Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:25 AM GMT

PDB ID	:	3APG
Title	:	Crystal structure of hyperthermophilic beta-glucosidase from pyrococcus furiosus
Authors	:	Kado, Y.; Inoue, T.; Ishikawa, K.
Deposited on	:	2010-10-15
Resolution	:	2.35 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:

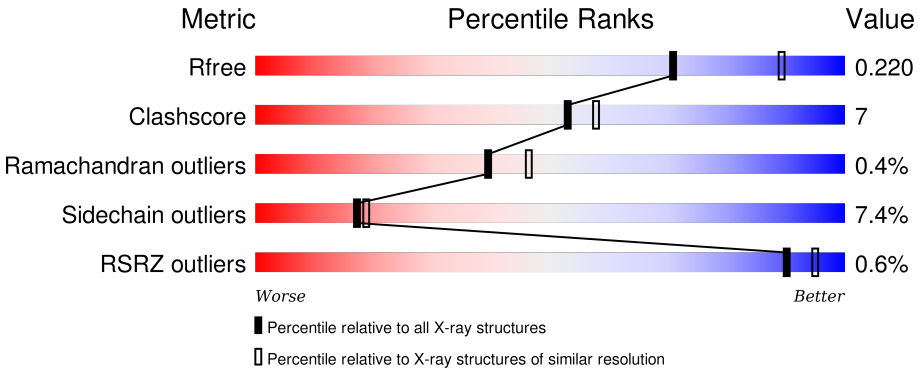
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	473	79% 17%
1	B	473	% 77% 19%
1	C	473	81% 16%
1	D	473	% 81% 17%

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	GOL	A	473	-	-	-	X
2	GOL	B	473	-	-	-	X
2	GOL	B	474	-	-	X	-
2	GOL	D	473	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15832 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.

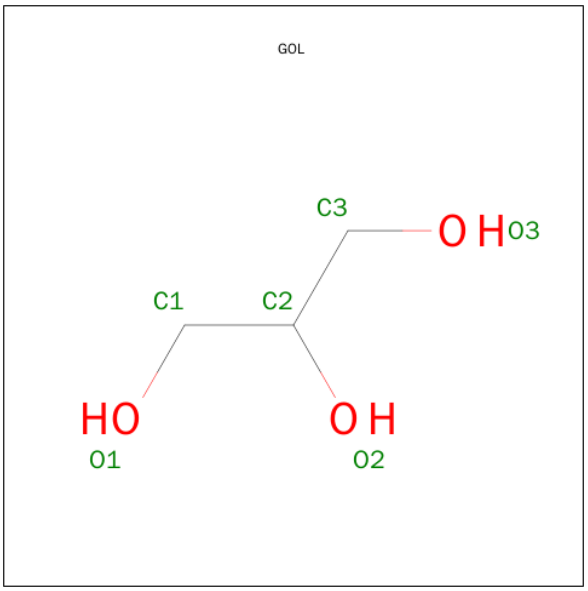
- Molecule 1 is a protein called Beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3861	2512	635	701	13			
1	B	471	Total	C	N	O	S	0	0	0
			3861	2512	635	701	13			
1	C	471	Total	C	N	O	S	0	0	0
			3861	2512	635	701	13			
1	D	471	Total	C	N	O	S	0	0	0
			3861	2512	635	701	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q51723
A	1	ALA	-	EXPRESSION TAG	UNP Q51723
B	0	MET	-	EXPRESSION TAG	UNP Q51723
B	1	ALA	-	EXPRESSION TAG	UNP Q51723
C	0	MET	-	EXPRESSION TAG	UNP Q51723
C	1	ALA	-	EXPRESSION TAG	UNP Q51723
D	0	MET	-	EXPRESSION TAG	UNP Q51723
D	1	ALA	-	EXPRESSION TAG	UNP Q51723

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

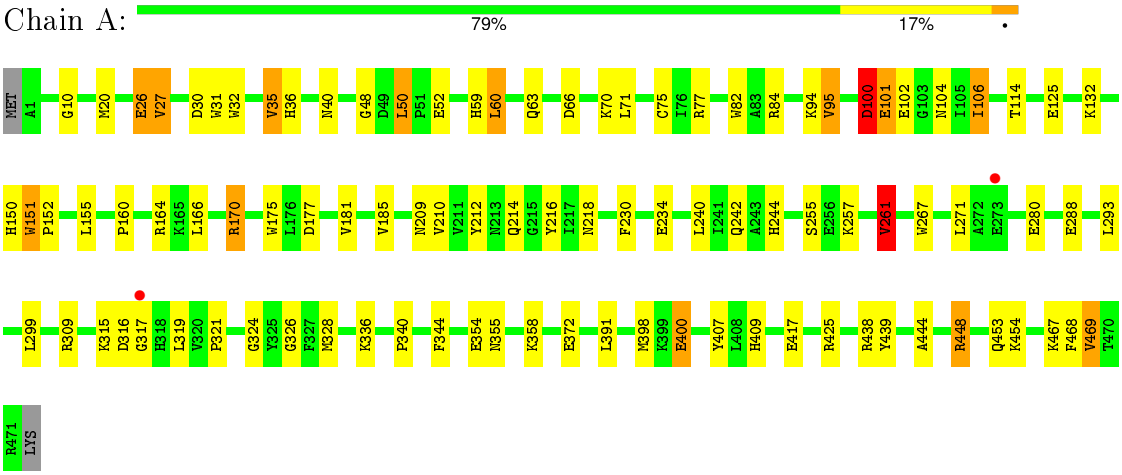
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	84	Total O 84 84	0	0
3	B	106	Total O 106 106	0	0
3	C	76	Total O 76 76	0	0
3	D	92	Total O 92 92	0	0

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.

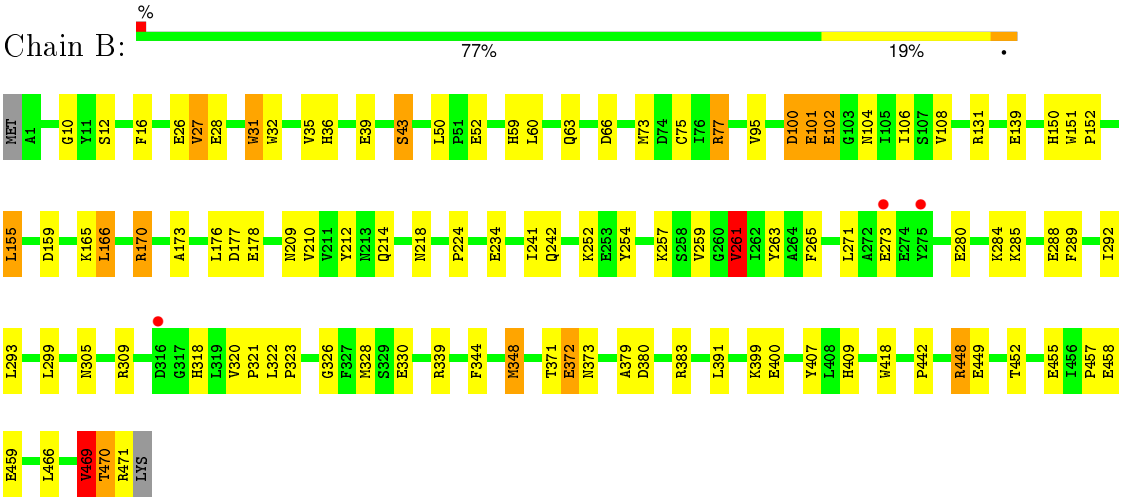
- Molecule 1: Beta-glucosidase

Chain A:



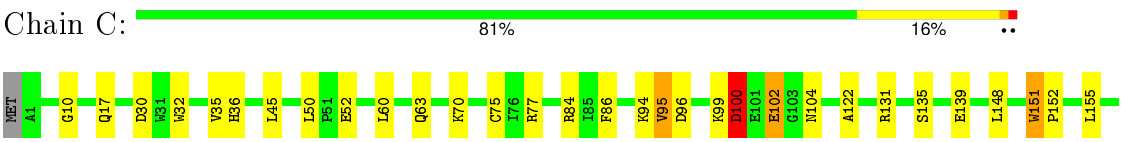
- Molecule 1: Beta-glucosidase

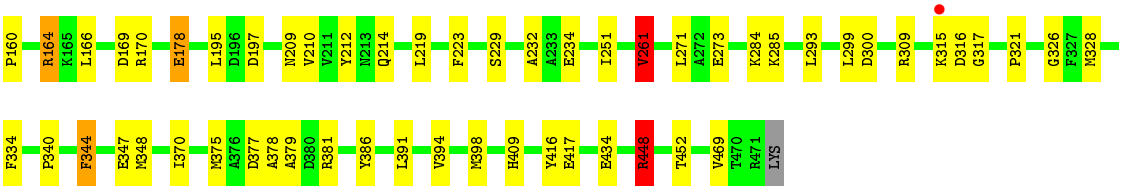
Chain B:



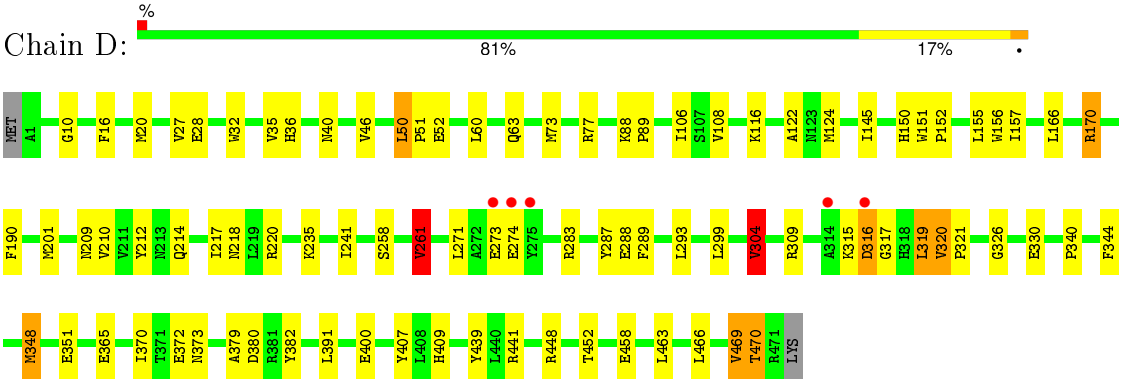
- Molecule 1: Beta-glucosidase

Chain C:





- Molecule 1: Beta-glucosidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.96Å 141.96Å 343.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.35 49.66 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.66-2.35) 97.6 (49.66-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.223 0.177 , 0.220	Depositor DCC
R_{free} test set	7130 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 30.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 141852 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: GOL

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	1.13	12/3984 (0.3%)	0.97	13/5404 (0.2%)
1	B	1.12	11/3984 (0.3%)	0.99	13/5404 (0.2%)
1	C	1.14	10/3984 (0.3%)	0.95	11/5404 (0.2%)
1	D	1.08	2/3984 (0.1%)	0.93	4/5404 (0.1%)
All	All	1.12	35/15936 (0.2%)	0.96	41/21616 (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	A	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	GLU	CG-CD	12.98	1.71	1.51
1	C	234	GLU	CG-CD	9.50	1.66	1.51
1	C	178	GLU	CD-OE1	7.53	1.33	1.25
1	B	139	GLU	CG-CD	7.49	1.63	1.51
1	C	386	TYR	CD1-CE1	-6.65	1.29	1.39
1	A	125	GLU	CD-OE1	6.25	1.32	1.25
1	A	234	GLU	CG-CD	6.18	1.61	1.51
1	A	125	GLU	CG-CD	5.96	1.60	1.51
1	B	178	GLU	CG-CD	5.92	1.60	1.51
1	C	234	GLU	CD-OE1	5.89	1.32	1.25
1	B	254	TYR	CD1-CE1	5.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	GLU	CG-CD	5.83	1.60	1.51
1	B	31	TRP	CE3-CZ3	5.76	1.48	1.38
1	A	101	GLU	CG-CD	5.68	1.60	1.51
1	A	280	GLU	CG-CD	5.66	1.60	1.51
1	A	439	TYR	CD1-CE1	5.65	1.47	1.39
1	D	304	VAL	CB-CG1	-5.64	1.41	1.52
1	B	139	GLU	CD-OE2	5.63	1.31	1.25
1	A	82	TRP	CB-CG	5.60	1.60	1.50
1	C	273	GLU	CG-CD	5.51	1.60	1.51
1	A	444	ALA	CA-CB	-5.51	1.40	1.52
1	A	125	GLU	CD-OE2	5.49	1.31	1.25
1	C	334	PHE	CE2-CZ	5.45	1.47	1.37
1	B	28	GLU	CB-CG	5.44	1.62	1.52
1	C	223	PHE	CE1-CZ	5.43	1.47	1.37
1	A	288	GLU	CG-CD	5.37	1.60	1.51
1	C	178	GLU	CB-CG	5.35	1.62	1.52
1	A	216	TYR	CD2-CE2	5.33	1.47	1.39
1	B	234	GLU	CG-CD	5.31	1.59	1.51
1	B	418	TRP	CB-CG	5.31	1.59	1.50
1	C	344	PHE	CD1-CE1	5.29	1.49	1.39
1	B	372	GLU	CB-CG	-5.28	1.42	1.52
1	A	425	ARG	CZ-NH1	5.16	1.39	1.33
1	D	365	GLU	CG-CD	5.12	1.59	1.51
1	B	469	VAL	CB-CG2	-5.12	1.42	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C	448	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	448	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C	261	VAL	CB-CA-C	-7.99	96.22	111.40
1	A	261	VAL	CB-CA-C	-7.96	96.28	111.40
1	B	261	VAL	CB-CA-C	-7.70	96.77	111.40
1	A	177	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	155	LEU	CB-CG-CD1	-6.84	99.38	111.00
1	D	170	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	381	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	C	164	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	B	170	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	448	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	170	ARG	NE-CZ-NH1	6.41	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	261	VAL	CB-CA-C	-6.40	99.24	111.40
1	B	348	MET	CG-SD-CE	-6.30	90.11	100.20
1	C	52	GLU	CB-CA-C	-6.29	97.83	110.40
1	B	27	VAL	CB-CA-C	-6.23	99.57	111.40
1	C	448	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	166	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	71	LEU	CB-CG-CD1	-6.17	100.51	111.00
1	B	66	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	438	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	100	ASP	CB-CA-C	-6.05	98.31	110.40
1	C	300	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	261	VAL	CG1-CB-CG2	5.92	120.37	110.90
1	C	317	GLY	N-CA-C	-5.92	98.30	113.10
1	A	35	VAL	CG1-CB-CG2	5.88	120.31	110.90
1	C	100	ASP	CB-CA-C	-5.76	98.87	110.40
1	C	300	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	D	319	LEU	CB-CG-CD2	5.59	120.51	111.00
1	C	45	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	66	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	B	159	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	155	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	383	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	339	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	448	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	60	LEU	CB-CG-CD1	5.12	119.71	111.00
1	A	448	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	170	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	ASP	Peptide
1	C	316	ASP	Peptide
1	C	99	LYS	Peptide
1	D	315	LYS	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	3861	0	3715	62	0
1	B	3861	0	3715	60	0
1	C	3861	0	3715	37	0
1	D	3861	0	3715	53	0
2	A	6	0	8	1	0
2	B	12	0	16	4	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
3	A	84	0	0	2	0
3	B	106	0	0	3	0
3	C	76	0	0	2	0
3	D	92	0	0	2	0
All	All	15832	0	14900	200	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 7.

All (200) 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:D:316:ASP:HB2	1:D:317:GLY:CA	1.75	1.17
1:B:348:MET:HE1	1:B:466:LEU:HD22	1.27	1.14
1:D:316:ASP:HB2	1:D:317:GLY:HA3	1.15	1.09
1:B:348:MET:CE	1:B:466:LEU:HD22	1.90	1.01
1:D:316:ASP:CB	1:D:317:GLY:HA3	1.97	0.95
1:D:261:VAL:HG22	1:D:299:LEU:HD21	1.51	0.91
1:A:104:ASN:HD22	1:A:242:GLN:HE22	1.17	0.88
1:A:20:MET:CE	1:A:27:VAL:H	1.88	0.87
1:B:466:LEU:O	1:B:470:THR:HG23	1.74	0.86
1:C:261:VAL:HG22	1:C:299:LEU:HD21	1.59	0.85
1:D:32:TRP:O	1:D:36:HIS:HD2	1.61	0.82
1:D:122:ALA:HB3	1:D:124:MET:HE3	1.59	0.82
1:B:131:ARG:HE	2:B:474:GOL:H12	1.42	0.82
1:A:372:GLU:OE1	2:A:473:GOL:H11	1.81	0.80
1:A:340:PRO:HG2	1:A:469:VAL:HG13	1.62	0.80
1:A:261:VAL:HG22	1:A:299:LEU:HD21	1.64	0.78
1:C:100:ASP:HB3	1:C:102:GLU:H	1.51	0.76
1:D:124:MET:HE1	1:D:190:PHE:HZ	1.52	0.75
1:A:20:MET:CE	1:A:26:GLU:HA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TRP:O	1:A:36:HIS:HD2	1.70	0.74
1:D:122:ALA:HB3	1:D:124:MET:CE	2.18	0.73
1:B:348:MET:CE	1:B:466:LEU:CD2	2.66	0.73
1:A:100:ASP:HB3	1:A:102:GLU:H	1.52	0.72
1:B:373:ASN:ND2	1:B:407:TYR:OH	2.20	0.72
1:A:104:ASN:ND2	1:A:242:GLN:HE22	1.88	0.72
1:D:288:GLU:HB3	3:D:480:HOH:O	1.89	0.71
1:B:32:TRP:O	1:B:36:HIS:HD2	1.74	0.70
1:A:340:PRO:CG	1:A:469:VAL:HG13	2.22	0.68
1:A:59:HIS:HB3	3:A:511:HOH:O	1.94	0.68
1:D:124:MET:CE	1:D:190:PHE:HZ	2.05	0.68
1:C:100:ASP:OD2	1:C:104:ASN:HB2	1.94	0.68
1:A:20:MET:HE1	1:A:26:GLU:HA	1.74	0.68
1:C:409:HIS:HE1	3:C:475:HOH:O	1.75	0.67
1:D:124:MET:HE1	1:D:190:PHE:CZ	2.30	0.66
1:A:20:MET:HE1	1:A:27:VAL:H	1.59	0.66
1:B:348:MET:HE1	1:B:466:LEU:CD2	2.17	0.65
1:C:30:ASP:HB2	1:C:160:PRO:HD3	1.78	0.65
1:B:471:ARG:HH11	1:B:471:ARG:CG	2.11	0.64
1:B:39:GLU:O	1:B:43:SER:HB3	1.97	0.63
1:D:316:ASP:CB	1:D:317:GLY:CA	2.62	0.63
1:B:261:VAL:HG22	1:B:299:LEU:HD21	1.79	0.63
1:D:372:GLU:OE1	2:D:473:GOL:H11	1.99	0.62
1:D:466:LEU:O	1:D:470:THR:CG2	2.47	0.62
1:A:170:ARG:HD2	1:B:170:ARG:CZ	2.29	0.62
1:B:131:ARG:NE	2:B:474:GOL:H12	2.13	0.61
1:C:340:PRO:HG2	1:C:348:MET:HE3	1.83	0.61
1:D:466:LEU:O	1:D:470:THR:HG23	2.01	0.60
1:A:36:HIS:HE1	1:A:52:GLU:OE1	1.85	0.59
1:B:104:ASN:HD22	1:B:242:GLN:HE22	1.49	0.59
1:C:32:TRP:O	1:C:36:HIS:HD2	1.84	0.59
1:B:409:HIS:HE1	3:B:475:HOH:O	1.85	0.58
1:B:36:HIS:HE1	1:B:52:GLU:OE2	1.86	0.58
1:B:131:ARG:HE	2:B:474:GOL:H31	1.67	0.58
1:B:466:LEU:O	1:B:470:THR:CG2	2.49	0.58
1:A:210:VAL:HG13	1:A:214:GLN:HG3	1.85	0.57
1:B:263:TYR:HB3	1:B:265:PHE:CE2	2.40	0.57
1:D:32:TRP:O	1:D:36:HIS:CD2	2.52	0.57
1:B:469:VAL:HG23	1:D:379:ALA:HB1	1.86	0.57
1:C:131:ARG:O	1:C:135:SER:HB2	2.05	0.57
1:C:409:HIS:CE1	3:C:475:HOH:O	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HH11	1:B:471:ARG:HG3	1.71	0.55
1:D:380:ASP:HB2	1:D:441:ARG:HD3	1.88	0.55
1:D:10:GLY:HA2	1:D:73:MET:HG2	1.88	0.55
1:C:10:GLY:HA3	1:C:75:CYS:O	2.07	0.55
1:B:409:HIS:CE1	3:B:475:HOH:O	2.60	0.55
1:A:104:ASN:HD22	1:A:242:GLN:NE2	1.95	0.55
1:B:252:LYS:HE2	1:B:259:VAL:HG23	1.88	0.54
1:A:151:TRP:N	1:A:151:TRP:CD1	2.74	0.54
1:A:354:GLU:HG2	1:A:358:LYS:HE3	1.90	0.54
1:C:151:TRP:HB2	1:C:152:PRO:HD3	1.90	0.54
1:A:20:MET:HE2	1:A:26:GLU:HA	1.89	0.53
1:C:309:ARG:O	1:C:326:GLY:HA3	2.07	0.53
1:D:261:VAL:HG22	1:D:299:LEU:CD2	2.32	0.53
1:A:32:TRP:O	1:A:36:HIS:CD2	2.57	0.53
1:A:214:GLN:HE22	1:A:218:ASN:HD22	1.55	0.52
1:A:27:VAL:HG11	1:A:84:ARG:HG2	1.92	0.52
1:A:309:ARG:O	1:A:326:GLY:HA3	2.10	0.52
1:D:16:PHE:HB2	1:D:152:PRO:HG2	1.91	0.52
1:A:453:GLN:O	1:A:454:LYS:HB2	2.10	0.52
1:D:150:HIS:O	1:D:152:PRO:HD3	2.10	0.52
1:B:261:VAL:HG22	1:B:299:LEU:CD2	2.39	0.52
1:C:394:VAL:O	1:C:398:MET:HG3	2.09	0.52
1:D:309:ARG:O	1:D:326:GLY:HA3	2.10	0.52
1:B:214:GLN:HE22	1:B:218:ASN:HD22	1.58	0.51
1:C:370:ILE:N	1:C:370:ILE:HD13	2.26	0.51
1:A:469:VAL:HG23	1:C:379:ALA:HB1	1.92	0.50
1:D:156:TRP:CE3	1:D:157:ILE:HG12	2.46	0.50
1:A:70:LYS:O	1:A:448:ARG:HD2	2.12	0.50
1:A:20:MET:CE	1:A:27:VAL:N	2.67	0.50
1:A:209:ASN:HA	1:A:212:TYR:CZ	2.47	0.50
1:C:100:ASP:HB3	1:C:102:GLU:N	2.25	0.50
1:D:316:ASP:HB2	1:D:317:GLY:HA2	1.83	0.49
1:B:16:PHE:HB2	1:B:152:PRO:HG2	1.94	0.49
1:A:100:ASP:HB3	1:A:102:GLU:N	2.25	0.49
1:C:229:SER:HB3	1:C:232:ALA:HB3	1.93	0.49
1:C:131:ARG:O	1:C:135:SER:CB	2.61	0.49
1:D:407:TYR:OH	1:D:409:HIS:HD2	1.96	0.49
1:B:321:PRO:HB2	1:B:328:MET:SD	2.53	0.48
1:A:59:HIS:HD2	3:A:474:HOH:O	1.96	0.48
1:A:48:GLY:O	1:A:50:LEU:HD13	2.14	0.48
1:A:175:TRP:CE2	1:A:240:LEU:HD21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:VAL:HG22	1:D:321:PRO:HD2	1.96	0.48
1:B:210:VAL:HG13	1:B:214:GLN:HG3	1.96	0.48
1:A:40:ASN:OD1	1:A:164:ARG:NH1	2.45	0.48
1:A:95:VAL:HG23	1:A:114:THR:HG21	1.96	0.47
1:C:326:GLY:HA2	1:C:347:GLU:HB3	1.96	0.47
1:D:36:HIS:HE1	1:D:52:GLU:OE1	1.98	0.47
1:C:135:SER:O	1:C:139:GLU:HB2	2.14	0.47
1:C:148:LEU:HD11	1:C:251:ILE:HD11	1.97	0.47
1:D:439:TYR:N	1:D:439:TYR:CD2	2.82	0.47
1:B:32:TRP:O	1:B:36:HIS:CD2	2.63	0.47
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.66	0.47
1:C:448:ARG:O	1:C:452:THR:HG23	2.15	0.47
1:C:417:GLU:O	1:C:417:GLU:HG3	2.15	0.46
1:A:324:GLY:HA3	1:A:336:LYS:HE2	1.97	0.46
1:B:348:MET:HE3	1:B:466:LEU:CD2	2.45	0.46
1:A:170:ARG:CZ	1:B:170:ARG:HD2	2.45	0.46
1:B:101:GLU:HA	1:B:101:GLU:OE2	2.14	0.46
1:D:448:ARG:O	1:D:452:THR:HG23	2.16	0.45
1:A:255:SER:HG	1:A:257:LYS:HG3	1.82	0.45
1:C:170:ARG:CZ	1:D:170:ARG:HD2	2.47	0.45
1:C:170:ARG:HD2	1:D:170:ARG:CZ	2.47	0.45
1:A:150:HIS:O	1:A:152:PRO:HD3	2.17	0.45
1:D:340:PRO:HG2	1:D:348:MET:HE3	1.99	0.45
1:A:468:PHE:CD1	1:C:378:ALA:HB1	2.51	0.44
1:D:150:HIS:HD2	3:D:519:HOH:O	2.00	0.44
1:B:150:HIS:O	1:B:152:PRO:HD3	2.18	0.44
1:B:209:ASN:HA	1:B:212:TYR:CE2	2.53	0.44
1:C:210:VAL:HG13	1:C:214:GLN:HG3	1.98	0.44
1:D:88:LYS:HB3	1:D:89:PRO:HD2	1.99	0.44
1:D:373:ASN:ND2	1:D:407:TYR:OH	2.38	0.44
1:D:209:ASN:HA	1:D:212:TYR:CZ	2.53	0.44
1:D:20:MET:HB3	1:D:52:GLU:HA	2.00	0.44
1:B:10:GLY:HA2	1:B:73:MET:HG2	1.99	0.44
1:B:131:ARG:HE	2:B:474:GOL:C1	2.22	0.44
1:A:10:GLY:HA3	1:A:75:CYS:O	2.17	0.44
1:D:210:VAL:HG13	1:D:214:GLN:HG3	1.99	0.44
1:A:255:SER:OG	1:A:257:LYS:HG3	2.17	0.44
1:B:77:ARG:NH2	1:B:372:GLU:HG3	2.33	0.44
1:C:321:PRO:HB2	1:C:328:MET:SD	2.58	0.44
1:A:209:ASN:HA	1:A:212:TYR:CE2	2.53	0.44
1:A:50:LEU:HB3	1:A:52:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:MET:CE	1:D:382:TYR:HB3	2.48	0.43
1:D:241:ILE:HG13	1:D:289:PHE:CE1	2.53	0.43
1:B:100:ASP:HB3	1:B:102:GLU:N	2.34	0.43
1:B:209:ASN:HA	1:B:212:TYR:CZ	2.53	0.43
1:B:12:SER:HA	1:B:77:ARG:O	2.19	0.43
1:A:417:GLU:O	1:A:417:GLU:HG3	2.18	0.43
1:A:321:PRO:HB2	1:A:328:MET:SD	2.58	0.43
1:A:267:TRP:CZ2	1:A:355:ASN:HB3	2.54	0.43
1:A:398:MET:C	1:A:400:GLU:N	2.72	0.43
1:A:170:ARG:HD2	1:B:170:ARG:NH1	2.33	0.43
1:B:288:GLU:HG3	1:B:292:ILE:CD1	2.48	0.43
1:A:398:MET:C	1:A:400:GLU:H	2.21	0.43
1:B:100:ASP:HB2	1:B:104:ASN:H	1.84	0.43
1:B:173:ALA:HB3	1:B:177:ASP:OD1	2.18	0.43
1:A:407:TYR:OH	1:A:409:HIS:HD2	2.02	0.43
1:B:59:HIS:HD2	3:B:520:HOH:O	2.01	0.43
1:A:209:ASN:N	1:A:209:ASN:OD1	2.52	0.43
1:A:230:PHE:CE2	1:B:39:GLU:HG2	2.54	0.42
1:C:131:ARG:NH2	1:C:197:ASP:OD2	2.44	0.42
1:C:375:MET:HG3	1:C:377:ASP:HB2	2.01	0.42
1:B:31:TRP:CZ2	1:B:224:PRO:HD2	2.54	0.42
1:A:26:GLU:HG2	1:A:26:GLU:H	1.27	0.42
1:A:30:ASP:OD1	1:A:31:TRP:N	2.52	0.42
1:B:10:GLY:HA2	1:B:73:MET:CG	2.49	0.42
1:A:150:HIS:O	1:A:151:TRP:HB2	2.20	0.42
1:B:10:GLY:HA3	1:B:75:CYS:O	2.20	0.42
1:C:209:ASN:HA	1:C:212:TYR:CZ	2.55	0.42
1:D:36:HIS:CE1	1:D:50:LEU:HG	2.55	0.42
1:C:70:LYS:O	1:C:448:ARG:CD	2.68	0.42
1:C:169:ASP:OD1	1:D:170:ARG:NH2	2.53	0.42
1:A:20:MET:HB3	1:A:52:GLU:HA	2.02	0.42
1:C:86:PHE:CE1	1:C:122:ALA:HB2	2.55	0.42
1:D:348:MET:HE1	1:D:382:TYR:HB3	2.02	0.41
1:A:244:HIS:CD2	1:A:244:HIS:C	2.93	0.41
1:C:164:ARG:HB3	1:C:164:ARG:HE	1.66	0.41
1:D:16:PHE:CZ	1:D:51:PRO:HG3	2.55	0.41
1:B:379:ALA:HB1	1:D:469:VAL:HG23	2.02	0.41
1:B:241:ILE:HG13	1:B:289:PHE:CE1	2.55	0.41
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.91	0.41
1:B:442:PRO:HD3	1:D:463:LEU:HD21	2.03	0.41
1:D:340:PRO:CD	1:D:469:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ARG:O	1:B:452:THR:HG23	2.20	0.41
1:B:455:GLU:O	1:B:457:PRO:HD3	2.20	0.41
1:B:348:MET:CE	1:B:466:LEU:HD13	2.51	0.41
1:A:30:ASP:HB2	1:A:160:PRO:HD3	2.03	0.41
1:D:283:ARG:HG3	1:D:287:TYR:CE1	2.56	0.41
1:D:304:VAL:HG13	1:D:370:ILE:HA	2.02	0.41
1:A:181:VAL:O	1:A:185:VAL:HG23	2.21	0.41
1:C:17:GLN:HG2	1:C:416:TYR:O	2.21	0.41
1:B:305:ASN:CG	1:B:372:GLU:HB2	2.41	0.40
1:C:95:VAL:HG13	1:C:96:ASP:N	2.36	0.40
1:B:173:ALA:HB1	1:B:176:LEU:HB2	2.02	0.40
1:D:40:ASN:HB3	1:D:46:VAL:HG22	2.03	0.40
1:A:104:ASN:HA	1:A:242:GLN:OE1	2.21	0.40
1:B:309:ARG:O	1:B:326:GLY:HA3	2.21	0.40
1:B:322:LEU:HA	1:B:323:PRO:HD3	1.97	0.40
1:D:145:ILE:HG12	1:D:201:MET:HB2	2.03	0.40
1:B:449:GLU:OE2	1:B:459:GLU:OE2	2.40	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	469/473 (99%)	446 (95%)	20 (4%)	3 (1%)	30	34
1	B	469/473 (99%)	453 (97%)	14 (3%)	2 (0%)	39	46
1	C	469/473 (99%)	449 (96%)	18 (4%)	2 (0%)	39	46
1	D	469/473 (99%)	457 (97%)	11 (2%)	1 (0%)	52	63
All	All	1876/1892 (99%)	1805 (96%)	63 (3%)	8 (0%)	39	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	151	TRP
1	B	100	ASP
1	B	151	TRP
1	C	151	TRP
1	D	151	TRP
1	A	317	GLY
1	C	100	ASP

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	399/401 (100%)	376 (94%)	23 (6%)	25 29
1	B	399/401 (100%)	363 (91%)	36 (9%)	12 12
1	C	399/401 (100%)	374 (94%)	25 (6%)	22 25
1	D	399/401 (100%)	365 (92%)	34 (8%)	13 14
All	All	1596/1604 (100%)	1478 (93%)	118 (7%)	17 19

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	27	VAL
1	A	35	VAL
1	A	50	LEU
1	A	60	LEU
1	A	63	GLN
1	A	77	ARG
1	A	94	LYS
1	A	95	VAL
1	A	101	GLU
1	A	106	ILE
1	A	132	LYS
1	A	166	LEU
1	A	261	VAL

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	293	LEU
1	A	315	LYS
1	A	319	LEU
1	A	344	PHE
1	A	391	LEU
1	A	400	GLU
1	A	467	LYS
1	A	469	VAL
1	B	26	GLU
1	B	27	VAL
1	B	35	VAL
1	B	43	SER
1	B	50	LEU
1	B	60	LEU
1	B	63	GLN
1	B	77	ARG
1	B	95	VAL
1	B	101	GLU
1	B	102	GLU
1	B	106	ILE
1	B	108	VAL
1	B	155	LEU
1	B	165	LYS
1	B	166	LEU
1	B	257	LYS
1	B	261	VAL
1	B	271	LEU
1	B	273	GLU
1	B	280	GLU
1	B	284	LYS
1	B	285	LYS
1	B	293	LEU
1	B	318	HIS
1	B	320	VAL
1	B	330	GLU
1	B	344	PHE
1	B	371	THR
1	B	380	ASP
1	B	391	LEU
1	B	399	LYS
1	B	400	GLU

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Mol	Chain	Res	Type
1	B	458	GLU
1	B	469	VAL
1	B	470	THR
1	C	35	VAL
1	C	50	LEU
1	C	60	LEU
1	C	63	GLN
1	C	77	ARG
1	C	84	ARG
1	C	94	LYS
1	C	95	VAL
1	C	102	GLU
1	C	155	LEU
1	C	166	LEU
1	C	178	GLU
1	C	195	LEU
1	C	219	LEU
1	C	261	VAL
1	C	271	LEU
1	C	284	LYS
1	C	285	LYS
1	C	293	LEU
1	C	315	LYS
1	C	344	PHE
1	C	391	LEU
1	C	434	GLU
1	C	448	ARG
1	C	469	VAL
1	D	27	VAL
1	D	28	GLU
1	D	35	VAL
1	D	50	LEU
1	D	60	LEU
1	D	63	GLN
1	D	77	ARG
1	D	106	ILE
1	D	108	VAL
1	D	116	LYS
1	D	166	LEU
1	D	217	ILE
1	D	218	ASN
1	D	220	ARG

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Mol	Chain	Res	Type
1	D	235	LYS
1	D	258	SER
1	D	261	VAL
1	D	271	LEU
1	D	273	GLU
1	D	274	GLU
1	D	293	LEU
1	D	304	VAL
1	D	316	ASP
1	D	319	LEU
1	D	320	VAL
1	D	330	GLU
1	D	344	PHE
1	D	348	MET
1	D	351	GLU
1	D	391	LEU
1	D	400	GLU
1	D	458	GLU
1	D	469	VAL
1	D	470	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	59	HIS
1	A	63	GLN
1	A	104	ASN
1	A	213	ASN
1	A	214	GLN
1	A	268	HIS
1	A	409	HIS
1	A	453	GLN
1	B	36	HIS
1	B	59	HIS
1	B	104	ASN
1	B	150	HIS
1	B	214	GLN
1	B	373	ASN
1	B	409	HIS
1	C	36	HIS
1	C	213	ASN

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Mol	Chain	Res	Type
1	C	214	GLN
1	C	268	HIS
1	C	409	HIS
1	C	453	GLN
1	D	36	HIS
1	D	150	HIS
1	D	213	ASN
1	D	214	GLN
1	D	218	ASN
1	D	409	HIS

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

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	GOL	A	473	-	5,5,5	0.35	0	5,5,5	0.76	0
2	GOL	B	473	-	5,5,5	0.29	0	5,5,5	1.43	1 (20%)
2	GOL	B	474	-	5,5,5	0.37	0	5,5,5	1.07	0
2	GOL	C	473	-	5,5,5	0.26	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	D	473	-	5,5,5	0.28	0	5,5,5	1.16	1 (20%)

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	GOL	A	473	-	-	0/4/4/4	0/0/0/0
2	GOL	B	473	-	-	0/4/4/4	0/0/0/0
2	GOL	B	474	-	-	0/4/4/4	0/0/0/0
2	GOL	C	473	-	-	0/4/4/4	0/0/0/0
2	GOL	D	473	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	473	GOL	O1-C1-C2	-2.31	98.97	110.18
2	D	473	GOL	O2-C2-C3	2.13	118.44	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	473	GOL	1	0
2	B	474	GOL	4	0
2	D	473	GOL	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, 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	471/473 (99%)	-0.54	2 (0%)	93	97	20, 31, 52, 80	0
1	B	471/473 (99%)	-0.51	3 (0%)	90	95	19, 29, 49, 77	0
1	C	471/473 (99%)	-0.50	1 (0%)	95	98	21, 31, 49, 75	0
1	D	471/473 (99%)	-0.36	5 (1%)	82	90	21, 34, 58, 81	0
All	All	1884/1892 (99%)	-0.48	11 (0%)	90	95	19, 31, 53, 81	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	GLY	3.7
1	D	275	TYR	3.3
1	D	273	GLU	3.3
1	D	274	GLU	2.9
1	D	314	ALA	2.7
1	B	316	ASP	2.7
1	D	316	ASP	2.6
1	B	275	TYR	2.5
1	A	273	GLU	2.4
1	C	315	LYS	2.2
1	B	273	GLU	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	GOL	D	473	6/6	0.95	0.16	4.15	42,43,44,44	0
2	GOL	B	473	6/6	0.96	0.14	2.39	32,33,35,36	0
2	GOL	A	473	6/6	0.98	0.12	2.21	29,32,32,33	0
2	GOL	C	473	6/6	0.99	0.14	1.97	28,33,35,35	0
2	GOL	B	474	6/6	0.96	0.14	0.97	30,35,37,39	0

6.5 Other polymers

There are no such residues in this entry.