



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:46 pm BST

PDB ID : 6D89
Title : Bacteroides uniformis beta-glucuronidase 1 with N-terminal loop deletion
Authors : Walton, W.G.; Pellock, S.J.; Redinbo, M.R.
Deposited on : 2018-04-26
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

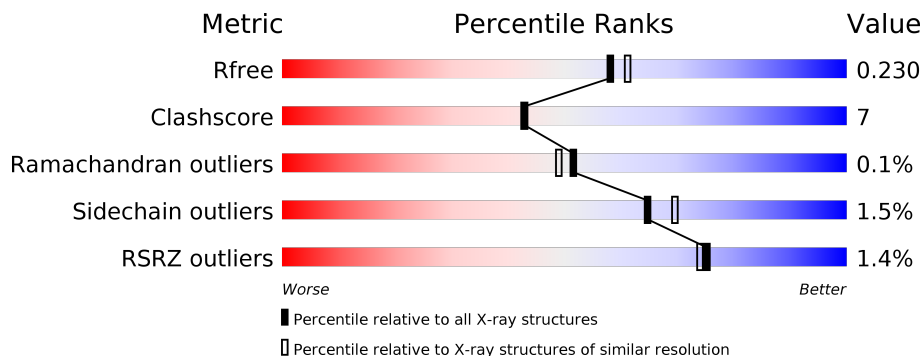
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	
1	B	595	
1	C	595	
1	D	595	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20593 atoms, of which 20 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-galactosidase/beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	571	4678	2994	801	869	14	0	1	0
1	D	571	4697	3009	803	871	14	0	1	0
1	A	571	4702	3012	804	872	14	0	2	0
1	B	568	4660	2987	796	863	14	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

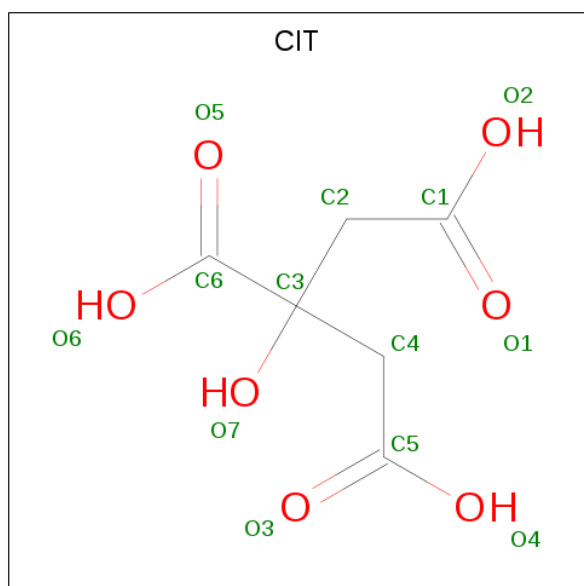
Chain	Residue	Modelled	Actual	Comment	Reference
C	54	ARG	-	linker	UNP A0A174CQK8
C	55	GLY	-	linker	UNP A0A174CQK8
C	56	MET	-	linker	UNP A0A174CQK8
C	57	LYS	-	linker	UNP A0A174CQK8
C	58	VAL	-	linker	UNP A0A174CQK8
C	59	TYR	-	linker	UNP A0A174CQK8
C	418	LYS	GLU	conflict	UNP A0A174CQK8
C	509	HIS	ARG	conflict	UNP A0A174CQK8
D	54	ARG	-	linker	UNP A0A174CQK8
D	55	GLY	-	linker	UNP A0A174CQK8
D	56	MET	-	linker	UNP A0A174CQK8
D	57	LYS	-	linker	UNP A0A174CQK8
D	58	VAL	-	linker	UNP A0A174CQK8
D	59	TYR	-	linker	UNP A0A174CQK8
D	418	LYS	GLU	conflict	UNP A0A174CQK8
D	509	HIS	ARG	conflict	UNP A0A174CQK8
A	54	ARG	-	linker	UNP A0A174CQK8
A	55	GLY	-	linker	UNP A0A174CQK8
A	56	MET	-	linker	UNP A0A174CQK8
A	57	LYS	-	linker	UNP A0A174CQK8
A	58	VAL	-	linker	UNP A0A174CQK8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	59	TYR	-	linker	UNP A0A174CQK8
A	418	LYS	GLU	conflict	UNP A0A174CQK8
A	509	HIS	ARG	conflict	UNP A0A174CQK8
B	54	ARG	-	linker	UNP A0A174CQK8
B	55	GLY	-	linker	UNP A0A174CQK8
B	56	MET	-	linker	UNP A0A174CQK8
B	57	LYS	-	linker	UNP A0A174CQK8
B	58	VAL	-	linker	UNP A0A174CQK8
B	59	TYR	-	linker	UNP A0A174CQK8
B	418	LYS	GLU	conflict	UNP A0A174CQK8
B	509	HIS	ARG	conflict	UNP A0A174CQK8

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	C	1	Total	C	H	O	0	0
			18	6	5	7		
2	D	1	Total	C	H	O	0	0
			18	6	5	7		
2	A	1	Total	C	H	O	0	0
			18	6	5	7		
2	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

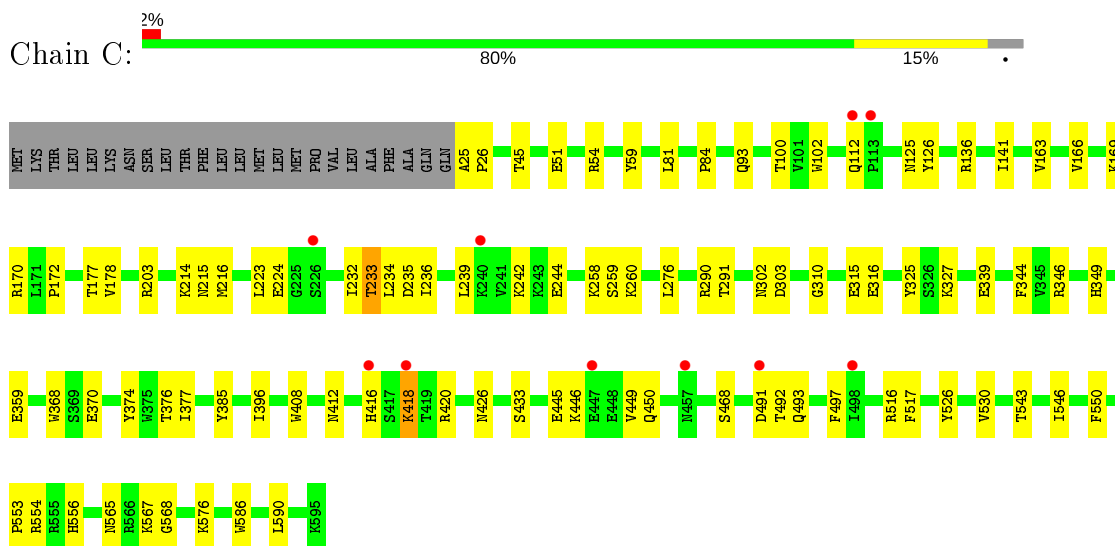
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	392	Total O 392 392	0	0
4	D	470	Total O 470 470	0	0
4	A	449	Total O 449 449	0	0
4	B	469	Total O 469 469	0	0

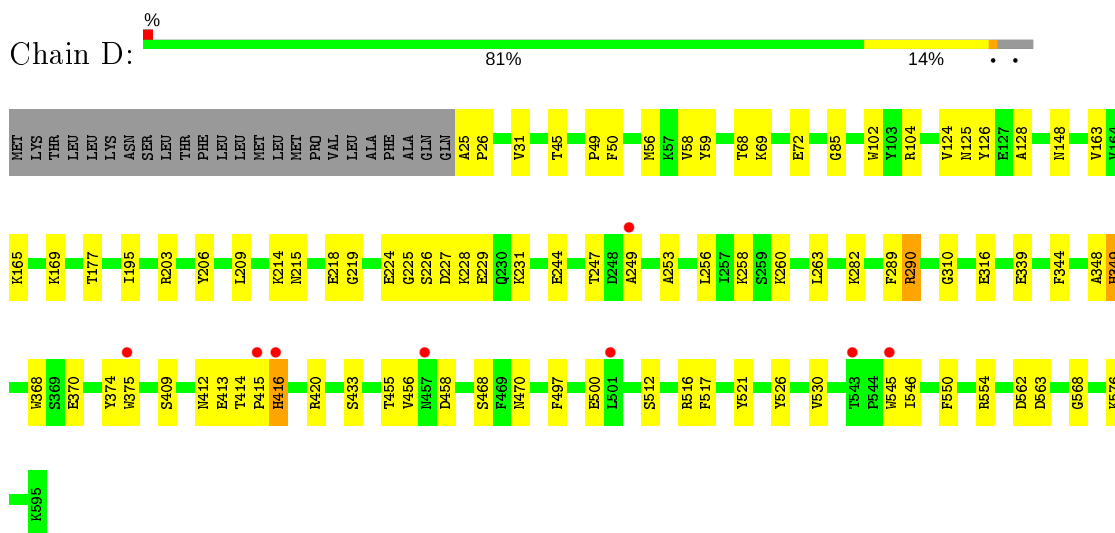
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

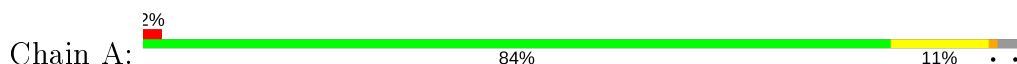
- Molecule 1: Beta-galactosidase/beta-glucuronidase

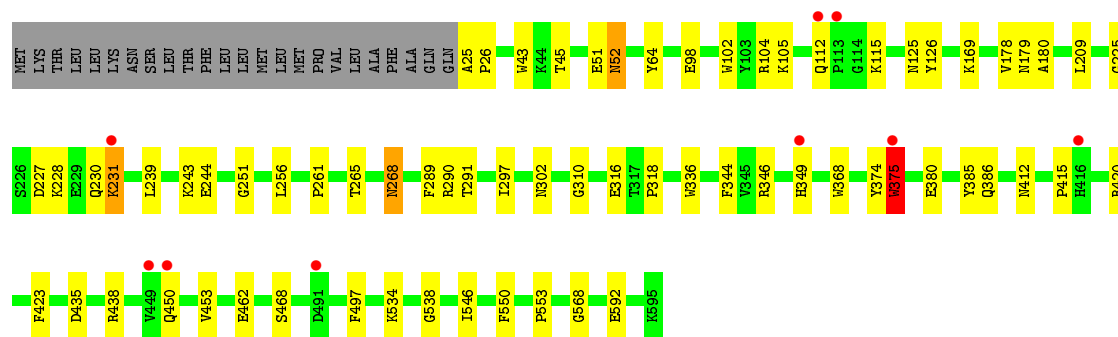


- Molecule 1: Beta-galactosidase/beta-glucuronidase

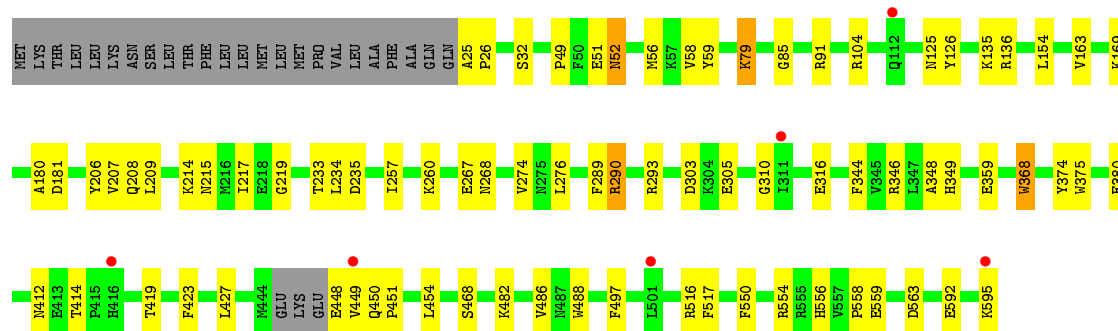
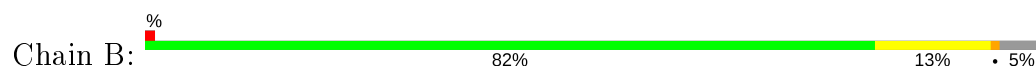


- Molecule 1: Beta-galactosidase/beta-glucuronidase





- Molecule 1: Beta-galactosidase/beta-glucuronidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.65Å 199.19Å 84.62Å 90.00° 102.81° 90.00°	Depositor
Resolution (Å)	29.34 – 2.00 29.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.34-2.00) 98.1 (29.34-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.176 , 0.230 0.176 , 0.230	Depositor DCC
R_{free} test set	1995 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.615	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20593	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.37	0/4829	0.53	0/6545
1	B	0.39	0/4782	0.56	0/6480
1	C	0.37	0/4802	0.55	0/6506
1	D	0.38	0/4821	0.54	0/6533
All	All	0.38	0/19234	0.55	0/26064

There are no bond length outliers.

There are no bond angle outliers.

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	4702	0	4610	52	0
1	B	4660	0	4571	63	0
1	C	4678	0	4589	78	0
1	D	4697	0	4603	65	0
2	A	13	5	5	0	0
2	B	13	5	5	0	0
2	C	13	5	5	0	0
2	D	13	5	5	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	449	0	0	7	1
4	B	469	0	0	10	0
4	C	392	0	0	11	1
4	D	470	0	0	7	0
All	All	20573	20	18393	254	1

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 (254) 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:418:LYS:H	1:C:418:LYS:HD2	1.30	0.97
1:C:233:THR:HG23	1:C:244:GLU:HG2	1.56	0.85
1:D:214:LYS:HG2	1:D:263:LEU:HD11	1.59	0.84
1:C:51:GLU:OE2	1:C:169:LYS:HE2	1.82	0.79
1:A:51:GLU:OE2	1:A:169:LYS:HE2	1.84	0.78
1:A:265:THR:HG23	1:A:268[A]:ASN:H	1.48	0.77
1:A:265:THR:HG23	1:A:268[B]:ASN:H	1.50	0.77
1:D:375:TRP:CE2	1:D:415:PRO:HG3	2.19	0.76
1:C:112:GLN:HG2	4:C:832:HOH:O	1.87	0.74
1:A:265:THR:CG2	1:A:268[B]:ASN:H	2.01	0.73
1:C:236:ILE:HG21	1:C:239:LEU:HD12	1.71	0.72
1:B:450:GLN:HG3	1:B:451:PRO:HD2	1.71	0.72
1:C:170:ARG:HD2	1:C:178:VAL:O	1.90	0.72
1:B:234:LEU:HD11	1:B:274:VAL:CG1	2.20	0.72
1:A:265:THR:CG2	1:A:268[A]:ASN:H	2.03	0.71
1:B:559:GLU:OE1	4:B:701:HOH:O	2.08	0.71
1:A:225:GLY:O	1:A:228:LYS:HE3	1.91	0.70
1:B:234:LEU:HD13	1:B:276:LEU:HG	1.74	0.69
1:D:554:ARG:NH1	4:D:703:HOH:O	2.25	0.69
1:C:26:PRO:HB2	1:C:203:ARG:HD2	1.75	0.69
1:B:32:SER:O	4:B:702:HOH:O	2.12	0.68
1:D:225:GLY:O	1:D:228:LYS:HG3	1.94	0.67
1:A:375:TRP:CZ3	1:A:415:PRO:HG3	2.30	0.66
1:A:462:GLU:N	4:A:704:HOH:O	2.28	0.66
1:B:449:VAL:HG23	1:B:450:GLN:H	1.59	0.66
1:C:54:ARG:HH21	1:C:136:ARG:HH11	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:TRP:CE3	1:A:375:TRP:HA	2.31	0.65
1:C:54:ARG:HH21	1:C:136:ARG:NH1	1.94	0.65
1:C:416:HIS:ND1	1:C:416:HIS:O	2.29	0.65
1:B:563:ASP:OD2	4:B:703:HOH:O	2.15	0.64
1:B:268:ASN:HB2	4:B:1060:HOH:O	1.98	0.63
1:B:234:LEU:HD11	1:B:274:VAL:HG13	1.79	0.63
1:B:450:GLN:CG	1:B:451:PRO:HD2	2.29	0.63
1:C:216:MET:CE	1:C:258:LYS:HG3	2.28	0.63
1:C:214:LYS:HE2	1:C:303:ASP:OD2	1.98	0.63
1:D:203:ARG:HD3	1:D:224:GLU:HG3	1.81	0.62
1:A:375:TRP:HE3	1:A:375:TRP:HA	1.64	0.62
1:C:310:GLY:HA2	1:C:344:PHE:O	1.99	0.62
1:A:349[B]:HIS:NE2	1:A:412:ASN:HB2	2.14	0.62
1:A:468:SER:HA	1:A:497:PHE:O	2.00	0.62
1:B:233:THR:HG22	1:B:235:ASP:OD1	2.00	0.62
1:B:293:ARG:NH2	1:B:303:ASP:OD1	2.33	0.61
1:B:214:LYS:HE3	1:B:303:ASP:OD2	2.00	0.61
1:C:565:ASN:OD1	1:C:567:LYS:HG3	2.00	0.61
1:B:412:ASN:O	1:B:414:THR:HG23	2.01	0.60
1:C:449:VAL:HG12	1:C:450:GLN:HG3	1.84	0.60
1:A:346:ARG:HH22	1:A:349[A]:HIS:CE1	2.19	0.60
1:C:233:THR:HG23	1:C:244:GLU:CG	2.30	0.59
1:B:468:SER:HA	1:B:497:PHE:O	2.03	0.59
1:C:203:ARG:HD3	1:C:224:GLU:HG3	1.85	0.59
1:C:234:LEU:HD23	1:C:276:LEU:CD2	2.33	0.59
1:D:31:VAL:HG13	1:D:195:ILE:HD11	1.85	0.59
1:B:346:ARG:HG3	1:B:368:TRP:CD1	2.38	0.59
1:C:54:ARG:NH2	1:C:136:ARG:HH11	2.01	0.59
1:A:346:ARG:HH22	1:A:349[A]:HIS:HE1	1.51	0.59
1:D:68:THR:O	4:D:701:HOH:O	2.17	0.59
1:B:85:GLY:HA2	4:B:884:HOH:O	2.01	0.59
1:B:449:VAL:HG23	1:B:450:GLN:N	2.17	0.58
1:C:468:SER:HA	1:C:497:PHE:O	2.03	0.58
1:C:346:ARG:HH22	1:C:349[A]:HIS:HE1	1.50	0.58
1:A:386:GLN:HG3	4:A:1030:HOH:O	2.04	0.58
1:C:349[B]:HIS:CE1	1:C:412:ASN:HB2	2.38	0.58
1:D:416:HIS:H	1:D:416:HIS:CD2	2.20	0.58
1:C:45:THR:HG21	1:C:81:LEU:HD12	1.85	0.58
1:B:310:GLY:HA2	1:B:344:PHE:O	2.04	0.57
1:C:349[B]:HIS:HA	1:C:370:GLU:OE2	2.05	0.57
1:D:468:SER:HA	1:D:497:PHE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LYS:O	1:B:486:VAL:HG13	2.06	0.56
1:C:349[A]:HIS:HA	1:C:370:GLU:OE2	2.06	0.56
1:C:234:LEU:HD23	1:C:276:LEU:HD21	1.88	0.56
1:D:349[A]:HIS:CE1	2:D:601:CIT:O3	2.59	0.56
1:D:45:THR:HA	1:D:102:TRP:O	2.07	0.55
1:B:180:ALA:HA	1:B:374:TYR:HE2	1.72	0.55
1:C:546:ILE:O	1:C:568:GLY:HA2	2.07	0.55
1:D:339:GLU:OE2	1:D:576:LYS:HE2	2.07	0.54
1:C:45:THR:HA	1:C:102:TRP:O	2.07	0.54
1:D:85:GLY:HA2	4:D:803:HOH:O	2.07	0.54
1:A:297:ILE:HD12	1:A:538:GLY:HA2	1.90	0.54
1:B:52:ASN:H	1:B:52:ASN:HD22	1.56	0.54
1:C:235:ASP:OD1	1:C:242:LYS:HG3	2.07	0.54
1:C:224:GLU:HG2	4:C:768:HOH:O	2.08	0.54
1:B:25:ALA:N	1:B:26:PRO:CD	2.70	0.54
1:A:385:TYR:HA	1:A:423:PHE:CZ	2.43	0.53
1:A:316:GLU:OE2	1:A:550:PHE:HA	2.10	0.52
1:B:79:LYS:HB2	4:B:1029:HOH:O	2.08	0.52
1:A:450:GLN:HG2	1:A:453:VAL:HB	1.91	0.52
1:B:448:GLU:HA	1:B:454:LEU:HD23	1.92	0.51
1:D:412:ASN:OD1	1:D:413:GLU:N	2.42	0.51
1:D:316:GLU:OE2	1:D:550:PHE:HA	2.11	0.51
1:D:31:VAL:HG13	1:D:195:ILE:CD1	2.40	0.51
1:C:54:ARG:HD2	4:C:990:HOH:O	2.09	0.51
1:B:181:ASP:OD1	1:B:554:ARG:HD3	2.11	0.51
1:C:136:ARG:NE	4:C:716:HOH:O	2.41	0.51
1:B:316:GLU:OE2	1:B:550:PHE:HA	2.11	0.51
1:B:56:MET:HG3	1:B:58:VAL:HG13	1.92	0.51
1:B:215:ASN:HB3	4:B:817:HOH:O	2.12	0.50
1:B:135:LYS:HE2	1:B:154:LEU:HD21	1.93	0.50
1:B:450:GLN:NE2	1:B:451:PRO:HD2	2.26	0.50
1:D:416:HIS:N	1:D:416:HIS:CD2	2.79	0.50
1:D:56:MET:HG3	1:D:58:VAL:HG13	1.93	0.50
1:A:25:ALA:N	1:A:26:PRO:CD	2.75	0.50
1:B:380:GLU:HG2	1:B:419:THR:HG21	1.93	0.50
1:B:215:ASN:OD1	1:B:260:LYS:HE3	2.12	0.50
1:C:385:TYR:OH	1:C:426:ASN:HB3	2.12	0.49
1:B:206:TYR:O	1:B:219:GLY:HA3	2.12	0.49
1:D:247:THR:HA	1:D:253:ALA:HB2	1.94	0.49
1:D:412:ASN:O	1:D:414:THR:HG23	2.13	0.49
1:D:370:GLU:HB3	1:D:409:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:HG2	4:A:951:HOH:O	2.12	0.49
1:C:316:GLU:OE2	1:C:550:PHE:HA	2.12	0.48
1:A:239:LEU:HD11	1:A:261:PRO:HB3	1.94	0.48
1:C:126:TYR:CE2	1:C:141:ILE:HG23	2.48	0.48
1:D:214:LYS:HE2	1:D:263:LEU:HD12	1.94	0.48
1:C:310:GLY:HA3	1:C:543:THR:HG22	1.95	0.48
1:C:418:LYS:N	1:C:418:LYS:HD2	2.13	0.48
1:D:177:THR:HG22	1:D:374:TYR:OH	2.12	0.48
1:A:228:LYS:O	1:A:251:GLY:HA2	2.14	0.48
1:A:180:ALA:HA	1:A:374:TYR:HE1	1.77	0.48
1:A:180:ALA:HA	1:A:374:TYR:CE1	2.49	0.48
1:A:534:LYS:NZ	4:A:703:HOH:O	2.28	0.48
1:A:98:GLU:HB2	4:A:1026:HOH:O	2.13	0.48
1:B:450:GLN:HG3	1:B:451:PRO:CD	2.43	0.48
1:C:327:LYS:NZ	4:C:723:HOH:O	2.46	0.48
1:C:554:ARG:NH2	4:C:727:HOH:O	2.47	0.48
1:C:216:MET:HE1	1:C:258:LYS:HG3	1.95	0.47
1:A:349[B]:HIS:NE2	1:A:374:TYR:HD2	2.13	0.47
1:B:359:GLU:OE1	1:B:359:GLU:HA	2.13	0.47
1:D:209:LEU:HG	1:D:289:PHE:HB3	1.95	0.47
1:A:52:ASN:H	1:A:52:ASN:HD22	1.61	0.47
1:D:339:GLU:OE1	4:D:702:HOH:O	2.20	0.47
1:D:546:ILE:O	1:D:568:GLY:HA2	2.13	0.47
1:A:380:GLU:HG3	4:A:706:HOH:O	2.14	0.47
1:C:93:GLN:HG2	4:C:1033:HOH:O	2.13	0.47
1:D:258:LYS:HE2	4:D:1031:HOH:O	2.15	0.47
1:A:346:ARG:NH2	1:A:349[A]:HIS:CE1	2.82	0.47
1:B:25:ALA:N	1:B:26:PRO:HD3	2.30	0.47
1:D:59:TYR:HA	1:D:163:VAL:HG11	1.95	0.47
1:B:59:TYR:HA	1:B:163:VAL:HG11	1.97	0.47
1:D:26:PRO:HB2	1:D:203:ARG:HD2	1.96	0.47
1:D:349[A]:HIS:CE1	2:D:601:CIT:C5	2.97	0.47
1:C:418:LYS:CD	1:C:418:LYS:H	2.03	0.47
1:B:303:ASP:OD2	4:B:704:HOH:O	2.20	0.47
1:C:25:ALA:N	1:C:26:PRO:CD	2.78	0.47
1:A:43:TRP:HB3	1:A:104:ARG:O	2.14	0.47
1:B:423:PHE:HE1	1:B:427:LEU:HD11	1.80	0.47
1:A:310:GLY:HA2	1:A:344:PHE:O	2.15	0.46
1:C:396:ILE:HG12	1:C:408:TRP:CE2	2.50	0.46
1:D:349[A]:HIS:CE1	1:D:545:TRP:CH2	3.03	0.46
1:D:215:ASN:OD1	1:D:260:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:LYS:HG2	1:D:263:LEU:CD1	2.39	0.46
1:D:229:GLU:HG3	1:D:249:ALA:HA	1.96	0.46
1:A:112:GLN:HG3	1:A:115:LYS:HG2	1.98	0.46
1:D:102:TRP:CZ2	1:D:165:LYS:HD2	2.50	0.46
1:D:500:GLU:OE2	2:D:601:CIT:H41	2.16	0.46
1:B:448:GLU:CA	1:B:454:LEU:HD23	2.46	0.45
1:D:125:ASN:HA	1:D:126:TYR:HA	1.64	0.45
1:C:169:LYS:NZ	4:C:728:HOH:O	2.47	0.45
1:D:69:LYS:HE2	4:D:962:HOH:O	2.16	0.45
1:A:231:LYS:HG2	1:A:244:GLU:CD	2.37	0.45
1:B:592:GLU:HG2	1:B:595:LYS:HZ3	1.82	0.45
1:C:291:THR:OG1	1:C:302:ASN:HA	2.16	0.45
1:B:268:ASN:HB2	4:B:1068:HOH:O	2.16	0.45
1:C:553:PRO:HB2	1:D:49:PRO:HG2	1.98	0.45
1:A:45:THR:HA	1:A:102:TRP:O	2.17	0.45
1:C:125:ASN:HA	1:C:126:TYR:HA	1.76	0.45
1:C:346:ARG:NH2	1:C:349[A]:HIS:CE1	2.85	0.45
1:A:291:THR:OG1	1:A:302:ASN:HA	2.17	0.45
1:D:218:GLU:HB2	1:D:256:LEU:HD23	1.99	0.45
1:C:177:THR:OG1	1:C:178:VAL:N	2.50	0.45
1:C:215:ASN:OD1	1:C:260:LYS:HG2	2.17	0.45
1:D:349[B]:HIS:HA	1:D:370:GLU:OE1	2.17	0.45
1:A:125:ASN:HA	1:A:126:TYR:HA	1.74	0.44
1:B:305:GLU:OE2	4:B:705:HOH:O	2.21	0.44
1:C:223:LEU:HD11	1:C:232:ILE:HD11	2.00	0.44
1:C:84:PRO:HG2	1:C:325:TYR:CZ	2.52	0.44
1:D:206:TYR:O	1:D:219:GLY:HA3	2.18	0.44
1:D:526:TYR:O	1:D:530:VAL:HG23	2.17	0.44
1:A:43:TRP:CD2	1:A:105:LYS:HB2	2.53	0.44
1:B:556:HIS:O	1:B:558:PRO:HD3	2.17	0.44
1:C:526:TYR:O	1:C:530:VAL:HG23	2.18	0.44
1:D:290:ARG:HD2	1:D:290:ARG:C	2.38	0.44
1:D:349[A]:HIS:HA	1:D:370:GLU:OE1	2.17	0.44
1:C:516:ARG:O	1:C:517:PHE:HB2	2.18	0.44
1:C:45:THR:HG21	1:C:81:LEU:CD1	2.47	0.44
1:B:558:PRO:O	1:B:559:GLU:HB2	2.17	0.44
1:D:226:SER:O	1:D:228:LYS:N	2.51	0.44
1:C:260:LYS:N	4:C:709:HOH:O	2.36	0.43
1:A:435:ASP:OD2	1:A:438:ARG:HD2	2.17	0.43
1:B:449:VAL:CG2	1:B:450:GLN:H	2.27	0.43
1:D:124:VAL:HG11	1:D:128:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLY:HA2	1:D:344:PHE:O	2.18	0.43
1:A:546:ILE:O	1:A:568:GLY:HA2	2.18	0.43
1:D:177:THR:HG22	1:D:374:TYR:CZ	2.53	0.43
1:B:267:GLU:CD	1:B:267:GLU:H	2.22	0.43
1:C:374:TYR:O	1:C:377:ILE:HG12	2.17	0.43
1:D:349[A]:HIS:HE1	2:D:601:CIT:C5	2.31	0.43
1:A:231:LYS:HG2	1:A:244:GLU:OE2	2.19	0.43
1:C:172:PRO:HA	1:C:178:VAL:HG13	1.99	0.43
1:C:215:ASN:HA	1:C:259:SER:O	2.19	0.43
1:C:346:ARG:NH2	1:C:349[A]:HIS:HE1	2.14	0.43
1:D:25:ALA:N	1:D:26:PRO:CD	2.82	0.43
1:D:348:ALA:HA	1:D:349[A]:HIS:HA	1.86	0.43
1:B:374:TYR:O	1:B:375:TRP:HB2	2.19	0.43
1:C:59:TYR:HA	1:C:163:VAL:HG11	2.01	0.43
1:A:178:VAL:HG23	1:A:179:ASN:N	2.34	0.42
1:A:318:PRO:HB3	1:A:336:TRP:CH2	2.54	0.42
1:B:276:LEU:HD12	1:B:276:LEU:N	2.34	0.42
1:D:562:ASP:O	1:D:563:ASP:HB2	2.20	0.42
1:C:359:GLU:HA	1:C:359:GLU:OE1	2.18	0.42
1:B:348:ALA:HA	1:B:349:HIS:HA	1.87	0.42
1:D:231:LYS:HE2	1:D:244:GLU:HB3	2.00	0.42
1:D:516:ARG:O	1:D:517:PHE:HB2	2.19	0.42
1:C:492:THR:HG22	1:C:493:GLN:N	2.34	0.42
1:D:102:TRP:CZ3	1:D:165:LYS:HB2	2.55	0.42
1:D:412:ASN:OD1	1:D:470:ASN:ND2	2.52	0.42
1:A:209:LEU:HG	1:A:289:PHE:HB3	2.02	0.42
1:B:207:VAL:O	1:B:208:GLN:HG2	2.20	0.42
1:B:516:ARG:O	1:B:517:PHE:HB2	2.20	0.42
1:A:227:ASP:HB3	1:A:230:GLN:HE21	1.85	0.42
1:C:339:GLU:OE1	1:C:576:LYS:HE3	2.20	0.42
1:D:25:ALA:HA	1:D:148:ASN:O	2.20	0.41
1:B:51:GLU:OE1	1:B:169:LYS:NZ	2.48	0.41
1:B:125:ASN:HA	1:B:126:TYR:HA	1.72	0.41
1:B:450:GLN:CD	1:B:451:PRO:HD2	2.40	0.41
1:C:346:ARG:HH22	1:C:349[A]:HIS:CE1	2.34	0.41
1:D:458:ASP:N	4:D:707:HOH:O	2.29	0.41
1:B:79:LYS:HG3	1:B:91:ARG:NH2	2.34	0.41
1:C:315:GLU:O	1:C:315:GLU:HG2	2.20	0.41
1:A:256:LEU:HD22	1:A:256:LEU:N	2.35	0.41
1:B:209:LEU:HG	1:B:289:PHE:HB3	2.02	0.41
1:C:349[B]:HIS:CE1	1:C:412:ASN:CB	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:GLU:HG2	1:C:446:LYS:O	2.20	0.41
1:C:468:SER:OG	4:C:701:HOH:O	2.07	0.41
1:C:556:HIS:HB2	1:D:72:GLU:O	2.20	0.41
1:D:214:LYS:HE2	1:D:263:LEU:CD1	2.51	0.41
1:D:339:GLU:CD	1:D:576:LYS:HE2	2.41	0.41
1:D:521:TYR:C	1:D:521:TYR:CD1	2.94	0.41
1:B:217:ILE:HB	1:B:257:ILE:HB	2.02	0.41
1:C:236:ILE:CG2	1:C:239:LEU:HD12	2.47	0.41
1:C:491:ASP:OD1	1:C:491:ASP:N	2.54	0.41
1:C:100:THR:HA	1:C:166:VAL:O	2.21	0.41
1:B:454:LEU:HD13	1:B:488:TRP:CZ2	2.56	0.41
1:C:553:PRO:HG2	1:D:50:PHE:CD2	2.56	0.41
1:A:112:GLN:HG3	1:A:115:LYS:CG	2.52	0.40
1:A:592:GLU:OE2	4:A:701:HOH:O	2.22	0.40
1:C:586:TRP:CZ2	1:C:590:LEU:HD11	2.56	0.40
1:B:180:ALA:HA	1:B:374:TYR:CE2	2.55	0.40
1:B:290:ARG:C	1:B:290:ARG:HD2	2.41	0.40
1:C:235:ASP:HB3	4:C:836:HOH:O	2.22	0.40
1:A:243:LYS:HE3	1:A:243:LYS:HB2	1.90	0.40
1:C:418:LYS:N	1:C:418:LYS:CD	2.80	0.40
1:A:553:PRO:HB2	1:B:49:PRO:HG2	2.01	0.40
1:D:455:THR:HG23	1:D:456:VAL:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:715:HOH:O	4:A:706:HOH:O 1_554	2.04	0.16

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	571/595 (96%)	552 (97%)	18 (3%)	1 (0%)	47	44
1	B	564/595 (95%)	543 (96%)	21 (4%)	0	100	100
1	C	570/595 (96%)	547 (96%)	23 (4%)	0	100	100
1	D	570/595 (96%)	549 (96%)	20 (4%)	1 (0%)	47	44
All	All	2275/2380 (96%)	2191 (96%)	82 (4%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	227	ASP
1	A	375	TRP

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	508/528 (96%)	499 (98%)	9 (2%)	59	63
1	B	503/528 (95%)	497 (99%)	6 (1%)	71	76
1	C	505/528 (96%)	498 (99%)	7 (1%)	67	72
1	D	507/528 (96%)	496 (98%)	11 (2%)	52	55
All	All	2023/2112 (96%)	1990 (98%)	33 (2%)	65	67

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	233	THR
1	C	290	ARG
1	C	368	TRP
1	C	376	THR
1	C	418	LYS
1	C	420	ARG
1	C	433	SER
1	D	104	ARG
1	D	169	LYS

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Mol	Chain	Res	Type
1	D	282	LYS
1	D	290	ARG
1	D	349[A]	HIS
1	D	349[B]	HIS
1	D	368	TRP
1	D	416	HIS
1	D	420	ARG
1	D	433	SER
1	D	512	SER
1	A	52	ASN
1	A	64	TYR
1	A	231	LYS
1	A	268[A]	ASN
1	A	268[B]	ASN
1	A	290	ARG
1	A	368	TRP
1	A	375	TRP
1	A	420	ARG
1	B	52	ASN
1	B	79	LYS
1	B	104	ARG
1	B	136	ARG
1	B	290	ARG
1	B	368	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	416	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	601	1	3,12,12	1.53	1 (33%)	3,17,17	1.15	0
2	CIT	B	601	1	3,12,12	1.07	0	3,17,17	0.95	0
2	CIT	C	601	1	3,12,12	1.62	0	3,17,17	1.87	2 (66%)
2	CIT	D	601	-	3,12,12	1.92	2 (66%)	3,17,17	2.99	2 (66%)

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	601	1	-	0/6/16/16	-
2	CIT	B	601	1	-	3/6/16/16	-
2	CIT	C	601	1	-	0/6/16/16	-
2	CIT	D	601	-	-	0/6/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	CIT	C4-C3	-2.13	1.51	1.54
2	A	601	CIT	O7-C3	2.05	1.46	1.43
2	D	601	CIT	C2-C3	-2.03	1.52	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	601	CIT	C3-C2-C1	-3.60	109.22	114.98
2	D	601	CIT	C3-C4-C5	-3.47	109.42	114.98
2	C	601	CIT	C3-C4-C5	-2.44	111.08	114.98
2	C	601	CIT	C3-C2-C1	-2.12	111.59	114.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	CIT	C6-C3-C4-C5
2	B	601	CIT	C2-C3-C4-C5
2	B	601	CIT	O7-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	CIT	4	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 [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	571/595 (95%)	-0.21	9 (1%) 72 70	18, 29, 48, 58	0
1	B	568/595 (95%)	-0.33	6 (1%) 80 79	17, 27, 42, 56	0
1	C	571/595 (95%)	-0.24	10 (1%) 68 66	17, 29, 46, 62	0
1	D	571/595 (95%)	-0.36	8 (1%) 75 74	17, 27, 42, 62	0
All	All	2281/2380 (95%)	-0.29	33 (1%) 75 74	17, 28, 45, 62	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	416	HIS	4.7
1	A	375	TRP	4.6
1	C	491	ASP	3.9
1	D	416	HIS	3.8
1	C	113	PRO	3.7
1	A	416	HIS	3.7
1	B	449	VAL	3.6
1	A	113	PRO	3.1
1	A	449	VAL	3.1
1	B	595	LYS	2.9
1	D	249	ALA	2.9
1	C	226	SER	2.8
1	C	240	LYS	2.8
1	C	457	ASN	2.7
1	A	491	ASP	2.7
1	C	418	LYS	2.7
1	B	112	GLN	2.7
1	C	112	GLN	2.6
1	D	375	TRP	2.4
1	A	112	GLN	2.4
1	D	501	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	501	LEU	2.3
1	D	545	TRP	2.3
1	A	231	LYS	2.2
1	B	416	HIS	2.2
1	A	450	GLN	2.2
1	D	543	THR	2.2
1	D	457	ASN	2.1
1	A	349[A]	HIS	2.1
1	C	447	GLU	2.1
1	B	311	ILE	2.1
1	C	498	ILE	2.0
1	D	415	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CIT	B	601	13/13	0.85	0.17	28,43,51,51	0
2	CIT	A	601	13/13	0.90	0.14	25,35,45,48	0
2	CIT	D	601	13/13	0.91	0.10	28,34,40,41	0
2	CIT	C	601	13/13	0.95	0.09	24,32,41,41	0
3	CL	B	602	1/1	0.99	0.04	27,27,27,27	0
3	CL	A	602	1/1	0.99	0.07	22,22,22,22	0
3	CL	C	602	1/1	0.99	0.05	20,20,20,20	0
3	CL	D	602	1/1	0.99	0.06	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.