



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:10 PM UTC

PDB ID : 2J4G / pdb_00002j4g
Title : Bacteroides thetaiotaomicron GH84 O-GlcNAcase in complex with n-butyl-thiazoline inhibitor
Authors : Dennis, R.J.; Davies, G.J.
Deposited on : 2006-08-31
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 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

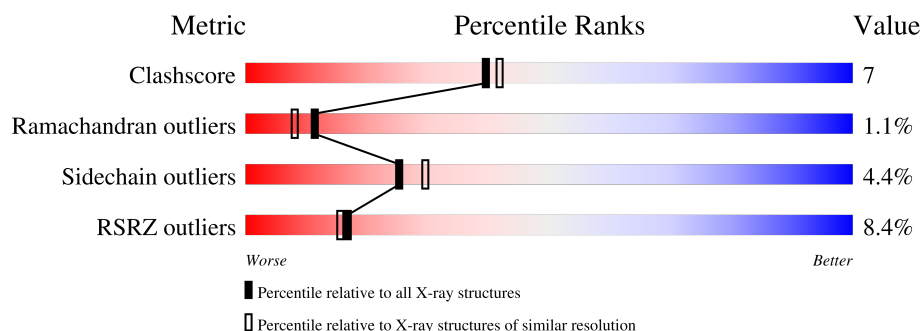
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	715	
1	B	715	

2 Entry composition [i](#)

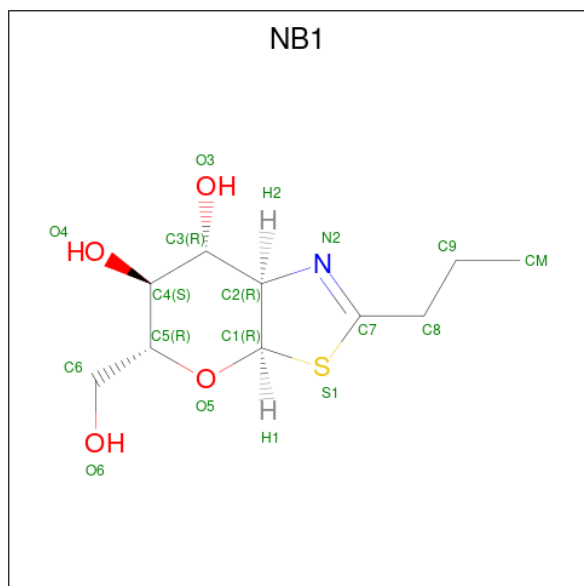
There are 5 unique types of molecules in this entry. The entry contains 10075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYALURONOGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4759	3040	806	897	16			
1	B	580	Total	C	N	O	S	0	0	0
			4706	3009	794	887	16			

- Molecule 2 is (3AR,5R,6S,7R,7AR)-5-(HYDROXYMETHYL)-2-PROPYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D][1,3]THIAZOLE-6,7-DIOL (CCD ID: NB1) (formula: $C_{10}H_{17}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			16	10	1	4	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

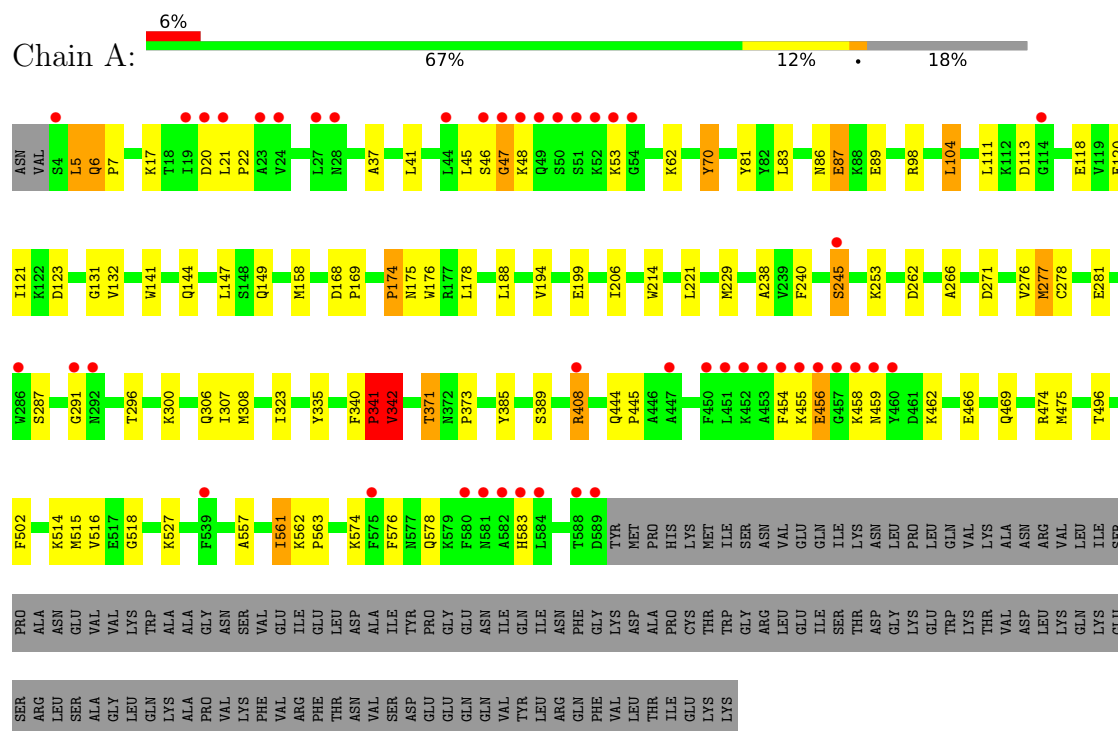
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	280	Total 280	O 280	0	0
5	B	278	Total 278	O 278	0	0

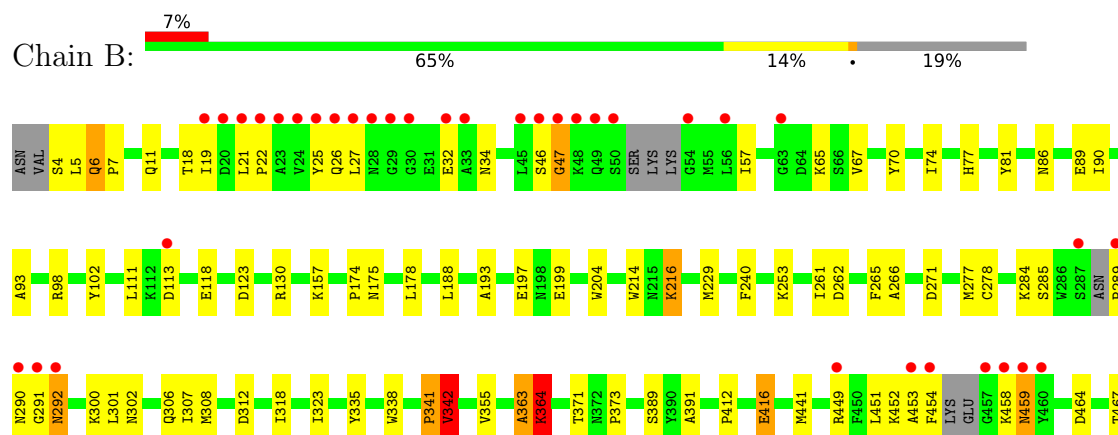
3 Residue-property plots

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: HYALURONOGLUCOSAMINIDASE



• Molecule 1: HYALURONOGLUCOSAMINIDASE



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.11Å 51.71Å 172.78Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	169.03 – 2.25 169.03 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (169.03-2.25) 99.6 (169.03-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.284 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10075	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 63.56 % 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 9.4882e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NB1, GOL, ACT

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	0.83	1/4886 (0.0%)	1.04	9/6626 (0.1%)
1	B	0.86	3/4827 (0.1%)	1.07	9/6544 (0.1%)
All	All	0.84	4/9713 (0.0%)	1.06	18/13170 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	VAL	CA-CB	5.88	1.60	1.54
1	B	556	THR	CA-CB	5.18	1.62	1.53
1	A	496	THR	CA-CB	5.09	1.58	1.54
1	B	342	VAL	CA-C	5.02	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	GLN	N-CA-C	20.81	136.29	110.07
1	B	364	LYS	N-CA-C	-11.19	86.96	110.80
1	B	342	VAL	N-CA-C	-9.74	95.97	109.21
1	B	175	ASN	N-CA-C	-9.24	100.91	113.30
1	A	175	ASN	N-CA-C	-9.13	99.92	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LEU	CA-C-N	7.42	139.89	121.80
1	A	5	LEU	C-N-CA	7.42	139.89	121.80
1	B	6	GLN	N-CA-CB	-7.27	100.47	110.29
1	A	291	GLY	N-CA-C	-5.68	103.35	111.42
1	A	342	VAL	N-CA-CB	5.58	120.43	111.23
1	A	5	LEU	O-C-N	-5.52	116.72	122.96
1	B	291	GLY	N-CA-C	-5.50	100.15	113.18
1	A	561	ILE	N-CA-C	5.40	115.61	110.53
1	B	341	PRO	N-CA-C	5.35	126.00	112.10
1	B	300	LYS	N-CA-C	5.34	117.18	111.36
1	B	318	ILE	CB-CA-C	5.04	117.69	110.84
1	A	291	GLY	CA-C-O	-5.03	116.89	121.47
1	A	245	SER	N-CA-C	5.00	117.01	109.41

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	PRO	Peptide
1	A	341	PRO	Peptide
1	A	5	LEU	Peptide
1	B	174	PRO	Peptide
1	B	341	PRO	Peptide
1	B	363	ALA	Peptide
1	B	5	LEU	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	4759	0	4642	60	0
1	B	4706	0	4583	66	0
2	A	16	0	17	0	0
2	B	16	0	17	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
5	A	280	0	0	9	0
5	B	278	0	0	10	0
All	All	10075	0	9281	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (126) 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:A:245:SER:HB3	5:A:2121:HOH:O	1.66	0.94
1:B:532:LYS:O	1:B:536:GLN:HG3	1.85	0.77
1:B:570:ALA:O	1:B:574:LYS:HE3	1.89	0.72
1:A:277:MET:HE2	1:A:307:ILE:HG23	1.73	0.71
1:A:277:MET:CE	1:A:307:ILE:HG23	2.20	0.71
1:A:6:GLN:H	1:A:7:PRO:C	1.99	0.69
1:B:441:MET:HB2	5:B:2222:HOH:O	1.95	0.67
1:B:6:GLN:HA	1:B:7:PRO:C	2.18	0.66
1:B:188:LEU:HD13	1:B:229:MET:HE1	1.78	0.64
1:A:62:LYS:HD3	5:A:2036:HOH:O	1.98	0.64
1:B:292:ASN:H	1:B:292:ASN:HD22	1.45	0.64
1:A:245:SER:CB	5:A:2121:HOH:O	2.34	0.64
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.81	0.61
1:A:83:LEU:HD22	1:A:121:ILE:HD12	1.81	0.60
1:A:46:SER:O	1:A:47:GLY:O	2.21	0.59
1:A:245:SER:CA	5:A:2121:HOH:O	2.50	0.58
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.40	0.57
1:B:515:MET:HG3	1:B:527:LYS:HB3	1.87	0.57
1:B:539:PHE:O	1:B:543:GLN:HG2	2.04	0.56
1:A:7:PRO:HB3	1:A:389:SER:HA	1.87	0.56
1:B:416:GLU:HB3	1:B:474:ARG:NH2	2.21	0.56
1:B:292:ASN:HD22	1:B:292:ASN:N	2.04	0.56
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.88	0.55
1:B:86:ASN:HA	1:B:118:GLU:HG3	1.89	0.55
1:B:306:GLN:HE21	1:B:306:GLN:HA	1.71	0.55
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.89	0.55
1:B:74:ILE:HD11	1:B:93:ALA:HB1	1.89	0.54
1:A:454:PHE:C	1:A:456:GLU:H	2.15	0.54
1:B:308:MET:HA	1:B:335:TYR:O	2.08	0.54
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:MET:HA	1:A:335:TYR:O	2.08	0.54
1:A:296:THR:O	1:A:300:LYS:HB2	2.09	0.53
1:A:188:LEU:HD13	1:A:229:MET:HE1	1.89	0.52
1:B:21:LEU:HD13	1:B:111:LEU:HD13	1.91	0.52
1:B:46:SER:O	1:B:47:GLY:O	2.28	0.52
1:A:70:TYR:OH	1:A:89:GLU:OE2	2.27	0.52
1:B:458:LYS:HE2	5:B:2226:HOH:O	2.09	0.51
1:B:306:GLN:HA	1:B:306:GLN:NE2	2.26	0.51
1:A:17:LYS:NZ	1:A:87:GLU:HG2	2.25	0.51
1:A:47:GLY:HA3	1:A:48:LYS:HD2	1.93	0.51
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.45	0.51
1:A:144:GLN:HG2	5:A:2068:HOH:O	2.10	0.51
1:B:277:MET:HG2	1:B:301:LEU:HD11	1.93	0.51
1:B:515:MET:CG	1:B:527:LYS:HB3	2.40	0.51
1:A:41:LEU:HB2	1:A:104:LEU:HD21	1.93	0.49
1:A:445:PRO:HD2	5:A:2225:HOH:O	2.12	0.49
1:B:240:PHE:HA	1:B:278:CYS:HB3	1.95	0.49
1:A:98:ARG:HG3	1:A:199:GLU:HB3	1.94	0.49
1:B:364:LYS:CB	5:B:2179:HOH:O	2.60	0.49
1:A:131:GLY:HA2	1:A:158:MET:HG2	1.95	0.49
1:A:515:MET:HG3	1:A:527:LYS:HB3	1.95	0.49
1:A:141:TRP:CZ3	1:A:149:GLN:HG3	2.48	0.48
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.94	0.48
1:B:458:LYS:O	1:B:459:ASN:HB2	2.14	0.48
1:A:132:VAL:HG22	1:A:371:THR:HG23	1.97	0.47
1:A:462:LYS:O	1:A:466:GLU:HG2	2.15	0.47
1:B:364:LYS:HB3	5:B:2179:HOH:O	2.14	0.47
1:A:527:LYS:HD3	1:A:527:LYS:HA	1.66	0.47
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.97	0.46
1:B:57:ILE:HG12	1:B:90:ILE:HB	1.98	0.46
1:B:22:PRO:HG2	1:B:57:ILE:HD11	1.96	0.46
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.50	0.46
1:B:536:GLN:OE1	5:B:2255:HOH:O	2.20	0.46
1:A:214:TRP:CD2	1:A:253:LYS:HB3	2.51	0.45
1:A:408[B]:ARG:NE	5:A:2209:HOH:O	2.43	0.45
1:A:514:LYS:NZ	5:A:2252:HOH:O	2.50	0.45
1:B:527:LYS:N	1:B:527:LYS:HD2	2.31	0.44
1:A:240:PHE:HA	1:A:278:CYS:HB3	1.99	0.44
1:A:306:GLN:HE21	1:A:306:GLN:HA	1.82	0.44
1:A:576:PHE:C	1:A:578:GLN:H	2.25	0.44
1:B:34:ASN:OD1	1:B:34:ASN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ALA:HB1	1:A:104:LEU:HD13	1.98	0.44
1:B:543:GLN:NE2	5:B:2257:HOH:O	2.50	0.44
1:B:262:ASP:HA	1:B:266:ALA:HB3	1.99	0.44
1:B:338:TRP:CH2	1:B:355:VAL:HG13	2.52	0.44
1:B:342:VAL:HA	1:B:373:PRO:C	2.43	0.44
1:B:533:ALA:O	1:B:537:GLN:HG3	2.18	0.44
1:A:176:TRP:HE3	1:A:206:ILE:HD11	1.83	0.44
1:A:262:ASP:HA	1:A:266:ALA:HB3	2.00	0.44
1:A:174:PRO:HD2	5:A:2082:HOH:O	2.19	0.43
1:B:364:LYS:HZ3	1:B:364:LYS:HB2	1.84	0.43
1:A:238:ALA:HA	1:A:276:VAL:O	2.19	0.43
1:B:261:ILE:O	1:B:265:PHE:HB3	2.18	0.43
1:A:6:GLN:HA	1:A:6:GLN:OE1	2.19	0.43
1:A:168:ASP:HA	1:A:169:PRO:HD2	1.82	0.43
1:B:302:ASN:HB3	5:B:2146:HOH:O	2.18	0.43
1:B:364:LYS:HZ2	1:B:364:LYS:HA	1.84	0.43
1:A:41:LEU:HB2	1:A:104:LEU:CD2	2.49	0.43
1:A:340:PHE:HA	1:A:341:PRO:HA	1.63	0.42
1:B:501:GLN:HA	1:B:501:GLN:OE1	2.19	0.42
1:B:102:TYR:CE1	1:B:157:LYS:HA	2.53	0.42
1:B:193:ALA:O	1:B:197:GLU:HG3	2.18	0.42
1:B:7:PRO:HB3	1:B:389:SER:HA	2.01	0.42
1:B:98:ARG:HG3	1:B:199:GLU:HB3	2.01	0.42
1:B:77:HIS:HB3	5:B:2030:HOH:O	2.20	0.42
1:A:17:LYS:HZ2	1:A:87:GLU:HG2	1.85	0.42
1:A:475:MET:HG2	1:A:502:PHE:CZ	2.55	0.42
1:B:214:TRP:CD2	1:B:253:LYS:HB3	2.54	0.42
1:A:6:GLN:HG3	1:A:385:TYR:OH	2.20	0.42
1:A:21:LEU:HD22	1:A:111:LEU:HD11	2.00	0.42
1:B:271:ASP:N	1:B:271:ASP:OD1	2.52	0.42
1:B:292:ASN:N	1:B:292:ASN:ND2	2.68	0.42
1:B:452:LYS:C	1:B:454:PHE:H	2.28	0.42
1:A:454:PHE:C	1:A:456:GLU:N	2.78	0.42
1:B:22:PRO:HB2	1:B:25:TYR:HB3	2.01	0.42
1:A:86:ASN:HA	1:A:118:GLU:HG3	2.02	0.41
1:A:147:LEU:HD22	1:A:194:VAL:HG21	2.02	0.41
1:A:271:ASP:OD1	1:A:271:ASP:N	2.53	0.41
1:B:364:LYS:HB2	5:B:2179:HOH:O	2.20	0.41
1:B:412:PRO:HD2	1:B:487:GLU:OE2	2.20	0.41
1:B:538:MET:HE2	1:B:538:MET:HB3	1.90	0.41
1:B:449:ARG:HD2	1:B:464:ASP:OD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TRP:CE3	1:A:206:ILE:HD11	2.56	0.41
1:A:281:GLU:CD	1:A:287:SER:HA	2.46	0.41
1:A:306:GLN:HA	1:A:306:GLN:NE2	2.36	0.41
1:A:341:PRO:HD2	1:A:373:PRO:HA	2.03	0.41
1:B:70:TYR:OH	1:B:89:GLU:OE1	2.38	0.41
1:B:130:ARG:HG2	1:B:391:ALA:HB1	2.03	0.41
1:B:204:TRP:CE3	1:B:229:MET:HG3	2.55	0.41
1:B:289:PRO:HD2	1:B:290:ASN:H	1.86	0.41
1:B:458:LYS:HB2	1:B:458:LYS:HE3	1.90	0.41
1:B:284:LYS:HB3	1:B:312:ASP:HA	2.02	0.40
1:B:451:LEU:HD21	1:B:567:ARG:HD2	2.03	0.40
1:A:6:GLN:HA	1:A:7:PRO:HA	1.93	0.40
1:B:4:SER:HA	5:B:2001:HOH:O	2.21	0.40
1:B:216:LYS:HE3	1:B:216:LYS:HB2	1.81	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	585/715 (82%)	553 (94%)	24 (4%)	8 (1%)	9	5
1	B	572/715 (80%)	544 (95%)	23 (4%)	5 (1%)	14	12
All	All	1157/1430 (81%)	1097 (95%)	47 (4%)	13 (1%)	11	8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	47	GLY
1	A	342	VAL
1	B	47	GLY

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Mol	Chain	Res	Type
1	A	455	LYS
1	A	518	GLY
1	B	363	ALA
1	B	518	GLY
1	B	453	ALA
1	A	459	ASN
1	A	53	LYS
1	A	456	GLU
1	B	459	ASN

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	513/629 (82%)	490 (96%)	23 (4%)	24	29
1	B	507/629 (81%)	484 (96%)	23 (4%)	24	29
All	All	1020/1258 (81%)	974 (96%)	46 (4%)	25	29

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	45	LEU
1	A	70	TYR
1	A	87	GLU
1	A	104	LEU
1	A	113	ASP
1	A	120	GLU
1	A	178	LEU
1	A	221	LEU
1	A	277	MET
1	A	323	ILE
1	A	341	PRO
1	A	342	VAL
1	A	371	THR

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Mol	Chain	Res	Type
1	A	408[A]	ARG
1	A	408[B]	ARG
1	A	444	GLN
1	A	458	LYS
1	A	469	GLN
1	A	474	ARG
1	A	516	VAL
1	A	574	LYS
1	A	583	HIS
1	B	11	GLN
1	B	18	THR
1	B	19	ILE
1	B	26	GLN
1	B	27	LEU
1	B	32	GLU
1	B	65	LYS
1	B	113	ASP
1	B	178	LEU
1	B	216	LYS
1	B	285	SER
1	B	292	ASN
1	B	323	ILE
1	B	342	VAL
1	B	364	LYS
1	B	371	THR
1	B	416	GLU
1	B	467	THR
1	B	469	GLN
1	B	527	LYS
1	B	564	LEU
1	B	574	LYS
1	B	581	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	49	GLN
1	A	156	ASN
1	A	231	GLN
1	A	254	GLN
1	A	274	GLN

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Mol	Chain	Res	Type
1	A	306	GLN
1	A	372	ASN
1	A	583	HIS
1	B	187	GLN
1	B	252	GLN
1	B	292	ASN
1	B	306	GLN
1	B	372	ASN
1	B	401	GLN
1	B	469	GLN
1	B	583	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	A	1591	-	3,3,3	0.88	0	3,3,3	1.36	0
2	NB1	B	1590	-	15,17,17	2.65	2 (13%)	15,24,24	2.26	4 (26%)
4	GOL	A	1719	-	5,5,5	0.39	0	5,5,5	1.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1719	-	5,5,5	0.58	0	5,5,5	0.41	0
3	ACT	B	1591	-	3,3,3	0.87	0	3,3,3	1.42	0
2	NB1	A	1590	-	15,17,17	2.27	2 (13%)	15,24,24	2.12	4 (26%)

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	NB1	B	1590	-	-	0/5/33/33	0/2/2/2
4	GOL	A	1719	-	-	0/4/4/4	-
4	GOL	B	1719	-	-	0/4/4/4	-
2	NB1	A	1590	-	-	0/5/33/33	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1590	NB1	C7-N2	9.62	1.35	1.27
2	A	1590	NB1	C7-N2	7.54	1.34	1.27
2	A	1590	NB1	C7-S1	-3.20	1.70	1.76
2	B	1590	NB1	C7-S1	-2.54	1.71	1.76

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1590	NB1	C8-C7-S1	7.00	130.31	121.58
2	A	1590	NB1	C8-C7-S1	5.88	128.91	121.58
2	A	1590	NB1	C1-O5-C5	3.62	119.05	112.56
2	B	1590	NB1	C1-O5-C5	3.09	118.11	112.56
2	A	1590	NB1	C9-C8-C7	-2.77	110.00	115.06
2	B	1590	NB1	O4-C4-C3	-2.70	104.01	110.38
2	B	1590	NB1	C9-C8-C7	-2.67	110.18	115.06
2	A	1590	NB1	O4-C4-C3	-2.45	104.61	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	586/715 (81%)	0.31	45 (7%)	19 17	13, 27, 63, 77	1 (0%)
1	B	580/715 (81%)	0.35	53 (9%)	15 14	13, 26, 63, 78	0
All	All	1166/1430 (81%)	0.33	98 (8%)	17 15	13, 27, 63, 78	1 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	LYS	5.5
1	B	291	GLY	5.2
1	B	454	PHE	5.0
1	B	47	GLY	4.7
1	A	291	GLY	4.7
1	B	50	SER	4.7
1	B	46	SER	4.6
1	B	457	GLY	4.5
1	A	47	GLY	4.4
1	A	46	SER	4.4
1	A	457	GLY	4.3
1	B	453	ALA	4.3
1	A	455	LYS	4.0
1	A	54	GLY	4.0
1	B	460	TYR	3.8
1	B	23	ALA	3.7
1	B	290	ASN	3.7
1	B	576	PHE	3.7
1	A	454	PHE	3.6
1	B	49	GLN	3.5
1	A	48	LYS	3.5
1	B	24	VAL	3.5
1	A	458	LYS	3.5
1	B	579	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	3.4
1	B	575	PHE	3.4
1	A	453	ALA	3.4
1	B	458	LYS	3.4
1	B	289	PRO	3.3
1	B	33	ALA	3.3
1	B	589	ASP	3.2
1	B	25	TYR	3.2
1	A	459	ASN	3.1
1	B	584	LEU	3.1
1	A	49	GLN	3.1
1	B	22	PRO	3.0
1	B	572	VAL	2.9
1	A	581	ASN	2.9
1	A	19	ILE	2.9
1	A	460	TYR	2.9
1	B	56	LEU	2.8
1	A	582	ALA	2.8
1	A	456	GLU	2.8
1	A	584	LEU	2.8
1	A	4	SER	2.8
1	B	580	PHE	2.8
1	B	578	GLN	2.7
1	B	586	ALA	2.7
1	A	114	GLY	2.7
1	B	21	LEU	2.7
1	B	583	HIS	2.7
1	B	29	GLY	2.7
1	B	63	GLY	2.7
1	A	51	SER	2.7
1	A	589	ASP	2.6
1	A	583	HIS	2.5
1	A	23	ALA	2.5
1	A	24	VAL	2.5
1	A	27	LEU	2.5
1	B	287	SER	2.5
1	A	447	ALA	2.5
1	B	28	ASN	2.4
1	A	50	SER	2.4
1	A	21	LEU	2.4
1	B	292	ASN	2.4
1	A	588	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	588	THR	2.4
1	A	575	PHE	2.4
1	A	451	LEU	2.3
1	B	19	ILE	2.3
1	A	539	PHE	2.3
1	B	470	TYR	2.3
1	B	582	ALA	2.3
1	A	44	LEU	2.3
1	B	27	LEU	2.3
1	B	20	ASP	2.3
1	A	28	ASN	2.2
1	A	452	LYS	2.2
1	A	450	PHE	2.2
1	B	539	PHE	2.2
1	B	113	ASP	2.2
1	B	459	ASN	2.2
1	B	587	THR	2.2
1	A	408[A]	ARG	2.2
1	B	518	GLY	2.2
1	A	20	ASP	2.1
1	B	32	GLU	2.1
1	A	245	SER	2.1
1	B	26	GLN	2.1
1	B	449	ARG	2.1
1	A	580	PHE	2.1
1	B	45	LEU	2.1
1	B	48	LYS	2.0
1	A	292	ASN	2.0
1	B	581	ASN	2.0
1	B	30	GLY	2.0
1	A	286	TRP	2.0
1	A	53	LYS	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	ACT	A	1591	4/4	0.65	0.28	56,56,56,56	0
3	ACT	B	1591	4/4	0.72	0.20	52,52,52,52	0
4	GOL	B	1719	6/6	0.89	0.11	35,37,42,44	0
4	GOL	A	1719	6/6	0.90	0.11	25,31,32,36	0
2	NB1	B	1590	16/16	0.95	0.08	15,19,20,20	0
2	NB1	A	1590	16/16	0.97	0.07	14,18,19,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.