Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:00 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

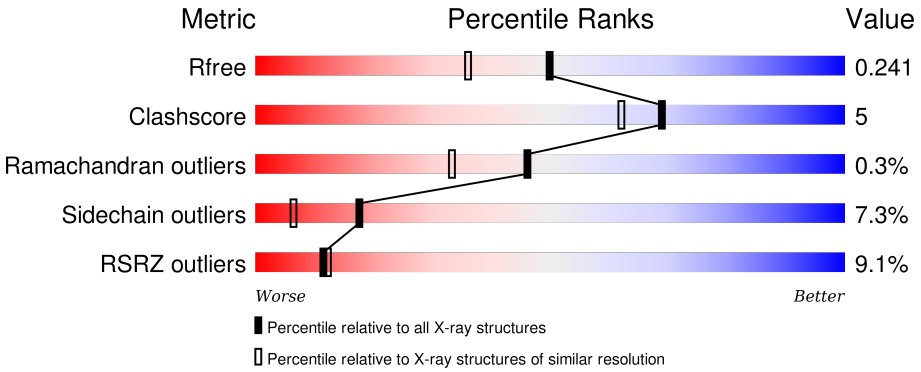
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (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 <=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	5% 86% 13%
1	B	432	12% 82% 16%
1	C	432	9% 85% 13%
1	D	432	8% 84% 14%
1	E	432	11% 88% 12%

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Mol	Chain	Length	Quality of chain
1	F	432	9% 87% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	1434	-	-	-	X

2 Entry composition

There are 5 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

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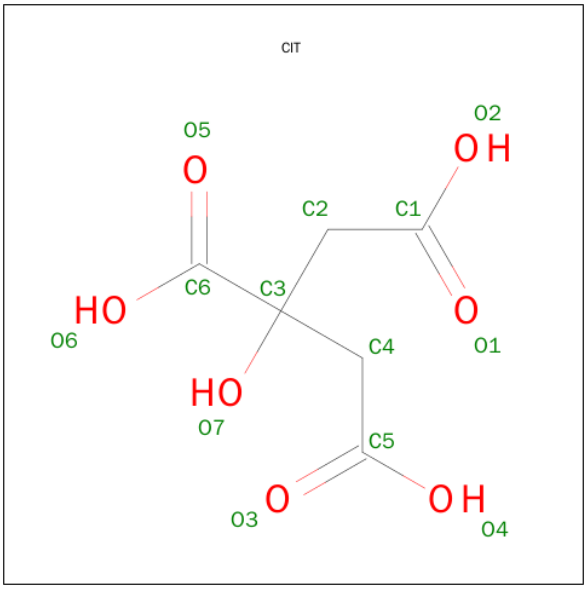
Chain	Residue	Modelled	Actual	Comment	Reference
F	179	ALA	VAL	CLONING ARTIFACT	UNP O33833

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

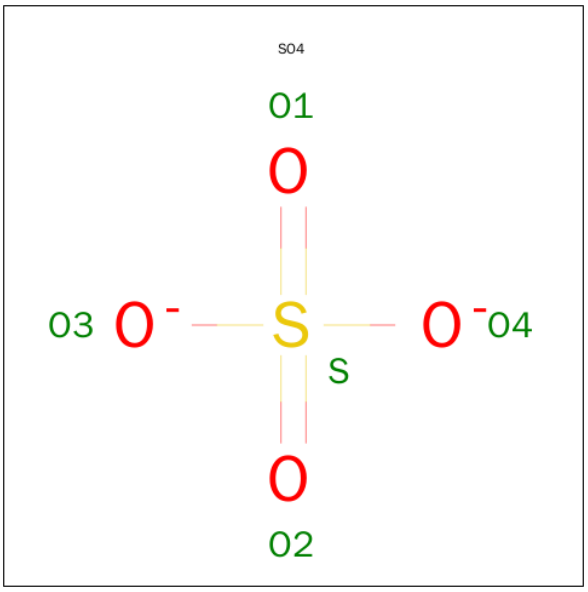


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total C O 34 18 16	0	0
3	B	2	Total C O 34 18 16	0	0
3	C	2	Total C O 34 18 16	0	0
3	D	2	Total C O 34 18 16	0	0
3	E	2	Total C O 34 18 16	0	0
3	F	2	Total C O 34 18 16	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

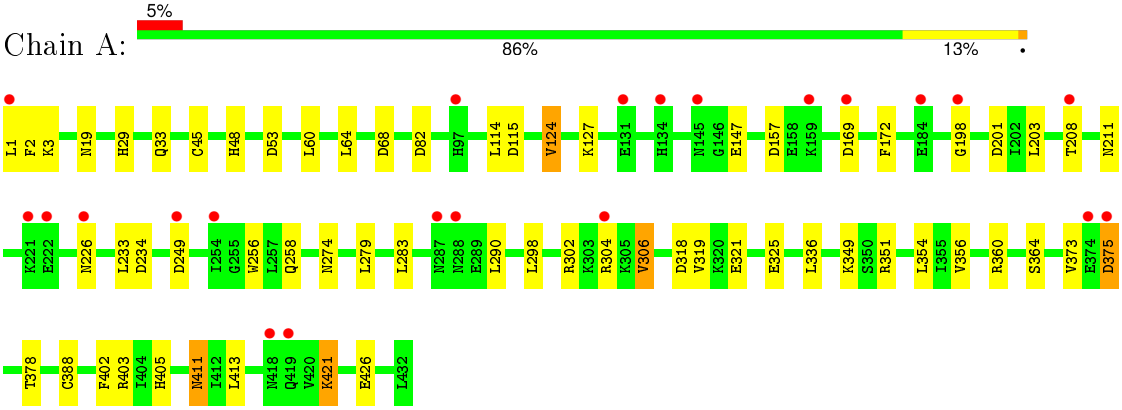
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	339	Total O 339 339	0	0
5	B	259	Total O 259 259	0	0
5	C	316	Total O 316 316	0	0
5	D	364	Total O 364 364	0	0
5	E	296	Total O 296 296	0	0
5	F	314	Total O 314 314	0	0

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 (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.

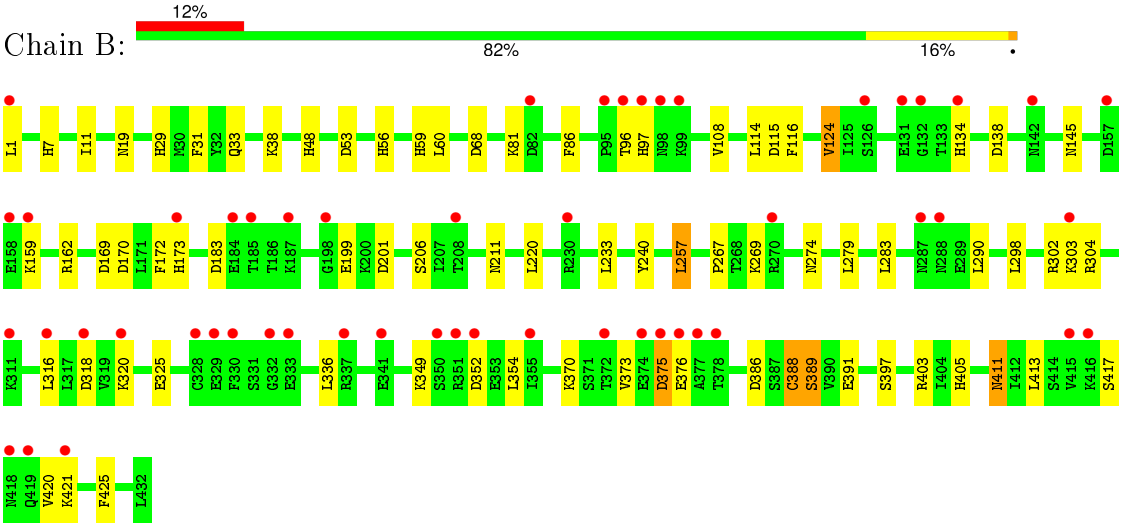
- Molecule 1: BETA FRUCTOSIDASE

Chain A:



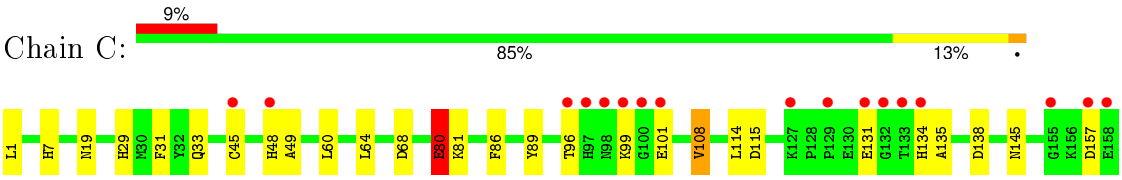
- Molecule 1: BETA FRUCTOSIDASE

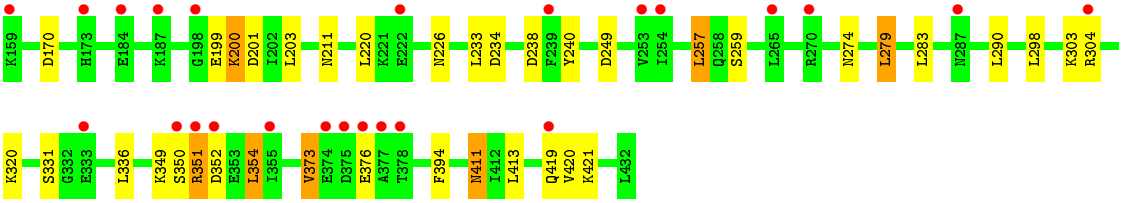
Chain B:



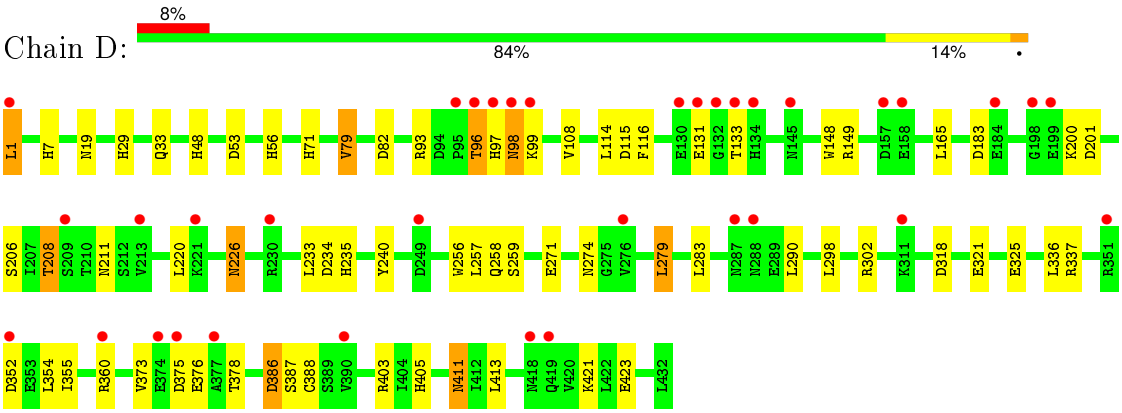
- Molecule 1: BETA FRUCTOSIDASE

Chain C:

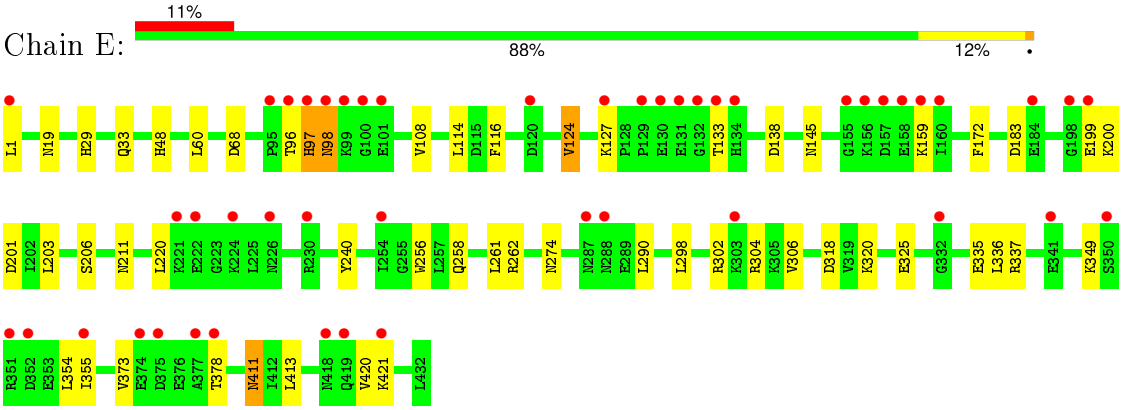




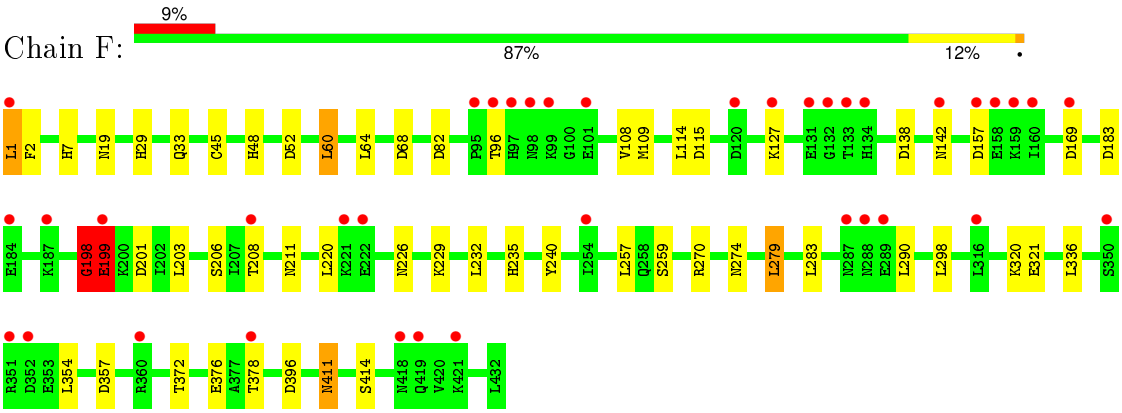
• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE



• Molecule 1: BETA FRUCTOSIDASE



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.28%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 220442 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (i)

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	34	0	30	0	0
3	B	34	0	30	0	0
3	C	34	0	30	0	0
3	D	34	0	30	0	0
3	E	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	34	0	30	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	E	5	0	0	0	0
5	A	339	0	0	16	0
5	B	259	0	0	1	0
5	C	316	0	0	5	0
5	D	364	0	0	4	0
5	E	296	0	0	4	0
5	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	5:A:2179:HOH:O	1.56	1.20
1:F:270:ARG:CZ	5: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	5: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	5:F:2203:HOH:O	2.04	0.83
2:A:1433:CIT:O3	5:A:2331:HOH:O	1.95	0.83
2:A:1433:CIT:C6	5:A:2336:HOH:O	2.27	0.82
2:A:1433:CIT:O5	5:A:2336:HOH:O	1.97	0.81
1:C:211:ASN:HD21	1:C:259:SER:CA	1.93	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:E:97:HIS:O	1:E:98:ASN:ND2	2.17	0.77
1:B:11:ILE:HG23	1:B:59:HIS:CE1	2.20	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	5:A:2333:HOH:O	2.06	0.73
1:E:262:ARG:NH2	5:E:2184:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	5:A:2002:HOH:O	2.04	0.70
1:A:360:ARG:NE	5:A:2281:HOH:O	2.25	0.70
1:E:97:HIS:C	1:E:98:ASN:HD22	1.95	0.69
1:D:7:HIS:CE1	1:D:279:LEU:HD13	2.27	0.69
1:C:211:ASN:CG	5: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:E:211:ASN:HD21	1:E:261:LEU:HG	1.58	0.67
1:D:208:THR:O	1:D:211:ASN:ND2	2.28	0.67
1:B:267:PRO:HD2	1:B:405:HIS:HD2	1.60	0.65
1:F:19:ASN:HD21	1:F:33:GLN:HE21	1.45	0.65
1:D:19:ASN:HD21	1:D: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	5:A:2281:HOH:O	2.48	0.60
1:A:360:ARG:CG	5: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	5:C:2163:HOH:O	2.35	0.58
1:C:351:ARG:NH2	5:C:2258:HOH:O	2.36	0.58
1:E:335:GLU:OE1	1:E:337:ARG:NE	2.37	0.58
1:D:1:LEU:HD12	1:D:1:LEU:H3	1.67	0.58
1:B:19:ASN:HD21	1:B:33:GLN:HE21	1.52	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
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:D:29:HIS:HD2	1:D:48:HIS:NE2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD11	1:A:413:LEU:HD11	1.88	0.56
1:E:29:HIS:HD2	1:E:48:HIS:NE2	2.04	0.55
1:E:1:LEU:HD23	5:E:2002:HOH:O	2.06	0.55
1:C:31:PHE:CZ	1:C:48:HIS:HE1	2.20	0.55
1:D:235:HIS:HD2	5: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:31:PHE:CE2	1:C:48:HIS:CE1	2.94	0.54
1:C:134:HIS:CD2	1:C:135:ALA:H	2.25	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	5: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	5:D:2130:HOH:O	2.08	0.54
1:A:360:ARG:HG2	5: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	5: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	5: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:B:336:LEU:HD11	1:B:413:LEU:HD11	1.92	0.51
1:A:351:ARG:NH2	1:C:220:LEU:O	2.42	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:F:270:ARG:NH2	5:F:2203:HOH:O	2.21	0.50
1:E:211:ASN:ND2	1:E:261:LEU:H	2.10	0.50
1:F:1:LEU:HD22	5:F:2287:HOH:O	2.11	0.50
1:A:403:ARG:HH21	1:A:405:HIS:HE1	1.58	0.50
1:C:81:LYS:HB3	1:C:86:PHE:CE1	2.46	0.49
1:C:134:HIS:CD2	1:C:135:ALA:N	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1:LEU:HB3	5:E:2002:HOH:O	2.13	0.48
1:A:375:ASP:OD2	1:C:200:LYS:NZ	2.46	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:D:97:HIS:O	1:D:98:ASN:ND2	2.47	0.48
1:B:29:HIS:HE1	5:B:2015:HOH:O	1.97	0.48
1:B:108:VAL:HG11	1:B:116:PHE:HB3	1.96	0.48
1:E:108:VAL:HG11	1:E:116:PHE:HB3	1.94	0.48
1:B:19:ASN:ND2	1:B:33:GLN:HE21	2.11	0.48
1:B:124:VAL:HG22	1:B:172:PHE:O	2.13	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:D:7:HIS:CD2	1:D:386:ASP:OD2	2.68	0.47
1:A:426:GLU:CD	5:A:2319:HOH:O	2.53	0.47
1:C:7:HIS:NE2	1:C:279:LEU:HD13	2.29	0.47
1:D:53:ASP:OD2	1:D:56:HIS:HD2	1.98	0.47
1:C:29:HIS:HE1	5:C:2020:HOH:O	1.98	0.47
1:F:1:LEU:HD13	1:F:2:PHE:CD1	2.49	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:C:351:ARG:CZ	5:C:2258:HOH:O	2.62	0.46
1:B:53:ASP:OD2	1:B:56:HIS:HD2	1.98	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:C:238:ASP:O	1:C:257:LEU:HD23	2.16	0.46
1:B:388:CYS:O	1:B:389:SER:HB3	2.15	0.46
1:D:96:THR:HB	1:D:97:HIS:H	1.58	0.46
1:F:270:ARG:NH2	5:F:2204:HOH:O	2.49	0.46
1:D:7:HIS:ND1	1:D:279:LEU:HD13	2.31	0.46
1:C:354:LEU:HB2	1:C:373:VAL:HG21	1.98	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:C:211:ASN:OD1	1:C:240:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:HD2	1:A:48:HIS:NE2	2.15	0.45
1:D:1:LEU:HD13	1:D:271:GLU:OE1	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: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:C:48:HIS:CD2	1:C:60:LEU:HD12	2.53	0.44
1:A:45:CYS:HB3	1:A:64:LEU:O	2.18	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:D:1:LEU:O	1:D:387:SER:HB3	2.18	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:360:ARG:HG2	5: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:C:7:HIS:CD2	1:C:279:LEU:HD13	2.54	0.42
1:A:124:VAL:HG22	1:A:172:PHE:O	2.18	0.42
1:F:206:SER:HB3	1:F:240:TYR:CE1	2.53	0.42
1:C:373:VAL:HG11	1:C:394:PHE:CD2	2.55	0.42
1:B:170:ASP:OD2	1:B:173:HIS:HD2	2.01	0.42
1:E:256:TRP:CE2	1:E:258:GLN:HB3	2.54	0.42
1:E:29:HIS:CD2	1:E:48:HIS:NE2	2.87	0.42
1:C:101:GLU:OE2	1:C:134:HIS:CE1	2.72	0.42
1:A:360:ARG:HG3	5: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
1:E:97:HIS:C	1:E:98:ASN:ND2	2.67	0.41
1:B:417:SER:HB3	1:B:420:VAL:CG1	2.50	0.41
1:E:145:ASN:ND2	5:E:2128:HOH:O	2.48	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	5:D:2018:HOH:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:LYS:NZ	5: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 (i)

5.3.1 Protein backbone (i)

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%)	52	40
1	B	430/432 (100%)	412 (96%)	17 (4%)	1 (0%)	52	40
1	C	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	52	40
1	D	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	52	40
1	E	430/432 (100%)	414 (96%)	15 (4%)	1 (0%)	52	40
1	F	430/432 (100%)	412 (96%)	16 (4%)	2 (0%)	34	20
All	All	2580/2592 (100%)	2477 (96%)	96 (4%)	7 (0%)	46	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	ARG
1	F	199	GLU
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 (i)

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%)	25	12
1	B	387/387 (100%)	352 (91%)	35 (9%)	12	4
1	C	387/387 (100%)	359 (93%)	28 (7%)	18	7
1	D	386/387 (100%)	358 (93%)	28 (7%)	17	6
1	E	387/387 (100%)	362 (94%)	25 (6%)	21	9
1	F	386/387 (100%)	355 (92%)	31 (8%)	15	5
All	All	2318/2322 (100%)	2149 (93%)	169 (7%)	17	6

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	F	411	ASN

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

12 carbohydrates 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	$\#\|Z\| > 2$
3	SUC	A	1434	3	24,24,24	1.38	1 (4%)	36,36,36	1.35	5 (13%)
3	GLA	A	1435	3	11,11,12	0.60	0	14,15,17	0.56	0
3	SUC	B	1434	3	24,24,24	1.35	1 (4%)	36,36,36	0.65	1 (2%)
3	GLA	B	1435	3	11,11,12	0.52	0	14,15,17	0.57	0
3	SUC	C	1435	3	24,24,24	1.35	1 (4%)	36,36,36	0.64	0
3	GLA	C	1436	3	11,11,12	0.55	0	14,15,17	0.59	0
3	SUC	D	1433	3	24,24,24	1.37	1 (4%)	36,36,36	1.48	8 (22%)
3	GLA	D	1434	3	11,11,12	0.58	0	14,15,17	0.54	0
3	SUC	E	1434	3	24,24,24	1.40	1 (4%)	36,36,36	1.33	4 (11%)
3	GLA	E	1435	3	11,11,12	0.52	0	14,15,17	0.49	0
3	SUC	F	1433	3	24,24,24	1.34	1 (4%)	36,36,36	0.95	2 (5%)
3	GLA	F	1434	3	11,11,12	0.53	0	14,15,17	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SUC	A	1434	3	-	0/12/51/51	0/2/2/2
3	GLA	A	1435	3	-	0/2/19/22	0/1/1/1
3	SUC	B	1434	3	-	0/12/51/51	0/2/2/2
3	GLA	B	1435	3	-	0/2/19/22	0/1/1/1
3	SUC	C	1435	3	-	0/12/51/51	0/2/2/2
3	GLA	C	1436	3	-	0/2/19/22	0/1/1/1
3	SUC	D	1433	3	-	0/12/51/51	0/2/2/2
3	GLA	D	1434	3	-	0/2/19/22	0/1/1/1
3	SUC	E	1434	3	-	0/12/51/51	0/2/2/2
3	GLA	E	1435	3	-	0/2/19/22	0/1/1/1
3	SUC	F	1433	3	-	0/12/51/51	0/2/2/2
3	GLA	F	1434	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1434	SUC	O6'-C6'	-6.36	1.14	1.42
3	C	1435	SUC	O6'-C6'	-6.33	1.15	1.42
3	B	1434	SUC	O6'-C6'	-6.26	1.15	1.42
3	A	1434	SUC	O6'-C6'	-6.24	1.15	1.42
3	F	1433	SUC	O6'-C6'	-6.21	1.15	1.42
3	D	1433	SUC	O6'-C6'	-6.09	1.16	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1433	SUC	C1-O5-C5	-4.08	105.82	113.75
3	A	1434	SUC	C1-O5-C5	-3.39	107.17	113.75
3	F	1433	SUC	O5-C1-C2	-3.17	103.77	110.28
3	E	1434	SUC	C1-O5-C5	-2.75	108.41	113.75
3	D	1433	SUC	C1-C2-C3	-2.72	104.62	109.97
3	A	1434	SUC	C1-C2-C3	-2.19	105.66	109.97
3	B	1434	SUC	O2'-C2'-C1'	2.06	113.59	107.98
3	D	1433	SUC	O5-C5-C4	2.11	113.64	109.68
3	D	1433	SUC	O1-C1-C2	2.17	115.60	108.36
3	A	1434	SUC	C2'-O1-C1	2.33	123.67	117.53
3	E	1434	SUC	C2'-O1-C1	2.33	123.68	117.53
3	D	1433	SUC	C2'-O1-C1	2.34	123.71	117.53
3	E	1434	SUC	O2'-C2'-C1'	2.44	114.63	107.98
3	A	1434	SUC	O2'-C2'-C1'	2.50	114.77	107.98
3	F	1433	SUC	O2'-C2'-C1'	2.57	114.98	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1433	SUC	O2'-C2'-C1'	2.60	115.05	107.98
3	D	1433	SUC	O5-C1-O1	2.62	118.76	109.96
3	D	1433	SUC	O5-C1-C2	3.33	117.11	110.28
3	A	1434	SUC	O5-C1-O1	3.92	123.14	109.96
3	E	1434	SUC	O5-C1-O1	4.46	124.94	109.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

5 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	1.32	0	3,17,17	2.02	1 (33%)
4	SO4	B	1433	-	4,4,4	0.23	0	6,6,6	0.21	0
4	SO4	C	1433	-	4,4,4	0.49	0	6,6,6	0.41	0
4	SO4	C	1434	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SO4	E	1433	-	4,4,4	1.18	0	6,6,6	0.80	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
4	SO4	B	1433	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1433	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1434	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	E	1433	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1433	CIT	C4-C3-C2	3.19	117.45	109.81

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)

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, 95^{th} 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%)	0.36	22 (5%) 32 33	7, 16, 28, 33	4 (0%)
1	B	432/432 (100%)	0.67	52 (12%) 6 6	8, 17, 28, 34	6 (1%)
1	C	432/432 (100%)	0.54	41 (9%) 10 11	7, 17, 28, 34	8 (1%)
1	D	432/432 (100%)	0.56	35 (8%) 15 16	8, 16, 28, 34	8 (1%)
1	E	432/432 (100%)	0.54	47 (10%) 7 8	8, 16, 28, 34	9 (2%)
1	F	432/432 (100%)	0.55	38 (8%) 12 13	7, 16, 28, 34	10 (2%)
All	All	2592/2592 (100%)	0.54	235 (9%) 11 12	7, 16, 28, 34	45 (1%)

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	98	ASN	12.0
1	D	98	ASN	11.0
1	E	97	HIS	10.7
1	B	97	HIS	10.4
1	C	97	HIS	10.4
1	E	96	THR	9.4
1	B	98	ASN	9.3
1	F	97	HIS	8.7
1	E	99	LYS	8.2
1	D	97	HIS	8.2
1	F	96	THR	7.8
1	B	99	LYS	7.5
1	F	98	ASN	6.4
1	B	96	THR	6.0
1	C	132	GLY	5.8
1	B	134	HIS	5.7
1	E	198	GLY	5.7
1	E	131	GLU	5.7
1	B	351	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	96	THR	5.5
1	D	134	HIS	5.4
1	E	134	HIS	5.4
1	C	134	HIS	5.3
1	B	287	ASN	5.2
1	C	131	GLU	5.2
1	F	287	ASN	5.2
1	A	418	ASN	5.2
1	E	95	PRO	5.1
1	D	418	ASN	5.0
1	F	134	HIS	5.0
1	C	351	ARG	5.0
1	B	352	ASP	4.8
1	C	270	ARG	4.8
1	D	199	GLU	4.7
1	B	131	GLU	4.7
1	E	100	GLY	4.6
1	B	350	SER	4.6
1	B	288	ASN	4.5
1	F	1	LEU	4.4
1	E	158	GLU	4.4
1	E	159	LYS	4.3
1	E	377	ALA	4.3
1	B	418	ASN	4.2
1	A	159	LYS	4.2
1	B	372	THR	4.2
1	E	157	ASP	4.1
1	B	230	ARG	4.0
1	B	1	LEU	4.0
1	B	332	GLY	3.9
1	C	99	LYS	3.9
1	F	159	LYS	3.9
1	C	377	ALA	3.8
1	A	419	GLN	3.8
1	E	351	ARG	3.8
1	E	352	ASP	3.8
1	F	352	ASP	3.8
1	F	288	ASN	3.8
1	C	352	ASP	3.7
1	E	101	GLU	3.7
1	F	158	GLU	3.7
1	D	287	ASN	3.7

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

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Mol	Chain	Res	Type	RSRZ
1	C	198	GLY	3.0
1	E	184	GLU	3.0
1	F	95	PRO	3.0
1	F	360	ARG	3.0
1	D	157	ASP	3.0
1	E	133	THR	2.9
1	E	199	GLU	2.9
1	F	133	THR	2.9
1	F	199	GLU	2.9
1	D	95	PRO	2.9
1	D	374	GLU	2.9
1	E	332	GLY	2.9
1	C	376	GLU	2.8
1	E	375	ASP	2.8
1	A	198	GLY	2.8
1	C	133	THR	2.8
1	E	350	SER	2.8
1	A	222	GLU	2.8
1	A	184	GLU	2.8
1	C	265	LEU	2.8
1	D	249	ASP	2.8
1	E	130	GLU	2.8
1	B	157	ASP	2.7
1	B	355	ILE	2.7
1	C	100	GLY	2.7
1	D	360	ARG	2.7
1	B	158	GLU	2.7
1	B	82	ASP	2.7
1	B	419	GLN	2.7
1	D	99	LYS	2.7
1	B	184	GLU	2.7
1	C	419	GLN	2.7
1	B	376	GLU	2.7
1	F	221	LYS	2.6
1	C	374	GLU	2.6
1	F	421	LYS	2.6
1	E	254	ILE	2.6
1	C	158	GLU	2.6
1	B	187	LYS	2.5
1	C	127	LYS	2.5
1	D	158	GLU	2.5
1	A	1	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	2.5
1	F	350	SER	2.5
1	F	142	ASN	2.5
1	A	374	GLU	2.5
1	B	95	PRO	2.5
1	C	101	GLU	2.5
1	E	421	LYS	2.5
1	A	131	GLU	2.5
1	B	328	CYS	2.5
1	E	419	GLN	2.5
1	C	222	GLU	2.5
1	E	160	ILE	2.4
1	E	230	ARG	2.4
1	B	333	GLU	2.4
1	E	418	ASN	2.4
1	B	416	LYS	2.4
1	C	187	LYS	2.4
1	D	209	SER	2.4
1	B	377	ALA	2.4
1	F	101	GLU	2.4
1	D	311	LYS	2.4
1	A	221	LYS	2.4
1	D	221	LYS	2.4
1	C	129	PRO	2.4
1	C	254	ILE	2.4
1	C	355	ILE	2.4
1	E	222	GLU	2.4
1	B	421	LYS	2.4
1	F	132	GLY	2.4
1	E	374	GLU	2.4
1	F	120	ASP	2.4
1	A	254	ILE	2.3
1	C	184	GLU	2.3
1	E	303	LYS	2.3
1	B	318	ASP	2.3
1	A	288	ASN	2.3
1	C	287	ASN	2.3
1	B	337	ARG	2.3
1	D	132	GLY	2.3
1	A	304	ARG	2.3
1	B	185	THR	2.3
1	C	98	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	169	ASP	2.3
1	D	213	VAL	2.3
1	B	198	GLY	2.3
1	B	316	LEU	2.2
1	C	253	VAL	2.2
1	C	173	HIS	2.2
1	C	304	ARG	2.2
1	A	97	HIS	2.2
1	B	173	HIS	2.2
1	D	133	THR	2.2
1	A	375	ASP	2.2
1	B	311	LYS	2.2
1	E	221	LYS	2.2
1	D	230	ARG	2.2
1	D	390	VAL	2.2
1	A	226	ASN	2.2
1	D	375	ASP	2.2
1	F	127	LYS	2.2
1	E	226	ASN	2.1
1	F	378	THR	2.1
1	D	130	GLU	2.1
1	E	287	ASN	2.1
1	B	208	THR	2.1
1	E	127	LYS	2.1
1	D	276	VAL	2.1
1	B	142	ASN	2.1
1	D	288	ASN	2.1
1	F	160	ILE	2.1
1	E	341	GLU	2.1
1	B	320	LYS	2.1
1	C	48	HIS	2.1
1	B	330	PHE	2.1
1	C	239	PHE	2.1
1	F	254	ILE	2.1
1	C	45	CYS	2.1
1	F	316	LEU	2.1
1	B	303	LYS	2.1
1	E	224	LYS	2.1
1	B	270	ARG	2.1
1	B	378	THR	2.1
1	B	126	SER	2.0
1	B	415	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	120	ASP	2.0
1	B	329	GLU	2.0
1	E	378	THR	2.0
1	D	184	GLU	2.0
1	F	169	ASP	2.0
1	E	355	ILE	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)

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, 95^{th} 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	SUC	C	1435	23/23	0.68	0.19	1.72	24,29,35,37	0
3	GLA	B	1435	11/12	0.68	0.22	1.58	41,42,42,43	0
3	SUC	B	1434	23/23	0.74	0.17	1.24	25,27,34,36	0
3	SUC	E	1434	23/23	0.82	0.13	0.26	21,25,29,30	0
3	SUC	D	1433	23/23	0.88	0.13	-0.10	16,18,22,24	0
3	SUC	F	1433	23/23	0.86	0.13	-0.34	18,20,25,26	0
3	SUC	A	1434	23/23	0.89	0.11	-0.42	17,20,25,27	0
3	GLA	D	1434	11/12	0.89	0.17	-	29,31,32,32	0
3	GLA	E	1435	11/12	0.81	0.17	-	35,36,37,38	0
3	GLA	F	1434	11/12	0.85	0.27	-	33,35,36,36	0
3	GLA	C	1436	11/12	0.72	0.27	-	43,44,45,45	0
3	GLA	A	1435	11/12	0.80	0.17	-	29,30,31,31	0

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, 95^{th} 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
4	SO4	C	1434	5/5	0.82	0.24	2.33	44,45,45,46	0
2	CIT	A	1433	13/13	0.75	0.23	1.53	50,51,51,52	0
4	SO4	C	1433	5/5	0.89	0.44	-	2,2,13,14	0
4	SO4	B	1433	5/5	0.85	0.19	-	43,44,44,45	0
4	SO4	E	1433	5/5	0.94	0.39	-	2,2,2,2	0

6.5 Other polymers

There are no such residues in this entry.