Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:17 AM EDT

PDB ID	:	6EUJ
Title	:	The GH43, Beta 1,3 Galactosidase, BT0265
Authors	:	Cartmell, A.; Gilbert, H.J.
Deposited on	:	2017-10-30
Resolution	:	2.75 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

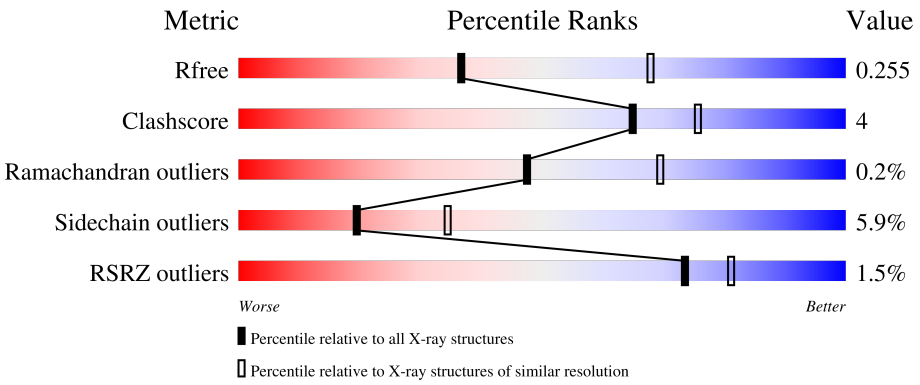
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	475	2% 86% 12% ••
1	B	475	% 88% 10% ••
1	C	475	% 89% 9% ••
1	D	475	% 86% 12% ••

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14732 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-glucanase.

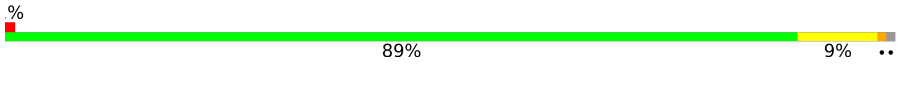
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	472	3680	2347	605	709	19	0	0	0
1	A	472	3684	2349	605	711	19	0	0	0
1	B	472	3688	2352	606	711	19	0	0	0
1	D	472	3680	2347	605	709	19	0	0	0

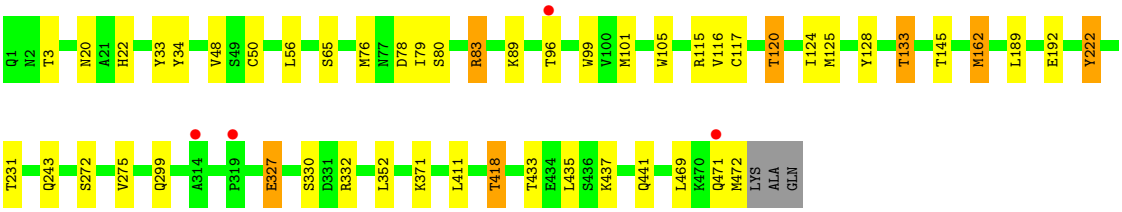
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta-glucanase

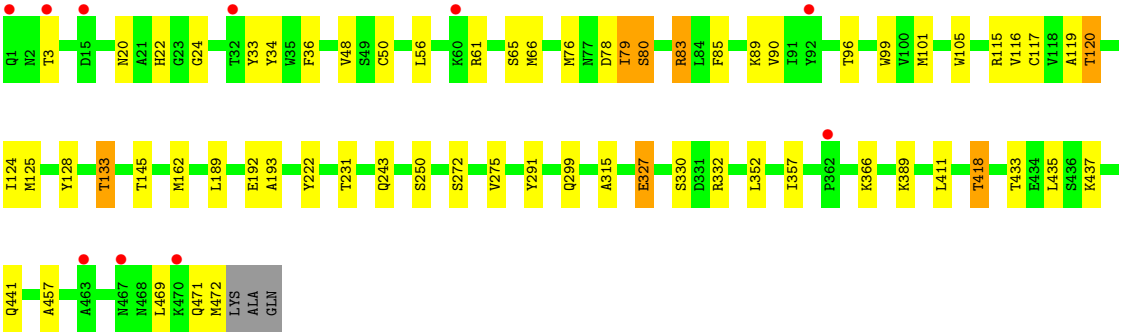
Chain C:





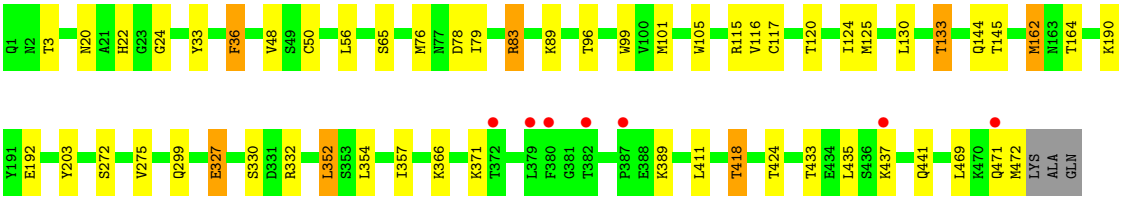
• Molecule 1: Beta-glucanase

Chain A:



• Molecule 1: Beta-glucanase

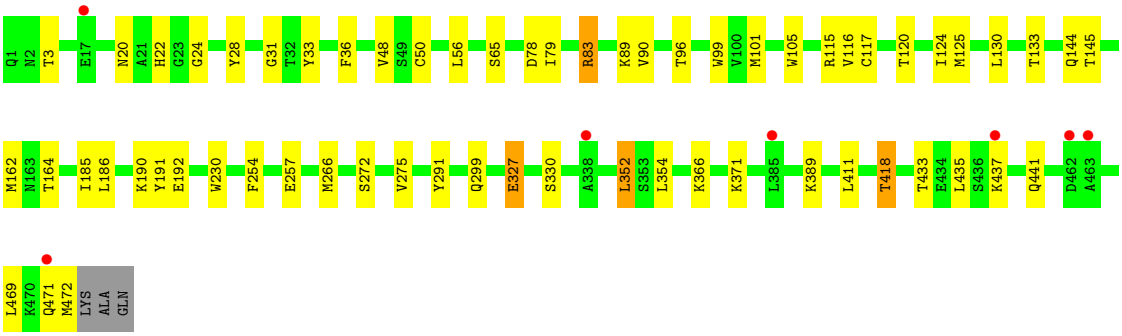
Chain B:



• Molecule 1: Beta-glucanase

Chain D:

%
86%
12%


Q1 N2 T3 E17 N20 A21 H22 G23 G24 Y28 G31 T32 Y33 F36 V48 S49 C50 L56 S65 D78 I79 R83 K89 V90 T96 W99 V100 M101 W105 R115 V116 C117 T120 I124 M125 L130 T133 Q144 T145
M162 M163 T164 I185 L186 K190 Y191 E192 W230 F254 E257 M266 S272 V275 Y291 Q299 E327 S330 A338 L352 S353 L354 K366 K371 L385 K389 L411 T418 T433 E434 L435 S436 K437 Q441 D462 A463
L469 K470 Q471 M472 LYS ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.32Å 73.33Å 116.46Å 91.04° 107.41° 99.93°	Depositor
Resolution (Å)	110.81 – 2.75 46.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (110.81-2.75) 98.3 (46.53-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.216 , 0.254 0.221 , 0.255	Depositor DCC
R_{free} test set	2886 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14732	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.58	0/3781	0.75	2/5144 (0.0%)
1	B	0.65	5/3785 (0.1%)	0.77	0/5148
1	C	0.58	0/3777	0.76	1/5139 (0.0%)
1	D	0.63	1/3777 (0.0%)	0.78	0/5139
All	All	0.61	6/15120 (0.0%)	0.77	3/20570 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	TYR	CE1-CZ	-7.68	1.28	1.38
1	B	203	TYR	CG-CD2	-6.53	1.30	1.39
1	B	36	PHE	CG-CD1	-5.62	1.30	1.38
1	B	36	PHE	CG-CD2	-5.30	1.30	1.38
1	D	291	TYR	CE1-CZ	-5.01	1.32	1.38
1	B	203	TYR	CG-CD1	-5.00	1.32	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	332	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	332	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3684	0	3364	35	0
1	B	3688	0	3375	27	0
1	C	3680	0	3360	27	0
1	D	3680	0	3360	27	0
All	All	14732	0	13459	115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASP:OD1	1:C:80:SER:OG	1.90	0.90
1:A:78:ASP:OD1	1:A:80:SER:OG	1.88	0.90
1:B:83:ARG:HD3	1:B:105:TRP:CZ2	2.17	0.79
1:D:115:ARG:HH11	1:D:133:THR:HG22	1.60	0.67
1:C:79:ILE:HD11	1:C:117:CYS:SG	2.35	0.66
1:D:48:VAL:HG21	1:D:101:MET:HE1	1.78	0.65
1:B:115:ARG:HH11	1:B:133:THR:HG22	1.62	0.64
1:A:99:TRP:CH2	1:A:124:ILE:HD12	2.33	0.63
1:D:79:ILE:HD11	1:D:117:CYS:SG	2.40	0.62
1:A:34:TYR:CE2	1:A:124:ILE:HG21	2.35	0.62
1:A:66:MET:HE3	1:A:119:ALA:HB2	1.83	0.61
1:C:222:TYR:CE1	1:C:231:THR:HB	2.36	0.60
1:C:34:TYR:CE2	1:C:124:ILE:HG21	2.37	0.60
1:A:83:ARG:HD3	1:A:105:TRP:CZ2	2.38	0.58
1:B:79:ILE:HD11	1:B:117:CYS:SG	2.43	0.58
1:A:79:ILE:HD12	1:A:85:PHE:CE1	2.40	0.56
1:C:48:VAL:HG21	1:C:101:MET:CE	2.35	0.56
1:C:34:TYR:HD2	1:C:124:ILE:HD13	1.70	0.56
1:B:20:ASN:HB2	1:B:22:HIS:NE2	2.21	0.55
1:A:222:TYR:CE2	1:A:291:TYR:HE2	2.25	0.55
1:A:115:ARG:HH11	1:A:133:THR:HG22	1.71	0.54
1:B:99:TRP:CH2	1:B:124:ILE:HD12	2.42	0.54
1:D:469:LEU:HA	1:D:472:MET:HE3	1.89	0.54
1:B:469:LEU:HA	1:B:472:MET:HE3	1.89	0.54
1:A:48:VAL:HG21	1:A:101:MET:HE1	1.91	0.53
1:A:66:MET:HE1	1:A:79:ILE:HG13	1.89	0.53
1:A:76:MET:O	1:A:133:THR:HG21	2.09	0.53
1:C:76:MET:O	1:C:133:THR:HG21	2.08	0.53
1:A:469:LEU:HA	1:A:472:MET:HE3	1.91	0.53
1:C:115:ARG:HH11	1:C:133:THR:HG22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ARG:HD3	1:D:105:TRP:CZ2	2.44	0.52
1:A:48:VAL:HG21	1:A:101:MET:CE	2.39	0.52
1:C:469:LEU:HA	1:C:472:MET:HE3	1.92	0.51
1:D:48:VAL:HG21	1:D:101:MET:CE	2.40	0.51
1:D:115:ARG:NH1	1:D:133:THR:HG22	2.24	0.51
1:A:20:ASN:HB2	1:A:22:HIS:NE2	2.26	0.51
1:B:76:MET:O	1:B:133:THR:HG21	2.11	0.50
1:C:33:TYR:CG	1:C:56:LEU:HD21	2.47	0.50
1:B:115:ARG:NH1	1:B:133:THR:HG22	2.26	0.50
1:D:186:LEU:HD13	1:D:191:TYR:CD2	2.46	0.50
1:D:366:LYS:NZ	1:D:389:LYS:O	2.44	0.49
1:C:48:VAL:HG21	1:C:101:MET:HE1	1.94	0.49
1:C:115:ARG:NH1	1:C:133:THR:HG22	2.26	0.49
1:A:34:TYR:HD2	1:A:124:ILE:HD13	1.78	0.49
1:D:418:THR:HG21	1:D:441:GLN:HE21	1.78	0.49
1:C:99:TRP:CH2	1:C:124:ILE:HD12	2.48	0.48
1:A:79:ILE:HD11	1:A:117:CYS:SG	2.53	0.48
1:C:162:MET:HG2	1:B:162:MET:HG2	1.94	0.48
1:C:20:ASN:HB2	1:C:22:HIS:NE2	2.28	0.48
1:D:28:TYR:CD2	1:D:257:GLU:HG3	2.48	0.48
1:A:120:THR:O	1:A:128:TYR:HA	2.14	0.48
1:A:222:TYR:CE1	1:A:231:THR:HB	2.49	0.48
1:A:327:GLU:HG3	1:A:330:SER:HB3	1.96	0.48
1:B:24:GLY:HA3	1:B:36:PHE:O	2.14	0.48
1:D:24:GLY:HA3	1:D:36:PHE:O	2.14	0.48
1:B:78:ASP:OD2	1:B:83:ARG:NH1	2.47	0.47
1:C:83:ARG:HD3	1:C:105:TRP:CZ2	2.48	0.47
1:B:48:VAL:HG21	1:B:101:MET:HE1	1.97	0.47
1:C:327:GLU:HG3	1:C:330:SER:HB3	1.97	0.46
1:A:418:THR:HG21	1:A:441:GLN:HE21	1.80	0.46
1:C:50:CYS:HB2	1:C:65:SER:OG	2.16	0.46
1:C:78:ASP:OD1	1:C:83:ARG:HD2	2.14	0.46
1:D:20:ASN:HB2	1:D:22:HIS:NE2	2.30	0.46
1:C:418:THR:HG21	1:C:441:GLN:HE21	1.80	0.45
1:C:33:TYR:CD2	1:C:56:LEU:HD21	2.51	0.45
1:D:79:ILE:HG12	1:D:130:LEU:HD22	1.97	0.45
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.82	0.45
1:A:24:GLY:HA3	1:A:36:PHE:O	2.17	0.45
1:A:33:TYR:CG	1:A:56:LEU:HD21	2.51	0.45
1:B:327:GLU:HG3	1:B:330:SER:HB3	1.99	0.45
1:B:418:THR:HG21	1:B:441:GLN:HE21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HB	1:A:366:LYS:HB2	1.99	0.45
1:D:50:CYS:HB2	1:D:65:SER:OG	2.17	0.45
1:A:115:ARG:NH1	1:A:133:THR:HG22	2.32	0.45
1:D:89:LYS:HG3	1:D:145:THR:HA	1.98	0.45
1:A:222:TYR:CE2	1:A:291:TYR:CE2	3.05	0.45
1:D:185:ILE:HG21	1:D:230:TRP:CD1	2.52	0.45
1:A:79:ILE:O	1:A:79:ILE:HG22	2.17	0.44
1:B:50:CYS:HB2	1:B:65:SER:OG	2.17	0.44
1:B:48:VAL:HG21	1:B:101:MET:CE	2.48	0.44
1:D:418:THR:CG2	1:D:441:GLN:HE21	2.31	0.44
1:B:33:TYR:CG	1:B:56:LEU:HD21	2.53	0.44
1:B:357:ILE:HB	1:B:366:LYS:HB2	2.00	0.44
1:B:366:LYS:NZ	1:B:389:LYS:O	2.50	0.44
1:D:352:LEU:HG	1:D:354:LEU:HD21	2.01	0.43
1:A:33:TYR:CD2	1:A:56:LEU:HD21	2.54	0.43
1:D:33:TYR:CG	1:D:56:LEU:HD21	2.54	0.43
1:D:327:GLU:HG3	1:D:330:SER:HB3	2.01	0.43
1:C:34:TYR:CD2	1:C:124:ILE:HD13	2.52	0.43
1:A:89:LYS:HG3	1:A:145:THR:HA	2.01	0.43
1:D:99:TRP:CH2	1:D:124:ILE:HD12	2.53	0.43
1:B:89:LYS:HG3	1:B:145:THR:HA	2.00	0.43
1:D:78:ASP:OD1	1:D:83:ARG:HD2	2.19	0.42
1:B:332:ARG:NH1	1:B:424:THR:O	2.52	0.42
1:D:28:TYR:OH	1:D:31:GLY:HA2	2.20	0.42
1:A:366:LYS:NZ	1:A:389:LYS:O	2.51	0.42
1:B:83:ARG:CD	1:B:105:TRP:CZ2	2.97	0.42
1:B:352:LEU:HG	1:B:354:LEU:HD21	2.01	0.41
1:D:90:VAL:HG22	1:D:101:MET:HB3	2.02	0.41
1:D:164:THR:HA	1:D:190:LYS:HG2	2.02	0.41
1:A:193:ALA:HB1	1:A:250:SER:O	2.21	0.41
1:B:164:THR:HA	1:B:190:LYS:HG2	2.02	0.41
1:B:79:ILE:HG12	1:B:130:LEU:HD22	2.03	0.41
1:A:79:ILE:O	1:A:79:ILE:CG2	2.67	0.41
1:C:79:ILE:HG22	1:C:79:ILE:O	2.20	0.41
1:C:418:THR:CG2	1:C:441:GLN:HE21	2.34	0.41
1:A:79:ILE:HA	1:A:79:ILE:HD13	1.54	0.41
1:B:418:THR:CG2	1:B:441:GLN:HE21	2.33	0.41
1:C:120:THR:O	1:C:128:TYR:HA	2.21	0.40
1:A:50:CYS:HB2	1:A:65:SER:OG	2.21	0.40
1:A:315:ALA:HA	1:A:457:ALA:HB2	2.03	0.40
1:D:254:PHE:CD1	1:D:266:MET:HE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:MET:HB3	1:C:105:TRP:CH2	2.57	0.40
1:C:89:LYS:HG3	1:C:145:THR:HA	2.03	0.40
1:A:36:PHE:CD2	1:A:90:VAL:HG21	2.57	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	470/475 (99%)	456 (97%)	14 (3%)	0	100	100
1	B	470/475 (99%)	452 (96%)	17 (4%)	1 (0%)	47	69
1	C	470/475 (99%)	451 (96%)	18 (4%)	1 (0%)	47	69
1	D	470/475 (99%)	453 (96%)	16 (3%)	1 (0%)	47	69
All	All	1880/1900 (99%)	1812 (96%)	65 (4%)	3 (0%)	47	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	LYS
1	C	371	LYS
1	D	371	LYS

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	371/417 (89%)	347 (94%)	24 (6%)	17	30
1	B	372/417 (89%)	351 (94%)	21 (6%)	21	36
1	C	370/417 (89%)	347 (94%)	23 (6%)	18	32
1	D	370/417 (89%)	350 (95%)	20 (5%)	22	38
All	All	1483/1668 (89%)	1395 (94%)	88 (6%)	19	34

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	THR
1	C	83	ARG
1	C	96	THR
1	C	116	VAL
1	C	120	THR
1	C	125	MET
1	C	133	THR
1	C	162	MET
1	C	189	LEU
1	C	192	GLU
1	C	222	TYR
1	C	243	GLN
1	C	272	SER
1	C	275	VAL
1	C	299	GLN
1	C	327	GLU
1	C	352	LEU
1	C	411	LEU
1	C	418	THR
1	C	433	THR
1	C	435	LEU
1	C	437	LYS
1	C	471	GLN
1	A	3	THR
1	A	79	ILE
1	A	80	SER
1	A	83	ARG
1	A	96	THR
1	A	116	VAL
1	A	120	THR
1	A	125	MET
1	A	133	THR
1	A	162	MET

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Mol	Chain	Res	Type
1	A	189	LEU
1	A	192	GLU
1	A	243	GLN
1	A	272	SER
1	A	275	VAL
1	A	299	GLN
1	A	327	GLU
1	A	352	LEU
1	A	411	LEU
1	A	418	THR
1	A	433	THR
1	A	435	LEU
1	A	437	LYS
1	A	471	GLN
1	B	3	THR
1	B	83	ARG
1	B	96	THR
1	B	116	VAL
1	B	120	THR
1	B	125	MET
1	B	133	THR
1	B	144	GLN
1	B	162	MET
1	B	192	GLU
1	B	272	SER
1	B	275	VAL
1	B	299	GLN
1	B	327	GLU
1	B	352	LEU
1	B	411	LEU
1	B	418	THR
1	B	433	THR
1	B	435	LEU
1	B	437	LYS
1	B	471	GLN
1	D	3	THR
1	D	83	ARG
1	D	96	THR
1	D	116	VAL
1	D	120	THR
1	D	125	MET
1	D	144	GLN

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Mol	Chain	Res	Type
1	D	162	MET
1	D	192	GLU
1	D	272	SER
1	D	275	VAL
1	D	299	GLN
1	D	327	GLU
1	D	352	LEU
1	D	411	LEU
1	D	418	THR
1	D	433	THR
1	D	435	LEU
1	D	437	LYS
1	D	471	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	ASN
1	C	81	GLN
1	A	52	GLN
1	D	52	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	472/475 (99%)	0.20	10 (2%)	63	72	20, 34, 52, 60	0
1	B	472/475 (99%)	0.11	7 (1%)	73	81	17, 29, 44, 60	0
1	C	472/475 (99%)	0.13	4 (0%)	86	90	18, 32, 45, 53	0
1	D	472/475 (99%)	-0.01	7 (1%)	73	81	13, 24, 40, 57	0
All	All	1888/1900 (99%)	0.11	28 (1%)	73	81	13, 30, 47, 60	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	471	GLN	3.5
1	A	3	THR	3.4
1	B	387	PRO	3.3
1	D	463	ALA	3.0
1	A	32	THR	2.9
1	B	471	GLN	2.7
1	A	362	PRO	2.7
1	A	467	ASN	2.6
1	D	437	LYS	2.5
1	C	319	PRO	2.4
1	A	15	ASP	2.4
1	A	92	TYR	2.4
1	A	463	ALA	2.3
1	B	382	THR	2.3
1	B	380	PHE	2.3
1	D	385	LEU	2.2
1	D	338	ALA	2.2
1	B	372	THR	2.2
1	A	1	GLN	2.2
1	D	462	ASP	2.2
1	B	379	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	96	THR	2.1
1	A	60	LYS	2.1
1	D	471	GLN	2.1
1	A	470	LYS	2.0
1	B	437	LYS	2.0
1	D	17	GLU	2.0
1	C	314	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.