



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 03:09 PM BST

PDB ID : 5WOA
Title : Crystal Structure of Transient Receptor Potential (TRP) channel TRPV6* in the presence of Gadolinium
Authors : Singh, A.K.; Saotome, K.; Sobolevsky, A.I.
Deposited on : 2017-08-01
Resolution : 3.90 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
Xtriage (Phenix) : 1.13
EDS : 2.13
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

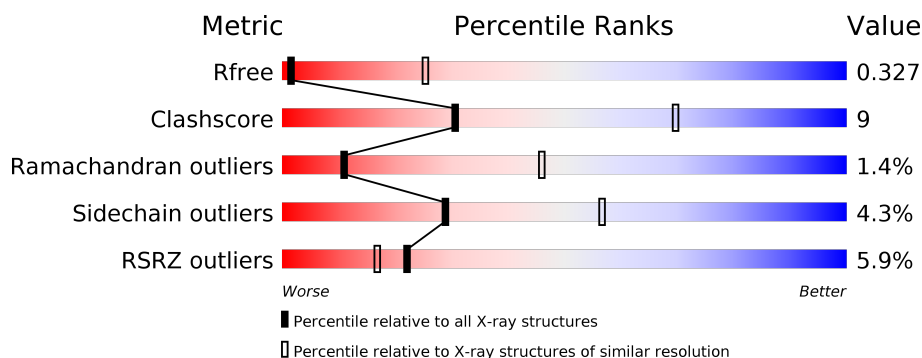
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	672	<div> <div>5%</div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GD	A	701	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4741 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4739	3070	790	845	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	engineered mutation	UNP Q9R186
A	92	ASN	LEU	engineered mutation	UNP Q9R186
A	96	GLN	MET	engineered mutation	UNP Q9R186
A	670	VAL	-	expression tag	UNP Q9R186
A	671	PRO	-	expression tag	UNP Q9R186
A	672	ARG	-	expression tag	UNP Q9R186

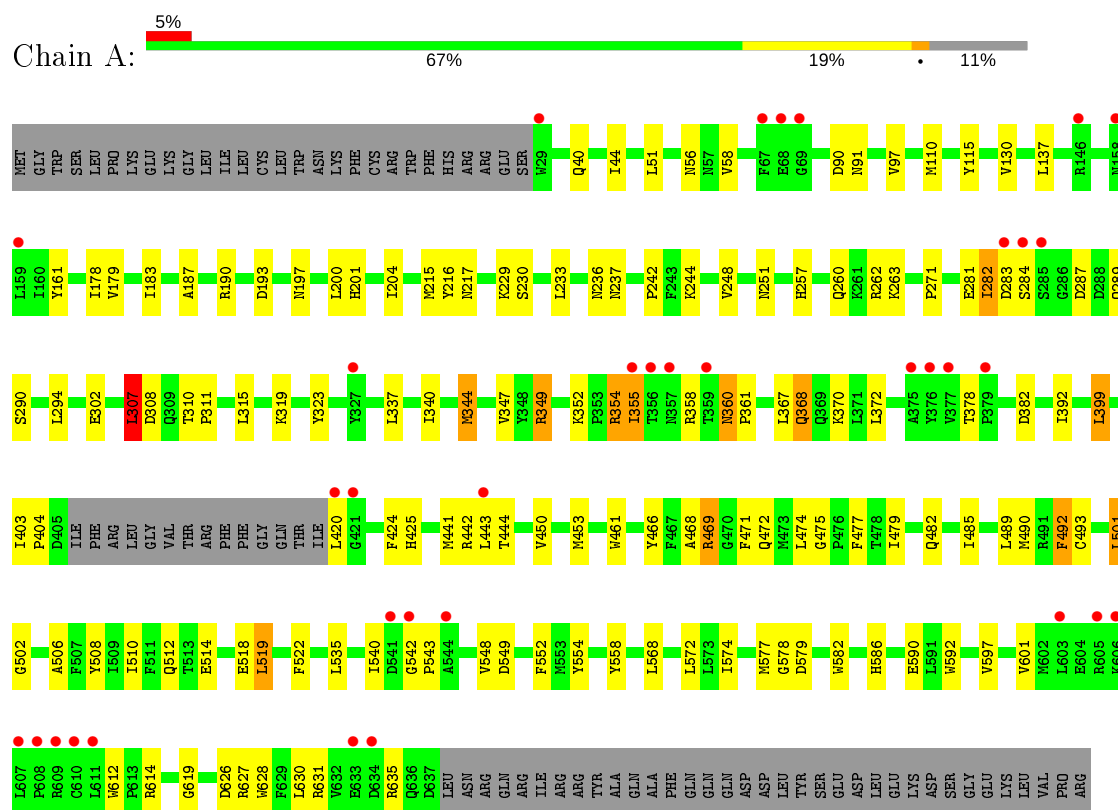
- Molecule 2 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

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

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: Transient receptor potential cation channel subfamily V member 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.08Å 146.08Å 116.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 3.90 47.18 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.18-3.90) 93.9 (47.18-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.88Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.271 , 0.316 0.280 , 0.327	Depositor DCC
R_{free} test set	535 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	158.8	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 136.8	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	0.83	EDS
Total number of atoms	4741	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: GD

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	0.27	1/4849 (0.0%)	0.56	11/6590 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	LEU	CA-C	6.43	1.69	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	GLN	N-CA-CB	-12.63	87.86	110.60
1	A	518	GLU	N-CA-C	11.84	142.97	111.00
1	A	471	PHE	N-CA-C	-9.94	84.17	111.00
1	A	471	PHE	CB-CA-C	9.38	129.16	110.40
1	A	519	LEU	N-CA-C	-7.06	91.94	111.00
1	A	492	PHE	CB-CA-C	-6.70	96.99	110.40
1	A	502	GLY	N-CA-C	5.85	127.73	113.10
1	A	501	LEU	CA-C-O	5.33	131.30	120.10
1	A	307	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	501	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	501	LEU	CA-C-N	-5.01	106.18	116.20

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	4739	0	4759	87	1
2	A	2	0	0	0	0
All	All	4741	0	4759	87	1

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 9.

All (87) 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:468:ALA:HB1	1:A:474:LEU:CD1	1.48	1.41
1:A:468:ALA:HB1	1:A:474:LEU:HD13	1.25	1.17
1:A:492:PHE:CE1	1:A:568:LEU:O	2.11	1.03
1:A:492:PHE:HE1	1:A:568:LEU:O	1.45	1.00
1:A:468:ALA:CB	1:A:474:LEU:CD1	2.40	0.99
1:A:468:ALA:HB1	1:A:474:LEU:HD11	1.49	0.92
1:A:548:VAL:HG22	1:A:549:ASP:H	1.38	0.89
1:A:492:PHE:O	1:A:492:PHE:CG	2.28	0.86
1:A:577:MET:O	1:A:579:ASP:N	2.10	0.84
1:A:492:PHE:O	1:A:492:PHE:CD2	2.31	0.83
1:A:378:THR:HG23	1:A:378:THR:O	1.86	0.73
1:A:352:LYS:HB3	1:A:370:LYS:HA	1.69	0.73
1:A:490:MET:HA	1:A:493:CYS:SG	2.29	0.73
1:A:548:VAL:HG22	1:A:549:ASP:N	2.03	0.71
1:A:468:ALA:CB	1:A:474:LEU:HD13	2.13	0.69
1:A:468:ALA:CB	1:A:474:LEU:HD11	2.14	0.67
1:A:577:MET:C	1:A:579:ASP:H	2.00	0.66
1:A:378:THR:OG1	1:A:382:ASP:N	2.28	0.64
1:A:492:PHE:CE2	1:A:572:LEU:HD22	2.33	0.64
1:A:540:ILE:HG22	1:A:542:GLY:H	1.63	0.63
1:A:468:ALA:HB1	1:A:474:LEU:HD12	1.69	0.62
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.18	0.61
1:A:479:ILE:HD13	1:A:592:TRP:HB2	1.84	0.60
1:A:490:MET:O	1:A:493:CYS:SG	2.58	0.60
1:A:349:ARG:HD3	1:A:453:MET:HE1	1.84	0.59
1:A:619:GLY:N	1:A:627:ARG:O	2.36	0.59
1:A:548:VAL:CG2	1:A:549:ASP:H	2.13	0.58
1:A:323:TYR:O	1:A:612:TRP:CZ3	2.56	0.58
1:A:230:SER:HB3	1:A:233:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:HD13	1:A:187:ALA:HB3	1.87	0.57
1:A:469:ARG:O	1:A:592:TRP:NE1	2.37	0.56
1:A:197:ASN:OD1	1:A:236:ASN:ND2	2.40	0.55
1:A:58:VAL:HG13	1:A:97:VAL:HG21	1.89	0.54
1:A:420:LEU:O	1:A:482:GLN:NE2	2.39	0.53
1:A:352:LYS:HD2	1:A:372:LEU:HB2	1.91	0.52
1:A:485:ILE:HG23	1:A:489:LEU:HD23	1.92	0.52
1:A:450:VAL:HA	1:A:453:MET:HE3	1.90	0.52
1:A:315:LEU:HG	1:A:319:LYS:HD2	1.92	0.52
1:A:378:THR:CG2	1:A:378:THR:O	2.58	0.51
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.92	0.51
1:A:307:LEU:H	1:A:307:LEU:HD13	1.76	0.51
1:A:260:GLN:HA	1:A:263:LYS:HE2	1.93	0.50
1:A:130:VAL:HG22	1:A:178:ILE:HD11	1.95	0.49
1:A:204:ILE:O	1:A:251:ASN:ND2	2.46	0.48
1:A:424:PHE:HB3	1:A:466:TYR:HB2	1.95	0.48
1:A:506:ALA:O	1:A:510:ILE:HG12	2.13	0.48
1:A:492:PHE:CD2	1:A:572:LEU:HD22	2.48	0.48
1:A:284:SER:HA	1:A:290:SER:HB3	1.95	0.48
1:A:403:ILE:HG22	1:A:404:PRO:HD3	1.96	0.47
1:A:475:GLY:O	1:A:479:ILE:HD12	2.14	0.47
1:A:262:ARG:HH12	1:A:281:GLU:HG3	1.79	0.47
1:A:282:ILE:HG22	1:A:283:ASP:H	1.80	0.47
1:A:40:GLN:O	1:A:44:ILE:HG12	2.15	0.46
1:A:354:ARG:HG2	1:A:368:GLN:HG3	1.97	0.46
1:A:442:ARG:C	1:A:444:THR:H	2.18	0.46
1:A:110:MET:HB2	1:A:115:TYR:O	2.17	0.45
1:A:360:ASN:H	1:A:361:PRO:HD2	1.81	0.45
1:A:535:LEU:HD13	1:A:558:TYR:HE1	1.81	0.45
1:A:190:ARG:NH1	1:A:229:LYS:O	2.44	0.45
1:A:614:ARG:HD3	1:A:628:TRP:CE2	2.51	0.45
1:A:354:ARG:O	1:A:355:ILE:HG22	2.16	0.45
1:A:352:LYS:HE2	1:A:355:ILE:HD12	1.98	0.45
1:A:586:HIS:O	1:A:590:GLU:HG2	2.18	0.44
1:A:344:MET:HA	1:A:347:VAL:HG22	2.00	0.44
1:A:179:VAL:HG21	1:A:215:MET:SD	2.57	0.43
1:A:358:ARG:HH12	1:A:367:LEU:HD12	1.82	0.43
1:A:442:ARG:HG3	1:A:443:LEU:H	1.84	0.43
1:A:399:LEU:HA	1:A:399:LEU:HD12	1.86	0.43
1:A:56:ASN:OD1	1:A:91:ASN:HB3	2.18	0.43
1:A:485:ILE:O	1:A:489:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:HD12	1:A:474:LEU:C	2.39	0.42
1:A:217:ASN:OD1	1:A:257:HIS:NE2	2.44	0.42
1:A:137:LEU:HA	1:A:137:LEU:HD13	1.89	0.42
1:A:236:ASN:OD1	1:A:237:ASN:N	2.52	0.42
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.91	0.42
1:A:543:PRO:O	1:A:554:TYR:OH	2.22	0.42
1:A:354:ARG:HH22	1:A:367:LEU:HB2	1.85	0.41
1:A:392:ILE:HA	1:A:392:ILE:HD13	1.93	0.41
1:A:248:VAL:HG22	1:A:294:LEU:HB3	2.02	0.41
1:A:574:ILE:HA	1:A:577:MET:HE2	2.02	0.41
1:A:466:TYR:O	1:A:469:ARG:HD2	2.21	0.41
1:A:201:HIS:CE1	1:A:242:PRO:HD3	2.56	0.40
1:A:271:PRO:HB2	1:A:635:ARG:HG3	2.02	0.40
1:A:508:TYR:O	1:A:512:GLN:N	2.53	0.40
1:A:597:VAL:O	1:A:601:VAL:HG23	2.22	0.40
1:A:337:LEU:HA	1:A:340:ILE:HG22	2.03	0.40
1:A:200:LEU:HB3	1:A:216:TYR:HE2	1.85	0.40

All (1) 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)
1:A:461:TRP:CE2	1:A:501:LEU:CD2[3_1045]	2.09	0.11

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	591/672 (88%)	528 (89%)	55 (9%)	8 (1%)	11 46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLY
1	A	90	ASP
1	A	360	ASN
1	A	311	PRO
1	A	355	ILE
1	A	626	ASP
1	A	310	THR
1	A	282	ILE

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	510/584 (87%)	488 (96%)	22 (4%)	29 57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	287	ASP
1	A	289	GLN
1	A	302	GLU
1	A	307	LEU
1	A	308	ASP
1	A	344	MET
1	A	349	ARG
1	A	354	ARG
1	A	368	GLN
1	A	399	LEU
1	A	425	HIS
1	A	441	MET
1	A	469	ARG
1	A	477	PHE
1	A	514	GLU
1	A	519	LEU
1	A	522	PHE
1	A	552	PHE

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Mol	Chain	Res	Type
1	A	582	TRP
1	A	630	LEU
1	A	631	ARG

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	595/672 (88%)	0.01	35 (5%) 22 17	103, 148, 218, 307	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	PRO	8.5
1	A	610	CYS	7.5
1	A	607	LEU	7.0
1	A	606	LYS	6.4
1	A	609	ARG	4.8
1	A	377	VAL	4.1
1	A	158	ASN	4.1
1	A	376	TYR	4.1
1	A	375	ALA	4.0
1	A	357	ASN	3.9
1	A	355	ILE	3.6
1	A	633	GLU	3.4
1	A	421	GLY	3.3
1	A	611	LEU	3.1
1	A	605	ARG	3.1
1	A	603	LEU	3.0
1	A	379	PRO	2.8
1	A	146	ARG	2.8
1	A	541	ASP	2.8
1	A	69	GLY	2.8
1	A	283	ASP	2.7
1	A	542	GLY	2.7
1	A	356	THR	2.7
1	A	634	ASP	2.7
1	A	544	ALA	2.6
1	A	285	SER	2.5
1	A	420	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	2.2
1	A	443	LEU	2.1
1	A	284	SER	2.1
1	A	68	GLU	2.1
1	A	29	TRP	2.0
1	A	327	TYR	2.0
1	A	359	THR	2.0
1	A	67	PHE	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(\AA^2)	Q<0.9
2	GD	A	701	1/1	-0.69	3.19	706,706,706,706	0
2	GD	A	702	1/1	0.99	0.06	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.