



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:18 pm GMT

PDB ID : 1YFO
Title : RECEPTOR PROTEIN TYROSINE PHOSPHATASE ALPHA, DOMAIN 1
FROM MOUSE
Authors : Bilwes, A.M.; Noel, J.P.
Deposited on : 1996-12-11
Resolution : 2.25 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

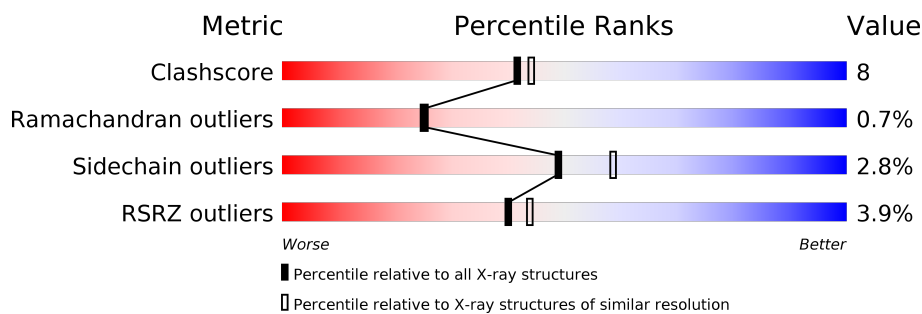
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	302	
1	B	302	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4839 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 RECEPTOR PROTEIN TYROSINE PHOSPHATASE ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2276	1454	389	415	18			
1	B	279	Total	C	N	O	S	0	0	0
			2276	1454	389	415	18			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	LEU	ILE	CONFLICT	UNP P18052
A	?	-	PHE	DELETION	UNP P18052
A	?	-	LEU	DELETION	UNP P18052
A	?	-	SER	DELETION	UNP P18052
A	?	-	LEU	DELETION	UNP P18052
A	?	-	ALA	DELETION	UNP P18052
A	?	-	VAL	DELETION	UNP P18052
A	?	-	SER	DELETION	UNP P18052
A	?	-	LYS	DELETION	UNP P18052
A	?	-	ASP	DELETION	UNP P18052
A	?	-	ALA	DELETION	UNP P18052
A	?	-	VAL	DELETION	UNP P18052
A	?	-	LYS	DELETION	UNP P18052
A	?	-	ALA	DELETION	UNP P18052
A	?	-	LEU	DELETION	UNP P18052
A	?	-	ASN	DELETION	UNP P18052
A	?	-	LYS	DELETION	UNP P18052
A	?	-	THR	DELETION	UNP P18052
A	?	-	THR	DELETION	UNP P18052
A	?	-	PRO	DELETION	UNP P18052
A	?	-	LEU	DELETION	UNP P18052
A	?	-	LEU	DELETION	UNP P18052
A	?	-	GLU	DELETION	UNP P18052
A	?	-	ARG	DELETION	UNP P18052

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	DELETION	UNP P18052
A	?	-	PHE	DELETION	UNP P18052
A	?	-	ILE	DELETION	UNP P18052
A	?	-	GLY	DELETION	UNP P18052
A	?	-	LYS	DELETION	UNP P18052
A	?	-	SER	DELETION	UNP P18052
A	?	-	ASN	DELETION	UNP P18052
A	?	-	SER	DELETION	UNP P18052
A	?	-	ARG	DELETION	UNP P18052
A	?	-	GLY	DELETION	UNP P18052
A	?	-	CYS	DELETION	UNP P18052
A	?	-	LEU	DELETION	UNP P18052
A	?	-	SER	DELETION	UNP P18052
A	268	TYR	ASP	CONFLICT	UNP P18052
B	231	LEU	ILE	CONFLICT	UNP P18052
B	?	-	PHE	DELETION	UNP P18052
B	?	-	LEU	DELETION	UNP P18052
B	?	-	SER	DELETION	UNP P18052
B	?	-	LEU	DELETION	UNP P18052
B	?	-	ALA	DELETION	UNP P18052
B	?	-	VAL	DELETION	UNP P18052
B	?	-	SER	DELETION	UNP P18052
B	?	-	LYS	DELETION	UNP P18052
B	?	-	ASP	DELETION	UNP P18052
B	?	-	ALA	DELETION	UNP P18052
B	?	-	VAL	DELETION	UNP P18052
B	?	-	LYS	DELETION	UNP P18052
B	?	-	ALA	DELETION	UNP P18052
B	?	-	LEU	DELETION	UNP P18052
B	?	-	ASN	DELETION	UNP P18052
B	?	-	LYS	DELETION	UNP P18052
B	?	-	THR	DELETION	UNP P18052
B	?	-	THR	DELETION	UNP P18052
B	?	-	PRO	DELETION	UNP P18052
B	?	-	LEU	DELETION	UNP P18052
B	?	-	LEU	DELETION	UNP P18052
B	?	-	GLU	DELETION	UNP P18052
B	?	-	ARG	DELETION	UNP P18052
B	?	-	ARG	DELETION	UNP P18052
B	?	-	PHE	DELETION	UNP P18052
B	?	-	ILE	DELETION	UNP P18052
B	?	-	GLY	DELETION	UNP P18052

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP P18052
B	?	-	SER	DELETION	UNP P18052
B	?	-	ASN	DELETION	UNP P18052
B	?	-	SER	DELETION	UNP P18052
B	?	-	ARG	DELETION	UNP P18052
B	?	-	GLY	DELETION	UNP P18052
B	?	-	CYS	DELETION	UNP P18052
B	?	-	LEU	DELETION	UNP P18052
B	?	-	SER	DELETION	UNP P18052
B	268	TYR	ASP	CONFLICT	UNP P18052

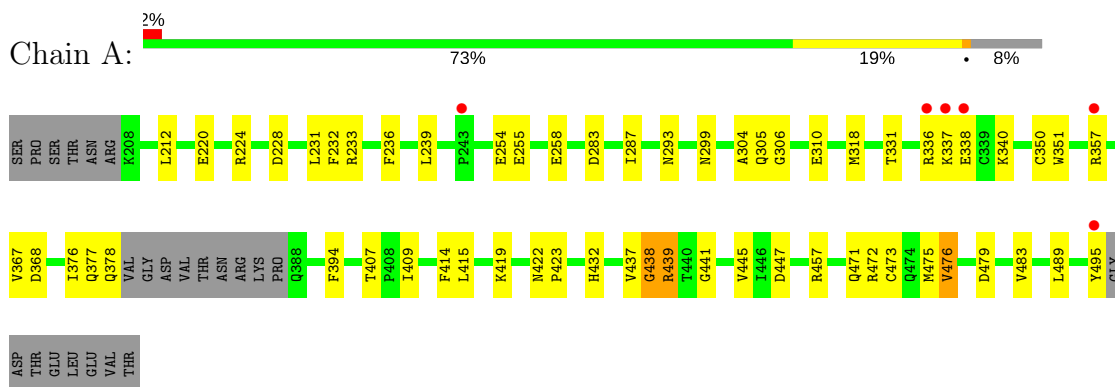
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	163	Total O 163 163	0	0
2	B	124	Total O 124 124	0	0

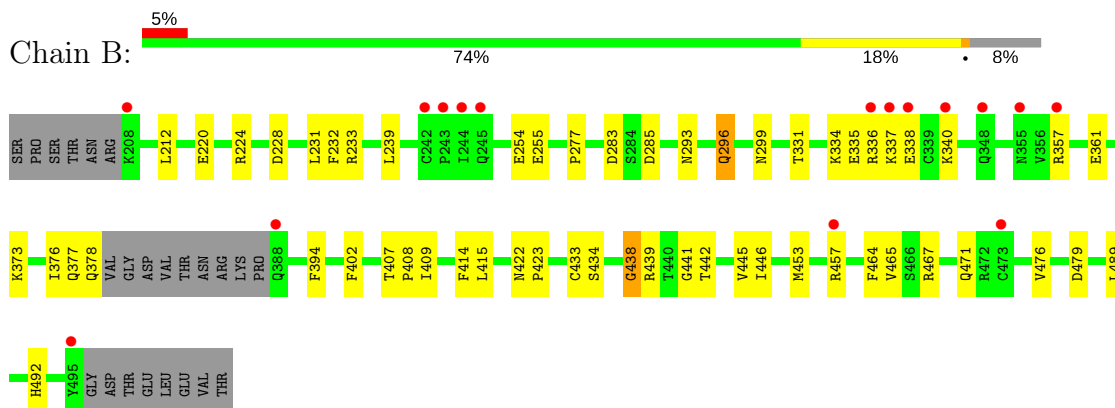
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: RECEPTOR PROTEIN TYROSINE PHOSPHATASE ALPHA



• Molecule 1: RECEPTOR PROTEIN TYROSINE PHOSPHATASE ALPHA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.19Å 119.84Å 61.18Å 90.00° 110.08° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 23.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	82.4 (20.00-2.25) 81.8 (23.90-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 2.26Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.251 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.257 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4839	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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

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	0.30	0/2332	0.56	0/3160
1	B	0.29	0/2332	0.57	0/3160
All	All	0.30	0/4664	0.56	0/6320

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	2276	0	2230	35	0
1	B	2276	0	2230	37	0
2	A	163	0	0	3	0
2	B	124	0	0	4	0
All	All	4839	0	4460	72	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 8.

All (72) 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:336:ARG:HH21	1:B:402:PHE:HE2	1.36	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:CYS:HA	2:A:606:HOH:O	1.92	0.69
1:B:340:LYS:HE3	1:B:434:SER:HB2	1.78	0.66
1:B:331:THR:OG1	1:B:433:CYS:HA	1.99	0.62
1:B:340:LYS:HG3	1:B:434:SER:HB2	1.82	0.61
1:B:438:GLY:HA3	2:B:552:HOH:O	2.01	0.61
1:A:438:GLY:HA3	2:A:659:HOH:O	1.99	0.60
1:B:340:LYS:HE3	1:B:434:SER:CB	2.31	0.59
1:B:293:ASN:ND2	1:B:299:ASN:H	2.01	0.59
1:A:293:ASN:ND2	1:A:299:ASN:H	2.02	0.56
1:B:373:LYS:HE3	2:B:606:HOH:O	2.04	0.56
1:B:293:ASN:ND2	1:B:471:GLN:HE22	2.05	0.54
1:A:336:ARG:O	1:A:337:LYS:HB2	2.08	0.53
1:B:407:THR:CG2	1:B:409:ILE:HD13	2.38	0.53
1:A:338:GLU:HB2	1:A:340:LYS:HE2	1.92	0.50
1:A:212:LEU:HD21	1:A:224:ARG:NH2	2.27	0.50
1:A:305:GLN:HG2	1:A:306:GLY:O	2.12	0.49
1:B:239:LEU:HD21	1:B:465:VAL:HG11	1.93	0.49
1:A:228:ASP:O	1:A:233:ARG:NH2	2.46	0.49
1:A:437:VAL:HG12	1:A:472:ARG:HE	1.78	0.48
1:B:296:GLN:O	1:B:296:GLN:HG2	2.13	0.48
1:B:331:THR:CG2	1:B:340:LYS:HG2	2.43	0.48
1:A:419:LYS:HE2	1:A:447:ASP:OD1	2.14	0.48
1:B:334:LYS:HE2	1:B:337:LYS:HA	1.95	0.47
1:A:258:GLU:HB3	1:A:310:GLU:OE1	2.14	0.47
1:B:277:PRO:HG3	1:B:285:ASP:HB3	1.96	0.47
1:A:236:PHE:O	1:A:239:LEU:HB2	2.15	0.47
1:A:407:THR:HB	1:A:409:ILE:HD13	1.97	0.47
1:A:331:THR:HG22	1:A:439:ARG:NH1	2.30	0.47
1:B:394:PHE:HB3	1:B:414:PHE:CE1	2.50	0.46
2:A:564:HOH:O	1:B:340:LYS:HD2	2.16	0.45
1:B:228:ASP:O	1:B:233:ARG:NH2	2.49	0.45
1:A:367:VAL:HG13	1:A:368:ASP:H	1.82	0.45
1:A:293:ASN:HD22	1:A:299:ASN:H	1.65	0.45
1:A:293:ASN:ND2	1:A:471:GLN:HE22	2.15	0.45
1:A:409:ILE:HD12	1:A:409:ILE:H	1.81	0.45
1:A:357:ARG:O	1:A:376:ILE:HA	2.18	0.44
1:A:287:ILE:HG21	1:A:318:MET:HE2	1.98	0.44
1:B:377:GLN:O	1:B:378:GLN:HB2	2.17	0.44
1:B:453:MET:O	1:B:457:ARG:HA	2.17	0.44
1:B:233:ARG:HD3	1:B:479:ASP:OD2	2.18	0.43
1:B:441:GLY:O	1:B:445:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:MET:O	1:A:476:VAL:HB	2.18	0.43
1:B:224:ARG:HA	1:B:231:LEU:HB2	2.00	0.43
1:A:304:ALA:O	1:A:432:HIS:HB2	2.19	0.43
1:B:336:ARG:C	1:B:338:GLU:H	2.22	0.43
1:A:233:ARG:HD3	1:A:479:ASP:OD2	2.19	0.43
1:B:357:ARG:O	1:B:376:ILE:HA	2.19	0.43
1:A:224:ARG:HA	1:A:231:LEU:HB2	2.01	0.42
1:B:407:THR:HA	1:B:408:PRO:HD3	1.90	0.42
1:B:407:THR:HG21	1:B:409:ILE:HD13	2.00	0.42
1:A:441:GLY:O	1:A:445:VAL:HG23	2.19	0.42
1:B:492:HIS:HD2	2:B:591:HOH:O	2.03	0.42
1:A:212:LEU:HD21	1:A:224:ARG:HH22	1.85	0.42
1:B:239:LEU:HD21	1:B:465:VAL:CG1	2.49	0.42
1:B:335:GLU:O	1:B:338:GLU:HB2	2.21	0.41
1:B:212:LEU:HD22	1:B:220:GLU:HG3	2.02	0.41
1:A:479:ASP:O	1:A:483:VAL:HG23	2.20	0.41
1:A:350:CYS:SG	1:A:357:ARG:HG2	2.61	0.41
1:B:442:THR:O	1:B:446:ILE:HG13	2.21	0.41
1:B:340:LYS:HG3	1:B:434:SER:CB	2.50	0.41
1:A:350:CYS:SG	1:A:351:TRP:N	2.94	0.41
1:B:422:ASN:HA	1:B:423:PRO:HD3	1.91	0.41
1:B:299:ASN:ND2	2:B:517:HOH:O	2.54	0.41
1:A:394:PHE:HB3	1:A:414:PHE:CE1	2.56	0.41
1:A:422:ASN:HA	1:A:423:PRO:HD3	1.93	0.41
1:A:255:GLU:CD	1:A:255:GLU:H	2.24	0.40
1:B:255:GLU:HG3	1:B:283:ASP:OD2	2.22	0.40
1:B:464:PHE:O	1:B:467:ARG:HB3	2.21	0.40
1:A:220:GLU:O	1:A:224:ARG:HG3	2.21	0.40
1:A:255:GLU:HG3	1:A:283:ASP:CG	2.42	0.40
1:A:377:GLN:O	1:A:378:GLN:HB2	2.22	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	275/302 (91%)	258 (94%)	15 (6%)	2 (1%)	25	25
1	B	275/302 (91%)	258 (94%)	15 (6%)	2 (1%)	25	25
All	All	550/604 (91%)	516 (94%)	30 (6%)	4 (1%)	25	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	VAL
1	A	438	GLY
1	B	438	GLY
1	B	476	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	249/270 (92%)	242 (97%)	7 (3%)	49	58
1	B	249/270 (92%)	242 (97%)	7 (3%)	49	58
All	All	498/540 (92%)	484 (97%)	14 (3%)	49	58

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

Mol	Chain	Res	Type
1	A	232	PHE
1	A	254	GLU
1	A	415	LEU
1	A	439	ARG
1	A	457	ARG
1	A	489	LEU
1	A	495	TYR
1	B	232	PHE
1	B	254	GLU

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Mol	Chain	Res	Type
1	B	296	GLN
1	B	361	GLU
1	B	415	LEU
1	B	439	ARG
1	B	489	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	293	ASN
1	A	299	ASN
1	A	323	ASN
1	A	492	HIS
1	B	229	ASN
1	B	293	ASN
1	B	296	GLN
1	B	299	ASN
1	B	323	ASN
1	B	378	GLN
1	B	492	HIS

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](#)

There are no ligands in this entry.

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

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	279/302 (92%)	-0.18	6 (2%) 62 65	4, 16, 42, 73	0
1	B	279/302 (92%)	-0.00	16 (5%) 24 27	6, 17, 48, 83	0
All	All	558/604 (92%)	-0.09	22 (3%) 40 44	4, 17, 45, 83	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ILE	6.0
1	B	495	TYR	5.8
1	A	495	TYR	4.4
1	A	336	ARG	4.4
1	B	245	GLN	3.8
1	B	243	PRO	3.7
1	B	348	GLN	3.7
1	B	242	CYS	3.5
1	A	337	LYS	2.9
1	B	337	LYS	2.8
1	B	338	GLU	2.5
1	B	336	ARG	2.4
1	B	457	ARG	2.4
1	B	357	ARG	2.4
1	A	338	GLU	2.4
1	B	473	CYS	2.3
1	B	355	ASN	2.3
1	A	243	PRO	2.2
1	B	208	LYS	2.1
1	B	388	GLN	2.1
1	B	340	LYS	2.1
1	A	357	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.