



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:42 AM UTC

PDB ID : 1H30 / pdb_00001h30
Title : C-terminal LG domain pair of human Gas6
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Deposited on : 2002-08-21
Resolution : 2.20 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

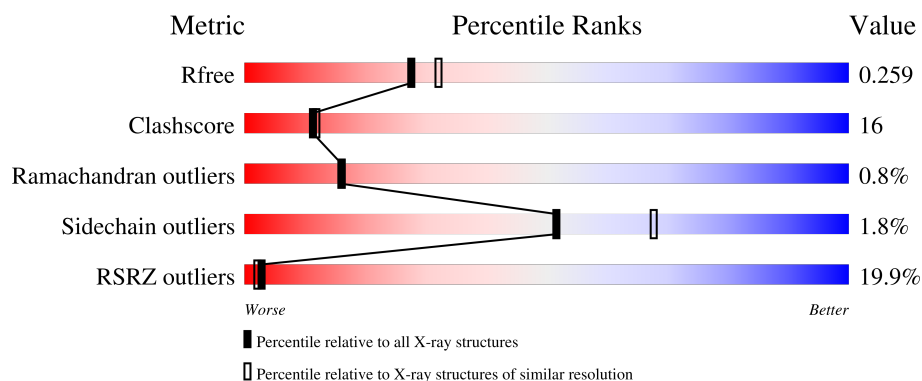
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	422	18% 64% 26% • 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3182 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.

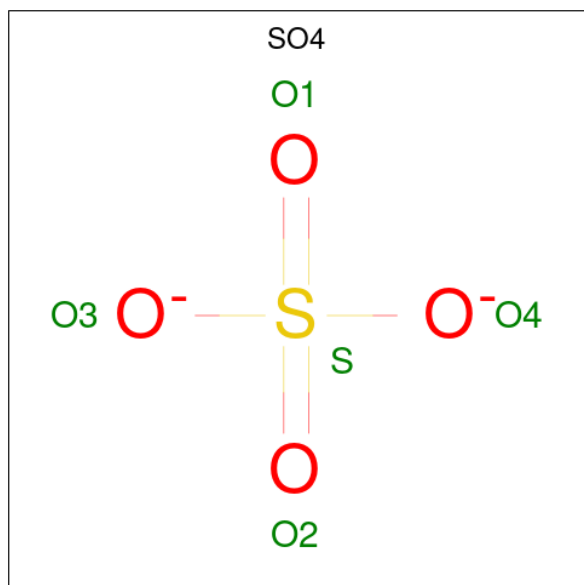
- Molecule 1 is a protein called GROWTH-ARREST-SPECIFIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3049	1937	542	554	16			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total 122	O 122	0	0

● Molecule 1: GROWTH-ARREST-SPECIFIC PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	111.31Å 111.31Å 217.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.7 (20.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.259 0.234 , 0.259	Depositor DCC
R_{free} test set	3471 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	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	0.93	EDS
Total number of atoms	3182	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CA, 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	0.39	0/3113	0.95	20/4225 (0.5%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	667	ALA	N-CA-C	7.33	119.28	111.28
1	A	328	PHE	N-CA-C	-6.77	104.92	113.72
1	A	438	ASN	CA-C-N	6.74	126.69	119.28
1	A	438	ASN	C-N-CA	6.74	126.69	119.28
1	A	663	SER	N-CA-C	6.03	120.18	112.34
1	A	335	LEU	N-CA-C	5.96	117.21	108.14
1	A	292	VAL	N-CA-C	5.92	116.58	110.36
1	A	677	ALA	N-CA-C	5.89	117.70	111.28
1	A	553	VAL	N-CA-C	-5.87	99.90	108.11
1	A	343	SER	CA-C-O	5.58	121.17	117.94
1	A	556	ALA	N-CA-C	5.54	117.61	109.24
1	A	552	LEU	N-CA-C	5.54	117.83	109.41
1	A	343	SER	CB-CA-C	-5.29	109.45	117.07
1	A	439	PRO	N-CA-C	5.24	120.73	113.65
1	A	272	GLN	CB-CA-C	-5.23	110.52	116.54
1	A	533	VAL	CA-C-N	5.08	125.11	119.32
1	A	533	VAL	C-N-CA	5.08	125.11	119.32
1	A	426	ILE	CA-C-N	5.08	125.15	119.87
1	A	426	ILE	C-N-CA	5.08	125.15	119.87
1	A	560	THR	N-CA-C	5.02	116.94	108.96

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	3049	0	3051	99	0
2	A	1	0	0	0	0
3	A	10	0	0	0	0
4	A	122	0	0	4	0
All	All	3182	0	3051	99	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 16.

All (99) 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:516:ALA:HB3	1:A:641:ARG:HG3	1.55	0.87
1:A:444:CYS:HB2	4:A:2010:HOH:O	1.78	0.83
1:A:272:GLN:HA	1:A:549:LYS:NZ	1.95	0.81
1:A:567:ILE:HG23	1:A:569:VAL:HG13	1.62	0.80
1:A:314:LEU:O	1:A:315:GLN:HB3	1.83	0.77
1:A:599:VAL:HB	1:A:603:GLN:HG3	1.64	0.76
1:A:650:ARG:HB2	1:A:650:ARG:HH11	1.49	0.76
1:A:313:ARG:HG2	1:A:317:THR:HG21	1.66	0.76
1:A:650:ARG:HB2	1:A:650:ARG:NH1	2.01	0.75
1:A:318:ARG:NH2	1:A:388:ALA:HB2	2.02	0.73
1:A:272:GLN:HA	1:A:549:LYS:HZ3	1.55	0.69
1:A:566:GLU:H	1:A:566:GLU:CD	2.01	0.68
1:A:540:VAL:HG22	1:A:636:VAL:HG21	1.75	0.67
1:A:314:LEU:HD13	1:A:416:LEU:HD13	1.75	0.67
1:A:415:GLY:C	1:A:416:LEU:HD22	2.24	0.62
1:A:341:GLN:HE21	1:A:360:ARG:NH1	1.98	0.62
1:A:402:LYS:HB3	1:A:402:LYS:NZ	2.16	0.61
1:A:677:ALA:O	1:A:678:ALA:HB3	2.02	0.60
1:A:374:ILE:HG23	1:A:380:GLN:NE2	2.17	0.60
1:A:307:ILE:HD13	1:A:461:THR:HB	1.85	0.59
1:A:355:LEU:HG	1:A:374:ILE:HG13	1.85	0.58
1:A:514:ARG:NH2	4:A:2062:HOH:O	2.37	0.58
1:A:298:GLY:O	1:A:299:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TYR:CZ	1:A:298:GLY:HA3	2.40	0.57
1:A:600:SER:OG	1:A:603:GLN:HG2	2.05	0.57
1:A:505:TRP:NE1	1:A:612:GLU:HG2	2.20	0.56
1:A:306:VAL:HG22	1:A:423:VAL:O	2.04	0.56
1:A:335:LEU:HD23	1:A:348:LEU:HB3	1.87	0.56
1:A:445:MET:HE2	1:A:448:TRP:CD1	2.41	0.56
1:A:318:ARG:HH21	1:A:388:ALA:HB2	1.70	0.56
1:A:357:LEU:HD22	1:A:393:ILE:HD11	1.87	0.55
1:A:265:ARG:HD3	4:A:2092:HOH:O	2.06	0.55
1:A:344:THR:HA	1:A:360:ARG:O	2.07	0.55
1:A:599:VAL:HB	1:A:603:GLN:CG	2.37	0.54
1:A:336:PHE:HB3	1:A:422:THR:OG1	2.08	0.54
1:A:310:ARG:HG2	1:A:420:ASN:OD1	2.07	0.54
1:A:288:VAL:O	1:A:288:VAL:HG12	2.09	0.53
1:A:341:GLN:HE21	1:A:360:ARG:HH11	1.56	0.53
1:A:370:SER:C	1:A:372:PRO:CD	2.82	0.52
1:A:600:SER:H	1:A:603:GLN:NE2	2.06	0.52
1:A:516:ALA:HB3	1:A:641:ARG:CG	2.34	0.52
1:A:357:LEU:HD23	1:A:403:ILE:HD12	1.92	0.51
1:A:505:TRP:CD1	1:A:612:GLU:HG2	2.46	0.50
1:A:305:PRO:HB3	1:A:422:THR:HB	1.94	0.50
1:A:557:VAL:HG21	1:A:607:ARG:HB3	1.93	0.50
1:A:341:GLN:NE2	1:A:360:ARG:NH1	2.61	0.49
1:A:374:ILE:HG23	1:A:380:GLN:HE22	1.76	0.49
1:A:312:LYS:N	1:A:312:LYS:HD2	2.28	0.48
1:A:374:ILE:HD12	1:A:380:GLN:NE2	2.28	0.48
1:A:429:HIS:CD2	1:A:431:LYS:H	2.31	0.48
1:A:314:LEU:O	1:A:315:GLN:CB	2.58	0.48
1:A:265:ARG:NH1	1:A:626:LEU:O	2.47	0.47
1:A:445:MET:HE2	1:A:448:TRP:HD1	1.79	0.47
1:A:540:VAL:HG22	1:A:636:VAL:CG2	2.44	0.47
1:A:373:VAL:HG13	1:A:373:VAL:O	2.13	0.47
1:A:371:GLY:N	1:A:372:PRO:HD3	2.29	0.47
1:A:413:GLU:O	1:A:414:ARG:HB2	2.15	0.47
1:A:445:MET:HB3	1:A:448:TRP:HE1	1.80	0.47
1:A:386:GLU:HA	1:A:391:LEU:HD23	1.96	0.46
1:A:272:GLN:HA	1:A:549:LYS:CE	2.45	0.46
1:A:359:LEU:HD12	1:A:359:LEU:N	2.30	0.46
1:A:416:LEU:HD22	1:A:416:LEU:N	2.31	0.46
1:A:368:THR:OG1	1:A:403:ILE:HD11	2.16	0.45
1:A:438:ASN:ND2	1:A:657:GLU:OE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:OE1	1:A:418:HIS:ND1	2.49	0.45
1:A:270:LEU:HD21	1:A:274:MET:HB3	1.98	0.45
1:A:306:VAL:O	1:A:307:ILE:HG13	2.16	0.45
1:A:421:LEU:C	1:A:421:LEU:HD23	2.42	0.45
1:A:354:ARG:NH1	1:A:371:GLY:O	2.50	0.45
1:A:465:ASN:O	1:A:467:ARG:N	2.50	0.45
1:A:543:HIS:HB2	1:A:552:LEU:HD11	1.98	0.44
1:A:566:GLU:CD	1:A:566:GLU:N	2.73	0.44
1:A:550:LYS:NZ	1:A:550:LYS:HB3	2.33	0.44
1:A:316:PRO:HG3	1:A:417:TYR:CZ	2.53	0.44
1:A:567:ILE:CG2	1:A:569:VAL:HG13	2.41	0.44
1:A:465:ASN:O	1:A:466:THR:C	2.60	0.44
1:A:557:VAL:O	1:A:557:VAL:HG23	2.18	0.43
1:A:463:LYS:HG3	1:A:463:LYS:O	2.18	0.43
1:A:677:ALA:O	1:A:678:ALA:CB	2.67	0.43
1:A:470:CYS:HB3	4:A:2010:HOH:O	2.17	0.43
1:A:350:LEU:HD12	1:A:354:ARG:C	2.44	0.43
1:A:396:ASN:O	1:A:397:ARG:HB2	2.18	0.43
1:A:298:GLY:O	1:A:299:ARG:CB	2.67	0.43
1:A:512:HIS:CD2	1:A:576:VAL:HG22	2.54	0.43
1:A:601:ALA:O	1:A:605:GLN:HG2	2.19	0.42
1:A:318:ARG:CZ	1:A:388:ALA:HB2	2.49	0.42
1:A:422:THR:HG21	1:A:427:PRO:HG3	2.01	0.42
1:A:323:PHE:CG	1:A:445:MET:HE3	2.55	0.41
1:A:329:ASP:HA	1:A:330:PRO:HD3	1.86	0.41
1:A:650:ARG:HH11	1:A:650:ARG:CB	2.24	0.41
1:A:374:ILE:HG23	1:A:380:GLN:CD	2.45	0.41
1:A:507:VAL:HG11	1:A:535:LEU:HD21	2.03	0.41
1:A:323:PHE:CD1	1:A:445:MET:HE3	2.55	0.41
1:A:357:LEU:HD23	1:A:403:ILE:CD1	2.51	0.41
1:A:371:GLY:N	1:A:372:PRO:CD	2.83	0.41
1:A:402:LYS:HB3	1:A:402:LYS:HZ2	1.84	0.40
1:A:607:ARG:HA	1:A:607:ARG:NE	2.35	0.40
1:A:410:PHE:CE1	1:A:419:LEU:HD22	2.56	0.40
1:A:504:THR:O	1:A:504:THR:HG22	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	381/422 (90%)	362 (95%)	16 (4%)	3 (1%)	16	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	THR
1	A	315	GLN
1	A	464	VAL

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	330/356 (93%)	324 (98%)	6 (2%)	51	68

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

Mol	Chain	Res	Type
1	A	359	LEU
1	A	430	GLU
1	A	550	LYS
1	A	555	LEU
1	A	564	LEU
1	A	604	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	341	GLN
1	A	380	GLN
1	A	429	HIS
1	A	469	GLN
1	A	543	HIS
1	A	551	GLN
1	A	603	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	SO4	A	703	-	4,4,4	0.37	0	6,6,6	0.07	0
3	SO4	A	702	-	4,4,4	0.38	0	6,6,6	0.10	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.

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	391/422 (92%)	0.73	78 (19%) 3 2	12, 35, 80, 94	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	6.0
1	A	363	GLY	5.6
1	A	312	LYS	5.4
1	A	411	GLN	5.4
1	A	462	VAL	5.3
1	A	270	LEU	4.9
1	A	464	VAL	4.7
1	A	306	VAL	4.6
1	A	542	TYR	4.4
1	A	371	GLY	4.1
1	A	559	HIS	4.1
1	A	418	HIS	4.0
1	A	315	GLN	4.0
1	A	271	SER	4.0
1	A	448	TRP	4.0
1	A	340	HIS	4.0
1	A	264	GLY	4.0
1	A	451	LEU	3.9
1	A	342	ASP	3.9
1	A	263	ASP	3.7
1	A	274	MET	3.6
1	A	314	LEU	3.6
1	A	543	HIS	3.6
1	A	412	PRO	3.6
1	A	272	GLN	3.6
1	A	299	ARG	3.5
1	A	549	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	3.5
1	A	372	PRO	3.5
1	A	261	HIS	3.4
1	A	370	SER	3.4
1	A	262	CYS	3.4
1	A	417	TYR	3.3
1	A	678	ALA	3.3
1	A	397	ARG	3.2
1	A	266	GLY	3.2
1	A	494	ARG	3.1
1	A	415	GLY	3.1
1	A	617	SER	3.0
1	A	265	ARG	3.0
1	A	268	LEU	2.9
1	A	313	ARG	2.9
1	A	278	GLU	2.9
1	A	273	ASP	2.9
1	A	616	ARG	2.8
1	A	582	ARG	2.8
1	A	461	THR	2.7
1	A	504	THR	2.7
1	A	467	ARG	2.6
1	A	276	THR	2.6
1	A	317	THR	2.5
1	A	410	PHE	2.5
1	A	463	LYS	2.5
1	A	311	PHE	2.5
1	A	369	SER	2.4
1	A	466	THR	2.4
1	A	414	ARG	2.4
1	A	388	ALA	2.4
1	A	362	ASN	2.4
1	A	403	ILE	2.4
1	A	291	SER	2.3
1	A	279	ASP	2.3
1	A	308	ARG	2.3
1	A	277	CYS	2.3
1	A	613	ARG	2.2
1	A	594	ARG	2.2
1	A	373	VAL	2.2
1	A	465	ASN	2.2
1	A	503	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	305	PRO	2.2
1	A	275	ASP	2.1
1	A	606	GLU	2.1
1	A	280	ILE	2.1
1	A	402	LYS	2.1
1	A	413	GLU	2.1
1	A	310	ARG	2.0
1	A	298	GLY	2.0
1	A	316	PRO	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
3	SO4	A	703	5/5	0.78	0.18	99,99,100,100	0
3	SO4	A	702	5/5	0.82	0.17	82,82,85,85	0
2	CA	A	701	1/1	0.99	0.09	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.