Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 08:15 pm BST

PDB ID	:	2V5C
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 (i) symbol.

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

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

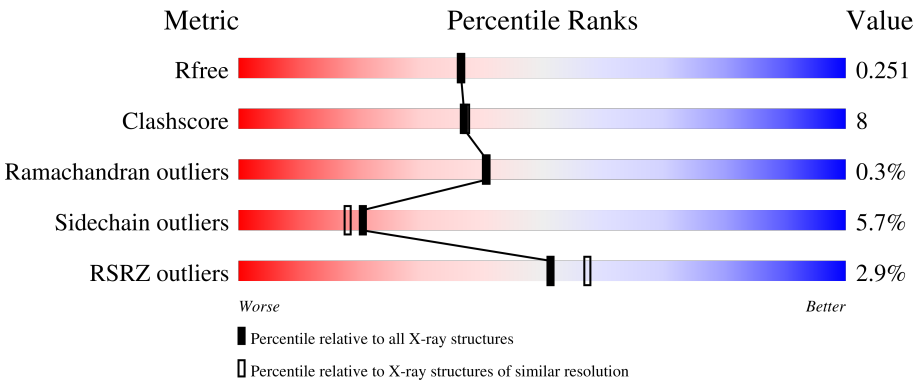
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

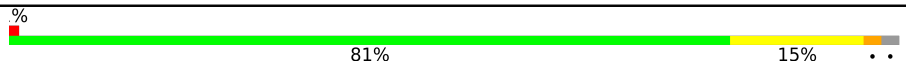
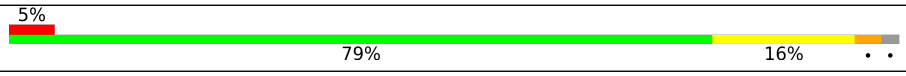
The reported resolution of this entry is 2.10 Å.

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	
1	B	594	

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.

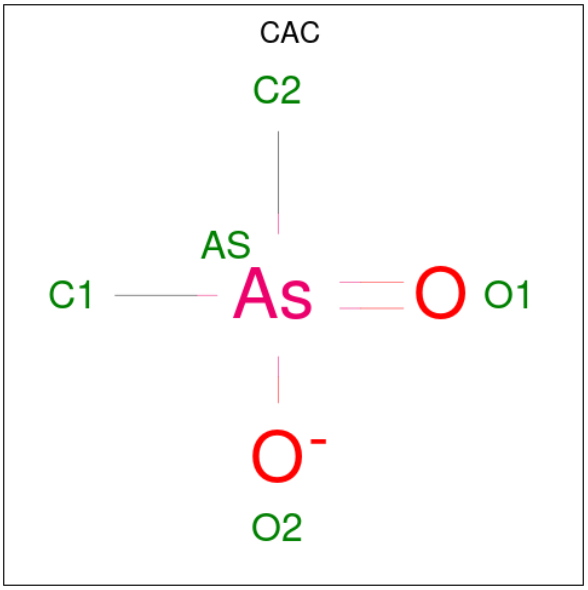
- Molecule 1 is a protein called O-GLCNACASE NAGJ.

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

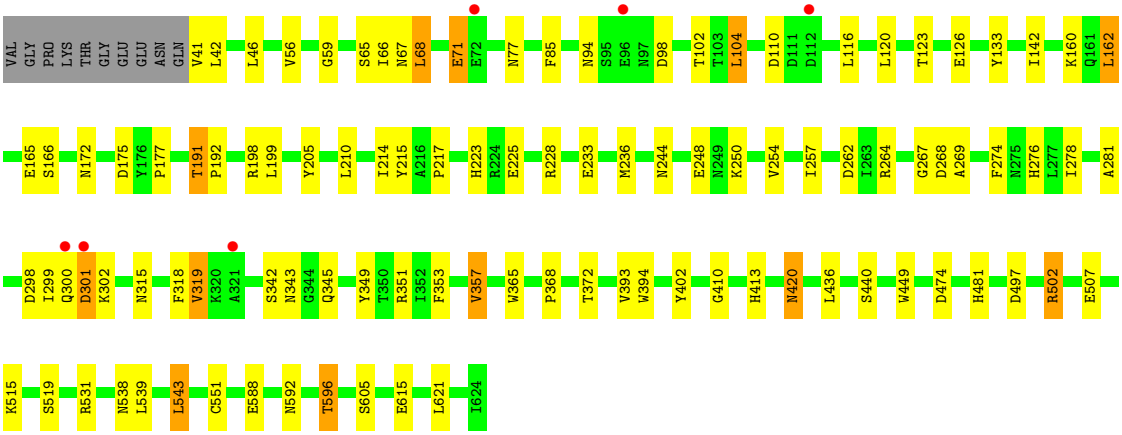
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	626	626	626	0	0
			Total	O		
5	B	565	565	565	0	0

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.

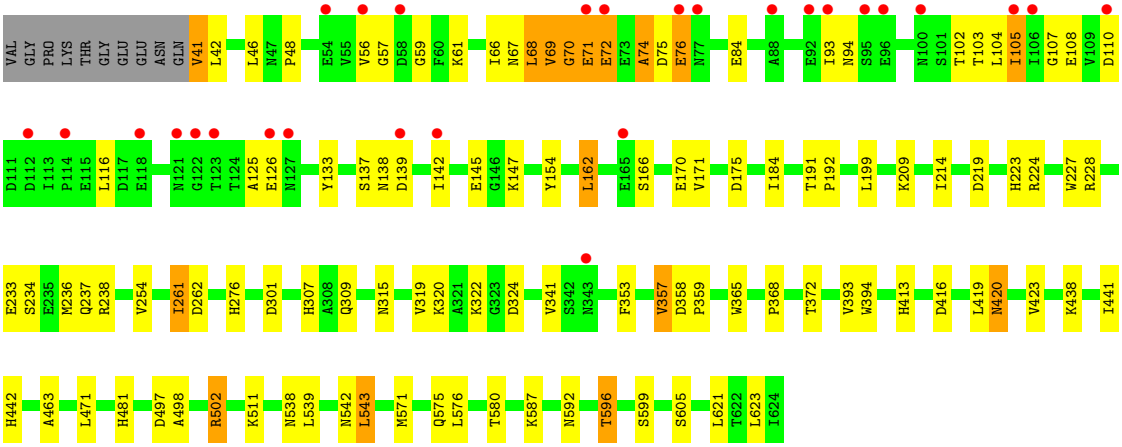
• Molecule 1: O-GLCNACASE NAGJ

Chain A:



• Molecule 1: O-GLCNACASE NAGJ

Chain B:



4 Data and refinement statistics (i)

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 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (105.41-2.10) 99.8 (20.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.59	1/4749 (0.0%)	0.64	3/6447 (0.0%)
1	B	0.55	0/4737	0.64	3/6432 (0.0%)
All	All	0.57	1/9486 (0.0%)	0.64	6/12879 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	TYR	CD1-CE1	-5.25	1.31	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	GLY	O-C-N	-7.99	109.92	122.70
1	B	70	GLY	C-N-CA	5.97	136.63	121.70
1	A	497	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	267	GLY	C-N-CA	-5.27	108.52	121.70
1	B	74	ALA	C-N-CA	5.25	134.83	121.70
1	A	268	ASP	N-CA-CB	5.12	119.82	110.60

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 (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	4641	0	4448	64	0
1	B	4632	0	4432	78	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	141	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 (141) 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	1.06
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:B:71:GLU:C	1:B:72:GLU:HG2	1.92	0.90
1:A:302:LYS:O	1:A:302:LYS:HG3	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:592[B]:ASN:ND2	5:B:2528:HOH:O	2.21	0.73
1:B:571:MET:HE3	1:B:587:LYS:HB2	1.71	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
1:A:67:ASN:HD21	1:A:98:ASP:H	1.42	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: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: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:571:MET:CE	1:B:587:LYS:HB2	2.32	0.59
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:228:ARG:HH22	1:B:262:ASP:CG	2.06	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:70:GLY:HA2	1:B:71:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:502:ARG:HD3	1:B:502:ARG:C	2.27	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: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
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:225:GLU:H	1:A:225:GLU:CD	2.14	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:B:497:ASP:O	1:B:498:ALA:C	2.51	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: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:228:ARG:HH22	1:A:262:ASP:CG	2.16	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:B:322:LYS:C	1:B:324:ASP:H	2.16	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:71:GLU:O	1:B:72:GLU:CD	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	1:A:502:ARG:HD3	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: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:502:ARG:HD3	1:A:502:ARG:C	2.38	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:416:ASP:HB3	1:B:419:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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%)	29	26
All	All	1171/1188 (99%)	1133 (97%)	35 (3%)	3 (0%)	41	41

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/507 (99%)	474 (94%)	29 (6%)	20	17
1	B	502/507 (99%)	474 (94%)	28 (6%)	21	18
All	All	1005/1014 (99%)	948 (94%)	57 (6%)	20	18

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	199	LEU
1	A	223	HIS
1	A	233	GLU
1	A	236	MET
1	A	257	ILE
1	A	319	VAL
1	A	357	VAL
1	A	365	TRP
1	A	393	VAL
1	A	394	TRP
1	A	420	ASN
1	A	502	ARG
1	A	519	SER
1	A	538	ASN
1	A	543	LEU

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Mol	Chain	Res	Type
1	A	596	THR
1	A	621	LEU
1	B	41	VAL
1	B	42	LEU
1	B	56	VAL
1	B	68	LEU
1	B	76	GLU
1	B	84	GLU
1	B	105	ILE
1	B	108	GLU
1	B	116	LEU
1	B	126	GLU
1	B	139	ASP
1	B	162	LEU
1	B	191	THR
1	B	199	LEU
1	B	223	HIS
1	B	237	GLN
1	B	261	ILE
1	B	309	GLN
1	B	341	VAL
1	B	357	VAL
1	B	365	TRP
1	B	394	TRP
1	B	420	ASN
1	B	471	LEU
1	B	502	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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	77	ASN
1	A	80	ASN
1	A	172	ASN
1	A	275	ASN
1	A	413	HIS
1	A	420	ASN
1	A	481	HIS

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Mol	Chain	Res	Type
1	B	67	ASN
1	B	196	GLN
1	B	275	ASN
1	B	300	GLN
1	B	309	GLN
1	B	343	ASN
1	B	345	GLN
1	B	413	HIS
1	B	420	ASN
1	B	481	HIS
1	B	538	ASN
1	B	575	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	1629	-	0,4,4	-	-	0,6,6	-	-
3	CAC	B	1627	-	0,4,4	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CAC	A	1627	-	0,4,4	-	-	0,6,6	-	-
3	CAC	B	1628	-	0,4,4	-	-	0,6,6	-	-
3	CAC	A	1628	-	0,4,4	-	-	0,6,6	-	-

There are no bond length outliers.

There are no bond angle outliers.

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	1627	CAC	1	0
3	A	1627	CAC	1	0
3	B	1628	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 (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	584/594 (98%)	-0.22	6 (1%)	82	85	12, 26, 48, 59	1 (0%)
1	B	584/594 (98%)	-0.05	28 (4%)	30	36	14, 29, 62, 71	0
All	All	1168/1188 (98%)	-0.13	34 (2%)	51	57	12, 28, 56, 71	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLN	5.5
1	B	93	ILE	5.0
1	A	301	ASP	4.9
1	B	112	ASP	4.9
1	B	100	ASN	4.5
1	B	122	GLY	4.4
1	B	95	SER	4.2
1	B	96	GLU	3.8
1	B	118	GLU	3.8
1	B	56	VAL	3.6
1	B	126	GLU	3.3
1	B	72	GLU	3.1
1	B	142	ILE	2.9
1	B	139	ASP	2.7
1	B	76	GLU	2.6
1	B	343	ASN	2.6
1	B	58	ASP	2.5
1	A	72	GLU	2.5
1	B	106	ILE	2.5
1	A	96	GLU	2.4
1	B	110	ASP	2.4
1	B	114	PRO	2.3
1	B	71	GLU	2.3
1	B	105	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	88	ALA	2.3
1	B	77	ASN	2.3
1	A	321	ALA	2.2
1	B	54	GLU	2.2
1	A	112	ASP	2.2
1	B	165	GLU	2.1
1	B	92	GLU	2.1
1	B	121	ASN	2.1
1	B	123	THR	2.1
1	B	127	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 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	CA	B	1625	1/1	0.89	0.07	35,35,35,35	0
3	CAC	A	1628	5/5	0.91	0.17	80,81,82,82	0
2	CA	B	1626	1/1	0.92	0.03	58,58,58,58	0
2	CA	A	1626	1/1	0.92	0.06	50,50,50,50	0
2	CA	A	1625	1/1	0.94	0.06	32,32,32,32	0
3	CAC	B	1628	5/5	0.94	0.14	78,78,79,79	0
3	CAC	B	1627	5/5	0.96	0.16	81,81,82,82	0
3	CAC	A	1627	5/5	0.97	0.22	66,67,68,68	0
3	CAC	A	1629	5/5	0.97	0.17	46,47,48,48	0
4	NA	B	1629	1/1	0.97	0.10	33,33,33,33	0
4	NA	A	1630	1/1	0.99	0.11	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.