



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:45 AM UTC

PDB ID : 8I16 / pdb_00008i16
Title : Crystal structure of the selenomethionine (SeMet)-derived Cas12g (D513A) mutant
Authors : Zhang, B.; Chen, J.; Ye, Y.M.; OuYang, S.Y.
Deposited on : 2023-01-12
Resolution : 2.24 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

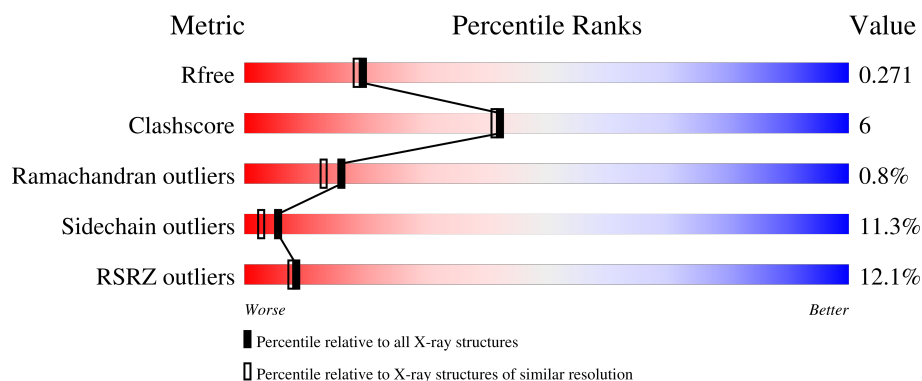
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	775	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5382 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 Cas12g.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	Se	0	0	0
			5338	3389	1008	927	9	5			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

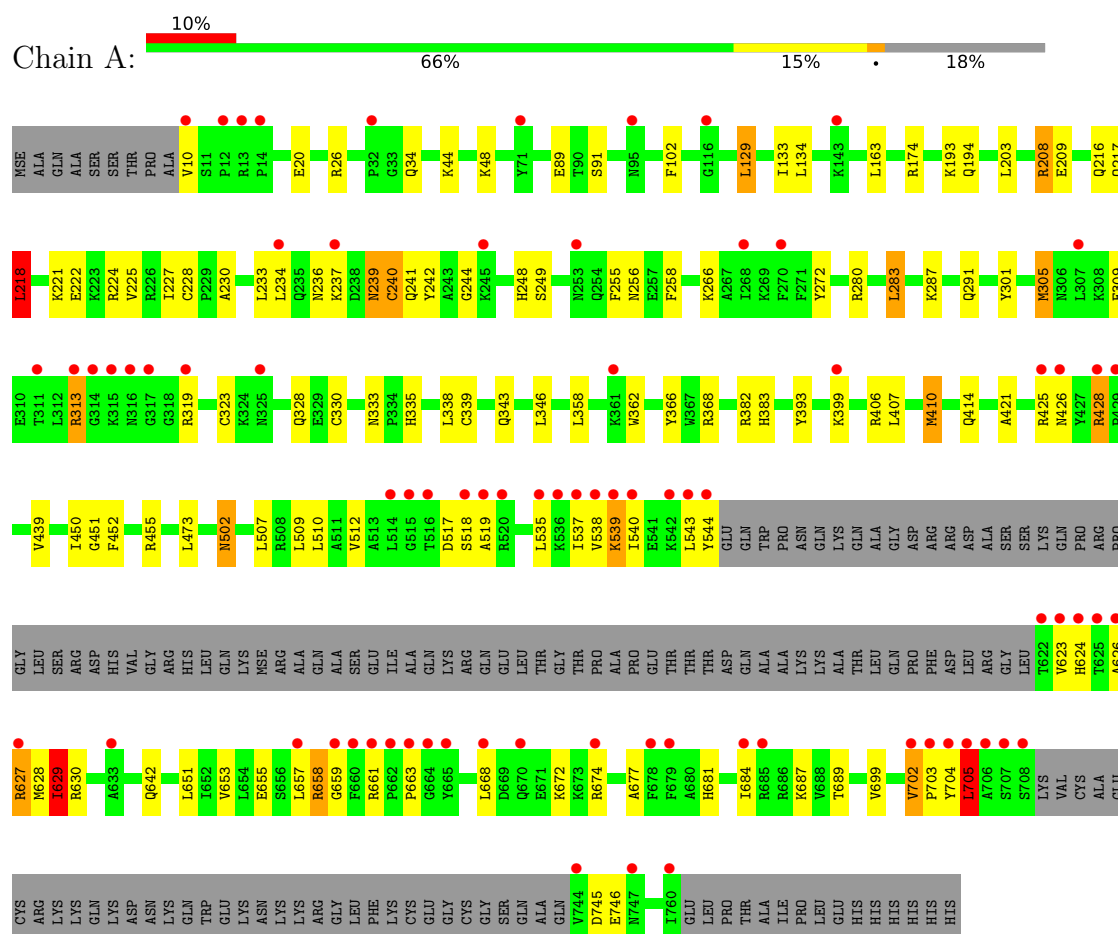
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		

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: Cas12g



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.07Å 95.12Å 167.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.86 – 2.24 62.86 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (62.86-2.24) 99.3 (62.86-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.268 0.231 , 0.271	Depositor DCC
R_{free} test set	2416 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5382	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	2/5467 (0.0%)	1.43	8/7353 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	ARG	C-O	6.87	1.32	1.24
1	A	208	ARG	C-O	-5.14	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	LEU	CA-C-N	-8.51	110.62	122.87
1	A	218	LEU	C-N-CA	-8.51	110.62	122.87
1	A	239	ASN	CA-C-O	-7.25	111.97	119.51
1	A	629	ILE	N-CA-C	-6.81	104.36	111.58
1	A	626	ALA	N-CA-C	-6.69	99.59	109.62
1	A	102	PHE	N-CA-C	-5.63	105.23	111.36
1	A	272	TYR	CA-C-N	5.51	127.61	120.44
1	A	272	TYR	C-N-CA	5.51	127.61	120.44

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	5338	0	5324	67	0
2	A	2	0	0	0	0
3	A	42	0	0	0	0
All	All	5382	0	5324	67	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 6.

All (67) 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:255:PHE:HA	1:A:305:MSE:HE1	1.31	1.12
1:A:702:VAL:HG12	1:A:703:PRO:HD2	1.22	1.11
1:A:702:VAL:HG12	1:A:703:PRO:CD	1.96	0.94
1:A:627:ARG:HH21	1:A:627:ARG:HG3	1.39	0.86
1:A:627:ARG:O	1:A:627:ARG:NH2	2.09	0.86
1:A:255:PHE:HA	1:A:305:MSE:CE	2.04	0.85
1:A:658:ARG:HG3	1:A:704:TYR:CE2	2.14	0.82
1:A:255:PHE:CA	1:A:305:MSE:HE1	2.09	0.81
1:A:26:ARG:HD3	1:A:421:ALA:O	1.81	0.81
1:A:627:ARG:HG3	1:A:627:ARG:NH2	1.97	0.75
1:A:240:CYS:SG	1:A:242:TYR:N	2.59	0.70
1:A:228:CYS:SG	1:A:240:CYS:HA	2.31	0.69
1:A:681:HIS:O	1:A:684:ILE:HG22	1.92	0.69
1:A:702:VAL:CG1	1:A:703:PRO:CD	2.72	0.67
1:A:702:VAL:CG1	1:A:703:PRO:HD2	2.13	0.66
1:A:629:ILE:HD13	1:A:629:ILE:N	2.12	0.63
1:A:407:LEU:HB2	1:A:410:MSE:HE3	1.81	0.61
1:A:657:LEU:HD21	1:A:677:ALA:HB1	1.82	0.61
1:A:233:LEU:O	1:A:343:GLN:NE2	2.34	0.61
1:A:217:GLN:C	1:A:218:LEU:O	2.42	0.59
1:A:248:HIS:ND1	1:A:330:CYS:HB2	2.17	0.59
1:A:323:CYS:SG	1:A:330:CYS:HA	2.42	0.59
1:A:20:GLU:O	1:A:455:ARG:HG3	2.04	0.58
1:A:283:LEU:HD22	1:A:291:GLN:HG2	1.86	0.57
1:A:248:HIS:CE1	1:A:328:GLN:O	2.59	0.55
1:A:208:ARG:HD3	1:A:362:TRP:CE2	2.40	0.55
1:A:224:ARG:HB3	1:A:663:PRO:HG3	1.89	0.55
1:A:519:ALA:HB1	1:A:535:LEU:O	2.07	0.55
1:A:428:ARG:NE	1:A:428:ARG:HA	2.22	0.54
1:A:653:VAL:HG13	1:A:702:VAL:CG2	2.39	0.53
1:A:502:ASN:C	1:A:502:ASN:HD22	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:VAL:CG1	1:A:702:VAL:CG2	2.89	0.51
1:A:658:ARG:HA	1:A:704:TYR:CG	2.46	0.50
1:A:309:GLU:OE2	1:A:313:ARG:NH1	2.45	0.49
1:A:216:GLN:O	1:A:218:LEU:O	2.31	0.49
1:A:627:ARG:HH21	1:A:627:ARG:CG	2.14	0.49
1:A:225:VAL:HG12	1:A:227:ILE:HG13	1.94	0.49
1:A:335:HIS:HB3	1:A:339:CYS:HB2	1.96	0.48
1:A:539:LYS:HA	1:A:539:LYS:HE2	1.96	0.47
1:A:240:CYS:SG	1:A:242:TYR:HB2	2.55	0.46
1:A:509:LEU:C	1:A:509:LEU:HD23	2.40	0.46
1:A:629:ILE:N	1:A:629:ILE:CD1	2.79	0.45
1:A:330:CYS:SG	1:A:333:ASN:HB2	2.56	0.45
1:A:705:LEU:HD12	1:A:705:LEU:HA	1.82	0.45
1:A:657:LEU:HD12	1:A:657:LEU:HA	1.85	0.45
1:A:240:CYS:HG	1:A:242:TYR:H	1.61	0.44
1:A:507:LEU:C	1:A:507:LEU:HD23	2.42	0.44
1:A:406:ARG:HG3	1:A:410:MSE:HG2	1.98	0.44
1:A:439:VAL:HA	1:A:451:GLY:O	2.18	0.44
1:A:258:PHE:HB2	1:A:305:MSE:HE2	2.00	0.43
1:A:230:ALA:HB1	1:A:346:LEU:HD13	2.01	0.43
1:A:509:LEU:HA	1:A:651:LEU:O	2.18	0.43
1:A:630:ARG:HE	1:A:630:ARG:HB2	1.68	0.43
1:A:240:CYS:SG	1:A:241:GLN:N	2.92	0.43
1:A:382:ARG:O	1:A:383:HIS:CG	2.72	0.43
1:A:627:ARG:HG3	1:A:627:ARG:O	2.18	0.42
1:A:129:LEU:HD22	1:A:133:ILE:CD1	2.49	0.42
1:A:450:ILE:HD12	1:A:452:PHE:CZ	2.55	0.42
1:A:255:PHE:N	1:A:305:MSE:HE1	2.35	0.42
1:A:393:TYR:HA	1:A:406:ARG:HB3	2.02	0.42
1:A:228:CYS:HB2	1:A:233:LEU:HD13	2.01	0.41
1:A:193:LYS:HG3	1:A:366:TYR:HB3	2.02	0.41
1:A:689:THR:HA	1:A:699:VAL:HG21	2.03	0.41
1:A:655:GLU:OE2	1:A:705:LEU:HB2	2.20	0.40
1:A:244:GLY:HA3	1:A:248:HIS:O	2.21	0.40
1:A:258:PHE:CE1	1:A:301:TYR:HA	2.57	0.40
1:A:230:ALA:HB1	1:A:346:LEU:CD1	2.51	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	633/775 (82%)	603 (95%)	25 (4%)	5 (1%)	16 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	LEU
1	A	518	SER
1	A	668	LEU
1	A	705	LEU
1	A	659	GLY

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	559/665 (84%)	496 (89%)	63 (11%)	5 3

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	34	GLN
1	A	44	LYS
1	A	48	LYS
1	A	89	GLU
1	A	91	SER

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Mol	Chain	Res	Type
1	A	129	LEU
1	A	134	LEU
1	A	163	LEU
1	A	194	GLN
1	A	203	LEU
1	A	209	GLU
1	A	221	LYS
1	A	222	GLU
1	A	234	LEU
1	A	236	ASN
1	A	237	LYS
1	A	239	ASN
1	A	240	CYS
1	A	249	SER
1	A	256	ASN
1	A	266	LYS
1	A	280	ARG
1	A	283	LEU
1	A	287	LYS
1	A	305	MSE
1	A	313	ARG
1	A	319	ARG
1	A	338	LEU
1	A	358	LEU
1	A	368	ARG
1	A	399	LYS
1	A	410	MSE
1	A	414	GLN
1	A	425	ARG
1	A	426	ASN
1	A	428	ARG
1	A	473	LEU
1	A	502	ASN
1	A	510	LEU
1	A	512	VAL
1	A	517	ASP
1	A	537	ILE
1	A	538	VAL
1	A	539	LYS
1	A	540	ILE
1	A	543	LEU
1	A	544	TYR

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Mol	Chain	Res	Type
1	A	623	VAL
1	A	624	HIS
1	A	627	ARG
1	A	628	MSE
1	A	629	ILE
1	A	642	GLN
1	A	658	ARG
1	A	661	ARG
1	A	672	LYS
1	A	674	ARG
1	A	687	LYS
1	A	702	VAL
1	A	705	LEU
1	A	745	ASP
1	A	746	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	239	ASN
1	A	241	GLN
1	A	254	GLN
1	A	264	GLN
1	A	341	GLN
1	A	343	GLN
1	A	344	GLN
1	A	430	GLN
1	A	485	GLN
1	A	502	ASN
1	A	505	GLN
1	A	636	ASN
1	A	639	GLN
1	A	670	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	634/775 (81%)	0.80	77 (12%) 8 8	35, 60, 129, 172	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	623	VAL	6.7
1	A	10	VAL	6.6
1	A	540	ILE	6.5
1	A	626	ALA	6.0
1	A	665	TYR	5.8
1	A	760	ILE	5.6
1	A	12	PRO	5.3
1	A	538	VAL	5.1
1	A	744	VAL	5.1
1	A	660	PHE	4.6
1	A	543	LEU	4.3
1	A	315	LYS	4.3
1	A	14	PRO	4.2
1	A	514	LEU	4.2
1	A	314	GLY	4.0
1	A	234	LEU	3.9
1	A	706	ALA	3.9
1	A	515	GLY	3.8
1	A	668	LEU	3.8
1	A	678	PHE	3.6
1	A	662	PRO	3.6
1	A	663	PRO	3.6
1	A	544	TYR	3.6
1	A	705	LEU	3.6
1	A	32	PRO	3.3
1	A	429	PRO	3.3
1	A	702	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	708	SER	3.2
1	A	622	THR	3.2
1	A	311	THR	3.0
1	A	317	GLY	3.0
1	A	399	LYS	3.0
1	A	679	PHE	2.9
1	A	657	LEU	2.9
1	A	535	LEU	2.9
1	A	625	THR	2.9
1	A	633	ALA	2.9
1	A	624	HIS	2.8
1	A	516	THR	2.6
1	A	659	GLY	2.6
1	A	313	ARG	2.6
1	A	519	ALA	2.6
1	A	747	ASN	2.6
1	A	539	LYS	2.6
1	A	116	GLY	2.5
1	A	537	ILE	2.5
1	A	316	ASN	2.5
1	A	237	LYS	2.4
1	A	428	ARG	2.4
1	A	518	SER	2.4
1	A	661	ARG	2.4
1	A	707	SER	2.4
1	A	684	ILE	2.4
1	A	542	LYS	2.3
1	A	520	ARG	2.3
1	A	325	ASN	2.3
1	A	685	ARG	2.3
1	A	703	PRO	2.3
1	A	268	ILE	2.3
1	A	71	TYR	2.3
1	A	270	PHE	2.2
1	A	13	ARG	2.2
1	A	425	ARG	2.2
1	A	704	TYR	2.2
1	A	670	GLN	2.2
1	A	245	LYS	2.2
1	A	307	LEU	2.2
1	A	664	GLY	2.2
1	A	627	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	361	LYS	2.2
1	A	536	LYS	2.2
1	A	143	LYS	2.2
1	A	426	ASN	2.1
1	A	674	ARG	2.1
1	A	95	ASN	2.1
1	A	319	ARG	2.1
1	A	253	ASN	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ZN	A	801	1/1	0.98	0.04	63,63,63,63	0
2	ZN	A	802	1/1	0.98	0.05	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.