



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:07 AM EDT

PDB ID : 7JZT
Title : Low resolution crystal structure of Zaire Ebola virus VP40 in space group P6422
Authors : Norris, M.J.; Bornholdt, Z.A.; Sapphire, E.O.
Deposited on : 2020-09-02
Resolution : 3.77 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

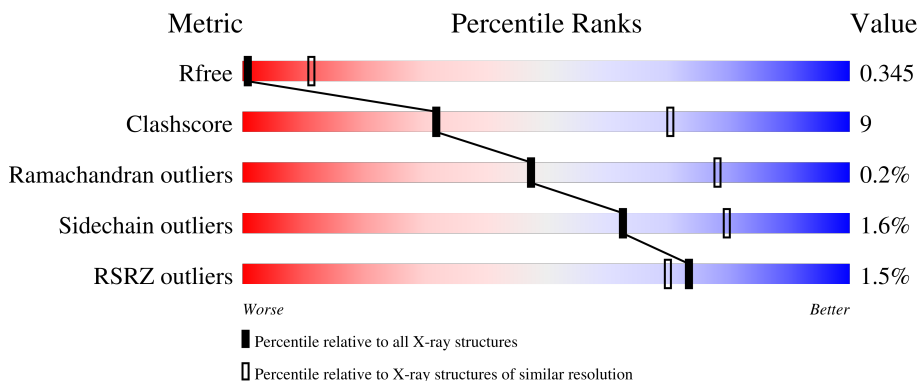
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.77 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	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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 of 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 $\leq 5\%$. 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	297	 2% 57% 19% 23%
1	B	297	 2% 65% 10% 25%
1	C	297	 0% 58% 20% 22%
1	D	297	 0% 60% 17% 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13677 atoms, of which 6882 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 Matrix protein VP40.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	230	3456	1117	1738	281	316	4	0	0	0
1	B	222	3290	1064	1655	267	298	6	0	0	0
1	C	233	3495	1121	1764	288	317	5	0	0	0
1	D	230	3436	1112	1725	278	316	5	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP Q05128
A	31	ALA	-	expression tag	UNP Q05128
A	32	HIS	-	expression tag	UNP Q05128
A	33	HIS	-	expression tag	UNP Q05128
A	34	HIS	-	expression tag	UNP Q05128
A	35	HIS	-	expression tag	UNP Q05128
A	36	HIS	-	expression tag	UNP Q05128
A	37	HIS	-	expression tag	UNP Q05128
A	38	VAL	-	expression tag	UNP Q05128
A	39	ASP	-	expression tag	UNP Q05128
A	40	ASP	-	expression tag	UNP Q05128
A	41	ASP	-	expression tag	UNP Q05128
A	42	ASP	-	expression tag	UNP Q05128
A	43	LYS	ASN	conflict	UNP Q05128
B	30	MET	-	initiating methionine	UNP Q05128
B	31	ALA	-	expression tag	UNP Q05128
B	32	HIS	-	expression tag	UNP Q05128
B	33	HIS	-	expression tag	UNP Q05128
B	34	HIS	-	expression tag	UNP Q05128
B	35	HIS	-	expression tag	UNP Q05128
B	36	HIS	-	expression tag	UNP Q05128

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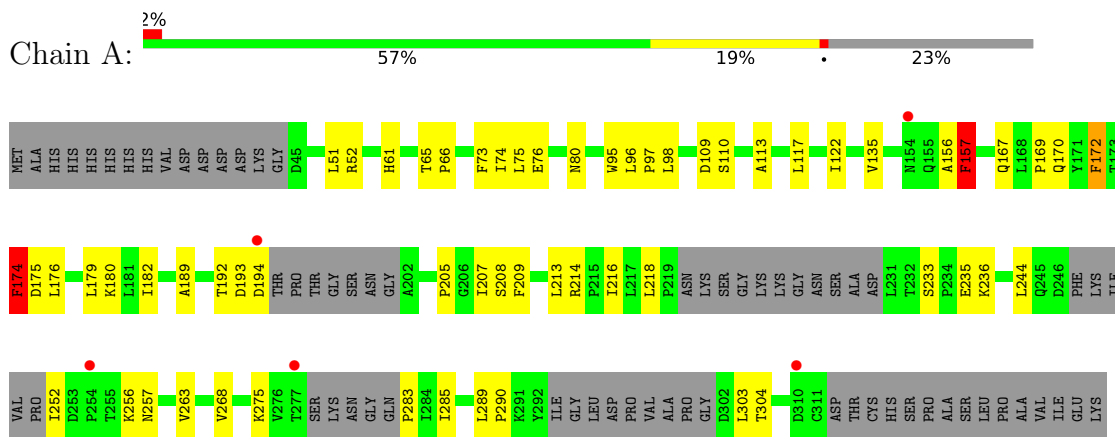
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Chain	Residue	Modelled	Actual	Comment	Reference
B	37	HIS	-	expression tag	UNP Q05128
B	38	VAL	-	expression tag	UNP Q05128
B	39	ASP	-	expression tag	UNP Q05128
B	40	ASP	-	expression tag	UNP Q05128
B	41	ASP	-	expression tag	UNP Q05128
B	42	ASP	-	expression tag	UNP Q05128
B	43	LYS	ASN	conflict	UNP Q05128
C	30	MET	-	initiating methionine	UNP Q05128
C	31	ALA	-	expression tag	UNP Q05128
C	32	HIS	-	expression tag	UNP Q05128
C	33	HIS	-	expression tag	UNP Q05128
C	34	HIS	-	expression tag	UNP Q05128
C	35	HIS	-	expression tag	UNP Q05128
C	36	HIS	-	expression tag	UNP Q05128
C	37	HIS	-	expression tag	UNP Q05128
C	38	VAL	-	expression tag	UNP Q05128
C	39	ASP	-	expression tag	UNP Q05128
C	40	ASP	-	expression tag	UNP Q05128
C	41	ASP	-	expression tag	UNP Q05128
C	42	ASP	-	expression tag	UNP Q05128
C	43	LYS	ASN	conflict	UNP Q05128
D	30	MET	-	initiating methionine	UNP Q05128
D	31	ALA	-	expression tag	UNP Q05128
D	32	HIS	-	expression tag	UNP Q05128
D	33	HIS	-	expression tag	UNP Q05128
D	34	HIS	-	expression tag	UNP Q05128
D	35	HIS	-	expression tag	UNP Q05128
D	36	HIS	-	expression tag	UNP Q05128
D	37	HIS	-	expression tag	UNP Q05128
D	38	VAL	-	expression tag	UNP Q05128
D	39	ASP	-	expression tag	UNP Q05128
D	40	ASP	-	expression tag	UNP Q05128
D	41	ASP	-	expression tag	UNP Q05128
D	42	ASP	-	expression tag	UNP Q05128
D	43	LYS	ASN	conflict	UNP Q05128

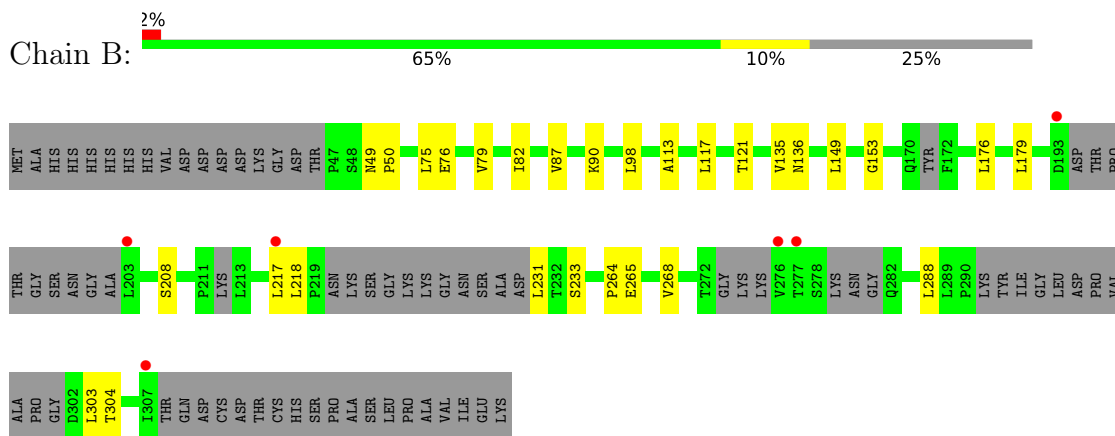
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

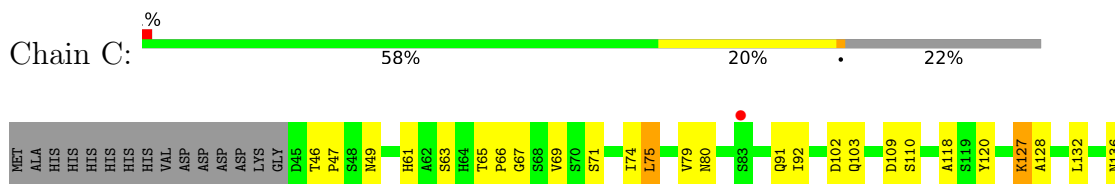
- Molecule 1: Matrix protein VP40

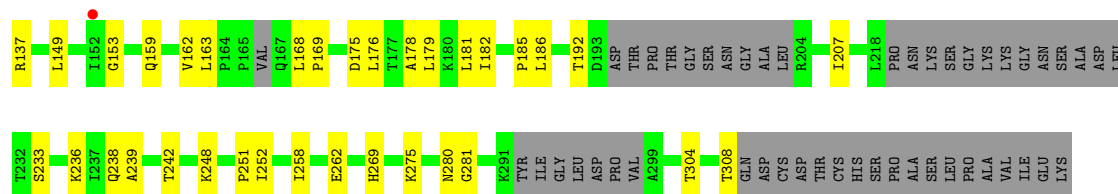


- Molecule 1: Matrix protein VP40



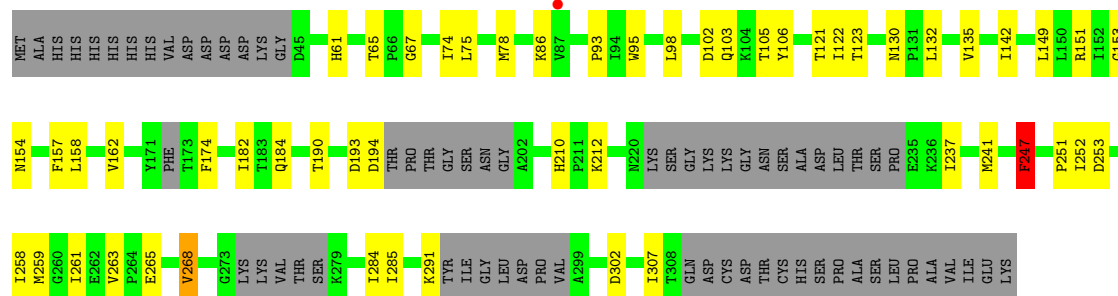
- Molecule 1: Matrix protein VP40





- Molecule 1: Matrix protein VP40

Chain D: 60% 17% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.28Å 105.28Å 463.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.77 19.90 – 3.77	Depositor EDS
% Data completeness (in resolution range)	45.7 (19.90-3.77) 45.7 (19.90-3.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.82Å)	Xtrriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.315 , 0.345 0.315 , 0.345	Depositor DCC
R_{free} test set	352 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	159.9	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 177.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13677	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.40 % 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 8.0429e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.31	0/1758	0.68	4/2412 (0.2%)
1	B	0.26	0/1671	0.53	0/2292
1	C	0.30	0/1771	0.63	0/2425
1	D	0.30	0/1752	0.72	4/2405 (0.2%)
All	All	0.29	0/6952	0.64	8/9534 (0.1%)

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	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	302	ASP	CB-CG-OD1	10.17	127.45	118.30
1	D	247	PHE	CB-CG-CD2	-9.58	114.10	120.80
1	A	157	PHE	CB-CG-CD2	-9.52	114.13	120.80
1	A	174	PHE	CB-CG-CD2	-8.69	114.72	120.80
1	D	302	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	D	247	PHE	CB-CG-CD1	6.83	125.58	120.80
1	A	157	PHE	CB-CG-CD1	6.31	125.22	120.80
1	A	174	PHE	CB-CG-CD1	6.09	125.06	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	PHE	Sidechain
1	C	127	LYS	Peptide
1	D	247	PHE	Sidechain

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	1718	1738	1738	40	2
1	B	1635	1655	1655	16	0
1	C	1731	1764	1764	35	1
1	D	1711	1725	1724	30	3
All	All	6795	6882	6881	121	3

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 (121) 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:C:176:LEU:HD11	1:C:179:LEU:HD11	1.63	0.81
1:C:238:GLN:O	1:C:242:THR:HG23	1.87	0.74
1:C:181:LEU:HD23	1:C:182:ILE:N	2.06	0.70
1:C:49:ASN:ND2	1:C:175:ASP:OD1	2.24	0.69
1:A:244:LEU:HD22	1:A:304:THR:HG21	1.75	0.67
1:D:61:HIS:O	1:D:65:THR:OG1	2.13	0.66
1:A:208:SER:HB3	1:A:303:LEU:HD22	1.78	0.65
1:D:251:PRO:HA	1:D:259:MET:SD	2.37	0.65
1:C:79:VAL:O	1:C:92:ILE:N	2.30	0.64
1:D:247:PHE:HD1	1:D:247:PHE:O	1.82	0.63
1:C:176:LEU:HD11	1:C:179:LEU:CD1	2.28	0.63
1:A:263:VAL:HG12	1:A:285:ILE:HG13	1.81	0.62
1:A:233:SER:O	1:A:236:LYS:HG2	2.00	0.62
1:A:209:PHE:HZ	1:A:213:LEU:HD23	1.63	0.62
1:A:76:GLU:OE1	1:A:180:LYS:HE2	2.00	0.61
1:A:233:SER:HB3	1:A:235:GLU:OE1	2.00	0.60
1:A:73:PHE:HB3	1:A:98:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:OD1	1:A:176:LEU:N	2.34	0.60
1:C:178:ALA:C	1:C:179:LEU:HD12	2.23	0.60
1:C:109:ASP:OD1	1:C:110:SER:N	2.33	0.58
1:B:113:ALA:O	1:B:117:LEU:N	2.36	0.58
1:C:61:HIS:O	1:C:65:THR:OG1	2.19	0.58
1:A:80:ASN:O	1:A:174:PHE:HA	2.03	0.58
1:A:205:PRO:HB2	1:A:218:LEU:HD12	1.85	0.57
1:C:118:ALA:O	1:C:137:ARG:NH1	2.36	0.57
1:A:207:ILE:HB	1:A:216:ILE:HB	1.87	0.56
1:A:109:ASP:OD1	1:A:110:SER:N	2.37	0.56
1:D:210:HIS:CE1	1:D:212:LYS:HE2	2.41	0.56
1:A:268:VAL:HG11	1:A:275:LYS:HB2	1.88	0.55
1:A:113:ALA:O	1:A:117:LEU:N	2.39	0.55
1:D:78:MET:SD	1:D:93:PRO:HB3	2.47	0.55
1:D:102:ASP:O	1:D:102:ASP:OD1	2.25	0.55
1:D:158:LEU:O	1:D:162:VAL:HG22	2.07	0.55
1:B:121:THR:OG1	1:B:136:ASN:OD1	2.25	0.55
1:B:303:LEU:H	1:B:303:LEU:HD23	1.72	0.54
1:D:193:ASP:OD1	1:D:194:ASP:N	2.41	0.53
1:A:174:PHE:HD1	1:A:174:PHE:O	1.92	0.52
1:D:74:ILE:HD11	1:D:182:ILE:HD12	1.91	0.52
1:C:233:SER:HB3	1:C:236:LYS:HB2	1.92	0.52
1:A:172:PHE:N	1:A:172:PHE:CD2	2.79	0.51
1:D:135:VAL:O	1:D:154:ASN:OD1	2.29	0.50
1:B:79:VAL:HA	1:B:176:LEU:HA	1.94	0.50
1:C:80:ASN:OD1	1:C:91:GLN:N	2.39	0.49
1:D:142:ILE:HB	1:D:151:ARG:HA	1.95	0.49
1:A:252:ILE:HG23	1:A:252:ILE:O	2.13	0.49
1:C:46:THR:HG22	1:C:47:PRO:HD2	1.95	0.49
1:D:78:MET:SD	1:D:93:PRO:CA	3.01	0.49
1:A:209:PHE:CZ	1:A:213:LEU:HD23	2.46	0.49
1:C:102:ASP:O	1:C:102:ASP:OD1	2.31	0.49
1:B:288:LEU:HD12	1:B:288:LEU:O	2.13	0.49
1:C:67:GLY:HA2	1:C:103:GLN:OE1	2.13	0.48
1:C:136:ASN:OD1	1:C:153:GLY:O	2.30	0.48
1:C:251:PRO:O	1:C:252:ILE:HD13	2.13	0.48
1:B:231:LEU:N	1:B:233:SER:HG	2.10	0.48
1:C:149:LEU:O	1:C:153:GLY:N	2.46	0.48
1:D:130:ASN:O	1:D:132:LEU:HD12	2.14	0.48
1:C:280:ASN:OD1	1:C:281:GLY:N	2.47	0.47
1:A:61:HIS:O	1:A:65:THR:OG1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:PHE:HB3	1:D:162:VAL:HG21	1.95	0.47
1:C:74:ILE:HG22	1:C:75:LEU:N	2.30	0.47
1:D:247:PHE:HB2	1:D:263:VAL:HA	1.97	0.47
1:A:75:LEU:HD21	1:A:179:LEU:HD11	1.96	0.47
1:B:264:PRO:O	1:B:268:VAL:HG13	2.15	0.46
1:B:121:THR:O	1:B:135:VAL:HG13	2.16	0.46
1:A:51:LEU:HD22	1:A:176:LEU:HD23	1.98	0.45
1:C:66:PRO:HB2	1:C:69:VAL:HG22	1.98	0.45
1:D:149:LEU:O	1:D:153:GLY:N	2.50	0.45
1:A:74:ILE:N	1:A:182:ILE:O	2.50	0.45
1:C:71:SER:HA	1:C:186:LEU:CB	2.47	0.44
1:B:208:SER:HB3	1:B:304:THR:HG23	2.00	0.44
1:A:122:ILE:HD12	1:A:122:ILE:N	2.32	0.44
1:D:78:MET:SD	1:D:93:PRO:CB	3.06	0.44
1:C:162:VAL:HG23	1:C:163:LEU:HG	1.98	0.44
1:A:65:THR:N	1:A:66:PRO:CD	2.80	0.44
1:A:257:ASN:O	1:A:289:LEU:HB2	2.16	0.44
1:B:217:LEU:HD23	1:B:218:LEU:N	2.32	0.44
1:A:189:ALA:HB1	1:A:283:PRO:N	2.33	0.44
1:A:156:ALA:O	1:A:157:PHE:HB3	2.17	0.44
1:A:193:ASP:O	1:A:194:ASP:CB	2.66	0.44
1:A:75:LEU:O	1:A:96:LEU:HB2	2.18	0.44
1:B:75:LEU:HD22	1:B:179:LEU:HD11	2.00	0.44
1:D:265:GLU:O	1:D:268:VAL:HG22	2.18	0.43
1:C:236:LYS:O	1:C:239:ALA:HB3	2.18	0.43
1:D:252:ILE:O	1:D:258:ILE:HB	2.18	0.43
1:C:304:THR:O	1:C:304:THR:HG23	2.18	0.43
1:A:97:PRO:HD2	1:A:157:PHE:CD2	2.53	0.43
1:A:61:HIS:O	1:A:65:THR:N	2.52	0.43
1:A:213:LEU:HG	1:A:214:ARG:H	1.84	0.43
1:B:76:GLU:O	1:B:179:LEU:HD12	2.19	0.43
1:C:269:HIS:O	1:C:275:LYS:HD3	2.18	0.43
1:D:95:TRP:HB2	1:D:291:LYS:HD2	2.00	0.43
1:A:122:ILE:HG13	1:A:135:VAL:HG22	2.01	0.43
1:D:190:THR:HA	1:D:284:ILE:O	2.19	0.43
1:D:252:ILE:O	1:D:258:ILE:O	2.37	0.43
1:D:261:ILE:HB	1:D:285:ILE:HB	2.01	0.43
1:C:120:TYR:CB	1:C:136:ASN:O	2.67	0.42
1:B:82:ILE:HA	1:B:87:VAL:HA	2.00	0.42
1:C:46:THR:CG2	1:C:47:PRO:HD2	2.50	0.42
1:D:67:GLY:HA2	1:D:103:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:THR:C	1:D:106:TYR:CD1	2.93	0.42
1:A:193:ASP:O	1:A:194:ASP:HB3	2.20	0.42
1:C:207:ILE:HG23	1:C:304:THR:HG23	2.02	0.42
1:D:121:THR:O	1:D:135:VAL:HA	2.20	0.42
1:D:184:GLN:HG2	1:D:253:ASP:OD2	2.20	0.42
1:C:102:ASP:OD2	1:C:192:THR:HG21	2.21	0.41
1:C:252:ILE:O	1:C:258:ILE:O	2.38	0.41
1:A:52:ARG:C	1:A:179:LEU:HD23	2.40	0.41
1:A:174:PHE:C	1:A:174:PHE:CD1	2.94	0.41
1:D:237:ILE:O	1:D:241:MET:N	2.54	0.41
1:A:213:LEU:HD22	1:A:290:PRO:CG	2.51	0.41
1:C:159:GLN:HA	1:C:162:VAL:HG22	2.02	0.41
1:D:98:LEU:HD23	1:D:149:LEU:HD11	2.02	0.41
1:B:265:GLU:O	1:B:268:VAL:HG22	2.21	0.41
1:C:248:LYS:HD3	1:C:262:GLU:OE2	2.21	0.41
1:B:49:ASN:HB3	1:B:50:PRO:HD2	2.04	0.40
1:B:149:LEU:O	1:B:153:GLY:N	2.54	0.40
1:A:95:TRP:CZ2	1:A:256:LYS:O	2.73	0.40
1:A:169:PRO:O	1:A:170:GLN:C	2.59	0.40
1:C:63:SER:HB3	1:C:185:PRO:HG3	2.02	0.40
1:D:122:ILE:HG22	1:D:123:THR:N	2.35	0.40
1:C:168:LEU:HB3	1:C:169:PRO:HD2	2.02	0.40

All (3) 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:C:308:THR:OG1	1:D:307:ILE:O[11_555]	1.81	0.39
1:A:167:GLN:OE1	1:D:86:LYS:NZ[10_665]	1.95	0.25
1:A:167:GLN:OE1	1:D:86:LYS:HZ3[10_665]	1.49	0.11

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	218/297 (73%)	206 (94%)	12 (6%)	0	100	100
1	B	206/297 (69%)	198 (96%)	8 (4%)	0	100	100
1	C	223/297 (75%)	210 (94%)	11 (5%)	2 (1%)	17	54
1	D	218/297 (73%)	208 (95%)	10 (5%)	0	100	100
All	All	865/1188 (73%)	822 (95%)	41 (5%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	ALA
1	C	127	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	190/259 (73%)	186 (98%)	4 (2%)	53	74
1	B	181/259 (70%)	179 (99%)	2 (1%)	73	85
1	C	192/259 (74%)	190 (99%)	2 (1%)	76	86
1	D	189/259 (73%)	185 (98%)	4 (2%)	53	74
All	All	752/1036 (73%)	740 (98%)	12 (2%)	62	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	PHE
1	A	172	PHE
1	A	174	PHE
1	A	192	THR
1	B	90	LYS
1	B	98	LEU
1	C	75	LEU

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Mol	Chain	Res	Type
1	C	132	LEU
1	D	75	LEU
1	D	174	PHE
1	D	247	PHE
1	D	268	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	230/297 (77%)	-0.10	5 (2%) 62 57	113, 181, 239, 280	0
1	B	222/297 (74%)	-0.13	6 (2%) 54 48	138, 187, 256, 355	0
1	C	233/297 (78%)	-0.10	2 (0%) 84 82	135, 180, 221, 245	0
1	D	230/297 (77%)	-0.16	1 (0%) 92 92	124, 178, 224, 259	0
All	All	915/1188 (77%)	-0.12	14 (1%) 73 70	113, 182, 236, 355	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	VAL	4.4
1	A	154	ASN	3.6
1	A	254	PRO	3.6
1	A	310	ASP	3.1
1	A	194	ASP	3.0
1	C	152	ILE	2.7
1	A	277	THR	2.4
1	B	277	THR	2.4
1	C	83	SER	2.3
1	D	87	VAL	2.1
1	B	307	ILE	2.1
1	B	193	ASP	2.1
1	B	203	LEU	2.1
1	B	217	LEU	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 monosaccharides 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.