



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2AO7 / pdb_00002ao7
Title : Adam10 Disintegrin and cysteine- rich domain
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Deposited on : 2005-08-12
Resolution : 2.90 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 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

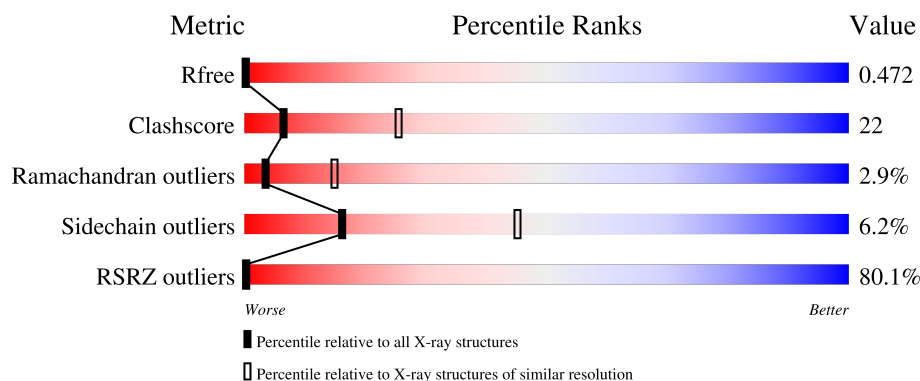
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	192	

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	SO4	A	648	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1109 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 ADAM 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1099	666	198	209	26	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

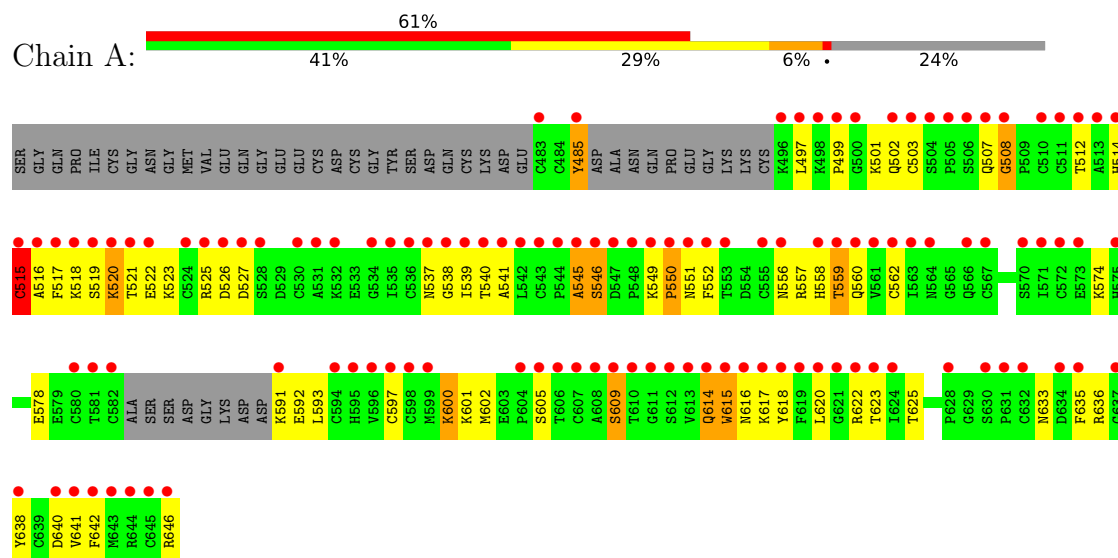


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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: ADAM 10



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	146.78Å 146.78Å 146.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90 8.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.90) 94.0 (8.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.289 0.477 , 0.472	Depositor DCC
R_{free} test set	574 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.53	EDS
Total number of atoms	1109	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: SO4

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	0.55	0/1119	1.06	7/1501 (0.5%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	VAL	N-CA-C	-9.36	100.25	113.07
1	A	614	GLN	N-CA-C	-7.14	101.63	110.41
1	A	592	GLU	N-CA-C	-6.24	105.72	113.15
1	A	600	LYS	N-CA-C	-6.17	101.80	110.50
1	A	515	CYS	N-CA-C	5.73	119.76	111.56
1	A	508	GLY	CA-C-N	5.54	126.27	120.12
1	A	508	GLY	C-N-CA	5.54	126.27	120.12

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	1099	0	1036	47	12
2	A	10	0	0	1	2
All	All	1109	0	1036	47	12

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 22.

All (47) 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:556:ASN:HD22	1:A:560:GLN:HE21	1.09	0.94
1:A:559:THR:HG22	1:A:560:GLN:HG3	1.55	0.88
1:A:556:ASN:HD22	1:A:560:GLN:NE2	1.75	0.84
1:A:545:ALA:O	1:A:546:SER:HB2	1.90	0.70
1:A:556:ASN:ND2	1:A:560:GLN:HE21	1.89	0.68
1:A:502:GLN:HE21	1:A:516:ALA:HA	1.61	0.65
1:A:518:LYS:HB3	1:A:522:GLU:HG3	1.82	0.61
1:A:545:ALA:O	1:A:546:SER:CB	2.51	0.59
1:A:519:SER:C	1:A:521:THR:H	2.10	0.58
1:A:508:GLY:HA3	1:A:541:ALA:O	2.04	0.58
1:A:523:LYS:NZ	1:A:526:ASP:HA	2.19	0.58
1:A:559:THR:HG22	1:A:560:GLN:CG	2.33	0.57
1:A:633:ASN:O	1:A:636:ARG:HB2	2.06	0.56
1:A:485:TYR:H	1:A:485:TYR:HD2	1.52	0.56
1:A:614:GLN:O	1:A:615:TRP:HB2	2.07	0.55
1:A:556:ASN:O	1:A:559:THR:HB	2.06	0.54
1:A:485:TYR:HA	1:A:497:LEU:HA	1.91	0.53
1:A:622:ARG:HG2	1:A:622:ARG:HH11	1.73	0.53
1:A:623:THR:HG22	1:A:623:THR:O	2.09	0.53
1:A:502:GLN:NE2	1:A:517:PHE:H	2.08	0.51
1:A:552:PHE:CD2	1:A:574:LYS:HA	2.47	0.50
1:A:525:ARG:NH1	2:A:648:SO4:S	2.86	0.49
1:A:518:LYS:O	1:A:538:GLY:HA2	2.13	0.48
1:A:578:GLU:HG3	1:A:601:LYS:HG2	1.96	0.48
1:A:537:ASN:HD21	1:A:540:THR:HG22	1.80	0.47
1:A:591:LYS:C	1:A:593:LEU:H	2.23	0.46
1:A:485:TYR:N	1:A:485:TYR:CD2	2.83	0.46
1:A:519:SER:C	1:A:521:THR:N	2.74	0.46
1:A:616:ASN:C	1:A:618:TYR:N	2.74	0.45
1:A:640:ASP:HB3	1:A:642:PHE:H	1.83	0.44
1:A:503:CYS:O	1:A:515:CYS:HB3	2.18	0.43
1:A:616:ASN:OD1	1:A:620:LEU:HA	2.18	0.43
1:A:646:ARG:HD2	1:A:646:ARG:HA	1.84	0.43
1:A:485:TYR:HD2	1:A:485:TYR:N	2.14	0.43
1:A:523:LYS:HZ1	1:A:526:ASP:HA	1.84	0.42
1:A:519:SER:O	1:A:521:THR:N	2.51	0.42
1:A:614:GLN:C	1:A:616:ASN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LYS:O	1:A:550:PRO:C	2.63	0.42
1:A:552:PHE:HB3	1:A:574:LYS:HG3	2.01	0.42
1:A:557:ARG:C	1:A:559:THR:H	2.28	0.42
1:A:551:ASN:O	1:A:562:CYS:O	2.38	0.42
1:A:640:ASP:CB	1:A:642:PHE:H	2.33	0.41
1:A:557:ARG:C	1:A:559:THR:N	2.76	0.41
1:A:597:CYS:SG	1:A:609:SER:HA	2.60	0.41
1:A:620:LEU:HB2	1:A:622:ARG:NH1	2.36	0.41
1:A:507:GLN:H	1:A:507:GLN:HG3	1.66	0.40
1:A:512:THR:C	1:A:514:HIS:N	2.79	0.40

All (12) 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:512:THR:OG1	1:A:605:SER:OG[33_554]	1.66	0.54
1:A:501:LYS:NZ	1:A:635:PHE:O[10_655]	1.96	0.24
1:A:502:GLN:CD	1:A:635:PHE:CZ[10_655]	1.99	0.21
1:A:525:ARG:CG	1:A:622:ARG:NH2[24_555]	2.03	0.17
1:A:622:ARG:NH2	2:A:648:SO4:O2[24_555]	2.03	0.17
1:A:521:THR:OG1	1:A:602:MET:SD[33_554]	2.07	0.13
1:A:502:GLN:CG	1:A:635:PHE:CE2[10_655]	2.09	0.11
1:A:502:GLN:CG	1:A:635:PHE:CZ[10_655]	2.12	0.08
1:A:600:LYS:CE	1:A:617:LYS:CE[43_655]	2.14	0.06
1:A:622:ARG:NE	2:A:648:SO4:O2[24_555]	2.17	0.03
1:A:499:PRO:CB	1:A:638:TYR:CD2[10_655]	2.18	0.02
1:A:527:ASP:O	1:A:558:HIS:NE2[24_555]	2.18	0.02

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	140/192 (73%)	123 (88%)	13 (9%)	4 (3%)	3	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	ALA
1	A	546	SER
1	A	520	LYS
1	A	550	PRO

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	128/165 (78%)	120 (94%)	8 (6%)	16	45

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	TYR
1	A	515	CYS
1	A	520	LYS
1	A	539	ILE
1	A	559	THR
1	A	609	SER
1	A	615	TRP
1	A	625	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	502	GLN
1	A	507	GLN
1	A	558	HIS
1	A	560	GLN

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Mol	Chain	Res	Type
1	A	614	GLN

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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	A	647	-	4,4,4	0.37	0	6,6,6	0.12	0
2	SO4	A	648	-	4,4,4	0.39	0	6,6,6	0.12	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	648	SO4	1	2

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	146/192 (76%)	3.19	117 (80%) 0 0	21, 40, 52, 60	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	611	GLY	10.4
1	A	546	SER	7.7
1	A	536	CYS	7.4
1	A	483	CYS	7.4
1	A	516	ALA	7.1
1	A	534	GLY	6.7
1	A	541	ALA	6.4
1	A	503	CYS	6.4
1	A	622	ARG	6.4
1	A	512	THR	5.6
1	A	535	ILE	5.3
1	A	508	GLY	5.3
1	A	551	ASN	5.2
1	A	515	CYS	4.9
1	A	525	ARG	4.8
1	A	519	SER	4.8
1	A	613	VAL	4.7
1	A	572	CYS	4.7
1	A	511	CYS	4.6
1	A	556	ASN	4.6
1	A	500	GLY	4.5
1	A	580	CYS	4.5
1	A	640	ASP	4.5
1	A	555	CYS	4.5
1	A	561	VAL	4.4
1	A	540	THR	4.3
1	A	513	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	524	CYS	4.3
1	A	506	SER	4.2
1	A	514	HIS	4.2
1	A	528	SER	4.2
1	A	637	GLY	4.2
1	A	624	ILE	4.0
1	A	526	ASP	4.0
1	A	597	CYS	3.9
1	A	598	CYS	3.8
1	A	543	CYS	3.8
1	A	594	CYS	3.8
1	A	547	ASP	3.7
1	A	616	ASN	3.7
1	A	614	GLN	3.7
1	A	505	PRO	3.6
1	A	566	GLN	3.5
1	A	553	THR	3.5
1	A	542	LEU	3.5
1	A	538	GLY	3.5
1	A	527	ASP	3.5
1	A	558	HIS	3.5
1	A	562	CYS	3.4
1	A	630	SER	3.4
1	A	644	ARG	3.4
1	A	499	PRO	3.4
1	A	608	ALA	3.4
1	A	522	GLU	3.3
1	A	618	TYR	3.3
1	A	498	LYS	3.3
1	A	485	TYR	3.3
1	A	548	PRO	3.3
1	A	641	VAL	3.3
1	A	591	LYS	3.2
1	A	595	HIS	3.2
1	A	507	GLN	3.2
1	A	520	LYS	3.2
1	A	582	CYS	3.2
1	A	607	CYS	3.2
1	A	510	CYS	3.2
1	A	544	PRO	3.2
1	A	549	LYS	3.1
1	A	621	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	517	PHE	3.1
1	A	619	PHE	3.1
1	A	497	LEU	3.0
1	A	620	LEU	3.0
1	A	518	LYS	3.0
1	A	532	LYS	3.0
1	A	560	GLN	3.0
1	A	563	ILE	3.0
1	A	581	THR	2.9
1	A	623	THR	2.9
1	A	631	PRO	2.9
1	A	617	LYS	2.9
1	A	545	ALA	2.9
1	A	642	PHE	2.8
1	A	570	SER	2.8
1	A	521	THR	2.7
1	A	502	GLN	2.7
1	A	567	CYS	2.6
1	A	645	CYS	2.6
1	A	643	MET	2.6
1	A	605	SER	2.6
1	A	537	ASN	2.6
1	A	612	SER	2.6
1	A	628	PRO	2.6
1	A	596	VAL	2.6
1	A	615	TRP	2.5
1	A	571	ILE	2.5
1	A	610	THR	2.5
1	A	634	ASP	2.5
1	A	604	PRO	2.5
1	A	573	GLU	2.5
1	A	646	ARG	2.5
1	A	530	CYS	2.4
1	A	539	ILE	2.4
1	A	564	ASN	2.4
1	A	638	TYR	2.4
1	A	635	PHE	2.3
1	A	531	ALA	2.3
1	A	632	CYS	2.3
1	A	559	THR	2.2
1	A	504	SER	2.2
1	A	550	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	552	PHE	2.2
1	A	496	LYS	2.1
1	A	609	SER	2.1
1	A	575	HIS	2.1
1	A	599	MET	2.1
1	A	606	THR	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](#)

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	SO4	A	648	5/5	0.22	0.23	87,87,88,88	0
2	SO4	A	647	5/5	0.55	0.31	61,62,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.