



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:31 PM UTC

PDB ID : 1ON0 / pdb_00001on0
Title : Crystal Structure of Putative Acetyltransferase (YycN) from *Bacillus subtilis*, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET SR144
Authors : Forouhar, F.; Shen, J.; Kuzin, A.; Chiang, Y.; Xiao, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2003-02-26
Resolution : 2.20 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)

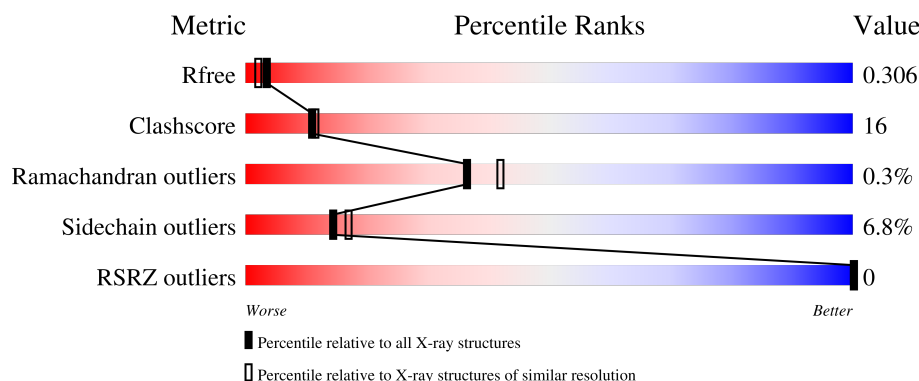
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	158	
1	B	158	
1	C	158	
1	D	158	

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5528 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 YycN protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	Se	0	0	0
			1283	829	218	232	4			
1	B	157	Total	C	N	O	Se	0	0	0
			1292	834	219	235	4			
1	C	156	Total	C	N	O	Se	0	0	0
			1283	829	218	232	4			
1	D	157	Total	C	N	O	Se	0	0	0
			1292	834	219	235	4			

There are 28 discrepancies between the modelled and reference sequences:

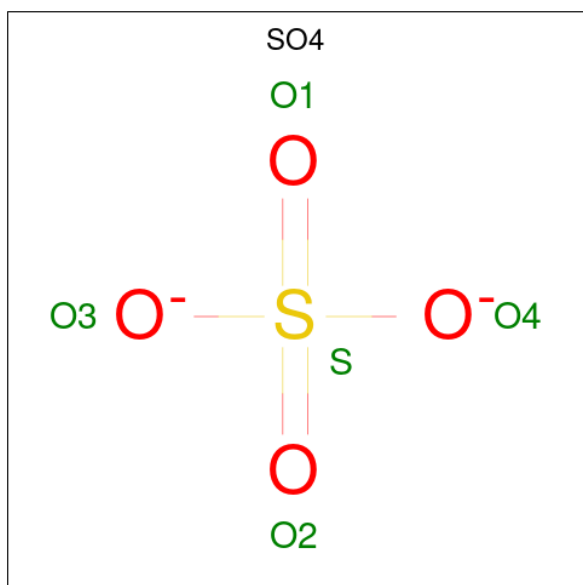
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O32293
A	4	MSE	MET	modified residue	UNP O32293
A	8	MSE	MET	modified residue	UNP O32293
A	120	MSE	MET	modified residue	UNP O32293
A	152	MSE	MET	modified residue	UNP O32293
A	157	LEU	-	cloning artifact	UNP O32293
A	158	GLU	-	cloning artifact	UNP O32293
B	1	MSE	MET	modified residue	UNP O32293
B	4	MSE	MET	modified residue	UNP O32293
B	8	MSE	MET	modified residue	UNP O32293
B	120	MSE	MET	modified residue	UNP O32293
B	152	MSE	MET	modified residue	UNP O32293
B	157	LEU	-	cloning artifact	UNP O32293
B	158	GLU	-	cloning artifact	UNP O32293
C	1	MSE	MET	modified residue	UNP O32293
C	4	MSE	MET	modified residue	UNP O32293
C	8	MSE	MET	modified residue	UNP O32293
C	120	MSE	MET	modified residue	UNP O32293
C	152	MSE	MET	modified residue	UNP O32293
C	157	LEU	-	cloning artifact	UNP O32293
C	158	GLU	-	cloning artifact	UNP O32293

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	modified residue	UNP O32293
D	4	MSE	MET	modified residue	UNP O32293
D	8	MSE	MET	modified residue	UNP O32293
D	120	MSE	MET	modified residue	UNP O32293
D	152	MSE	MET	modified residue	UNP O32293
D	157	LEU	-	cloning artifact	UNP O32293
D	158	GLU	-	cloning artifact	UNP O32293

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

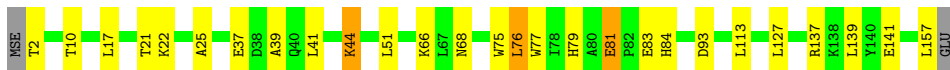
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total 88	O 88	0	0
4	B	96	Total 96	O 96	0	0
4	C	90	Total 90	O 90	0	0
4	D	83	Total 83	O 83	0	0

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.

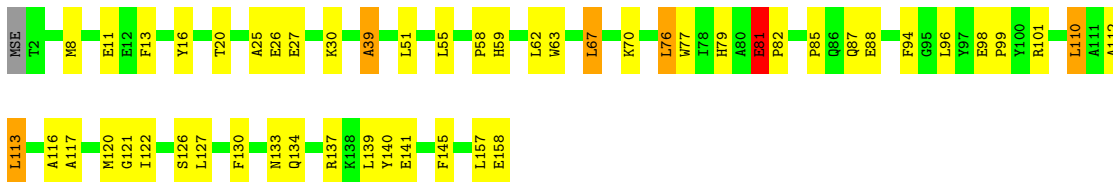
- Molecule 1: YycN protein

Chain A: 



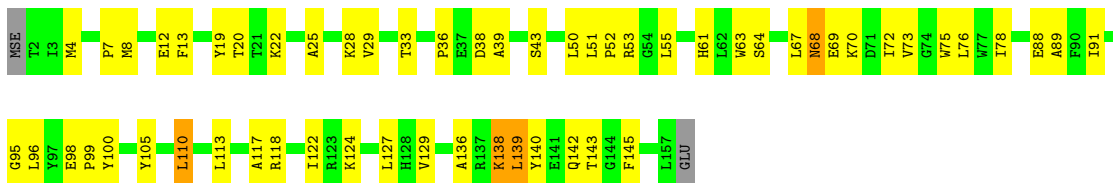
- Molecule 1: YycN protein

Chain B: 



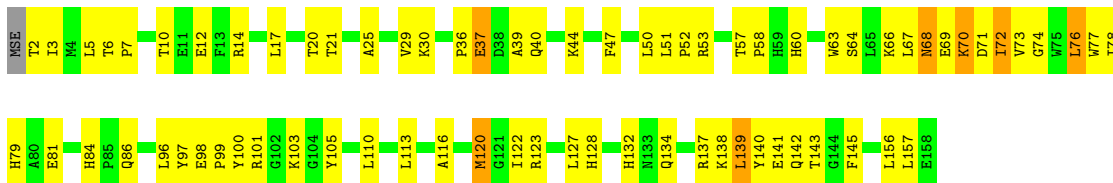
- Molecule 1: YycN protein

Chain C: 



- Molecule 1: YycN protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.89Å 101.59Å 62.12Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.20 29.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	9.9 (29.68-2.20) 97.0 (29.68-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.289 0.241 , 0.306	Depositor DCC
R_{free} test set	7541 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.278 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5528	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, CL

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	0.48	0/1315	0.86	0/1775
1	B	0.48	0/1324	0.87	2/1787 (0.1%)
1	C	0.44	0/1315	0.83	1/1775 (0.1%)
1	D	0.43	0/1324	0.77	0/1787
All	All	0.46	0/5278	0.83	3/7124 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	LEU	N-CA-C	-7.55	103.69	113.12
1	B	67	LEU	N-CA-C	-6.59	104.26	112.90
1	B	112	ALA	N-CA-C	-5.48	106.10	112.89

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	1283	0	1266	20	0
1	B	1292	0	1272	40	0
1	C	1283	0	1266	60	0
1	D	1292	0	1272	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
4	A	88	0	0	3	0
4	B	96	0	0	5	0
4	C	90	0	0	3	0
4	D	83	0	0	2	0
All	All	5528	0	5076	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 16.

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:A:81:GLU:HB3	1:A:84:HIS:HB2	1.37	1.02
1:B:87:GLN:HG2	1:B:121:GLY:O	1.71	0.90
1:B:87:GLN:HB2	4:B:419:HOH:O	1.75	0.86
1:C:70:LYS:HG3	1:D:36:PRO:HB3	1.57	0.85
1:D:120:MSE:HG3	1:D:122:ILE:HD13	1.61	0.80
1:C:64:SER:HB3	1:C:72:ILE:HG21	1.64	0.79
1:C:110:LEU:HD23	1:C:143:THR:HG21	1.67	0.76
1:D:68:ASN:H	1:D:68:ASN:HD22	1.30	0.76
1:D:116:ALA:O	1:D:120:MSE:HG2	1.86	0.76
1:C:8:MSE:HE2	1:C:55:LEU:HD21	1.66	0.75
1:A:21:THR:HG21	1:A:44:LYS:HD2	1.68	0.75
1:C:63:TRP:HE3	1:C:76:LEU:HD12	1.53	0.73
1:A:76:LEU:HD11	1:A:113:LEU:HD13	1.70	0.72
1:B:127:LEU:C	1:B:127:LEU:HD12	2.15	0.72
1:C:138:LYS:O	1:C:142:GLN:HG2	1.91	0.70
1:B:110:LEU:HD22	1:B:139:LEU:HD11	1.74	0.69
1:C:8:MSE:HE3	1:C:13:PHE:HB2	1.73	0.69
1:A:10:THR:HG22	4:A:450:HOH:O	1.92	0.69
1:B:70:LYS:HB3	1:C:53:ARG:HH11	1.58	0.68
1:A:44:LYS:HE2	1:C:7:PRO:HD3	1.77	0.66
1:C:8:MSE:CE	1:C:55:LEU:HD21	2.24	0.66
1:B:8:MSE:HE1	1:B:13:PHE:HD1	1.60	0.66
1:B:117:ALA:HB1	1:B:122:ILE:HB	1.77	0.65
1:C:63:TRP:CE3	1:C:76:LEU:HD12	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LYS:CG	1:D:36:PRO:HB3	2.28	0.64
1:A:137:ARG:O	1:A:141:GLU:HG3	1.99	0.63
1:A:21:THR:CG2	1:A:44:LYS:HD2	2.29	0.62
1:D:66:LYS:HD3	1:D:69:GLU:HA	1.80	0.62
1:D:76:LEU:HD11	1:D:113:LEU:HG	1.80	0.62
1:A:81:GLU:HG2	1:A:84:HIS:HD2	1.64	0.61
1:B:116:ALA:O	1:B:120:MSE:HG2	2.00	0.61
1:D:84:HIS:CD2	1:D:86:GLN:H	2.19	0.61
1:B:25:ALA:HB1	1:B:39:ALA:HB1	1.83	0.60
1:C:64:SER:HB3	1:C:72:ILE:CG2	2.30	0.60
1:B:81:GLU:HB2	4:B:479:HOH:O	2.01	0.59
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.66	0.59
1:D:37:GLU:CD	1:D:37:GLU:H	2.10	0.59
1:D:110:LEU:HD13	1:D:143:THR:HG21	1.85	0.58
1:D:123:ARG:HG3	1:D:123:ARG:HH11	1.69	0.58
1:C:25:ALA:HB1	1:C:39:ALA:HB1	1.86	0.58
1:B:79:HIS:NE2	1:B:81:GLU:HG3	2.19	0.57
1:A:127:LEU:C	1:A:127:LEU:HD12	2.29	0.57
1:D:2:THR:HB	4:D:477:HOH:O	2.03	0.57
1:A:25:ALA:HB1	1:A:39:ALA:HB1	1.85	0.57
1:D:3:ILE:HD12	1:D:3:ILE:N	2.19	0.57
1:C:140:TYR:O	1:C:145:PHE:HB2	2.05	0.57
1:C:88:GLU:CB	1:C:124:LYS:HB3	2.35	0.56
1:C:89:ALA:HB2	1:C:122:ILE:HD13	1.87	0.56
1:C:95:GLY:C	1:C:96:LEU:HD12	2.30	0.56
1:C:76:LEU:CD1	1:C:78:ILE:HG23	2.35	0.56
1:B:8:MSE:HE2	1:B:62:LEU:CB	2.36	0.55
1:D:25:ALA:HB1	1:D:39:ALA:HB1	1.89	0.55
1:B:137:ARG:O	1:B:141:GLU:HG3	2.06	0.55
1:C:68:ASN:HA	4:C:438:HOH:O	2.06	0.55
1:C:138:LYS:HB3	1:C:138:LYS:NZ	2.22	0.55
1:D:50:LEU:C	1:D:52:PRO:HD3	2.32	0.55
1:B:8:MSE:HE2	1:B:62:LEU:HB3	1.89	0.55
1:D:138:LYS:O	1:D:142:GLN:HG3	2.07	0.55
1:C:91:ILE:HD12	1:C:127:LEU:HD23	1.89	0.54
1:C:76:LEU:HD11	1:C:78:ILE:HG23	1.87	0.54
1:B:26:GLU:O	1:B:30:LYS:HG3	2.08	0.54
1:B:8:MSE:HE3	1:B:55:LEU:HD21	1.90	0.54
1:C:28:LYS:NZ	1:C:33:THR:HG21	2.23	0.54
1:D:68:ASN:HD22	1:D:68:ASN:N	1.94	0.54
1:C:96:LEU:CD2	1:C:105:TYR:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:MSE:HE1	1:C:13:PHE:HD1	1.72	0.53
1:C:76:LEU:HD13	1:C:76:LEU:C	2.33	0.53
1:D:63:TRP:HZ3	1:D:78:ILE:HD12	1.73	0.53
1:C:73:VAL:HG12	1:C:100:TYR:CG	2.43	0.53
1:D:68:ASN:H	1:D:68:ASN:ND2	2.04	0.53
1:D:137:ARG:O	1:D:141:GLU:HG3	2.09	0.53
1:C:139:LEU:C	1:C:139:LEU:HD13	2.33	0.52
1:D:73:VAL:HG12	1:D:100:TYR:CG	2.44	0.52
1:A:37:GLU:HG3	4:C:490:HOH:O	2.08	0.52
1:C:96:LEU:HD21	1:C:105:TYR:HB2	1.90	0.52
1:C:8:MSE:CE	1:C:13:PHE:HD1	2.23	0.52
1:B:101:ARG:HG2	4:B:442:HOH:O	2.11	0.51
1:B:11:GLU:H	1:B:11:GLU:CD	2.19	0.50
1:B:139:LEU:C	1:B:139:LEU:HD13	2.36	0.50
1:C:88:GLU:HA	1:C:124:LYS:O	2.12	0.50
1:D:64:SER:HB3	1:D:72:ILE:HG22	1.93	0.50
1:B:127:LEU:C	1:B:127:LEU:CD1	2.85	0.49
1:C:8:MSE:HE3	1:C:13:PHE:CB	2.40	0.49
1:C:70:LYS:C	1:C:70:LYS:HD3	2.37	0.49
1:C:110:LEU:CD2	1:C:139:LEU:HD11	2.42	0.49
1:A:41:LEU:HD21	1:C:4:MSE:SE	2.63	0.49
1:A:77:TRP:C	1:A:77:TRP:CD1	2.90	0.49
1:C:117:ALA:HB1	1:C:122:ILE:HB	1.93	0.49
1:C:96:LEU:HD12	1:C:96:LEU:N	2.28	0.48
1:D:30:LYS:HE3	1:D:132:HIS:CD2	2.48	0.48
1:D:98:GLU:N	1:D:99:PRO:HD2	2.28	0.48
1:B:27:GLU:HB3	1:B:130:PHE:CE1	2.48	0.48
1:C:28:LYS:HZ2	1:C:33:THR:HG21	1.78	0.48
1:B:140:TYR:O	1:B:145:PHE:HB2	2.14	0.48
1:C:22:LYS:HE3	1:D:99:PRO:HG3	1.96	0.48
1:B:11:GLU:OE1	1:B:11:GLU:N	2.40	0.47
1:D:134:GLN:O	1:D:138:LYS:HG2	2.14	0.47
1:A:157:LEU:HD12	1:A:157:LEU:H	1.79	0.47
1:B:110:LEU:HD22	1:B:139:LEU:CD1	2.43	0.47
1:B:63:TRP:CE3	1:B:76:LEU:HD13	2.50	0.46
1:D:57:THR:O	1:D:60:HIS:HB2	2.15	0.46
1:D:156:LEU:C	1:D:157:LEU:HD12	2.41	0.46
1:C:8:MSE:CE	1:C:13:PHE:CD1	2.98	0.46
1:B:77:TRP:C	1:B:77:TRP:CD1	2.92	0.46
1:D:127:LEU:HD12	1:D:127:LEU:C	2.41	0.46
1:D:77:TRP:C	1:D:77:TRP:CD1	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:O	1:D:113:LEU:HD23	2.15	0.46
1:D:53:ARG:NH2	1:D:58:PRO:HD3	2.31	0.45
1:D:140:TYR:O	1:D:145:PHE:HB2	2.16	0.45
1:B:16:TYR:O	1:B:20:THR:HG22	2.16	0.45
1:B:58:PRO:O	1:B:59:HIS:HB2	2.16	0.45
1:D:86:GLN:HG2	4:D:484:HOH:O	2.16	0.45
1:C:25:ALA:O	1:C:29:VAL:HG23	2.15	0.45
1:C:88:GLU:HB3	1:C:124:LYS:HB3	1.97	0.45
1:C:91:ILE:HB	1:C:127:LEU:HB3	1.98	0.45
1:D:10:THR:O	1:D:14:ARG:HG3	2.17	0.45
1:C:50:LEU:C	1:C:52:PRO:HD3	2.41	0.45
1:D:73:VAL:HG12	1:D:100:TYR:CD1	2.51	0.45
1:D:110:LEU:CD1	1:D:143:THR:HG21	2.46	0.45
1:A:37:GLU:H	1:A:37:GLU:CD	2.24	0.45
1:B:13:PHE:HB2	1:B:55:LEU:HD11	1.99	0.45
1:D:53:ARG:HH21	1:D:58:PRO:HG3	1.81	0.45
1:C:29:VAL:HG13	1:C:36:PRO:HG3	1.99	0.45
1:A:81:GLU:HG2	1:A:84:HIS:CD2	2.49	0.44
1:C:70:LYS:HE3	1:D:29:VAL:HG21	1.99	0.44
1:D:97:TYR:HB3	1:D:99:PRO:HD2	2.00	0.44
1:B:157:LEU:HB3	1:B:158:GLU:OE1	2.17	0.44
1:D:70:LYS:HE3	1:D:71:ASP:OD1	2.17	0.44
1:C:25:ALA:HB2	1:C:43:SER:OG	2.17	0.44
1:C:98:GLU:N	1:C:99:PRO:HD2	2.33	0.44
1:C:19:TYR:HE2	1:C:75:TRP:CH2	2.36	0.44
1:D:68:ASN:N	1:D:68:ASN:ND2	2.65	0.44
1:D:76:LEU:HD11	1:D:113:LEU:CG	2.46	0.44
1:B:85:PRO:HG2	4:B:489:HOH:O	2.18	0.44
1:C:118:ARG:HG3	1:C:118:ARG:NH1	2.32	0.44
1:D:128:HIS:ND1	1:D:128:HIS:C	2.76	0.43
1:C:8:MSE:HE3	1:C:13:PHE:CD1	2.53	0.43
1:D:5:LEU:HD22	1:D:5:LEU:N	2.33	0.43
1:B:98:GLU:N	1:B:99:PRO:HD2	2.34	0.43
1:B:127:LEU:HD12	1:B:127:LEU:O	2.18	0.43
1:A:75:TRP:HE1	1:A:93:ASP:CG	2.26	0.43
1:C:75:TRP:CZ2	1:C:95:GLY:HA3	2.54	0.43
1:D:2:THR:C	1:D:67:LEU:HD22	2.43	0.43
1:B:82:PRO:HA	4:B:493:HOH:O	2.19	0.43
1:D:17:LEU:O	1:D:20:THR:HG22	2.18	0.43
1:D:110:LEU:CD1	1:D:139:LEU:HD12	2.49	0.43
1:A:17:LEU:HD21	4:A:473:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLU:OE1	1:B:126:SER:HB2	2.20	0.42
1:D:40:GLN:HA	1:D:40:GLN:HE21	1.83	0.42
1:D:69:GLU:N	1:D:69:GLU:OE2	2.52	0.42
1:D:79:HIS:NE2	1:D:81:GLU:HG2	2.34	0.42
1:C:61:HIS:HE1	4:C:410:HOH:O	2.03	0.42
1:D:6:THR:O	1:D:7:PRO:C	2.63	0.42
1:C:29:VAL:CG1	1:C:36:PRO:HG3	2.50	0.42
1:C:127:LEU:C	1:C:127:LEU:HD12	2.45	0.42
1:A:79:HIS:CD2	4:A:440:HOH:O	2.72	0.41
1:D:96:LEU:HD11	1:D:105:TYR:HB2	2.02	0.41
1:D:21:THR:HA	1:D:47:PHE:CE2	2.56	0.41
1:A:66:LYS:HB3	1:A:68:ASN:O	2.19	0.41
1:B:94:PHE:CZ	1:B:110:LEU:HD13	2.55	0.41
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.88	0.41
1:C:70:LYS:HD3	1:C:70:LYS:O	2.21	0.41
1:B:8:MSE:HE1	1:B:13:PHE:CD1	2.48	0.41
1:B:8:MSE:CE	1:B:55:LEU:HD21	2.50	0.41
1:C:136:ALA:HB1	1:C:140:TYR:CE2	2.57	0.41
1:D:74:GLY:HA2	1:D:96:LEU:HA	2.03	0.40
1:C:129:VAL:O	1:C:129:VAL:HG13	2.21	0.40
1:D:101:ARG:C	1:D:103:LYS:H	2.28	0.40
1:B:76:LEU:HD11	1:B:113:LEU:HG	2.03	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	154/158 (98%)	143 (93%)	11 (7%)	0	100	100
1	B	155/158 (98%)	148 (96%)	5 (3%)	2 (1%)	9	8
1	C	154/158 (98%)	144 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	155/158 (98%)	141 (91%)	14 (9%)	0	100	100
All	All	618/632 (98%)	576 (93%)	40 (6%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	ALA
1	B	81	GLU

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	135/132 (102%)	127 (94%)	8 (6%)	18	22
1	B	136/132 (103%)	127 (93%)	9 (7%)	15	18
1	C	135/132 (102%)	125 (93%)	10 (7%)	13	14
1	D	136/132 (103%)	126 (93%)	10 (7%)	13	14
All	All	542/528 (103%)	505 (93%)	37 (7%)	14	17

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	22	LYS
1	A	44	LYS
1	A	51	LEU
1	A	76	LEU
1	A	81	GLU
1	A	83	GLU
1	A	139	LEU
1	B	51	LEU
1	B	67	LEU
1	B	76	LEU
1	B	81	GLU

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Mol	Chain	Res	Type
1	B	96	LEU
1	B	110	LEU
1	B	113	LEU
1	B	133	ASN
1	B	134	GLN
1	C	12	GLU
1	C	20	THR
1	C	38	ASP
1	C	51	LEU
1	C	68	ASN
1	C	69	GLU
1	C	110	LEU
1	C	113	LEU
1	C	138	LYS
1	C	139	LEU
1	D	12	GLU
1	D	37	GLU
1	D	44	LYS
1	D	51	LEU
1	D	68	ASN
1	D	70	LYS
1	D	72	ILE
1	D	76	LEU
1	D	120	MSE
1	D	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	79	HIS
1	A	115	GLN
1	A	133	ASN
1	A	142	GLN
1	B	45	GLN
1	B	61	HIS
1	B	86	GLN
1	B	108	GLN
1	B	115	GLN
1	B	133	ASN
1	C	59	HIS
1	C	61	HIS

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Mol	Chain	Res	Type
1	C	68	ASN
1	C	134	GLN
1	C	146	GLN
1	D	40	GLN
1	D	68	ASN
1	D	84	HIS
1	D	87	GLN
1	D	133	ASN
1	D	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	B	400	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	C	402	-	4,4,4	0.40	0	6,6,6	0.16	0
2	SO4	D	403	-	4,4,4	0.36	0	6,6,6	0.09	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.

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 [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	152/158 (96%)	-1.37	0 100 100	16, 28, 49, 76	0
1	B	153/158 (96%)	-1.33	0 100 100	15, 29, 52, 83	0
1	C	152/158 (96%)	-1.26	0 100 100	17, 35, 64, 90	0
1	D	153/158 (96%)	-1.19	0 100 100	18, 38, 72, 92	0
All	All	610/632 (96%)	-1.29	0 100 100	15, 33, 64, 92	0

There are no RSRZ outliers to report.

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	400	5/5	0.99	0.04	30,30,31,33	0
2	SO4	C	402	5/5	0.99	0.04	46,50,51,51	0
2	SO4	D	403	5/5	0.99	0.04	64,64,65,65	0
3	CL	A	405	1/1	0.99	0.03	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	401	5/5	1.00	0.02	25,26,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.