



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 05:55 PM EDT

PDB ID : 3KFH  
Title : Major mouse urinary protein IV complexed with 2-ethylhexanol  
Authors : Perez-Miller, S.; Zou, Q.; Hurley, T.D.  
Deposited on : unknown  
Resolution : 1.02 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](mailto: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.

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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 : rb-20030345  
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) : rb-20030345

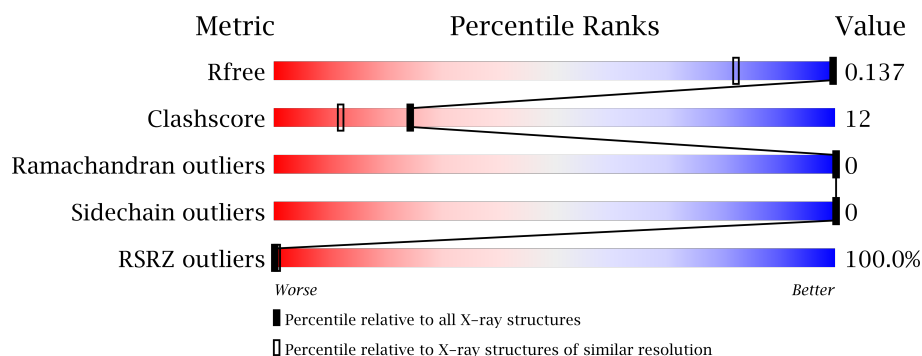
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.02 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	1313 (1.10-0.94)
Clashscore	112137	1404 (1.10-0.94)
Ramachandran outliers	110173	1318 (1.10-0.94)
Sidechain outliers	110143	1317 (1.10-0.94)
RSRZ outliers	101464	1320 (1.10-0.94)

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  $\geq 3$ , 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	A	162	<div> <div>94%</div> <div> <div>79%</div> <div>14%</div> <div>6%</div> </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
3	2EH	A	301	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1633 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.

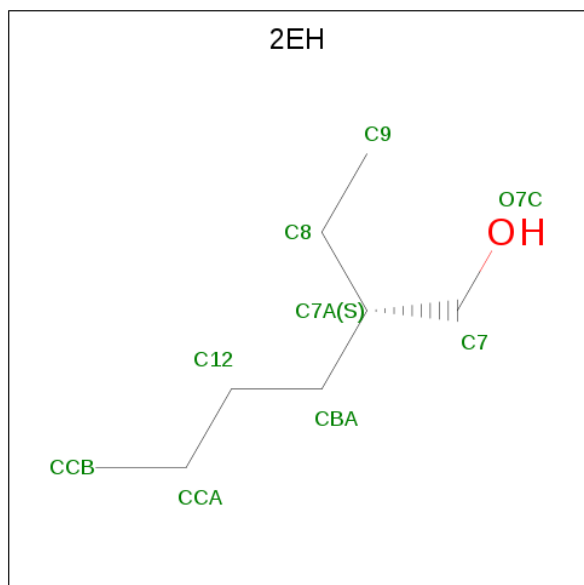
- Molecule 1 is a protein called Major urinary protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	6	25	0
			1353	862	217	266	8			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is (2S)-2-ethylhexan-1-ol (three-letter code: 2EH) (formula: C<sub>8</sub>H<sub>18</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		

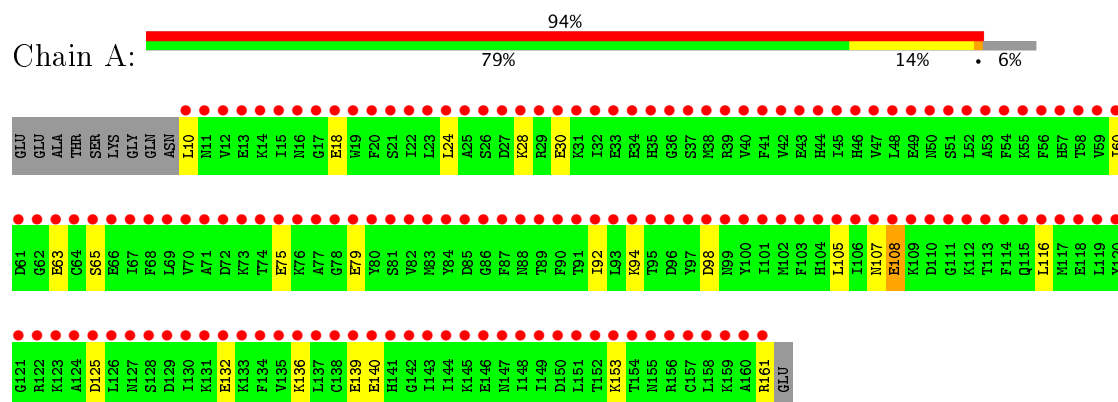
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total 270	O 270	0	14

### 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 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 ( $\text{RSRZ} > 2$ ). 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: Major urinary protein 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.78Å 54.12Å 61.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.60 – 1.02 20.59 – 1.02	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.60-1.02) 91.8 (20.59-1.02)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 1.02Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, $R_{free}$	0.130 , 0.162 0.138 , 0.137	Depositor DCC
$R_{free}$ test set	3670 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 2EH, CL

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	0.82	2/1476 (0.1%)	1.13	5/1978 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108[A]	GLU	CD-OE2	5.62	1.31	1.25
1	A	108[B]	GLU	CD-OE2	5.62	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	63	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	A	161	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	98[A]	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	98[B]	ASP	CB-CG-OD2	-5.09	113.72	118.30

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	A	1353	0	1323	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	9	0	17	0	0
4	A	270	0	0	27	0
All	All	1633	0	1340	34	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 12.

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:A:139[A]:GLU:HG3	4:A:581:HOH:O	1.30	1.27
1:A:136[B]:LYS:HD3	4:A:803:HOH:O	1.18	1.25
1:A:140[B]:GLU:OE1	4:A:587:HOH:O	1.62	1.17
1:A:136[B]:LYS:NZ	4:A:803:HOH:O	1.80	1.13
1:A:139[A]:GLU:CG	4:A:581:HOH:O	1.96	0.97
1:A:18[B]:GLU:CD	4:A:696:HOH:O	2.04	0.95
1:A:136[B]:LYS:CD	4:A:803:HOH:O	1.86	0.80
1:A:108[B]:GLU:OE1	4:A:692:HOH:O	2.02	0.78
1:A:18[B]:GLU:CG	4:A:696:HOH:O	2.37	0.71
1:A:18[B]:GLU:HG3	4:A:696:HOH:O	1.92	0.67
1:A:140[B]:GLU:CD	4:A:587:HOH:O	2.14	0.67
1:A:79:GLU:OE1	4:A:656[A]:HOH:O	2.14	0.65
1:A:132[A]:GLU:OE1	4:A:678[A]:HOH:O	2.15	0.63
1:A:132[B]:GLU:HG3	4:A:594:HOH:O	2.00	0.62
1:A:136[B]:LYS:HE3	4:A:611:HOH:O	2.04	0.58
1:A:132[B]:GLU:OE2	1:A:136[B]:LYS:HE2	2.10	0.52
1:A:24:LEU:HD11	1:A:116[B]:LEU:HD11	1.93	0.50
1:A:136[B]:LYS:HE2	4:A:594:HOH:O	2.13	0.49
1:A:10:LEU:HD21	1:A:92[A]:ILE:HD12	1.96	0.47
1:A:28:LYS:HE3	1:A:30:GLU:OE2	2.15	0.47
1:A:153:LYS:NZ	4:A:651:HOH:O	2.46	0.46
1:A:136[B]:LYS:CE	4:A:803:HOH:O	2.15	0.46
1:A:108[B]:GLU:CD	4:A:692:HOH:O	2.50	0.45
1:A:136[A]:LYS:HE2	4:A:612:HOH:O	2.16	0.44
1:A:94:LYS:HE3	4:A:795:HOH:O	2.18	0.43
1:A:60:ILE:HB	4:A:674:HOH:O	2.18	0.43
1:A:65[A]:SER:HB3	4:A:674:HOH:O	2.19	0.42
1:A:136[A]:LYS:CE	4:A:614:HOH:O	2.68	0.41
1:A:140[B]:GLU:HG3	4:A:614:HOH:O	2.21	0.41
1:A:105:LEU:HB3	1:A:116[B]:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140[B]:GLU:HG2	4:A:702:HOH:O	2.20	0.41
1:A:136[A]:LYS:HE3	4:A:614:HOH:O	2.21	0.41

There are no symmetry-related clashes.

## 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	175/162 (108%)	168 (96%)	7 (4%)	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	A	162/146 (111%)	162 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	147	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	2EH	A	301	-	8,8,8	1.18	1 (12%)	8,8,8	1.22	1 (12%)

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
3	2EH	A	301	-	-	0/8/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	2EH	O7C-C7	2.37	1.52	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	301	2EH	CCA-C12-CBA	-2.17	101.06	114.77

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	152/162 (93%)	9.25	152 (100%) 0 0	9, 13, 23, 30	5 (3%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	TRP	15.8
1	A	10	LEU	15.4
1	A	48[A]	LEU	14.9
1	A	137[A]	LEU	14.2
1	A	116[A]	LEU	13.9
1	A	67	ILE	13.7
1	A	148	ILE	13.2
1	A	106	ILE	13.1
1	A	119	LEU	12.9
1	A	111[A]	GLY	12.9
1	A	41	PHE	12.8
1	A	138	CYS	12.8
1	A	101	ILE	12.7
1	A	22	ILE	12.7
1	A	134	PHE	12.6
1	A	23	LEU	12.6
1	A	69	LEU	12.4
1	A	90	PHE	12.4
1	A	59	VAL	12.4
1	A	24	LEU	12.4
1	A	20	PHE	12.4
1	A	105	LEU	12.3
1	A	143	ILE	12.3
1	A	40	VAL	12.2
1	A	52	LEU	12.2
1	A	149	ILE	12.2
1	A	42	VAL	12.2

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Mol	Chain	Res	Type	RSRZ
1	A	45	ILE	12.2
1	A	120	TYR	12.1
1	A	15	ILE	12.1
1	A	114	PHE	12.1
1	A	92[A]	ILE	12.0
1	A	84	TYR	12.0
1	A	103	PHE	11.8
1	A	87	PHE	11.8
1	A	130	ILE	11.7
1	A	144	ILE	11.7
1	A	151	LEU	11.6
1	A	100	TYR	11.6
1	A	70	VAL	11.6
1	A	158	LEU	11.5
1	A	32	ILE	11.5
1	A	97	TYR	11.5
1	A	93	LEU	11.4
1	A	47	VAL	11.3
1	A	25	ALA	11.2
1	A	135	VAL	11.2
1	A	54	PHE	11.1
1	A	126	LEU	11.1
1	A	60	ILE	11.1
1	A	80	TYR	11.1
1	A	56	PHE	11.0
1	A	68	PHE	11.0
1	A	64	CYS	10.9
1	A	77	ALA	10.9
1	A	71	ALA	10.6
1	A	12	VAL	10.5
1	A	82	VAL	10.4
1	A	53	ALA	10.3
1	A	124	ALA	10.3
1	A	160	ALA	10.0
1	A	157	CYS	9.9
1	A	91	THR	9.7
1	A	113[A]	THR	9.6
1	A	35[A]	HIS	9.5
1	A	121	GLY	9.3
1	A	142	GLY	9.1
1	A	75[A]	GLU	9.1
1	A	89	THR	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	62	GLY	8.9
1	A	117[A]	MET	8.9
1	A	17	GLY	8.6
1	A	74	THR	8.6
1	A	95	THR	8.5
1	A	94	LYS	8.5
1	A	141	HIS	8.3
1	A	58	THR	8.3
1	A	152	THR	8.3
1	A	21	SER	8.2
1	A	38	MET	8.2
1	A	104	HIS	8.2
1	A	112	LYS	8.2
1	A	36	GLY	8.2
1	A	86	GLY	8.1
1	A	154	THR	8.1
1	A	147	ASN	8.1
1	A	26	SER	8.0
1	A	88	ASN	8.0
1	A	44	HIS	7.9
1	A	50	ASN	7.8
1	A	107	ASN	7.8
1	A	110	ASP	7.7
1	A	102	MET	7.7
1	A	159	LYS	7.7
1	A	39[A]	ARG	7.7
1	A	57	HIS	7.7
1	A	99[A]	ASN	7.6
1	A	98[A]	ASP	7.6
1	A	65[A]	SER	7.6
1	A	11	ASN	7.6
1	A	16[A]	ASN	7.5
1	A	127	ASN	7.5
1	A	81	SER	7.5
1	A	136[A]	LYS	7.5
1	A	34[A]	GLU	7.5
1	A	129[A]	ASP	7.4
1	A	76	LYS	7.4
1	A	46	HIS	7.4
1	A	125	ASP	7.3
1	A	145	LYS	7.3
1	A	83	MET	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	78	GLY	7.2
1	A	122	ARG	7.2
1	A	49	GLU	7.2
1	A	115	GLN	7.1
1	A	128[A]	SER	7.1
1	A	155	ASN	7.1
1	A	123	LYS	7.1
1	A	61	ASP	7.0
1	A	51	SER	7.0
1	A	18[A]	GLU	7.0
1	A	161	ARG	6.9
1	A	37	SER	6.8
1	A	156	ARG	6.8
1	A	108[A]	GLU	6.5
1	A	85	ASP	6.4
1	A	72	ASP	6.4
1	A	13[A]	GLU	6.4
1	A	150	ASP	6.3
1	A	96	ASP	6.3
1	A	79	GLU	6.3
1	A	28	LYS	6.3
1	A	133	LYS	6.3
1	A	146	GLU	6.2
1	A	27	ASP	6.2
1	A	132[A]	GLU	6.2
1	A	139[A]	GLU	6.2
1	A	153	LYS	6.2
1	A	140[A]	GLU	6.1
1	A	14	LYS	6.1
1	A	66	GLU	6.1
1	A	31	LYS	6.1
1	A	73	LYS	6.1
1	A	131	LYS	6.1
1	A	43[A]	GLU	6.1
1	A	118	GLU	6.0
1	A	55	LYS	6.0
1	A	30	GLU	5.9
1	A	109	LYS	5.9
1	A	29	ARG	5.9
1	A	33	GLU	5.5
1	A	63	GLU	5.3

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	2EH	A	301	9/9	0.73	0.49	2.59	15,19,25,28	0
2	CL	A	201	1/1	0.99	0.32	-2.22	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.