



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2018 – 12:17 PM EST

PDB ID : 3HMK
Title : Crystal Structure of Serine Racemase
Authors : Smith, M.A.; Barker, J.; Mack, V.; Ebner, A.; Felicetti, B.; Woods, M.
Deposited on : 2009-05-29
Resolution : 2.10 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 : rb-20030736
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-20030736

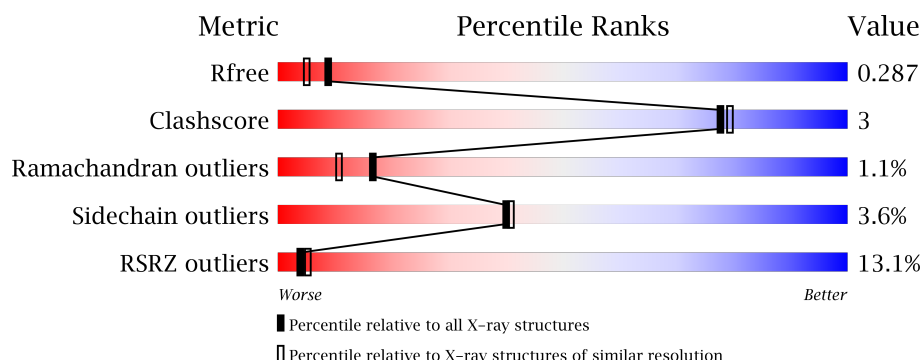
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	A	339	<div> <div>8%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>
1	B	339	<div> <div>17%</div> <div>84%</div> <div>9%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5078 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 Serine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2415	1537	406	466	6			
1	B	322	Total	C	N	O	S	0	0	0
			2429	1548	408	467	6			

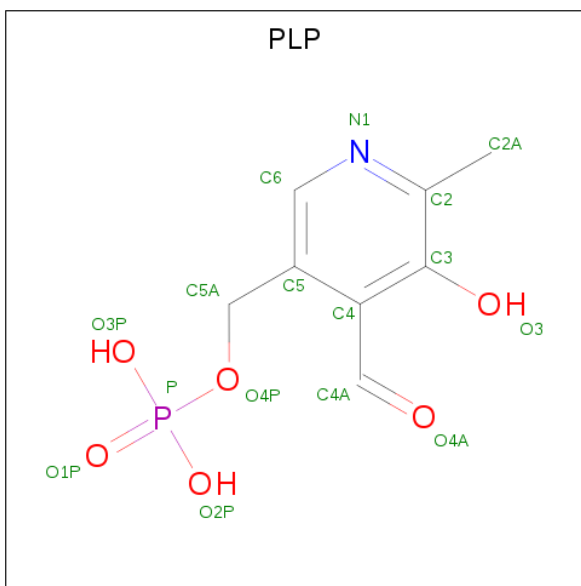
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	CYS	ENGINEERED	UNP Q76EQ0
A	6	ASP	CYS	ENGINEERED	UNP Q76EQ0
A	334	HIS	-	EXPRESSION TAG	UNP Q76EQ0
A	335	HIS	-	EXPRESSION TAG	UNP Q76EQ0
A	336	HIS	-	EXPRESSION TAG	UNP Q76EQ0
A	337	HIS	-	EXPRESSION TAG	UNP Q76EQ0
A	338	HIS	-	EXPRESSION TAG	UNP Q76EQ0
A	339	HIS	-	EXPRESSION TAG	UNP Q76EQ0
B	2	ASP	CYS	ENGINEERED	UNP Q76EQ0
B	6	ASP	CYS	ENGINEERED	UNP Q76EQ0
B	334	HIS	-	EXPRESSION TAG	UNP Q76EQ0
B	335	HIS	-	EXPRESSION TAG	UNP Q76EQ0
B	336	HIS	-	EXPRESSION TAG	UNP Q76EQ0
B	337	HIS	-	EXPRESSION TAG	UNP Q76EQ0
B	338	HIS	-	EXPRESSION TAG	UNP Q76EQ0
B	339	HIS	-	EXPRESSION TAG	UNP Q76EQ0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

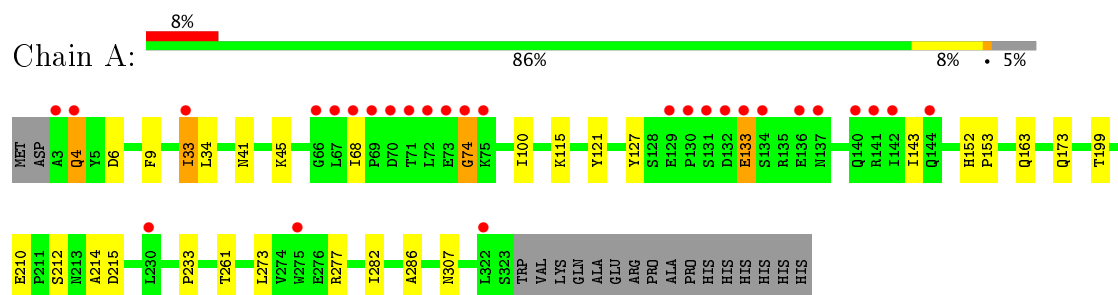
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	84	Total	O	0	0
			84	84		

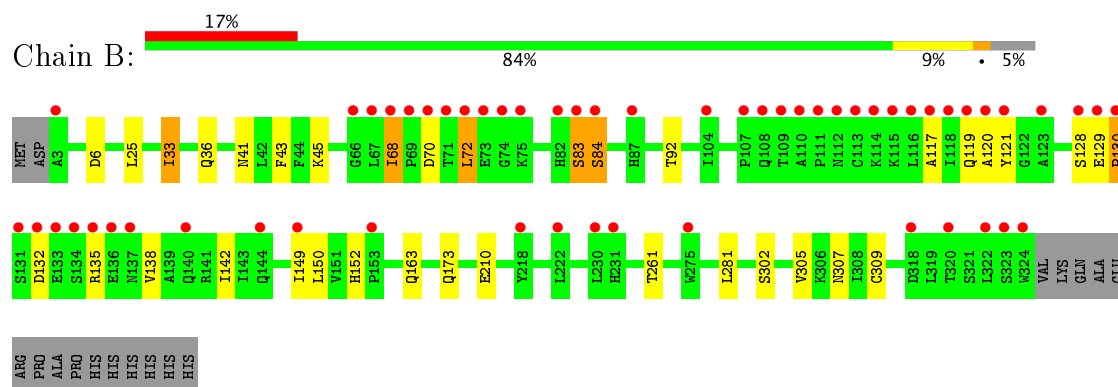
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: Serine racemase



• Molecule 1: Serine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.26Å 102.96Å 120.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 2.10 41.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.10-2.10) 95.8 (41.10-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.241 , 0.289 0.240 , 0.287	Depositor DCC
R_{free} test set	1795 reflections (5.50%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5078	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: MN, PLP

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	0.35	0/2459	0.50	0/3354
1	B	0.33	0/2475	0.49	0/3377
All	All	0.34	0/4934	0.50	0/6731

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	A	2415	0	2463	14	0
1	B	2429	0	2473	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	6	0	0
4	A	118	0	0	1	0
4	B	84	0	0	2	0
All	All	5078	0	4949	33	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 3.

All (33) 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:B:72:LEU:HD22	1:B:72:LEU:N	2.06	0.70
1:B:92:THR:HG22	1:B:121:TYR:HB2	1.72	0.70
1:B:41:ASN:HB2	1:B:307:ASN:HD22	1.64	0.61
1:B:119:GLN:HA	4:B:378:HOH:O	2.01	0.60
1:B:92:THR:HG21	4:B:378:HOH:O	2.00	0.60
1:B:33:ILE:O	1:B:36:GLN:HG2	2.07	0.53
1:B:72:LEU:N	1:B:72:LEU:CD2	2.74	0.50
1:B:138:VAL:O	1:B:142:ILE:HG12	2.11	0.50
1:B:41:ASN:HD22	1:B:307:ASN:HD21	1.60	0.50
1:B:302:SER:HB3	1:B:305:VAL:HG23	1.95	0.48
1:A:214:ALA:HB2	1:A:233:PRO:HB3	1.95	0.48
1:B:83:SER:O	1:B:84:SER:HB3	2.14	0.47
1:A:9:PHE:CG	1:A:199:THR:HG21	2.50	0.47
1:B:210:GLU:O	1:B:261:THR:HA	2.15	0.47
1:A:212:SER:HA	1:A:215:ASP:HB3	1.97	0.47
1:A:45:LYS:NZ	1:A:173:GLN:HE22	2.13	0.47
1:B:117:ALA:HA	1:B:120:ALA:HB2	1.98	0.46
1:B:68:ILE:H	1:B:68:ILE:HG13	1.58	0.46
1:A:41:ASN:HB2	1:A:307:ASN:HD22	1.81	0.45
1:A:115:LYS:HE2	1:A:127:TYR:HE1	1.82	0.45
1:B:43:PHE:O	1:B:309:CYS:HA	2.18	0.44
1:A:282:ILE:HB	1:A:286:ALA:HB3	1.99	0.43
1:A:68:ILE:HG23	1:A:74:GLY:O	2.19	0.43
1:A:45:LYS:HZ3	1:A:173:GLN:HE22	1.67	0.43
1:B:41:ASN:HD22	1:B:307:ASN:ND2	2.17	0.42
1:A:4:GLN:HA	1:A:4:GLN:HE21	1.83	0.42
1:B:128:SER:HB3	1:B:135:ARG:HG2	2.02	0.41
1:A:210:GLU:O	1:A:261:THR:HA	2.20	0.41
1:A:273:LEU:O	1:A:277:ARG:HB2	2.20	0.41
1:A:33:ILE:HG22	4:A:392:HOH:O	2.21	0.41
1:B:45:LYS:NZ	1:B:173:GLN:HE22	2.18	0.41
1:A:152:HIS:CG	1:A:153:PRO:HD2	2.57	0.40
1:B:129:GLU:HA	1:B:130:PRO:HD3	1.88	0.40

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	319/339 (94%)	306 (96%)	11 (3%)	2 (1%)	28	24
1	B	320/339 (94%)	301 (94%)	14 (4%)	5 (2%)	11	5
All	All	639/678 (94%)	607 (95%)	25 (4%)	7 (1%)	17	11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	ASP
1	B	83	SER
1	A	74	GLY
1	B	132	ASP
1	A	133	GLU
1	B	84	SER
1	B	130	PRO

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	267/283 (94%)	258 (97%)	9 (3%)	42	43
1	B	268/283 (95%)	258 (96%)	10 (4%)	39	39
All	All	535/566 (94%)	516 (96%)	19 (4%)	40	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	ASP
1	A	33	ILE
1	A	34	LEU
1	A	100	ILE
1	A	121	TYR
1	A	133	GLU
1	A	143	ILE
1	A	163	GLN
1	B	6	ASP
1	B	25	LEU
1	B	33	ILE
1	B	68	ILE
1	B	72	LEU
1	B	149	ILE
1	B	150	LEU
1	B	152	HIS
1	B	163	GLN
1	B	281	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	89	GLN
1	A	173	GLN
1	A	296	GLN
1	A	307	ASN
1	B	36	GLN
1	B	82	HIS
1	B	87	HIS
1	B	108	GLN
1	B	152	HIS
1	B	173	GLN
1	B	307	ASN

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 2 are 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	PLP	A	350	1	15,15,16	0.77	1 (6%)	20,22,23	1.00	1 (5%)
3	PLP	B	350	1	15,15,16	2.47	5 (33%)	20,22,23	2.13	4 (20%)

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	PLP	A	350	1	-	0/6/6/8	0/1/1/1
3	PLP	B	350	1	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	350	PLP	C3-C2	-6.53	1.36	1.40
3	B	350	PLP	P-O2P	-3.52	1.40	1.54
3	B	350	PLP	P-O3P	-3.34	1.41	1.54
3	B	350	PLP	O3-C3	-2.80	1.30	1.37
3	B	350	PLP	P-O1P	-2.79	1.41	1.50
3	A	350	PLP	C3-C2	-2.14	1.39	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	350	PLP	C4A-C4-C3	-2.90	115.54	120.54
3	B	350	PLP	C5A-C5-C6	-2.66	114.75	119.33
3	A	350	PLP	C5-C6-N1	-2.00	120.48	123.87
3	B	350	PLP	O4P-C5A-C5	5.13	119.64	109.32
3	B	350	PLP	C4A-C4-C5	5.42	126.33	120.86

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 [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	321/339 (94%)	0.52	28 (8%) 11 14	14, 21, 48, 56	3 (0%)
1	B	322/339 (94%)	1.49	56 (17%) 2 2	17, 29, 73, 78	5 (1%)
All	All	643/678 (94%)	1.01	84 (13%) 4 5	14, 24, 61, 78	8 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	LEU	21.4
1	B	71	THR	19.7
1	B	113	CYS	19.3
1	B	110	ALA	15.6
1	B	70	ASP	15.1
1	B	109	THR	14.9
1	B	131	SER	14.6
1	B	120	ALA	14.3
1	B	69	PRO	14.1
1	B	116	LEU	12.8
1	B	68	ILE	12.4
1	B	132	ASP	11.4
1	B	111	PRO	11.0
1	A	72	LEU	10.7
1	A	67	LEU	10.6
1	A	71	THR	10.5
1	A	69	PRO	10.2
1	A	68	ILE	9.1
1	A	70	ASP	9.0
1	B	130	PRO	8.4
1	B	114	LYS	8.0
1	A	3	ALA	8.0
1	B	118	ILE	7.7
1	B	67	LEU	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	112	ASN	7.5
1	B	66	GLY	7.5
1	B	108	GLN	6.3
1	B	117	ALA	6.2
1	B	119	GLN	6.1
1	A	73	GLU	5.9
1	B	133	GLU	5.9
1	B	73	GLU	5.8
1	B	135	ARG	5.8
1	B	134	SER	5.8
1	B	115	LYS	5.7
1	B	322	LEU	5.7
1	B	121	TYR	5.4
1	B	129	GLU	5.2
1	B	324	TRP	5.2
1	B	84	SER	4.7
1	A	66	GLY	4.4
1	B	74	GLY	4.3
1	B	3	ALA	4.1
1	A	74	GLY	4.0
1	B	230	LEU	4.0
1	B	107	PRO	3.9
1	B	128	SER	3.7
1	A	132	ASP	3.6
1	B	136	GLU	3.4
1	B	231	HIS	3.4
1	A	4	GLN	3.3
1	A	133	GLU	3.2
1	B	140	GLN	3.1
1	B	137	ASN	3.0
1	A	322	LEU	3.0
1	A	130	PRO	3.0
1	B	75	LYS	2.9
1	B	144	GLN	2.8
1	A	134	SER	2.7
1	B	82	HIS	2.7
1	B	153	PRO	2.7
1	A	230	LEU	2.7
1	A	129	GLU	2.6
1	B	83	SER	2.5
1	B	149	ILE	2.5
1	A	137	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	33	ILE	2.5
1	A	131	SER	2.5
1	B	87	HIS	2.5
1	A	75	LYS	2.5
1	A	141	ARG	2.4
1	B	320	THR	2.4
1	B	318	ASP	2.4
1	A	136	GLU	2.3
1	A	140	GLN	2.3
1	A	142	ILE	2.3
1	B	323	SER	2.3
1	B	123	ALA	2.2
1	A	144	GLN	2.2
1	A	275	TRP	2.2
1	B	218	TYR	2.2
1	B	104	ILE	2.1
1	B	222	LEU	2.1
1	B	275	TRP	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	PLP	B	350	15/16	0.95	0.11	-0.63	21,22,23,23	0
3	PLP	A	350	15/16	0.97	0.10	-0.95	15,16,17,17	0
2	MN	B	340	1/1	0.96	0.05	-3.54	28,28,28,28	1
2	MN	A	340	1/1	0.93	0.04	-5.53	19,19,19,19	1

6.5 Other polymers

There are no such residues in this entry.