



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2016 – 12:10 PM EDT

PDB ID : 5HDT
Title : Human cohesin regulator Pds5B bound to a Wapl peptide
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Deposited on : 2016-01-05
Resolution : 2.71 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-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

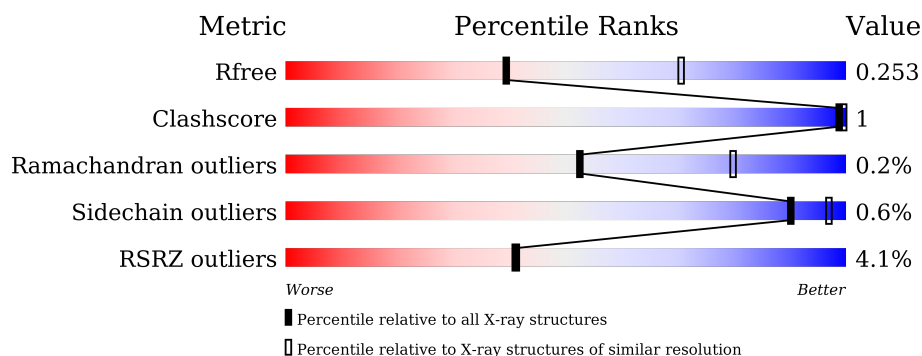
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	1111	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	B	1111	<div> <div>6%</div> <div>93%</div> <div>..</div> </div>
2	E	33	<div> <div>3%</div> <div>15%</div> <div>85%</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	IHP	A	1201	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35400 atoms, of which 17896 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 Sister chromatid cohesion protein PDS5 homolog B.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	1085	Total	C	H	N	O	S	Se		0	0	0
			17689	5589	8955	1490	1599	22	34				
1	B	1073	Total	C	H	N	O	S	Se		0	0	0
			17536	5543	8883	1475	1579	22	34				

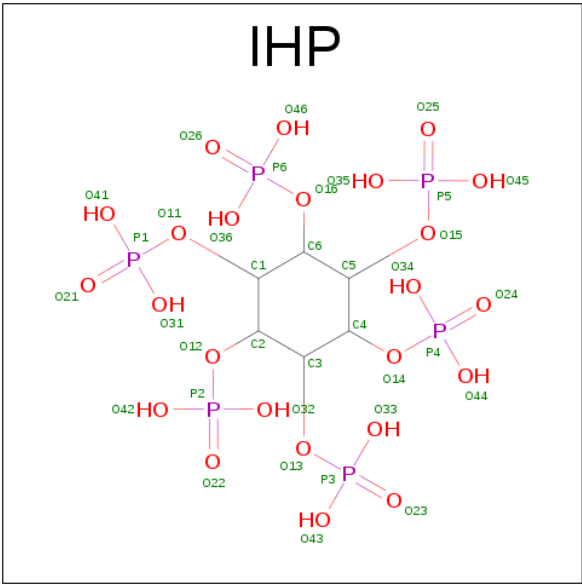
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP Q9NTI5
A	11	ALA	-	expression tag	UNP Q9NTI5
A	12	MSE	-	expression tag	UNP Q9NTI5
A	13	ASP	-	expression tag	UNP Q9NTI5
A	14	PRO	-	expression tag	UNP Q9NTI5
A	15	GLU	-	expression tag	UNP Q9NTI5
A	16	PHE	-	expression tag	UNP Q9NTI5
A	17	GLY	-	expression tag	UNP Q9NTI5
A	18	ARG	-	expression tag	UNP Q9NTI5
A	19	PRO	-	expression tag	UNP Q9NTI5
A	20	MSE	-	expression tag	UNP Q9NTI5
A	97	HIS	TYR	engineered mutation	UNP Q9NTI5
B	10	GLY	-	expression tag	UNP Q9NTI5
B	11	ALA	-	expression tag	UNP Q9NTI5
B	12	MSE	-	expression tag	UNP Q9NTI5
B	13	ASP	-	expression tag	UNP Q9NTI5
B	14	PRO	-	expression tag	UNP Q9NTI5
B	15	GLU	-	expression tag	UNP Q9NTI5
B	16	PHE	-	expression tag	UNP Q9NTI5
B	17	GLY	-	expression tag	UNP Q9NTI5
B	18	ARG	-	expression tag	UNP Q9NTI5
B	19	PRO	-	expression tag	UNP Q9NTI5
B	20	MSE	-	expression tag	UNP Q9NTI5
B	97	HIS	TYR	engineered mutation	UNP Q9NTI5

- Molecule 2 is a protein called Wings apart-like protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	E	5	91	28	46	9	8	0	0	0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆).

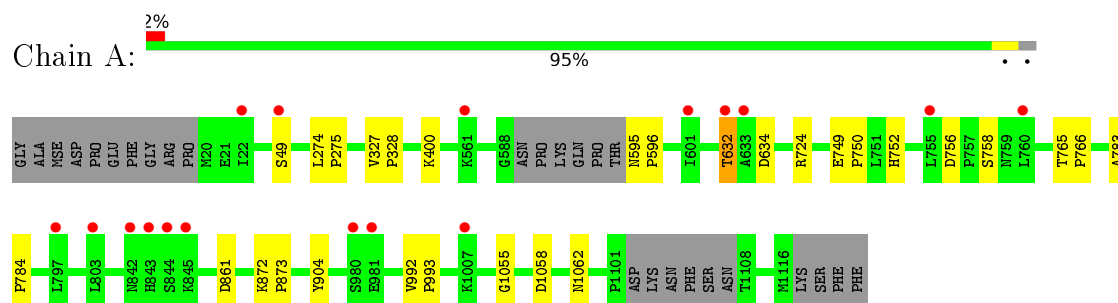


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
3	A	1	42	6	6	24	6	0	0
3	B	1	42	6	6	24	6	0	0

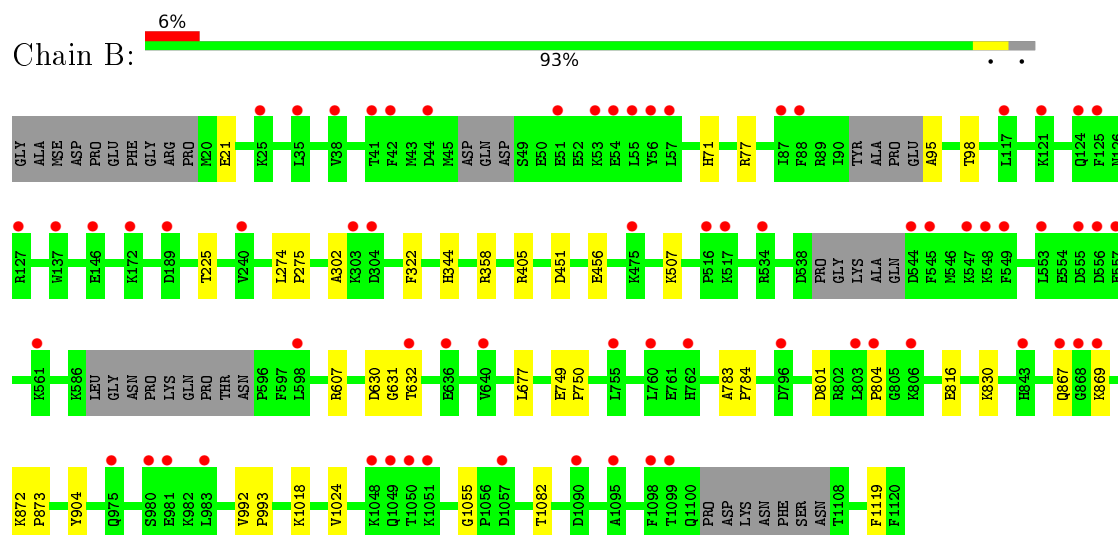
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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.

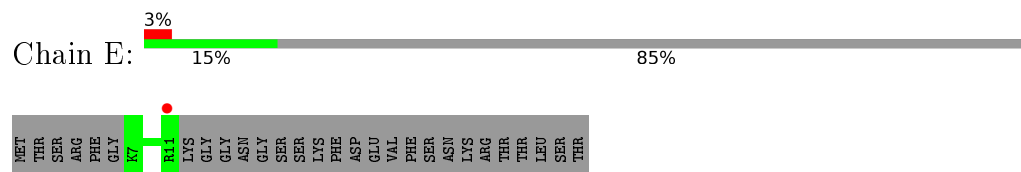
- Molecule 1: Sister chromatid cohesion protein PDS5 homolog B



- Molecule 1: Sister chromatid cohesion protein PDS5 homolog B



- Molecule 2: Wings apart-like protein homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.76Å 162.37Å 173.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.60 – 2.71 40.59 – 2.71	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.60-2.71) 87.4 (40.59-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.216 , 0.253 0.217 , 0.253	Depositor DCC
R_{free} test set	1994 reflections (2.46%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 12.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 81111 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	35400	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IHP

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	0.22	0/8870	0.37	0/11929
1	B	0.21	0/8784	0.36	0/11801
2	E	0.22	0/45	0.34	0/58
All	All	0.22	0/17699	0.36	0/23788

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	8734	8955	8955	13	0
1	B	8653	8883	8883	16	0
2	E	45	46	46	0	0
3	A	36	6	5	1	0
3	B	36	6	5	1	0
All	All	17504	17896	17894	29	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 1.

All (29) 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:322:PHE:O	1:B:358:ARG:NH1	2.29	0.65
1:B:405:ARG:NH2	1:B:451:ASP:OD1	2.34	0.61
1:B:1018:LYS:NZ	1:B:1119:PHE:O	2.40	0.53
1:A:1058:ASP:O	1:A:1062:ASN:ND2	2.41	0.53
1:B:71:HIS:O	1:B:77:ARG:NH1	2.42	0.53
1:A:724:ARG:NH2	3:A:1201:IHP:O26	2.43	0.52
1:B:302:ALA:O	1:B:344:HIS:NE2	2.41	0.50
1:B:630:ASP:O	1:B:632:THR:N	2.45	0.49
1:A:749:GLU:HB2	1:A:750:PRO:HD3	1.98	0.46
1:A:632:THR:HG23	1:A:634:ASP:H	1.81	0.46
1:B:872:LYS:HB2	1:B:873:PRO:HD3	1.99	0.45
1:B:95:ALA:O	1:B:98:THR:OG1	2.31	0.45
1:B:992:VAL:HB	1:B:993:PRO:HD3	1.99	0.45
1:A:756:ASP:OD2	1:A:758:SER:OG	2.26	0.44
1:A:992:VAL:HB	1:A:993:PRO:HD3	1.99	0.44
1:B:816:GLU:OE1	1:B:816:GLU:N	2.48	0.43
1:A:783:ALA:HB3	1:A:784:PRO:HD3	2.01	0.43
1:B:456:GLU:OE1	1:B:607:ARG:NH1	2.52	0.42
1:B:749:GLU:HB3	1:B:750:PRO:HD3	2.00	0.42
1:A:274:LEU:HB2	1:A:275:PRO:HD3	2.02	0.42
1:A:327:VAL:HB	1:A:328:PRO:HD3	2.02	0.42
1:A:595:ASN:HB3	1:A:596:PRO:HD3	2.02	0.42
1:B:274:LEU:HB2	1:B:275:PRO:HD3	2.02	0.41
1:B:783:ALA:HB3	1:B:784:PRO:HD3	2.02	0.41
1:A:765:THR:HB	1:A:766:PRO:HD3	2.02	0.41
1:B:867:GLN:O	1:B:869:LYS:N	2.50	0.41
1:A:400:LYS:N	1:A:400:LYS:HD2	2.36	0.41
1:B:830:LYS:NZ	3:B:1201:IHP:O35	2.50	0.40
1:A:872:LYS:HB2	1:A:873:PRO:HD3	2.04	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	1079/1111 (97%)	1052 (98%)	25 (2%)	2 (0%)	52	80
1	B	1061/1111 (96%)	1028 (97%)	30 (3%)	3 (0%)	46	74
2	E	3/33 (9%)	3 (100%)	0	0	100	100
All	All	2143/2255 (95%)	2083 (97%)	55 (3%)	5 (0%)	52	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	B	804	PRO
1	B	1055	GLY
1	B	631	GLY
1	A	1055	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	981/969 (101%)	977 (100%)	4 (0%)	93	98
1	B	973/969 (100%)	965 (99%)	8 (1%)	86	95
2	E	5/29 (17%)	5 (100%)	0	100	100
All	All	1959/1967 (100%)	1947 (99%)	12 (1%)	90	97

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

Mol	Chain	Res	Type
1	A	632	THR
1	A	752	HIS
1	A	861	ASP
1	A	904	TYR
1	B	21	GLU

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Mol	Chain	Res	Type
1	B	225	THR
1	B	507	LYS
1	B	677	LEU
1	B	801	ASP
1	B	904	TYR
1	B	1024	VAL
1	B	1082	THR

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](#)

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	$\# Z > 2$
3	IHP	A	1201	-	30,36,36	0.69	0	60,60,60	1.59	9 (15%)
3	IHP	B	1201	-	30,36,36	0.68	0	60,60,60	1.57	6 (10%)

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	IHP	A	1201	-	-	0/30/54/54	0/1/1/1
3	IHP	B	1201	-	-	0/30/54/54	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	IHP	P5-O15-C5	-2.06	116.29	121.56
3	A	1201	IHP	C5-C4-C3	-2.02	106.03	110.48
3	A	1201	IHP	O36-P6-O16	2.05	112.75	106.62
3	A	1201	IHP	C4-C3-C2	2.19	115.31	110.48
3	B	1201	IHP	C4-C3-C2	2.59	116.18	110.48
3	B	1201	IHP	C3-C2-C1	2.99	117.08	110.48
3	A	1201	IHP	C3-C2-C1	3.21	117.55	110.48
3	A	1201	IHP	C6-C1-C2	3.72	118.68	110.48
3	B	1201	IHP	C6-C1-C2	3.90	119.09	110.48
3	A	1201	IHP	C6-C5-C4	4.30	119.96	110.48
3	B	1201	IHP	C6-C5-C4	4.65	120.73	110.48
3	B	1201	IHP	O15-C5-C6	5.15	119.08	108.54
3	A	1201	IHP	O15-C5-C6	5.23	119.25	108.54
3	B	1201	IHP	O15-C5-C4	5.41	119.61	108.54
3	A	1201	IHP	O15-C5-C4	5.79	120.39	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	IHP	1	0
3	B	1201	IHP	1	0

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	1051/1111 (94%)	0.11	17 (1%) 74 75	11, 34, 89, 162	0
1	B	1039/1111 (93%)	0.49	68 (6%) 22 21	14, 55, 123, 259	0
2	E	5/33 (15%)	1.34	1 (20%) 1 1	86, 86, 96, 98	0
All	All	2095/2255 (92%)	0.30	86 (4%) 41 41	11, 44, 111, 259	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1090	ASP	5.9
1	A	843	HIS	5.8
1	B	632	THR	5.0
1	A	803	LEU	4.9
1	B	806	LYS	4.9
1	A	980	SER	4.7
1	A	760	LEU	4.4
1	B	516	PRO	4.2
1	B	556	ASP	4.1
1	A	981	GLU	4.1
1	B	983	LEU	4.0
1	A	844	SER	3.8
1	B	42	PHE	3.7
1	B	124	GLN	3.7
1	A	632	THR	3.5
1	B	57	LEU	3.5
1	B	869	LYS	3.5
1	B	51	GLU	3.4
1	B	1050	THR	3.4
1	B	636	GLU	3.4
1	B	980	SER	3.3
1	B	555	ASP	3.3
1	B	981	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	517	LYS	3.2
1	B	137	TRP	3.1
1	B	54	GLU	3.1
1	B	304	ASP	3.1
1	B	557	GLU	3.1
1	B	1095	ALA	3.1
1	B	189	ASP	3.1
1	B	25	LYS	3.0
1	B	1048	LYS	3.0
1	B	1057	ASP	3.0
1	B	146	GLU	2.9
1	A	845	LYS	2.9
1	B	127	ARG	2.9
1	B	55	LEU	2.8
1	A	842	ASN	2.8
1	B	121	LYS	2.8
1	A	797	LEU	2.8
1	A	755	LEU	2.7
1	B	303	LYS	2.7
1	B	803	LEU	2.6
1	A	633	ALA	2.6
1	B	534	ARG	2.6
1	B	547	LYS	2.5
1	B	35	LEU	2.5
1	B	561	LYS	2.5
1	B	125	PHE	2.5
1	B	755	LEU	2.5
1	B	553	LEU	2.4
1	B	975	GLN	2.4
1	B	843	HIS	2.4
1	B	640	VAL	2.4
1	B	1049	GLN	2.4
1	A	22	ILE	2.4
1	B	172	LYS	2.4
2	E	11	ARG	2.4
1	B	598	LEU	2.3
1	B	38	VAL	2.3
1	B	544	ASP	2.3
1	B	545	PHE	2.3
1	B	88	PHE	2.3
1	B	41	THR	2.3
1	B	240	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	796	ASP	2.3
1	A	1007	LYS	2.2
1	B	56	TYR	2.2
1	B	475	LYS	2.2
1	B	1051	LYS	2.2
1	B	760	LEU	2.2
1	B	548	LYS	2.2
1	B	1099	THR	2.2
1	A	49	SER	2.2
1	B	87	ILE	2.2
1	B	53	LYS	2.1
1	B	867	GLN	2.1
1	B	44	ASP	2.1
1	B	868	GLY	2.1
1	A	601	ILE	2.1
1	B	117	LEU	2.1
1	B	804	PRO	2.1
1	A	561	LYS	2.1
1	B	549	PHE	2.1
1	B	1098	PHE	2.1
1	B	762	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	IHP	A	1201	36/36	0.96	0.27	3.92	19,33,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	IHP	B	1201	36/36	0.95	0.19	0.23	16,44,80,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.