



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:10 PM BST

PDB ID : 6NCX
Title : Crystal structure of GH2 beta-galacturonidase from Eisenbergiella tayi bound to galacturonate
Authors : Walton, W.G.; Pellock, S.J.; Redinbo, M.R.
Deposited on : 2018-12-12
Resolution : 2.25 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 : 2.13.1
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) : 2.13.1

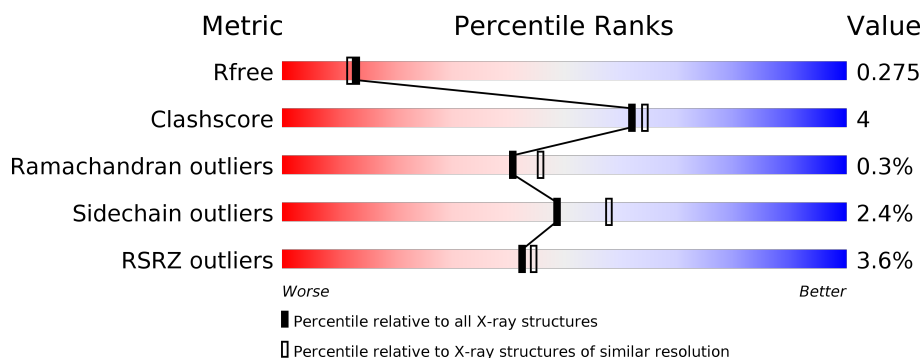
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	574	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	574	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	574	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>••</div> </div> </div>
1	D	574	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19071 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-galacturonidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	555	Total	C	N	O	S	0	0	0
			4481	2849	764	846	22			
1	A	554	Total	C	N	O	S	0	0	0
			4474	2845	763	844	22			
1	B	559	Total	C	N	O	S	0	0	0
			4503	2861	768	852	22			
1	C	559	Total	C	N	O	S	0	0	0
			4503	2861	768	852	22			

There are 60 discrepancies between the modelled and reference sequences:

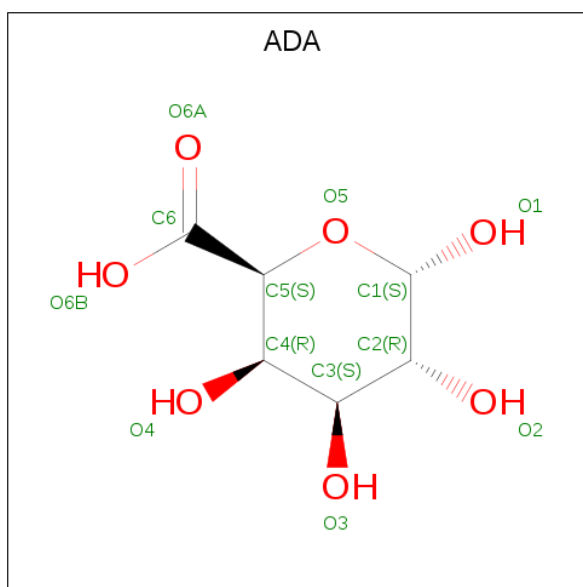
Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLU	-	expression tag	UNP A0A1E3AEY6
A	561	ASN	-	expression tag	UNP A0A1E3AEY6
A	562	LEU	-	expression tag	UNP A0A1E3AEY6
A	563	TYR	-	expression tag	UNP A0A1E3AEY6
A	564	PHE	-	expression tag	UNP A0A1E3AEY6
A	565	GLN	-	expression tag	UNP A0A1E3AEY6
A	566	SER	-	expression tag	UNP A0A1E3AEY6
A	567	GLY	-	expression tag	UNP A0A1E3AEY6
A	568	SER	-	expression tag	UNP A0A1E3AEY6
A	569	HIS	-	expression tag	UNP A0A1E3AEY6
A	570	HIS	-	expression tag	UNP A0A1E3AEY6
A	571	HIS	-	expression tag	UNP A0A1E3AEY6
A	572	HIS	-	expression tag	UNP A0A1E3AEY6
A	573	HIS	-	expression tag	UNP A0A1E3AEY6
A	574	HIS	-	expression tag	UNP A0A1E3AEY6
B	560	GLU	-	expression tag	UNP A0A1E3AEY6
B	561	ASN	-	expression tag	UNP A0A1E3AEY6
B	562	LEU	-	expression tag	UNP A0A1E3AEY6
B	563	TYR	-	expression tag	UNP A0A1E3AEY6
B	564	PHE	-	expression tag	UNP A0A1E3AEY6
B	565	GLN	-	expression tag	UNP A0A1E3AEY6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	SER	-	expression tag	UNP A0A1E3AEY6
B	567	GLY	-	expression tag	UNP A0A1E3AEY6
B	568	SER	-	expression tag	UNP A0A1E3AEY6
B	569	HIS	-	expression tag	UNP A0A1E3AEY6
B	570	HIS	-	expression tag	UNP A0A1E3AEY6
B	571	HIS	-	expression tag	UNP A0A1E3AEY6
B	572	HIS	-	expression tag	UNP A0A1E3AEY6
B	573	HIS	-	expression tag	UNP A0A1E3AEY6
B	574	HIS	-	expression tag	UNP A0A1E3AEY6
C	560	GLU	-	expression tag	UNP A0A1E3AEY6
C	561	ASN	-	expression tag	UNP A0A1E3AEY6
C	562	LEU	-	expression tag	UNP A0A1E3AEY6
C	563	TYR	-	expression tag	UNP A0A1E3AEY6
C	564	PHE	-	expression tag	UNP A0A1E3AEY6
C	565	GLN	-	expression tag	UNP A0A1E3AEY6
C	566	SER	-	expression tag	UNP A0A1E3AEY6
C	567	GLY	-	expression tag	UNP A0A1E3AEY6
C	568	SER	-	expression tag	UNP A0A1E3AEY6
C	569	HIS	-	expression tag	UNP A0A1E3AEY6
C	570	HIS	-	expression tag	UNP A0A1E3AEY6
C	571	HIS	-	expression tag	UNP A0A1E3AEY6
C	572	HIS	-	expression tag	UNP A0A1E3AEY6
C	573	HIS	-	expression tag	UNP A0A1E3AEY6
C	574	HIS	-	expression tag	UNP A0A1E3AEY6
D	560	GLU	-	expression tag	UNP A0A1E3AEY6
D	561	ASN	-	expression tag	UNP A0A1E3AEY6
D	562	LEU	-	expression tag	UNP A0A1E3AEY6
D	563	TYR	-	expression tag	UNP A0A1E3AEY6
D	564	PHE	-	expression tag	UNP A0A1E3AEY6
D	565	GLN	-	expression tag	UNP A0A1E3AEY6
D	566	SER	-	expression tag	UNP A0A1E3AEY6
D	567	GLY	-	expression tag	UNP A0A1E3AEY6
D	568	SER	-	expression tag	UNP A0A1E3AEY6
D	569	HIS	-	expression tag	UNP A0A1E3AEY6
D	570	HIS	-	expression tag	UNP A0A1E3AEY6
D	571	HIS	-	expression tag	UNP A0A1E3AEY6
D	572	HIS	-	expression tag	UNP A0A1E3AEY6
D	573	HIS	-	expression tag	UNP A0A1E3AEY6
D	574	HIS	-	expression tag	UNP A0A1E3AEY6

- Molecule 2 is alpha-D-galactopyranuronic acid (three-letter code: ADA) (formula: C₆H₁₀O₇).



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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	268	Total	O	0	0
			268	268		

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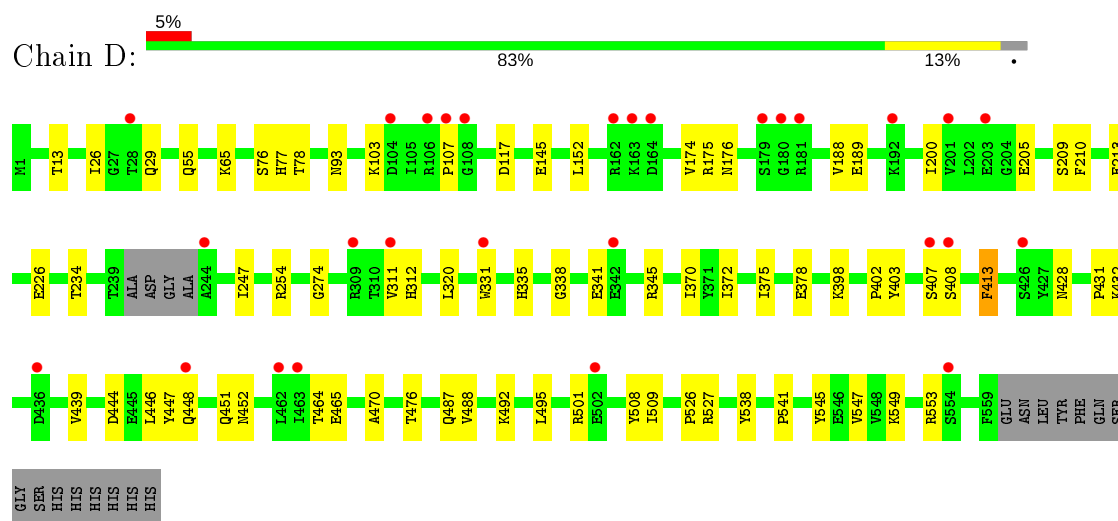
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	245	Total 245	O 245	0	0
4	B	255	Total 255	O 255	0	0
4	C	286	Total 286	O 286	0	0

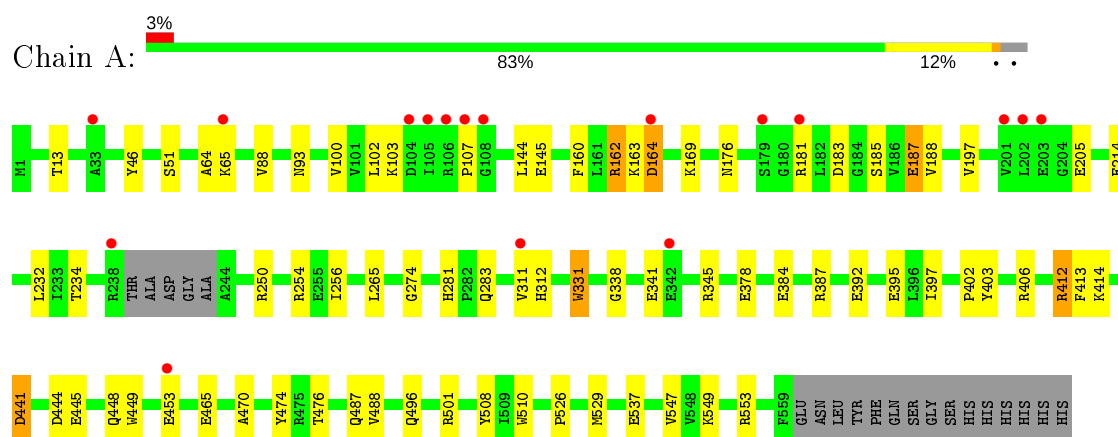
3 Residue-property plots [i](#)

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.

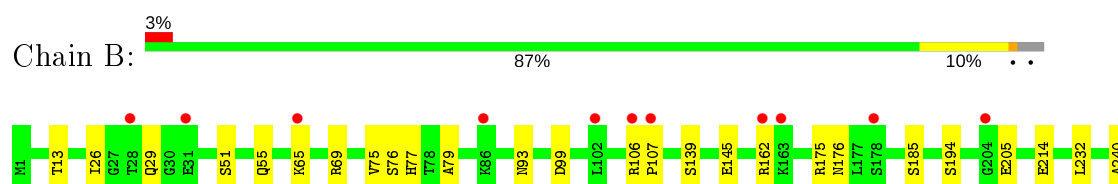
• Molecule 1: Beta-galacturonidase

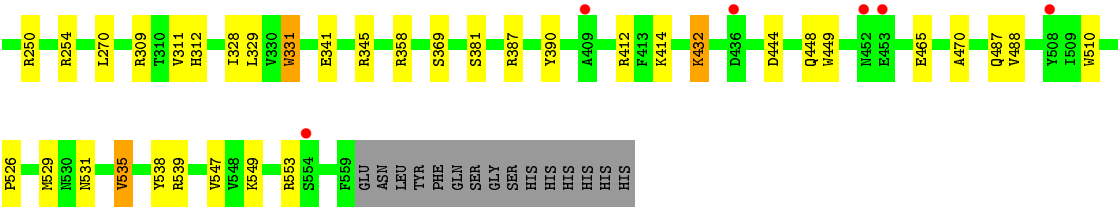


• Molecule 1: Beta-galacturonidase

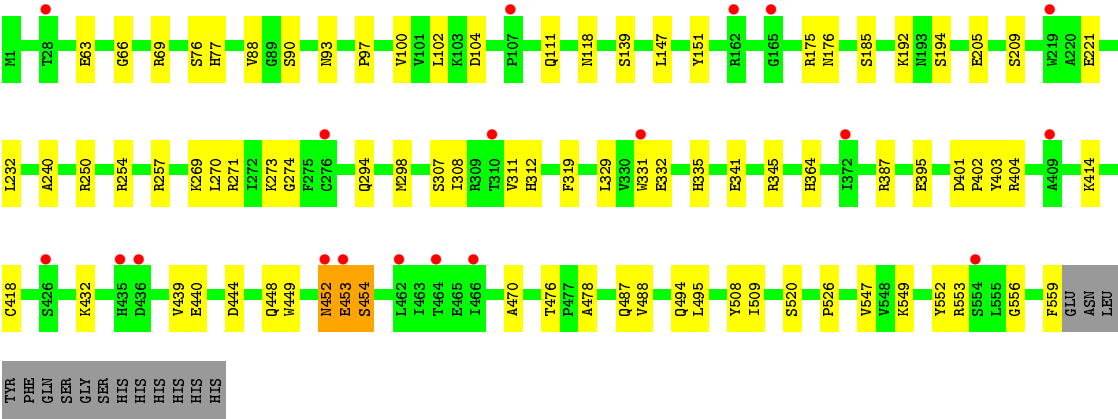
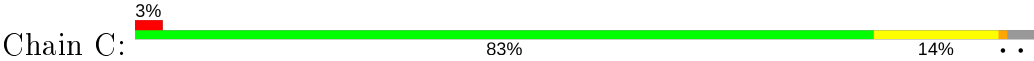


• Molecule 1: Beta-galacturonidase





● Molecule 1: Beta-galacturonidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.34Å 156.04Å 124.28Å 90.00° 101.27° 90.00°	Depositor
Resolution (Å)	29.88 – 2.25 29.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.88-2.25) 99.3 (29.88-2.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.221 , 0.275 0.221 , 0.275	Depositor DCC
R_{free} test set	1987 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.62$, $\langle L^2 \rangle = 0.47$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19071	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7575e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, ADA

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	0.43	0/4596	0.58	0/6236
1	B	0.43	0/4626	0.58	0/6279
1	C	0.44	0/4626	0.59	0/6279
1	D	0.42	0/4603	0.58	0/6246
All	All	0.43	0/18451	0.58	0/25040

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	4474	0	4281	40	0
1	B	4503	0	4306	34	2
1	C	4503	0	4306	45	2
1	D	4481	0	4288	41	0
2	A	13	0	9	1	0
2	B	13	0	9	2	0
2	C	13	0	9	0	0
2	D	13	0	9	2	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	245	0	0	2	0
4	B	255	0	0	4	1
4	C	286	0	0	5	1
4	D	268	0	0	3	0
All	All	19071	0	17217	155	3

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 (155) 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:488:VAL:HG13	1:D:547:VAL:HG21	1.71	0.73
1:C:232:LEU:HD23	1:C:250:ARG:HG2	1.73	0.70
1:D:189:GLU:OE1	4:D:701:HOH:O	2.09	0.69
1:B:232:LEU:HD23	1:B:250:ARG:HG2	1.74	0.69
1:C:97:PRO:O	4:C:701:HOH:O	2.11	0.68
1:C:476:THR:HG22	1:C:478:ALA:H	1.58	0.67
1:B:444:ASP:O	1:B:448:GLN:HG2	1.96	0.66
1:D:444:ASP:O	1:D:448:GLN:HG2	1.96	0.65
1:C:332:GLU:OE2	1:C:364:HIS:ND1	2.26	0.65
1:B:526:PRO:HG3	1:C:526:PRO:HG3	1.80	0.64
1:A:488:VAL:HG13	1:A:547:VAL:HG21	1.81	0.62
1:C:444:ASP:O	1:C:448:GLN:HG2	2.00	0.62
1:C:488:VAL:HG13	1:C:547:VAL:HG21	1.80	0.62
1:D:465:GLU:OE2	2:D:601:ADA:O1	2.14	0.61
1:A:88:VAL:CG2	1:A:102:LEU:HD21	2.30	0.61
1:C:341:GLU:OE2	1:C:345:ARG:NH1	2.35	0.60
1:A:444:ASP:O	1:A:448:GLN:HG2	2.02	0.60
1:D:103:LYS:NZ	4:D:705:HOH:O	2.35	0.59
1:A:414:LYS:HG2	1:A:449:TRP:CG	2.37	0.59
1:A:341:GLU:OE2	1:A:345:ARG:NH1	2.34	0.59
1:B:535:VAL:HG13	1:B:539:ARG:HA	1.83	0.59
1:A:88:VAL:HG21	1:A:102:LEU:HD21	1.85	0.57
1:B:488:VAL:HG13	1:B:547:VAL:HG21	1.86	0.57
1:C:274:GLY:HA2	1:C:307:SER:O	2.05	0.56
1:A:162:ARG:NH2	1:A:214:GLU:OE1	2.27	0.56
1:B:465:GLU:OE2	2:B:601:ADA:O1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:HG12	1:C:100:VAL:HG11	1.88	0.56
1:A:181:ARG:NH2	1:A:183:ASP:OD2	2.36	0.56
1:A:232:LEU:HD23	1:A:250:ARG:HG2	1.88	0.56
1:D:452:ASN:OD1	4:D:703:HOH:O	2.18	0.55
1:D:13:THR:HG22	1:D:145:GLU:HG2	1.89	0.55
1:B:414:LYS:HG2	1:B:449:TRP:CG	2.42	0.54
1:A:13:THR:HG22	1:A:145:GLU:HG2	1.90	0.54
1:A:465:GLU:OE2	2:A:601:ADA:O1	2.16	0.54
1:C:470:ALA:HB2	1:C:487:GLN:HB2	1.91	0.53
1:C:495:LEU:HD21	1:C:509:ILE:HD11	1.89	0.53
1:A:402:PRO:HG2	1:A:403:TYR:CE1	2.43	0.53
1:A:187:GLU:HG2	1:A:197:VAL:HG22	1.90	0.53
1:A:444:ASP:OD1	1:A:501:ARG:NH1	2.40	0.53
1:C:308:ILE:HD13	1:C:319:PHE:HE2	1.73	0.53
1:A:281:HIS:CE1	1:A:283:GLN:HB2	2.44	0.52
1:B:309:ARG:HG3	1:B:331:TRP:CD1	2.44	0.52
1:D:176:ASN:O	1:D:205:GLU:HA	2.09	0.52
1:C:274:GLY:HA3	1:C:508:TYR:CD2	2.45	0.52
1:D:274:GLY:HA3	1:D:508:TYR:CD2	2.45	0.51
1:C:88:VAL:HG13	1:C:102:LEU:HD21	1.93	0.51
1:C:414:LYS:HG2	1:C:449:TRP:CG	2.45	0.51
1:D:402:PRO:HG2	1:D:403:TYR:CE1	2.46	0.51
1:C:269:LYS:HE3	1:C:559:PHE:CD2	2.45	0.51
1:D:541:PRO:HB3	1:D:545:TYR:CD2	2.46	0.51
1:D:444:ASP:OD1	1:D:501:ARG:NH1	2.43	0.50
1:B:387:ARG:NH1	4:B:712:HOH:O	2.45	0.50
1:A:65:LYS:HD3	1:A:107:PRO:HB3	1.92	0.50
1:A:549:LYS:HE2	1:A:553:ARG:CZ	2.42	0.50
1:C:401:ASP:OD1	1:C:404:ARG:HD2	2.11	0.50
1:B:470:ALA:HB2	1:B:487:GLN:HB2	1.93	0.50
1:D:447:TYR:O	1:D:451:GLN:HG2	2.11	0.50
1:C:88:VAL:CG1	1:C:100:VAL:HG11	2.42	0.50
1:C:221:GLU:OE2	4:C:702:HOH:O	2.19	0.49
1:D:26:ILE:HG13	1:D:55:GLN:HB2	1.95	0.49
1:C:111:GLN:OE1	4:C:703:HOH:O	2.20	0.48
1:B:65:LYS:HD3	1:B:107:PRO:HB3	1.95	0.48
1:D:65:LYS:HD3	1:D:107:PRO:HB3	1.95	0.48
1:B:529:MET:O	1:B:531:ASN:ND2	2.47	0.48
1:A:164:ASP:OD2	1:A:164:ASP:N	2.42	0.47
1:D:428:ASN:HB3	1:D:465:GLU:HB2	1.95	0.47
1:A:441:ASP:OD1	1:A:441:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:TRP:CZ2	2:B:601:ADA:H4	2.48	0.47
1:C:341:GLU:O	1:C:345:ARG:HG3	2.15	0.47
1:D:470:ALA:HB2	1:D:487:GLN:HB2	1.96	0.47
1:B:26:ILE:HG13	1:B:55:GLN:HB2	1.97	0.47
1:D:431:PRO:HG2	1:D:439:VAL:HG13	1.96	0.47
1:D:375:ILE:O	1:D:408:SER:OG	2.14	0.47
1:D:320:LEU:HD13	1:D:370:ILE:HD11	1.97	0.47
1:B:341:GLU:OE2	1:B:345:ARG:NH1	2.48	0.46
1:C:192:LYS:HB3	4:C:704:HOH:O	2.14	0.46
1:B:77:HIS:HB3	4:B:832:HOH:O	2.15	0.46
1:C:549:LYS:HE2	1:C:553:ARG:NH1	2.29	0.46
1:A:274:GLY:HA3	1:A:508:TYR:CD2	2.51	0.46
1:D:312:HIS:O	1:D:335:HIS:HA	2.15	0.46
1:C:549:LYS:HE2	1:C:553:ARG:CZ	2.45	0.46
1:D:341:GLU:O	1:D:345:ARG:HG3	2.15	0.46
1:A:338:GLY:HA2	1:A:378:GLU:O	2.16	0.45
1:D:76:SER:HA	1:D:77:HIS:HA	1.71	0.45
1:C:273:LYS:NZ	1:C:552:TYR:O	2.45	0.45
1:C:270:LEU:HD21	1:C:329:LEU:HD13	1.99	0.45
1:A:470:ALA:HB2	1:A:487:GLN:HB2	1.99	0.45
1:B:311:VAL:HA	1:B:312:HIS:HA	1.71	0.45
1:B:341:GLU:O	1:B:345:ARG:HG3	2.16	0.45
1:C:311:VAL:HA	1:C:312:HIS:HA	1.72	0.45
1:D:338:GLY:HA2	1:D:378:GLU:O	2.17	0.45
1:A:384:GLU:OE1	1:A:387:ARG:NH2	2.41	0.45
1:C:402:PRO:HG2	1:C:403:TYR:CE1	2.52	0.45
1:A:176:ASN:O	1:A:205:GLU:HA	2.16	0.44
1:B:162:ARG:NH2	1:B:214:GLU:OE1	2.50	0.44
1:B:432:LYS:HA	1:B:432:LYS:HD2	1.62	0.44
1:C:312:HIS:O	1:C:335:HIS:HA	2.17	0.44
1:A:188:VAL:HA	1:A:234:THR:O	2.18	0.44
1:A:465:GLU:HG2	1:A:510:TRP:HB2	1.99	0.44
1:C:257:ARG:HD2	4:C:706:HOH:O	2.18	0.44
1:C:452:ASN:O	1:C:454:SER:N	2.50	0.44
1:B:13:THR:HG22	1:B:145:GLU:HG2	2.00	0.44
1:B:270:LEU:HD21	1:B:329:LEU:HD13	2.00	0.44
1:A:392:GLU:O	1:A:395:GLU:HG2	2.18	0.44
1:C:294:GLN:O	1:C:298:MET:HG3	2.17	0.43
1:D:226:GLU:CD	1:D:226:GLU:H	2.21	0.43
1:D:378:GLU:OE1	2:D:601:ADA:H1	2.18	0.43
1:D:200:ILE:HD12	1:D:210:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ALA:HB2	1:A:144:LEU:HD21	2.00	0.43
1:B:526:PRO:HB3	1:C:526:PRO:HB3	2.00	0.43
1:D:495:LEU:HD11	1:D:509:ILE:HD11	1.99	0.43
1:A:88:VAL:HG13	1:A:100:VAL:HG11	2.00	0.43
1:A:103:LYS:NZ	4:A:720:HOH:O	2.52	0.43
1:B:381:SER:HB3	1:B:390:TYR:CZ	2.54	0.43
1:B:75:VAL:HG11	1:B:79:ALA:HB2	2.01	0.43
1:A:412:ARG:NH2	4:A:719:HOH:O	2.51	0.43
1:C:271:ARG:NH1	1:C:556:GLY:O	2.47	0.43
1:D:413:PHE:CE2	1:D:446:LEU:HB2	2.54	0.43
1:D:526:PRO:HG3	1:A:526:PRO:HG3	2.01	0.42
1:D:538:TYR:HB3	1:B:538:TYR:CE1	2.54	0.42
1:C:176:ASN:O	1:C:205:GLU:HA	2.19	0.42
1:A:256:ILE:HD11	1:A:265:LEU:HD12	2.01	0.42
1:B:69:ARG:NE	1:B:99:ASP:OD2	2.46	0.42
1:A:414:LYS:NZ	1:A:445:GLU:OE1	2.47	0.42
1:B:176:ASN:O	1:B:205:GLU:HA	2.19	0.42
1:D:549:LYS:O	1:D:553:ARG:HB2	2.20	0.42
1:B:549:LYS:HE2	1:B:553:ARG:NH1	2.35	0.41
1:B:76:SER:HA	1:B:77:HIS:HA	1.79	0.41
1:C:387:ARG:HA	1:C:418:CYS:SG	2.60	0.41
1:D:372:ILE:HD11	1:D:407:SER:HB2	2.02	0.41
1:A:311:VAL:HA	1:A:312:HIS:HA	1.75	0.41
1:B:535:VAL:CG1	1:B:539:ARG:HA	2.50	0.41
1:C:77:HIS:CD2	1:C:118:ASN:HA	2.55	0.41
1:C:147:LEU:HD13	1:C:151:TYR:CD2	2.55	0.41
1:C:66:GLY:HA2	1:C:104:ASP:HA	2.01	0.41
1:D:188:VAL:HA	1:D:234:THR:O	2.20	0.41
1:D:311:VAL:HA	1:D:312:HIS:HA	1.67	0.41
1:C:69:ARG:HB2	1:C:147:LEU:HD11	2.03	0.41
1:A:160:PHE:HE2	1:A:169:LYS:HG2	1.85	0.41
1:B:358:ARG:NH1	4:B:711:HOH:O	2.44	0.41
1:C:449:TRP:O	1:C:452:ASN:O	2.38	0.41
1:B:106:ARG:HG2	4:B:885:HOH:O	2.20	0.41
1:A:397:ILE:HG21	1:A:406:ARG:HG2	2.03	0.41
1:D:432:LYS:HD2	1:D:432:LYS:HA	1.65	0.41
1:A:529:MET:HE1	1:A:537:GLU:HB3	2.03	0.41
1:D:527:ARG:HB3	1:A:474:TYR:CE2	2.55	0.41
1:C:439:VAL:HG11	1:C:494:GLN:HA	2.03	0.41
1:B:328:ILE:O	1:B:369:SER:HB2	2.20	0.41
1:D:492:LYS:HB3	1:D:492:LYS:HE2	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:THR:HB	1:D:117:ASP:HB3	2.03	0.40
1:A:331:TRP:CD1	1:A:331:TRP:C	2.94	0.40
1:C:76:SER:HA	1:C:77:HIS:HA	1.76	0.40
1:D:398:LYS:HD2	1:D:398:LYS:HA	1.93	0.40
1:D:152:LEU:HD23	1:D:174:VAL:HG22	2.03	0.40
1:C:432:LYS:HG2	1:C:439:VAL:CG2	2.51	0.40

All (3) 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)
1:B:240:ALA:O	1:C:194:SER:OG[1_656]	2.03	0.17
1:B:194:SER:OG	1:C:240:ALA:O[1_656]	2.06	0.14
4:B:949:HOH:O	4:C:968:HOH:O[1_655]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/574 (96%)	532 (97%)	16 (3%)	2 (0%)	34	37
1	B	557/574 (97%)	537 (96%)	19 (3%)	1 (0%)	47	55
1	C	557/574 (97%)	537 (96%)	18 (3%)	2 (0%)	34	37
1	D	551/574 (96%)	537 (98%)	12 (2%)	2 (0%)	34	37
All	All	2215/2296 (96%)	2143 (97%)	65 (3%)	7 (0%)	41	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	93	ASN
1	A	93	ASN

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Mol	Chain	Res	Type
1	A	413	PHE
1	B	93	ASN
1	C	93	ASN
1	C	453	GLU
1	D	413	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/499 (97%)	469 (97%)	14 (3%)	42	51
1	B	485/499 (97%)	475 (98%)	10 (2%)	53	62
1	C	485/499 (97%)	471 (97%)	14 (3%)	42	51
1	D	484/499 (97%)	475 (98%)	9 (2%)	57	66
All	All	1937/1996 (97%)	1890 (98%)	47 (2%)	49	58

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	29	GLN
1	D	175	ARG
1	D	209	SER
1	D	213	GLU
1	D	247	ILE
1	D	254	ARG
1	D	331	TRP
1	D	464	THR
1	D	476	THR
1	A	46	TYR
1	A	51	SER
1	A	162	ARG
1	A	163	LYS
1	A	164	ASP
1	A	185	SER
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	254	ARG
1	A	331	TRP
1	A	412	ARG
1	A	441	ASP
1	A	453	GLU
1	A	476	THR
1	A	496	GLN
1	B	29	GLN
1	B	51	SER
1	B	139	SER
1	B	175	ARG
1	B	185	SER
1	B	254	ARG
1	B	331	TRP
1	B	412	ARG
1	B	432	LYS
1	B	535	VAL
1	C	63	GLU
1	C	90	SER
1	C	139	SER
1	C	175	ARG
1	C	185	SER
1	C	209	SER
1	C	254	ARG
1	C	331	TRP
1	C	395	GLU
1	C	440	GLU
1	C	452	ASN
1	C	453	GLU
1	C	454	SER
1	C	520	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	HIS
1	C	489	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	ADA	B	601	-	10,13,13	1.06	0	15,19,19	1.21	2 (13%)
2	ADA	C	601	-	10,13,13	1.21	1 (10%)	15,19,19	1.33	2 (13%)
2	ADA	A	601	-	10,13,13	1.33	1 (10%)	15,19,19	1.28	3 (20%)
2	ADA	D	601	-	10,13,13	1.39	2 (20%)	15,19,19	1.08	1 (6%)

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	ADA	B	601	-	-	0/0/24/24	0/1/1/1
2	ADA	C	601	-	-	0/0/24/24	0/1/1/1
2	ADA	A	601	-	-	0/0/24/24	0/1/1/1
2	ADA	D	601	-	-	0/0/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ADA	O5-C5	2.50	1.47	1.44
2	A	601	ADA	O5-C5	2.42	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	ADA	O5-C5	2.41	1.47	1.44
2	D	601	ADA	C4-C3	-2.30	1.46	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ADA	C1-C2-C3	2.80	116.12	110.31
2	B	601	ADA	C1-C2-C3	2.69	115.89	110.31
2	A	601	ADA	C1-C2-C3	2.56	115.62	110.31
2	D	601	ADA	C1-C2-C3	2.47	115.44	110.31
2	C	601	ADA	O5-C1-C2	2.38	114.54	110.28
2	A	601	ADA	O5-C1-C2	2.36	114.50	110.28
2	B	601	ADA	C4-C3-C2	2.21	114.68	110.82
2	A	601	ADA	O4-C4-C5	-2.18	105.89	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADA	2	0
2	A	601	ADA	1	0
2	D	601	ADA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/574 (96%)	0.25	17 (3%) 49 52	15, 24, 44, 58	0
1	B	559/574 (97%)	0.20	17 (3%) 50 53	16, 25, 39, 58	0
1	C	559/574 (97%)	0.24	19 (3%) 45 47	15, 25, 39, 52	0
1	D	555/574 (96%)	0.33	28 (5%) 28 31	16, 25, 46, 63	0
All	All	2227/2296 (96%)	0.26	81 (3%) 42 44	15, 25, 42, 63	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	163	LYS	4.7
1	A	106	ARG	4.7
1	D	107	PRO	4.4
1	D	106	ARG	4.2
1	D	180	GLY	3.9
1	D	448	GLN	3.8
1	D	408	SER	3.7
1	C	331	TRP	3.6
1	B	436	ASP	3.4
1	B	107	PRO	3.3
1	D	502	GLU	3.2
1	A	108	GLY	3.2
1	B	163	LYS	3.2
1	A	179	SER	3.2
1	C	436	ASP	3.1
1	D	426	SER	3.1
1	C	462	LEU	2.9
1	D	179	SER	2.9
1	C	464	THR	2.9
1	D	331	TRP	2.9
1	D	181	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	105	ILE	2.8
1	D	311	VAL	2.8
1	D	436	ASP	2.8
1	D	201	VAL	2.8
1	D	104	ASP	2.7
1	C	107	PRO	2.7
1	D	162	ARG	2.7
1	D	407	SER	2.7
1	B	28	THR	2.7
1	B	453	GLU	2.6
1	D	192	LYS	2.6
1	D	28	THR	2.6
1	A	181	ARG	2.6
1	C	409	ALA	2.6
1	D	108	GLY	2.6
1	C	452	ASN	2.6
1	B	178	SER	2.5
1	D	309	ARG	2.5
1	C	453	GLU	2.5
1	A	65	LYS	2.5
1	A	311	VAL	2.5
1	C	28	THR	2.5
1	C	276	CYS	2.5
1	A	201	VAL	2.4
1	D	203	GLU	2.4
1	B	162	ARG	2.4
1	A	202	LEU	2.4
1	A	33	ALA	2.4
1	A	238	ARG	2.4
1	C	310	THR	2.4
1	D	462	LEU	2.3
1	D	244	ALA	2.3
1	B	102	LEU	2.3
1	C	426	SER	2.3
1	C	554	SER	2.3
1	B	106	ARG	2.3
1	D	342	GLU	2.3
1	A	104	ASP	2.3
1	B	554	SER	2.3
1	A	107	PRO	2.2
1	B	31	GLU	2.2
1	C	466	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	162	ARG	2.2
1	A	203	GLU	2.2
1	D	463	ILE	2.2
1	B	409	ALA	2.1
1	C	435	HIS	2.1
1	D	554	SER	2.1
1	D	164	ASP	2.1
1	A	453	GLU	2.1
1	B	452	ASN	2.1
1	C	372	ILE	2.1
1	B	65	LYS	2.1
1	B	86	LYS	2.1
1	A	164	ASP	2.1
1	C	219	TRP	2.1
1	C	165	GLY	2.0
1	A	342	GLU	2.0
1	B	508	TYR	2.0
1	B	204	GLY	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](#)

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	ADA	C	601	13/13	0.93	0.12	17,22,27,27	0
2	ADA	A	601	13/13	0.94	0.13	20,22,24,26	0
2	ADA	D	601	13/13	0.95	0.12	14,19,23,29	0
2	ADA	B	601	13/13	0.95	0.11	16,22,26,28	0
3	CL	B	602	1/1	0.99	0.13	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	A	602	1/1	0.99	0.13	23,23,23,23	0
3	CL	C	602	1/1	0.99	0.13	22,22,22,22	0
3	CL	D	602	1/1	0.99	0.07	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.