WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:46 pm BST

PDB ID	:	4N0Q
Title	:	Crystal Structure of an ABC transporter, substrate-binding protein from Brucella melitensis 16M in complex with L-Leucine using a crystal grown in a Crystal Former (Microlytic)
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2013-10-02
Resolution	:	2.30 Å(reported)

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 2.30 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.
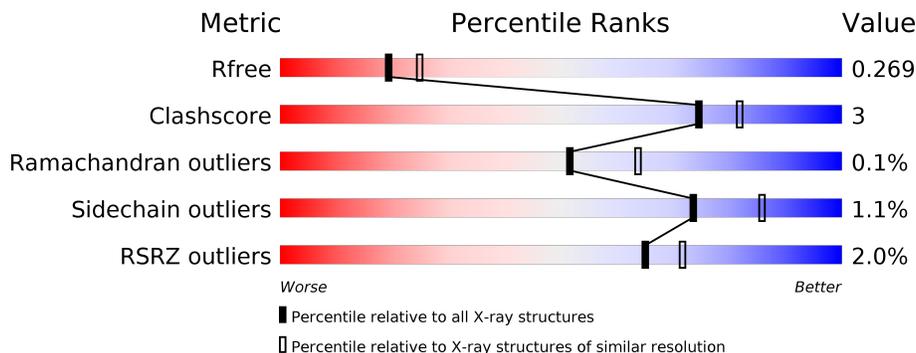
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	354	90% 7% ·
1	B	354	88% 9% ·
1	C	354	87% 10% ·
1	D	354	91% 6% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10258 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 Leu/Ile/Val-binding protein homolog 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	2	0
			2432	1529	408	489	6			
1	B	345	Total	C	N	O	S	0	2	0
			2486	1565	418	497	6			
1	C	344	Total	C	N	O	S	0	0	0
			2391	1505	402	478	6			
1	D	344	Total	C	N	O	S	0	0	0
			2416	1521	406	483	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	EXPRESSION TAG	UNP Q8YEE8
A	16	ALA	-	EXPRESSION TAG	UNP Q8YEE8
A	17	HIS	-	EXPRESSION TAG	UNP Q8YEE8
A	18	HIS	-	EXPRESSION TAG	UNP Q8YEE8
A	19	HIS	-	EXPRESSION TAG	UNP Q8YEE8
A	20	HIS	-	EXPRESSION TAG	UNP Q8YEE8
A	21	HIS	-	EXPRESSION TAG	UNP Q8YEE8
A	22	HIS	-	EXPRESSION TAG	UNP Q8YEE8
B	15	MET	-	EXPRESSION TAG	UNP Q8YEE8
B	16	ALA	-	EXPRESSION TAG	UNP Q8YEE8
B	17	HIS	-	EXPRESSION TAG	UNP Q8YEE8
B	18	HIS	-	EXPRESSION TAG	UNP Q8YEE8
B	19	HIS	-	EXPRESSION TAG	UNP Q8YEE8
B	20	HIS	-	EXPRESSION TAG	UNP Q8YEE8
B	21	HIS	-	EXPRESSION TAG	UNP Q8YEE8
B	22	HIS	-	EXPRESSION TAG	UNP Q8YEE8
C	15	MET	-	EXPRESSION TAG	UNP Q8YEE8
C	16	ALA	-	EXPRESSION TAG	UNP Q8YEE8
C	17	HIS	-	EXPRESSION TAG	UNP Q8YEE8
C	18	HIS	-	EXPRESSION TAG	UNP Q8YEE8
C	19	HIS	-	EXPRESSION TAG	UNP Q8YEE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	HIS	-	EXPRESSION TAG	UNP Q8YEE8
C	21	HIS	-	EXPRESSION TAG	UNP Q8YEE8
C	22	HIS	-	EXPRESSION TAG	UNP Q8YEE8
D	15	MET	-	EXPRESSION TAG	UNP Q8YEE8
D	16	ALA	-	EXPRESSION TAG	UNP Q8YEE8
D	17	HIS	-	EXPRESSION TAG	UNP Q8YEE8
D	18	HIS	-	EXPRESSION TAG	UNP Q8YEE8
D	19	HIS	-	EXPRESSION TAG	UNP Q8YEE8
D	20	HIS	-	EXPRESSION TAG	UNP Q8YEE8
D	21	HIS	-	EXPRESSION TAG	UNP Q8YEE8
D	22	HIS	-	EXPRESSION TAG	UNP Q8YEE8

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).
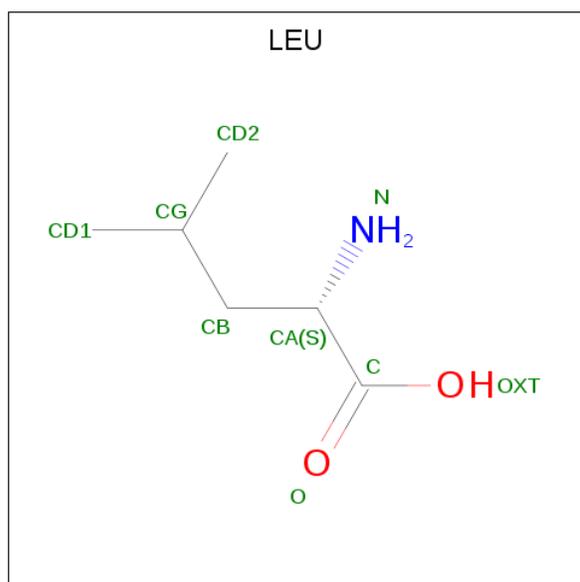
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9	C 6	N 1	O 2	0	0
2	B	1	Total 9	C 6	N 1	O 2	0	0
2	C	1	Total 9	C 6	N 1	O 2	0	0
2	D	1	Total 9	C 6	N 1	O 2	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total 74	O 74	0	0
3	B	229	Total 229	O 229	0	0
3	C	70	Total 70	O 70	0	0
3	D	124	Total 124	O 124	0	0

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 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.
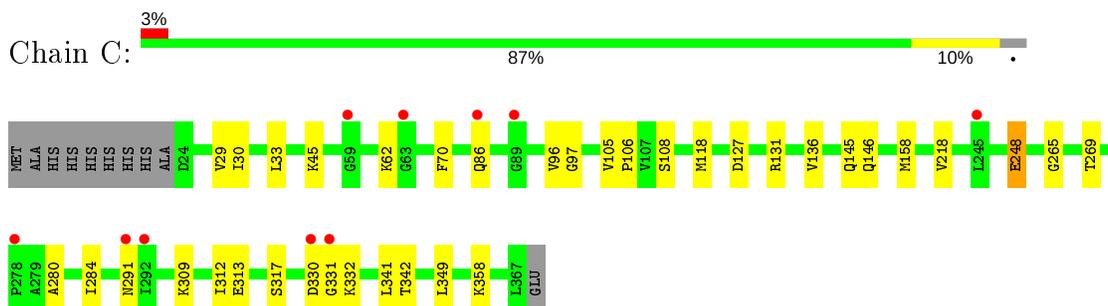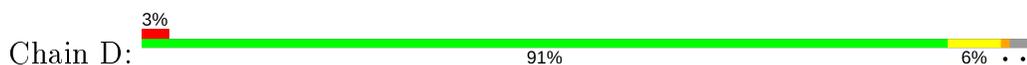
- Molecule 1: Leu/Ile/Val-binding protein homolog 3
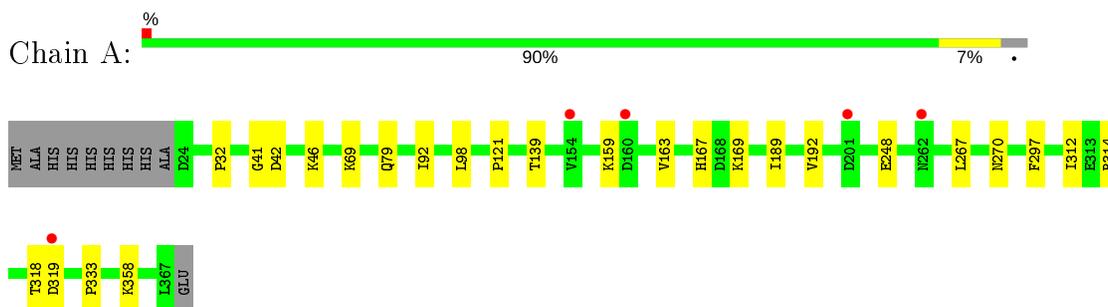
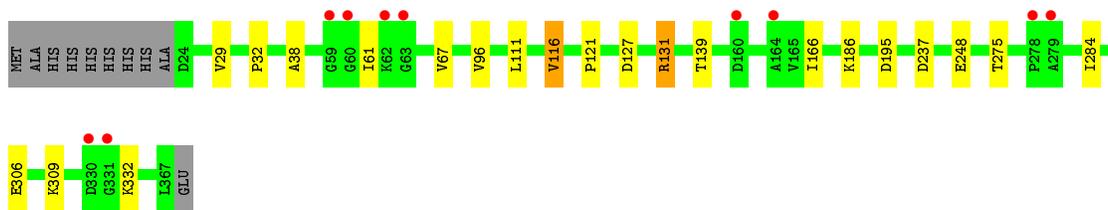- Molecule 1: Leu/Ile/Val-binding protein homolog 3
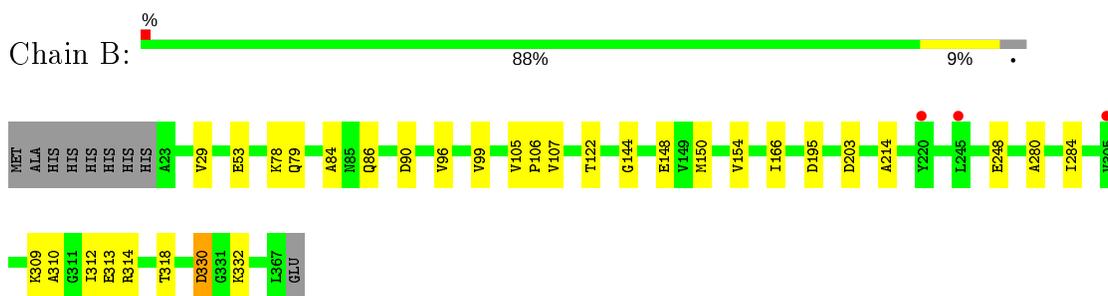
- Molecule 1: Leu/Ile/Val-binding protein homolog 3

- Molecule 1: Leu/Ile/Val-binding protein homolog 3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.50Å 59.85Å 147.90Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	19.93 – 2.30 19.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.93-2.30) 98.1 (19.93-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.67 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0049, PHENIX	Depositor
R, R_{free}	0.212 , 0.269 0.218 , 0.269	Depositor DCC
R_{free} test set	2727 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10258	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5495e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 (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	0.51	0/2476	0.63	0/3374
1	B	0.75	0/2527	0.80	2/3430 (0.1%)
1	C	0.51	0/2429	0.65	0/3314
1	D	0.66	0/2454	0.73	2/3343 (0.1%)
All	All	0.62	0/9886	0.71	4/13461 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

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	203	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	330	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	131	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	237	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	330	ASP	Peptide

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	2432	0	2346	16	0
1	B	2486	0	2454	16	1
1	C	2391	0	2278	17	1
1	D	2416	0	2330	13	0
2	A	9	0	10	2	0
2	B	9	0	10	0	0
2	C	9	0	10	1	0
2	D	9	0	10	0	0
3	A	74	0	0	1	0
3	B	229	0	0	3	0
3	C	70	0	0	2	0
3	D	124	0	0	1	0
All	All	10258	0	9448	62	1

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 3.

All (62) 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:144:GLY:O	1:B:148:GLU:HG2	1.73	0.89
1:A:248:GLU:OE2	2:A:500:LEU:N	2.26	0.69
1:B:309[B]:LYS:NZ	1:B:313:GLU:OE2	2.20	0.69
1:D:111:LEU:HB3	1:D:116:VAL:HG13	1.73	0.68
1:A:314:ARG:NH2	1:A:333:PRO:O	2.31	0.64
1:A:32:PRO:O	1:A:41:GLY:HA3	2.00	0.62
1:B:53[B]:GLU:OE1	3:B:897:HOH:O	2.17	0.58
1:A:167:HIS:HD2	1:A:169:LYS:H	1.50	0.58
1:C:280:ALA:O	1:C:284:ILE:HG12	2.04	0.57
1:C:146:GLN:HG3	1:C:269:THR:OG1	2.07	0.55
1:C:105:VAL:HB	1:C:106:PRO:HD3	1.89	0.54
1:A:42:ASP:OD2	1:A:46:LYS:HE2	2.07	0.54
1:C:312:ILE:HG23	1:C:317:SER:O	2.08	0.53
1:C:331:GLY:O	1:C:332:LYS:C	2.44	0.53
1:C:45:LYS:HG3	1:C:70:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLY:HA2	1:C:358:LYS:HE3	1.90	0.52
1:A:69:LYS:HD2	1:A:92:ILE:HD11	1.92	0.51
1:C:158:MET:HE1	1:C:218:VAL:HG11	1.93	0.51
1:C:248:GLU:OE2	2:C:700:LEU:N	2.44	0.51
1:D:127:ASP:O	1:D:131:ARG:HD3	2.11	0.51
1:B:280:ALA:O	1:B:284:ILE:HG12	2.13	0.49
1:D:186:LYS:HE2	3:D:948:HOH:O	2.13	0.49
1:D:127:ASP:OD1	1:D:131:ARG:HD2	2.12	0.48
1:A:163:VAL:O	1:A:192:VAL:HG22	2.13	0.48
1:A:248:GLU:HG2	1:A:297:PHE:HZ	1.78	0.47
1:C:127:ASP:O	1:C:131:ARG:NE	2.43	0.47
1:C:309:LYS:O	1:C:313:GLU:HG2	2.14	0.47
1:B:214:ALA:O	3:B:763:HOH:O	2.21	0.46
1:D:306:GLU:O	1:D:309:LYS:HB3	2.16	0.46
1:B:84:ALA:HB2	1:B:107:VAL:HG13	1.98	0.46
1:A:248:GLU:HG2	1:A:297:PHE:CZ	2.51	0.46
1:D:186:LYS:HE2	1:D:186:LYS:HB3	1.79	0.45
1:B:99:VAL:HA	1:B:122:THR:OG1	2.17	0.45
1:B:105:VAL:HB	1:B:106:PRO:HD3	1.99	0.45
1:D:275:THR:HA	1:D:284:ILE:HD11	1.98	0.45
1:A:297:PHE:CE2	2:A:500:LEU:HD11	2.52	0.44
1:B:330:ASP:OD2	1:B:332:LYS:NZ	2.46	0.44
1:D:121:PRO:HA	1:D:139:THR:OG1	2.17	0.44
1:D:29:VAL:HA	1:D:96:VAL:O	2.18	0.44
1:C:118:MET:SD	1:C:136:VAL:HG22	2.57	0.44
1:D:61:ILE:HD12	1:D:309:LYS:HG3	2.00	0.44
1:D:32:PRO:O	1:D:38:ALA:HA	2.18	0.43
1:C:30:ILE:O	1:C:97:GLY:HA3	2.19	0.43
1:C:145:GLN:OE1	3:C:809:HOH:O	2.21	0.43
1:C:29:VAL:HA	1:C:96:VAL:O	2.19	0.43
1:C:105:VAL:O	1:C:108:SER:OG	2.29	0.42
1:B:29:VAL:HA	1:B:96:VAL:O	2.20	0.42
1:B:312:ILE:HG21	1:B:318:THR:HG22	2.01	0.42
1:A:312:ILE:HG21	1:A:318:THR:HG22	2.01	0.42
1:B:86:GLN:HG3	3:B:898:HOH:O	2.20	0.42
1:C:341:LEU:HD22	1:C:349:LEU:HD22	2.02	0.42
1:B:150:MET:O	1:B:154:VAL:HG23	2.20	0.41
1:B:310:ALA:O	1:B:314:ARG:HG2	2.20	0.41
1:A:159:LYS:HA	1:A:189:ILE:HD11	2.00	0.41
1:A:121:PRO:HA	1:A:139:THR:OG1	2.20	0.41
1:B:166:ILE:HA	1:B:195:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:CD2	1:A:358:LYS:HB3	2.51	0.41
1:B:78:LYS:HG3	1:B:79:GLN:N	2.37	0.40
3:C:828:HOH:O	1:D:332:LYS:CB	2.70	0.40
1:A:270:ASN:ND2	3:A:632:HOH:O	2.40	0.40
1:A:98:LEU:N	1:A:98:LEU:HD12	2.35	0.40
1:D:166:ILE:HA	1:D:195:ASP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASP:OD1	1:C:291:ASN:ND2[2_647]	2.14	0.06

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	344/354 (97%)	337 (98%)	7 (2%)	0	100	100
1	B	345/354 (98%)	339 (98%)	6 (2%)	0	100	100
1	C	342/354 (97%)	334 (98%)	7 (2%)	1 (0%)	41	50
1	D	342/354 (97%)	334 (98%)	8 (2%)	0	100	100
All	All	1373/1416 (97%)	1344 (98%)	28 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	62	LYS

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	236/261 (90%)	233 (99%)	3 (1%)	69	82
1	B	247/261 (95%)	246 (100%)	1 (0%)	91	96
1	C	225/261 (86%)	221 (98%)	4 (2%)	59	75
1	D	232/261 (89%)	229 (99%)	3 (1%)	69	82
All	All	940/1044 (90%)	929 (99%)	11 (1%)	73	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79[A]	GLN
1	A	79[B]	GLN
1	A	319	ASP
1	B	248	GLU
1	C	33	LEU
1	C	86	GLN
1	C	248	GLU
1	C	342	THR
1	D	67	VAL
1	D	116	VAL
1	D	248	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	B	157	ASN
1	C	264	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	344/354 (97%)	0.21	5 (1%)	73	79	25, 32, 48, 63	0
1	B	345/354 (97%)	0.21	3 (0%)	84	88	2, 17, 20, 27	0
1	C	344/354 (97%)	0.29	10 (2%)	51	58	20, 32, 48, 59	0
1	D	344/354 (97%)	0.07	10 (2%)	51	58	12, 18, 41, 56	0
All	All	1377/1416 (97%)	0.19	28 (2%)	65	71	2, 26, 45, 63	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	GLN	3.2
1	D	278	PRO	3.2
1	D	279	ALA	3.1
1	D	63	GLY	3.1
1	A	160	ASP	3.0
1	D	330	ASP	2.9
1	C	63	GLY	2.8
1	B	245	LEU	2.5
1	C	59	GLY	2.4
1	A	154	VAL	2.4
1	C	292	ILE	2.3
1	B	220	TYR	2.3
1	B	305	VAL	2.3
1	C	89	GLY	2.3
1	A	201	ASP	2.3
1	D	60	GLY	2.2
1	A	262	ASN	2.2
1	C	330	ASP	2.2
1	D	160	ASP	2.2
1	C	245	LEU	2.2
1	A	319	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	59	GLY	2.1
1	D	331	GLY	2.1
1	D	62	LYS	2.1
1	C	278	PRO	2.1
1	C	291	ASN	2.1
1	C	331	GLY	2.0
1	D	164	ALA	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)

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	LEU	C	700	9/9	0.88	0.18	16,21,23,23	0
2	LEU	A	500	9/9	0.94	0.12	18,22,25,26	0
2	LEU	D	800	9/9	0.95	0.12	2,2,2,2	0
2	LEU	B	600	9/9	0.96	0.12	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.