



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:58 pm BST

PDB ID : 4UWX
Title : Structure of liprin-alpha3 in complex with mDia1 Diaphanous- inhibitory domain
Authors : Brenig, J.; de Boor, S.; Knyphausen, P.; Kuhlmann, N.; Wroblowski, S.; Baldus, L.; Scislowski, L.; Artz, O.; Trauschies, P.; Baumann, U.; Neundorf, I.; Lammers, M.
Deposited on : 2014-08-15
Resolution : 1.65 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 : 2.11
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

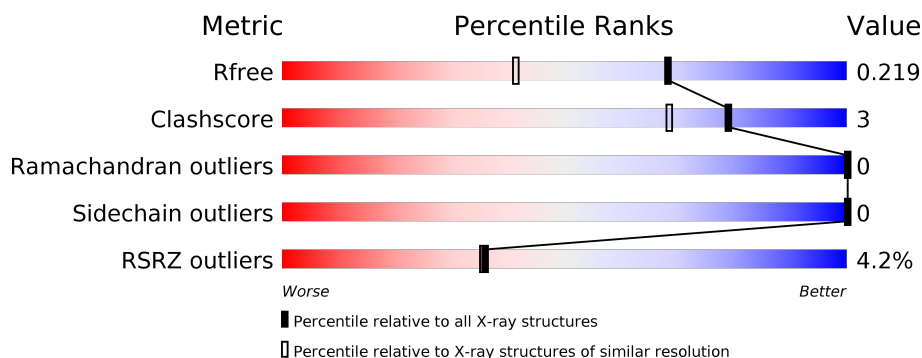
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	239	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	239	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
2	C	21	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>19%</div> <div>29%</div> </div> </div>
2	D	21	<div> <div>10%</div> <div> <div></div> <div>52%</div> <div>24%</div> <div>24%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4337 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 PROTEIN DIAPHANOUS HOMOLOG 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1859	1167	318	356	18			
1	B	230	Total	C	N	O	S	0	0	0
			1829	1148	314	349	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLY	-	expression tag	UNP O08808
A	132	SER	-	expression tag	UNP O08808
A	133	GLU	-	expression tag	UNP O08808
A	134	PHE	-	expression tag	UNP O08808
B	131	GLY	-	expression tag	UNP O08808
B	132	SER	-	expression tag	UNP O08808
B	133	GLU	-	expression tag	UNP O08808
B	134	PHE	-	expression tag	UNP O08808

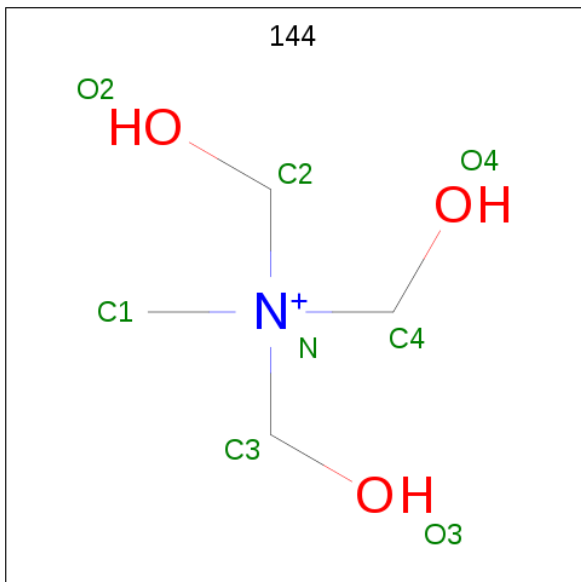
- Molecule 2 is a protein called LIPRIN-ALPHA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	0	0	0
			115	69	25	20	1			
2	D	16	Total	C	N	O	S	0	0	0
			123	75	26	21	1			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (three-letter code: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

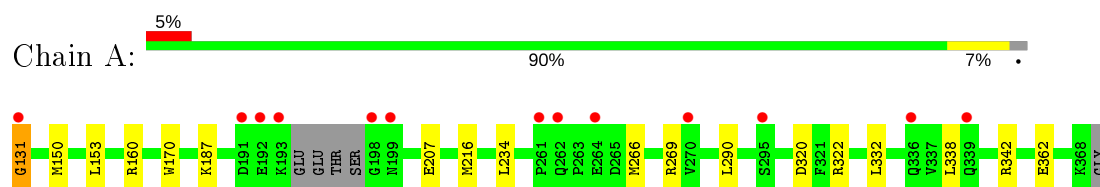
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	185	Total	O	0	0
			185	185		
5	B	189	Total	O	0	0
			189	189		
5	C	6	Total	O	0	0
			6	6		
5	D	13	Total	O	0	0
			13	13		

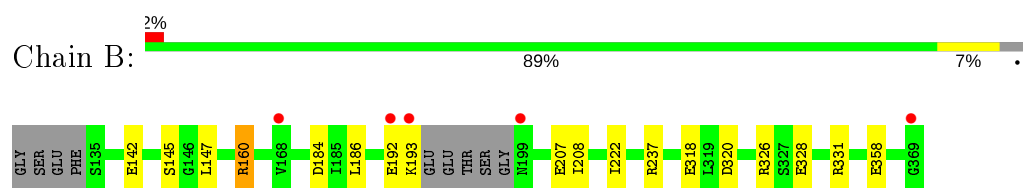
3 Residue-property plots [i](#)

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: PROTEIN DIAPHANOUS HOMOLOG 1



• Molecule 1: PROTEIN DIAPHANOUS HOMOLOG 1



• Molecule 2: LIPRIN-ALPHA-3



• Molecule 2: LIPRIN-ALPHA-3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.09 Å 49.38 Å 106.37 Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	32.32 – 1.65 32.30 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.32-1.65) 99.7 (32.30-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.65 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.210 0.187 , 0.219	Depositor DCC
R_{free} test set	3777 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4337	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 7.61% 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: NI, 144

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	1.06	5/1882 (0.3%)	1.04	7/2530 (0.3%)
1	B	1.01	2/1851 (0.1%)	1.08	12/2489 (0.5%)
2	C	0.84	0/115	1.47	3/153 (2.0%)
2	D	1.20	1/123 (0.8%)	1.90	5/164 (3.0%)
All	All	1.04	8/3971 (0.2%)	1.11	27/5336 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	MET	SD-CE	-8.92	1.27	1.77
1	A	131	GLY	C-O	7.83	1.36	1.23
1	B	160	ARG	CD-NE	-7.31	1.34	1.46
1	B	318	GLU	CG-CD	6.15	1.61	1.51
2	D	574	GLU	CG-CD	5.70	1.60	1.51
1	A	207	GLU	CD-OE1	-5.45	1.19	1.25
1	A	362	GLU	CD-OE2	5.16	1.31	1.25
1	A	269	ARG	CD-NE	-5.07	1.37	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	572	ARG	NE-CZ-NH1	14.12	127.36	120.30
1	A	216	MET	CG-SD-CE	-10.92	82.73	100.20
1	B	160	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	B	331	ARG	NE-CZ-NH1	10.15	125.37	120.30
2	C	572	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	B	160	ARG	NE-CZ-NH1	9.35	124.98	120.30
2	C	572	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	269	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	B	326	ARG	NE-CZ-NH1	8.33	124.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	D	572	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	237	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	331	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	D	576	MET	CG-SD-CE	-6.34	90.06	100.20
1	A	320	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	269	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	326	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	160	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	322	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	331	ARG	CD-NE-CZ	5.30	131.01	123.60
2	D	569	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	320	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	320	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	184	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	237	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	C	575	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	D	572	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1859	0	1872	8	0
1	B	1829	0	1849	11	0
2	C	115	0	122	1	0
2	D	123	0	133	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	9	0	0
4	B	8	0	10	1	0
5	A	185	0	0	5	3
5	B	189	0	0	5	3
5	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	13	0	0	0	0
All	All	4337	0	3995	22	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 3.

All (22) 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:A:266:MET:SD	5:A:2120:HOH:O	1.91	1.25
1:B:145:SER:HB3	5:B:2002:HOH:O	1.75	0.85
5:A:2160:HOH:O	4:B:1371:144:O3	2.09	0.68
1:B:145:SER:CB	5:B:2002:HOH:O	2.42	0.59
5:B:2175:HOH:O	2:D:575:ARG:NH1	2.37	0.53
1:A:131:GLY:N	5:A:2001:HOH:O	2.42	0.53
1:B:160:ARG:HD2	1:B:207:GLU:OE2	2.10	0.52
1:B:192:GLU:O	1:B:193:LYS:HG3	2.12	0.49
1:A:187:LYS:HE2	1:A:234:LEU:HD11	1.93	0.49
1:B:142:GLU:HG3	1:B:147:LEU:HD21	1.97	0.46
1:A:290:LEU:HD22	1:A:332:LEU:HG	1.98	0.46
1:B:192:GLU:O	1:B:193:LYS:CB	2.66	0.43
1:B:328:GLU:OE2	5:B:2155:HOH:O	2.21	0.42
1:B:186:LEU:HG	1:B:208:ILE:HG21	2.02	0.42
1:A:338:LEU:O	1:A:342:ARG:HG3	2.20	0.41
1:A:150:MET:CE	5:A:2023:HOH:O	2.67	0.41
1:B:358:GLU:OE1	2:D:575:ARG:NH2	2.51	0.41
1:A:131:GLY:HA2	1:A:170:TRP:CD1	2.56	0.40
1:B:222:ILE:HD11	5:B:2061:HOH:O	2.21	0.40
1:A:153:LEU:HD21	5:A:2025:HOH:O	2.22	0.40
1:B:142:GLU:CG	1:B:147:LEU:HD21	2.51	0.40
2:C:567:THR:N	2:C:570:SER:HG	2.19	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)
5:A:2025:HOH:O	5:B:2114:HOH:O[3_545]	1.80	0.40
5:A:2023:HOH:O	5:B:2125:HOH:O[3_545]	1.92	0.28
5:A:2176:HOH:O	5:B:2008:HOH:O[2_758]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	230/239 (96%)	228 (99%)	2 (1%)	0	100	100
1	B	226/239 (95%)	225 (100%)	1 (0%)	0	100	100
2	C	13/21 (62%)	13 (100%)	0	0	100	100
2	D	14/21 (67%)	14 (100%)	0	0	100	100
All	All	483/520 (93%)	480 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	208/212 (98%)	208 (100%)	0	100	100
1	B	205/212 (97%)	205 (100%)	0	100	100
2	C	11/15 (73%)	11 (100%)	0	100	100
2	D	12/15 (80%)	12 (100%)	0	100	100
All	All	436/454 (96%)	436 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	144	A	1370	3	1,7,7	0.13	0	3,9,9	1.55	1 (33%)
4	144	B	1371	3	1,7,7	0.93	0	3,9,9	0.43	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
4	144	A	1370	3	-	0/0/9/9	-
4	144	B	1371	3	-	0/0/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1370	144	C1-N-C3	-2.50	92.77	108.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1371	144	1	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	234/239 (97%)	-0.01	13 (5%) 24 23	14, 24, 47, 70	0
1	B	230/239 (96%)	-0.06	5 (2%) 62 63	14, 23, 43, 75	0
2	C	15/21 (71%)	0.48	1 (6%) 17 16	29, 40, 46, 52	0
2	D	16/21 (76%)	0.21	2 (12%) 3 3	20, 24, 43, 66	0
All	All	495/520 (95%)	-0.01	21 (4%) 36 35	14, 24, 45, 75	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	6.5
2	D	582	LEU	5.5
1	B	193	LYS	4.8
1	B	192	GLU	4.0
1	A	262	GLN	3.7
1	A	295	SER	3.2
1	B	199	ASN	3.1
2	C	567	THR	2.9
1	A	199	ASN	2.9
1	B	369	GLY	2.8
1	A	261	PRO	2.8
1	A	339	GLN	2.7
1	A	192	GLU	2.6
1	A	193	LYS	2.5
2	D	581	ALA	2.4
1	A	264	GLU	2.4
1	A	336	GLN	2.4
1	A	131	GLY	2.3
1	B	168	VAL	2.3
1	A	191	ASP	2.2
1	A	270	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](#)

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
4	144	B	1371	8/8	0.86	0.13	24,29,35,50	0
4	144	A	1370	8/8	0.87	0.13	25,28,35,41	0
3	NI	A	1369	1/1	0.99	0.02	23,23,23,23	0
3	NI	B	1370	1/1	1.00	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.