W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2023 – 03:08 PM EDT

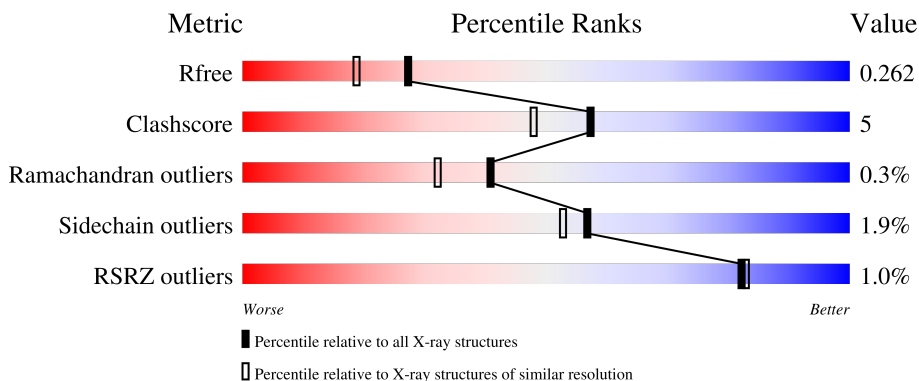|		
PDB ID	:	7UXJ
Title	:	Structure of PPIA in complex with FP29102, a Helicon Polypeptide
Authors	:	Li, K.; Agarwal, S.; Tokareva, O.; Thomson, T.; Wahl, S.; Verdine, G.; McGee, J.
Deposited on	:	2022-05-05
Resolution	:	2.07 Å(reported)

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 2.07 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		1.9%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	166	93% 7%
1	B	166	87% 11% ••
1	C	166	90% 10% •
1	D	166	86% 13% ••
2	E	12	100%

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Mol	Chain	Length	Quality of chain
2	F	12	83% 17%
2	G	12	67% 33%
2	H	12	8% 67% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5881 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 Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	1	0
			1276	809	220	238	9			
1	B	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			
1	C	166	Total	C	N	O	S	0	0	0
			1270	804	219	238	9			
1	D	165	Total	C	N	O	S	0	0	0
			1266	802	218	237	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P62937
B	0	GLY	-	expression tag	UNP P62937
C	0	GLY	-	expression tag	UNP P62937
D	0	GLY	-	expression tag	UNP P62937

- Molecule 2 is a protein called FP29102.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	S	0	0	0
			97	64	14	17	2			
2	F	12	Total	C	N	O	S	0	0	0
			97	64	14	17	2			
2	G	12	Total	C	N	O	S	0	0	0
			97	64	14	17	2			
2	H	12	Total	C	N	O	S	0	0	0
			97	64	14	17	2			

- Molecule 3 is AMINO GROUP (three-letter code: NH2) (formula: H_2N).

NH2
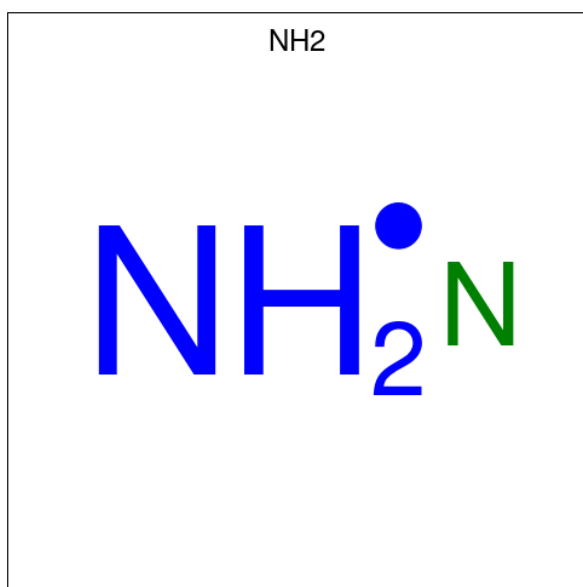
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	N 1	0	0
3	F	1	Total 1	N 1	0	0
3	G	1	Total 1	N 1	0	0
3	H	1	Total 1	N 1	0	0

- Molecule 4 is N,N'-(1,4-phenylene)diacetamide (three-letter code: WHL) (formula: $C_{10}H_{12}N_2O_2$).

WHL
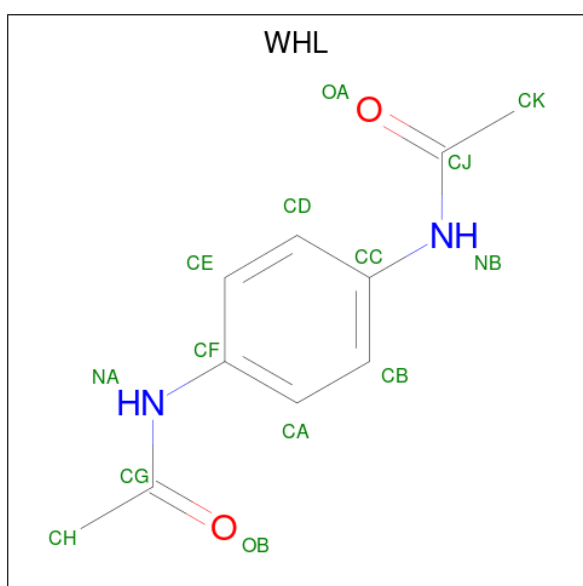
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total 14	C 10	N 2	O 2	0	0
4	F	1	Total 14	C 10	N 2	O 2	0	0
4	G	1	Total 14	C 10	N 2	O 2	0	0
4	H	1	Total 14	C 10	N 2	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total 107	O 107	0	0
5	B	103	Total 103	O 103	0	0
5	C	73	Total 73	O 73	0	0
5	D	44	Total 44	O 44	0	0
5	E	9	Total 9	O 9	0	0
5	F	6	Total 6	O 6	0	0
5	G	7	Total 7	O 7	0	0
5	H	6	Total 6	O 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Peptidyl-prolyl cis-trans isomerase A
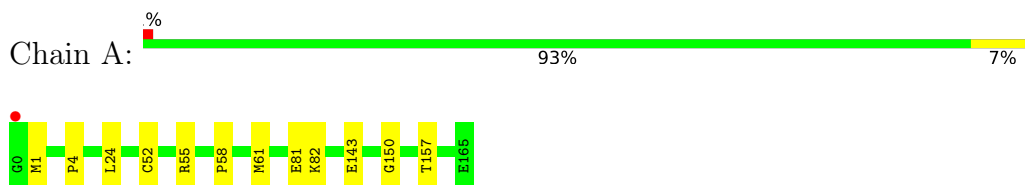
Chain A:

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A
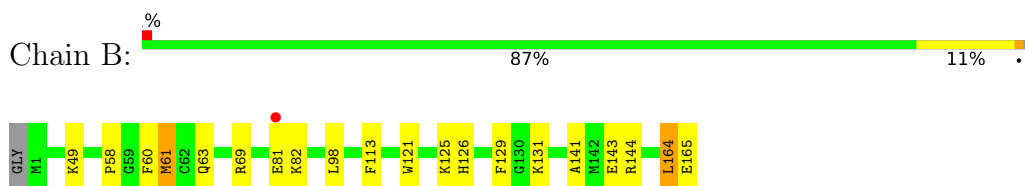
Chain B:

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain C:

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain D:

• Molecule 2: FP29102

Chain E:

100%
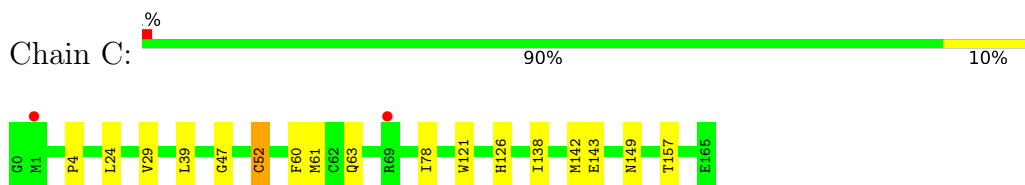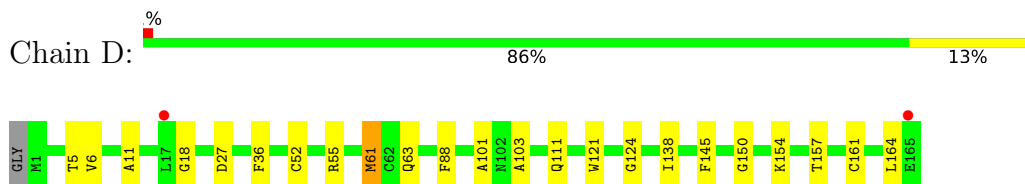
There are no outlier residues recorded for this chain.

• Molecule 2: FP29102

Chain F:

83%   17%

ACE0 H4 W9 C10 I11

• Molecule 2: FP29102

Chain G:

67%   33%

ACE0 P1 E2 C3 H4 I11

• Molecule 2: FP29102

8%

Chain H:

67%   33%

ACE0 P1 A7 I11
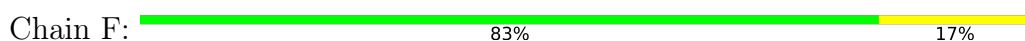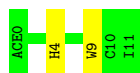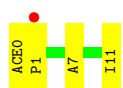
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.77Å 74.53Å 73.77Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	47.73 – 2.07 47.72 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.73-2.07) 94.9 (47.72-2.07)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.262 0.224 , 0.262	Depositor DCC
R_{free} test set	1851 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.001 for -h,l,k 0.329 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5881	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: WHL, ACE, NH2

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	0.28	0/1307	0.48	0/1749
1	B	0.28	0/1294	0.51	0/1733
1	C	0.28	0/1298	0.49	0/1738
1	D	0.27	0/1294	0.48	0/1733
2	E	0.26	0/99	0.44	0/136
2	F	0.24	0/99	0.44	0/136
2	G	0.30	0/99	0.47	0/136
2	H	0.28	0/99	0.51	0/136
All	All	0.28	0/5589	0.49	0/7497

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 ⓘ

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	1276	0	1253	5	0
1	B	1266	0	1237	15	0
1	C	1270	0	1240	11	0
1	D	1266	0	1237	19	0
2	E	97	0	83	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	97	0	83	2	0
2	G	97	0	83	3	0
2	H	97	0	83	9	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	E	14	0	0	0	0
4	F	14	0	0	0	0
4	G	14	0	0	0	0
4	H	14	0	0	0	0
5	A	107	0	0	1	0
5	B	103	0	0	5	0
5	C	73	0	0	1	0
5	D	44	0	0	0	0
5	E	9	0	0	0	0
5	F	6	0	0	0	0
5	G	7	0	0	0	0
5	H	6	0	0	0	0
All	All	5881	0	5299	53	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 5.

The worst 5 of 53 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:D:103:ALA:HB2	2:H:0:ACE:O	1.64	0.97
1:B:61:MET:HG2	1:B:113:PHE:HB2	1.52	0.90
1:B:81:GLU:HG2	1:B:82:LYS:HG2	1.67	0.75
1:D:103:ALA:CB	2:H:0:ACE:O	2.36	0.73
1:B:61:MET:CG	1:B:113:PHE:HB2	2.18	0.72

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	165/166 (99%)	159 (96%)	5 (3%)	1 (1%)	25	15
1	B	163/166 (98%)	158 (97%)	5 (3%)	0	100	100
1	C	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
1	D	163/166 (98%)	153 (94%)	10 (6%)	0	100	100
2	E	10/12 (83%)	10 (100%)	0	0	100	100
2	F	10/12 (83%)	10 (100%)	0	0	100	100
2	G	10/12 (83%)	9 (90%)	0	1 (10%)	0	0
2	H	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
All	All	695/712 (98%)	665 (96%)	28 (4%)	2 (0%)	41	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	1	PRO
1	A	1	MET

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	134/133 (101%)	132 (98%)	2 (2%)	65	62
1	B	133/133 (100%)	130 (98%)	3 (2%)	50	45
1	C	133/133 (100%)	130 (98%)	3 (2%)	50	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	133/133 (100%)	130 (98%)	3 (2%)	50	45
2	E	10/10 (100%)	10 (100%)	0	100	100
2	F	10/10 (100%)	10 (100%)	0	100	100
2	G	10/10 (100%)	10 (100%)	0	100	100
2	H	10/10 (100%)	10 (100%)	0	100	100
All	All	573/572 (100%)	562 (98%)	11 (2%)	57	53

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	TRP
1	D	61	MET
1	D	161	CYS
1	D	121	TRP
1	B	164	LEU

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are modelled with single atom - 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	#$|Z| > 2$
4	WHL	G	102	2	14,14,14	2.41	4 (28%)	18,18,18	1.24	3 (16%)
4	WHL	E	102	2	14,14,14	2.42	5 (35%)	18,18,18	1.03	2 (11%)
4	WHL	H	102	2	14,14,14	2.44	5 (35%)	18,18,18	1.50	3 (16%)
4	WHL	F	102	2	14,14,14	2.46	4 (28%)	18,18,18	1.28	2 (11%)

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
4	WHL	G	102	2	-	0/8/8/8	0/1/1/1
4	WHL	E	102	2	-	0/8/8/8	0/1/1/1
4	WHL	H	102	2	-	0/8/8/8	0/1/1/1
4	WHL	F	102	2	-	0/8/8/8	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	102	WHL	CG-NA	5.61	1.46	1.36
4	H	102	WHL	CG-NA	5.60	1.46	1.36
4	G	102	WHL	CG-NA	5.42	1.46	1.36
4	G	102	WHL	CJ-NB	5.39	1.46	1.36
4	E	102	WHL	CJ-NB	5.38	1.46	1.36

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	102	WHL	CK-CJ-NB	3.79	120.54	114.98
4	G	102	WHL	CK-CJ-NB	3.06	119.48	114.98
4	F	102	WHL	CH-CG-NA	3.00	119.39	114.98
4	H	102	WHL	CH-CG-NA	2.85	119.16	114.98
4	F	102	WHL	CK-CJ-NB	2.56	118.74	114.98

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(Å²)	Q<0.9
1	A	166/166 (100%)	-0.07	1 (0%)	89	90	26, 34, 45, 56	0
1	B	165/166 (99%)	-0.01	1 (0%)	89	90	27, 33, 43, 66	0
1	C	166/166 (100%)	0.14	2 (1%)	79	80	31, 40, 57, 79	0
1	D	165/166 (99%)	0.22	2 (1%)	79	80	32, 50, 65, 84	0
2	E	11/12 (91%)	0.34	0	100	100	36, 41, 48, 51	0
2	F	11/12 (91%)	0.17	0	100	100	32, 35, 44, 46	0
2	G	11/12 (91%)	0.12	0	100	100	34, 37, 46, 53	0
2	H	11/12 (91%)	0.18	1 (9%)	9	9	33, 37, 57, 58	0
All	All	706/712 (99%)	0.08	7 (0%)	82	83	26, 37, 60, 84	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	LEU	3.6
1	B	81	GLU	3.2
1	C	1	MET	2.6
1	D	165	GLU	2.4
1	A	0	GLY	2.4

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 monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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. 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	B-factors(Å^2)	Q<0.9
4	WHL	G	102	14/14	0.88	0.16	34,44,52,58	0
4	WHL	H	102	14/14	0.89	0.12	41,46,51,55	0
4	WHL	E	102	14/14	0.91	0.12	36,40,53,56	0
4	WHL	F	102	14/14	0.91	0.16	28,37,50,53	0
3	NH2	G	101	1/1	0.94	0.23	39,39,39,39	0
3	NH2	H	101	1/1	0.97	0.19	31,31,31,31	0
3	NH2	E	101	1/1	0.98	0.35	46,46,46,46	0
3	NH2	F	101	1/1	0.99	0.36	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.