



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 11:35 pm BST

PDB ID : 9T5Q / pdb_00009t5q
Title : LRR domain Structure of LRRC8A in complex with synthetic nanobody Sb4
Authors : Lehmann, E.F.; Deneka, D.; Stierli, F.; Rutz, S.; Dutzler, R.
Deposited on : 2025-11-05
Resolution : 1.60 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

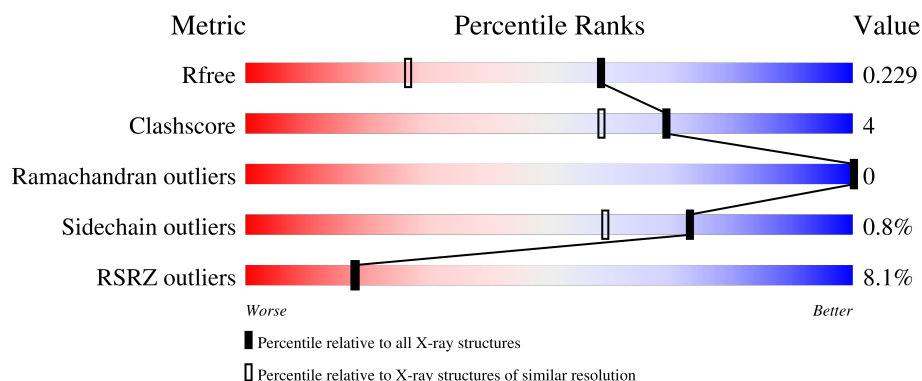
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	415	11% 84% 11% 5%
1	B	415	7% 87% 9% .
2	C	128	5% 96% . .
2	I	128	5% 95% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9261 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 Volume-regulated anion channel subunit LRRC8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3222	2075	566	573	8			
1	B	400	Total	C	N	O	S	0	0	0
			3258	2099	573	578	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	811	ALA	-	expression tag	UNP Q80WG5
A	812	LEU	-	expression tag	UNP Q80WG5
A	813	GLU	-	expression tag	UNP Q80WG5
A	814	VAL	-	expression tag	UNP Q80WG5
A	815	LEU	-	expression tag	UNP Q80WG5
A	816	PHE	-	expression tag	UNP Q80WG5
A	817	GLN	-	expression tag	UNP Q80WG5
B	811	ALA	-	expression tag	UNP Q80WG5
B	812	LEU	-	expression tag	UNP Q80WG5
B	813	GLU	-	expression tag	UNP Q80WG5
B	814	VAL	-	expression tag	UNP Q80WG5
B	815	LEU	-	expression tag	UNP Q80WG5
B	816	PHE	-	expression tag	UNP Q80WG5
B	817	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Sb4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	126	Total	C	N	O	S	0	0	0
			969	613	158	195	3			
2	C	127	Total	C	N	O	S	0	0	0
			974	616	159	196	3			

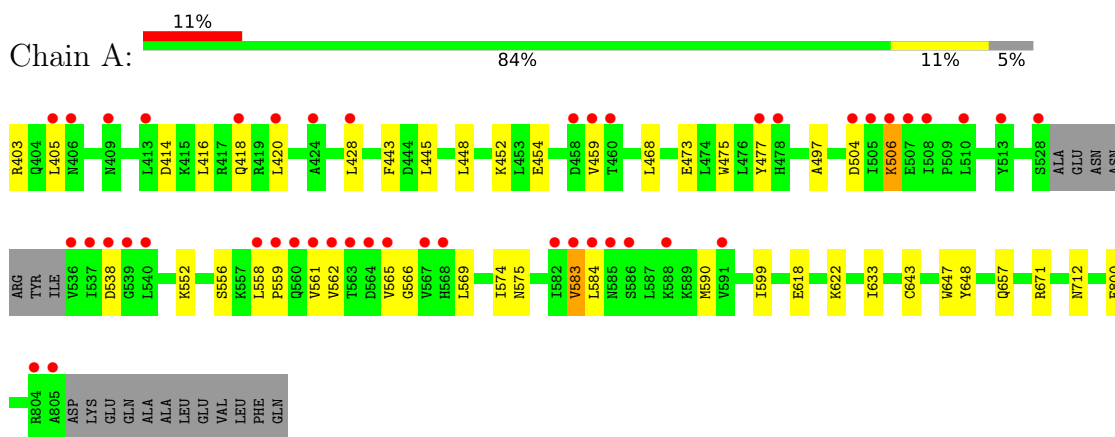
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total 310	O 310	0	0
3	I	117	Total 117	O 117	0	0
3	B	287	Total 287	O 287	0	0
3	C	124	Total 124	O 124	0	0

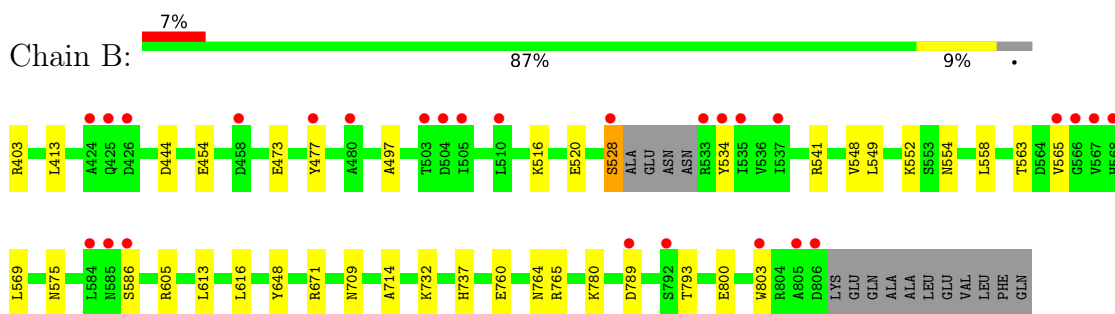
3 Residue-property plots [i](#)

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.

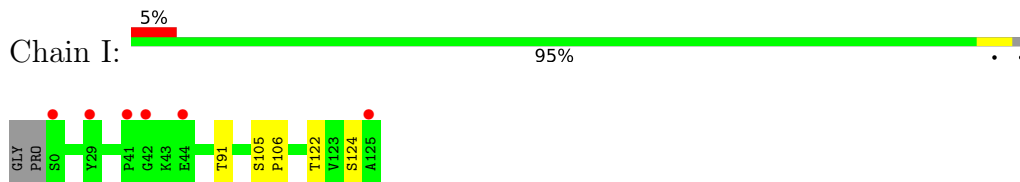
- Molecule 1: Volume-regulated anion channel subunit LRRC8A



- Molecule 1: Volume-regulated anion channel subunit LRRC8A

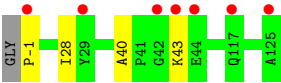


- Molecule 2: Sb4



- Molecule 2: Sb4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.95Å 73.49Å 81.92Å 111.04° 94.35° 110.31°	Depositor
Resolution (Å)	40.08 – 1.60 40.08 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.08-1.60) 97.0 (40.08-1.60)	Depositor EDS
R_{merge}	9.99	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, R_{free}	0.198 , 0.229 0.198 , 0.229	Depositor DCC
R_{free} test set	7111 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9261	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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](#)

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	0.25	0/3277	0.49	0/4443
1	B	0.25	0/3314	0.47	0/4493
2	C	0.29	0/997	0.54	1/1356 (0.1%)
2	I	0.28	0/992	0.51	0/1349
All	All	0.26	0/8580	0.49	1/11641 (0.0%)

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
2	I	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	-1	PRO	N-CA-CB	6.80	110.48	103.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	124	SER	Mainchain

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	3222	0	3396	27	0
1	B	3258	0	3431	30	0
2	C	974	0	907	2	0
2	I	969	0	908	2	0
3	A	310	0	0	2	0
3	B	287	0	0	2	0
3	C	124	0	0	1	0
3	I	117	0	0	0	0
All	All	9261	0	8642	60	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 4.

All (60) 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:454:GLU:HG2	1:B:477:TYR:HB2	1.70	0.74
1:A:454:GLU:HG2	1:A:477:TYR:HB2	1.70	0.73
1:B:737:HIS:HA	1:B:760:GLU:HG2	1.72	0.71
2:C:28:ILE:HG22	3:C:201:HOH:O	1.90	0.70
1:B:473:GLU:HG2	1:B:497:ALA:HB3	1.76	0.67
1:B:528:SER:HA	1:B:534:TYR:HE2	1.60	0.67
1:A:420:LEU:HD13	1:A:428:LEU:HD21	1.79	0.64
1:B:413:LEU:HD11	1:B:444:ASP:HB2	1.81	0.62
1:A:452:LYS:HE2	1:A:454:GLU:OE2	2.00	0.61
1:A:712:ASN:HB2	3:A:1130:HOH:O	2.02	0.58
1:B:800:GLU:HA	1:B:803:TRP:CD1	2.40	0.57
1:A:583:VAL:HG13	1:A:584:LEU:H	1.69	0.57
1:B:737:HIS:HA	1:B:760:GLU:CG	2.35	0.56
1:B:528:SER:HA	1:B:534:TYR:CE2	2.41	0.55
1:B:800:GLU:HA	1:B:803:TRP:HD1	1.71	0.55
1:A:403:ARG:HA	3:A:972:HOH:O	2.10	0.52
2:C:40:ALA:HB3	2:C:43:LYS:HE3	1.92	0.52
1:A:405:LEU:H	1:A:405:LEU:HD12	1.75	0.51
1:A:452:LYS:HE3	1:A:475:TRP:CE3	2.47	0.50
1:A:473:GLU:HG2	1:A:497:ALA:HB3	1.94	0.49
1:A:618:GLU:HG2	1:A:643:CYS:HB3	1.93	0.49
1:A:538:ASP:HA	1:A:561:VAL:HG11	1.94	0.48
1:A:428:LEU:HD22	1:A:448:LEU:HA	1.96	0.48
1:A:559:PRO:HG2	1:A:562:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:THR:HG21	1:B:586:SER:HB2	1.96	0.48
1:B:605:ARG:HD2	3:B:932:HOH:O	2.14	0.47
1:B:709:ASN:HA	1:B:732:LYS:HD3	1.95	0.47
1:B:648:TYR:CE1	1:B:671:ARG:HG3	2.49	0.47
1:B:613:LEU:HB3	1:B:616:LEU:HG	1.97	0.46
1:B:732:LYS:HE2	1:B:732:LYS:HB3	1.65	0.46
1:A:414:ASP:O	1:A:418:GLN:HG3	2.16	0.46
1:A:443:PHE:HA	1:A:468:LEU:HD21	1.98	0.46
1:A:416:LEU:HB3	1:A:445:LEU:HD11	1.98	0.45
1:A:558:LEU:HD21	1:A:574:ILE:HD11	1.98	0.45
1:A:648:TYR:CE1	1:A:671:ARG:HG3	2.52	0.45
1:B:760:GLU:O	1:B:760:GLU:HG3	2.17	0.44
1:B:789:ASP:O	1:B:793:THR:HG23	2.18	0.44
1:B:714:ALA:HA	1:B:737:HIS:HB2	1.99	0.44
1:B:403:ARG:N	3:B:903:HOH:O	2.51	0.43
1:A:583:VAL:O	1:A:584:LEU:HD12	2.18	0.43
1:A:599:ILE:HD12	1:A:622:LYS:HB3	2.00	0.43
1:A:504:ASP:OD1	1:A:506:LYS:HB3	2.19	0.43
1:B:541:ARG:HA	1:B:565:VAL:HG12	2.00	0.43
1:B:516:LYS:HE3	1:B:516:LYS:HB3	1.84	0.43
1:A:552:LYS:HA	1:A:575:ASN:O	2.19	0.42
1:B:780:LYS:HA	1:B:780:LYS:HD3	1.54	0.42
1:A:633:ILE:HD12	1:A:657:GLN:HG2	2.01	0.42
1:A:800:GLU:OE1	1:B:803:TRP:CH2	2.73	0.42
1:A:566:GLY:HA3	1:A:590:MET:HE3	2.02	0.42
1:A:566:GLY:HA2	1:A:569:LEU:HB2	2.01	0.42
1:B:520:GLU:HG2	1:B:548:VAL:HB	2.01	0.41
1:B:558:LEU:HA	1:B:558:LEU:HD23	1.79	0.41
2:I:105:SER:HA	2:I:106:PRO:HD3	1.93	0.41
1:B:549:LEU:HB3	1:B:569:LEU:HD21	2.03	0.41
1:B:528:SER:HB2	1:B:554:ASN:ND2	2.35	0.41
2:I:91:THR:HG23	2:I:122:THR:HA	2.03	0.41
1:B:541:ARG:HA	1:B:565:VAL:CG1	2.51	0.41
1:B:552:LYS:HA	1:B:575:ASN:O	2.21	0.41
1:A:420:LEU:HD11	1:A:445:LEU:HD22	2.03	0.41
1:B:764:ASN:O	1:B:765:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

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	392/415 (94%)	376 (96%)	16 (4%)	0	100	100
1	B	396/415 (95%)	381 (96%)	15 (4%)	0	100	100
2	C	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
2	I	124/128 (97%)	122 (98%)	2 (2%)	0	100	100
All	All	1037/1086 (96%)	1002 (97%)	35 (3%)	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	367/384 (96%)	361 (98%)	6 (2%)	55	33
1	B	370/384 (96%)	369 (100%)	1 (0%)	86	78
2	C	97/98 (99%)	97 (100%)	0	100	100
2	I	97/98 (99%)	97 (100%)	0	100	100
All	All	931/964 (97%)	924 (99%)	7 (1%)	73	59

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	VAL
1	A	506	LYS

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Mol	Chain	Res	Type
1	A	556	SER
1	A	565	VAL
1	A	583	VAL
1	A	647	TRP
1	B	528	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	478	HIS
1	A	758	GLN
1	B	608	HIS
1	B	639	HIS
1	B	709	ASN
2	C	1	GLN
2	C	74	ASN

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 oligosaccharides 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 ⓘ

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	396/415 (95%)	0.48	45 (11%) 10 9	12, 20, 46, 85	0
1	B	400/415 (96%)	0.43	27 (6%) 23 24	13, 22, 37, 55	0
2	C	127/128 (99%)	0.08	7 (5%) 30 31	13, 16, 31, 55	0
2	I	126/128 (98%)	0.08	6 (4%) 35 37	12, 16, 29, 57	0
All	All	1049/1086 (96%)	0.36	85 (8%) 18 18	12, 20, 39, 85	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	VAL	7.7
2	C	42	GLY	7.6
1	A	583	VAL	6.9
1	A	505	ILE	6.5
2	I	42	GLY	5.7
1	A	584	LEU	5.6
1	A	537	ILE	5.5
1	B	567	VAL	5.3
1	A	563	THR	5.0
1	B	803	TRP	4.7
1	B	510	LEU	4.7
1	A	565	VAL	4.5
2	C	43	LYS	4.5
1	A	560	GLN	4.4
1	A	562	VAL	4.3
1	A	585	ASN	4.2
2	I	41	PRO	3.9
1	B	584	LEU	3.8
1	B	504	ASP	3.8
1	B	586	SER	3.7
1	A	510	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	424	ALA	3.7
1	B	528	SER	3.7
1	B	537	ILE	3.6
1	A	586	SER	3.5
1	A	591	VAL	3.4
1	B	566	GLY	3.4
1	A	540	LEU	3.3
1	B	534	TYR	3.1
1	A	538	ASP	3.1
1	A	504	ASP	3.1
1	A	805	ALA	3.0
2	C	44	GLU	3.0
1	A	567	VAL	3.0
1	B	535	ILE	3.0
2	C	125	ALA	2.9
1	B	806	ASP	2.9
1	B	565	VAL	2.9
1	A	405	LEU	2.8
1	A	568	HIS	2.8
1	A	508	ILE	2.8
1	A	561	VAL	2.8
1	B	585	ASN	2.8
1	B	533	ARG	2.8
1	B	505	ILE	2.8
1	A	507	GLU	2.7
1	A	409	ASN	2.7
1	A	506	LYS	2.6
1	B	568	HIS	2.6
2	I	125	ALA	2.6
1	A	539	GLY	2.5
1	A	582	ILE	2.5
1	A	588	LYS	2.5
2	C	-1	PRO	2.4
2	I	29	TYR	2.4
1	B	480	ALA	2.4
1	A	528	SER	2.4
1	A	559	PRO	2.4
2	I	44	GLU	2.4
1	A	477	TYR	2.4
1	B	477	TYR	2.4
1	A	460	THR	2.3
1	B	426	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	0	SER	2.3
1	B	805	ALA	2.3
1	A	513	TYR	2.2
2	C	29	TYR	2.2
2	C	117	GLN	2.1
1	A	478	HIS	2.1
1	A	804	ARG	2.1
1	A	424	ALA	2.1
1	A	420	LEU	2.1
1	A	406	ASN	2.1
1	A	564	ASP	2.1
1	B	425	GLN	2.1
1	A	558	LEU	2.1
1	B	458	ASP	2.0
1	A	413	LEU	2.0
1	A	428	LEU	2.0
1	B	503	THR	2.0
1	A	418	GLN	2.0
1	A	458	ASP	2.0
1	B	789	ASP	2.0
1	B	792	SER	2.0
1	A	459	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 oligosaccharides 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.