



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H72
Title : CRYSTAL STRUCTURE OF HOMOSERINE KINASE COMPLEXED WITH HSE
Authors : Krishna, S.S.; Zhou, T.; Daugherty, M.; Osterman, A.L.; Zhang, H.
Deposited on : 2001-07-02
Resolution : 1.80 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

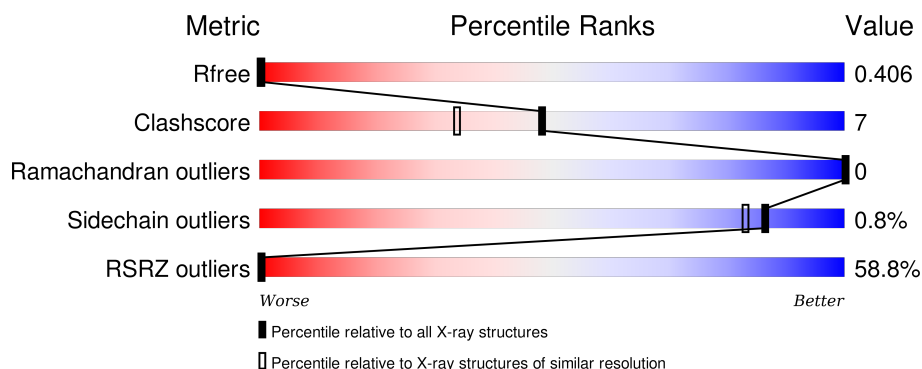
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	C	296	<div> <div>59%</div> <div>86%</div> <div>14%</div> </div>

2 Entry composition [i](#)

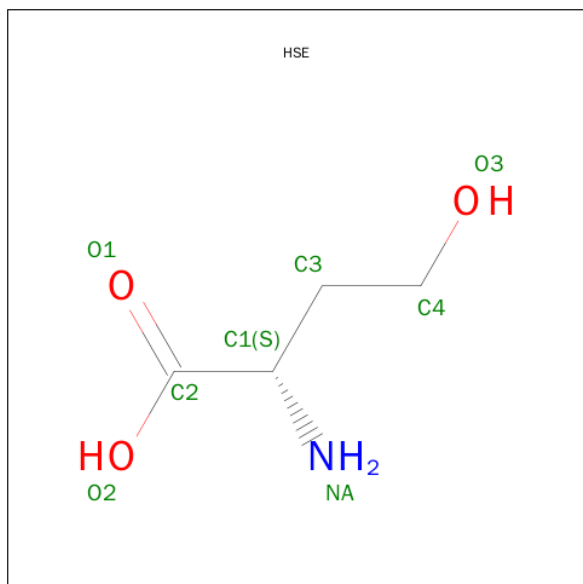
There are 5 unique types of molecules in this entry. The entry contains 2669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HOMOSERINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	296	Total	C	N	O	S	0	7	0
			2314	1484	373	448	9			

- Molecule 2 is L-HOMOSERINE (three-letter code: HSE) (formula: $C_4H_9NO_3$).



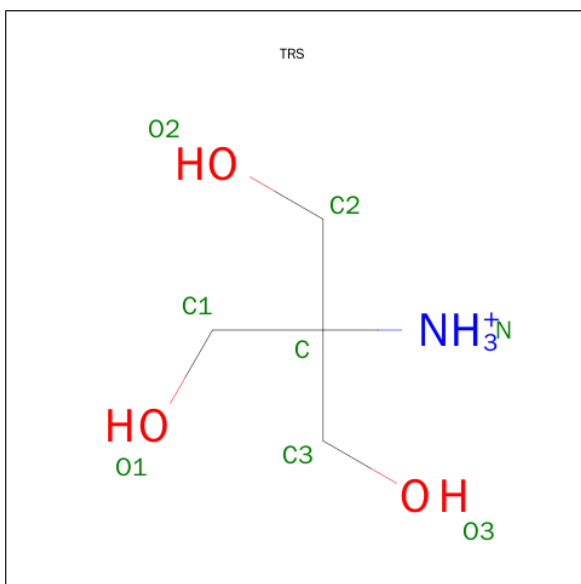
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

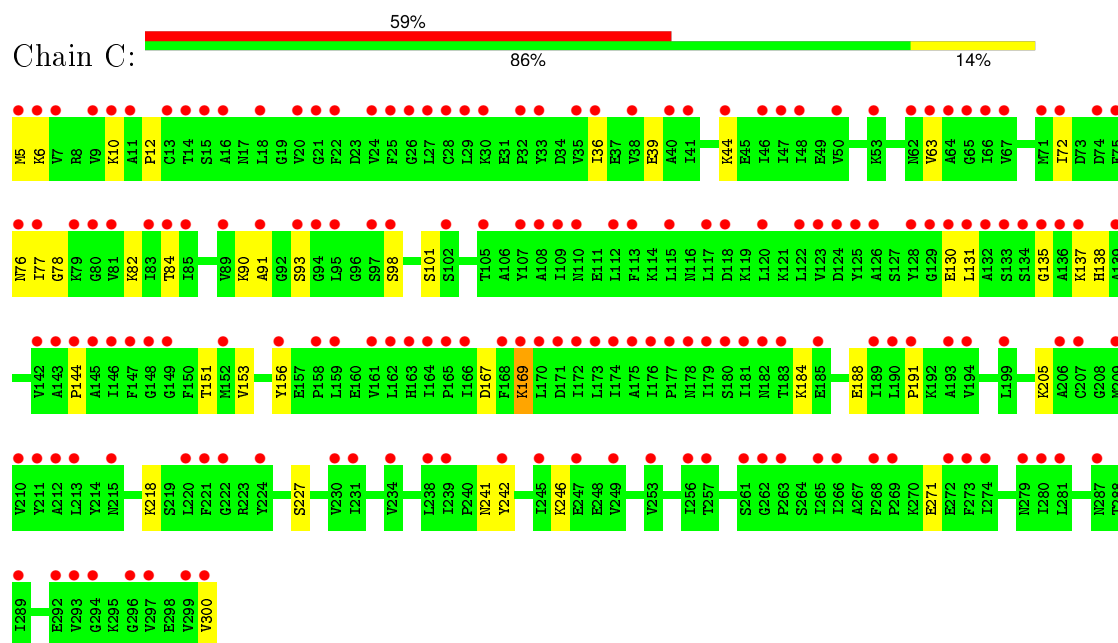
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	308	Total 308	O 308	0	0

3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: HOMOSERINE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.99 Å 87.99 Å 99.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 40.22 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.80) 98.7 (40.22-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 1.81 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.207 0.388 , 0.406	Depositor DCC
R_{free} test set	1709 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36244 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2669	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TRS, ANP, HSE

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	C	0.68	0/2350	0.80	0/3169

There are no bond length outliers.

There are no bond angle outliers.

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	C	2314	0	2374	33	1
2	C	8	0	9	0	0
3	C	31	0	13	4	0
4	C	8	0	12	1	1
5	C	308	0	0	15	1
All	All	2669	0	2408	34	2

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 7.

All (34) 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:C:91:ALA:HB1	3:C:1301:ANP:H5'2	1.68	0.75
1:C:5:MET:N	5:C:2001:HOH:O	2.23	0.72
1:C:184:LYS:O	1:C:188:GLU:HG3	1.92	0.69
1:C:5:MET:HB3	5:C:2002:HOH:O	1.92	0.69
1:C:137:LYS:O	1:C:137:LYS:HG2	1.98	0.64
1:C:242:TYR:CZ	1:C:246:LYS:HD2	2.34	0.62
1:C:138:HIS:HB2	5:C:2167:HOH:O	2.02	0.59
1:C:169:LYS:HA	5:C:2187:HOH:O	2.01	0.59
1:C:98[B]:SER:HB2	3:C:1301:ANP:O5'	2.03	0.58
1:C:169:LYS:O	1:C:218:LYS:HE2	2.06	0.55
4:C:1302:TRS:H31	5:C:2122:HOH:O	2.05	0.55
1:C:271:GLU:HG3	5:C:2188:HOH:O	2.08	0.53
1:C:167:ASP:HB3	5:C:2183:HOH:O	2.09	0.52
1:C:72:ILE:HA	1:C:77:ILE:HD12	1.92	0.52
1:C:169:LYS:NZ	5:C:2185:HOH:O	2.45	0.50
1:C:63:VAL:HG11	1:C:98[B]:SER:OG	2.11	0.50
1:C:130:GLU:OE1	5:C:2163:HOH:O	2.20	0.48
1:C:6:LYS:HG2	1:C:39:GLU:HB2	1.96	0.47
1:C:191:PRO:HG3	5:C:2121:HOH:O	2.15	0.47
1:C:98[A]:SER:HB3	3:C:1301:ANP:O5'	2.14	0.47
1:C:184:LYS:HG3	5:C:2198:HOH:O	2.15	0.47
1:C:36:ILE:HD11	1:C:101:SER:HA	1.96	0.47
1:C:205:LYS:HG3	1:C:227[A]:SER:OG	2.15	0.47
1:C:10:LYS:HG2	1:C:300[B]:VAL:HG13	1.96	0.46
1:C:82:LYS:NZ	5:C:2111:HOH:O	2.49	0.45
1:C:84[B]:THR:HG23	5:C:2112:HOH:O	2.18	0.44
1:C:153:VAL:HG11	1:C:156:TYR:CZ	2.53	0.43
1:C:44:LYS:HE2	1:C:78:GLY:O	2.18	0.42
1:C:241:ASN:ND2	5:C:2245:HOH:O	2.28	0.42
1:C:91:ALA:HA	3:C:1301:ANP:O2A	2.19	0.42
1:C:138:HIS:CB	5:C:2167:HOH:O	2.65	0.42
1:C:90:LYS:HG3	1:C:93[B]:SER:OG	2.19	0.41
1:C:131:LEU:O	1:C:135:GLY:N	2.50	0.41
1:C:144:PRO:HD3	1:C:151:THR:OG1	2.21	0.40

All (2) 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)
5:C:2197:HOH:O	5:C:2197:HOH:O[8_665]	2.04	0.16
1:C:76:ASN:OD1	4:C:1302:TRS:O3[3_644]	2.18	0.02

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	C	300/296 (101%)	296 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	C	255/248 (103%)	253 (99%)	2 (1%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	PRO
1	C	169	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	155	ASN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	HSE	C	1300	-	4,7,7	0.41	0	2,8,8	1.54	0
3	ANP	C	1301	1	27,33,33	2.03	6 (22%)	30,52,52	2.89	12 (40%)
4	TRS	C	1302	-	7,7,7	2.24	2 (28%)	9,9,9	2.96	6 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HSE	C	1300	-	-	0/3/7/7	0/0/0/0
3	ANP	C	1301	1	-	0/12/38/38	0/3/3/3
4	TRS	C	1302	-	-	0/9/9/9	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1302	TRS	C-N	-3.33	1.45	1.50
3	C	1301	ANP	PB-O2B	-3.33	1.47	1.56
3	C	1301	ANP	C2-N1	2.18	1.38	1.33
3	C	1301	ANP	PB-O1B	2.76	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1301	ANP	O4'-C1'	4.03	1.46	1.41
4	C	1302	TRS	C1-C	4.20	1.61	1.53
3	C	1301	ANP	PG-O1G	4.72	1.51	1.46
3	C	1301	ANP	PG-N3B	5.33	1.77	1.63

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	ANP	N3-C2-N1	-7.40	123.23	128.89
3	C	1301	ANP	O1B-PB-N3B	-5.80	103.00	111.90
4	C	1302	TRS	C2-C-C1	-4.24	101.60	110.78
4	C	1302	TRS	O1-C1-C	-4.12	102.84	111.18
3	C	1301	ANP	O1G-PG-N3B	-3.33	106.79	111.90
3	C	1301	ANP	O4'-C4'-C3'	-3.31	98.47	105.15
3	C	1301	ANP	O3'-C3'-C4'	-2.62	103.18	111.05
4	C	1302	TRS	O2-C2-C	-2.31	106.51	111.18
3	C	1301	ANP	O3A-PA-O5'	-2.30	96.85	102.94
3	C	1301	ANP	O4'-C4'-C5'	2.30	117.56	109.32
4	C	1302	TRS	O3-C3-C	2.37	115.98	111.18
3	C	1301	ANP	O2'-C2'-C3'	2.49	119.91	111.83
3	C	1301	ANP	O3A-PB-N3B	2.74	113.98	106.44
3	C	1301	ANP	PA-O3A-PB	3.22	143.46	132.67
4	C	1302	TRS	C3-C-N	3.34	114.16	108.09
4	C	1302	TRS	C2-C-N	3.96	115.30	108.09
3	C	1301	ANP	O4'-C1'-N9	5.29	119.18	108.10
3	C	1301	ANP	C4'-O4'-C1'	7.22	117.66	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	ANP	4	0
4	C	1302	TRS	1	1

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	C	296/296 (100%)	2.36	174 (58%) 0 0	14, 22, 42, 55	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	GLY	8.1
1	C	136	ALA	6.4
1	C	5	MET	6.1
1	C	7	VAL	6.1
1	C	168	PHE	4.9
1	C	300[A]	VAL	4.9
1	C	189	ILE	4.8
1	C	28	CYS	4.7
1	C	134	SER	4.7
1	C	148	GLY	4.7
1	C	109	ILE	4.5
1	C	179	ILE	4.4
1	C	115	LEU	4.4
1	C	83	ILE	4.3
1	C	231	ILE	4.3
1	C	25	PHE	4.1
1	C	35	VAL	4.1
1	C	170	LEU	4.1
1	C	132	ALA	4.1
1	C	16	ALA	4.1
1	C	299	VAL	4.0
1	C	91	ALA	4.0
1	C	89	VAL	4.0
1	C	131	LEU	3.9
1	C	93[A]	SER	3.9
1	C	46	ILE	3.7
1	C	33	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	77	ILE	3.7
1	C	85	ILE	3.7
1	C	75	PHE	3.7
1	C	280	ILE	3.6
1	C	169	LYS	3.6
1	C	84[A]	THR	3.6
1	C	129	GLY	3.6
1	C	173	LEU	3.6
1	C	181	ILE	3.5
1	C	274	ILE	3.5
1	C	221	PHE	3.5
1	C	125	TYR	3.5
1	C	50	VAL	3.5
1	C	20	VAL	3.4
1	C	162	LEU	3.4
1	C	253	VAL	3.3
1	C	27	LEU	3.3
1	C	113	PHE	3.3
1	C	147	PHE	3.3
1	C	180	SER	3.3
1	C	190	LEU	3.3
1	C	249	VAL	3.3
1	C	212	ALA	3.3
1	C	145	ALA	3.2
1	C	174	ILE	3.2
1	C	296	GLY	3.2
1	C	135	GLY	3.2
1	C	158	PRO	3.2
1	C	117	LEU	3.1
1	C	81	VAL	3.1
1	C	66	ILE	3.1
1	C	41	ILE	3.1
1	C	166	ILE	3.1
1	C	95	LEU	3.1
1	C	79	LYS	3.1
1	C	80	GLY	3.1
1	C	44	LYS	3.1
1	C	161	VAL	3.1
1	C	14	THR	3.0
1	C	152	MET	3.0
1	C	183	THR	3.0
1	C	268	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	156	TYR	3.0
1	C	211	TYR	3.0
1	C	273	PHE	3.0
1	C	29	LEU	3.0
1	C	245	ILE	3.0
1	C	191	PRO	3.0
1	C	263	PRO	2.9
1	C	164	ILE	2.9
1	C	98[A]	SER	2.9
1	C	63	VAL	2.9
1	C	146	ILE	2.9
1	C	107	TYR	2.9
1	C	177	PRO	2.8
1	C	185	GLU	2.8
1	C	22	PHE	2.8
1	C	123	VAL	2.8
1	C	97	SER	2.8
1	C	94	GLY	2.8
1	C	234	VAL	2.8
1	C	133	SER	2.8
1	C	72	ILE	2.8
1	C	210	VAL	2.8
1	C	130	GLU	2.8
1	C	47	ILE	2.7
1	C	110	ASN	2.7
1	C	120	LEU	2.7
1	C	38	VAL	2.7
1	C	142	VAL	2.7
1	C	65	GLY	2.7
1	C	293	VAL	2.7
1	C	74	ASP	2.7
1	C	178	ASN	2.6
1	C	9	VAL	2.6
1	C	24	VAL	2.6
1	C	194	VAL	2.6
1	C	6	LYS	2.6
1	C	265	ILE	2.6
1	C	239	ILE	2.6
1	C	18	LEU	2.6
1	C	182	ASN	2.6
1	C	220	LEU	2.6
1	C	13	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	53	LYS	2.5
1	C	272	GLU	2.5
1	C	224	TYR	2.5
1	C	262	GLY	2.5
1	C	126	ALA	2.5
1	C	199	LEU	2.5
1	C	21	GLY	2.5
1	C	172	ILE	2.5
1	C	112	LEU	2.5
1	C	238	LEU	2.4
1	C	11	ALA	2.4
1	C	26	GLY	2.4
1	C	71	MET	2.4
1	C	247	GLU	2.4
1	C	206	ALA	2.4
1	C	32	PRO	2.4
1	C	165	PRO	2.4
1	C	15[A]	SER	2.4
1	C	176	ILE	2.3
1	C	76	ASN	2.3
1	C	144	PRO	2.3
1	C	62	ASN	2.3
1	C	124	ASP	2.3
1	C	266	ILE	2.3
1	C	128	TYR	2.3
1	C	193	ALA	2.3
1	C	297	VAL	2.3
1	C	36	ILE	2.3
1	C	122	LEU	2.3
1	C	163	HIS	2.3
1	C	64	ALA	2.3
1	C	215	ASN	2.2
1	C	149	GLY	2.2
1	C	102	SER	2.2
1	C	242	TYR	2.2
1	C	118	ASP	2.2
1	C	256	ILE	2.2
1	C	207	CYS	2.2
1	C	261	SER	2.2
1	C	171	ASP	2.1
1	C	30	LYS	2.1
1	C	143	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	230	VAL	2.1
1	C	10	LYS	2.1
1	C	137	LYS	2.1
1	C	175	ALA	2.1
1	C	67	VAL	2.1
1	C	292	GLU	2.1
1	C	289	ILE	2.1
1	C	159	LEU	2.1
1	C	40	ALA	2.1
1	C	257	THR	2.1
1	C	209	MET	2.1
1	C	222	GLY	2.1
1	C	269	PRO	2.1
1	C	213	LEU	2.1
1	C	105	THR	2.1
1	C	108	ALA	2.0
1	C	279	ASN	2.0
1	C	48	ILE	2.0
1	C	281	LEU	2.0
1	C	287	ASN	2.0
1	C	139	ALA	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ANP	C	1301	31/31	0.71	0.27	0.58	18,41,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	TRS	C	1302	8/8	0.60	0.25	0.34	20,33,36,36	0
2	HSE	C	1300	8/8	0.76	0.23	0.18	26,28,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.