



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2017 – 03:15 PM EST

PDB ID : 5LYH
Title : Human PARP14 (ARTD8), catalytic fragment in complex with inhibitor H10
Authors : Karlberg, T.; Thorsell, A.G.; Schuler, H.
Deposited on : 2016-09-28
Resolution : 2.17 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

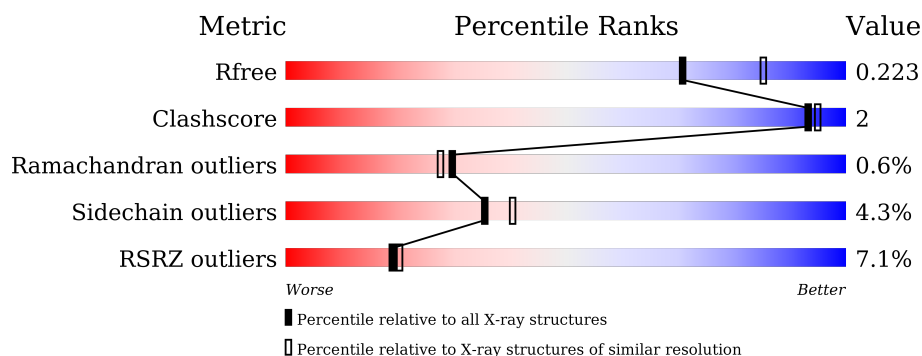
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	193	
1	B	193	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3090 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.

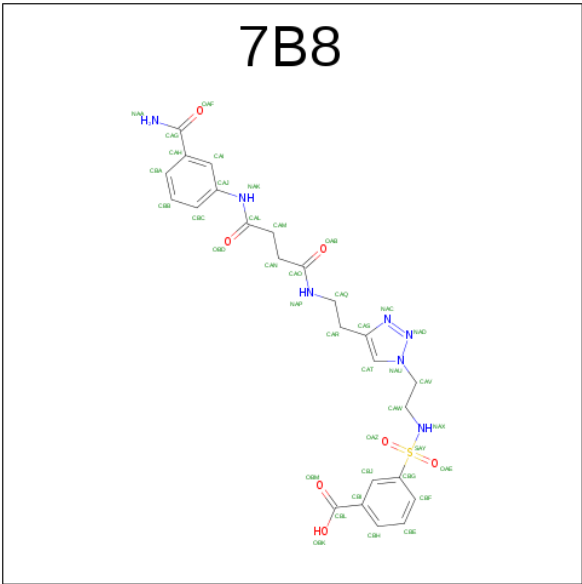
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1500	948	265	282	5			
1	B	182	Total	C	N	O	S	0	1	0
			1493	945	263	281	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1609	SER	-	expression tag	UNP Q460N5
A	1610	MET	-	expression tag	UNP Q460N5
B	1609	SER	-	expression tag	UNP Q460N5
B	1610	MET	-	expression tag	UNP Q460N5

- Molecule 2 is 3-[2-[4-[2-[[4-[(3-aminocarbonylphenyl)amino]-4-oxidanylidene-butanoyl]amino]ethyl]-1,2,3-triazol-1-yl]ethylsulfamoyl]benzoic acid (three-letter code: 7B8) (formula: C₂₄H₂₇N₇O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			39	24	7	7	1		
2	B	1	Total	C	N	O	S	0	0
			39	24	7	7	1		

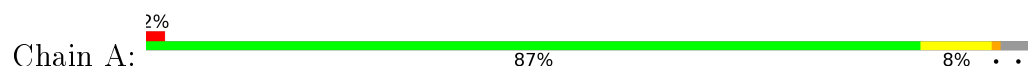
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	9	Total	O	0	0
			9	9		

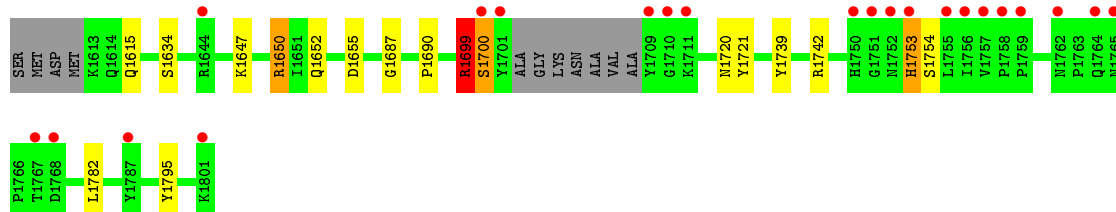
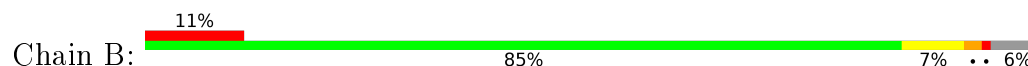
3 Residue-property plots [i](#)

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: Poly [ADP-ribose] polymerase 14



- Molecule 1: Poly [ADP-ribose] polymerase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.03Å 83.03Å 122.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.50 – 2.17 46.53 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.50-2.17) 99.6 (46.53-2.17)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.195 , 0.218 0.197 , 0.223	Depositor DCC
R_{free} test set	1999 reflections (8.22%)	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.348 for -h,-k,l	Xtriage
Reported twinning fraction	0.658 for H, K, L 0.342 for -H, -K, L	Depositor
Outliers	0 of 26408 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3090	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: 7B8

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	0.67	0/1542	0.83	2/2095 (0.1%)
1	B	0.72	0/1539	0.86	3/2091 (0.1%)
All	All	0.70	0/3081	0.84	5/4186 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1742	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	1644	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	1699	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	B	1650	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	1729	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1612	MET	Peptide

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Mol	Chain	Res	Type	Group
1	B	1699	ARG	Peptide

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	1500	0	1425	3	0
1	B	1493	0	1414	8	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
3	A	10	0	0	0	0
3	B	9	0	0	0	0
All	All	3090	0	2839	11	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 2.

All (11) 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:1628:GLU:OE1	1:A:1650:ARG:NH1	2.28	0.65
1:B:1699:ARG:CG	1:B:1700:SER:HA	2.29	0.62
1:B:1650:ARG:NH2	1:B:1652:GLN:OE1	2.33	0.60
1:B:1699:ARG:HG3	1:B:1700:SER:HA	1.90	0.54
1:B:1615:GLN:HG3	1:B:1655:ASP:HB2	1.94	0.49
1:B:1753:HIS:CG	1:B:1754:SER:N	2.87	0.43
1:A:1687:GLY:O	1:A:1690:PRO:HD2	2.19	0.42
1:B:1687:GLY:O	1:B:1690:PRO:HD2	2.19	0.42
1:B:1739:TYR:HA	1:B:1795:TYR:O	2.20	0.41
1:A:1679:GLN:HB3	1:A:1740:TYR:CZ	2.55	0.41
1:B:1699:ARG:HB3	1:B:1700:SER:CB	2.52	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	181/193 (94%)	176 (97%)	4 (2%)	1 (1%)	30	27
1	B	179/193 (93%)	167 (93%)	11 (6%)	1 (1%)	30	27
All	All	360/386 (93%)	343 (95%)	15 (4%)	2 (1%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1698	ASN
1	B	1753	HIS

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	164/170 (96%)	156 (95%)	8 (5%)	31	34
1	B	164/170 (96%)	158 (96%)	6 (4%)	41	47
All	All	328/340 (96%)	314 (96%)	14 (4%)	35	40

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1615	GLN
1	A	1647	LYS
1	A	1650	ARG
1	A	1663	LYS

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Mol	Chain	Res	Type
1	A	1700	SER
1	A	1707	VAL
1	A	1762	ASN
1	A	1782	LEU
1	B	1634	SER
1	B	1647	LYS
1	B	1700	SER
1	B	1720	ASN
1	B	1721	TYR
1	B	1782	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1693	ASN
1	B	1642	HIS
1	B	1693	ASN
1	B	1724	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](#)

2 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	7B8	A	1901	-	36,41,41	4.19	10 (27%)	49,56,56	2.30	21 (42%)
2	7B8	B	1901	-	36,41,41	3.35	10 (27%)	49,56,56	1.96	9 (18%)

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	7B8	A	1901	-	-	0/31/36/36	0/3/3/3
2	7B8	B	1901	-	-	0/31/36/36	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	7B8	CBG-SAY	-7.38	1.65	1.76
2	A	1901	7B8	NAC-NAD	-5.86	1.25	1.34
2	B	1901	7B8	NAC-NAD	-5.38	1.26	1.34
2	A	1901	7B8	CAH-CAG	-5.19	1.42	1.50
2	B	1901	7B8	CAH-CAG	-5.06	1.42	1.50
2	A	1901	7B8	NAD-NAU	-4.65	1.25	1.34
2	A	1901	7B8	CAJ-NAK	-4.27	1.33	1.41
2	B	1901	7B8	NAD-NAU	-3.50	1.27	1.34
2	B	1901	7B8	CAR-CAS	2.12	1.56	1.51
2	A	1901	7B8	CAN-CAM	2.23	1.58	1.52
2	B	1901	7B8	CAI-CAH	2.35	1.42	1.39
2	A	1901	7B8	CAM-CAL	2.37	1.56	1.51
2	B	1901	7B8	CAL-NAK	2.75	1.42	1.35
2	B	1901	7B8	CAN-CAO	3.20	1.57	1.51
2	A	1901	7B8	OAZ-SAY	9.19	1.53	1.43
2	B	1901	7B8	OAZ-SAY	9.40	1.53	1.43
2	B	1901	7B8	OAE-SAY	9.44	1.53	1.43
2	A	1901	7B8	OAE-SAY	9.48	1.54	1.43
2	B	1901	7B8	SAY-NAX	10.49	1.75	1.61
2	A	1901	7B8	SAY-NAX	16.40	1.83	1.61

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1901	7B8	OAZ-SAY-OAE	-7.71	109.32	119.54
2	A	1901	7B8	OAZ-SAY-OAE	-6.89	110.40	119.54
2	B	1901	7B8	CBC-CAJ-CAI	-3.76	115.21	119.68
2	B	1901	7B8	OBD-CAL-CAM	-3.19	116.43	121.97
2	A	1901	7B8	OAF-CAG-NAA	-3.15	118.09	122.58
2	A	1901	7B8	OAZ-SAY-CBG	-2.98	104.15	107.94
2	B	1901	7B8	CAJ-NAK-CAL	-2.91	121.91	127.49
2	A	1901	7B8	CBF-CBG-SAY	-2.89	116.49	119.79
2	B	1901	7B8	CAT-CAS-NAC	-2.69	107.10	111.42
2	A	1901	7B8	CAI-CAJ-NAK	-2.68	111.44	120.14
2	A	1901	7B8	CAT-CAS-NAC	-2.67	107.13	111.42
2	A	1901	7B8	CBH-CBI-CBL	-2.55	117.07	120.43
2	A	1901	7B8	CAM-CAL-NAK	-2.18	110.72	114.52
2	B	1901	7B8	OAF-CAG-NAA	-2.17	119.49	122.58
2	A	1901	7B8	CBA-CAH-CAI	-2.14	116.69	119.25
2	A	1901	7B8	OAB-CAO-CAN	-2.00	118.50	121.97
2	A	1901	7B8	OBD-CAL-NAK	2.05	127.36	123.77
2	A	1901	7B8	CBH-CBI-CBJ	2.21	120.98	118.17
2	A	1901	7B8	CAH-CAI-CAJ	2.44	124.27	120.45
2	A	1901	7B8	OAE-SAY-CBG	2.52	111.15	107.94
2	B	1901	7B8	CAH-CAI-CAJ	2.58	124.50	120.45
2	A	1901	7B8	CBC-CAJ-NAK	2.88	130.04	120.40
2	A	1901	7B8	OAE-SAY-NAX	2.94	111.97	107.00
2	A	1901	7B8	CAQ-NAP-CAO	3.03	128.80	122.79
2	A	1901	7B8	CBJ-CBG-SAY	3.91	123.37	119.00
2	A	1901	7B8	OAZ-SAY-NAX	3.91	113.62	107.00
2	B	1901	7B8	OAF-CAG-CAH	4.07	124.11	119.60
2	B	1901	7B8	NAC-NAD-NAU	4.34	110.59	107.31
2	A	1901	7B8	OAF-CAG-CAH	4.42	124.49	119.60
2	A	1901	7B8	NAC-NAD-NAU	5.33	111.33	107.31

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	185/193 (95%)	0.30	4 (2%) 65 66	34, 53, 89, 115	0
1	B	182/193 (94%)	0.93	22 (12%) 6 6	34, 57, 126, 185	0
All	All	367/386 (95%)	0.61	26 (7%) 19 20	34, 54, 114, 185	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1756	ILE	9.4
1	B	1700	SER	8.2
1	B	1764	GLN	7.2
1	B	1765	ASN	7.2
1	B	1710	GLY	6.6
1	A	1707	VAL	5.8
1	B	1762	ASN	5.7
1	B	1755	LEU	4.6
1	B	1758	PRO	4.4
1	B	1751	GLY	4.4
1	B	1701	TYR	4.3
1	B	1759	PRO	4.0
1	B	1709	TYR	4.0
1	B	1757	VAL	3.8
1	B	1787	TYR	3.3
1	B	1711	LYS	3.1
1	B	1767	THR	3.1
1	A	1764	GLN	2.8
1	B	1752	ASN	2.7
1	A	1754	SER	2.5
1	A	1766	PRO	2.1
1	B	1801	LYS	2.1
1	B	1753	HIS	2.1
1	B	1750	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1768	ASP	2.0
1	B	1644	ARG	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
2	7B8	A	1901	39/39	0.81	0.24	1.53	35,86,116,122	0
2	7B8	B	1901	39/39	0.86	0.26	0.61	38,85,126,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.