



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2020 – 06:06 PM EDT

PDB ID : 7JZJ
Title : Crystal structure demonstrating CTD-CTD interactions of Zaire Ebola virus VP40 dimer
Authors : Norris, M.J.; Bornholdt, Z.A.; Saphire, E.O.
Deposited on : 2020-09-02
Resolution : 2.46 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

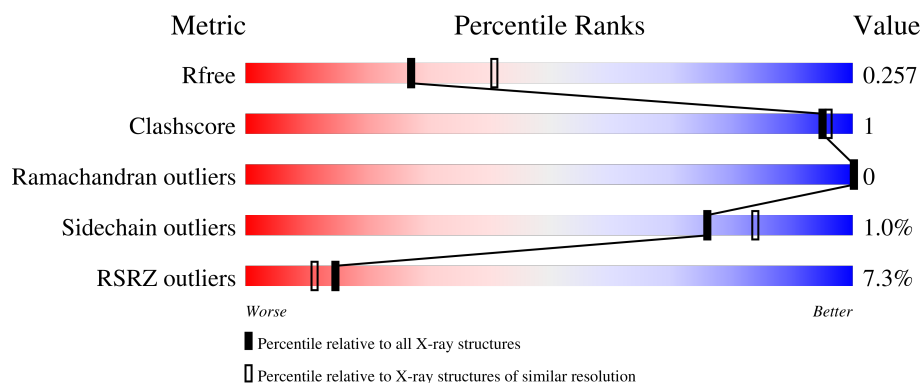
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 $\leq 5\%$. 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	<div> <div>4%</div> <div>80%</div> <div>16%</div> </div>
1	B	297	<div> <div>4%</div> <div>87%</div> <div>10%</div> </div>
1	C	297	<div> <div>8%</div> <div>78%</div> <div>19%</div> </div>
1	D	297	<div> <div>8%</div> <div>80%</div> <div>17%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14511 atoms, of which 7064 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
1	A	249	Total	C	H	N	O	S	0	0	0
			3611	1180	1777	308	339	7			
1	B	267	Total	C	H	N	O	S	0	0	0
			3943	1275	1961	329	370	8			
1	C	240	Total	C	H	N	O	S	0	0	0
			3300	1098	1587	292	316	7			
1	D	246	Total	C	H	N	O	S	0	0	0
			3540	1162	1739	301	330	8			

There are 52 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
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
B	37	HIS	-	expression tag	UNP Q05128

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

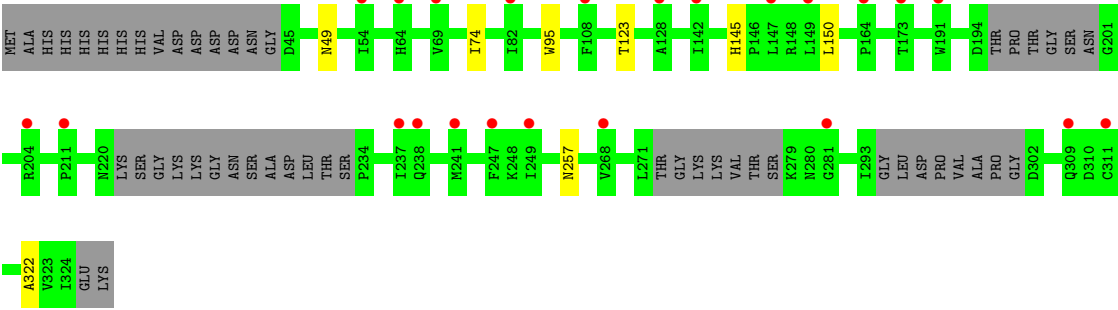
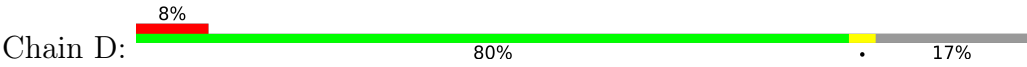
- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	21	Total	O	0	0
			21	21		
3	C	17	Total	O	0	0
			17	17		
3	D	16	Total	O	0	0
			16	16		



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	159.94Å 159.94Å 89.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.17 – 2.46 79.97 – 2.46	Depositor EDS
% Data completeness (in resolution range)	91.7 (46.17-2.46) 91.9 (79.97-2.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.249 , 0.258 0.248 , 0.257	Depositor DCC
R_{free} test set	2191 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14511	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE

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	0.63	0/1880	0.88	0/2582
1	B	0.62	0/2034	0.89	0/2796
1	C	0.66	0/1755	0.89	0/2414
1	D	0.61	0/1847	0.85	0/2541
All	All	0.63	0/7516	0.88	0/10333

There are no bond length outliers.

There are no bond angle outliers.

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	1834	1777	1777	5	0
1	B	1982	1961	1961	5	5
1	C	1713	1587	1589	4	0
1	D	1801	1739	1746	4	5
2	A	16	0	22	1	0
2	B	16	0	22	2	0
2	D	16	0	22	2	0
3	A	15	0	0	0	0
3	B	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	17	0	0	0	0
3	D	16	0	0	0	0
All	All	7447	7064	7139	18	5

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 1.

All (18) 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:95:TRP:CZ3	2:B:401:1PE:H261	2.39	0.58
1:C:249:ILE:HD11	1:C:303:LEU:HD21	1.85	0.57
1:B:291:LYS:HG3	2:B:401:1PE:H142	1.89	0.55
1:D:257:ASN:HB2	2:D:401:1PE:H131	1.90	0.54
1:A:94:ILE:HD12	1:A:163:LEU:CD2	2.39	0.53
1:C:75:LEU:HG	1:C:98:LEU:HD11	1.92	0.52
1:A:219:PRO:O	1:A:220:ASN:C	2.50	0.49
1:D:145:HIS:CE1	1:D:150:LEU:HD12	2.48	0.49
1:A:145:HIS:CE1	1:A:150:LEU:HD12	2.48	0.49
1:C:81:VAL:HB	1:C:89:MET:CB	2.44	0.47
1:B:94:ILE:HD12	1:B:163:LEU:CD2	2.47	0.45
1:B:145:HIS:CE1	1:B:150:LEU:HD12	2.53	0.44
1:D:74:ILE:HG21	1:D:95:TRP:CE2	2.53	0.43
1:B:94:ILE:HD12	1:B:163:LEU:HD23	2.01	0.41
1:D:95:TRP:CZ3	2:D:401:1PE:H222	2.56	0.41
1:A:108:PHE:HE1	1:A:183:THR:HG21	1.86	0.40
1:C:213:LEU:HD11	1:C:293:ILE:HD13	2.04	0.40
1:A:95:TRP:CE3	2:A:401:1PE:H222	2.56	0.40

All (5) 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:274:LYS:NZ	1:D:322:ALA:O[5_554]	1.38	0.82
1:B:274:LYS:CE	1:D:322:ALA:O[5_554]	1.72	0.48
1:B:274:LYS:HZ1	1:D:322:ALA:O[5_554]	1.23	0.37
1:B:274:LYS:HE3	1:D:322:ALA:O[5_554]	1.47	0.13
1:B:274:LYS:HZ2	1:D:322:ALA:O[5_554]	1.48	0.12

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	239/297 (80%)	237 (99%)	2 (1%)	0	100	100
1	B	261/297 (88%)	258 (99%)	3 (1%)	0	100	100
1	C	224/297 (75%)	219 (98%)	5 (2%)	0	100	100
1	D	236/297 (80%)	235 (100%)	1 (0%)	0	100	100
All	All	960/1188 (81%)	949 (99%)	11 (1%)	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	195/259 (75%)	193 (99%)	2 (1%)	76	84
1	B	218/259 (84%)	215 (99%)	3 (1%)	67	77
1	C	171/259 (66%)	170 (99%)	1 (1%)	86	91
1	D	191/259 (74%)	189 (99%)	2 (1%)	76	84
All	All	775/1036 (75%)	767 (99%)	8 (1%)	76	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	SER
1	A	287	VAL

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Mol	Chain	Res	Type
1	B	65	THR
1	B	296	ASP
1	B	313	THR
1	C	119	SER
1	D	49	ASN
1	D	123	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	124	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	1PE	B	401	-	15,15,15	0.37	0	14,14,14	0.42	0
2	1PE	A	401	-	15,15,15	0.55	0	14,14,14	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1PE	D	401	-	15,15,15	0.40	0	14,14,14	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1PE	B	401	-	-	8/13/13/13	-
2	1PE	A	401	-	-	5/13/13/13	-
2	1PE	D	401	-	-	5/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	1PE	C13-C23-OH3-C22
2	D	401	1PE	C14-C24-OH4-C13
2	A	401	1PE	OH5-C14-C24-OH4
2	A	401	1PE	OH7-C16-C26-OH6
2	B	401	1PE	OH5-C14-C24-OH4
2	D	401	1PE	OH5-C14-C24-OH4
2	A	401	1PE	OH4-C13-C23-OH3
2	B	401	1PE	C14-C24-OH4-C13
2	A	401	1PE	OH6-C15-C25-OH5
2	D	401	1PE	C12-C22-OH3-C23
2	A	401	1PE	C23-C13-OH4-C24
2	B	401	1PE	C24-C14-OH5-C25
2	B	401	1PE	OH6-C15-C25-OH5
2	D	401	1PE	C16-C26-OH6-C15
2	B	401	1PE	OH7-C16-C26-OH6
2	B	401	1PE	C16-C26-OH6-C15
2	B	401	1PE	OH4-C13-C23-OH3
2	D	401	1PE	OH7-C16-C26-OH6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	1PE	2	0
2	A	401	1PE	1	0
2	D	401	1PE	2	0

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

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	249/297 (83%)	0.68	12 (4%) 30 28	59, 90, 130, 156	0
1	B	267/297 (89%)	0.67	13 (4%) 29 27	51, 77, 130, 154	0
1	C	240/297 (80%)	0.72	25 (10%) 6 4	60, 92, 150, 172	0
1	D	246/297 (82%)	0.75	23 (9%) 8 5	61, 90, 147, 179	0
All	All	1002/1188 (84%)	0.70	73 (7%) 15 11	51, 88, 140, 179	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	TRP	4.2
1	B	200	ASN	4.0
1	C	151	ARG	3.9
1	D	238	GLN	3.6
1	C	132	LEU	3.5
1	C	252	ILE	3.5
1	D	268	VAL	3.4
1	A	138	LEU	3.3
1	B	209	PHE	3.3
1	C	126	GLY	3.3
1	A	209	PHE	3.2
1	B	203	LEU	3.2
1	C	54	ILE	3.1
1	D	69	VAL	3.1
1	C	87	VAL	3.0
1	D	241	MET	3.0
1	C	312	ASP	2.9
1	B	315	HIS	2.9
1	C	268	VAL	2.9
1	D	309	GLN	2.8
1	D	249	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	173	THR	2.8
1	D	247	PHE	2.8
1	C	174	PHE	2.7
1	A	111	THR	2.7
1	A	284	ILE	2.7
1	B	297	PRO	2.7
1	C	162	VAL	2.6
1	D	64	HIS	2.6
1	C	264	PRO	2.6
1	A	218	LEU	2.6
1	D	82	ILE	2.6
1	C	160	GLU	2.6
1	C	189	ALA	2.5
1	D	54	ILE	2.5
1	B	158	LEU	2.5
1	C	241	MET	2.4
1	D	147	LEU	2.4
1	C	93	PRO	2.4
1	A	175	ASP	2.4
1	D	142	ILE	2.4
1	A	258	ILE	2.3
1	B	92	ILE	2.3
1	C	204	ARG	2.3
1	D	108	PHE	2.3
1	B	69	VAL	2.3
1	D	311	CYS	2.3
1	C	283	PRO	2.3
1	C	258	ILE	2.3
1	D	237	ILE	2.2
1	C	146	PRO	2.2
1	C	282	GLN	2.2
1	C	203	LEU	2.2
1	D	164	PRO	2.2
1	A	142	ILE	2.2
1	A	207	ILE	2.2
1	D	281	GLY	2.1
1	B	197	THR	2.1
1	B	266	THR	2.1
1	A	293	ILE	2.1
1	D	149	LEU	2.1
1	A	60	ASP	2.1
1	C	306	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	284	ILE	2.1
1	C	307	ILE	2.1
1	C	157	PHE	2.1
1	C	74	ILE	2.1
1	D	204	ARG	2.1
1	D	128	ALA	2.0
1	A	216	ILE	2.0
1	B	217	LEU	2.0
1	B	258	ILE	2.0
1	D	211	PRO	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](#)

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(\AA^2)	Q<0.9
2	1PE	A	401	16/16	0.77	0.20	102,103,105,105	0
2	1PE	D	401	16/16	0.84	0.23	114,117,119,119	0
2	1PE	B	401	16/16	0.96	0.15	67,71,73,74	16

6.5 Other polymers [i](#)

There are no such residues in this entry.