



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:35 pm GMT

PDB ID : 1H72
Title : CRYSTAL STRUCTURE OF HOMOSERINE KINASE COMPLEXED WITH HSE
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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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

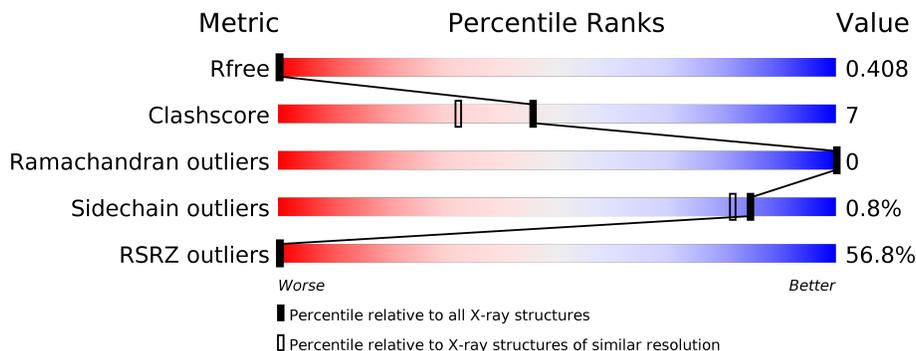
1 Overall quality at a glance

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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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	

2 Entry composition [i](#)

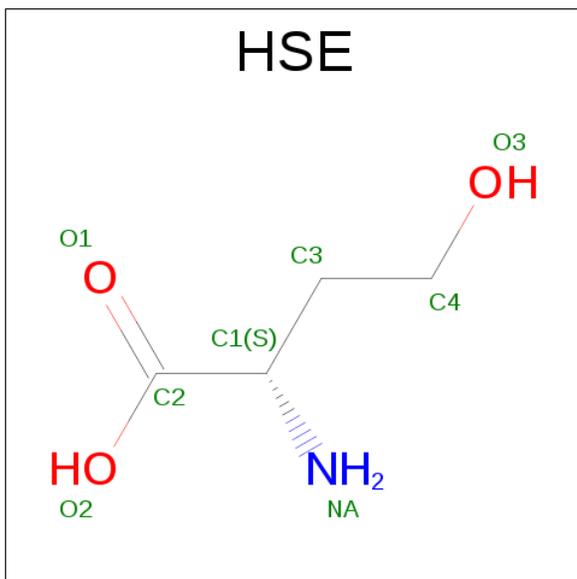
There are 5 unique types of molecules in this entry. The entry contains 2669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	C	296	2314	1484	373	448	9	0	7	0

- Molecule 2 is L-HOMOSERINE (three-letter code: HSE) (formula: C₄H₉NO₃).



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

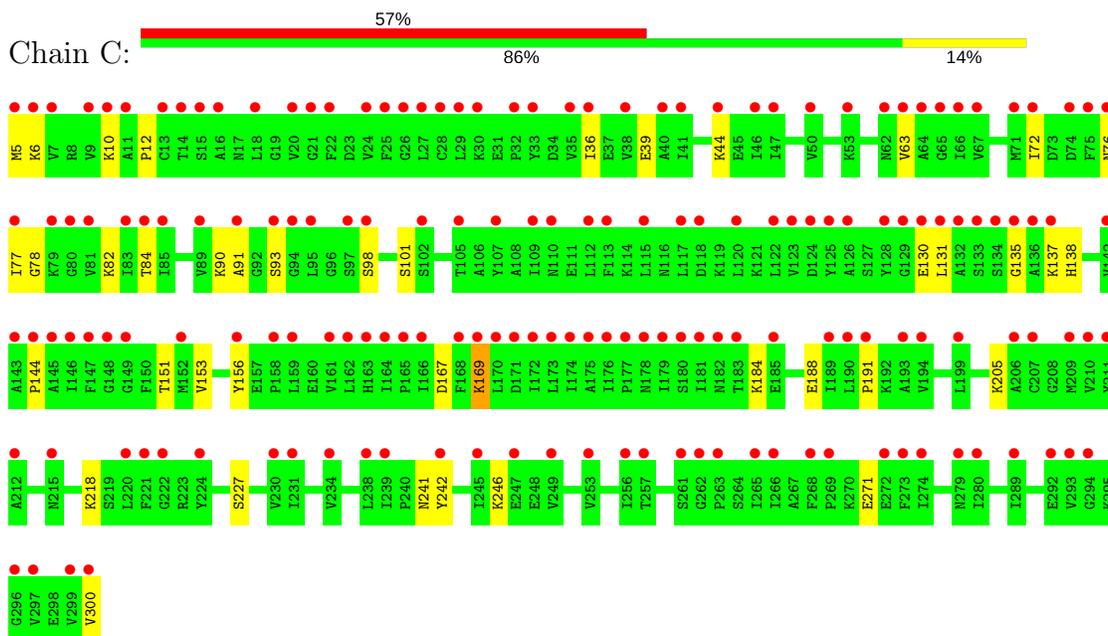
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

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

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 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: 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	87.99Å 87.99Å 99.30Å 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 1.81Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.207 0.387 , 0.408	Depositor DCC
R_{free} test set	1706 reflections (4.71%)	DCC
Wilson B-factor (Å ²)	21.0	Xtrriage
Anisotropy	0.646	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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:36:ILE:HD11	1:C:101:SER:HA	1.96	0.47
1:C:184:LYS:HG3	5:C:2198:HOH:O	2.15	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%)	85 81

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	-	2,7,7	0.28	0	1,8,8	1.06	0
3	ANP	C	1301	1	29,33,33	2.10	7 (24%)	28,52,52	2.72	11 (39%)
4	TRS	C	1302	-	7,7,7	1.66	1 (14%)	9,9,9	2.33	4 (44%)

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	-	0/13/38/38	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)
3	C	1301	ANP	C2'-C1'	-4.09	1.47	1.53
3	C	1301	ANP	PB-O2B	-3.39	1.47	1.56
3	C	1301	ANP	C2-N1	2.20	1.38	1.33
3	C	1301	ANP	PB-O1B	2.77	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1302	TRS	C1-C	3.50	1.61	1.52
3	C	1301	ANP	O4'-C1'	3.64	1.46	1.41
3	C	1301	ANP	PG-O1G	4.76	1.51	1.46
3	C	1301	ANP	PG-N3B	5.33	1.77	1.63

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	ANP	N3-C2-N1	-6.46	123.23	128.86
3	C	1301	ANP	O1B-PB-N3B	-5.88	103.00	111.79
3	C	1301	ANP	O4'-C4'-C3'	-3.37	98.47	105.17
3	C	1301	ANP	O1G-PG-N3B	-3.34	106.79	111.79
4	C	1302	TRS	C2-C-C1	-3.34	101.60	111.06
3	C	1301	ANP	O3'-C3'-C4'	-2.71	103.18	111.09
4	C	1302	TRS	O1-C1-C	-2.63	102.84	110.47
3	C	1301	ANP	O5'-C5'-C4'	2.07	116.35	109.00
3	C	1301	ANP	O4'-C4'-C5'	2.42	117.56	109.40
3	C	1301	ANP	O2'-C2'-C3'	2.52	119.91	111.83
3	C	1301	ANP	O3A-PB-N3B	2.67	113.98	106.59
4	C	1302	TRS	C3-C-N	3.02	114.16	107.73
3	C	1301	ANP	PA-O3A-PB	3.14	143.46	132.38
4	C	1302	TRS	C2-C-N	3.56	115.30	107.73
3	C	1301	ANP	C4'-O4'-C1'	7.41	117.66	109.77

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 [i](#)

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%)	2.30	168 (56%) 0 0	14, 22, 42, 55	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	GLY	7.9
1	C	136	ALA	6.3
1	C	5	MET	6.1
1	C	7	VAL	5.9
1	C	168	PHE	4.8
1	C	300[A]	VAL	4.8
1	C	189	ILE	4.7
1	C	28	CYS	4.6
1	C	134	SER	4.6
1	C	148	GLY	4.6
1	C	109	ILE	4.4
1	C	115	LEU	4.3
1	C	179	ILE	4.3
1	C	83	ILE	4.2
1	C	231	ILE	4.2
1	C	25	PHE	4.0
1	C	170	LEU	4.0
1	C	35	VAL	4.0
1	C	132	ALA	4.0
1	C	16	ALA	4.0
1	C	91	ALA	3.9
1	C	299	VAL	3.9
1	C	89	VAL	3.8
1	C	131	LEU	3.8
1	C	93[A]	SER	3.8
1	C	46	ILE	3.6
1	C	33	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	169	LYS	3.6
1	C	77	ILE	3.6
1	C	85	ILE	3.6
1	C	75	PHE	3.5
1	C	280	ILE	3.5
1	C	84[A]	THR	3.5
1	C	129	GLY	3.5
1	C	173	LEU	3.5
1	C	181	ILE	3.4
1	C	274	ILE	3.4
1	C	125	TYR	3.4
1	C	221	PHE	3.4
1	C	50	VAL	3.4
1	C	20	VAL	3.3
1	C	162	LEU	3.3
1	C	180	SER	3.2
1	C	27	LEU	3.2
1	C	253	VAL	3.2
1	C	113	PHE	3.2
1	C	147	PHE	3.2
1	C	190	LEU	3.2
1	C	212	ALA	3.2
1	C	249	VAL	3.2
1	C	145	ALA	3.2
1	C	174	ILE	3.1
1	C	296	GLY	3.1
1	C	135	GLY	3.1
1	C	158	PRO	3.1
1	C	79	LYS	3.0
1	C	117	LEU	3.0
1	C	44	LYS	3.0
1	C	81	VAL	3.0
1	C	66	ILE	3.0
1	C	80	GLY	3.0
1	C	152	MET	3.0
1	C	95	LEU	3.0
1	C	41	ILE	3.0
1	C	166	ILE	3.0
1	C	14	THR	3.0
1	C	183	THR	3.0
1	C	156	TYR	3.0
1	C	211	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	161	VAL	3.0
1	C	268	PHE	2.9
1	C	191	PRO	2.9
1	C	273	PHE	2.9
1	C	29	LEU	2.9
1	C	263	PRO	2.9
1	C	245	ILE	2.9
1	C	164	ILE	2.8
1	C	98[A]	SER	2.8
1	C	107	TYR	2.8
1	C	185	GLU	2.8
1	C	177	PRO	2.8
1	C	63	VAL	2.8
1	C	146	ILE	2.8
1	C	97	SER	2.7
1	C	22	PHE	2.7
1	C	94	GLY	2.7
1	C	130	GLU	2.7
1	C	123	VAL	2.7
1	C	133	SER	2.7
1	C	110	ASN	2.7
1	C	234	VAL	2.7
1	C	72	ILE	2.7
1	C	210	VAL	2.7
1	C	47	ILE	2.6
1	C	65	GLY	2.6
1	C	120	LEU	2.6
1	C	38	VAL	2.6
1	C	142	VAL	2.6
1	C	74	ASP	2.6
1	C	6	LYS	2.6
1	C	178	ASN	2.6
1	C	293	VAL	2.6
1	C	9	VAL	2.5
1	C	24	VAL	2.5
1	C	194	VAL	2.5
1	C	182	ASN	2.5
1	C	53	LYS	2.5
1	C	265	ILE	2.5
1	C	272	GLU	2.5
1	C	239	ILE	2.5
1	C	13	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	18	LEU	2.5
1	C	220	LEU	2.5
1	C	224	TYR	2.5
1	C	262	GLY	2.5
1	C	126	ALA	2.4
1	C	199	LEU	2.4
1	C	21	GLY	2.4
1	C	71	MET	2.4
1	C	172	ILE	2.4
1	C	112	LEU	2.4
1	C	26	GLY	2.4
1	C	247	GLU	2.4
1	C	238	LEU	2.3
1	C	11	ALA	2.3
1	C	206	ALA	2.3
1	C	32	PRO	2.3
1	C	165	PRO	2.3
1	C	15[A]	SER	2.3
1	C	76	ASN	2.3
1	C	62	ASN	2.3
1	C	144	PRO	2.3
1	C	176	ILE	2.3
1	C	124	ASP	2.3
1	C	128	TYR	2.2
1	C	193	ALA	2.2
1	C	163	HIS	2.2
1	C	266	ILE	2.2
1	C	297	VAL	2.2
1	C	36	ILE	2.2
1	C	215	ASN	2.2
1	C	122	LEU	2.2
1	C	64	ALA	2.2
1	C	149	GLY	2.2
1	C	242	TYR	2.2
1	C	102	SER	2.1
1	C	118	ASP	2.1
1	C	30	LYS	2.1
1	C	207	CYS	2.1
1	C	256	ILE	2.1
1	C	10	LYS	2.1
1	C	261	SER	2.1
1	C	171	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	137	LYS	2.1
1	C	292	GLU	2.1
1	C	143	ALA	2.1
1	C	209	MET	2.0
1	C	230	VAL	2.0
1	C	175	ALA	2.0
1	C	257	THR	2.0
1	C	67	VAL	2.0
1	C	40	ALA	2.0
1	C	222	GLY	2.0
1	C	269	PRO	2.0
1	C	159	LEU	2.0
1	C	279	ASN	2.0
1	C	289	ILE	2.0
1	C	105	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 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(\AA^2)	Q<0.9
3	ANP	C	1301	31/31	0.71	0.27	0.58	18,41,73,73	0
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.