WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:53 am BST

PDB ID	:	4ZXV
Title	:	Streptomyces peucetius nitrososynthase DnmZ in ligand-free state
Authors	:	Sartor, L.M.; Vey, J.L.
Deposited on	:	2015-05-20
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

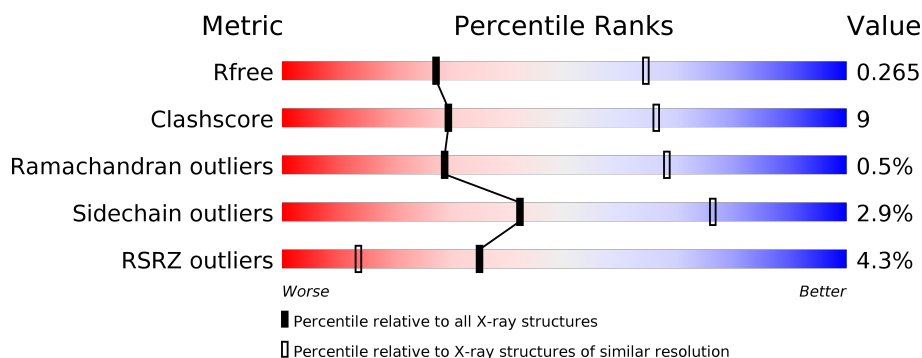|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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		0.265
Clashscore		9
Ramachandran outliers		0.5%
Sidechain outliers		2.9%
RSRZ outliers		4.3%

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 <=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	425	2%　73%　19%　•　7%
1	B	425	8%　75%　16%　•　8%
1	C	425	2%　73%　18%　•　8%
1	D	425	5%　76%　16%　•　7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11465 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 DnmZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total 2901	C 1805	N 532	O 549	S 15	0	0	0
1	B	391	Total 2808	C 1745	N 512	O 536	S 15	0	0	0
1	C	391	Total 2849	C 1778	N 514	O 542	S 15	0	0	0
1	D	395	Total 2880	C 1798	N 523	O 544	S 15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	6	Total 6	O 6	0	0
2	C	6	Total 6	O 6	0	0
2	D	8	Total 8	O 8	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 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.
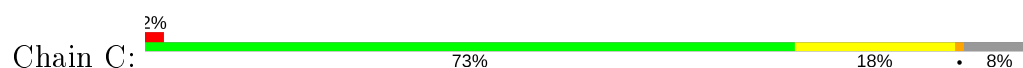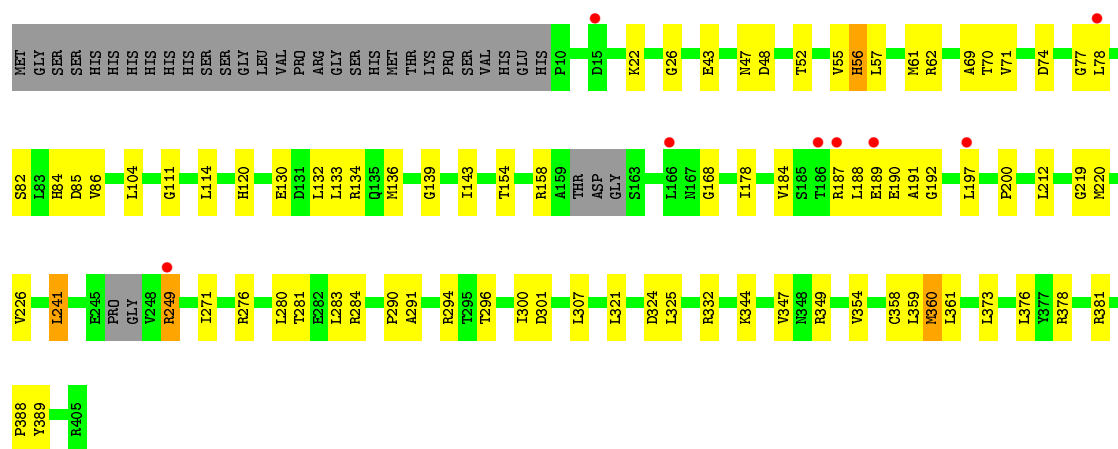
- Molecule 1: DnmZ

- Molecule 1: DnmZ

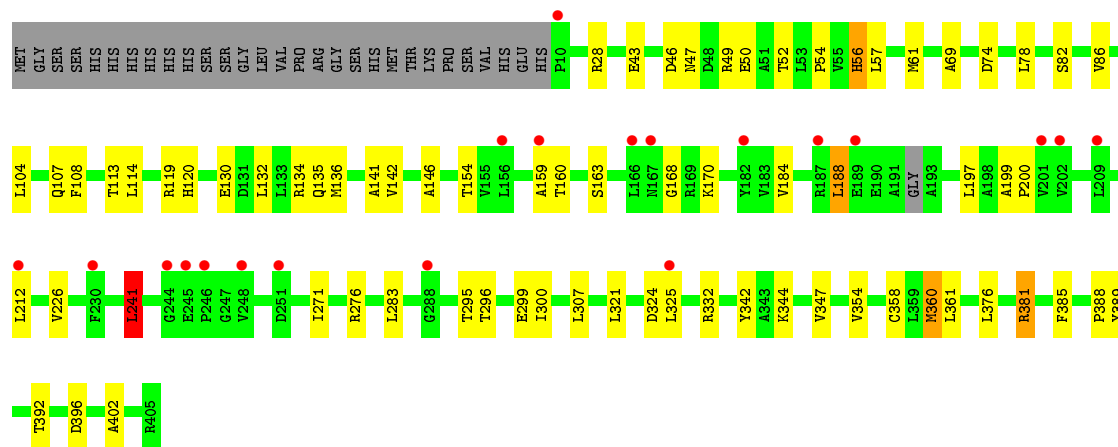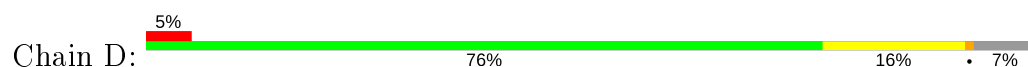- Molecule 1: DnmZ

• Molecule 1: DnmZ

Chain D:
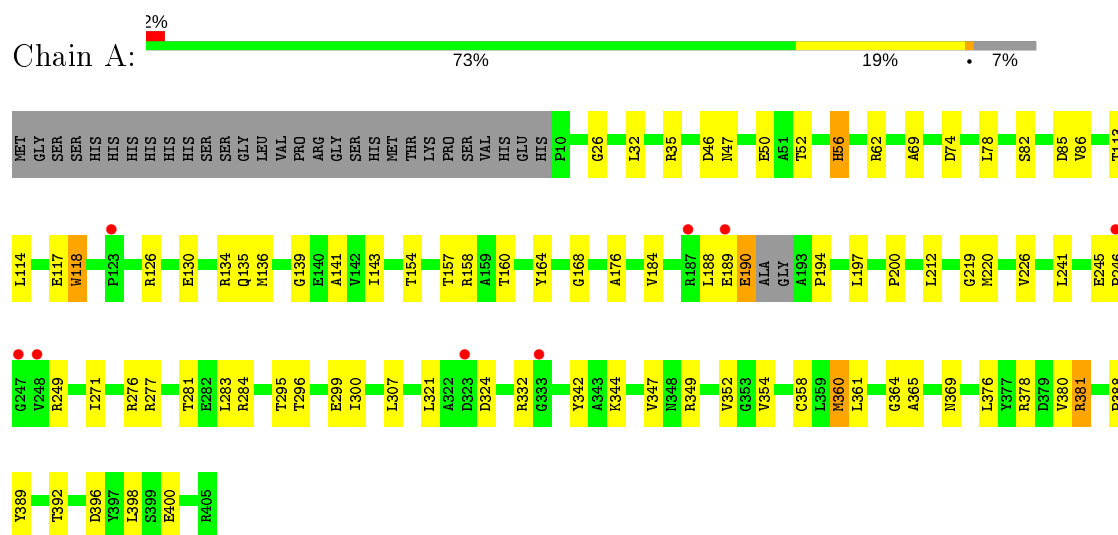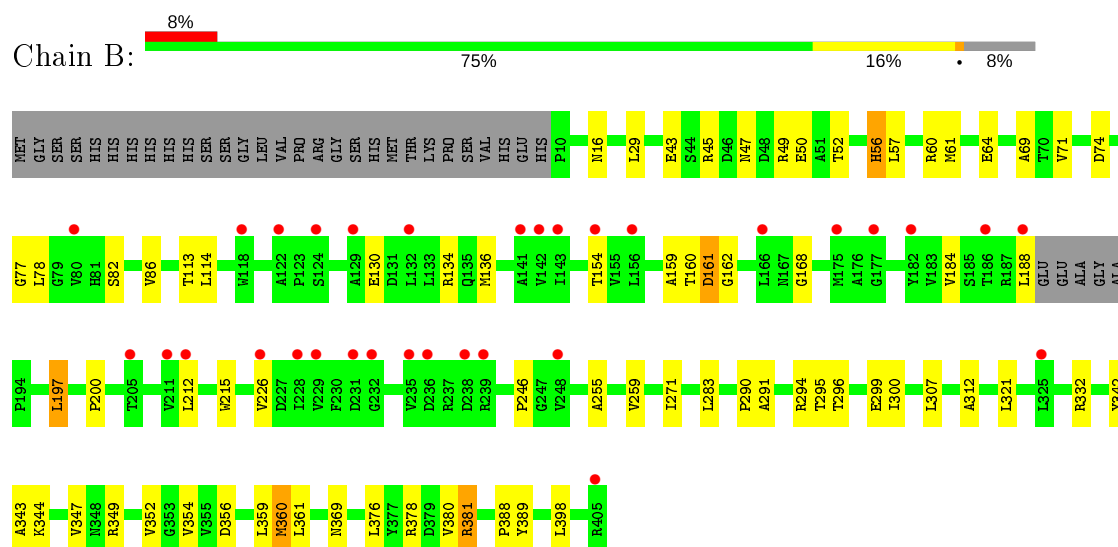
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.84Å 134.49Å 142.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.00 48.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.97-3.00) 97.7 (48.97-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.265 0.206 , 0.265	Depositor DCC
R_{free} test set	1937 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	91.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.3	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11465	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.61	1/2948 (0.0%)	0.78	2/4006 (0.0%)
1	B	0.57	1/2855 (0.0%)	0.73	1/3887 (0.0%)
1	C	0.62	0/2894	0.78	2/3935 (0.1%)
1	D	0.60	0/2927	0.77	5/3980 (0.1%)
All	All	0.60	2/11624 (0.0%)	0.76	10/15808 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	TRP	CD2-CE2	5.27	1.47	1.41
1	B	215	TRP	CD2-CE2	5.18	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	241	LEU	CA-CB-CG	6.69	130.70	115.30
1	D	241	LEU	CA-CB-CG	6.16	129.47	115.30
1	D	381	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	C	104	LEU	CA-CB-CG	-5.27	103.18	115.30
1	D	381	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	241	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	381	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	381	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	396	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	188	LEU	CA-CB-CG	5.00	126.80	115.30

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	2901	0	2879	59	0
1	B	2808	0	2716	55	0
1	C	2849	0	2810	64	0
1	D	2880	0	2854	60	0
2	A	7	0	0	0	0
2	B	6	0	0	2	0
2	C	6	0	0	0	0
2	D	8	0	0	1	0
All	All	11465	0	11259	215	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 9.

All (215) 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:D:120:HIS:HD2	1:D:325:LEU:CD1	1.55	1.19
1:D:120:HIS:CD2	1:D:325:LEU:CD1	2.38	1.05
1:C:120:HIS:HD2	1:C:325:LEU:CD1	1.71	1.03
1:C:120:HIS:HD2	1:C:325:LEU:HD11	1.22	1.00
1:D:120:HIS:HD2	1:D:325:LEU:HD11	1.27	0.99
1:D:120:HIS:CD2	1:D:325:LEU:HD11	1.98	0.97
1:C:120:HIS:CD2	1:C:325:LEU:HD11	2.07	0.90
1:B:291:ALA:CB	1:C:294:ARG:HD3	2.05	0.86
1:D:120:HIS:CD2	1:D:325:LEU:HD12	2.08	0.84
1:A:271:ILE:HG23	1:A:376:LEU:HD22	1.60	0.83
1:C:120:HIS:CD2	1:C:325:LEU:CD1	2.61	0.82
1:C:271:ILE:HG23	1:C:376:LEU:HD22	1.63	0.80
1:B:360:MET:HB3	1:D:381:ARG:HH12	1.49	0.77
1:B:271:ILE:HG23	1:B:376:LEU:HD22	1.65	0.76
1:C:82:SER:O	1:C:86:VAL:HG23	1.86	0.76
1:B:130:GLU:O	1:B:134:ARG:HG3	1.87	0.75
1:D:54:PRO:HB2	1:D:57:LEU:HD23	1.69	0.74
1:C:158:ARG:CB	1:C:190:GLU:HG3	2.21	0.71
1:D:271:ILE:HG23	1:D:376:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:O	1:A:134:ARG:HG3	1.91	0.71
1:D:46:ASP:O	1:D:50:GLU:HG2	1.91	0.71
1:B:159:ALA:O	1:B:161:ASP:N	2.25	0.70
1:B:349:ARG:NH2	2:B:501:HOH:O	1.90	0.70
1:A:396:ASP:O	1:A:400:GLU:HG3	1.92	0.70
1:C:130:GLU:O	1:C:134:ARG:HG3	1.92	0.70
1:B:294:ARG:HD3	1:C:291:ALA:CB	2.21	0.69
1:D:130:GLU:O	1:D:134:ARG:HG3	1.90	0.69
1:A:381:ARG:NH1	1:C:360:MET:HB3	2.07	0.69
1:B:291:ALA:HB3	1:C:294:ARG:HD3	1.75	0.68
1:A:381:ARG:HH12	1:C:360:MET:HB3	1.59	0.67
1:B:360:MET:HB3	1:D:381:ARG:NH1	2.09	0.67
1:C:120:HIS:HD2	1:C:325:LEU:HD12	1.58	0.67
1:B:154:THR:HG23	1:B:168:GLY:HA3	1.77	0.67
1:A:190:GLU:HG2	1:A:194:PRO:HD2	1.77	0.67
1:C:344:LYS:HE2	1:C:389:TYR:O	1.95	0.66
1:D:47:ASN:HD22	1:D:52:THR:HG23	1.61	0.65
1:C:300:ILE:HG23	1:C:354:VAL:HG13	1.79	0.65
1:C:190:GLU:O	1:C:192:GLY:N	2.29	0.65
1:A:158:ARG:HH21	1:A:190:GLU:HB2	1.62	0.64
1:B:45:ARG:HE	1:B:49:ARG:HH22	1.42	0.64
1:B:381:ARG:HH12	1:D:360:MET:HB3	1.61	0.64
1:A:184:VAL:O	1:A:200:PRO:HD2	1.98	0.64
1:A:360:MET:HB3	1:C:381:ARG:NH1	2.14	0.63
1:C:283:LEU:HD11	1:C:361:LEU:HG	1.79	0.63
1:C:154:THR:HG23	1:C:168:GLY:HA3	1.80	0.62
1:A:114:LEU:HD12	1:A:136:MET:CE	2.30	0.62
1:A:376:LEU:O	1:A:380:VAL:HG12	2.00	0.61
1:D:47:ASN:HA	1:D:52:THR:HG22	1.83	0.61
1:A:47:ASN:HA	1:A:52:THR:HG22	1.82	0.61
1:B:82:SER:O	1:B:86:VAL:HG23	2.00	0.61
1:A:360:MET:HB3	1:C:381:ARG:HH12	1.64	0.61
1:A:190:GLU:HG2	1:A:194:PRO:CD	2.32	0.60
1:D:184:VAL:O	1:D:200:PRO:HD2	2.02	0.60
1:D:47:ASN:HA	1:D:52:THR:CG2	2.32	0.60
1:A:47:ASN:HA	1:A:52:THR:CG2	2.32	0.59
1:B:381:ARG:NH1	1:D:360:MET:HB3	2.16	0.59
1:C:296:THR:HG21	1:C:360:MET:HE3	1.84	0.59
1:A:82:SER:O	1:A:86:VAL:HG23	2.03	0.59
1:C:120:HIS:CD2	1:C:325:LEU:HD12	2.35	0.58
1:D:114:LEU:HD12	1:D:136:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:HE2	1:A:389:TYR:O	2.03	0.58
1:D:146:ALA:HB1	1:D:170:LYS:HG3	1.86	0.58
1:A:47:ASN:HD22	1:A:52:THR:HG23	1.68	0.58
1:A:56:HIS:N	1:A:56:HIS:ND1	2.52	0.58
1:D:82:SER:O	1:D:86:VAL:HG23	2.04	0.57
1:A:114:LEU:HD12	1:A:136:MET:HE3	1.87	0.57
1:A:300:ILE:HG23	1:A:354:VAL:HG13	1.87	0.57
1:A:69:ALA:HA	1:A:78:LEU:HB2	1.88	0.56
1:B:60:ARG:HG2	1:B:64:GLU:OE2	2.04	0.56
1:A:154:THR:HG23	1:A:168:GLY:HA3	1.87	0.56
1:C:114:LEU:HD12	1:C:136:MET:CE	2.35	0.56
1:D:104:LEU:HD22	1:D:108:PHE:CZ	2.41	0.56
1:B:294:ARG:HD3	1:C:291:ALA:HB2	1.85	0.56
1:D:57:LEU:HD22	1:D:57:LEU:H	1.71	0.55
1:C:56:HIS:N	1:C:56:HIS:ND1	2.55	0.54
1:B:283:LEU:HD11	1:B:361:LEU:HG	1.90	0.54
1:D:56:HIS:N	1:D:56:HIS:ND1	2.54	0.54
1:A:135:GLN:HB3	1:A:141:ALA:HB2	1.90	0.54
1:B:47:ASN:HD22	1:B:52:THR:HG23	1.72	0.54
1:B:69:ALA:HA	1:B:78:LEU:HB2	1.90	0.53
1:C:281:THR:HG22	1:C:284:ARG:HH12	1.73	0.53
1:D:296:THR:HG21	1:D:360:MET:HE3	1.90	0.53
1:B:47:ASN:HA	1:B:52:THR:CG2	2.39	0.53
1:D:154:THR:HG23	1:D:168:GLY:HA3	1.91	0.53
1:A:158:ARG:HG2	1:A:164:TYR:HE1	1.73	0.53
1:B:56:HIS:ND1	1:B:56:HIS:N	2.56	0.53
1:B:47:ASN:HA	1:B:52:THR:HG22	1.89	0.53
1:C:344:LYS:CE	1:C:389:TYR:O	2.57	0.53
1:C:301:ASP:HB3	1:D:342:TYR:CZ	2.44	0.53
1:A:158:ARG:HG2	1:A:164:TYR:CE1	2.44	0.52
1:A:381:ARG:HH12	1:C:360:MET:CB	2.22	0.52
1:B:184:VAL:O	1:B:200:PRO:HD2	2.09	0.52
1:D:50:GLU:HB2	1:D:52:THR:CG2	2.39	0.52
1:A:113:THR:O	1:A:117:GLU:HG2	2.10	0.52
1:B:255:ALA:O	1:B:259:VAL:HG23	2.08	0.52
1:D:57:LEU:N	1:D:57:LEU:HD22	2.25	0.52
1:C:249:ARG:CZ	1:C:249:ARG:HB2	2.39	0.52
1:B:290:PRO:HB2	1:D:392:THR:CG2	2.40	0.52
1:B:300:ILE:HG23	1:B:354:VAL:HG13	1.92	0.52
1:C:69:ALA:HA	1:C:78:LEU:HB2	1.92	0.52
1:D:283:LEU:HD11	1:D:361:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HG	1:D:385:PHE:HZ	1.75	0.52
1:A:349:ARG:NH2	2:B:501:HOH:O	2.18	0.51
1:C:47:ASN:HA	1:C:52:THR:CG2	2.41	0.51
1:D:107:GLN:HE22	1:D:142:VAL:HA	1.76	0.51
1:A:342:TYR:CE1	1:A:398:LEU:HD22	2.45	0.51
1:A:26:GLY:HA3	1:A:85:ASP:OD2	2.11	0.50
1:B:342:TYR:CE1	1:B:398:LEU:HD22	2.46	0.50
1:A:50:GLU:HB2	1:A:52:THR:CG2	2.41	0.50
1:B:212:LEU:O	1:B:226:VAL:HB	2.12	0.50
1:C:70:THR:OG1	1:C:111:GLY:HA3	2.11	0.50
1:B:114:LEU:HD12	1:B:136:MET:CE	2.42	0.50
1:B:295:THR:O	1:B:299:GLU:HG2	2.12	0.50
1:D:47:ASN:ND2	1:D:52:THR:HG23	2.26	0.50
1:A:283:LEU:HD11	1:A:361:LEU:HG	1.94	0.50
1:A:295:THR:O	1:A:299:GLU:HG2	2.11	0.49
1:D:212:LEU:O	1:D:226:VAL:HB	2.12	0.49
1:C:301:ASP:HB3	1:D:342:TYR:CE1	2.47	0.49
1:B:296:THR:HG21	1:B:360:MET:HE3	1.93	0.49
1:C:47:ASN:HA	1:C:52:THR:HG22	1.94	0.49
1:D:135:GLN:HB3	1:D:141:ALA:HB2	1.95	0.49
1:A:46:ASP:O	1:A:50:GLU:HG2	2.12	0.49
1:B:50:GLU:HB2	1:B:52:THR:CG2	2.43	0.49
1:B:57:LEU:O	1:B:61:MET:HG3	2.12	0.49
1:C:132:LEU:O	1:C:136:MET:HG3	2.14	0.48
1:C:307:LEU:CD2	1:C:347:VAL:HA	2.43	0.48
1:C:360:MET:C	1:C:360:MET:SD	2.92	0.48
1:B:360:MET:CB	1:D:381:ARG:HH12	2.21	0.48
1:A:296:THR:HG21	1:A:360:MET:HE3	1.95	0.48
1:D:295:THR:O	1:D:299:GLU:HG2	2.14	0.48
1:B:197:LEU:HB3	1:B:246:PRO:HD3	1.96	0.48
1:A:307:LEU:CD2	1:A:347:VAL:HA	2.44	0.47
1:C:43:GLU:HB3	1:C:47:ASN:OD1	2.14	0.47
1:C:349:ARG:NH2	2:D:501:HOH:O	2.43	0.47
1:C:280:LEU:HD11	1:D:402:ALA:HB1	1.95	0.47
1:C:57:LEU:O	1:C:61:MET:HG3	2.13	0.47
1:A:219:GLY:O	1:A:220:MET:HB2	2.15	0.47
1:C:321:LEU:O	1:C:332:ARG:NH2	2.47	0.47
1:C:184:VAL:O	1:C:200:PRO:HD2	2.14	0.47
1:D:300:ILE:HG23	1:D:354:VAL:HG13	1.96	0.47
1:A:276:ARG:HA	1:A:358:CYS:SG	2.55	0.47
1:C:71:VAL:HG22	1:C:133:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HB	1:B:77:GLY:HA3	1.97	0.47
1:C:55:VAL:HG23	1:C:178:ILE:HG21	1.96	0.47
1:B:50:GLU:HB2	1:B:52:THR:HG22	1.96	0.46
1:A:344:LYS:CE	1:A:389:TYR:O	2.62	0.46
1:D:69:ALA:HA	1:D:78:LEU:HB2	1.97	0.46
1:A:32:LEU:HG	1:A:35:ARG:HH12	1.81	0.46
1:B:307:LEU:CD2	1:B:347:VAL:HA	2.46	0.46
1:D:388:PRO:HA	1:D:389:TYR:HA	1.78	0.46
1:C:47:ASN:HD22	1:C:52:THR:HG23	1.80	0.46
1:C:114:LEU:HD12	1:C:136:MET:HE3	1.96	0.46
1:C:388:PRO:HA	1:C:389:TYR:HA	1.82	0.46
1:B:344:LYS:HE2	1:B:389:TYR:O	2.15	0.46
1:A:245:GLU:HB2	1:A:246:PRO:HD2	1.97	0.45
1:C:43:GLU:OE1	1:C:57:LEU:HD21	2.15	0.45
1:D:321:LEU:O	1:D:332:ARG:NH2	2.50	0.45
1:D:344:LYS:HE2	1:D:389:TYR:O	2.16	0.45
1:B:369:ASN:OD1	1:B:378:ARG:NH2	2.50	0.45
1:D:199:ALA:O	1:D:241:LEU:HD22	2.17	0.45
1:D:50:GLU:HB2	1:D:52:THR:HG22	1.99	0.45
1:C:26:GLY:HA3	1:C:85:ASP:OD2	2.16	0.45
1:B:356:ASP:OD1	1:D:381:ARG:NE	2.50	0.45
1:A:352:VAL:HG22	1:A:380:VAL:HG22	1.99	0.44
1:B:43:GLU:HB3	1:B:47:ASN:OD1	2.17	0.44
1:C:359:LEU:HA	1:C:373:LEU:HD13	2.00	0.44
1:D:307:LEU:CD2	1:D:347:VAL:HA	2.48	0.44
1:A:281:THR:HG22	1:A:284:ARG:HH12	1.83	0.43
1:C:212:LEU:O	1:C:226:VAL:HB	2.18	0.43
1:D:132:LEU:O	1:D:136:MET:HG3	2.18	0.43
1:B:47:ASN:ND2	1:B:52:THR:HG23	2.32	0.43
1:A:47:ASN:ND2	1:A:52:THR:HG23	2.32	0.43
1:C:48:ASP:OD2	1:C:378:ARG:NH1	2.52	0.43
1:D:159:ALA:O	1:D:160:THR:C	2.57	0.43
1:B:321:LEU:O	1:B:332:ARG:NH2	2.51	0.43
1:D:52:THR:O	1:D:52:THR:HG23	2.19	0.43
1:A:62:ARG:NE	1:A:139:GLY:O	2.41	0.43
1:D:43:GLU:HB3	1:D:47:ASN:OD1	2.19	0.43
1:A:118:TRP:O	1:A:126:ARG:HG3	2.19	0.42
1:A:190:GLU:CG	1:A:194:PRO:HD2	2.46	0.42
1:A:307:LEU:HD22	1:A:347:VAL:HG22	2.01	0.42
1:A:364:GLY:O	1:A:365:ALA:C	2.56	0.42
1:C:219:GLY:O	1:C:220:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:VAL:HG22	1:B:380:VAL:HG22	2.01	0.42
1:D:159:ALA:HB3	1:D:163:SER:O	2.20	0.42
1:A:369:ASN:OD1	1:A:378:ARG:NH2	2.52	0.42
1:D:43:GLU:OE1	1:D:57:LEU:HD21	2.20	0.42
1:B:29:LEU:HD12	1:B:29:LEU:O	2.20	0.42
1:D:119:ARG:HB3	1:D:120:HIS:CE1	2.55	0.42
1:A:388:PRO:HA	1:A:389:TYR:HA	1.78	0.42
1:A:360:MET:CB	1:C:381:ARG:HH12	2.29	0.42
1:B:321:LEU:HD22	1:B:321:LEU:N	2.35	0.41
1:C:296:THR:O	1:C:300:ILE:HG13	2.20	0.41
1:B:376:LEU:O	1:B:380:VAL:HG12	2.20	0.41
1:A:321:LEU:O	1:A:332:ARG:NH2	2.53	0.41
1:A:212:LEU:O	1:A:226:VAL:HB	2.21	0.41
1:B:114:LEU:HA	1:B:114:LEU:HD23	1.89	0.41
1:C:136:MET:HE1	1:C:143:ILE:HD13	2.03	0.41
1:C:276:ARG:HA	1:C:358:CYS:SG	2.61	0.41
1:D:114:LEU:HD12	1:D:136:MET:HE1	2.03	0.41
1:A:176:ALA:HB3	1:A:226:VAL:CG2	2.51	0.41
1:A:392:THR:CG2	1:C:290:PRO:HB2	2.51	0.41
1:B:52:THR:HG23	1:B:52:THR:O	2.21	0.41
1:C:62:ARG:NE	1:C:139:GLY:O	2.42	0.41
1:A:136:MET:CE	1:A:143:ILE:HD13	2.51	0.41
1:A:157:THR:HG22	1:A:189:GLU:HB2	2.03	0.41
1:B:343:ALA:O	1:B:347:VAL:HG23	2.21	0.41
1:C:22:LYS:HE2	1:C:84:HIS:CG	2.56	0.41
1:B:16:ASN:O	1:B:312:ALA:HB3	2.22	0.40
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.83	0.40
1:D:276:ARG:HA	1:D:358:CYS:SG	2.61	0.40
1:D:57:LEU:O	1:D:61:MET:HG3	2.21	0.40
1:B:388:PRO:HA	1:B:389:TYR:HA	1.76	0.40
1:C:71:VAL:HB	1:C:77:GLY:HA3	2.02	0.40
1:B:359:LEU:HG	1:D:385:PHE:CZ	2.55	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	390/425 (92%)	367 (94%)	21 (5%)	2 (0%)	29	68
1	B	387/425 (91%)	368 (95%)	17 (4%)	2 (0%)	29	68
1	C	385/425 (91%)	364 (94%)	19 (5%)	2 (0%)	29	68
1	D	391/425 (92%)	375 (96%)	15 (4%)	1 (0%)	41	76
All	All	1553/1700 (91%)	1474 (95%)	72 (5%)	7 (0%)	29	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	191	ALA
1	B	160	THR
1	C	324	ASP
1	B	162	GLY
1	D	324	ASP
1	A	324	ASP
1	A	160	THR

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	292/327 (89%)	284 (97%)	8 (3%)	44	77
1	B	273/327 (84%)	266 (97%)	7 (3%)	46	78
1	C	284/327 (87%)	275 (97%)	9 (3%)	39	74
1	D	287/327 (88%)	278 (97%)	9 (3%)	40	75
All	All	1136/1308 (87%)	1103 (97%)	33 (3%)	42	76

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	74	ASP
1	A	188	LEU
1	A	190	GLU
1	A	197	LEU
1	A	249	ARG
1	A	277	ARG
1	A	360	MET
1	B	56	HIS
1	B	74	ASP
1	B	113	THR
1	B	161	ASP
1	B	188	LEU
1	B	197	LEU
1	B	360	MET
1	C	56	HIS
1	C	74	ASP
1	C	187	ARG
1	C	188	LEU
1	C	189	GLU
1	C	197	LEU
1	C	241	LEU
1	C	249	ARG
1	C	360	MET
1	D	28	ARG
1	D	49	ARG
1	D	56	HIS
1	D	74	ASP
1	D	113	THR
1	D	188	LEU
1	D	197	LEU
1	D	241	LEU
1	D	360	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	HIS
1	D	120	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	394/425 (92%)	-0.05	8 (2%)	65	36	59, 88, 148, 175	0
1	B	391/425 (92%)	0.43	32 (8%)	11	3	64, 111, 163, 195	0
1	C	391/425 (92%)	-0.04	8 (2%)	65	36	55, 95, 158, 188	0
1	D	395/425 (92%)	0.23	20 (5%)	28	10	64, 96, 158, 194	0
All	All	1571/1700 (92%)	0.14	68 (4%)	35	13	55, 97, 158, 195	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156	LEU	5.1
1	D	248	VAL	4.5
1	D	166	LEU	4.1
1	B	228	ILE	3.9
1	D	325	LEU	3.8
1	D	288	GLY	3.6
1	D	212	LEU	3.4
1	B	205	THR	3.3
1	D	10	PRO	3.3
1	B	212	LEU	3.3
1	D	189	GLU	3.3
1	D	245	GLU	3.3
1	B	177	GLY	3.3
1	B	325	LEU	3.3
1	B	141	ALA	3.2
1	A	248	VAL	3.2
1	B	248	VAL	3.2
1	B	124	SER	3.1
1	C	15	ASP	3.0
1	D	230	PHE	3.0
1	B	118	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	246	PRO	3.0
1	D	182	TYR	2.9
1	B	182	TYR	2.9
1	D	244	GLY	2.9
1	A	246	PRO	2.9
1	D	187	ARG	2.8
1	B	239	ARG	2.8
1	D	159	ALA	2.7
1	B	236	ASP	2.7
1	C	166	LEU	2.7
1	B	231	ASP	2.7
1	B	232	GLY	2.7
1	D	251	ASP	2.6
1	A	247	GLY	2.6
1	B	142	VAL	2.4
1	C	197	LEU	2.4
1	B	238	ASP	2.4
1	B	186	THR	2.4
1	B	166	LEU	2.4
1	C	189	GLU	2.4
1	B	122	ALA	2.4
1	B	132	LEU	2.4
1	A	323	ASP	2.3
1	B	226	VAL	2.3
1	C	187	ARG	2.3
1	B	211	VAL	2.3
1	B	154	THR	2.3
1	A	333	GLY	2.3
1	B	188	LEU	2.3
1	A	189	GLU	2.3
1	D	167	ASN	2.2
1	D	202	VAL	2.2
1	C	186	THR	2.2
1	B	175	MET	2.2
1	B	235	VAL	2.2
1	C	78	LEU	2.1
1	A	123	PRO	2.1
1	C	249	ARG	2.1
1	A	187	ARG	2.1
1	B	80	VAL	2.1
1	B	143	ILE	2.0
1	D	209	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	156	LEU	2.0
1	B	229	VAL	2.0
1	B	405	ARG	2.0
1	B	129	ALA	2.0
1	D	201	VAL	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.