



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 04:47 pm GMT

PDB ID : 5JPT
Title : CRYSTAL STRUCTURE OF THE PRP43P DEAH-BOX RNA HELICASE
IN COMPLEX WITH CDP
Authors : Robert-Paganin, J.; Rety, S.; Leulliot, N.
Deposited on : 2016-05-04
Resolution : 2.94 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 : recalc29047
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) : recalc29047

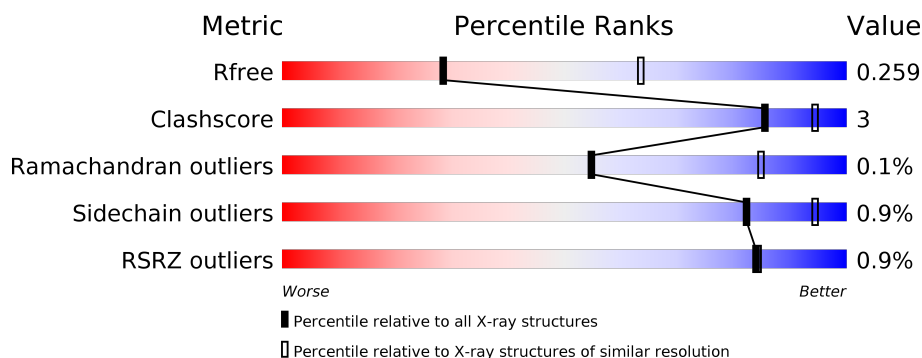
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.94 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	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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	767	
1	B	767	

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
4	GOL	A	803	-	-	-	X

2 Entry composition [i](#)

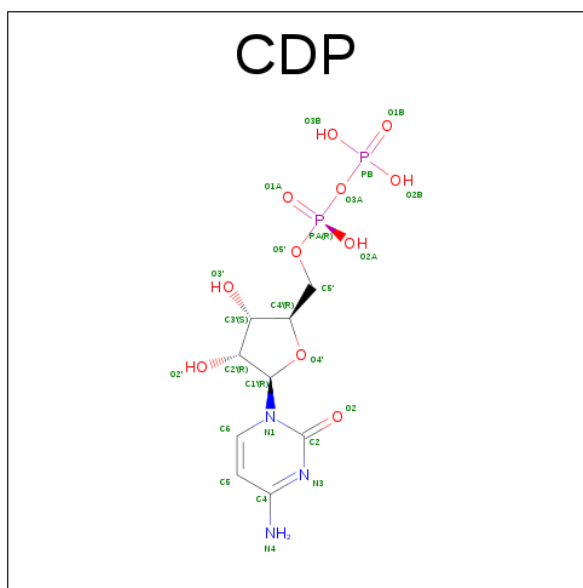
There are 7 unique types of molecules in this entry. The entry contains 12040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	745	Total	C	N	O	S	0	0	0
			5990	3793	1034	1139	24			
1	B	741	Total	C	N	O	S	0	0	0
			5961	3778	1027	1132	24			

- Molecule 2 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

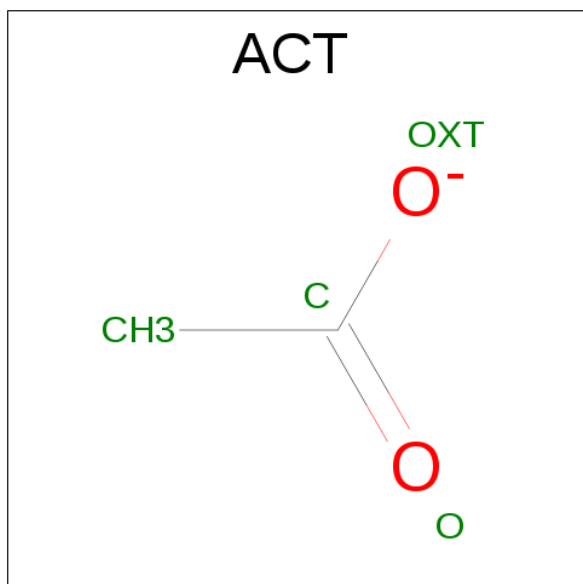
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ni 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	15	Total O 15 15	0	0
7	B	11	Total O 11 11	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.07Å 118.07Å 252.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.31 – 2.94 48.31 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.31-2.94) 99.6 (48.31-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.203 , 0.257 0.206 , 0.259	Depositor DCC
R_{free} test set	2208 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12040	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: GOL, MG, ACT, CDP, NI

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	0.27	0/6117	0.49	0/8280
1	B	0.27	0/6088	0.51	1/8242 (0.0%)
All	All	0.27	0/12205	0.50	1/16522 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	597	TYR	N-CA-C	-5.22	96.91	111.00

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	5990	0	5946	22	1
1	B	5961	0	5921	39	0
2	A	25	0	12	1	0
2	B	25	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0
5	A	4	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	15	0	0	1	0
7	B	11	0	0	0	0
All	All	12040	0	11902	61	1

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 (61) 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:662:LYS:NZ	1:B:692:GLU:OE2	2.07	0.88
1:B:557:ARG:NH1	1:B:566:ASP:OD1	2.14	0.81
1:B:109:ASN:O	1:B:242:LYS:NZ	2.18	0.76
1:B:407:ARG:NH1	1:B:675:ASP:OD1	2.19	0.76
1:B:561:ASP:OD1	1:B:564:ARG:NH1	2.21	0.73
1:B:598:GLY:O	1:B:602:TRP:N	2.32	0.62
1:B:490:THR:OG1	1:B:493:ARG:NH2	2.33	0.62
1:A:476:ASP:OD2	1:A:479:HIS:ND1	2.29	0.62
1:B:746:LYS:NZ	1:B:747:VAL:O	2.33	0.61
2:A:801:CDP:O1B	7:A:901:HOH:O	2.15	0.59
1:B:698:GLU:OE2	1:B:708:ARG:NH1	2.37	0.58
1:A:577:GLY:O	1:A:580:ILE:N	2.37	0.56
1:B:476:ASP:OD2	1:B:479:HIS:ND1	2.35	0.56
1:A:149:ARG:NH1	1:A:377:ASN:OD1	2.40	0.54
1:A:198:ARG:NH2	1:A:518:SER:O	2.44	0.51
1:B:365:ASN:O	1:B:365:ASN:ND2	2.44	0.50
1:B:556:ILE:HG22	1:B:558:PRO:HD3	1.94	0.50
1:B:558:PRO:HG2	1:B:561:ASP:HB3	1.95	0.49
1:A:556:ILE:HG22	1:A:558:PRO:HD3	1.94	0.48
1:A:150:ARG:NH2	1:A:346:GLY:O	2.45	0.47
1:B:406:ILE:H	1:B:406:ILE:HD12	1.80	0.47
1:B:664:ARG:NH2	1:B:678:ASP:OD1	2.47	0.46
1:A:714:ARG:HD3	1:A:717:TRP:CZ2	2.50	0.46
1:A:466:VAL:HG11	1:A:495:LEU:HD23	1.97	0.46
1:B:579:HIS:CG	1:B:652:LEU:HD11	2.51	0.46
1:A:701:LEU:O	1:A:701:LEU:HD12	2.15	0.46
1:A:11:HIS:ND1	1:A:727:ASP:OD2	2.43	0.46
1:B:365:ASN:O	1:B:367:ARG:N	2.49	0.46
1:A:432:ARG:HB2	1:A:433:PRO:HD2	1.99	0.45
1:B:739:SER:O	1:B:743:ILE:HD12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLU:N	1:A:593:GLU:OE1	2.50	0.44
1:B:174:TYR:HA	1:B:190:TYR:O	2.17	0.44
1:B:252:ALA:HB1	1:B:255:PHE:HD2	1.81	0.44
1:A:664:ARG:HG2	1:A:671:ILE:CD1	2.47	0.44
1:B:489:GLU:HG3	1:B:493:ARG:NH1	2.32	0.44
1:B:670:TYR:N	1:B:679:VAL:O	2.42	0.44
1:A:277:TYR:CE1	1:A:435:LYS:HD3	2.53	0.43
1:A:432:ARG:HB2	1:A:433:PRO:CD	2.48	0.43
1:B:86:ILE:HG21	1:B:163:GLU:HG2	2.01	0.43
1:B:564:ARG:CZ	1:B:564:ARG:HB2	2.48	0.43
1:B:576:ASP:HA	1:B:687:LEU:HD21	2.01	0.43
1:A:332:ARG:HG2	1:B:355:ARG:NH1	2.32	0.43
1:B:427:ARG:NE	1:B:427:ARG:HA	2.33	0.43
1:B:731:PHE:HB2	1:B:737:LYS:HD2	1.99	0.43
1:A:170:GLU:O	1:A:186:THR:HA	2.19	0.43
1:B:106:TYR:O	1:B:242:LYS:NZ	2.51	0.43
1:B:407:ARG:HE	1:B:493:ARG:HD3	1.84	0.42
1:B:564:ARG:NH1	1:B:564:ARG:HB2	2.34	0.42
1:B:125:GLN:O	1:B:128:GLN:N	2.53	0.42
1:B:403:ASN:HB3	1:B:404:PRO:HD2	2.02	0.42
1:A:572:PHE:CG	1:A:585:VAL:HG12	2.55	0.41
1:A:650:LYS:HE2	1:A:717:TRP:CD1	2.56	0.41
1:B:174:TYR:N	1:B:181:LYS:O	2.51	0.41
1:A:386:ASP:OD1	1:A:430:ARG:NH1	2.54	0.41
1:B:400:LYS:HE2	1:B:409:GLU:OE2	2.21	0.41
1:A:736:VAL:HG13	1:A:737:LYS:N	2.36	0.40
1:B:733:LYS:HD2	1:B:737:LYS:HD3	2.03	0.40
1:B:739:SER:HA	1:B:742:ARG:HH21	1.86	0.40
1:B:148:PRO:HB3	1:B:221:THR:HG21	2.03	0.40
1:B:222:LEU:HD13	1:B:457:ILE:HA	2.03	0.40
1:A:311:THR:HG21	1:A:413:VAL:HG13	2.04	0.40

All (1) 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)
1:A:68:ASP:O	1:A:70:LYS:NZ[5_555]	2.00	0.20

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	741/767 (97%)	717 (97%)	24 (3%)	0	100	100
1	B	737/767 (96%)	710 (96%)	25 (3%)	2 (0%)	44	75
All	All	1478/1534 (96%)	1427 (96%)	49 (3%)	2 (0%)	55	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	597	TYR
1	B	366	GLY

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	660/679 (97%)	654 (99%)	6 (1%)	82	94
1	B	657/679 (97%)	651 (99%)	6 (1%)	82	94
All	All	1317/1358 (97%)	1305 (99%)	12 (1%)	82	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	182	THR
1	A	325	LEU
1	A	382	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	410	SER
1	A	478	VAL
1	B	80	THR
1	B	167	LYS
1	B	264	LEU
1	B	382	SER
1	B	452	GLN
1	B	570	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
2	CDP	A	801	3	22,26,26	3.72	10 (45%)	23,40,40	0.96	2 (8%)
4	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	804	-	1,3,3	1.32	0	0,3,3	0.00	-
2	CDP	B	801	3	22,26,26	3.73	10 (45%)	23,40,40	0.93	0

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	CDP	A	801	3	-	0/12/32/32	0/2/2/2
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
5	ACT	A	804	-	-	0/0/0/0	0/0/0/0
2	CDP	B	801	3	-	0/12/32/32	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CDP	C3'-C4'	-9.00	1.29	1.53
2	B	801	CDP	C3'-C4'	-8.80	1.30	1.53
2	A	801	CDP	O4'-C1'	-7.00	1.31	1.41
2	B	801	CDP	O4'-C1'	-6.89	1.31	1.41
2	A	801	CDP	O2'-C2'	-2.15	1.38	1.43
2	B	801	CDP	O2'-C2'	-2.07	1.38	1.43
2	A	801	CDP	C5-C4	2.43	1.47	1.41
2	B	801	CDP	C5-C4	2.46	1.47	1.41
2	A	801	CDP	O3'-C3'	2.87	1.49	1.43
2	B	801	CDP	O3'-C3'	3.03	1.49	1.43
2	A	801	CDP	C4-N3	4.16	1.42	1.35
2	B	801	CDP	C4-N3	4.25	1.42	1.35
2	A	801	CDP	C6-C5	4.59	1.48	1.38
2	B	801	CDP	C6-C5	4.61	1.48	1.38
2	A	801	CDP	C2-N3	4.91	1.47	1.38
2	B	801	CDP	C2-N3	4.93	1.47	1.38
2	A	801	CDP	C6-N1	5.86	1.43	1.35
2	B	801	CDP	C6-N1	6.15	1.44	1.35
2	A	801	CDP	O4'-C4'	7.16	1.61	1.45
2	B	801	CDP	O4'-C4'	7.21	1.61	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CDP	C2'-C3'-C4'	2.03	106.57	102.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CDP	N4-C4-N3	2.10	120.17	116.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CDP	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	745/767 (97%)	-0.15	2 (0%) 93 94	33, 48, 72, 114	0
1	B	741/767 (96%)	0.05	12 (1%) 72 72	36, 56, 88, 142	0
All	All	1486/1534 (96%)	-0.05	14 (0%) 84 84	33, 52, 83, 142	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	PHE	2.9
1	B	404	PRO	2.8
1	B	407	ARG	2.8
1	B	250	LEU	2.7
1	B	559	THR	2.7
1	B	634	LEU	2.6
1	B	690	ASP	2.6
1	B	733	LYS	2.6
1	B	104	LYS	2.4
1	A	740	LEU	2.2
1	B	100	ASP	2.1
1	B	632	LEU	2.1
1	B	251	ASP	2.1
1	A	250	LEU	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
4	GOL	A	803	6/6	0.86	0.25	3.02	46,51,52,61	0
5	ACT	A	804	4/4	0.94	0.21	0.38	32,35,36,40	0
2	CDP	A	801	25/25	0.98	0.18	-0.26	31,41,45,51	0
2	CDP	B	801	25/25	0.98	0.15	-1.03	37,47,51,52	0
3	MG	B	802	1/1	0.99	0.13	-1.47	34,34,34,34	0
3	MG	A	802	1/1	0.98	0.14	-2.61	32,32,32,32	0
6	NI	A	805	1/1	0.58	0.38	-	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.