	F	82	ASP
1	F	84	ASN
1	F	194	GLU
1	F	199	TRP
1	F	245	GLU
1	F	251	LYS
1	F	410	LYS
1	F	413	THR
1	G	26	THR
1	G	82	ASP
1	G	84	ASN
1	G	128	THR
1	G	194	GLU
1	G	199	TRP
1	G	240	VAL
1	G	371	TRP
1	H	26	THR
1	H	82	ASP
1	H	84	ASN
1	H	194	GLU
1	H	199	TRP
1	H	231	GLU
1	H	245	GLU
1	H	410	LYS

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

Mol	Chain	Res	Type
1	A	20	HIS
1	A	343	ASN
1	A	347	GLN
1	B	5	ASN
1	B	20	HIS
1	B	347	GLN
1	D	343	ASN
1	D	347	GLN
1	E	20	HIS
1	E	234	GLN
1	E	347	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	20	HIS
1	F	347	GLN
1	G	347	GLN
1	H	343	ASN
1	H	347	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	FRU	A	1415	-	11,12,12	0.43	0	10,18,18	0.68	0
3	GLC	A	1416	-	12,12,12	0.41	0	17,17,17	0.81	0
2	FRU	B	1415	-	11,12,12	0.44	0	10,18,18	0.74	0
3	GLC	B	1416	-	12,12,12	0.41	0	17,17,17	0.72	0
2	FRU	C	1415	-	11,12,12	0.36	0	10,18,18	0.56	0
3	GLC	C	1416	-	12,12,12	0.42	0	17,17,17	1.03	2 (11%)
2	FRU	D	1415	-	11,12,12	0.44	0	10,18,18	0.70	0
3	GLC	D	1416	-	12,12,12	0.44	0	17,17,17	0.51	0
2	FRU	E	1415	-	11,12,12	0.43	0	10,18,18	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	E	1416	-	12,12,12	0.42	0	17,17,17	0.77	0
2	FRU	F	1415	-	11,12,12	0.38	0	10,18,18	0.70	0
3	GLC	F	1416	-	12,12,12	0.43	0	17,17,17	0.70	0
2	FRU	G	1415	-	11,12,12	0.45	0	10,18,18	0.65	0
3	GLC	G	1416	-	12,12,12	0.43	0	17,17,17	0.77	1 (5%)
2	FRU	H	1415	-	11,12,12	0.48	0	10,18,18	0.59	0
3	GLC	H	1416	-	12,12,12	0.42	0	17,17,17	0.97	2 (11%)

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	FRU	A	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	A	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	B	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	B	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	C	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	C	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	D	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	D	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	E	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	E	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	F	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	F	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	G	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	G	1416	-	-	0/2/22/22	0/1/1/1
2	FRU	H	1415	-	-	0/5/24/24	0/1/1/1
3	GLC	H	1416	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1416	GLC	C3-C4-C5	-2.57	105.65	110.23
3	H	1416	GLC	C3-C4-C5	-2.03	106.61	110.23
3	G	1416	GLC	O5-C5-C6	2.08	111.76	106.38
3	H	1416	GLC	O5-C5-C6	2.13	111.90	106.38
3	C	1416	GLC	O5-C5-C6	2.18	112.04	106.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1415	FRU	1	0
2	E	1415	FRU	1	0
2	F	1415	FRU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/415 (99%)	0.42	10 (2%) 62 55	14, 25, 42, 72	0
1	B	411/415 (99%)	0.58	17 (4%) 41 33	15, 31, 57, 104	0
1	C	411/415 (99%)	1.09	61 (14%) 3 2	17, 36, 56, 82	0
1	D	411/415 (99%)	0.83	35 (8%) 13 8	19, 44, 84, 129	0
1	E	411/415 (99%)	0.85	49 (11%) 6 3	17, 28, 47, 68	0
1	F	411/415 (99%)	0.74	25 (6%) 25 17	13, 30, 54, 82	0
1	G	411/415 (99%)	0.62	32 (7%) 16 10	16, 30, 53, 82	0
1	H	411/415 (99%)	0.23	8 (1%) 70 63	12, 21, 38, 67	0
All	All	3288/3320 (99%)	0.67	237 (7%) 18 12	12, 30, 57, 129	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	84	ASN	8.2
1	G	4	TYR	7.4
1	D	84	ASN	7.0
1	B	371	TRP	6.4
1	D	76	ASP	5.1
1	D	86	ASN	5.1
1	G	5	ASN	4.9
1	E	228	GLY	4.9
1	B	84	ASN	4.7
1	E	229	SER	4.6
1	D	93	TRP	4.6
1	B	82	ASP	4.5
1	D	78	PRO	4.4
1	G	372	LYS	4.4
1	D	85	GLY	4.4
1	C	86	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	85	GLY	4.1
1	E	179	VAL	4.1
1	C	314	THR	4.1
1	C	231	GLU	4.0
1	D	87	TYR	4.0
1	C	373	GLY	4.0
1	G	86	ASN	4.0
1	D	81	GLN	3.9
1	F	85	GLY	3.9
1	B	76	ASP	3.9
1	D	169	GLN	3.9
1	G	371	TRP	3.9
1	D	80	PHE	3.8
1	C	247	VAL	3.8
1	G	84	ASN	3.8
1	F	169	GLN	3.8
1	H	373	GLY	3.7
1	C	372	LYS	3.7
1	E	98	GLY	3.6
1	E	160	VAL	3.6
1	G	373	GLY	3.6
1	E	371	TRP	3.6
1	E	82	ASP	3.5
1	D	376	TYR	3.5
1	B	86	ASN	3.5
1	H	5	ASN	3.5
1	C	374	LYS	3.4
1	G	374	LYS	3.4
1	B	78	PRO	3.3
1	D	346	SER	3.3
1	C	240	VAL	3.2
1	C	29	PRO	3.2
1	C	158	ALA	3.2
1	C	371	TRP	3.2
1	E	157	ILE	3.2
1	G	82	ASP	3.2
1	C	310	ALA	3.2
1	B	4	TYR	3.1
1	F	86	ASN	3.1
1	C	157	ILE	3.1
1	D	252	TYR	3.1
1	C	243	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	272	ILE	3.1
1	E	84	ASN	3.1
1	C	6	TYR	3.1
1	D	83	GLU	3.1
1	C	375	ASP	3.0
1	D	79	GLN	3.0
1	G	83	GLU	3.0
1	G	271	GLN	3.0
1	E	86	ASN	3.0
1	D	31	ILE	3.0
1	E	4	TYR	3.0
1	F	168	ASP	3.0
1	F	139	ASN	3.0
1	G	298	TYR	3.0
1	D	25	THR	3.0
1	A	83	GLU	3.0
1	D	30	VAL	3.0
1	F	83	GLU	2.9
1	D	374	LYS	2.9
1	C	141	ARG	2.9
1	F	76	ASP	2.9
1	B	83	GLU	2.9
1	D	88	ASP	2.9
1	G	6	TYR	2.9
1	F	93	TRP	2.9
1	F	353	SER	2.9
1	C	223	VAL	2.9
1	C	367	ASP	2.8
1	D	77	ASN	2.8
1	E	159	LYS	2.8
1	C	84	ASN	2.8
1	E	78	PRO	2.8
1	C	346	SER	2.8
1	C	177	GLN	2.8
1	C	126	PRO	2.8
1	F	87	TYR	2.8
1	C	4	TYR	2.7
1	C	342	GLY	2.7
1	E	131	TRP	2.7
1	C	252	TYR	2.7
1	G	212	ASP	2.7
1	C	222	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	152	THR	2.7
1	D	375	ASP	2.7
1	F	78	PRO	2.6
1	E	97	HIS	2.6
1	E	223	VAL	2.6
1	E	74	ASN	2.6
1	D	75	THR	2.6
1	C	237	MET	2.6
1	E	272	ILE	2.6
1	E	230	HIS	2.6
1	A	84	ASN	2.6
1	G	79	GLN	2.6
1	E	194	GLU	2.6
1	E	342	GLY	2.6
1	C	179	VAL	2.6
1	A	75	THR	2.5
1	C	178	GLN	2.5
1	E	156	THR	2.5
1	G	263	LYS	2.5
1	F	373	GLY	2.5
1	C	234	GLN	2.5
1	C	376	TYR	2.5
1	C	139	ASN	2.5
1	C	33	ILE	2.5
1	D	90	THR	2.5
1	F	82	ASP	2.5
1	G	85	GLY	2.5
1	H	84	ASN	2.5
1	F	376	TYR	2.5
1	A	374	LYS	2.5
1	C	312	ASN	2.5
1	H	231	GLU	2.5
1	C	344	PRO	2.5
1	G	154	GLY	2.5
1	B	80	PHE	2.5
1	C	219	PHE	2.4
1	D	151	VAL	2.4
1	B	374	LYS	2.4
1	C	85	GLY	2.4
1	C	229	SER	2.4
1	C	268	SER	2.4
1	C	148	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	375	ASP	2.4
1	E	192	THR	2.4
1	B	272	ILE	2.4
1	E	5	ASN	2.4
1	E	198	PHE	2.4
1	H	252	TYR	2.4
1	C	245	GLU	2.4
1	E	81	GLN	2.4
1	G	266	SER	2.4
1	D	37	VAL	2.4
1	C	269	GLU	2.4
1	A	4	TYR	2.4
1	G	211	ASN	2.4
1	C	159	LYS	2.4
1	D	371	TRP	2.4
1	E	236	GLU	2.4
1	E	148	TYR	2.3
1	C	180	THR	2.3
1	C	185	ALA	2.3
1	E	178	GLN	2.3
1	D	71	ALA	2.3
1	E	247	VAL	2.3
1	E	373	GLY	2.3
1	G	76	ASP	2.3
1	F	375	ASP	2.3
1	C	205	SER	2.3
1	C	230	HIS	2.3
1	C	34	ALA	2.3
1	D	385	THR	2.3
1	A	231	GLU	2.3
1	C	280	VAL	2.3
1	C	343	ASN	2.3
1	F	307	TYR	2.3
1	C	272	ILE	2.3
1	E	183	PHE	2.3
1	D	398	VAL	2.3
1	C	162	GLY	2.2
1	D	228	GLY	2.2
1	E	197	ALA	2.2
1	B	373	GLY	2.2
1	G	194	GLU	2.2
1	B	184	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	259	LEU	2.2
1	F	374	LYS	2.2
1	A	79	GLN	2.2
1	D	4	TYR	2.2
1	E	271	GLN	2.2
1	F	231	GLU	2.2
1	B	181	SER	2.2
1	E	139	ASN	2.2
1	E	397	ILE	2.2
1	F	61	ASN	2.2
1	C	254	ALA	2.2
1	G	155	ALA	2.2
1	G	197	ALA	2.2
1	C	307	TYR	2.2
1	G	78	PRO	2.2
1	H	194	GLU	2.2
1	F	244	TYR	2.1
1	F	194	GLU	2.1
1	C	198	PHE	2.1
1	B	265	LEU	2.1
1	C	315	GLY	2.1
1	D	123	GLY	2.1
1	E	153	PRO	2.1
1	C	155	ALA	2.1
1	G	261	VAL	2.1
1	E	184	SER	2.1
1	E	102	ILE	2.1
1	E	162	GLY	2.1
1	E	180	THR	2.1
1	F	75	THR	2.1
1	E	221	GLY	2.1
1	G	77	ASN	2.1
1	C	145	ASP	2.1
1	E	130	GLU	2.1
1	E	103	CYS	2.1
1	B	177	GLN	2.1
1	G	152	THR	2.1
1	E	83	GLU	2.1
1	E	154	GLY	2.1
1	G	273	LEU	2.1
1	A	271	GLN	2.1
1	G	89	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	374	LYS	2.1
1	F	342	GLY	2.1
1	D	241	PRO	2.0
1	A	373	GLY	2.0
1	D	82	ASP	2.0
1	A	8	PRO	2.0
1	F	80	PHE	2.0
1	E	364	SER	2.0
1	C	278	THR	2.0
1	H	79	GLN	2.0
1	G	53	PHE	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GLC	A	1416	12/12	0.88	0.32	6.78	44,48,70,70	0
3	GLC	H	1416	12/12	0.89	0.40	6.67	44,47,76,83	0
3	GLC	G	1416	12/12	0.85	0.35	5.59	45,53,64,71	0
3	GLC	B	1416	12/12	0.83	0.33	5.35	45,57,67,70	0
2	FRU	H	1415	12/12	0.87	0.31	4.36	29,33,43,48	0
3	GLC	E	1416	12/12	0.80	0.43	2.90	45,51,58,58	0
2	FRU	A	1415	12/12	0.91	0.25	2.63	29,38,45,49	0
3	GLC	D	1416	12/12	0.84	0.33	2.13	54,60,72,78	0
3	GLC	C	1416	12/12	0.88	0.38	2.11	45,50,57,60	0
2	FRU	G	1415	12/12	0.91	0.25	1.94	32,37,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FRU	B	1415	12/12	0.92	0.24	1.77	30,38,48,52	0
3	GLC	F	1416	12/12	0.79	0.31	1.76	45,55,78,80	0
2	FRU	E	1415	12/12	0.86	0.31	0.94	31,41,58,59	0
2	FRU	C	1415	12/12	0.93	0.26	0.53	32,41,59,60	0
2	FRU	F	1415	12/12	0.91	0.22	-0.36	31,38,53,53	0
2	FRU	D	1415	12/12	0.88	0.19	-2.23	32,49,58,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.