



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2014 – 07:46 PM EDT

PDB ID : 4N4Q
Title : Crystal Structure of N-acetylneuraminate lyase from Mycoplasma synoviae, crystal form II
Authors : Georgescauld, F.; Popova, K.; Gupta, A.J.; Bracher, A.; Engen, J.R.; Hayer-Hartl, M.; Hartl, F.U.
Deposited on : 2013-10-08
Resolution : 2.00 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>

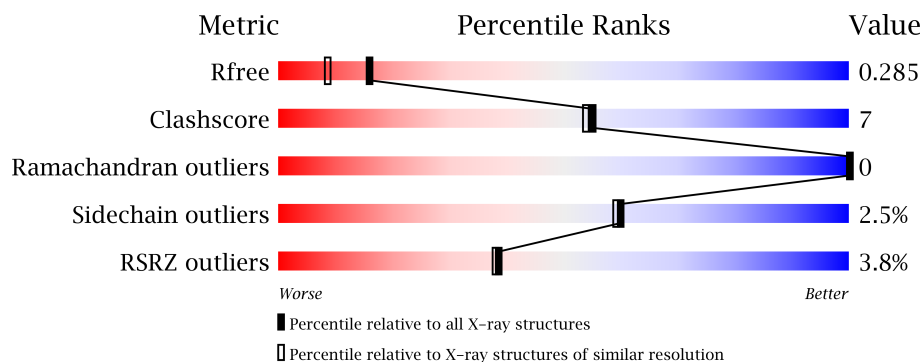
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	296	
1	B	296	
1	C	296	
1	D	296	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9824 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 Acylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2336	1523	372	431	10			
1	B	294	Total	C	N	O	S	0	0	0
			2339	1526	372	431	10			
1	C	292	Total	C	N	O	S	0	0	0
			2331	1520	371	430	10			
1	D	293	Total	C	N	O	S	0	0	0
			2336	1523	372	431	10			

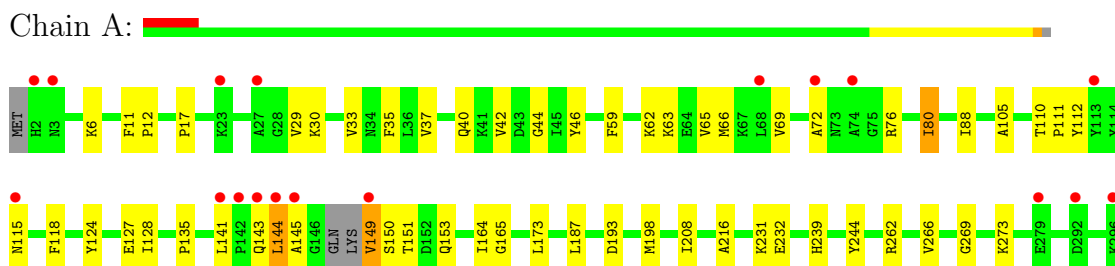
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	125	Total	O	0	0
			125	125		
2	C	143	Total	O	0	0
			143	143		
2	D	132	Total	O	0	0
			132	132		

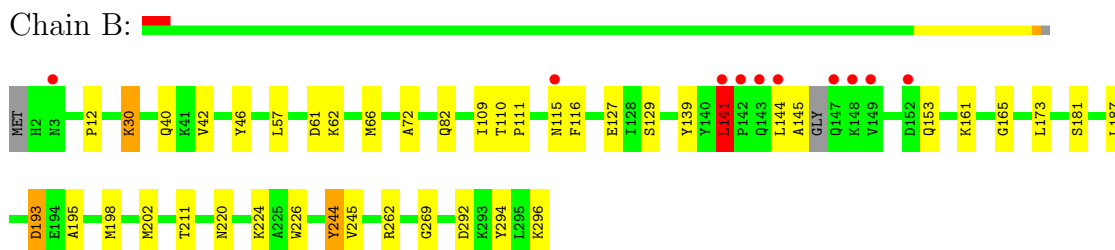
3 Residue-property plots

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.

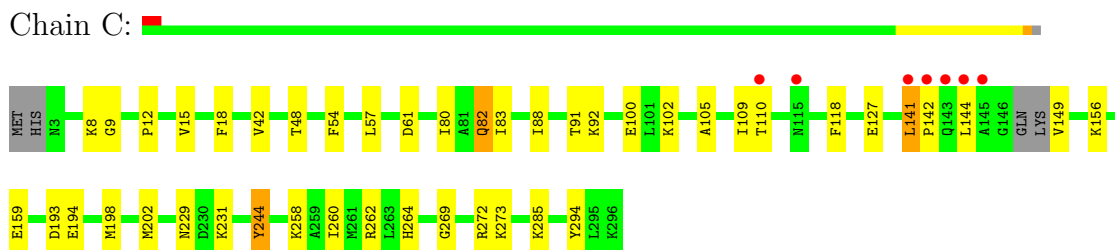
• Molecule 1: Acylneuraminate lyase



• Molecule 1: Acylneuraminate lyase



• Molecule 1: Acylneuraminate lyase



• Molecule 1: Acylneuraminate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.23Å 142.44Å 80.79Å 90.00° 108.27° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.00) 98.9 (29.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.283 0.240 , 0.285	Depositor DCC
R_{free} test set	4294 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 85788 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9824	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.55	0/2387	0.62	0/3212
1	B	0.60	0/2390	0.65	1/3217 (0.0%)
1	C	0.63	0/2382	0.66	1/3205 (0.0%)
1	D	0.66	0/2387	0.67	2/3212 (0.1%)
All	All	0.61	0/9546	0.65	4/12846 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	LEU	CA-CB-CG	6.09	129.32	115.30
1	D	243	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	172	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	61	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2336	0	2348	46	0
1	B	2339	0	2345	32	0
1	C	2331	0	2346	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2336	0	2348	35	0
2	A	82	0	0	3	0
2	B	125	0	0	3	0
2	C	143	0	0	3	0
2	D	132	0	0	1	0
All	All	9824	0	9387	125	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 7.

All (125) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:115:ASN:HB3	1:B:145:ALA:HB3	1.20	1.17
1:A:173:LEU:HD13	1:A:198:MET:HE1	1.45	0.99
1:B:115:ASN:HB3	1:B:145:ALA:CB	1.97	0.94
1:B:30:LYS:HG3	1:B:72:ALA:HB2	1.48	0.93
1:D:110:THR:HG21	1:D:141:LEU:HD21	1.51	0.92
1:D:110:THR:CG2	1:D:141:LEU:HD21	2.10	0.82
1:A:143:GLN:HA	1:A:149:VAL:HG21	1.65	0.78
1:A:111:PRO:O	2:A:347:HOH:O	2.02	0.77
1:C:102:LYS:HE3	2:C:312:HOH:O	1.85	0.75
1:A:198:MET:HE3	1:B:173:LEU:HD13	1.70	0.73
1:B:115:ASN:CB	1:B:145:ALA:HB3	2.11	0.73
1:D:62:LYS:O	1:D:66:MET:HG3	1.90	0.71
1:A:110:THR:O	2:A:339:HOH:O	2.10	0.68
1:A:141:LEU:CD2	1:A:144:LEU:HG	2.24	0.67
1:C:100:GLU:OE2	2:C:386:HOH:O	2.11	0.67
1:D:23:LYS:HA	1:D:23:LYS:HE2	1.76	0.66
1:A:65:VAL:O	1:A:69:VAL:HG23	1.95	0.65
1:D:143:GLN:HA	1:D:148:LYS:HA	1.77	0.65
1:A:80:ILE:HG23	1:A:105:ALA:HB3	1.79	0.65
1:C:12:PRO:HG3	1:C:42:VAL:HG11	1.80	0.64
1:C:231:LYS:HD3	1:D:226:TRP:CH2	2.32	0.64
1:A:173:LEU:CD1	1:A:198:MET:HE1	2.24	0.63
1:D:12:PRO:HG3	1:D:42:VAL:HG11	1.80	0.63
1:A:118:PHE:HA	1:A:144:LEU:HD22	1.82	0.62
1:A:173:LEU:HD13	1:A:198:MET:CE	2.27	0.59
1:A:262:ARG:HA	1:A:266:VAL:O	2.02	0.59
1:A:198:MET:CE	1:B:173:LEU:HD13	2.33	0.58
1:A:72:ALA:O	1:A:76:ARG:NH2	2.36	0.58
1:A:124:TYR:O	1:A:128:ILE:HG13	2.03	0.58
1:C:260:ILE:O	1:C:264:HIS:HD2	1.87	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:LEU:HD21	1:A:144:LEU:HG	1.86	0.57
1:A:173:LEU:HD12	1:B:173:LEU:HD12	1.86	0.57
1:A:173:LEU:CD1	1:B:173:LEU:HD12	2.34	0.57
1:A:198:MET:CE	1:B:198:MET:HB3	2.35	0.57
1:C:198:MET:HE1	1:D:173:LEU:HB3	1.88	0.56
1:B:116:PHE:O	1:B:144:LEU:HD12	2.06	0.56
1:D:30:LYS:HD3	1:D:72:ALA:HB2	1.87	0.55
1:A:17:PRO:HD2	1:A:29:VAL:HG22	1.89	0.55
1:A:33:VAL:O	1:A:37:VAL:HG23	2.07	0.55
1:C:118:PHE:HA	1:C:144:LEU:HD13	1.88	0.55
1:A:141:LEU:HD22	1:A:144:LEU:HG	1.88	0.54
1:D:149:VAL:HG13	1:D:153:GLN:HB3	1.88	0.54
1:D:65:VAL:O	1:D:69:VAL:HG23	2.07	0.54
1:C:198:MET:HG2	2:C:305:HOH:O	2.08	0.53
1:C:231:LYS:HD3	1:D:226:TRP:CZ2	2.43	0.53
1:B:139:TYR:O	1:B:141:LEU:HD23	2.09	0.53
1:A:30:LYS:HG2	1:A:72:ALA:HB2	1.90	0.52
1:C:8:LYS:HG2	1:C:9:GLY:N	2.23	0.52
1:B:40:GLN:NE2	2:B:350:HOH:O	2.41	0.52
1:A:62:LYS:O	1:A:66:MET:HG3	2.11	0.51
1:D:126:GLU:HG2	1:D:130:LYS:NZ	2.26	0.51
1:B:12:PRO:HG3	1:B:42:VAL:HG11	1.93	0.50
1:C:202:MET:HG2	1:D:198:MET:CE	2.41	0.50
1:B:129:SER:HB2	1:B:161:LYS:O	2.12	0.50
1:D:260:ILE:O	1:D:264:HIS:HD2	1.95	0.49
1:C:92:LYS:HE3	1:C:127:GLU:HG2	1.95	0.49
1:D:141:LEU:HD22	1:D:144:LEU:HG	1.94	0.49
1:B:292:ASP:HA	1:B:296:LYS:HE2	1.95	0.49
1:A:239:HIS:ND1	1:B:181:SER:HB2	2.28	0.48
1:C:141:LEU:HD13	1:C:144:LEU:HD11	1.95	0.48
1:B:220:ASN:O	1:B:224:LYS:HD3	2.12	0.48
1:A:165:GLY:HA3	1:A:187:LEU:O	2.14	0.48
1:B:115:ASN:HA	2:B:425:HOH:O	2.14	0.48
1:B:111:PRO:O	2:B:407:HOH:O	2.19	0.48
1:B:244:TYR:HB2	1:B:294:TYR:CD1	2.49	0.48
1:D:169:GLY:O	2:D:403:HOH:O	2.19	0.48
1:C:54:PHE:HA	1:C:57:LEU:HD12	1.96	0.47
1:B:211:THR:HG21	1:B:245:VAL:HG22	1.95	0.47
1:C:198:MET:CE	1:D:173:LEU:HB3	2.44	0.47
1:A:198:MET:HE2	1:B:198:MET:HB3	1.97	0.47
1:C:285:LYS:HA	1:C:285:LYS:HD3	1.74	0.47
1:A:11:PHE:CE2	1:A:44:GLY:HA3	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:57:LEU:HD22	1:B:61:ASP:HB3	1.96	0.46
1:A:150:SER:HB3	1:A:153:GLN:H	1.80	0.46
1:B:62:LYS:O	1:B:66:MET:HG3	2.15	0.46
1:A:273:LYS:HB3	1:C:88:ILE:HG13	1.97	0.46
1:B:195:ALA:HB1	1:B:198:MET:HG3	1.97	0.46
1:A:198:MET:HE3	1:B:198:MET:HB3	1.98	0.46
1:A:231:LYS:HD2	1:B:226:TRP:CZ2	2.50	0.46
1:C:229:ASN:OD1	1:D:231:LYS:NZ	2.48	0.45
1:A:12:PRO:HD2	1:A:44:GLY:O	2.16	0.45
1:C:141:LEU:HA	1:C:142:PRO:HD2	1.87	0.45
1:A:11:PHE:O	1:A:208:ILE:HA	2.17	0.45
1:A:115:ASN:HB3	1:A:145:ALA:HA	1.98	0.45
1:A:262:ARG:NH1	1:A:269:GLY:O	2.50	0.45
1:A:232:GLU:N	1:A:232:GLU:CD	2.70	0.44
1:B:46:TYR:HH	1:B:139:TYR:HH	1.58	0.44
1:C:202:MET:HG2	1:D:198:MET:HE2	1.99	0.44
1:C:83:ILE:O	1:C:91:THR:HG23	2.17	0.44
1:A:135:PRO:HB3	1:A:164:ILE:CG2	2.48	0.44
1:C:202:MET:CG	1:D:198:MET:HE3	2.47	0.44
1:A:112:TYR:HB3	2:A:339:HOH:O	2.18	0.43
1:C:262:ARG:NH1	1:C:269:GLY:O	2.51	0.43
1:D:57:LEU:HD22	1:D:61:ASP:HB3	2.00	0.43
1:A:35:PHE:CD1	1:A:266:VAL:HG21	2.54	0.43
1:A:59:PHE:CZ	1:A:63:LYS:HE3	2.53	0.43
1:D:244:TYR:HA	1:D:294:TYR:CE2	2.53	0.43
1:A:88:ILE:HG13	1:C:273:LYS:HB3	2.01	0.43
1:B:262:ARG:NH1	1:B:269:GLY:O	2.51	0.43
1:C:80:ILE:HG12	1:C:105:ALA:HB3	2.00	0.43
1:D:33:VAL:O	1:D:37:VAL:HG23	2.19	0.43
1:D:165:GLY:HA3	1:D:187:LEU:O	2.18	0.43
1:B:193:ASP:OD1	1:B:193:ASP:N	2.52	0.42
1:C:144:LEU:HD12	1:C:149:VAL:HG21	2.00	0.42
1:C:18:PHE:CD2	1:C:272:ARG:HG3	2.54	0.42
1:A:239:HIS:CE1	1:B:202:MET:CE	3.03	0.42
1:D:155:GLY:HA3	1:D:183:TYR:OH	2.20	0.42
1:A:12:PRO:HG3	1:A:42:VAL:HG11	2.02	0.42
1:D:116:PHE:O	1:D:144:LEU:HD22	2.20	0.42
1:A:46:TYR:HD1	1:A:80:ILE:HB	1.85	0.42
1:B:165:GLY:HA3	1:B:187:LEU:O	2.20	0.42
1:D:12:PRO:CG	1:D:42:VAL:HG11	2.48	0.41
1:D:73:ASN:OD1	1:D:77:VAL:HG22	2.19	0.41
1:D:155:GLY:HA2	1:D:158:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:109:ILE:H	1:D:109:ILE:HG13	1.68	0.41
1:D:137:LEU:HD21	1:D:187:LEU:HD23	2.03	0.41
1:C:48:THR:O	1:C:82:GLN:HB3	2.21	0.41
1:D:196:LEU:C	1:D:196:LEU:HD23	2.42	0.41
1:D:18:PHE:CD2	1:D:272:ARG:HG3	2.55	0.41
1:A:40:GLN:NE2	1:A:216:ALA:H	2.19	0.41
1:C:244:TYR:HA	1:C:294:TYR:CE2	2.55	0.41
1:C:109:ILE:HD12	1:C:110:THR:O	2.22	0.40
1:D:88:ILE:HD12	1:D:124:TYR:CD1	2.57	0.40
1:C:15:VAL:HB	1:C:258:LYS:HE3	2.04	0.40
1:C:156:LYS:HD2	1:C:159:GLU:OE1	2.22	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	289/296 (98%)	285 (99%)	4 (1%)	0	100	100
1	B	290/296 (98%)	285 (98%)	5 (2%)	0	100	100
1	C	288/296 (97%)	283 (98%)	5 (2%)	0	100	100
1	D	289/296 (98%)	281 (97%)	8 (3%)	0	100	100
All	All	1156/1184 (98%)	1134 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	243/248 (98%)	235 (97%)	8 (3%)	50	46
1	B	242/248 (98%)	233 (96%)	9 (4%)	45	40
1	C	243/248 (98%)	238 (98%)	5 (2%)	66	67
1	D	243/248 (98%)	241 (99%)	2 (1%)	89	92
All	All	971/992 (98%)	947 (98%)	24 (2%)	60	59

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	80	ILE
1	A	127	GLU
1	A	144	LEU
1	A	149	VAL
1	A	151	THR
1	A	193	ASP
1	A	244	TYR
1	B	30	LYS
1	B	82	GLN
1	B	109	ILE
1	B	110	THR
1	B	127	GLU
1	B	141	LEU
1	B	153	GLN
1	B	193	ASP
1	B	244	TYR
1	C	82	GLN
1	C	141	LEU
1	C	193	ASP
1	C	194	GLU
1	C	244	TYR
1	D	82	GLN
1	D	193	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	213	ASN
1	A	220	ASN

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Mol	Chain	Res	Type
1	B	40	GLN
1	C	40	GLN
1	C	220	ASN
1	C	264	HIS
1	D	3	ASN
1	D	220	ASN
1	D	264	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	293/296 (98%)	0.59	18 (6%)	21 20	20, 33, 45, 55	0
1	B	294/296 (99%)	0.18	10 (3%)	43 43	16, 25, 39, 51	0
1	C	292/296 (98%)	0.12	7 (2%)	56 56	13, 22, 40, 51	0
1	D	293/296 (98%)	0.15	9 (3%)	47 46	13, 23, 40, 53	0
All	All	1172/1184 (98%)	0.26	44 (3%)	38 38	13, 26, 43, 55	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	ALA	4.9
1	A	141	LEU	4.8
1	A	145	ALA	4.6
1	A	144	LEU	4.5
1	D	141	LEU	4.3
1	C	144	LEU	4.3
1	C	141	LEU	4.2
1	B	144	LEU	3.9
1	D	27	ALA	3.8
1	C	115	ASN	3.8
1	B	143	GLN	3.7
1	D	144	LEU	3.5
1	C	143	GLN	3.5
1	B	148	LYS	3.3
1	C	110	THR	3.3
1	B	149	VAL	3.1
1	C	145	ALA	3.0
1	A	113	TYR	3.0
1	A	2	HIS	2.9
1	A	296	LYS	2.9
1	C	142	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	110	THR	2.8
1	A	27	ALA	2.8
1	A	143	GLN	2.8
1	A	279	GLU	2.6
1	B	3	ASN	2.6
1	A	292	ASP	2.6
1	B	152	ASP	2.5
1	A	142	PRO	2.5
1	A	115	ASN	2.4
1	B	115	ASN	2.4
1	D	115	ASN	2.4
1	B	147	GLN	2.4
1	A	72	ALA	2.3
1	D	296	LYS	2.3
1	B	141	LEU	2.3
1	B	142	PRO	2.3
1	A	149	VAL	2.2
1	A	68	LEU	2.1
1	A	3	ASN	2.1
1	A	74	ALA	2.1
1	D	142	PRO	2.1
1	D	143	GLN	2.1
1	A	23	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.