



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:47 PM GMT

PDB ID : 1GXR
Title : WD40 Region of Human Groucho/TLE1
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Deposited on : 2002-04-10
Resolution : 1.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

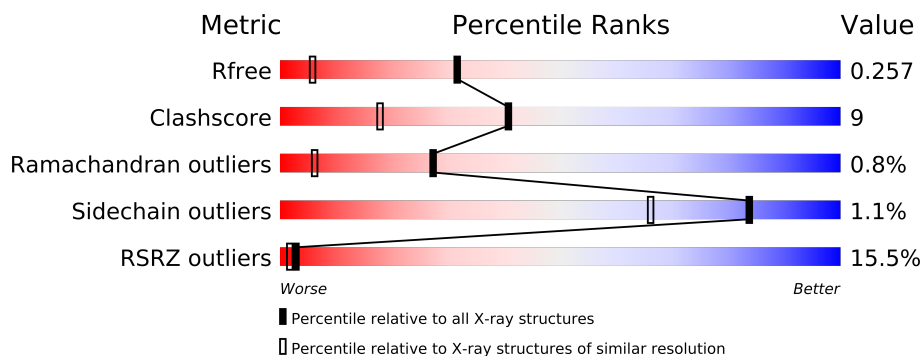
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	1003	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5594 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRANSDUCIN-LIKE ENHANCER PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2562	1613	442	490	17			
1	B	324	Total	C	N	O	S	0	0	0
			2467	1558	422	471	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	ASP	THR	SEE REMARK 999	UNP Q04724
A	465	ALA	PRO	SEE REMARK 999	UNP Q04724
B	464	ASP	THR	SEE REMARK 999	UNP Q04724
B	465	ALA	PRO	SEE REMARK 999	UNP Q04724

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

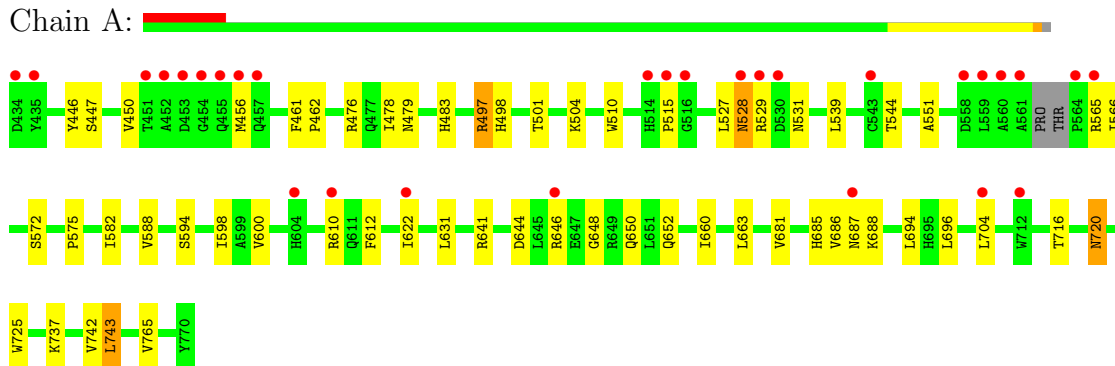
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	335	Total	O	0	0
			335	335		
3	B	229	Total	O	0	0
			229	229		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

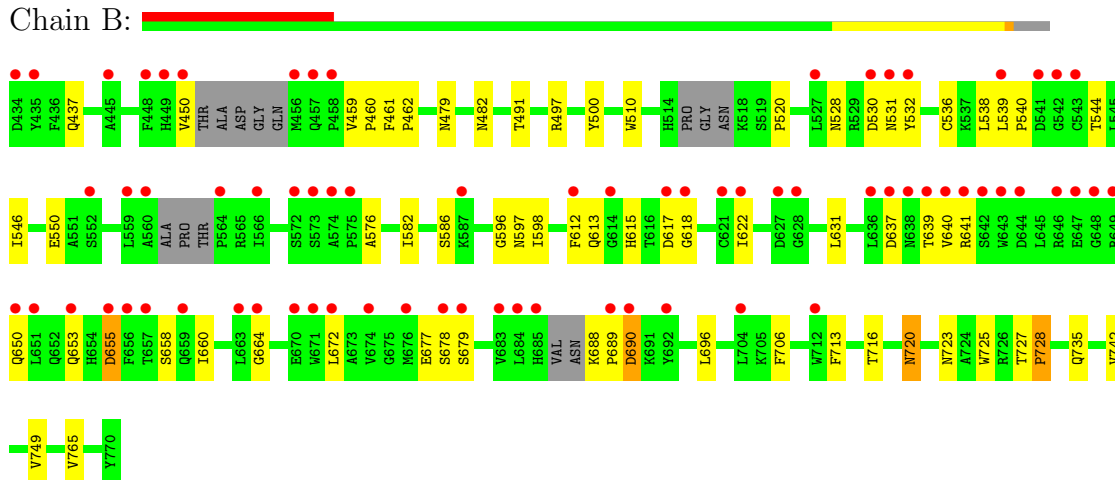
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain A:



• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.41Å 56.66Å 102.03Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	40.45 – 1.65 40.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.45-1.65) 100.0 (40.45-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.256 0.233 , 0.257	Depositor DCC
R_{free} test set	3977 reflections (4.74%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 92054 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5594	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.31	0/2626	0.64	0/3573
1	B	0.29	0/2525	0.57	0/3429
All	All	0.30	0/5151	0.61	0/7002

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2562	0	2471	46	0
1	B	2467	0	2357	48	0
2	A	1	0	0	0	0
3	A	335	0	0	9	0
3	B	229	0	0	4	0
All	All	5594	0	4828	92	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:447:SER:H	1:B:437:GLN:HE22	1.24	0.84
1:B:658:SER:HB2	1:B:677:GLU:HB3	1.59	0.83
1:B:749:VAL:HG22	3:B:2053:HOH:O	1.79	0.80
1:B:622:ILE:HD11	1:B:631:LEU:HD11	1.65	0.76
1:B:528:ASN:HB3	1:B:531:ASN:ND2	2.10	0.65
1:B:720:ASN:HD22	1:B:720:ASN:N	1.95	0.65
1:A:483:HIS:HD2	1:A:501:THR:OG1	1.81	0.62
1:B:696:LEU:HB2	1:B:725:TRP:HH2	1.66	0.61
1:B:491:THR:HG22	1:B:500:TYR:HB2	1.84	0.60
1:A:641:ARG:HH11	1:A:650:GLN:HE22	1.50	0.60
1:A:446:TYR:H	1:B:437:GLN:NE2	2.00	0.59
1:B:696:LEU:HB2	1:B:725:TRP:CH2	2.37	0.59
1:A:572:SER:HB2	3:A:2198:HOH:O	2.01	0.59
1:A:720:ASN:HD22	1:A:720:ASN:N	2.01	0.58
1:A:716:THR:HB	1:A:742:VAL:HB	1.86	0.58
1:A:598:ILE:HB	1:A:612:PHE:HB2	1.86	0.58
1:A:644:ASP:OD1	1:A:646:ARG:HG2	2.05	0.57
1:A:504:LYS:HG2	1:A:529:ARG:O	2.05	0.56
1:B:550:GLU:HA	1:B:576:ALA:HB1	1.88	0.56
1:A:528:ASN:HB3	1:A:531:ASN:ND2	2.21	0.55
1:A:622:ILE:HD11	1:A:631:LEU:HD11	1.88	0.55
1:B:598:ILE:HB	1:B:612:PHE:HB2	1.89	0.54
1:B:528:ASN:HD21	1:B:530:ASP:HB2	1.72	0.54
1:B:639:THR:HB	1:B:653:GLN:NE2	2.23	0.54
1:B:479:ASN:HB2	1:B:765:VAL:HB	1.89	0.54
1:A:483:HIS:HE1	3:A:2059:HOH:O	1.90	0.53
1:A:660:ILE:N	1:A:660:ILE:HD12	2.23	0.53
1:A:539:LEU:HD13	1:A:582:ILE:HG21	1.91	0.53
1:B:716:THR:HB	1:B:742:VAL:HB	1.90	0.53
1:B:639:THR:HB	1:B:653:GLN:HE22	1.73	0.52
1:A:478:ILE:HG13	1:A:479:ASN:HD22	1.75	0.52
1:A:575:PRO:HG2	1:A:594:SER:OG	2.10	0.52
1:A:539:LEU:HD23	1:A:544:THR:HB	1.91	0.51
1:B:617:ASP:HB2	1:B:637:ASP:HB3	1.92	0.51
1:B:660:ILE:HD12	1:B:660:ILE:N	2.26	0.51
1:B:615:HIS:HB3	1:B:617:ASP:O	2.11	0.51
1:B:510:TRP:CH2	1:B:520:PRO:HG3	2.45	0.51
1:A:743:LEU:HD22	1:A:743:LEU:N	2.26	0.51
1:A:663:LEU:HA	1:A:704:LEU:HD21	1.92	0.50
1:B:640:VAL:CG2	1:B:660:ILE:HG12	2.42	0.50
1:B:655:ASP:HA	3:B:2143:HOH:O	2.11	0.50
1:A:479:ASN:HB2	1:A:765:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:532:TYR:HB2	1:B:550:GLU:OE1	2.13	0.49
1:A:696:LEU:HB2	1:A:725:TRP:CH2	2.48	0.49
1:A:652:GLN:HG2	3:A:2194:HOH:O	2.13	0.49
1:B:546:ILE:HD12	1:B:582:ILE:HD11	1.95	0.48
1:B:640:VAL:HG23	1:B:660:ILE:HG12	1.94	0.48
1:B:596:GLY:N	1:B:618:GLY:HA2	2.29	0.48
1:A:565:ARG:HA	3:A:2113:HOH:O	2.15	0.47
1:B:531:ASN:HA	3:B:2071:HOH:O	2.13	0.47
1:B:500:TYR:CE1	1:B:538:LEU:HD11	2.50	0.47
1:B:641:ARG:HD3	1:B:650:GLN:CD	2.35	0.47
1:B:550:GLU:HA	1:B:576:ALA:CB	2.44	0.47
1:A:663:LEU:C	1:A:663:LEU:HD12	2.35	0.46
1:B:641:ARG:HD3	1:B:650:GLN:OE1	2.15	0.46
1:B:536:CYS:HA	1:B:546:ILE:O	2.16	0.46
1:B:540:PRO:HG2	1:B:586:SER:OG	2.16	0.46
1:A:450:VAL:HG22	1:A:456:MET:HG2	1.97	0.46
1:A:743:LEU:H	1:A:743:LEU:HD22	1.81	0.45
1:A:476:ARG:NH1	1:A:478:ILE:HG22	2.32	0.45
1:A:528:ASN:HD22	1:A:529:ARG:H	1.64	0.45
1:A:588:VAL:HG11	1:A:600:VAL:HG13	1.98	0.45
1:A:497:ARG:HB3	3:A:2055:HOH:O	2.17	0.45
1:A:479:ASN:ND2	3:A:2037:HOH:O	2.42	0.45
1:A:685:HIS:NE2	1:A:688:LYS:HD2	2.32	0.45
1:B:539:LEU:HD12	1:B:544:THR:HB	1.99	0.44
1:B:688:LYS:HG2	1:B:689:PRO:N	2.33	0.44
1:A:515:PRO:HB3	3:A:2068:HOH:O	2.16	0.44
1:B:723:ASN:ND2	1:B:735:GLN:HG2	2.32	0.44
1:B:450:VAL:O	1:B:690:ASP:HA	2.18	0.44
1:B:664:GLY:O	1:B:672:LEU:HD12	2.18	0.44
1:B:637:ASP:O	1:B:639:THR:HG23	2.18	0.44
1:A:737:LYS:HE3	3:A:2304:HOH:O	2.17	0.44
1:B:720:ASN:N	1:B:720:ASN:ND2	2.61	0.44
1:A:566:ILE:HG23	1:A:566:ILE:O	2.18	0.44
1:B:482:ASN:ND2	3:B:2040:HOH:O	2.50	0.44
1:A:461:PHE:HA	1:A:462:PRO:HD3	1.89	0.44
1:A:527:LEU:HD22	1:A:551:ALA:HB3	2.00	0.43
1:B:723:ASN:HD22	1:B:735:GLN:HG2	1.83	0.43
1:B:461:PHE:HA	1:B:462:PRO:HD3	1.90	0.43
1:B:459:VAL:HA	1:B:460:PRO:HD3	1.89	0.43
1:A:497:ARG:HE	1:A:498:HIS:CE1	2.36	0.43
1:A:504:LYS:HE2	3:A:2043:HOH:O	2.19	0.42
1:A:681:VAL:HB	1:A:694:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:597:ASN:OD1	1:B:613:GLN:HG2	2.20	0.42
1:B:727:THR:HA	1:B:728:PRO:HA	1.88	0.41
1:A:610:ARG:CZ	1:A:648:GLY:HA3	2.50	0.41
1:B:706:PHE:HA	1:B:713:PHE:CB	2.51	0.41
1:A:498:HIS:HA	1:A:510:TRP:O	2.20	0.41
1:A:686:VAL:HG12	1:A:687:ASN:ND2	2.36	0.41
1:A:610:ARG:HH11	1:A:610:ARG:HG2	1.85	0.41
1:A:497:ARG:HG3	1:A:498:HIS:ND1	2.37	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	331/337 (98%)	317 (96%)	13 (4%)	1 (0%)	50	24
1	B	314/337 (93%)	292 (93%)	18 (6%)	4 (1%)	18	2
All	All	645/674 (96%)	609 (94%)	31 (5%)	5 (1%)	27	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	679	SER
1	B	678	SER
1	B	497	ARG
1	B	690	ASP
1	A	497	ARG

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	283/288 (98%)	280 (99%)	3 (1%)	84	66
1	B	268/288 (93%)	265 (99%)	3 (1%)	84	66
All	All	551/576 (96%)	545 (99%)	6 (1%)	84	66

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	ASN
1	A	720	ASN
1	A	743	LEU
1	B	655	ASP
1	B	720	ASN
1	B	728	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	479	ASN
1	A	483	HIS
1	A	528	ASN
1	A	531	ASN
1	A	650	GLN
1	A	652	GLN
1	A	680	ASN
1	A	687	ASN
1	A	720	ASN
1	A	735	GLN
1	B	437	GLN
1	B	449	HIS
1	B	482	ASN
1	B	528	ASN
1	B	531	ASN
1	B	605	ASN
1	B	606	GLN
1	B	652	GLN
1	B	720	ASN
1	B	723	ASN
1	B	735	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 1 ligands modelled in this entry, 1 is 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.

5.7 Other polymers ⓘ

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	335/337 (99%)	0.60	29 (8%) 10 8	15, 24, 47, 59	0
1	B	324/337 (96%)	1.21	72 (22%) 1 1	16, 35, 50, 58	0
All	All	659/674 (97%)	0.90	101 (15%) 3 2	15, 29, 50, 59	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	ALA	12.4
1	A	454	GLY	10.0
1	A	452	ALA	8.5
1	B	655	ASP	8.2
1	B	649	ARG	6.8
1	A	435	TYR	6.6
1	B	651	LEU	6.1
1	B	647	GLU	6.1
1	B	646	ARG	6.0
1	B	456	MET	5.9
1	B	617	ASP	5.2
1	B	689	PRO	5.2
1	B	614	GLY	4.8
1	B	628	GLY	4.5
1	A	453	ASP	4.5
1	B	450	VAL	4.3
1	A	646	ARG	4.2
1	B	527	LEU	4.1
1	B	678	SER	4.0
1	B	532	TYR	3.9
1	B	683	VAL	3.8
1	A	559	LEU	3.8
1	B	690	ASP	3.6
1	B	657	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	565	ARG	3.5
1	B	435	TYR	3.5
1	B	653	GLN	3.5
1	B	637	ASP	3.5
1	B	449	HIS	3.4
1	B	644	ASP	3.4
1	A	451	THR	3.4
1	A	604	HIS	3.4
1	B	552	SER	3.4
1	B	636	LEU	3.3
1	A	515	PRO	3.3
1	A	564	PRO	3.3
1	B	648	GLY	3.2
1	B	656	PHE	3.2
1	A	434	ASP	3.2
1	B	572	SER	3.2
1	B	559	LEU	3.2
1	A	514	HIS	3.2
1	B	573	SER	3.2
1	A	516	GLY	3.2
1	B	704	LEU	3.1
1	B	543	CYS	3.1
1	B	560	ALA	3.1
1	A	528	ASN	3.1
1	B	640	VAL	3.0
1	A	456	MET	3.0
1	B	575	PRO	3.0
1	A	529	ARG	3.0
1	A	560	ALA	2.9
1	A	530	ASP	2.9
1	B	530	ASP	2.9
1	B	566	ILE	2.9
1	B	445	ALA	2.8
1	A	455	GLN	2.8
1	B	650	GLN	2.8
1	B	685	HIS	2.8
1	B	643	TRP	2.8
1	B	638	ASN	2.8
1	A	457	GLN	2.7
1	A	712	TRP	2.7
1	B	663	LEU	2.7
1	B	672	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	627	ASP	2.7
1	A	704	LEU	2.7
1	A	610	ARG	2.7
1	B	587	LYS	2.6
1	B	541	ASP	2.6
1	B	674	VAL	2.6
1	B	641	ARG	2.6
1	B	612	PHE	2.5
1	B	564	PRO	2.5
1	B	664	GLY	2.4
1	A	558	ASP	2.4
1	B	457	GLN	2.4
1	B	659	GLN	2.4
1	B	684	LEU	2.4
1	B	434	ASP	2.4
1	B	692	TYR	2.4
1	A	543	CYS	2.4
1	B	639	THR	2.3
1	B	621	CYS	2.3
1	B	531	ASN	2.3
1	B	458	PRO	2.3
1	B	622	ILE	2.3
1	B	671	TRP	2.3
1	B	642	SER	2.3
1	B	574	ALA	2.3
1	B	712	TRP	2.3
1	A	687	ASN	2.2
1	B	618	GLY	2.2
1	B	539	LEU	2.2
1	B	679	SER	2.2
1	A	622	ILE	2.2
1	B	448	PHE	2.2
1	B	542	GLY	2.2
1	B	670	GLU	2.0
1	B	676	MET	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	A	1003	1/1	0.27	3.71	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.