



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 PM UTC

PDB ID : 2V5C / pdb_00002v5c
Title : Family 84 glycoside hydrolase from Clostridium perfringens, 2.1 Angstrom structure
Authors : Ficko-Blean, E.; Gregg, K.J.; Adams, J.J.; Hehemann, J.H.; Smith, S.J.; Czjzek, M.; Boraston, A.B.
Deposited on : 2008-10-02
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

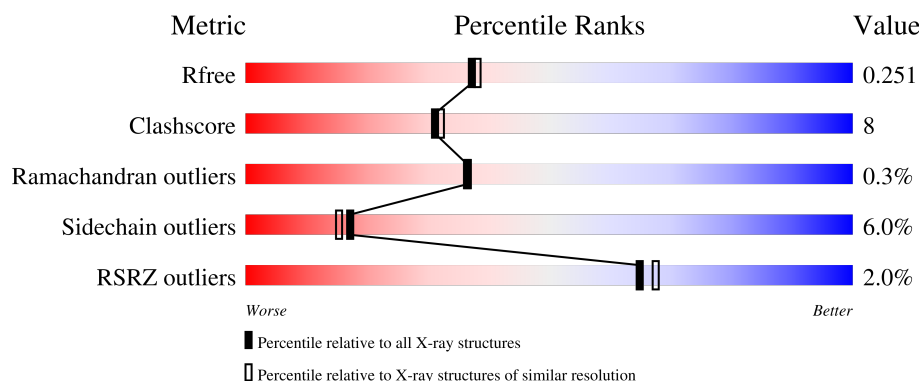
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	594	% 80% 16% . .
1	B	594	3% 78% 18% . .

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
3	CAC	A	1628	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10495 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.

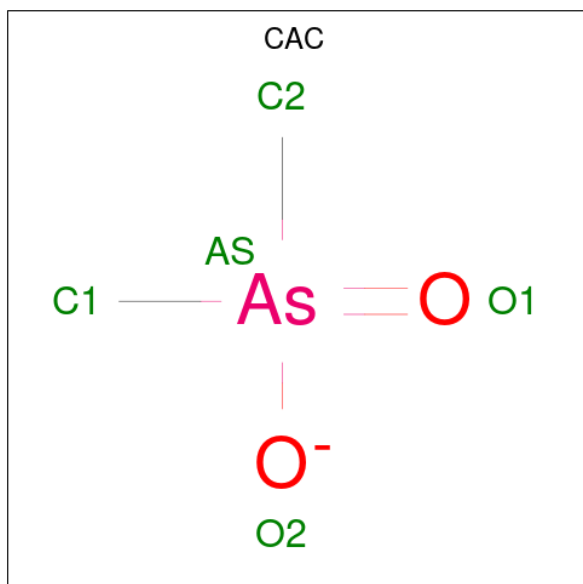
- Molecule 1 is a protein called O-GLCNACASE NAGJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	3	0
			4641	2922	762	940	17			
1	B	584	Total	C	N	O	S	0	3	0
			4632	2917	757	940	18			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

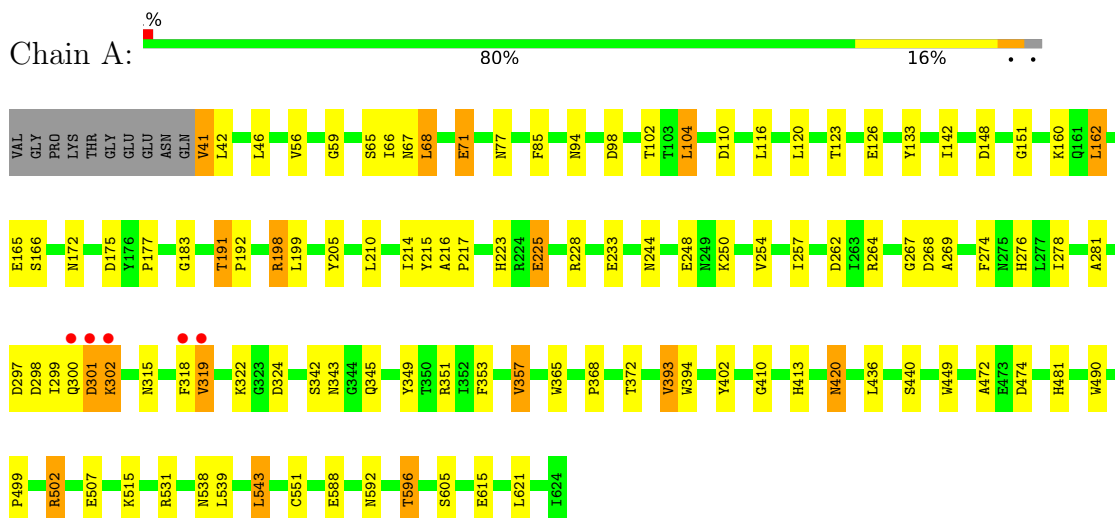
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	626	Total	O	0	0
			626	626		
5	B	565	Total	O	0	0
			565	565		

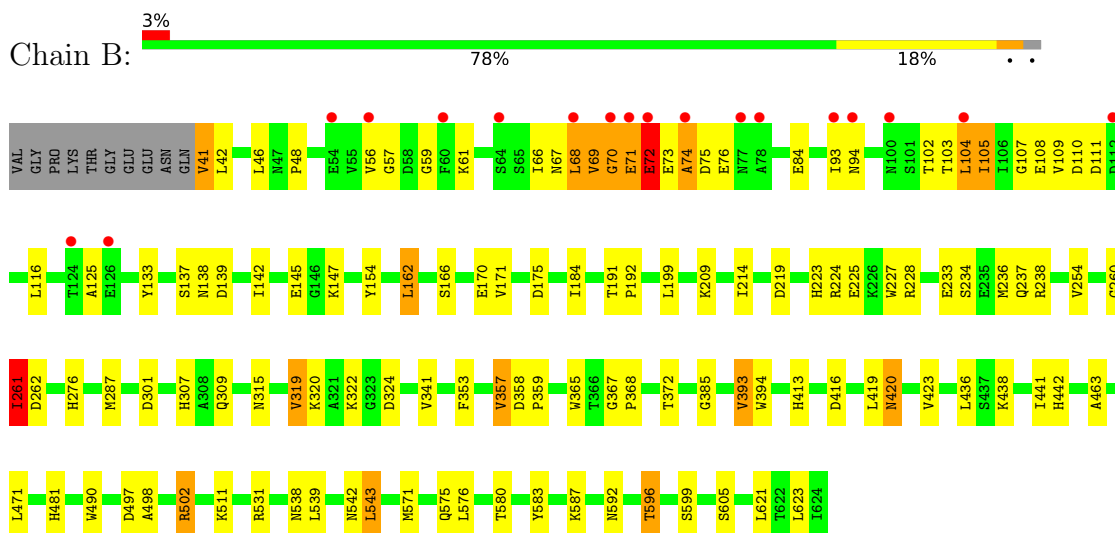
3 Residue-property plots [i](#)

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: O-GLCNACASE NAGJ



• Molecule 1: O-GLCNACASE NAGJ



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.38Å 150.05Å 155.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.41 – 2.10 105.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (105.41-2.10) 99.7 (105.41-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.75 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.255 0.195 , 0.251	Depositor DCC
R_{free} test set	4440 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10495	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, CA, NA

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	0.74	4/4749 (0.1%)	0.94	14/6447 (0.2%)
1	B	0.72	0/4737	0.98	15/6432 (0.2%)
All	All	0.73	4/9486 (0.0%)	0.96	29/12879 (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	1	1
1	B	0	1
All	All	1	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	PRO	C-O	-6.29	1.16	1.24
1	A	215	TYR	C-O	-5.44	1.17	1.24
1	A	216	ALA	CA-CB	-5.43	1.44	1.53
1	A	297	ASP	C-O	-5.11	1.18	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	GLY	O-C-N	-14.84	109.92	123.42
1	B	70	GLY	CA-C-N	8.29	136.63	121.70
1	B	70	GLY	C-N-CA	8.29	136.63	121.70
1	B	385	GLY	CA-C-N	8.03	130.84	120.56
1	B	385	GLY	C-N-CA	8.03	130.84	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLY	CA-C-N	-7.94	108.52	122.26
1	A	267	GLY	C-N-CA	-7.94	108.52	122.26
1	A	302	LYS	N-CA-C	-7.58	101.72	113.02
1	B	261	ILE	CB-CA-C	-7.31	102.46	112.04
1	B	74	ALA	CA-C-N	7.29	134.83	121.70
1	B	74	ALA	C-N-CA	7.29	134.83	121.70
1	B	490	TRP	N-CA-C	6.73	120.75	112.54
1	B	260	GLY	N-CA-C	6.47	120.72	112.83
1	A	267	GLY	O-C-N	-6.41	116.91	123.19
1	B	73	GLU	N-CA-C	-6.26	104.55	111.82
1	A	268	ASP	N-CA-CB	6.24	119.82	110.53
1	A	183	GLY	N-CA-C	5.78	121.02	111.59
1	A	148	ASP	CA-C-N	5.77	126.39	119.98
1	A	148	ASP	C-N-CA	5.77	126.39	119.98
1	A	490	TRP	N-CA-C	5.68	120.05	113.18
1	A	268	ASP	CB-CA-C	5.58	119.35	109.65
1	B	367	GLY	CA-C-N	5.45	125.12	119.56
1	B	367	GLY	C-N-CA	5.45	125.12	119.56
1	A	268	ASP	N-CA-C	5.39	120.01	113.38
1	A	393	VAL	N-CA-C	5.25	116.14	108.53
1	B	72	GLU	CA-C-N	5.22	128.24	120.31
1	B	72	GLU	C-N-CA	5.22	128.24	120.31
1	A	472	ALA	N-CA-C	5.07	116.49	111.07
1	A	151	GLY	CA-C-O	-5.03	115.57	120.75

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	268	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ASP	Peptide
1	B	69	VAL	Peptide

5.2 Too-close contacts ⓘ

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	4641	0	4448	66	0
1	B	4632	0	4432	84	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	15	0	0	1	0
3	B	10	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	626	0	0	10	0
5	B	565	0	0	11	0
All	All	10495	0	8880	149	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 8.

All (149) 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:B:71:GLU:O	1:B:72:GLU:HG2	1.47	1.14
1:B:74:ALA:HB1	1:B:75:ASP:C	1.75	1.11
1:B:571:MET:HE3	1:B:587:LYS:HB2	1.36	1.06
1:B:71:GLU:C	1:B:72:GLU:HG2	1.92	0.94
1:A:315:ASN:HA	1:A:319:VAL:HG13	1.49	0.94
1:A:507:GLU:HG3	5:A:2212:HOH:O	1.67	0.91
1:B:71:GLU:O	1:B:72:GLU:CG	2.17	0.91
1:A:302:LYS:O	1:A:302:LYS:HG3	1.73	0.89
1:A:299:ILE:HG12	1:A:301:ASP:HB2	1.54	0.87
1:A:68:LEU:HD13	1:A:71:GLU:HG2	1.61	0.83
1:B:74:ALA:HB3	5:B:2018:HOH:O	1.78	0.81
1:A:596:THR:HG21	5:A:2590:HOH:O	1.81	0.80
1:A:315:ASN:HA	1:A:319:VAL:CG1	2.12	0.79
1:B:74:ALA:HB1	1:B:75:ASP:CA	2.15	0.77
1:B:580:THR:HG22	5:B:2508:HOH:O	1.84	0.76
1:B:592[A]:ASN:ND2	5:B:2527:HOH:O	2.18	0.75
1:B:571:MET:HE3	1:B:587:LYS:CB	2.15	0.74
1:B:592[B]:ASN:ND2	5:B:2528:HOH:O	2.21	0.73
1:B:413:HIS:HE1	3:B:1627:CAC:O1	1.72	0.71
1:B:596:THR:HG21	5:B:2529:HOH:O	1.89	0.71
1:B:69:VAL:O	1:B:105:ILE:HA	1.91	0.69
1:B:74:ALA:HB1	1:B:76:GLU:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:HD21	1:A:98:ASP:H	1.42	0.67
1:B:571:MET:HE2	1:B:583:TYR:CE1	2.29	0.67
1:B:502:ARG:O	1:B:502:ARG:HD3	1.94	0.67
1:B:228:ARG:HG2	1:B:276:HIS:HB3	1.76	0.66
1:B:104:LEU:HD22	1:B:142:ILE:HB	1.80	0.64
3:B:1628:CAC:C1	5:B:2265:HOH:O	2.46	0.63
1:B:315:ASN:HA	1:B:319:VAL:HG13	1.80	0.63
1:B:228:ARG:HH22	1:B:262:ASP:CG	2.06	0.63
1:A:353:PHE:O	1:A:357:VAL:HG22	1.99	0.63
1:A:592:ASN:O	1:A:596:THR:HG23	2.00	0.62
1:B:571:MET:HE2	1:B:583:TYR:CZ	2.35	0.61
1:B:133:TYR:CE2	1:B:175:ASP:HB3	2.34	0.61
1:A:351:ARG:NH2	5:A:2330:HOH:O	2.33	0.61
1:B:110:ASP:HB3	5:B:2042:HOH:O	2.01	0.61
1:B:353:PHE:O	1:B:357:VAL:HG22	2.01	0.60
1:B:137:SER:HB3	1:B:171:VAL:H	1.67	0.60
1:B:538:ASN:ND2	1:B:542:ASN:HD22	2.00	0.60
1:B:481:HIS:HD2	1:B:605:SER:OG	1.85	0.59
1:A:264:ARG:CZ	1:A:269:ALA:HB1	2.33	0.58
1:B:502:ARG:HD3	1:B:502:ARG:C	2.27	0.58
1:A:502:ARG:NH2	1:A:615:GLU:OE2	2.38	0.56
1:A:413:HIS:HE1	3:A:1627:CAC:O2	1.89	0.56
1:A:539:LEU:O	1:A:543:LEU:HB2	2.05	0.56
1:B:74:ALA:CB	1:B:75:ASP:CA	2.83	0.56
1:A:413:HIS:HD2	5:A:2460:HOH:O	1.88	0.56
1:B:41:VAL:HG13	1:B:59:GLY:HA3	1.88	0.55
1:A:228:ARG:HG2	1:A:276:HIS:HB3	1.89	0.55
1:A:596:THR:CG2	5:A:2590:HOH:O	2.46	0.55
1:B:497:ASP:O	1:B:498:ALA:C	2.51	0.54
1:B:70:GLY:HA2	1:B:71:GLU:HB2	1.90	0.54
1:B:322:LYS:C	1:B:324:ASP:H	2.16	0.54
1:A:228:ARG:HH22	1:A:262:ASP:CG	2.16	0.54
1:A:225:GLU:H	1:A:225:GLU:CD	2.14	0.54
1:A:46:LEU:HD21	1:A:162:LEU:HD13	1.89	0.54
1:B:227:TRP:HD1	1:B:261:ILE:HD11	1.72	0.54
1:B:320:LYS:HG2	5:B:2088:HOH:O	2.09	0.53
1:B:66:ILE:HG22	1:B:102:THR:HB	1.91	0.52
1:A:539:LEU:HB3	1:A:543:LEU:HD22	1.92	0.52
1:B:71:GLU:O	1:B:72:GLU:CD	2.52	0.52
1:A:402:TYR:HA	1:B:623:LEU:CD1	2.40	0.52
1:A:436:LEU:HD21	1:A:551:CYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:HD22	1:A:250:LYS:NZ	2.08	0.51
1:A:368:PRO:HD2	1:A:372:THR:HG21	1.92	0.51
1:A:481:HIS:HE1	5:A:2190:HOH:O	1.94	0.51
1:A:315:ASN:CA	1:A:319:VAL:HG13	2.32	0.51
1:B:67:ASN:ND2	1:B:94:ASN:HD22	2.08	0.51
1:A:300:GLN:O	1:A:301:ASP:OD2	2.30	0.50
1:A:133:TYR:CE2	1:A:175:ASP:HB3	2.47	0.49
1:B:71:GLU:O	1:B:71:GLU:HG2	2.12	0.49
1:A:198:ARG:NH2	1:A:217:PRO:HB3	2.27	0.49
1:A:474:ASP:OD2	1:A:531[A]:ARG:NH1	2.38	0.49
1:B:236:MET:HE1	1:B:287:MET:HG2	1.94	0.49
1:A:596:THR:HG22	5:A:2591:HOH:O	2.13	0.49
1:A:274:PHE:CE2	1:A:278:ILE:HD11	2.47	0.49
1:A:298:ASP:OD2	1:A:298:ASP:O	2.30	0.49
1:B:576:LEU:HD23	1:B:621:LEU:HD11	1.93	0.49
1:A:41:VAL:HG22	1:A:59:GLY:HA3	1.95	0.49
1:B:48:PRO:HD2	1:B:209:LYS:HD2	1.93	0.49
1:A:481:HIS:HD2	1:A:605:SER:OG	1.95	0.49
1:A:588:GLU:OE2	1:A:592:ASN:ND2	2.45	0.48
1:A:592:ASN:O	1:A:596:THR:CG2	2.61	0.48
1:B:413:HIS:HD2	5:B:2305:HOH:O	1.96	0.48
1:B:301:ASP:OD1	1:B:307:HIS:NE2	2.47	0.48
1:B:420:ASN:H	1:B:420:ASN:HD22	1.60	0.48
1:A:345:GLN:NE2	5:A:2323:HOH:O	2.40	0.47
1:B:511:LYS:NZ	5:B:2419:HOH:O	2.46	0.47
1:B:575:GLN:NE2	1:B:621:LEU:H	2.12	0.47
1:A:502:ARG:C	1:A:502:ARG:HD3	2.38	0.47
1:B:125:ALA:O	1:B:147:LYS:HG2	2.14	0.47
1:A:205:TYR:HB3	1:A:210:LEU:HB2	1.97	0.47
1:A:302:LYS:O	1:A:349:TYR:HD1	1.98	0.47
1:A:420:ASN:H	1:A:420:ASN:HD22	1.63	0.46
1:B:227:TRP:CD1	1:B:261:ILE:HD11	2.51	0.46
1:A:66:ILE:HG22	1:A:102:THR:HB	1.97	0.46
1:B:438:LYS:O	1:B:442:HIS:HB2	2.16	0.46
1:B:67:ASN:HB2	1:B:103:THR:HG23	1.97	0.46
1:A:67:ASN:ND2	1:A:94:ASN:HD22	2.13	0.46
1:A:104:LEU:HD22	1:A:142:ILE:HB	1.98	0.46
1:A:402:TYR:HA	1:B:623:LEU:HD13	1.98	0.45
1:A:177:PRO:HB3	1:A:449:TRP:CE3	2.51	0.45
1:B:368:PRO:HD2	1:B:372:THR:HG21	1.98	0.45
1:B:539:LEU:HB3	1:B:543:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:HA	1:B:170:GLU:HG2	1.98	0.45
1:B:261:ILE:H	1:B:261:ILE:HG13	1.60	0.45
1:A:410:GLY:O	1:A:440[A]:SER:HB3	2.17	0.45
1:A:502:ARG:HD3	1:A:502:ARG:O	2.17	0.45
1:B:70:GLY:CA	1:B:71:GLU:CB	2.94	0.45
1:B:233:GLU:HA	1:B:236:MET:HG2	1.99	0.45
1:A:502:ARG:HD3	1:A:502:ARG:HA	1.66	0.44
1:A:531[A]:ARG:NH2	5:A:2523:HOH:O	2.49	0.44
1:B:70:GLY:HA2	1:B:71:GLU:CB	2.46	0.44
1:A:342:SER:O	1:A:343:ASN:HB2	2.17	0.44
1:B:61:LYS:HE3	1:B:166:SER:HB2	1.99	0.44
1:B:107:GLY:O	1:B:145:GLU:HA	2.17	0.44
1:B:228:ARG:NH2	1:B:262:ASP:CG	2.75	0.44
1:A:394:TRP:C	1:A:394:TRP:CD1	2.95	0.44
1:B:46:LEU:HD21	1:B:162:LEU:HD13	1.99	0.44
1:B:238:ARG:HG2	5:B:2186:HOH:O	2.17	0.44
1:B:228:ARG:NH2	1:B:262:ASP:OD1	2.49	0.44
1:A:515:LYS:HA	5:A:2491:HOH:O	2.18	0.43
1:A:299:ILE:HG23	1:A:301:ASP:H	1.82	0.43
1:B:104:LEU:CD2	1:B:142:ILE:HB	2.46	0.43
1:B:224:ARG:O	1:B:261:ILE:HD11	2.18	0.43
1:B:442:HIS:CE1	1:B:463:ALA:HA	2.54	0.43
1:A:191:THR:HA	1:A:192:PRO:HD3	1.89	0.42
1:A:120:LEU:HB3	1:A:123:THR:O	2.19	0.42
1:A:281:ALA:HB1	1:A:318:PHE:CZ	2.54	0.42
1:A:85:PHE:CD1	1:A:160:LYS:HG2	2.55	0.42
1:A:322:LYS:C	1:A:324:ASP:H	2.27	0.42
1:B:538:ASN:ND2	1:B:542:ASN:ND2	2.66	0.42
1:B:214:ILE:HA	1:B:254:VAL:HB	2.01	0.42
1:B:192:PRO:HG3	1:B:219:ASP:HB3	2.02	0.42
1:A:214:ILE:HA	1:A:254:VAL:HB	2.03	0.41
1:B:109:VAL:C	1:B:111:ASP:H	2.28	0.41
1:B:416:ASP:HB3	1:B:419:LEU:HD13	2.02	0.41
1:A:244:ASN:O	1:A:248:GLU:HG3	2.20	0.41
1:B:358:ASP:HA	1:B:359:PRO:HD3	1.92	0.41
1:B:393:VAL:HG13	1:B:423:VAL:HG11	2.03	0.41
1:A:165:GLU:O	1:A:166:SER:HB2	2.21	0.41
1:B:539:LEU:O	1:B:543:LEU:HB2	2.20	0.41
1:B:154:TYR:HB3	1:B:209:LYS:HE3	2.01	0.41
1:B:184:ILE:HD11	1:B:441:ILE:HG23	2.03	0.41
1:A:67:ASN:ND2	1:A:98:ASP:H	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLY:HA3	1:B:170:GLU:OE1	2.22	0.40
1:B:68:LEU:HB2	1:B:93:ILE:HG23	2.04	0.40
1:B:394:TRP:C	1:B:394:TRP:CD1	2.99	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	586/594 (99%)	570 (97%)	16 (3%)	0	100	100
1	B	585/594 (98%)	563 (96%)	19 (3%)	3 (0%)	24	22
All	All	1171/1188 (99%)	1133 (97%)	35 (3%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLU
1	B	72	GLU
1	B	234	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/507 (99%)	474 (94%)	29 (6%)	18	16
1	B	502/507 (99%)	471 (94%)	31 (6%)	16	14
All	All	1005/1014 (99%)	945 (94%)	60 (6%)	17	15

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	42	LEU
1	A	56	VAL
1	A	65	SER
1	A	68	LEU
1	A	71	GLU
1	A	104	LEU
1	A	110	ASP
1	A	116	LEU
1	A	126	GLU
1	A	162	LEU
1	A	172	ASN
1	A	191	THR
1	A	198	ARG
1	A	199	LEU
1	A	223	HIS
1	A	225	GLU
1	A	233	GLU
1	A	257	ILE
1	A	319	VAL
1	A	357	VAL
1	A	365	TRP
1	A	393	VAL
1	A	420	ASN
1	A	502	ARG
1	A	538	ASN
1	A	543	LEU
1	A	596	THR
1	A	621	LEU
1	B	41	VAL
1	B	42	LEU
1	B	56	VAL

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Mol	Chain	Res	Type
1	B	68	LEU
1	B	84	GLU
1	B	104	LEU
1	B	105	ILE
1	B	108	GLU
1	B	116	LEU
1	B	139	ASP
1	B	162	LEU
1	B	191	THR
1	B	199	LEU
1	B	223	HIS
1	B	225	GLU
1	B	237	GLN
1	B	261	ILE
1	B	309	GLN
1	B	319	VAL
1	B	341	VAL
1	B	357	VAL
1	B	365	TRP
1	B	393	VAL
1	B	420	ASN
1	B	436	LEU
1	B	471	LEU
1	B	502	ARG
1	B	531	ARG
1	B	543	LEU
1	B	596	THR
1	B	599	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	77	ASN
1	A	80	ASN
1	A	167	ASN
1	A	172	ASN
1	A	240	GLN
1	A	275	ASN
1	A	345	GLN
1	A	413	HIS
1	A	420	ASN

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Mol	Chain	Res	Type
1	A	481	HIS
1	A	614	GLN
1	B	52	ASN
1	B	67	ASN
1	B	80	ASN
1	B	275	ASN
1	B	343	ASN
1	B	413	HIS
1	B	420	ASN
1	B	481	HIS
1	B	538	ASN
1	B	542	ASN
1	B	575	GLN
1	B	614	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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
3	CAC	B	1628	-	2,4,4	2.43	2 (100%)	4,6,6	1.47	1 (25%)
3	CAC	B	1627	-	2,4,4	2.85	2 (100%)	4,6,6	1.52	1 (25%)
3	CAC	A	1629	-	2,4,4	3.02	2 (100%)	4,6,6	1.54	0
3	CAC	A	1628	-	2,4,4	2.71	2 (100%)	4,6,6	2.37	2 (50%)
3	CAC	A	1627	-	2,4,4	2.85	2 (100%)	4,6,6	1.91	1 (25%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1629	CAC	AS-C2	3.13	1.97	1.90
3	A	1629	CAC	AS-C1	2.90	1.97	1.90
3	B	1627	CAC	AS-C2	2.87	1.97	1.90
3	A	1627	CAC	AS-C1	2.87	1.97	1.90
3	A	1628	CAC	AS-C2	2.87	1.97	1.90
3	B	1627	CAC	AS-C1	2.84	1.97	1.90
3	A	1627	CAC	AS-C2	2.83	1.97	1.90
3	B	1628	CAC	AS-C2	2.61	1.96	1.90
3	A	1628	CAC	AS-C1	2.54	1.96	1.90
3	B	1628	CAC	AS-C1	2.24	1.95	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1628	CAC	O1-AS-C1	-3.34	107.35	111.50
3	B	1628	CAC	O1-AS-C1	-2.39	108.53	111.50
3	A	1627	CAC	O1-AS-C2	-2.34	108.58	111.50
3	A	1628	CAC	O1-AS-C2	-2.26	108.69	111.50
3	B	1627	CAC	O1-AS-C2	-2.23	108.72	111.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1628	CAC	1	0
3	B	1627	CAC	1	0
3	A	1627	CAC	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, 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	584/594 (98%)	-0.21	5 (0%) 81 83	8, 26, 48, 59	3 (0%)
1	B	584/594 (98%)	0.04	18 (3%) 51 54	11, 29, 62, 71	3 (0%)
All	All	1168/1188 (98%)	-0.08	23 (1%) 65 67	8, 28, 56, 71	6 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	VAL	4.2
1	A	301	ASP	3.8
1	B	74	ALA	3.3
1	B	104	LEU	2.9
1	A	300	GLN	2.8
1	B	78	ALA	2.8
1	B	126	GLU	2.7
1	B	93	ILE	2.7
1	B	112	ASP	2.7
1	B	100	ASN	2.5
1	B	68	LEU	2.4
1	B	70	GLY	2.4
1	B	64	SER	2.4
1	A	319	VAL	2.3
1	A	302	LYS	2.3
1	B	60	PHE	2.2
1	B	72	GLU	2.2
1	A	318	PHE	2.2
1	B	71	GLU	2.1
1	B	54	GLU	2.1
1	B	77	ASN	2.1
1	B	124	THR	2.0
1	B	94	ASN	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	CAC	A	1628	5/5	0.85	0.21	80,81,82,82	0
2	CA	A	1625	1/1	0.87	0.07	32,32,32,32	0
2	CA	B	1625	1/1	0.89	0.06	35,35,35,35	0
3	CAC	B	1628	5/5	0.91	0.17	78,78,79,79	0
3	CAC	B	1627	5/5	0.93	0.13	81,81,82,82	0
2	CA	A	1626	1/1	0.94	0.06	50,50,50,50	0
3	CAC	A	1627	5/5	0.95	0.15	66,67,68,68	0
2	CA	B	1626	1/1	0.95	0.05	58,58,58,58	0
4	NA	B	1629	1/1	0.95	0.06	33,33,33,33	0
4	NA	A	1630	1/1	0.97	0.03	10,10,10,10	0
3	CAC	A	1629	5/5	0.97	0.16	46,47,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.