



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:10 PM UTC

PDB ID : 1V4V / pdb_00001v4v
Title : Crystal Structure Of UDP-N-Acetylglucosamine 2-Epimerase From Thermus
Thermophilus HB8
Authors : Bagautdinov, B.; Tahirov, T.H.; RIKEN Structural Genomics/Proteomics Ini-
tiative (RSGI)
Deposited on : 2003-11-19
Resolution : 1.80 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

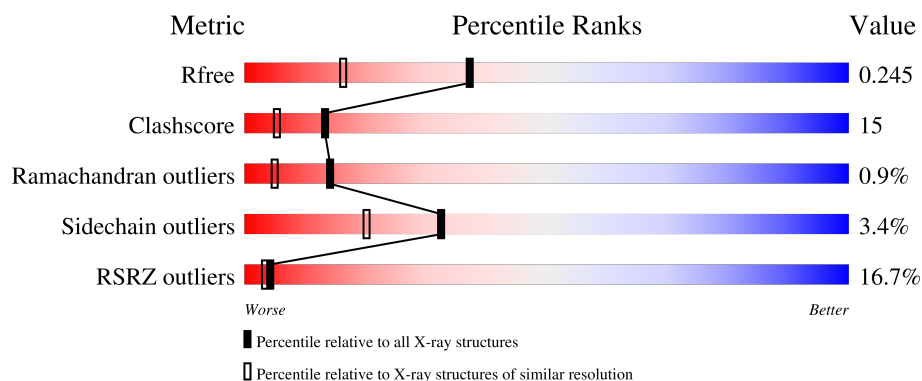
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	376	6% 77% 21% ..
1	B	376	25% 68% 27% ..

2 Entry composition [i](#)

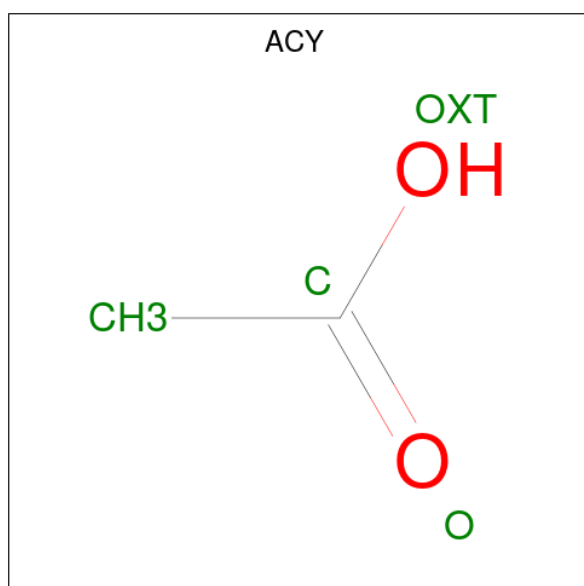
There are 4 unique types of molecules in this entry. The entry contains 6736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-Acetylglucosamine 2-Epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	Se	0	4	0
			2868	1834	511	513	10			
1	B	372	Total	C	N	O	Se	182	5	0
			2878	1841	512	516	9			

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

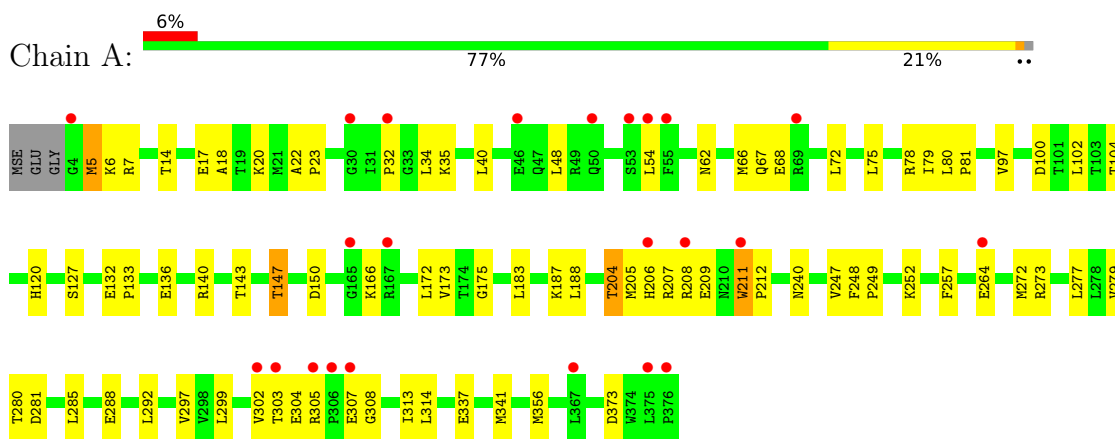
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	609	Total	O	0	0
			609	609		
4	B	365	Total	O	0	0
			365	365		

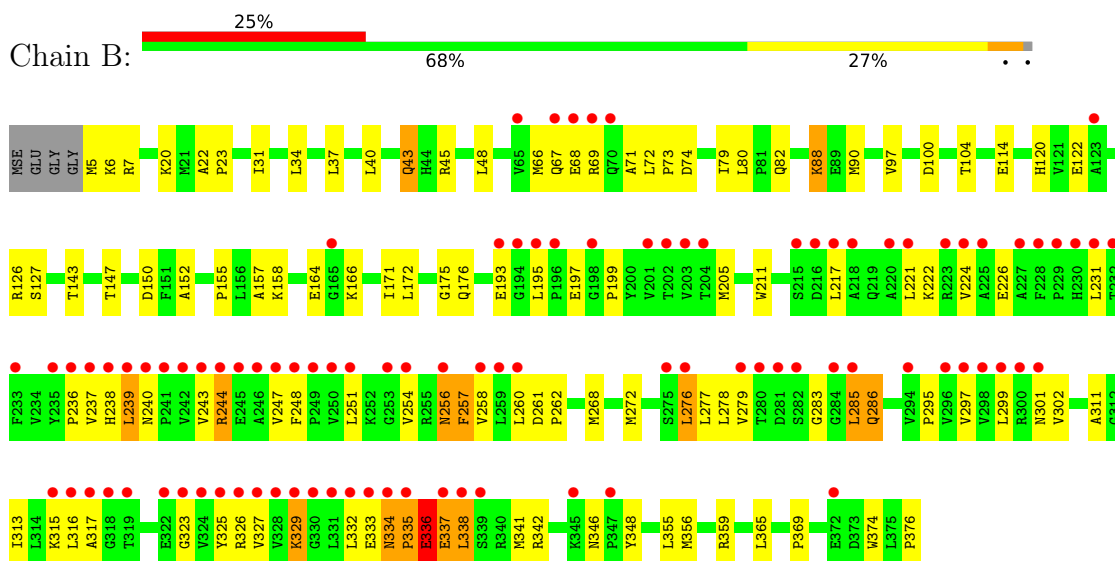
3 Residue-property plots

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: UDP-N-Acetylglucosamine 2-Epimerase



• Molecule 1: UDP-N-Acetylglucosamine 2-Epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.73Å 51.45Å 105.51Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.00-1.80) 96.4 (40.00-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.235 0.220 , 0.245	Depositor DCC
R_{free} test set	7814 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.5	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	0.95	EDS
Total number of atoms	6736	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: ACY, GOL

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	0.35	0/2940	0.88	6/3977 (0.2%)
1	B	0.34	0/2948	0.87	8/3992 (0.2%)
All	All	0.35	0/5888	0.87	14/7969 (0.2%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	GLU	N-CA-C	-10.12	101.06	113.41
1	A	247	VAL	N-CA-C	6.63	118.61	111.58
1	A	175	GLY	N-CA-C	-6.07	102.51	112.83
1	B	338	LEU	N-CA-C	-5.71	105.81	112.89
1	B	175	GLY	N-CA-C	-5.65	103.23	112.83
1	A	136	GLU	N-CA-C	5.57	118.06	111.33
1	B	336	GLU	N-CA-C	-5.52	99.05	110.80
1	A	127	SER	N-CA-C	-5.52	106.91	113.97
1	B	127	SER	N-CA-C	-5.38	107.09	113.97
1	A	147	THR	N-CA-C	5.34	118.19	110.28
1	A	79	ILE	N-CA-C	5.22	115.89	110.82
1	B	79	ILE	N-CA-C	5.10	115.33	110.53
1	B	43[A]	GLN	N-CA-C	-5.06	102.97	110.46
1	B	43[B]	GLN	N-CA-C	-5.06	102.97	110.46

There are no chirality outliers.

There are no planarity outliers.

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	2868	0	2968	71	0
1	B	2878	0	2980	98	0
2	A	4	0	3	0	0
3	A	6	0	8	0	0
3	B	6	0	8	3	0
4	A	609	0	0	17	0
4	B	365	0	0	14	0
All	All	6736	0	5967	169	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 15.

All (169) 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:244:ARG:HH11	1:B:244:ARG:HB3	1.21	1.00
1:B:40:LEU:HD22	1:B:48[A]:LEU:HD13	1.43	0.99
1:A:204:THR:HG21	1:A:285:LEU:HD12	1.49	0.93
1:A:204:THR:HG21	1:A:285:LEU:CD1	2.08	0.83
1:A:66:MSE:HE3	1:A:68:GLU:HG3	1.61	0.80
1:B:66:MSE:HE2	1:B:68:GLU:OE1	1.80	0.80
1:A:205[B]:MSE:HE1	1:A:281:ASP:HB3	1.64	0.79
1:B:238:HIS:C	1:B:239:LEU:HD23	2.14	0.73
1:A:6:LYS:HB2	1:A:34:LEU:HD23	1.70	0.72
1:A:172:LEU:HD12	1:A:373[A]:ASP:OD1	1.91	0.71
1:A:204:THR:O	1:A:205[B]:MSE:SE	2.59	0.70
1:B:150:ASP:OD2	1:B:166:LYS:HE2	1.91	0.69
1:B:334:ASN:N	1:B:335:PRO:HD3	2.08	0.68
1:A:66:MSE:HE3	1:A:68:GLU:CG	2.24	0.68
1:A:208:ARG:HH11	1:A:208:ARG:HG2	1.59	0.66
1:B:244:ARG:HB3	1:B:244:ARG:NH1	2.03	0.66
1:B:240:ASN:HD22	1:B:243:VAL:HG23	1.60	0.65
1:A:80:LEU:HB3	1:A:81:PRO:HD3	1.79	0.65
1:B:301:ASN:HA	1:B:316:LEU:HD23	1.78	0.64
1:B:283:GLY:O	1:B:286:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MSE:HE2	1:B:299:LEU:HD11	1.80	0.63
1:B:334:ASN:N	1:B:335:PRO:CD	2.62	0.63
1:B:172:LEU:HD21	1:B:356:MSE:HG2	1.81	0.62
1:A:54:LEU:HD22	4:A:1803:HOH:O	2.00	0.61
1:B:20:LYS:HE3	4:B:1693:HOH:O	1.99	0.61
1:B:88:LYS:HD3	1:B:114:GLU:HB3	1.80	0.61
1:B:315:LYS:HG3	1:B:341:MSE:HE3	1.83	0.61
1:B:346:ASN:ND2	1:B:348:TYR:H	1.99	0.61
1:B:48[A]:LEU:HD12	4:B:1575:HOH:O	2.00	0.61
1:B:205:MSE:HE1	1:B:217:LEU:HB3	1.84	0.59
1:B:323:GLY:O	1:B:327:VAL:HG23	2.01	0.59
1:B:205:MSE:HE2	1:B:299:LEU:CD1	2.32	0.59
1:B:67:GLN:HB3	4:B:1855:HOH:O	2.03	0.59
1:B:329:LYS:NZ	1:B:329:LYS:HB3	2.17	0.59
1:B:359:ARG:HG2	3:B:1501:GOL:H11	1.84	0.59
1:B:315:LYS:HG3	1:B:341:MSE:CE	2.32	0.58
1:A:277:LEU:HD11	1:A:297[A]:VAL:HG23	1.84	0.58
1:B:143:THR:O	1:B:147[B]:THR:HG23	2.02	0.58
1:B:122:GLU:HG3	1:B:176:GLN:NE2	2.18	0.58
1:A:337:GLU:O	1:A:341:MSE:HG3	2.03	0.58
1:A:143:THR:O	1:A:147:THR:HG23	2.03	0.58
1:A:314:LEU:C	1:A:314:LEU:HD12	2.30	0.56
1:A:208:ARG:HG2	1:A:208:ARG:NH1	2.19	0.55
1:B:295:PRO:HD3	1:B:342:ARG:HG2	1.87	0.55
1:B:268:MSE:HE2	1:B:285:LEU:HD21	1.89	0.55
1:A:205[B]:MSE:CE	1:A:281:ASP:HB3	2.37	0.54
1:B:254:VAL:HB	1:B:257:PHE:HB2	1.88	0.54
1:B:82:GLN:HG3	4:B:1754:HOH:O	2.07	0.54
1:B:244:ARG:HH11	1:B:244:ARG:CB	2.09	0.54
1:A:211:TRP:CE3	1:A:211:TRP:HA	2.42	0.54
1:B:236:PRO:HA	1:B:260:LEU:O	2.08	0.54
1:A:206:HIS:HA	1:A:211:TRP:HZ3	1.73	0.54
1:B:68:GLU:N	1:B:68:GLU:OE2	2.40	0.54
1:B:205:MSE:HE3	1:B:221:LEU:HD11	1.90	0.53
1:B:268:MSE:O	1:B:272:MSE:HG3	2.08	0.53
1:B:199:PRO:HB3	1:B:276:LEU:HD23	1.91	0.53
1:A:14:THR:OG1	1:A:17:GLU:HG3	2.08	0.53
1:B:97:VAL:HB	1:B:104:THR:HG23	1.89	0.53
1:B:222:LYS:O	1:B:226:GLU:HG3	2.07	0.53
1:B:43[A]:GLN:HG2	1:B:66:MSE:O	2.08	0.53
1:A:303:THR:HA	4:A:1883:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:H	1:A:307:GLU:CD	2.16	0.53
1:A:279:VAL:HG22	1:A:297[B]:VAL:CG1	2.39	0.53
1:B:277:LEU:HD11	1:B:297:VAL:HG13	1.91	0.53
1:A:150:ASP:OD1	1:A:166:LYS:HE2	2.09	0.53
1:A:40:LEU:HD12	1:A:62:ASN:ND2	2.24	0.52
1:A:75:LEU:HD23	1:A:102:LEU:HD23	1.91	0.52
1:B:238:HIS:O	1:B:239:LEU:HD23	2.10	0.52
1:A:211:TRP:HA	1:A:211:TRP:HE3	1.74	0.52
1:A:304:GLU:O	1:A:304:GLU:HG2	2.10	0.52
1:A:72:LEU:HD22	1:A:102:LEU:HD22	1.90	0.52
1:A:173:VAL:O	1:A:356:MSE:HE1	2.10	0.52
1:A:22:ALA:HB3	1:A:23:PRO:HD3	1.92	0.51
1:B:301:ASN:CA	1:B:316:LEU:HD23	2.41	0.51
1:A:40:LEU:HD12	1:A:62:ASN:HD21	1.76	0.51
1:B:297:VAL:HG23	1:B:297:VAL:O	2.10	0.50
1:B:6:LYS:HB2	1:B:34:LEU:HD23	1.94	0.50
1:B:279:VAL:HG22	1:B:297:VAL:HG21	1.94	0.50
1:B:317:ALA:HA	1:B:327:VAL:HG21	1.92	0.50
1:A:7:ARG:HH11	1:A:7:ARG:HG2	1.77	0.49
1:A:40:LEU:HD22	1:A:48:LEU:HD23	1.93	0.49
1:A:204:THR:O	1:A:280:THR:HA	2.12	0.49
1:B:7:ARG:NE	1:B:90:MSE:O	2.39	0.49
1:B:237:VAL:O	1:B:262:PRO:HD3	2.13	0.49
1:B:332:LEU:C	1:B:335:PRO:HD3	2.37	0.49
1:A:80:LEU:HD22	4:A:1892:HOH:O	2.11	0.49
1:A:264:GLU:HG2	4:A:2029:HOH:O	2.11	0.49
1:A:18:ALA:HB2	1:A:48:LEU:HD11	1.94	0.49
1:A:187:LYS:HE3	4:A:1937:HOH:O	2.13	0.48
1:B:279:VAL:HA	1:B:297:VAL:HG23	1.95	0.48
1:B:34:LEU:HD21	1:B:365:LEU:HD12	1.96	0.48
1:B:329:LYS:HB3	1:B:329:LYS:HZ3	1.76	0.48
1:B:31:ILE:HG23	3:B:1501:GOL:H32	1.96	0.48
1:A:54:LEU:O	1:A:188:LEU:HD13	2.13	0.48
1:B:279:VAL:HG22	1:B:297:VAL:CG2	2.44	0.47
1:B:376:PRO:HD3	4:B:1860:HOH:O	2.13	0.47
1:A:120:HIS:HB2	1:A:147:THR:HG21	1.95	0.47
1:B:120:HIS:HB2	1:B:147[B]:THR:HG21	1.97	0.47
1:B:338:LEU:O	1:B:342:ARG:HG3	2.14	0.47
1:B:71:ALA:HB3	1:B:74:ASP:OD2	2.15	0.47
1:A:206:HIS:HA	1:A:211:TRP:CZ3	2.51	0.46
1:B:45:ARG:HA	4:B:1588:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LYS:NZ	1:B:254:VAL:HG22	2.31	0.46
1:A:20:LYS:HE3	4:A:1750:HOH:O	2.14	0.46
1:B:334:ASN:H	1:B:335:PRO:HD3	1.77	0.46
1:B:48[A]:LEU:HD12	4:B:1588:HOH:O	2.16	0.46
1:B:195:LEU:HD23	1:B:258:VAL:HG11	1.97	0.46
1:B:48[A]:LEU:CD1	4:B:1575:HOH:O	2.59	0.46
1:A:273:ARG:HG3	4:A:1560:HOH:O	2.16	0.45
1:B:197:GLU:HG3	4:B:1792:HOH:O	2.16	0.45
1:B:5:MSE:N	4:B:1850:HOH:O	2.48	0.45
1:B:279:VAL:HA	1:B:297:VAL:CG2	2.47	0.45
1:B:346:ASN:C	1:B:346:ASN:HD22	2.23	0.45
1:A:207:ARG:HG2	1:A:209:GLU:HG2	1.98	0.45
1:B:329:LYS:O	1:B:333:GLU:HG3	2.17	0.45
1:A:32:PRO:HG3	4:A:1964:HOH:O	2.15	0.45
1:B:69:ARG:HD3	1:B:69:ARG:H	1.82	0.44
1:A:272:MSE:HE1	1:A:288:GLU:HB3	1.99	0.44
1:A:240:ASN:HB3	4:A:1578:HOH:O	2.17	0.44
1:A:304:GLU:O	1:A:305:ARG:HG3	2.17	0.44
1:A:7:ARG:NH1	1:A:35:LYS:HE2	2.33	0.44
1:A:183:LEU:HD23	1:A:292:LEU:HD23	1.99	0.44
1:B:247:VAL:HG23	1:B:248:PHE:N	2.32	0.44
1:B:72:LEU:HB2	1:B:73:PRO:HD3	2.00	0.44
1:B:356:MSE:HE1	1:B:374:TRP:HB2	1.99	0.44
1:A:5:MSE:SE	1:A:6:LYS:HG2	2.68	0.43
1:A:132:GLU:HA	1:A:133:PRO:HA	1.87	0.43
1:B:126:ARG:NE	1:B:164:GLU:OE1	2.42	0.43
1:A:7:ARG:NH1	1:A:35:LYS:CE	2.82	0.43
1:B:335:PRO:O	1:B:336:GLU:HB2	2.19	0.43
1:A:305:ARG:HB3	1:A:307:GLU:OE1	2.17	0.43
1:A:356:MSE:HG3	4:A:1898:HOH:O	2.18	0.43
1:B:325:TYR:C	1:B:325:TYR:CD1	2.96	0.43
1:B:316:LEU:HD12	1:B:316:LEU:N	2.33	0.43
1:B:122:GLU:HG3	1:B:176:GLN:HE22	1.84	0.43
1:B:222:LYS:HZ3	1:B:254:VAL:HG22	1.83	0.43
1:B:152:ALA:HB1	1:B:157:ALA:HB3	2.00	0.42
1:B:158:LYS:HG3	1:B:171:ILE:HG21	2.00	0.42
1:B:238:HIS:HA	1:B:262:PRO:HG3	2.01	0.42
1:A:248:PHE:N	1:A:249:PRO:HD2	2.35	0.42
1:B:251:LEU:HD13	1:B:257:PHE:CE2	2.54	0.42
1:A:5:MSE:HE1	4:A:1826:HOH:O	2.19	0.42
1:A:211:TRP:HB2	1:A:212:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:HD23	4:B:1543:HOH:O	2.19	0.42
1:A:97:VAL:HB	1:A:104:THR:HG23	2.02	0.42
1:B:369:PRO:HD2	3:B:1501:GOL:O1	2.20	0.41
1:A:308:GLY:HA2	1:A:313:ILE:HD11	2.02	0.41
1:B:205:MSE:CE	1:B:217:LEU:HB3	2.47	0.41
1:A:17:GLU:HG2	4:A:1567:HOH:O	2.21	0.41
1:B:155:PRO:HD2	4:B:1733:HOH:O	2.20	0.41
1:A:252:LYS:NZ	4:A:1692:HOH:O	2.51	0.41
1:A:264:GLU:HG3	4:A:1630:HOH:O	2.20	0.41
1:A:272:MSE:HE1	1:A:288:GLU:OE1	2.21	0.41
1:B:7:ARG:CZ	1:B:37:LEU:HD11	2.51	0.41
1:A:100:ASP:CG	1:A:140:ARG:HD3	2.45	0.41
1:B:22:ALA:HB3	1:B:23:PRO:HD3	2.03	0.41
1:B:88:LYS:HE3	4:B:1859:HOH:O	2.21	0.41
1:B:355:LEU:HD21	1:B:359:ARG:NH1	2.35	0.41
1:A:279:VAL:HG22	1:A:297[B]:VAL:HG11	2.02	0.41
1:A:279:VAL:HA	1:A:297[B]:VAL:HG13	2.03	0.41
1:A:303:THR:HG22	4:A:1883:HOH:O	2.20	0.41
1:B:221:LEU:HA	1:B:224:VAL:HG22	2.03	0.40
1:B:88:LYS:HG3	4:B:1859:HOH:O	2.21	0.40
1:B:326:ARG:HA	1:B:329:LYS:NZ	2.36	0.40
1:A:78:ARG:HD2	4:A:1555:HOH:O	2.21	0.40
1:A:302:VAL:HG23	4:A:1724:HOH:O	2.19	0.40
1:B:238:HIS:O	1:B:239:LEU:C	2.63	0.40
1:B:277:LEU:HD12	1:B:278:LEU:H	1.87	0.40
1:B:231:LEU:O	1:B:256:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

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	375/376 (100%)	370 (99%)	5 (1%)	0	100	100
1	B	375/376 (100%)	352 (94%)	16 (4%)	7 (2%)	6	1
All	All	750/752 (100%)	722 (96%)	21 (3%)	7 (1%)	14	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	GLU
1	B	239	LEU
1	B	313	ILE
1	B	302	VAL
1	B	335	PRO
1	B	311	ALA
1	B	334	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	301/289 (104%)	295 (98%)	6 (2%)	48	38
1	B	302/289 (104%)	287 (95%)	15 (5%)	22	10
All	All	603/578 (104%)	582 (96%)	21 (4%)	32	19

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MSE
1	A	67	GLN
1	A	204	THR
1	A	211	TRP
1	A	257	PHE
1	A	299	LEU
1	B	80	LEU
1	B	88	LYS
1	B	100[A]	ASP

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Mol	Chain	Res	Type
1	B	100[B]	ASP
1	B	193	GLU
1	B	211	TRP
1	B	244	ARG
1	B	256	ASN
1	B	257	PHE
1	B	261	ASP
1	B	276	LEU
1	B	285	LEU
1	B	286	GLN
1	B	329	LYS
1	B	337	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	58	GLN
1	A	62	ASN
1	A	67	GLN
1	A	176	GLN
1	A	238	HIS
1	A	301	ASN
1	B	47	GLN
1	B	58	GLN
1	B	160	ASN
1	B	176	GLN
1	B	240	ASN
1	B	256	ASN
1	B	286	GLN
1	B	334	ASN
1	B	346	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
2	ACY	A	1400	-	3,3,3	2.81	1 (33%)	3,3,3	1.40	0
3	GOL	B	1501	-	5,5,5	0.58	0	5,5,5	0.30	0
3	GOL	A	1500	-	5,5,5	0.55	0	5,5,5	0.31	0

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
3	GOL	B	1501	-	-	2/4/4/4	-
3	GOL	A	1500	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1400	ACY	O-C	4.52	1.41	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1500	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	1501	GOL	O1-C1-C2-C3
3	A	1500	GOL	O1-C1-C2-O2
3	B	1501	GOL	O1-C1-C2-O2
3	A	1500	GOL	C1-C2-C3-O3
3	A	1500	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	GOL	3	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	364/376 (96%)	0.46	23 (6%) 26 24	16, 29, 51, 70	2 (0%)
1	B	341/376 (90%)	1.10	95 (27%) 1 1	16, 34, 86, 93	5 (1%)
All	All	705/752 (93%)	0.77	118 (16%) 4 3	16, 30, 81, 93	7 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	LEU	5.9
1	B	282	SER	5.2
1	B	220	ALA	5.0
1	B	246	ALA	4.9
1	B	218	ALA	4.8
1	A	211	TRP	4.6
1	B	237	VAL	4.5
1	B	217	LEU	4.5
1	B	335	PRO	4.4
1	B	254	VAL	4.3
1	B	328	VAL	4.3
1	B	325	TYR	4.2
1	B	194	GLY	4.2
1	B	339	SER	4.2
1	B	248	PHE	4.2
1	A	4	GLY	4.2
1	B	165	GLY	4.1
1	B	332	LEU	4.0
1	B	224	VAL	4.0
1	B	327	VAL	4.0
1	B	227	ALA	3.9
1	B	239	LEU	3.8
1	B	216	ASP	3.7
1	B	329	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	250	VAL	3.6
1	B	65	VAL	3.6
1	B	225	ALA	3.5
1	B	330	GLY	3.5
1	B	242	VAL	3.5
1	B	317	ALA	3.5
1	B	319	THR	3.4
1	B	316	LEU	3.4
1	B	243	VAL	3.3
1	B	324	VAL	3.3
1	B	238	HIS	3.3
1	A	208	ARG	3.3
1	B	275	SER	3.3
1	B	235	TYR	3.3
1	B	229	PRO	3.2
1	A	50	GLN	3.2
1	A	206	HIS	3.1
1	B	69	ARG	3.1
1	A	307	GLU	3.1
1	B	201	VAL	3.1
1	B	259	LEU	3.1
1	B	232	THR	3.1
1	A	54	LEU	3.0
1	B	337	GLU	3.0
1	B	241	PRO	3.0
1	B	68	GLU	3.0
1	A	302	VAL	2.9
1	B	203	VAL	2.9
1	A	46	GLU	2.9
1	B	279	VAL	2.9
1	B	204	THR	2.9
1	B	280	THR	2.9
1	B	297	VAL	2.9
1	B	244	ARG	2.9
1	B	296	VAL	2.8
1	A	306	PRO	2.8
1	B	284	GLY	2.7
1	B	281	ASP	2.7
1	A	69	ARG	2.7
1	B	294	VAL	2.7
1	B	240	ASN	2.7
1	B	215	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	298	VAL	2.7
1	B	315	LYS	2.7
1	B	247	VAL	2.7
1	B	233	PHE	2.6
1	A	376	PRO	2.6
1	B	195	LEU	2.6
1	B	251	LEU	2.6
1	B	258	VAL	2.6
1	B	318	GLY	2.6
1	B	256	ASN	2.6
1	B	276	LEU	2.6
1	B	331	LEU	2.6
1	B	228	PHE	2.5
1	B	299	LEU	2.5
1	B	245	GLU	2.5
1	B	260	LEU	2.5
1	B	326	ARG	2.5
1	B	202	THR	2.5
1	B	249	PRO	2.5
1	B	193	GLU	2.4
1	A	53	SER	2.4
1	B	236	PRO	2.4
1	B	334	ASN	2.4
1	B	323	GLY	2.4
1	A	167	ARG	2.4
1	B	231	LEU	2.3
1	B	285	LEU	2.3
1	B	230	HIS	2.3
1	B	123	ALA	2.3
1	B	347	PRO	2.3
1	B	253	GLY	2.3
1	A	264	GLU	2.3
1	B	221	LEU	2.3
1	B	198	GLY	2.2
1	B	223	ARG	2.2
1	A	375	LEU	2.2
1	B	301	ASN	2.2
1	B	67	GLN	2.2
1	A	55	PHE	2.2
1	B	372	GLU	2.2
1	A	367	LEU	2.1
1	B	345	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	305	ARG	2.1
1	B	322	GLU	2.1
1	B	333	GLU	2.1
1	A	165	GLY	2.1
1	B	196	PRO	2.1
1	A	303	THR	2.0
1	A	30	GLY	2.0
1	B	70	GLN	2.0
1	A	32	PRO	2.0
1	B	300	ARG	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
2	ACY	A	1400	4/4	0.60	0.16	55,55,55,55	0
3	GOL	B	1501	6/6	0.79	0.16	69,69,70,70	0
3	GOL	A	1500	6/6	0.94	0.10	42,44,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.