WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 09:22 AM GMT

PDB ID : 3GWP
Title : Crystal structure of carbon-sulfur lyase involved in aluminum resistance (YP_878183.1) from CLOSTRIDIUM NOVYI NT at 2.90 A resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-04-01
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.271
Clashscore		9
Ramachandran outliers		0.4%
Sidechain outliers		0.4%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
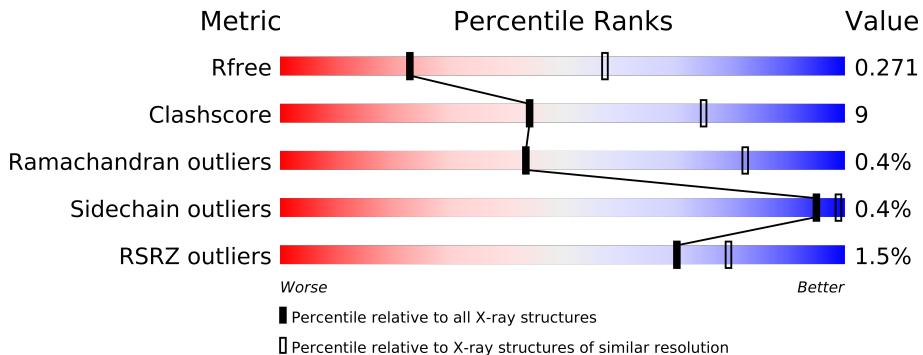
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	
1	C	427	
1	D	427	
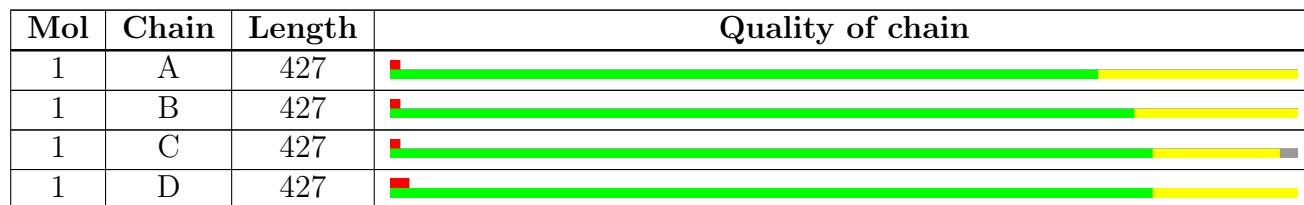
2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 12910 atoms, of which 0 are hydrogen and 0 are deuterium.

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 carbon-sulfur lyase involved in aluminum resistance.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	P	S	Se	0	0	0
			3223	2042	529	631	1	9	11			
1	B	427	Total	C	N	O	P	S	Se	0	2	0
			3272	2079	535	637	1	9	11			
1	C	418	Total	C	N	O	P	S	Se	0	1	0
			3149	1999	523	607	1	9	10			
1	D	427	Total	C	N	O	P	S	Se	0	2	0
			3266	2074	539	632	1	9	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP A0Q0N1
B	0	GLY	-	leader sequence	UNP A0Q0N1
C	0	GLY	-	leader sequence	UNP A0Q0N1
D	0	GLY	-	leader sequence	UNP A0Q0N1

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: carbon-sulfur lyase involved in aluminum resistance

Chain A:
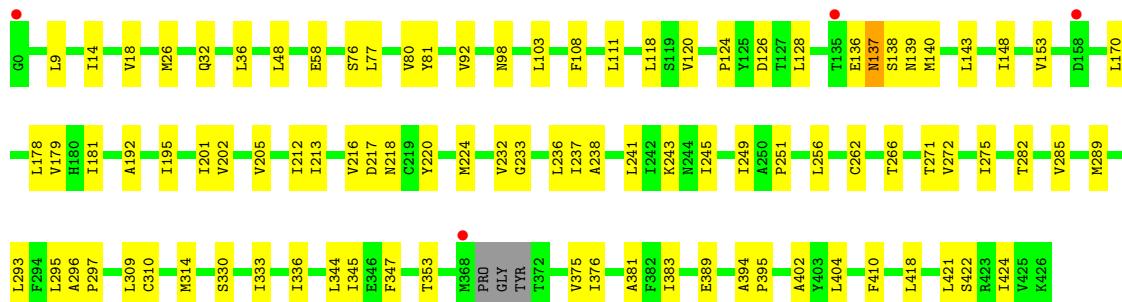
• Molecule 1: carbon-sulfur lyase involved in aluminum resistance

Chain B:
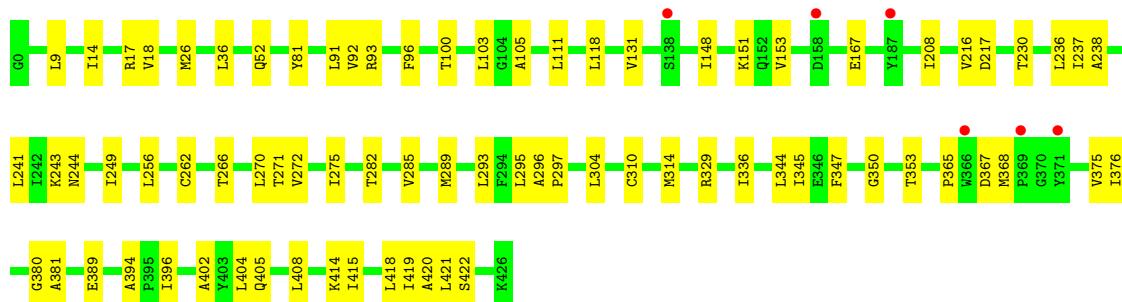
• Molecule 1: carbon-sulfur lyase involved in aluminum resistance

Chain C:

• Molecule 1: carbon-sulfur lyase involved in aluminum resistance

Chain D:
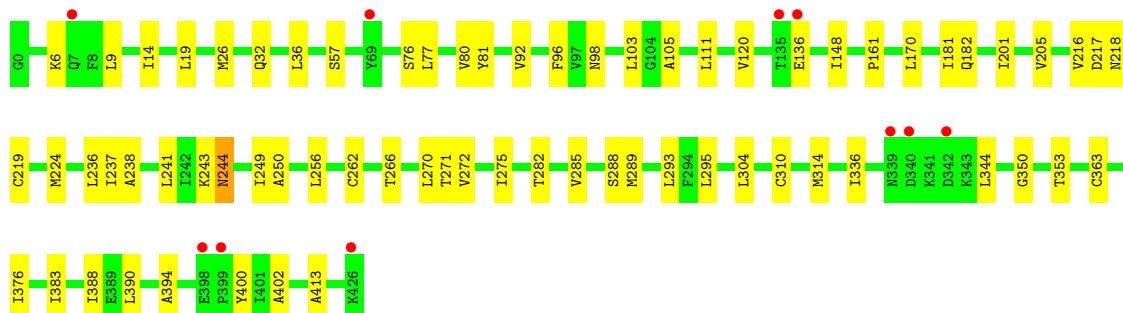
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.74Å 108.95Å 207.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.90 29.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.77-2.90) 100.0 (29.77-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.271 0.228 , 0.271	Depositor DCC
R_{free} test set	2022 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , -0.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Outliers	1 of 40368 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0/3241	0.55	0/4364
1	B	0.54	0/3301	0.54	0/4445
1	C	0.53	0/3169	0.54	0/4277
1	D	0.54	0/3295	0.54	0/4442
All	All	0.53	0/13006	0.54	0/17528

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3223	0	3103	67	0
1	B	3272	0	3169	56	0
1	C	3149	0	3004	48	0
1	D	3266	0	3151	59	0
All	All	12910	0	12427	219	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (219) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:18:VAL:HG23	1:C:425:VAL:HG21	1.52	0.92
1:D:256:LEU:HD13	1:D:266:THR:HG21	1.52	0.91
1:B:368:MSE:HE2	1:B:375:VAL:HG21	1.57	0.87
1:C:103:LEU:HD23	1:C:238:ALA:HB3	1.61	0.82
1:B:275:ILE:HD13	1:D:98:ASN:HD21	1.46	0.80
1:C:256:LEU:HD13	1:C:266:THR:HG21	1.67	0.77
1:B:256:LEU:HD13	1:B:266:THR:HG21	1.66	0.77
1:C:118:LEU:HD11	1:C:153:VAL:HG23	1.66	0.76
1:A:98:ASN:HD21	1:C:275:ILE:HD13	1.52	0.73
1:C:111:LEU:HD13	1:C:148:ILE:HG21	1.69	0.73
1:D:256:LEU:CD1	1:D:266:THR:HG21	2.21	0.70
1:C:15:ASN:HD21	1:C:425:VAL:HG23	1.57	0.68
1:A:310:CYS:SG	1:A:336:ILE:HD11	2.34	0.68
1:B:344:LEU:CD1	1:B:402:ALA:HB2	2.24	0.67
1:A:256:LEU:HD13	1:A:266:THR:HG21	1.75	0.67
1:D:238:ALA:HB2	1:D:256:LEU:HD23	1.78	0.66
1:C:256:LEU:CD1	1:C:266:THR:HG21	2.26	0.65
1:A:77:LEU:HD21	1:A:289:MSE:HE2	1.80	0.64
1:D:103:LEU:HD23	1:D:238:ALA:HB3	1.79	0.63
1:B:18:VAL:HG21	1:B:422:SER:HA	1.79	0.62
1:C:81:TYR:CE1	1:C:293:LEU:HD22	2.34	0.62
1:B:103:LEU:HD23	1:B:238:ALA:HB3	1.81	0.61
1:B:310:CYS:SG	1:B:336:ILE:HD11	2.40	0.61
1:A:344:LEU:CD1	1:A:402:ALA:HB2	2.31	0.61
1:B:230:THR:HG23	1:B:237:ILE:HD13	1.82	0.61
1:A:81:TYR:CE1	1:A:293:LEU:HD22	2.35	0.61
1:B:241:LEU:HD11	1:B:289:MSE:HE3	1.83	0.60
1:A:347:PHE:HB2	1:A:424:ILE:HD11	1.84	0.60
1:A:218:ASN:HD22	1:A:237:ILE:HD12	1.67	0.58
1:D:249:ILE:HD11	1:D:295:LEU:HD12	1.86	0.58
1:A:118:LEU:HD11	1:A:153:VAL:HG23	1.86	0.57
1:B:118:LEU:HD11	1:B:153:VAL:HG23	1.86	0.57
1:B:238:ALA:HB2	1:B:256:LEU:HD23	1.87	0.57
1:D:249:ILE:HG22	1:D:288:SER:HB2	1.86	0.57
1:B:238:ALA:HB2	1:B:256:LEU:CD2	2.35	0.57
1:B:241:LEU:CD1	1:B:289:MSE:HE3	2.34	0.57
1:D:271:THR:HG22	1:D:272:VAL:HG22	1.87	0.56
1:B:256:LEU:CD1	1:B:266:THR:HG21	2.35	0.56
1:C:224:MSE:HE2	1:C:224:MSE:HA	1.88	0.56
1:C:1:MSE:SE	1:C:19:LEU:HD11	2.55	0.56
1:C:18:VAL:HG23	1:C:425:VAL:CG2	2.30	0.56
1:A:220:TYR:CE2	1:A:333:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:241:LEU:HD23	1:A:245:ILE:HG23	1.87	0.55
1:C:9:LEU:HD22	1:C:14:ILE:HD12	1.87	0.55
1:A:256:LEU:CD1	1:A:266:THR:HG21	2.37	0.55
1:A:275:ILE:HD13	1:C:98:ASN:HD21	1.70	0.55
1:D:81:TYR:CE1	1:D:293:LEU:HD22	2.42	0.54
1:A:217:ASP:OD2	1:A:243:LLP:N1	2.41	0.54
1:C:178:LEU:HD12	1:C:213:ILE:O	2.07	0.53
1:D:250:ALA:O	1:D:383:ILE:HD13	2.08	0.53
1:C:249:ILE:HG22	1:C:288:SER:HB2	1.91	0.53
1:D:224:MSE:HA	1:D:224:MSE:HE2	1.91	0.53
1:A:103:LEU:HD23	1:A:238:ALA:HB3	1.89	0.53
1:A:314:MSE:SE	1:A:421:LEU:HD13	2.59	0.53
1:D:96:PHE:CZ	1:D:270:LEU:HD22	2.44	0.53
1:D:238:ALA:HB2	1:D:256:LEU:CD2	2.40	0.52
1:D:111:LEU:CB	1:D:148:ILE:HD13	2.40	0.52
1:B:296:ALA:HB3	1:B:297:PRO:HD3	1.90	0.52
1:C:310:CYS:SG	1:C:336:ILE:HD11	2.50	0.52
1:C:9:LEU:HB3	1:C:14:ILE:HD12	1.92	0.52
1:B:96:PHE:CE1	1:B:270:LEU:HD13	2.45	0.52
1:B:394:ALA:HB2	1:B:402:ALA:HA	1.91	0.51
1:D:241:LEU:HD11	1:D:289:MSE:HE3	1.92	0.51
1:B:345:ILE:CD1	1:B:376:ILE:HD12	2.40	0.51
1:B:92:VAL:HG12	1:B:289:MSE:CE	2.41	0.51
1:B:345:ILE:HD13	1:B:376:ILE:HD12	1.92	0.51
1:C:26:MSE:HE3	1:C:26:MSE:HA	1.93	0.51
1:A:92:VAL:HG12	1:A:289:MSE:CE	2.41	0.51
1:A:9:LEU:HD22	1:A:14:ILE:HD12	1.93	0.51
1:A:241:LEU:HD23	1:A:245:ILE:CG2	2.42	0.50
1:B:365:PRO:HB3	1:B:396:ILE:HD11	1.94	0.50
1:D:236:LEU:HD22	1:D:262:CYS:HB3	1.92	0.50
1:B:344:LEU:HD13	1:B:402:ALA:HB2	1.92	0.50
1:D:26:MSE:HE3	1:D:26:MSE:HA	1.93	0.50
1:A:192:ALA:HB1	1:A:330:SER:CB	2.42	0.50
1:A:124:PRO:HB2	1:A:128:LEU:HD23	1.94	0.50
1:C:394:ALA:HB2	1:C:402:ALA:HA	1.94	0.49
1:C:241:LEU:CD1	1:C:289:MSE:HE3	2.43	0.49
1:C:344:LEU:CD1	1:C:402:ALA:HB2	2.42	0.49
1:A:32:GLN:O	1:A:36:LEU:HD13	2.13	0.49
1:D:6:LYS:HG3	1:D:19:LEU:HD21	1.95	0.49
1:D:238:ALA:CB	1:D:256:LEU:HD23	2.41	0.49
1:D:9:LEU:HD22	1:D:14:ILE:HD12	1.95	0.49
1:C:111:LEU:CB	1:C:148:ILE:HD13	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:216:VAL:HB	1:C:237:ILE:HG22	1.95	0.49
1:B:111:LEU:CB	1:B:148:ILE:HD13	2.43	0.49
1:A:136:GLU:C	1:A:137:ASN:HD22	2.16	0.49
1:A:296:ALA:HB3	1:A:297:PRO:HD3	1.95	0.49
1:A:170:LEU:HD11	1:A:205:VAL:HG12	1.95	0.48
1:A:238:ALA:HB2	1:A:256:LEU:HD23	1.94	0.48
1:D:120:VAL:HG21	1:D:201:ILE:HG21	1.95	0.48
1:A:181:ILE:HB	1:A:216:VAL:HG22	1.95	0.48
1:C:238:ALA:HB2	1:C:256:LEU:HD23	1.96	0.48
1:D:394:ALA:HB2	1:D:402:ALA:HA	1.96	0.48
1:D:241:LEU:CD1	1:D:289:MSE:HE3	2.44	0.48
1:B:236:LEU:HD22	1:B:262:CYS:HB3	1.96	0.48
1:A:179:VAL:HG23	1:A:212:ILE:HG21	1.96	0.48
1:A:111:LEU:HB2	1:A:148:ILE:HD13	1.96	0.48
1:D:314:MSE:HG2	1:D:336:ILE:HD13	1.95	0.48
1:B:304:LEU:HD11	1:B:329:ARG:HD2	1.96	0.47
1:A:314:MSE:HG2	1:A:336:ILE:HD13	1.95	0.47
1:B:100:THR:HB	1:D:275:ILE:HD11	1.96	0.47
1:D:77:LEU:HD21	1:D:289:MSE:HE2	1.96	0.47
1:C:314:MSE:SE	1:C:421:LEU:HD13	2.64	0.47
1:D:182:GLN:HA	1:D:217:ASP:HB3	1.95	0.47
1:A:81:TYR:CG	1:A:92:VAL:HG21	2.49	0.47
1:D:92:VAL:HG12	1:D:289:MSE:CE	2.45	0.47
1:C:314:MSE:HG3	1:C:336:ILE:HD13	1.96	0.47
1:D:170:LEU:HD11	1:D:205:VAL:HG12	1.97	0.47
1:B:81:TYR:CG	1:B:92:VAL:HG21	2.50	0.47
1:A:220:TYR:O	1:A:224:MSE:HE3	2.15	0.47
1:D:111:LEU:HB3	1:D:148:ILE:HD13	1.97	0.47
1:D:81:TYR:CD1	1:D:92:VAL:HG21	2.50	0.46
1:A:238:ALA:HB2	1:A:256:LEU:CD2	2.45	0.46
1:A:241:LEU:CD1	1:A:289:MSE:HE3	2.45	0.46
1:B:111:LEU:HB3	1:B:148:ILE:HD13	1.97	0.46
1:C:345:ILE:HD11	1:C:396:ILE:HD11	1.97	0.46
1:D:344:LEU:HD22	1:D:400:TYR:HB3	1.96	0.46
1:B:282:THR:O	1:B:285:VAL:HG22	2.15	0.46
1:D:310:CYS:SG	1:D:336:ILE:HD11	2.56	0.46
1:A:249:ILE:CD1	1:A:295:LEU:HD12	2.46	0.46
1:A:76:SER:O	1:A:80:VAL:HG23	2.16	0.46
1:A:271:THR:HG22	1:A:272:VAL:N	2.31	0.46
1:B:36:LEU:CD2	1:B:304:LEU:HD23	2.46	0.46
1:B:381:ALA:HB1	1:B:389:GLU:CD	2.36	0.46
1:D:350:GLY:HA2	1:D:353:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:LEU:HD22	1:A:262:CYS:HB3	1.98	0.46
1:C:96:PHE:CE1	1:C:270:LEU:HD13	2.51	0.46
1:B:350:GLY:O	1:B:353:THR:HG22	2.16	0.46
1:A:381:ALA:HB1	1:A:389:GLU:CD	2.36	0.46
1:D:350:GLY:O	1:D:353:THR:HG22	2.16	0.45
1:C:167:GLU:HG2	1:C:208:ILE:HD11	1.98	0.45
1:C:365:PRO:HG3	1:C:396:ILE:HD11	1.99	0.45
1:A:26:MSE:HA	1:A:26:MSE:HE3	1.97	0.45
1:D:181:ILE:HB	1:D:216:VAL:HG22	1.99	0.45
1:C:236:LEU:HD22	1:C:262:CYS:HB3	1.98	0.45
1:D:344:LEU:CD1	1:D:402:ALA:HB2	2.46	0.45
1:B:26:MSE:HE3	1:B:26:MSE:HA	1.99	0.45
1:D:111:LEU:HD13	1:D:148:ILE:HG21	1.98	0.45
1:C:296:ALA:HB3	1:C:297:PRO:HD3	1.98	0.44
1:B:404:LEU:HD23	1:B:405:GLN:N	2.31	0.44
1:A:18:VAL:HG21	1:A:422:SER:HA	1.98	0.44
1:A:282:THR:O	1:A:285:VAL:HG22	2.17	0.44
1:A:271:THR:HG22	1:A:272:VAL:HG22	1.99	0.44
1:C:347:PHE:CD1	1:C:420:ALA:HB1	2.52	0.44
1:B:105:ALA:C	1:B:266:THR:HG23	2.38	0.44
1:D:9:LEU:HD22	1:D:14:ILE:CD1	2.47	0.44
1:A:353:THR:O	1:B:52:GLN:NE2	2.50	0.44
1:A:375:VAL:HG12	1:A:395:PRO:HA	2.00	0.44
1:C:111:LEU:HB2	1:C:148:ILE:HD13	1.99	0.44
1:C:32:GLN:O	1:C:36:LEU:HD13	2.18	0.44
1:D:76:SER:O	1:D:80:VAL:HG23	2.18	0.44
1:A:404:LEU:HD23	1:A:404:LEU:C	2.38	0.44
1:A:143:LEU:HD22	1:A:148:ILE:HD12	2.00	0.44
1:A:295:LEU:HD21	1:B:408:LEU:HB3	1.99	0.44
1:D:282:THR:O	1:D:285:VAL:HG22	2.18	0.44
1:D:9:LEU:HB3	1:D:14:ILE:HD12	1.99	0.43
1:A:202:VAL:HG11	1:A:233:GLY:HA3	2.00	0.43
1:D:81:TYR:CG	1:D:92:VAL:HG21	2.53	0.43
1:A:9:LEU:HB3	1:A:14:ILE:HD12	2.00	0.43
1:D:32:GLN:O	1:D:36:LEU:HD13	2.18	0.43
1:A:195:ILE:HG22	1:A:232:VAL:HG11	2.00	0.43
1:B:216:VAL:HB	1:B:237:ILE:HG22	2.00	0.43
1:B:353:THR:HG23	1:B:419:ILE:HG21	2.01	0.43
1:B:9:LEU:HB3	1:B:14:ILE:HD12	2.01	0.43
1:D:271:THR:HG21	1:D:275:ILE:HG21	2.01	0.42
1:A:138:SER:O	1:A:140:MSE:N	2.49	0.42
1:B:271:THR:HG22	1:B:272:VAL:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:271:THR:HG22	1:D:272:VAL:N	2.33	0.42
1:D:271:THR:HG21	1:D:275:ILE:CG2	2.49	0.42
1:D:111:LEU:HB2	1:D:148:ILE:HD13	2.00	0.42
1:B:314:MSE:HG2	1:B:336:ILE:HD13	1.99	0.42
1:D:219:CYS:HB3	1:D:243:LLP:HZ1	1.83	0.42
1:A:275:ILE:HD11	1:C:100:THR:HB	2.01	0.42
1:C:92:VAL:HG12	1:C:289:MSE:CE	2.50	0.42
1:D:363:CYS:HB3	1:D:376:ILE:HD11	2.01	0.42
1:C:238:ALA:HB2	1:C:256:LEU:CD2	2.49	0.42
1:C:111:LEU:HD13	1:C:148:ILE:CG2	2.45	0.42
1:B:81:TYR:CE1	1:B:293:LEU:HD22	2.54	0.42
1:B:118:LEU:HD13	1:B:151:LYS:HB3	2.02	0.42
1:B:217:ASP:OD2	1:B:243:LLP:N1	2.53	0.42
1:B:350:GLY:HA2	1:B:353:THR:HG22	2.02	0.41
1:A:14:ILE:HD13	1:A:418:LEU:HB3	2.02	0.41
1:A:111:LEU:HD21	1:A:178:LEU:CB	2.49	0.41
1:A:178:LEU:HD12	1:A:213:ILE:O	2.19	0.41
1:C:259:THR:HG23	1:C:262:CYS:H	1.86	0.41
1:C:357:ILE:HG23	1:D:57:SER:HA	2.03	0.41
1:B:167:GLU:HG2	1:B:208:ILE:HD11	2.01	0.41
1:A:251:PRO:HA	1:A:383:ILE:HD12	2.01	0.41
1:B:111:LEU:HD13	1:B:148:ILE:HG21	2.02	0.41
1:C:341:LYS:HE3	1:C:396:ILE:HG21	2.01	0.41
1:C:213:ILE:HG23	1:C:235:ASP:HB2	2.01	0.41
1:A:345:ILE:HD12	1:A:376:ILE:HD12	2.01	0.41
1:A:344:LEU:HD12	1:A:402:ALA:HB2	1.99	0.41
1:D:249:ILE:CD1	1:D:295:LEU:HD12	2.50	0.41
1:B:131:VAL:HG22	1:D:272:VAL:HB	2.03	0.41
1:A:120:VAL:HG21	1:A:201:ILE:HG21	2.02	0.41
1:A:394:ALA:HB2	1:A:402:ALA:HA	2.01	0.41
1:D:161:PRO:HB3	1:D:201:ILE:HD11	2.02	0.41
1:D:244:ASN:HA	1:D:388:ILE:HD13	2.03	0.41
1:B:314:MSE:SE	1:B:421:LEU:HD13	2.71	0.41
1:C:304:LEU:HD11	1:C:329:ARG:HD2	2.03	0.41
1:B:347:PHE:CD1	1:B:420:ALA:HB1	2.55	0.41
1:D:105:ALA:C	1:D:266:THR:HG23	2.41	0.41
1:A:111:LEU:CB	1:A:148:ILE:HD13	2.50	0.41
1:B:36:LEU:HD21	1:B:304:LEU:HD23	2.02	0.41
1:B:249:ILE:CD1	1:B:295:LEU:HD12	2.51	0.41
1:A:275:ILE:CD1	1:C:98:ASN:HD21	2.34	0.41
1:A:48:LEU:HD23	1:B:415:ILE:HG21	2.02	0.41
1:D:218:ASN:HD22	1:D:237:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:81:TYR:CG	1:C:92:VAL:HG21	2.55	0.40
1:D:390:LEU:HD22	1:D:413:ALA:HA	2.03	0.40
1:B:414:LYS:O	1:B:418:LEU:HD13	2.22	0.40
1:D:224:MSE:SE	1:D:304:LEU:HD22	2.71	0.40
1:A:108:PHE:CE1	1:A:143:LEU:HD23	2.56	0.40
1:A:111:LEU:HD21	1:A:178:LEU:HB2	2.03	0.40
1:B:91:LEU:HD12	1:B:93:ARG:NH1	2.35	0.40
1:C:111:LEU:HB3	1:C:148:ILE:HD13	2.02	0.40
1:A:309:LEU:HD22	1:A:410:PHE:CZ	2.56	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	419/427 (98%)	398 (95%)	19 (4%)	2 (0%)	38	79
1	B	426/427 (100%)	405 (95%)	19 (4%)	2 (0%)	38	79
1	C	412/427 (96%)	389 (94%)	22 (5%)	1 (0%)	56	89
1	D	426/427 (100%)	405 (95%)	19 (4%)	2 (0%)	38	79
All	All	1683/1708 (98%)	1597 (95%)	79 (5%)	7 (0%)	43	82

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASP
1	B	244	ASN
1	D	244	ASN
1	C	244	ASN
1	A	139	ASN
1	D	136	GLU
1	B	380	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	333/348 (96%)	331 (99%)	2 (1%)	92	98
1	B	340/348 (98%)	338 (99%)	2 (1%)	92	98
1	C	318/348 (91%)	317 (100%)	1 (0%)	96	99
1	D	336/348 (97%)	336 (100%)	0	100	100
All	All	1327/1392 (95%)	1322 (100%)	5 (0%)	95	99

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	137	ASN
1	B	17	ARG
1	B	367	ASP
1	C	137	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	C	30	GLN
1	C	137	ASN
1	D	98	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	LLP	A	243	1	24,24,25	4.03	6 (25%)	30,32,34	1.82	4 (13%)
1	LLP	B	243	1	24,24,25	4.01	5 (20%)	30,32,34	1.99	5 (16%)
1	LLP	C	243	1	24,24,25	4.26	5 (20%)	30,32,34	1.98	5 (16%)
1	LLP	D	243	1	24,24,25	4.00	5 (20%)	30,32,34	1.77	5 (16%)

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
1	LLP	A	243	1	-	0/15/17/19	0/1/1/1
1	LLP	B	243	1	-	0/15/17/19	0/1/1/1
1	LLP	C	243	1	-	0/15/17/19	0/1/1/1
1	LLP	D	243	1	-	0/15/17/19	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	LLP	O-C	19.00	1.24	1.11
1	A	243	LLP	O-C	17.86	1.23	1.11
1	D	243	LLP	O-C	17.60	1.23	1.11
1	B	243	LLP	O-C	17.52	1.23	1.11
1	B	243	LLP	O3-C3	-5.95	1.22	1.37
1	D	243	LLP	O3-C3	-5.74	1.23	1.37
1	C	243	LLP	O3-C3	-5.61	1.23	1.37
1	A	243	LLP	O3-C3	-5.47	1.23	1.37
1	D	243	LLP	CA-C	3.88	1.55	1.48
1	A	243	LLP	CA-C	3.87	1.55	1.48
1	C	243	LLP	CA-C	3.67	1.55	1.48
1	B	243	LLP	CA-C	3.58	1.55	1.48
1	A	243	LLP	C2-N1	2.65	1.38	1.33
1	B	243	LLP	C2-N1	2.52	1.38	1.33
1	C	243	LLP	C2-N1	2.50	1.38	1.33
1	D	243	LLP	C4'-NZ	-2.32	1.33	1.45
1	D	243	LLP	C2-N1	2.31	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	LLP	C4'-NZ	-2.30	1.33	1.45
1	C	243	LLP	C4'-NZ	-2.21	1.34	1.45
1	B	243	LLP	C4'-NZ	-2.17	1.34	1.45
1	A	243	LLP	C6-N1	2.06	1.39	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	243	LLP	C-CA-N	-7.10	106.74	113.83
1	B	243	LLP	C-CA-N	-6.87	106.97	113.83
1	A	243	LLP	C-CA-N	-5.77	108.06	113.83
1	D	243	LLP	OP4-C5'-C5	5.51	120.47	109.26
1	C	243	LLP	OP4-C5'-C5	5.23	119.90	109.26
1	B	243	LLP	OP4-C5'-C5	5.14	119.71	109.26
1	A	243	LLP	OP4-C5'-C5	5.12	119.67	109.26
1	D	243	LLP	C-CA-N	-4.67	109.17	113.83
1	A	243	LLP	C6-C5-C4	3.44	120.72	118.10
1	D	243	LLP	C6-C5-C4	3.13	120.47	118.10
1	C	243	LLP	C6-C5-C4	3.03	120.40	118.10
1	B	243	LLP	C6-C5-C4	2.97	120.36	118.10
1	B	243	LLP	C4-C4'-NZ	-2.79	106.33	111.52
1	B	243	LLP	CD-CE-NZ	-2.45	105.58	112.09
1	A	243	LLP	C5-C6-N1	-2.40	119.53	123.86
1	D	243	LLP	C4-C4'-NZ	-2.35	107.15	111.52
1	C	243	LLP	C4-C4'-NZ	-2.20	107.44	111.52
1	D	243	LLP	C5-C6-N1	-2.08	120.11	123.86
1	C	243	LLP	C5-C6-N1	-2.08	120.11	123.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	424/427 (99%)	-0.21	4 (0%)	81	88	20, 24, 31, 46	0
1	B	427/427 (100%)	-0.25	6 (1%)	72	80	20, 24, 32, 44	0
1	C	418/427 (97%)	-0.11	5 (1%)	75	83	20, 24, 30, 37	0
1	D	427/427 (100%)	-0.17	10 (2%)	57	66	19, 24, 32, 41	0
All	All	1696/1708 (99%)	-0.19	25 (1%)	70	79	19, 24, 32, 46	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	THR	4.0
1	D	398	GLU	3.8
1	A	0	GLY	3.7
1	B	369	PRO	3.2
1	D	135	THR	3.1
1	D	136	GLU	3.0
1	C	69	TYR	2.8
1	C	70	GLY	2.8
1	A	368	MSE	2.8
1	A	158	ASP	2.8
1	C	373	ASP	2.8
1	B	371	TYR	2.6
1	D	339	ASN	2.6
1	B	187	TYR	2.5
1	C	375	VAL	2.5
1	B	158	ASP	2.4
1	B	366	TRP	2.3
1	D	7	GLN	2.3
1	D	340	ASP	2.3
1	D	342	ASP	2.3
1	B	138	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	399	PRO	2.2
1	C	397	ARG	2.1
1	D	69	TYR	2.1
1	D	426	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	B	243	24/25	0.19	1.25	25,32,34,34	0
1	LLP	A	243	24/25	0.20	1.09	25,32,33,33	0
1	LLP	C	243	24/25	0.15	-0.26	25,32,32,33	0
1	LLP	D	243	24/25	0.14	-0.42	25,32,33,33	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.