



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:02 pm BST

PDB ID : 2J9Q
Title : A novel conformation for the TPR domain of pex5p
Authors : Stanley, W.A.; Wilmanns, M.; Kursula, P.
Deposited on : 2006-11-15
Resolution : 2.65 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

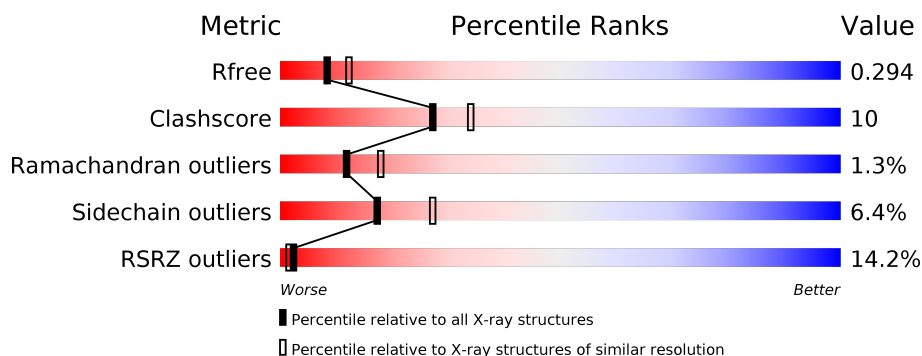
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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 $\leq 5\%$. 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	328	<div> <div>5%</div> <div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	328	<div> <div>19%</div> <div> <div>58%</div> <div>21%</div> <div>•</div> <div>18%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4468 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 PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2356	1482	409	452	13			
1	B	269	Total	C	N	O	S	0	0	0
			2092	1316	365	400	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	-	expression tag	UNP P50542
A	313	MET	-	expression tag	UNP P50542
A	314	GLY	-	expression tag	UNP P50542
A	425	ILE	THR	conflict	UNP P50542
B	312	GLY	-	expression tag	UNP P50542
B	313	MET	-	expression tag	UNP P50542
B	314	GLY	-	expression tag	UNP P50542
B	425	ILE	THR	conflict	UNP P50542

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

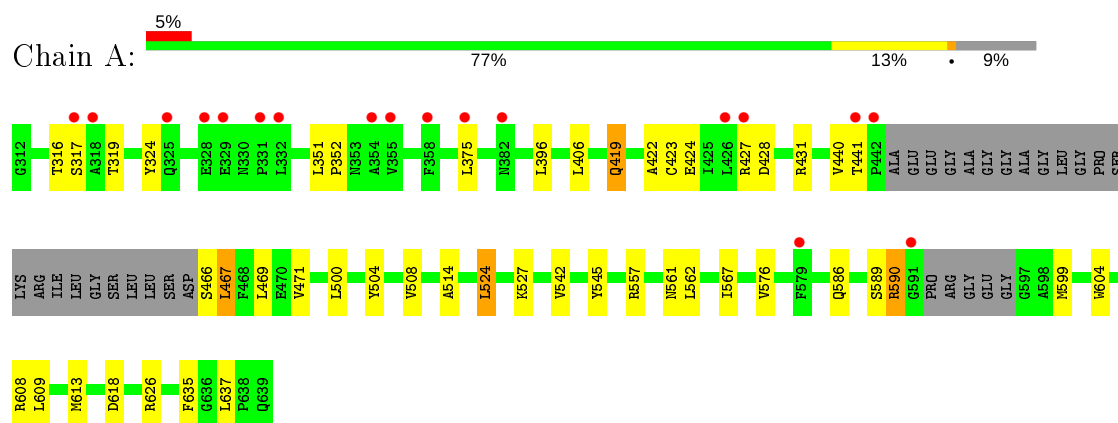
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	5	Total	O	0	0
			5	5		

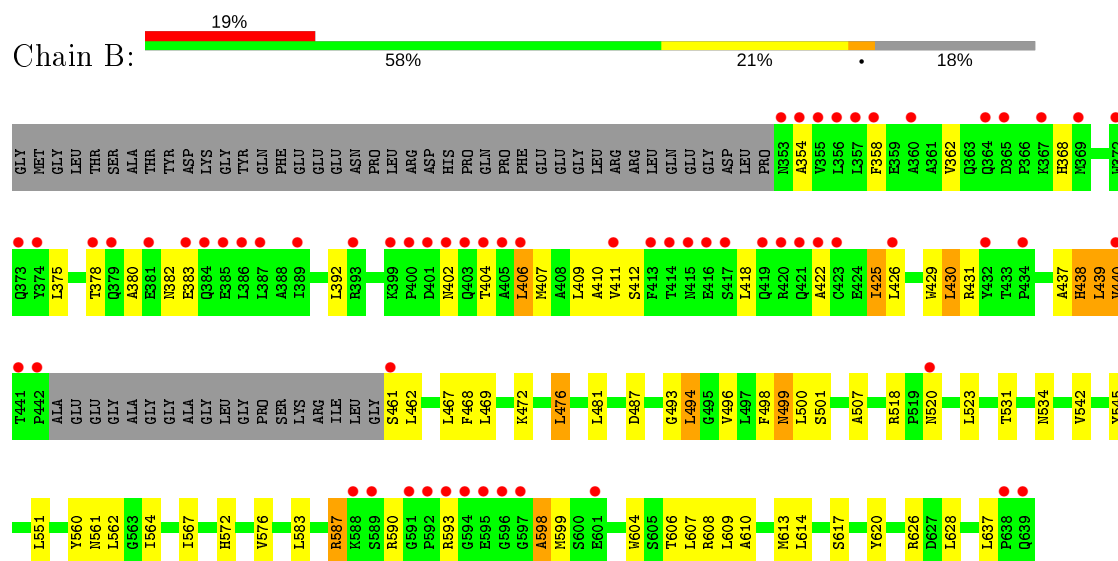
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR



• Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.67Å 91.41Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.65) 94.0 (19.53-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.300 0.239 , 0.294	Depositor DCC
R_{free} test set	833 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: SR

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	0.32	0/2403	0.48	0/3256
1	B	0.32	0/2129	0.49	0/2887
All	All	0.32	0/4532	0.49	0/6143

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	2356	0	2308	38	0
1	B	2092	0	2068	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	0	1	0
3	B	5	0	0	0	0
All	All	4468	0	4376	89	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 10.

All (89) 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:468:PHE:CE1	1:B:500:LEU:HD11	1.96	0.99
1:B:411:VAL:HG11	1:B:523:LEU:HD22	1.66	0.78
1:A:440:VAL:HG12	1:A:441:THR:H	1.51	0.76
1:A:609:LEU:HD23	1:B:609:LEU:HD23	1.70	0.72
1:B:392:LEU:HD13	1:B:409:LEU:HB3	1.74	0.70
1:B:409:LEU:HD12	1:B:410:ALA:N	2.07	0.70
1:A:609:LEU:HD21	1:B:606:THR:HG23	1.73	0.69
1:A:422:ALA:HB3	1:A:500:LEU:HD11	1.76	0.68
1:B:468:PHE:CD1	1:B:500:LEU:HD11	2.30	0.66
1:B:410:ALA:HB2	1:B:426:LEU:HD21	1.81	0.63
1:B:422:ALA:O	1:B:425:ILE:HG22	1.99	0.63
1:B:392:LEU:HD13	1:B:409:LEU:CB	2.30	0.60
1:B:418:LEU:O	1:B:422:ALA:HB3	2.01	0.60
1:B:520:ASN:O	1:B:551:LEU:HD13	2.02	0.59
1:A:604:TRP:CE2	1:A:626:ARG:HG3	2.37	0.59
1:B:499:ASN:HD21	1:B:534:ASN:HD22	1.50	0.59
1:B:380:ALA:HB1	1:B:412:SER:CB	2.33	0.59
1:A:316:THR:HG22	1:A:317:SER:H	1.69	0.57
1:A:567:ILE:CG2	1:B:613:MET:CE	2.83	0.57
1:A:567:ILE:HG21	1:B:613:MET:CE	2.35	0.57
1:B:576:VAL:HG13	1:B:607:LEU:HD11	1.87	0.56
1:B:500:LEU:HD12	1:B:500:LEU:C	2.26	0.56
1:B:429:TRP:HE3	1:B:430:LEU:HD12	1.71	0.55
1:B:567:ILE:HD11	1:B:610:ALA:HB2	1.87	0.55
1:B:439:LEU:HD22	1:B:440:VAL:N	2.23	0.54
1:B:410:ALA:CB	1:B:426:LEU:HD21	2.37	0.54
1:A:567:ILE:CG2	1:B:613:MET:HE2	2.38	0.53
1:B:406:LEU:HD13	1:B:429:TRP:HE1	1.72	0.53
1:B:545:TYR:CZ	1:B:561:ASN:HB3	2.44	0.53
1:A:419:GLN:NE2	3:A:2005:HOH:O	2.42	0.52
1:B:583:LEU:HD13	1:B:604:TRP:CZ2	2.44	0.52
1:A:613:MET:CE	1:B:613:MET:CE	2.88	0.52
1:B:476:LEU:HD13	1:B:494:LEU:HD11	1.91	0.52
1:A:567:ILE:HG21	1:B:613:MET:HE3	1.92	0.52
1:A:545:TYR:CZ	1:A:561:ASN:HB3	2.46	0.51
1:B:587:ARG:HG3	1:B:628:LEU:HD23	1.92	0.51
1:B:494:LEU:HD22	1:B:498:PHE:CD2	2.46	0.50
1:A:576:VAL:HG11	1:A:635:PHE:CE2	2.46	0.50
1:B:358:PHE:HB2	1:B:375:LEU:HD13	1.93	0.49
1:B:409:LEU:HD12	1:B:410:ALA:HB2	1.93	0.49
1:B:383:GLU:CD	1:B:598:ALA:HB1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LEU:HD12	1:B:501:SER:N	2.28	0.49
1:A:428:ASP:HA	1:A:431:ARG:HG2	1.94	0.49
1:B:499:ASN:HD21	1:B:534:ASN:ND2	2.11	0.49
1:B:407:MET:CE	1:B:410:ALA:HB3	2.44	0.48
1:B:542:VAL:HG13	1:B:562:LEU:HD11	1.95	0.48
1:A:467:LEU:HD22	1:A:471:VAL:HG23	1.95	0.48
1:B:378:THR:O	1:B:378:THR:HG22	2.14	0.47
1:A:422:ALA:CB	1:A:500:LEU:HD11	2.44	0.47
1:A:557:ARG:HA	1:A:599:MET:HE1	1.96	0.47
1:A:351:LEU:N	1:A:352:PRO:CD	2.78	0.47
1:A:316:THR:HG22	1:A:317:SER:N	2.29	0.47
1:B:493:GLY:O	1:B:496:VAL:HG22	2.15	0.47
1:B:358:PHE:O	1:B:362:VAL:HG13	2.14	0.46
1:B:617:SER:HA	1:B:620:TYR:CE1	2.51	0.46
1:A:419:GLN:HB3	1:A:500:LEU:HD22	1.98	0.46
1:A:324:TYR:OH	1:A:375:LEU:HD11	2.16	0.45
1:A:424:GLU:HG3	1:A:467:LEU:HD11	1.98	0.45
1:B:380:ALA:HB1	1:B:412:SER:OG	2.17	0.44
1:B:409:LEU:HD13	1:B:425:ILE:HG23	2.00	0.44
1:B:437:ALA:O	1:B:439:LEU:HD12	2.19	0.43
1:A:466:SER:OG	1:A:469:LEU:HD13	2.18	0.43
1:A:423:CYS:HB3	1:A:471:VAL:HG21	2.01	0.43
1:A:504:TYR:O	1:A:508:VAL:HG23	2.18	0.43
1:A:604:TRP:CZ2	1:A:626:ARG:HG3	2.53	0.43
1:A:586:GLN:O	1:A:590:ARG:HG3	2.18	0.43
1:B:572:HIS:HB2	1:B:614:LEU:HD13	2.00	0.43
1:B:354:ALA:CB	1:B:378:THR:HG21	2.49	0.42
1:A:567:ILE:CG2	1:B:613:MET:HE3	2.48	0.42
1:B:507:ALA:HB3	1:B:531:THR:HG21	2.02	0.42
1:B:467:LEU:HD13	1:B:467:LEU:C	2.40	0.42
1:B:468:PHE:CZ	1:B:501:SER:HB3	2.55	0.42
1:A:514:ALA:CB	1:A:524:LEU:HD11	2.50	0.41
1:A:396:LEU:HD21	1:A:406:LEU:HG	2.02	0.41
1:B:560:TYR:CZ	1:B:564:ILE:HD11	2.55	0.41
1:A:431:ARG:HB3	1:A:440:VAL:HG21	2.02	0.41
1:B:609:LEU:HG	1:B:613:MET:CE	2.50	0.41
1:A:542:VAL:HG13	1:A:562:LEU:HD11	2.03	0.41
1:B:407:MET:HE1	1:B:410:ALA:HB3	2.02	0.41
1:A:467:LEU:HD22	1:A:471:VAL:CG2	2.51	0.41
1:B:438:HIS:CG	1:B:438:HIS:O	2.74	0.41
1:A:423:CYS:HB2	1:A:467:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ASP:OD2	1:A:618:ASP:N	2.54	0.40
1:B:409:LEU:HD22	1:B:425:ILE:HD12	2.02	0.40
1:A:613:MET:HE1	1:B:613:MET:HE2	2.04	0.40
1:B:469:LEU:HD12	1:B:472:LYS:HE3	2.03	0.40
1:B:437:ALA:O	1:B:439:LEU:N	2.54	0.40
1:A:613:MET:CE	1:B:613:MET:HE2	2.51	0.40
1:B:609:LEU:HG	1:B:613:MET:HE3	2.03	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	295/328 (90%)	280 (95%)	13 (4%)	2 (1%)	22	33
1	B	265/328 (81%)	236 (89%)	24 (9%)	5 (2%)	8	11
All	All	560/656 (85%)	516 (92%)	37 (7%)	7 (1%)	12	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	SER
1	A	590	ARG
1	B	368	HIS
1	B	402	ASN
1	B	438	HIS
1	B	598	ALA
1	B	440	VAL

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	248/264 (94%)	240 (97%)	8 (3%)	39 56
1	B	220/264 (83%)	198 (90%)	22 (10%)	7 10
All	All	468/528 (89%)	438 (94%)	30 (6%)	17 27

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	THR
1	A	419	GLN
1	A	427	ARG
1	A	467	LEU
1	A	524	LEU
1	A	527	LYS
1	A	608	ARG
1	A	637	LEU
1	B	382	ASN
1	B	404	THR
1	B	406	LEU
1	B	425	ILE
1	B	430	LEU
1	B	431	ARG
1	B	439	LEU
1	B	461	SER
1	B	462	LEU
1	B	476	LEU
1	B	481	LEU
1	B	487	ASP
1	B	494	LEU
1	B	499	ASN
1	B	518	ARG
1	B	587	ARG
1	B	590	ARG
1	B	593	ARG
1	B	599	MET

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Mol	Chain	Res	Type
1	B	608	ARG
1	B	626	ARG
1	B	637	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	B	353	ASN
1	B	382	ASN
1	B	415	ASN
1	B	499	ASN
1	B	616	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	300/328 (91%)	0.45	18 (6%) 21 18	39, 44, 47, 52	0
1	B	269/328 (82%)	1.16	63 (23%) 0 0	39, 44, 50, 57	0
All	All	569/656 (86%)	0.79	81 (14%) 2 1	39, 44, 48, 57	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	ASP	8.7
1	B	594	GLY	8.1
1	B	591	GLY	7.9
1	B	403	GLN	6.6
1	B	415	ASN	6.4
1	A	441	THR	6.4
1	B	354	ALA	6.1
1	B	405	ALA	5.9
1	B	595	GLU	5.3
1	B	593	ARG	5.0
1	B	386	LEU	4.6
1	B	404	THR	4.4
1	B	596	GLY	4.3
1	B	369	MET	4.3
1	B	353	ASN	4.2
1	B	389	ILE	4.1
1	B	442	PRO	4.1
1	B	402	ASN	4.1
1	B	440	VAL	4.1
1	B	414	THR	4.1
1	B	419	GLN	4.0
1	B	441	THR	4.0
1	A	331	PRO	3.9
1	B	413	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	358	PHE	3.8
1	B	355	VAL	3.7
1	B	592	PRO	3.6
1	B	432	TYR	3.6
1	B	357	LEU	3.5
1	B	416	GLU	3.4
1	B	374	TYR	3.4
1	B	589	SER	3.4
1	B	367	LYS	3.3
1	A	442	PRO	3.3
1	A	317	SER	3.3
1	B	411	VAL	3.3
1	B	420	ARG	3.3
1	B	638	PRO	3.2
1	A	375	LEU	3.2
1	B	406	LEU	3.2
1	B	356	LEU	3.2
1	B	387	LEU	3.2
1	A	328	GLU	3.1
1	B	364	GLN	3.1
1	A	355	VAL	3.1
1	B	381	GLU	3.1
1	B	399	LYS	3.0
1	B	422	ALA	3.0
1	A	591	GLY	3.0
1	B	417	SER	2.9
1	A	318	ALA	2.9
1	B	358	PHE	2.9
1	B	400	PRO	2.8
1	B	426	LEU	2.8
1	B	421	GLN	2.7
1	B	597	GLY	2.6
1	B	385	GLU	2.6
1	A	332	LEU	2.6
1	A	329	GLU	2.6
1	A	426	LEU	2.5
1	B	601	GLU	2.5
1	B	378	THR	2.5
1	B	423	CYS	2.4
1	B	384	GLN	2.4
1	B	588	LYS	2.4
1	B	360	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	354	ALA	2.4
1	A	427	ARG	2.3
1	B	365	ASP	2.3
1	B	639	GLN	2.3
1	B	379	GLN	2.2
1	B	393	ARG	2.2
1	A	382	ASN	2.2
1	B	372	TRP	2.1
1	B	461	SER	2.1
1	B	373	GLN	2.1
1	B	520	ASN	2.1
1	A	579	PHE	2.1
1	B	434	PRO	2.1
1	A	325	GLN	2.0
1	B	383	GLU	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. 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(\AA^2)	Q<0.9
2	SR	B	1640	1/1	0.98	0.09	44,44,44,44	0
2	SR	A	1640	1/1	0.99	0.13	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.