



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:01 AM UTC

PDB ID : 3TOV / pdb_00003tov
Title : The crystal structure of the glycosyl transferase family 9 from *Veillonella parvula* DSM 2008
Authors : Tan, K.; Marshall, N.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2011-09-06
Resolution : 2.98 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

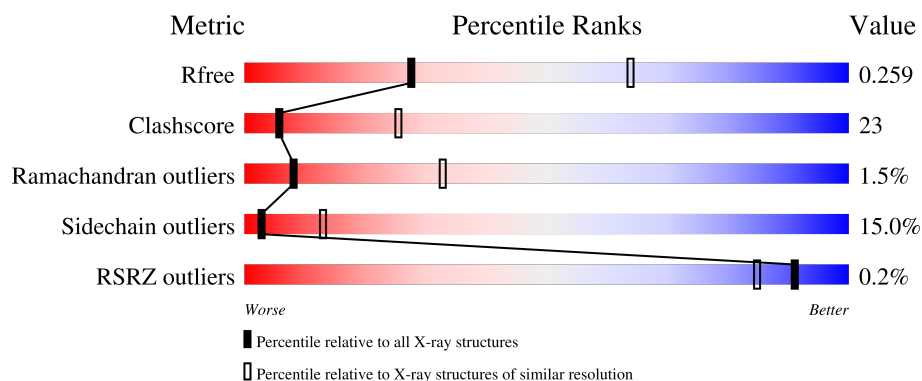
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	349	
1	B	349	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5539 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.

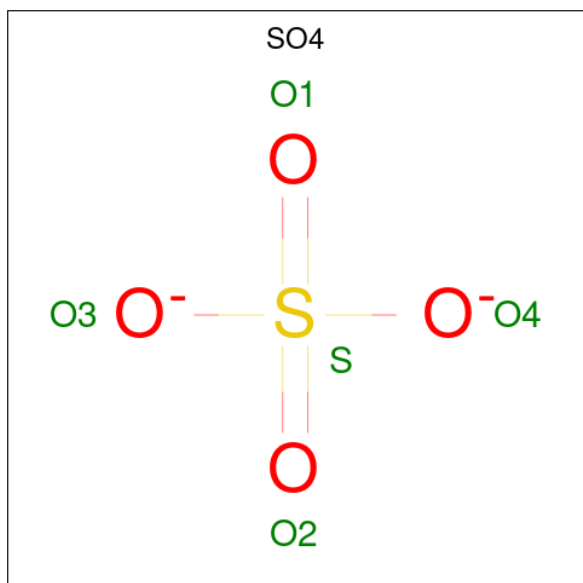
- Molecule 1 is a protein called Glycosyl transferase family 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2752	1761	466	509	3	13			
1	B	344	Total	C	N	O	S	Se	0	0	0
			2705	1732	459	499	3	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D1BM34
A	-1	ASN	-	expression tag	UNP D1BM34
A	0	ALA	-	expression tag	UNP D1BM34
B	-2	SER	-	expression tag	UNP D1BM34
B	-1	ASN	-	expression tag	UNP D1BM34
B	0	ALA	-	expression tag	UNP D1BM34

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

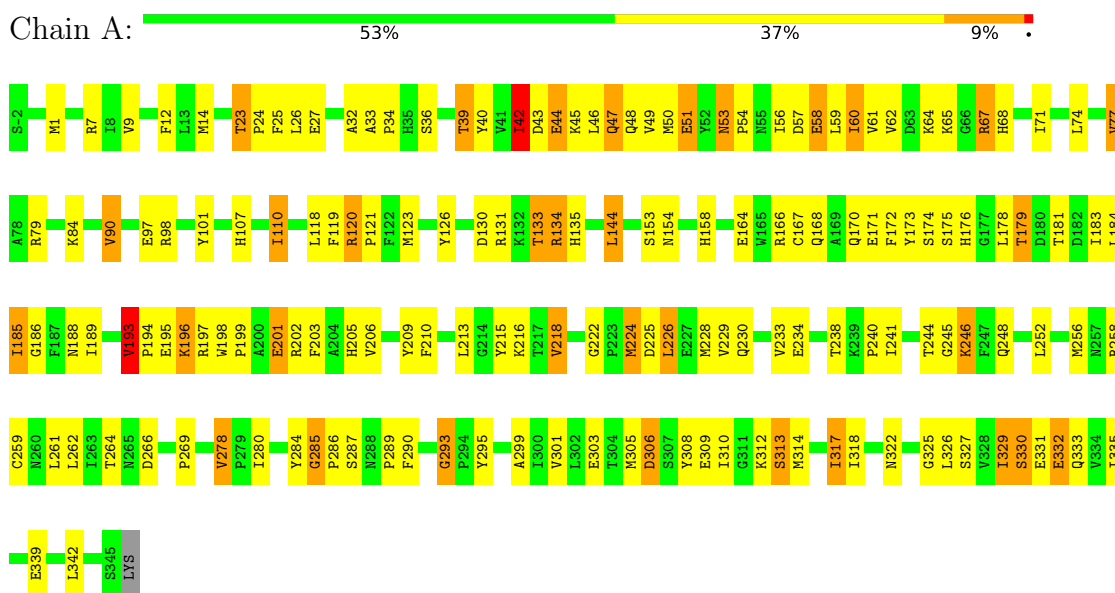
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	12	Total	O	0	0
			12	12		

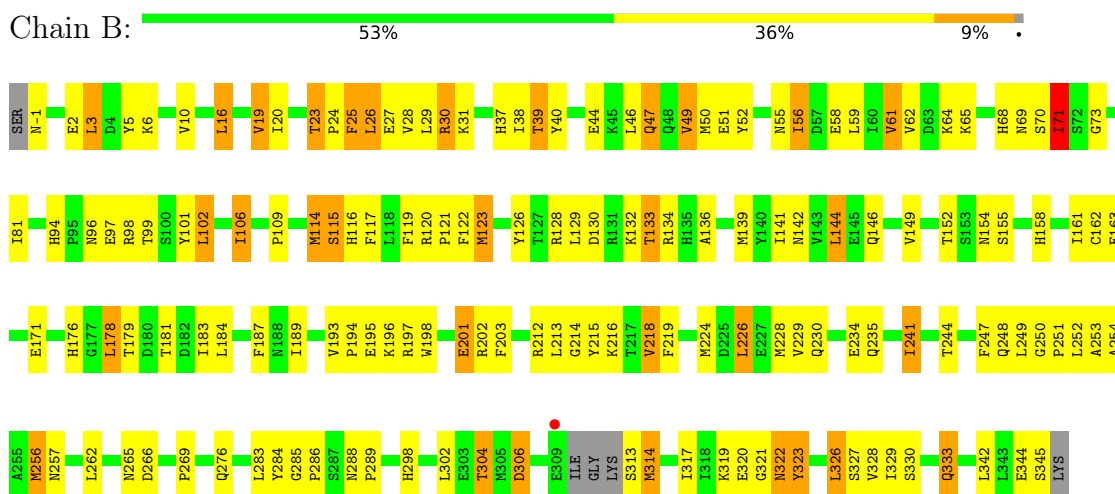
3 Residue-property plots

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: Glycosyl transferase family 9



• Molecule 1: Glycosyl transferase family 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.71Å 95.39Å 121.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.79 – 2.98 40.79 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.79-2.98) 97.3 (40.79-2.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.171 , 0.267 0.172 , 0.259	Depositor DCC
R_{free} test set	962 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.3	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	0.96	EDS
Total number of atoms	5539	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: SO4

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	0.53	0/2802	0.96	10/3776 (0.3%)
1	B	0.53	0/2754	0.90	3/3716 (0.1%)
All	All	0.53	0/5556	0.93	13/7492 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLY	CA-C-N	6.81	128.35	119.84
1	A	293	GLY	C-N-CA	6.81	128.35	119.84
1	A	285	GLY	CA-C-N	6.58	128.07	119.84
1	A	285	GLY	C-N-CA	6.58	128.07	119.84
1	A	193	VAL	CA-C-N	6.26	126.45	119.32
1	A	193	VAL	C-N-CA	6.26	126.45	119.32
1	B	47	GLN	N-CA-C	6.09	118.72	111.71
1	A	42	ILE	CB-CA-C	-5.69	101.96	111.29
1	B	123	MSE	N-CA-C	5.41	117.48	108.99
1	A	53	ASN	CA-C-N	5.31	124.81	119.19
1	A	53	ASN	C-N-CA	5.31	124.81	119.19
1	A	325	GLY	N-CA-C	5.22	120.47	110.86
1	B	71	ILE	N-CA-C	-5.08	105.55	110.42

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	2752	0	2754	132	0
1	B	2705	0	2681	124	0
2	A	25	0	0	1	0
2	B	30	0	0	2	0
3	A	15	0	0	1	0
3	B	12	0	0	3	0
All	All	5539	0	5435	254	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 23.

All (254) 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:42:ILE:HD11	1:A:59:LEU:HD11	1.43	0.97
1:B:23:THR:HG22	1:B:24:PRO:HD3	1.55	0.85
1:B:65:LYS:HA	1:B:69:ASN:HD22	1.42	0.84
1:B:23:THR:HG21	1:B:158:HIS:H	1.42	0.84
1:A:171:GLU:HG3	1:A:172:PHE:H	1.43	0.82
1:A:67:ARG:HA	1:A:98:ARG:NH1	1.95	0.81
1:A:209:TYR:O	1:A:213:LEU:HD23	1.79	0.81
1:A:172:PHE:O	1:A:175:SER:HB3	1.83	0.79
1:A:120:ARG:HA	1:A:123:MSE:HE2	1.66	0.78
1:B:123:MSE:HE3	1:B:126:TYR:HD1	1.47	0.78
1:A:67:ARG:HA	1:A:98:ARG:HH11	1.50	0.77
1:A:40:TYR:HB2	1:A:56:ILE:HD13	1.66	0.77
1:B:65:LYS:HA	1:B:69:ASN:ND2	1.99	0.77
1:A:42:ILE:CD1	1:A:59:LEU:HD11	2.15	0.77
1:A:184:LEU:HD11	1:A:218:VAL:HG22	1.66	0.76
1:A:60:ILE:HD11	1:A:77:VAL:HG13	1.66	0.75
1:B:114:MSE:HE3	1:B:129:LEU:H	1.52	0.75
1:B:114:MSE:HE3	1:B:129:LEU:N	2.03	0.74
1:A:305:MSE:CE	1:A:309:GLU:HG2	2.18	0.73
1:A:123:MSE:HE1	1:A:126:TYR:CD1	2.23	0.73
1:A:135:HIS:NE2	1:A:295:TYR:HB2	2.04	0.72
1:A:130:ASP:OD2	1:A:133:THR:HG22	1.90	0.72
1:B:-1:ASN:N	2:B:351:SO4:O4	2.22	0.71
1:B:44:GLU:HG3	1:B:61:VAL:HG21	1.73	0.70
1:B:26:LEU:HG	1:B:50:MSE:CE	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:THR:CG2	1:B:158:HIS:H	2.07	0.68
1:A:171:GLU:HG3	1:A:172:PHE:N	2.09	0.67
1:B:26:LEU:HD11	1:B:56:ILE:HG13	1.76	0.67
1:B:64:LYS:O	1:B:69:ASN:ND2	2.26	0.67
1:B:194:PRO:HA	1:B:197:ARG:HD2	1.75	0.67
1:B:224:MSE:HB2	3:B:363:HOH:O	1.93	0.67
1:A:1:MSE:SE	1:A:110:ILE:HD11	2.45	0.67
1:A:305:MSE:HE2	1:A:309:GLU:HG2	1.73	0.67
1:A:123:MSE:HE1	1:A:126:TYR:HD1	1.60	0.66
1:B:284:TYR:CZ	1:B:289:PRO:HA	2.29	0.66
1:A:39:THR:HB	1:A:58:GLU:HB3	1.78	0.66
1:B:19:VAL:HG11	1:B:46:LEU:HD13	1.78	0.65
1:B:120:ARG:HA	1:B:123:MSE:HE2	1.78	0.65
1:B:184:LEU:HD11	1:B:218:VAL:HG22	1.78	0.65
1:A:7:ARG:HH12	1:A:84:LYS:HE3	1.62	0.64
1:B:321:GLY:O	1:B:323:TYR:N	2.30	0.64
1:A:305:MSE:HE3	1:A:305:MSE:O	1.98	0.64
1:B:197:ARG:C	1:B:326:LEU:HD11	2.23	0.64
1:B:330:SER:OG	1:B:333:GLN:HG2	1.97	0.64
1:A:44:GLU:HG2	1:A:45:LYS:N	2.13	0.63
1:A:23:THR:HG21	1:A:158:HIS:H	1.63	0.63
1:A:317:ILE:HD12	1:A:318:ILE:N	2.14	0.63
1:B:115:SER:HB2	1:B:123:MSE:HE1	1.80	0.62
1:A:317:ILE:HD12	1:A:318:ILE:H	1.65	0.62
1:A:195:GLU:HA	3:A:358:HOH:O	1.99	0.61
1:A:33:ALA:HB1	1:A:36:SER:OG	2.01	0.61
1:A:330:SER:HB2	1:A:333:GLN:H	1.66	0.61
1:A:332:GLU:CD	1:A:332:GLU:H	2.08	0.61
1:B:189:ILE:HG22	1:B:203:PHE:CE1	2.35	0.61
1:A:199:PRO:HB2	1:A:202:ARG:HG3	1.82	0.61
1:B:194:PRO:HG2	1:B:195:GLU:OE1	2.01	0.60
1:A:195:GLU:O	1:A:326:LEU:HD13	2.01	0.60
1:B:202:ARG:NH1	1:B:329:ILE:O	2.34	0.60
1:A:322:ASN:HB3	1:A:327:SER:O	2.02	0.60
1:B:101:TYR:HA	1:B:119:PHE:CE1	2.36	0.60
1:A:42:ILE:HD11	1:A:59:LEU:CD1	2.26	0.59
1:B:266:ASP:HB3	1:B:284:TYR:CD2	2.38	0.59
1:A:290:PHE:CZ	1:B:109:PRO:HG3	2.37	0.59
1:A:188:ASN:ND2	1:A:269:PRO:HB2	2.17	0.59
1:B:152:THR:HG22	1:B:152:THR:O	2.02	0.59
1:B:37:HIS:CE1	1:B:39:THR:HG22	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLU:CD	1:B:201:GLU:H	2.10	0.59
1:A:310:ILE:HA	1:A:313:SER:HB2	1.84	0.59
1:A:39:THR:HG21	1:A:84:LYS:NZ	2.17	0.59
1:B:3:LEU:N	1:B:3:LEU:CD2	2.65	0.58
1:A:198:TRP:CD1	1:A:199:PRO:HD2	2.39	0.58
1:A:244:THR:O	1:A:246:LYS:N	2.36	0.58
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.69	0.58
1:A:33:ALA:N	1:A:34:PRO:HD3	2.18	0.58
1:B:3:LEU:HD23	1:B:3:LEU:H	1.68	0.58
1:B:123:MSE:CE	1:B:126:TYR:HD1	2.17	0.57
1:A:284:TYR:OH	1:A:293:GLY:HA2	2.04	0.57
1:B:3:LEU:CD2	1:B:3:LEU:H	2.17	0.57
1:B:115:SER:HB2	1:B:123:MSE:CE	2.35	0.57
1:A:134:ARG:NH1	2:A:348:SO4:O2	2.38	0.57
1:A:39:THR:HG21	1:A:84:LYS:HZ1	1.70	0.56
1:B:102:LEU:HD22	1:B:102:LEU:O	2.05	0.56
1:A:170:GLN:NE2	1:A:174:SER:HB2	2.21	0.55
1:A:23:THR:HG22	1:A:24:PRO:HD3	1.88	0.55
1:B:123:MSE:HE3	1:B:126:TYR:CD1	2.33	0.55
1:A:331:GLU:O	1:A:335:ILE:HG12	2.06	0.55
1:B:179:THR:C	1:B:181:THR:H	2.14	0.55
1:B:226:LEU:CD1	1:B:244:THR:HG22	2.37	0.55
1:A:230:GLN:NE2	1:A:234:GLU:OE2	2.38	0.55
1:B:68:HIS:HA	1:B:73:GLY:HA3	1.89	0.54
1:A:1:MSE:CE	1:A:110:ILE:HD11	2.36	0.54
1:A:225:ASP:OD1	1:A:228:MSE:HE3	2.08	0.54
1:A:44:GLU:O	1:A:47:GLN:HB3	2.07	0.54
1:A:193:VAL:HB	1:A:196:LYS:HG3	1.89	0.54
1:B:136:ALA:HA	1:B:139:MSE:HG2	1.88	0.54
1:B:142:ASN:O	1:B:146:GLN:HG3	2.08	0.54
1:B:302:LEU:HB3	1:B:329:ILE:HD11	1.90	0.54
1:A:185:ILE:HD12	1:A:186:GLY:N	2.23	0.54
1:B:26:LEU:HG	1:B:50:MSE:HE1	1.90	0.53
1:A:120:ARG:N	1:A:121:PRO:CD	2.71	0.53
1:A:123:MSE:HE3	1:A:126:TYR:HB2	1.90	0.53
1:B:184:LEU:HD11	1:B:218:VAL:CG2	2.40	0.52
1:A:9:VAL:HB	1:A:90:VAL:HG22	1.92	0.52
1:B:286:PRO:HB2	1:B:317:ILE:HG21	1.91	0.52
1:B:288:ASN:C	1:B:288:ASN:OD1	2.52	0.52
1:A:23:THR:N	1:A:24:PRO:CD	2.72	0.52
1:B:40:TYR:HB2	1:B:56:ILE:HD11	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:NH1	1:A:126:TYR:CD2	2.78	0.52
1:B:198:TRP:HB3	1:B:203:PHE:CE2	2.45	0.52
1:B:319:LYS:C	1:B:321:GLY:H	2.16	0.52
1:A:50:MSE:HB3	1:A:59:LEU:HD22	1.91	0.52
1:B:189:ILE:HD11	1:B:229:VAL:HA	1.90	0.52
1:A:26:LEU:HD11	1:A:40:TYR:CE1	2.45	0.52
1:A:50:MSE:O	1:A:51:GLU:C	2.53	0.52
1:A:335:ILE:O	1:A:339:GLU:HG3	2.09	0.51
1:B:187:PHE:HB2	1:B:219:PHE:CD1	2.44	0.51
1:A:225:ASP:O	1:A:229:VAL:HG23	2.11	0.51
1:B:5:TYR:C	1:B:6:LYS:HD2	2.36	0.51
1:B:194:PRO:HA	1:B:197:ARG:CD	2.40	0.51
1:A:12:PHE:CZ	1:A:14:MSE:SE	3.13	0.51
1:B:319:LYS:C	1:B:321:GLY:N	2.68	0.51
1:B:304:THR:HG23	1:B:328:VAL:HB	1.93	0.51
1:A:306:ASP:OD1	1:A:306:ASP:N	2.42	0.51
1:A:185:ILE:HD12	1:A:185:ILE:C	2.36	0.51
1:A:309:GLU:OE1	1:A:309:GLU:HA	2.12	0.50
1:B:40:TYR:CB	1:B:56:ILE:HD11	2.41	0.49
1:A:120:ARG:N	1:A:121:PRO:HD2	2.28	0.49
1:A:238:THR:O	1:A:240:PRO:HD3	2.12	0.49
1:B:94:HIS:NE2	2:B:352:SO4:O1	2.43	0.49
1:B:306:ASP:N	1:B:306:ASP:OD2	2.45	0.49
1:A:309:GLU:HB3	1:B:71:ILE:HG12	1.93	0.49
1:B:20:ILE:O	1:B:23:THR:HB	2.12	0.49
1:B:184:LEU:HD12	1:B:216:LYS:O	2.12	0.49
1:A:42:ILE:CG1	1:A:59:LEU:HD11	2.43	0.49
1:A:176:HIS:CD2	1:A:241:ILE:HG23	2.47	0.49
1:B:116:HIS:CE1	1:B:117:PHE:CE2	3.01	0.49
1:B:256:MSE:HE1	1:B:269:PRO:HB3	1.95	0.49
1:A:305:MSE:HE1	1:A:308:TYR:HD2	1.77	0.49
1:A:206:VAL:O	1:A:209:TYR:HB3	2.13	0.49
1:A:222:GLY:HA3	1:A:224:MSE:HE3	1.95	0.48
1:B:136:ALA:O	1:B:139:MSE:HG2	2.14	0.48
1:B:284:TYR:CE1	1:B:289:PRO:HA	2.48	0.48
1:A:40:TYR:CZ	1:A:50:MSE:HE3	2.48	0.48
1:A:305:MSE:HE3	1:A:305:MSE:CA	2.42	0.48
1:B:28:VAL:HG21	1:B:141:ILE:HD13	1.93	0.48
1:B:248:GLN:HG3	3:B:357:HOH:O	2.12	0.48
1:B:120:ARG:N	1:B:121:PRO:CD	2.77	0.48
1:A:244:THR:C	1:A:246:LYS:N	2.72	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PRO:HG3	1:A:301:VAL:HG11	1.94	0.47
1:B:302:LEU:HB3	1:B:329:ILE:CD1	2.43	0.47
1:B:46:LEU:O	1:B:49:VAL:HB	2.13	0.47
1:B:116:HIS:CE1	1:B:117:PHE:CD2	3.02	0.47
1:B:134:ARG:HH21	1:B:134:ARG:HG3	1.79	0.47
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.62	0.47
1:A:56:ILE:HG22	1:A:58:GLU:H	1.79	0.47
1:A:210:PHE:HB3	1:A:215:TYR:HB2	1.97	0.47
1:B:70:SER:HB3	1:B:73:GLY:H	1.80	0.47
1:B:162:CYS:O	1:B:163:GLU:C	2.57	0.47
1:B:189:ILE:HD11	1:B:229:VAL:HG22	1.97	0.47
1:B:215:TYR:N	1:B:215:TYR:CD1	2.82	0.47
1:A:226:LEU:HD13	1:A:244:THR:CG2	2.44	0.47
1:B:29:LEU:HB2	1:B:144:LEU:HD21	1.96	0.47
1:A:312:LYS:O	1:A:313:SER:C	2.58	0.47
1:B:189:ILE:HG22	1:B:203:PHE:CZ	2.49	0.47
1:B:247:PHE:HD1	1:B:251:PRO:CB	2.28	0.47
1:A:27:GLU:OE1	1:A:154:ASN:HB2	2.14	0.46
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.75	0.46
1:A:171:GLU:O	1:A:172:PHE:C	2.58	0.46
1:B:96:ASN:OD1	1:B:99:THR:HB	2.16	0.46
1:A:305:MSE:HE3	1:A:305:MSE:C	2.41	0.46
1:A:198:TRP:HB3	1:A:203:PHE:CE2	2.51	0.46
1:A:317:ILE:HD13	1:A:317:ILE:HA	1.71	0.46
1:B:26:LEU:HD22	1:B:26:LEU:HA	1.79	0.46
1:B:5:TYR:O	1:B:6:LYS:HD2	2.15	0.46
1:B:230:GLN:NE2	1:B:234:GLU:OE1	2.47	0.46
1:B:152:THR:O	1:B:152:THR:CG2	2.63	0.45
1:B:254:ALA:O	1:B:257:ASN:HB3	2.16	0.45
1:B:25:PHE:CD2	1:B:25:PHE:C	2.95	0.45
1:B:130:ASP:OD2	1:B:133:THR:HG22	2.17	0.45
1:A:280:ILE:HB	1:A:299:ALA:HB2	1.99	0.45
1:B:144:LEU:O	1:B:149:VAL:HB	2.17	0.45
1:A:258:ARG:HD2	1:A:258:ARG:O	2.17	0.45
1:A:101:TYR:HA	1:A:119:PHE:CE1	2.51	0.45
1:A:183:ILE:HG22	1:A:215:TYR:HD1	1.82	0.45
1:B:39:THR:HB	1:B:58:GLU:HB3	1.99	0.45
1:B:176:HIS:ND1	1:B:241:ILE:HG23	2.31	0.45
1:A:48:GLN:HE22	1:A:248:GLN:HB3	1.80	0.45
1:A:167:CYS:O	1:A:168:GLN:C	2.60	0.45
1:A:210:PHE:O	1:A:213:LEU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:O	1:A:310:ILE:HG13	2.16	0.44
1:B:197:ARG:HG2	1:B:228:MSE:HE1	1.98	0.44
1:A:226:LEU:HD13	1:A:244:THR:HG21	1.99	0.44
1:B:122:PHE:CD2	1:B:122:PHE:N	2.85	0.44
1:A:33:ALA:HB1	1:A:36:SER:CB	2.48	0.44
1:B:30:ARG:CZ	1:B:38:ILE:HD12	2.47	0.44
1:A:25:PHE:CD2	1:A:25:PHE:C	2.96	0.44
1:A:201:GLU:HG2	1:A:202:ARG:N	2.33	0.44
1:A:308:TYR:CZ	1:A:312:LYS:HD2	2.53	0.43
1:B:250:GLY:O	1:B:253:ALA:N	2.51	0.43
1:B:322:ASN:O	1:B:323:TYR:C	2.61	0.43
1:A:32:ALA:C	1:A:34:PRO:HD3	2.43	0.43
1:A:252:LEU:O	1:A:252:LEU:HD12	2.18	0.43
1:B:212:ARG:C	1:B:214:GLY:H	2.26	0.43
1:B:27:GLU:HA	1:B:55:ASN:OD1	2.19	0.43
1:B:313:SER:O	1:B:314:MSE:C	2.61	0.43
1:A:198:TRP:O	1:A:199:PRO:C	2.62	0.43
1:B:256:MSE:HE2	1:B:262:LEU:CD2	2.48	0.43
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.84	0.43
1:A:184:LEU:HD21	1:A:218:VAL:HG21	1.99	0.43
1:A:261:LEU:HG	1:A:262:LEU:N	2.34	0.43
1:A:53:ASN:HA	1:A:54:PRO:HD3	1.73	0.43
1:A:194:PRO:HA	1:A:197:ARG:HD2	2.00	0.43
1:A:202:ARG:NH1	1:A:329:ILE:O	2.52	0.43
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.90	0.43
1:B:19:VAL:CG1	1:B:46:LEU:HD13	2.49	0.43
1:B:44:GLU:HG3	1:B:61:VAL:CG2	2.46	0.43
1:A:229:VAL:O	1:A:233:VAL:HG22	2.19	0.42
1:A:46:LEU:O	1:A:49:VAL:HB	2.19	0.42
1:B:319:LYS:O	1:B:321:GLY:N	2.53	0.42
1:A:56:ILE:HG22	1:A:57:ASP:N	2.35	0.42
1:A:193:VAL:HA	1:A:194:PRO:HD2	1.74	0.42
1:A:259:CYS:O	1:A:278:VAL:HG13	2.20	0.42
1:B:81:ILE:HD12	1:B:106:ILE:HD11	2.00	0.42
1:B:249:LEU:HA	1:B:249:LEU:HD23	1.83	0.42
1:B:283:LEU:HB3	1:B:326:LEU:HD22	2.01	0.42
1:A:201:GLU:O	1:A:205:HIS:ND1	2.53	0.42
1:B:16:LEU:O	1:B:19:VAL:HG13	2.19	0.42
1:B:250:GLY:O	1:B:251:PRO:C	2.63	0.42
1:B:114:MSE:CE	1:B:128:ARG:HG3	2.50	0.42
1:A:284:TYR:CD2	1:A:301:VAL:HG13	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:VAL:HB	1:B:196:LYS:HB2	2.01	0.41
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.69	0.41
1:B:51:GLU:HG2	1:B:52:TYR:CE2	2.55	0.41
1:A:33:ALA:N	1:A:34:PRO:CD	2.83	0.41
1:A:285:GLY:HA3	1:A:286:PRO:HD2	1.82	0.41
1:B:30:ARG:HA	1:B:30:ARG:HD3	1.52	0.41
1:A:179:THR:OG1	1:A:181:THR:HG22	2.21	0.41
1:B:235:GLN:O	1:B:235:GLN:HG2	2.20	0.41
1:A:71:ILE:HA	1:A:74:LEU:HD12	2.03	0.41
1:A:135:HIS:CD2	1:A:295:TYR:CD1	3.08	0.41
1:A:184:LEU:HD12	1:A:216:LYS:O	2.20	0.41
1:B:24:PRO:HB3	1:B:154:ASN:OD1	2.21	0.41
1:A:64:LYS:HD2	1:A:64:LYS:O	2.21	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.83	0.40
1:A:314:MSE:HE2	1:A:314:MSE:HB3	1.91	0.40
1:B:329:ILE:HD13	1:B:329:ILE:HA	1.92	0.40
1:A:1:MSE:HE3	1:A:1:MSE:HB2	2.00	0.40
1:A:173:TYR:HB3	1:A:178:LEU:HD23	2.03	0.40
1:B:265:ASN:OD1	1:B:265:ASN:N	2.54	0.40
1:B:133:THR:O	1:B:133:THR:HG23	2.21	0.40
1:B:298:HIS:CE1	3:B:355:HOH:O	2.74	0.40
1:A:26:LEU:HD11	1:A:40:TYR:CD1	2.56	0.40
1:B:161:ILE:HD11	1:B:276:GLN:OE1	2.22	0.40
1:B:179:THR:C	1:B:181:THR:N	2.77	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	346/349 (99%)	311 (90%)	31 (9%)	4 (1%)	10 38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/349 (97%)	305 (90%)	29 (8%)	6 (2%)	6	28
All	All	686/698 (98%)	616 (90%)	60 (9%)	10 (2%)	8	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	GLY
1	B	322	ASN
1	A	51	GLU
1	A	153	SER
1	B	314	MSE
1	A	65	LYS
1	B	16	LEU
1	B	323	TYR
1	B	320	GLU
1	B	285	GLY

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%)	256 (85%)	45 (15%)	3	13
1	B	292/289 (101%)	248 (85%)	44 (15%)	3	13
All	All	593/578 (103%)	504 (85%)	89 (15%)	3	13

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	39	THR
1	A	42	ILE
1	A	43	ASP
1	A	44	GLU
1	A	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	58	GLU
1	A	60	ILE
1	A	61	VAL
1	A	62	VAL
1	A	67	ARG
1	A	68	HIS
1	A	77	VAL
1	A	79	ARG
1	A	90	VAL
1	A	97	GLU
1	A	107	HIS
1	A	110	ILE
1	A	120	ARG
1	A	133	THR
1	A	134	ARG
1	A	144	LEU
1	A	164	GLU
1	A	179	THR
1	A	185	ILE
1	A	189	ILE
1	A	193	VAL
1	A	196	LYS
1	A	201	GLU
1	A	218	VAL
1	A	224	MSE
1	A	226	LEU
1	A	246	LYS
1	A	256	MSE
1	A	264	THR
1	A	266	ASP
1	A	278	VAL
1	A	287	SER
1	A	303	GLU
1	A	306	ASP
1	A	313	SER
1	A	317	ILE
1	A	329	ILE
1	A	330	SER
1	A	332	GLU
1	B	2	GLU
1	B	3	LEU
1	B	10	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	19	VAL
1	B	23	THR
1	B	25	PHE
1	B	26	LEU
1	B	30	ARG
1	B	31	LYS
1	B	39	THR
1	B	47	GLN
1	B	49	VAL
1	B	56	ILE
1	B	59	LEU
1	B	61	VAL
1	B	62	VAL
1	B	71	ILE
1	B	97	GLU
1	B	98	ARG
1	B	102	LEU
1	B	106	ILE
1	B	114	MSE
1	B	115	SER
1	B	132	LYS
1	B	133	THR
1	B	144	LEU
1	B	155	SER
1	B	171	GLU
1	B	178	LEU
1	B	183	ILE
1	B	201	GLU
1	B	213	LEU
1	B	218	VAL
1	B	226	LEU
1	B	241	ILE
1	B	252	LEU
1	B	256	MSE
1	B	304	THR
1	B	306	ASP
1	B	326	LEU
1	B	327	SER
1	B	333	GLN
1	B	344	GLU
1	B	345	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	94	HIS
1	A	188	ASN
1	A	248	GLN
1	A	271	HIS
1	A	333	GLN
1	B	37	HIS
1	B	55	ASN
1	B	69	ASN
1	B	168	GLN
1	B	257	ASN

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](#)

11 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	SO4	B	348	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	A	347	-	4,4,4	0.27	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	347	-	4,4,4	0.25	0	6,6,6	0.23	0
2	SO4	B	349	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	351	-	4,4,4	0.28	0	6,6,6	0.32	0
2	SO4	A	350	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	B	352	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	B	351	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	B	350	-	4,4,4	0.22	0	6,6,6	0.14	0
2	SO4	A	349	-	4,4,4	0.27	0	6,6,6	0.26	0
2	SO4	A	348	-	4,4,4	0.28	0	6,6,6	0.13	0

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
2	B	352	SO4	1	0
2	B	351	SO4	1	0
2	A	348	SO4	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	335/349 (95%)	-0.55	0 100 100	33, 57, 98, 166	0
1	B	331/349 (94%)	-0.55	1 (0%) 90 82	37, 61, 100, 182	0
All	All	666/698 (95%)	-0.55	1 (0%) 91 85	33, 60, 99, 182	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	GLU	2.6

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(Å ²)	Q<0.9
2	SO4	B	351	5/5	0.63	0.11	116,116,118,119	5
2	SO4	A	350	5/5	0.65	0.09	107,108,110,114	5
2	SO4	B	348	5/5	0.73	0.21	97,102,105,111	5
2	SO4	B	352	5/5	0.77	0.16	105,105,106,109	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	348	5/5	0.83	0.07	92,92,98,100	5
2	SO4	A	347	5/5	0.84	0.09	100,100,104,108	5
2	SO4	B	349	5/5	0.86	0.10	98,100,103,106	5
2	SO4	A	351	5/5	0.88	0.10	92,95,95,96	5
2	SO4	B	347	5/5	0.88	0.12	80,83,89,92	5
2	SO4	B	350	5/5	0.90	0.16	99,100,103,105	5
2	SO4	A	349	5/5	0.92	0.08	77,87,90,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.