



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:52 AM BST

PDB ID : 6B4F
Title : Crystal structure of human Gle1 CTD-Nup42 GBM complex
Authors : Lin, D.H.; Correia, A.R.; Cai, S.W.; Huber, F.M.; Jette, C.A.; Hoelz, A.
Deposited on : 2017-09-26
Resolution : 2.81 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 : 2.13.1
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) : 2.13.1

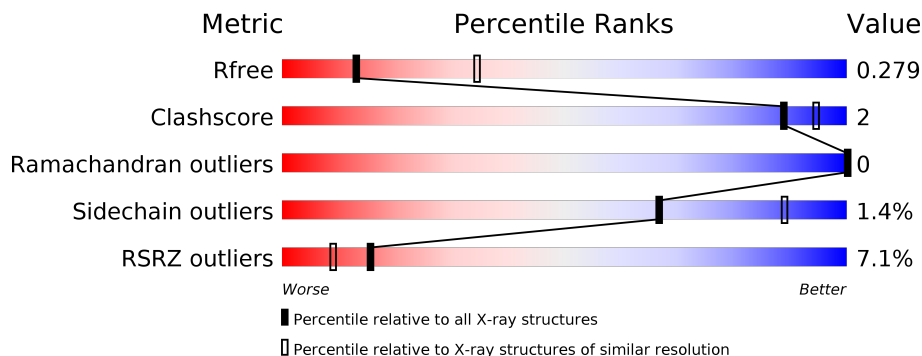
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	317	
1	B	317	
2	C	50	
2	D	50	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11711 atoms, of which 5876 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 Nucleoporin GLE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	B	315	5100	1640	2559	432	454	15	0	0	0
1	A	313	5068	1632	2541	429	451	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	382	MET	-	initiating methionine	UNP Q53GS7
A	382	MET	-	initiating methionine	UNP Q53GS7

- Molecule 2 is a protein called Nucleoporin like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	45	751	239	388	57	67	0	0	0
2	D	45	751	239	388	57	67	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

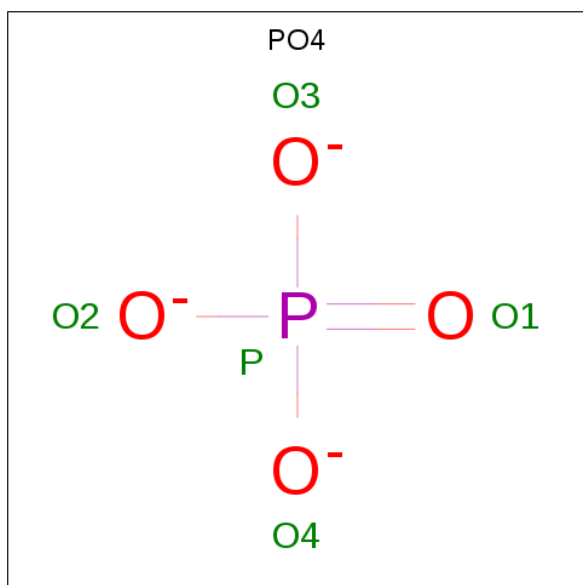
Chain	Residue	Modelled	Actual	Comment	Reference
C	374	GLY	-	expression tag	UNP Q3B7J4
C	375	PRO	-	expression tag	UNP Q3B7J4
C	376	SER	-	expression tag	UNP Q3B7J4
C	377	GLY	-	expression tag	UNP Q3B7J4
C	378	SER	-	expression tag	UNP Q3B7J4
C	379	ILE	-	expression tag	UNP Q3B7J4
C	380	ILE	-	expression tag	UNP Q3B7J4
D	374	GLY	-	expression tag	UNP Q3B7J4
D	375	PRO	-	expression tag	UNP Q3B7J4
D	376	SER	-	expression tag	UNP Q3B7J4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	377	GLY	-	expression tag	UNP Q3B7J4
D	378	SER	-	expression tag	UNP Q3B7J4
D	379	ILE	-	expression tag	UNP Q3B7J4
D	380	ILE	-	expression tag	UNP Q3B7J4

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	12	Total O 12 12	0	0

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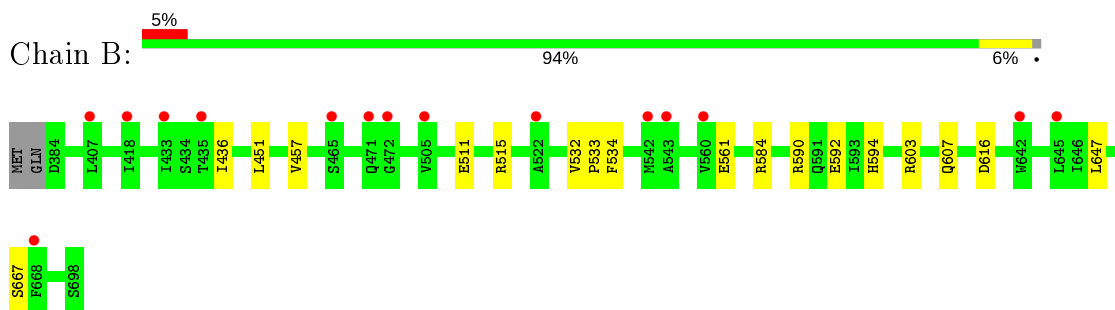
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		

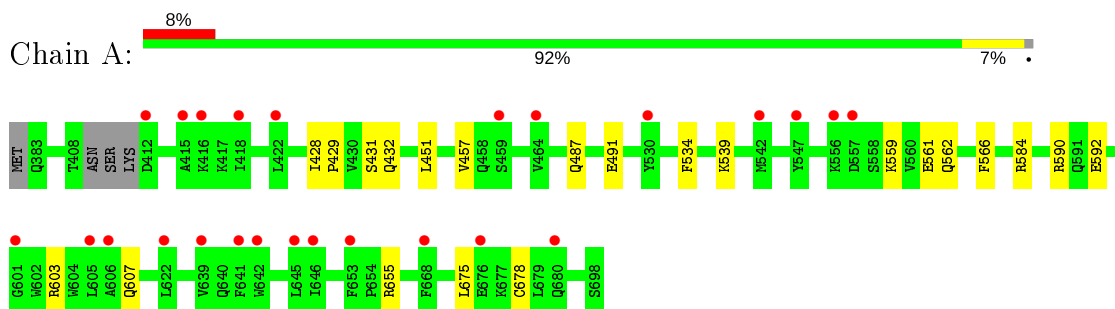
3 Residue-property plots [i](#)

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.

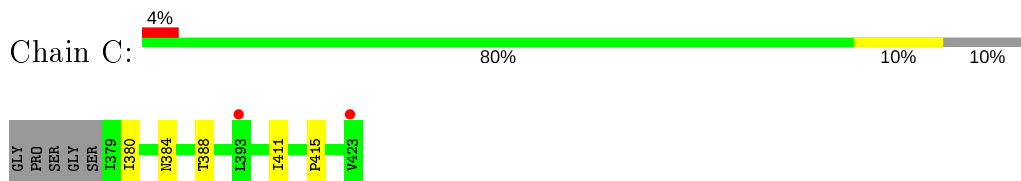
- Molecule 1: Nucleoporin GLE1



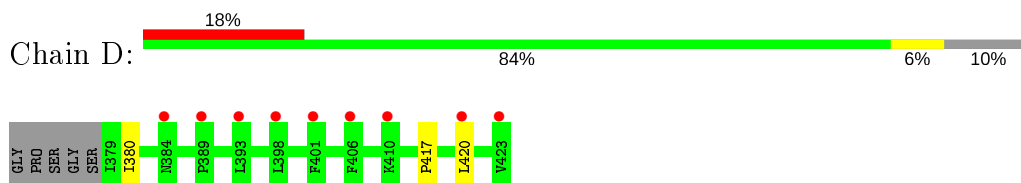
- Molecule 1: Nucleoporin GLE1



- Molecule 2: Nucleoporin like 2



- Molecule 2: Nucleoporin like 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.66Å 69.71Å 93.57Å 90.00° 90.66° 90.00°	Depositor
Resolution (Å)	46.78 – 2.81 46.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	79.9 (46.78-2.81) 96.2 (46.78-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.245 , 0.274 0.252 , 0.279	Depositor DCC
R_{free} test set	1328 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtrriage
Anisotropy	0.482	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.176 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11711	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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: PO4, CL

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	0.26	0/2589	0.41	0/3493
1	B	0.26	0/2604	0.42	0/3514
2	C	0.29	0/370	0.47	0/501
2	D	0.28	0/370	0.50	0/501
All	All	0.26	0/5933	0.43	0/8009

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	2527	2541	2541	10	0
1	B	2541	2559	2558	8	0
2	C	363	388	388	4	0
2	D	363	388	388	2	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	17	0	0	0	0
5	B	12	0	0	0	0
All	All	5835	5876	5875	22	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 2.

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:487:GLN:NE2	1:A:491:GLU:OE1	2.30	0.65
1:A:561:GLU:OE1	1:A:566:PHE:N	2.37	0.56
1:B:590:ARG:NH2	1:B:592:GLU:OE1	2.41	0.52
1:A:584:ARG:NH2	1:A:592:GLU:O	2.46	0.48
1:B:603:ARG:O	1:B:607:GLN:N	2.45	0.48
1:B:647:LEU:HD23	2:C:411:ILE:HD11	1.95	0.48
1:B:594:HIS:O	2:C:384:ASN:ND2	2.48	0.47
1:A:561:GLU:HG2	1:A:562:GLN:N	2.30	0.46
1:A:675:LEU:O	1:A:678:CYS:N	2.49	0.46
1:B:451:LEU:HB2	1:B:457:VAL:HG21	1.97	0.46
1:B:511:GLU:OE2	1:B:584:ARG:NH2	2.50	0.45
1:A:590:ARG:NH2	1:A:592:GLU:OE2	2.51	0.44
2:C:380:ILE:N	2:C:380:ILE:HD12	2.32	0.43
1:A:428:ILE:O	1:A:431:SER:OG	2.28	0.43
2:D:417:PRO:HG2	2:D:420:LEU:HD12	2.00	0.43
1:A:603:ARG:O	1:A:607:GLN:N	2.49	0.42
2:D:380:ILE:N	2:D:380:ILE:HD12	2.33	0.42
1:A:451:LEU:HB2	1:A:457:VAL:HG21	2.03	0.41
1:B:532:VAL:N	1:B:533:PRO:HA	2.35	0.41
1:A:428:ILE:N	1:A:429:PRO:CD	2.84	0.41
2:C:388:THR:OG1	2:C:415:PRO:O	2.37	0.41
1:B:616:ASP:OD1	1:B:667:SER:OG	2.26	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	309/317 (98%)	295 (96%)	14 (4%)	0	100	100
1	B	313/317 (99%)	297 (95%)	16 (5%)	0	100	100
2	C	43/50 (86%)	41 (95%)	2 (5%)	0	100	100
2	D	43/50 (86%)	41 (95%)	2 (5%)	0	100	100
All	All	708/734 (96%)	674 (95%)	34 (5%)	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	275/279 (99%)	270 (98%)	5 (2%)	59	85
1	B	277/279 (99%)	273 (99%)	4 (1%)	67	89
2	C	43/46 (94%)	43 (100%)	0	100	100
2	D	43/46 (94%)	43 (100%)	0	100	100
All	All	638/650 (98%)	629 (99%)	9 (1%)	67	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	436	ILE
1	B	515	ARG
1	B	534	PHE
1	B	561	GLU
1	A	432	GLN
1	A	534	PHE
1	A	539	LYS
1	A	559	LYS
1	A	655	ARG

Some 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](#)

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	$\# Z > 2$
3	PO4	A	702	-	4,4,4	0.90	0	6,6,6	0.37	0
3	PO4	A	701	-	4,4,4	0.84	0	6,6,6	0.41	0

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

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	313/317 (98%)	0.68	25 (7%) 12 7	19, 58, 107, 129	0
1	B	315/317 (99%)	0.57	15 (4%) 30 21	18, 44, 103, 127	0
2	C	45/50 (90%)	0.51	2 (4%) 34 24	28, 47, 76, 147	0
2	D	45/50 (90%)	1.07	9 (20%) 1 0	68, 97, 123, 178	0
All	All	718/734 (97%)	0.64	51 (7%) 16 9	18, 53, 109, 178	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	639	VAL	5.6
1	A	642	TRP	5.4
1	A	645	LEU	5.3
1	A	641	PHE	5.2
1	A	542	MET	5.0
1	B	642	TRP	4.9
1	A	668	PHE	4.7
2	C	423	VAL	4.6
2	D	423	VAL	4.6
1	B	465	SER	4.5
2	D	420	LEU	4.4
1	A	418	ILE	4.0
2	D	393	LEU	3.8
1	A	415	ALA	3.8
1	A	556	LYS	3.6
1	B	472	GLY	3.5
1	B	645	LEU	3.4
1	A	605	LEU	3.2
1	A	459	SER	3.0
2	D	389	PRO	3.0
1	A	622	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	464	VAL	2.9
1	A	416	LYS	2.9
1	B	433	ILE	2.9
2	D	384	ASN	2.8
1	B	543	ALA	2.7
1	A	557	ASP	2.6
2	D	398	LEU	2.6
1	B	418	ILE	2.6
2	D	401	PHE	2.5
2	D	406	PHE	2.5
1	B	668	PHE	2.4
1	B	560	VAL	2.4
1	B	505	VAL	2.4
1	B	542	MET	2.4
1	B	471	GLN	2.3
1	A	422	LEU	2.3
1	B	435	THR	2.3
1	A	601	GLY	2.3
2	D	410	LYS	2.3
1	A	646	ILE	2.3
1	A	412	ASP	2.2
1	A	606	ALA	2.2
1	A	680	GLN	2.2
1	A	653	PHE	2.2
1	A	547	TYR	2.1
2	C	393	LEU	2.1
1	A	530	TYR	2.1
1	A	676	GLU	2.1
1	B	407	LEU	2.0
1	B	522	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 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(Å ²)	Q<0.9
4	CL	A	703	1/1	0.91	0.29	56,56,56,56	0
3	PO4	A	701	5/5	0.91	0.11	49,52,77,89	0
3	PO4	A	702	5/5	0.95	0.20	54,63,75,79	0
4	CL	C	501	1/1	0.95	0.30	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.