Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:54 PM GMT

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 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

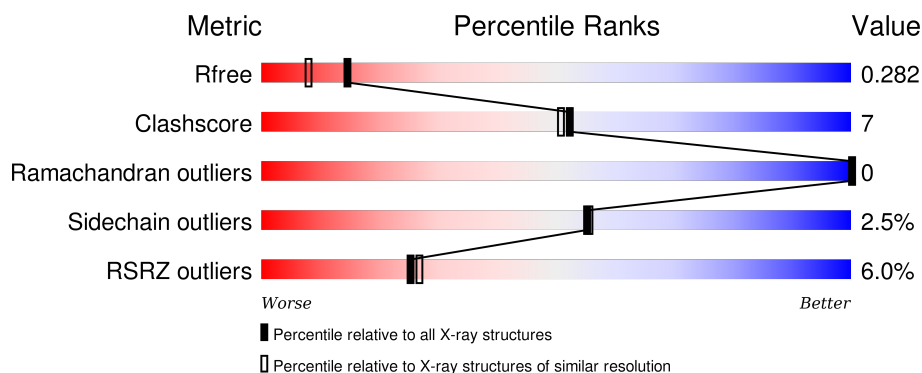|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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 | Percentile Ranks | Value

Rfree | | 0.282
Clashscore | | 7
Ramachandran outliers | | 0
Sidechain outliers | | 2.5%
RSRZ outliers | | 6.0%

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$_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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 <=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	296	10% 80% 18% ••
1	B	296	5% 85% 13% ••
1	C	296	4% 83% 14% ••
1	D	296	4% 82% 17% •

2 Entry composition (i)

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

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

- Molecule 2 is water.

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

3 Residue-property plots (i)

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.
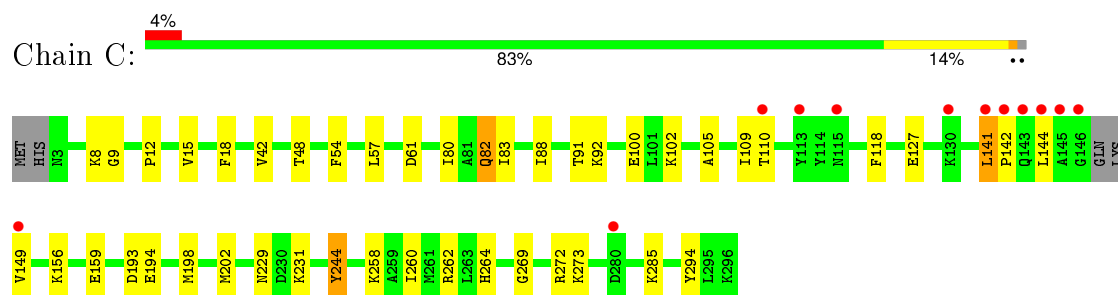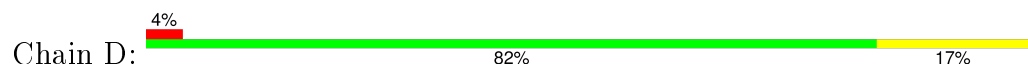
- Molecule 1: Acylneuraminate lyase
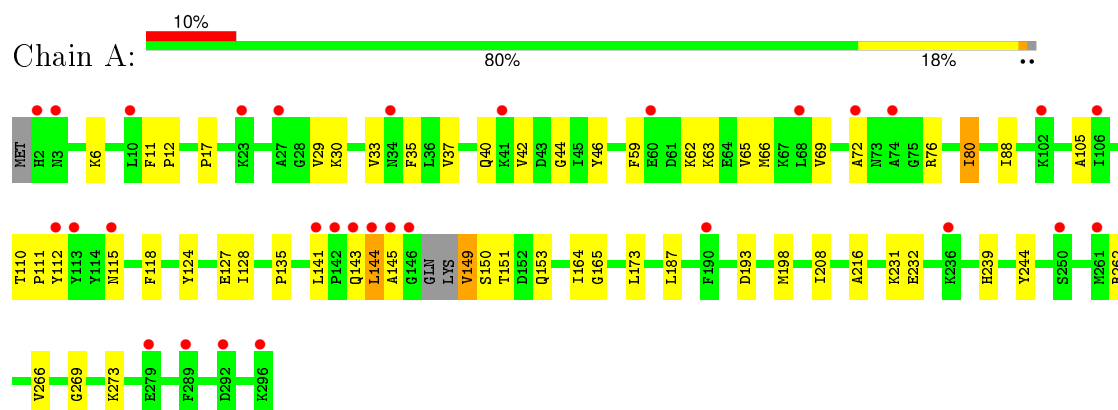
- Molecule 1: Acylneuraminate lyase
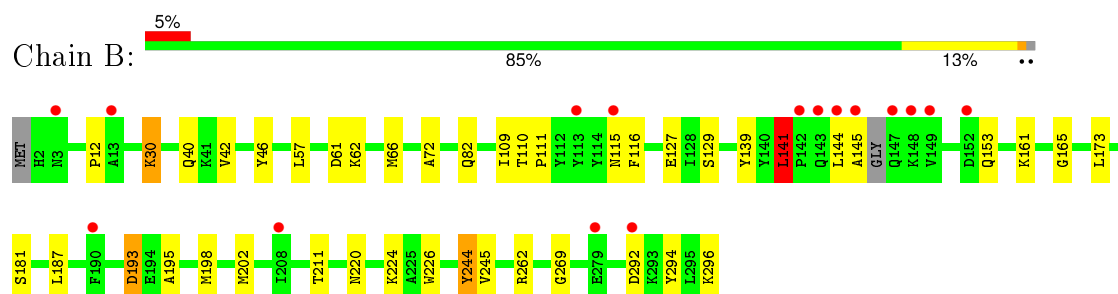
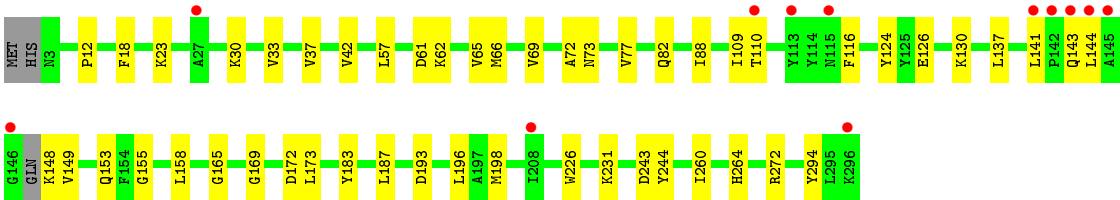- Molecule 1: Acylneuraminate lyase

- Molecule 1: Acylneuraminate lyase

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.283 0.240 , 0.282	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)	0.32 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	2336	0	2348	46	0
1	B	2339	0	2345	32	0
1	C	2331	0	2346	32	0
1	D	2336	0	2348	35	0
2	A	82	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 7.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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:D:143:GLN:HA	1:D:148:LYS:HA	1.77	0.65
1:A:65:VAL:O	1:A:69:VAL:HG23	1.95	0.65
1:A:80:ILE:HG23	1:A:105:ALA:HB3	1.79	0.65
1:C:231:LYS:HD3	1:D:226:TRP:CH2	2.32	0.64
1:C:12:PRO:HG3	1:C:42:VAL:HG11	1.80	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	Interatomic distance (Å)	Clash overlap (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:B:115:ASN:HA	2:B:425:HOH:O	2.14	0.48
1:A:165:GLY:HA3	1:A:187:LEU: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CE2	1:A:44:GLY:HA3	2.50	0.46
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:C:141:LEU:HA	1:C:142:PRO:HD2	1.87	0.45
1:A:12:PRO:HD2	1:A:44:GLY:O	2.16	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:B:46:TYR:HH	1:B:139:TYR:HH	1.58	0.44
1:A:232:GLU:N	1:A:232:GLU:CD	2.70	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:D:57:LEU:HD22	1:D:61:ASP:HB3	2.00	0.43
1:C:262:ARG:NH1	1:C:269:GLY:O	2.51	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:C:80:ILE:HG12	1:C:105:ALA:HB3	2.00	0.43
1:B:262:ARG:NH1	1:B:269:GLY:O	2.51	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: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:B:193:ASP:OD1	1:B:193:ASP:N	2.52	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:D:116:PHE:O	1:D:144:LEU:HD22	2.20	0.42
1:A:12:PRO:HG3	1:A:42:VAL:HG11	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:18:PHE:CD2	1:D:272:ARG:HG3	2.55	0.41
1:D:196:LEU:C	1:D:196:LEU:HD23	2.42	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 (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	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 (i)

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%)	45	43
1	B	242/248 (98%)	233 (96%)	9 (4%)	41	38
1	C	243/248 (98%)	238 (98%)	5 (2%)	61	63
1	D	243/248 (98%)	241 (99%)	2 (1%)	86	89
All	All	971/992 (98%)	947 (98%)	24 (2%)	55	55

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
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 (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 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 (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	293/296 (98%)	0.83	30 (10%)	9	9	20, 33, 45, 55	0
1	B	294/296 (99%)	0.39	16 (5%)	29	31	16, 25, 39, 51	0
1	C	292/296 (98%)	0.30	12 (4%)	41	42	13, 22, 40, 51	0
1	D	293/296 (98%)	0.34	12 (4%)	41	42	13, 23, 40, 53	0
All	All	1172/1184 (98%)	0.46	70 (5%)	25	27	13, 26, 43, 55	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	ALA	5.5
1	A	145	ALA	5.2
1	A	141	LEU	5.1
1	A	144	LEU	5.1
1	C	144	LEU	4.6
1	D	27	ALA	4.4
1	B	144	LEU	4.4
1	C	141	LEU	4.3
1	D	144	LEU	4.3
1	A	113	TYR	4.3
1	B	149	VAL	4.3
1	D	141	LEU	4.3
1	C	115	ASN	4.1
1	A	142	PRO	4.0
1	C	142	PRO	4.0
1	B	148	LYS	4.0
1	A	143	GLN	4.0
1	B	143	GLN	3.8
1	A	279	GLU	3.7
1	C	143	GLN	3.5
1	A	296	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	115	ASN	3.4
1	A	2	HIS	3.4
1	C	110	THR	3.2
1	D	143	GLN	3.2
1	A	68	LEU	3.1
1	A	27	ALA	3.1
1	A	3	ASN	3.0
1	B	115	ASN	3.0
1	A	292	ASP	3.0
1	B	145	ALA	3.0
1	C	149	VAL	2.9
1	B	3	ASN	2.9
1	B	142	PRO	2.9
1	C	145	ALA	2.8
1	A	74	ALA	2.8
1	B	152	ASP	2.7
1	A	289	PHE	2.7
1	D	110	THR	2.6
1	D	142	PRO	2.6
1	A	236	LYS	2.5
1	A	72	ALA	2.5
1	A	146	GLY	2.5
1	B	147	GLN	2.4
1	D	146	GLY	2.4
1	B	292	ASP	2.4
1	D	113	TYR	2.4
1	D	115	ASN	2.4
1	A	261	MET	2.4
1	C	280	ASP	2.3
1	D	296	LYS	2.3
1	A	23	LYS	2.3
1	A	60	GLU	2.3
1	C	113	TYR	2.2
1	A	102	LYS	2.2
1	A	34	ASN	2.2
1	B	208	ILE	2.2
1	B	279	GLU	2.2
1	B	113	TYR	2.2
1	C	146	GLY	2.1
1	B	13	ALA	2.1
1	A	10	LEU	2.1
1	B	190	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	208	ILE	2.1
1	A	190	PHE	2.1
1	A	106	ILE	2.1
1	A	250	SER	2.0
1	A	112	TYR	2.0
1	C	130	LYS	2.0
1	A	41	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.