



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:30 pm BST

PDB ID : 2AHS
Title : Crystal Structure of the Catalytic Domain of Human Tyrosine Receptor Phosphatase Beta
Authors : Ugochukwu, E.; Eswaran, J.; Barr, A.; Gileadi, O.; Sobott, F.; Burgess, N.; Ball, L.; Bray, J.; von Delft, F.; Debreczeni, J.; Bunkoczi, G.; Turnbull, A.; Das, S.; Weigelt, J.; Edwards, A.; Arrowsmith, C.; Sundstrom, M.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2005-07-28
Resolution : 2.10 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

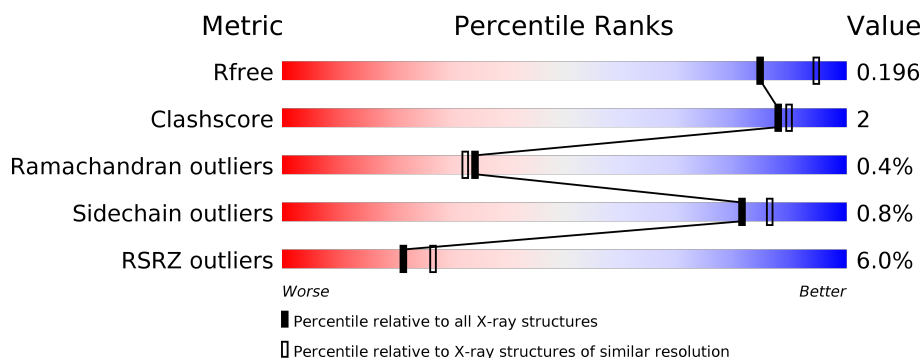
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	295	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	295	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5023 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-type tyrosine-protein phosphatase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	4	0
			2293	1450	409	419	15			
1	B	272	Total	C	N	O	S	0	6	0
			2209	1393	394	408	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1677	GLY	-	CLONING ARTIFACT	UNP P23467
A	1678	PRO	-	CLONING ARTIFACT	UNP P23467
A	1679	LEU	-	CLONING ARTIFACT	UNP P23467
A	1680	GLY	-	CLONING ARTIFACT	UNP P23467
A	1681	SER	-	CLONING ARTIFACT	UNP P23467
A	1682	PRO	-	CLONING ARTIFACT	UNP P23467
A	1683	GLY	-	CLONING ARTIFACT	UNP P23467
A	1684	ILE	-	CLONING ARTIFACT	UNP P23467
A	1685	PRO	-	CLONING ARTIFACT	UNP P23467
B	1677	GLY	-	CLONING ARTIFACT	UNP P23467
B	1678	PRO	-	CLONING ARTIFACT	UNP P23467
B	1679	LEU	-	CLONING ARTIFACT	UNP P23467
B	1680	GLY	-	CLONING ARTIFACT	UNP P23467
B	1681	SER	-	CLONING ARTIFACT	UNP P23467
B	1682	PRO	-	CLONING ARTIFACT	UNP P23467
B	1683	GLY	-	CLONING ARTIFACT	UNP P23467
B	1684	ILE	-	CLONING ARTIFACT	UNP P23467
B	1685	PRO	-	CLONING ARTIFACT	UNP P23467

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Cl	0	0
			6	6		

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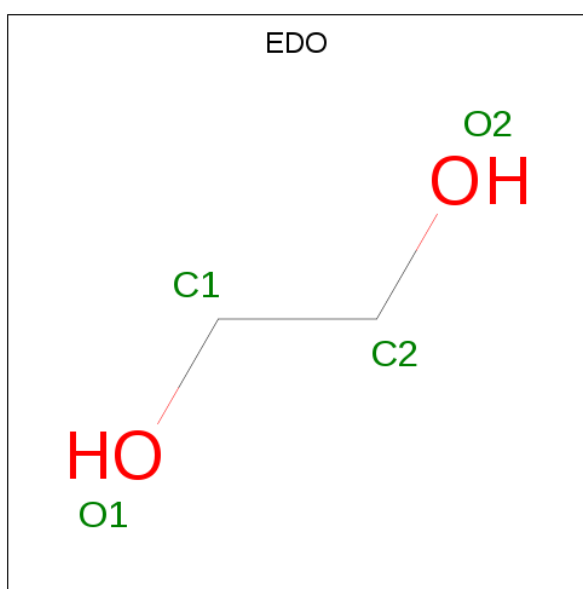
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

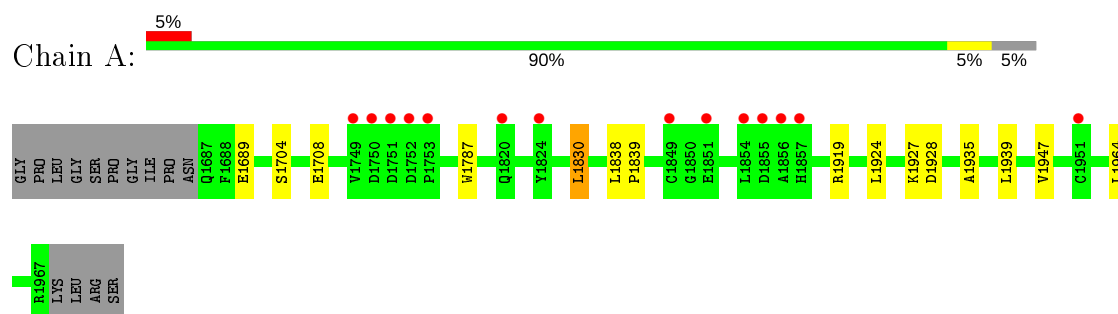
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	270	Total	O	0	0
			270	270		
5	B	209	Total	O	0	0
			209	209		

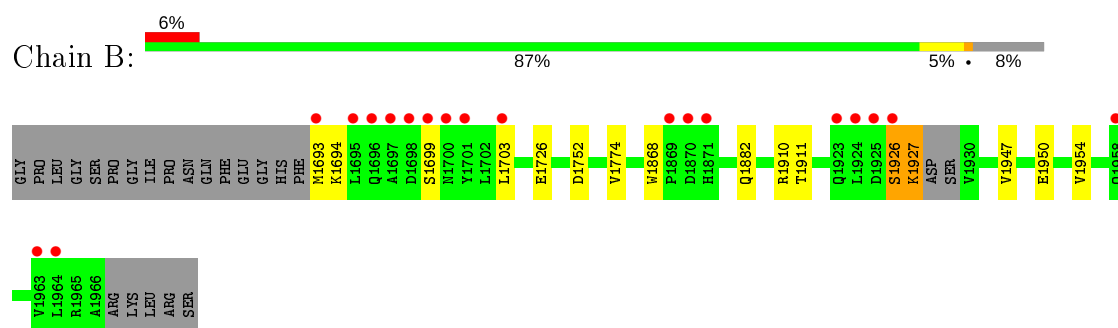
3 Residue-property plots [i](#)

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-type tyrosine-protein phosphatase beta



- Molecule 1: Receptor-type tyrosine-protein phosphatase beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.37Å 123.37Å 179.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.40 – 2.10 53.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (53.40-2.10) 99.2 (53.42-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.152 , 0.206 0.198 , 0.196	Depositor DCC
R_{free} test set	2347 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5023	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EDO, CL

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	0.62	0/2361	0.69	2/3207 (0.1%)
1	B	0.59	0/2278	0.67	0/3098
All	All	0.61	0/4639	0.68	2/6305 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1927	LYS	N-CA-C	5.66	126.29	111.00
1	A	1919	ARG	NE-CZ-NH2	-5.60	117.50	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1927	LYS	CA

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	2293	0	2212	7	0
1	B	2209	0	2119	11	0
2	A	3	0	0	0	0
2	B	6	0	0	1	0
3	A	1	0	0	0	0
4	A	16	0	24	0	0
4	B	16	0	24	0	0
5	A	270	0	0	1	6
5	B	209	0	0	1	4
All	All	5023	0	4379	18	6

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 2.

All (18) 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:1752:ASP:HB3	5:B:74:HOH:O	1.83	0.78
1:B:1774:VAL:HG13	1:B:1911:THR:HG21	1.74	0.68
1:B:1699:SER:O	1:B:1703:LEU:HG	1.94	0.67
1:B:1693:MET:CG	1:B:1694:LYS:H	2.20	0.54
1:A:1924:LEU:HD11	1:A:1964:LEU:HD21	1.91	0.53
1:A:1689:GLU:HG3	5:A:158:HOH:O	2.10	0.52
1:B:1726:GLU:HB2	2:B:801:CL:CL	2.48	0.51
1:B:1950:GLU:O	1:B:1954:VAL:HG13	2.12	0.49
1:A:1935:ALA:O	1:A:1939:LEU:HG	2.16	0.46
1:A:1924:LEU:O	1:A:1928:ASP:CB	2.65	0.45
1:B:1693:MET:HG2	1:B:1694:LYS:H	1.82	0.45
1:B:1868:TRP:CE2	1:B:1910[A]:ARG:HG2	2.52	0.45
1:A:1787:TRP:CZ2	1:A:1830:LEU:HD11	2.54	0.43
1:A:1838:LEU:HB3	1:A:1839:PRO:HD2	2.00	0.42
1:B:1926:SER:O	1:B:1927:LYS:C	2.58	0.42
1:B:1774:VAL:CG1	1:B:1911:THR:HG21	2.46	0.42
1:A:1704:SER:O	1:A:1708:GLU:HG2	2.21	0.41
1:B:1868:TRP:CZ2	1:B:1910[A]:ARG:HG2	2.56	0.41

All (6) 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)
5:A:171:HOH:O	5:A:624:HOH:O[12_565]	1.56	0.64
5:A:624:HOH:O	5:A:624:HOH:O[12_565]	1.75	0.45
5:A:616:HOH:O	5:B:114:HOH:O[8_665]	1.83	0.37
5:A:616:HOH:O	5:B:204:HOH:O[8_665]	2.02	0.18
5:A:191:HOH:O	5:B:40:HOH:O[8_665]	2.02	0.18
5:A:195:HOH:O	5:B:643:HOH:O[10_664]	2.16	0.04

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	283/295 (96%)	274 (97%)	8 (3%)	1 (0%)	34	32
1	B	274/295 (93%)	264 (96%)	9 (3%)	1 (0%)	34	32
All	All	557/590 (94%)	538 (97%)	17 (3%)	2 (0%)	34	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1947	VAL
1	B	1947	VAL

5.3.2 Protein sidechains [i](#)

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	248/265 (94%)	247 (100%)	1 (0%)	91	94
1	B	239/265 (90%)	236 (99%)	3 (1%)	69	75
All	All	487/530 (92%)	483 (99%)	4 (1%)	81	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1830	LEU
1	B	1882	GLN
1	B	1926	SER
1	B	1927	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1945	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](#)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	EDO	A	725	-	3,3,3	0.41	0	2,2,2	0.25	0
4	EDO	A	729	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	B	734	-	3,3,3	0.35	0	2,2,2	0.35	0
4	EDO	B	728	-	3,3,3	0.40	0	2,2,2	0.43	0
4	EDO	B	737	-	3,3,3	0.43	0	2,2,2	0.33	0
4	EDO	A	722	-	3,3,3	0.29	0	2,2,2	0.44	0
4	EDO	A	726	-	3,3,3	0.35	0	2,2,2	0.40	0
4	EDO	B	741	-	3,3,3	0.27	0	2,2,2	0.67	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
4	EDO	A	725	-	-	1/1/1/1	-
4	EDO	A	729	-	-	0/1/1/1	-
4	EDO	B	734	-	-	0/1/1/1	-
4	EDO	B	728	-	-	1/1/1/1	-
4	EDO	B	737	-	-	0/1/1/1	-
4	EDO	A	722	-	-	0/1/1/1	-
4	EDO	A	726	-	-	1/1/1/1	-
4	EDO	B	741	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	728	EDO	O1-C1-C2-O2
4	A	725	EDO	O1-C1-C2-O2
4	A	726	EDO	O1-C1-C2-O2

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	281/295 (95%)	0.10	14 (4%)	28 34	16, 23, 47, 67	0
1	B	272/295 (92%)	0.24	19 (6%)	16 20	15, 23, 43, 70	0
All	All	553/590 (93%)	0.17	33 (5%)	21 27	15, 23, 46, 70	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1869	PRO	4.2
1	B	1964	LEU	4.2
1	A	1855	ASP	4.1
1	B	1701	TYR	4.1
1	A	1854	LEU	3.9
1	A	1749	VAL	3.9
1	B	1925	ASP	3.6
1	B	1698	ASP	3.4
1	B	1693	MET	3.3
1	A	1856	ALA	3.3
1	B	1699	SER	3.2
1	A	1751	ASP	3.2
1	B	1703	LEU	3.2
1	B	1697	ALA	3.2
1	A	1752	ASP	3.1
1	B	1926	SER	3.1
1	B	1696	GLN	3.1
1	B	1924	LEU	3.0
1	B	1963	VAL	2.9
1	B	1871	HIS	2.9
1	A	1857	HIS	2.8
1	B	1870	ASP	2.7
1	A	1851	GLU	2.7
1	A	1824	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1849	CYS	2.5
1	B	1695	LEU	2.3
1	B	1700	ASN	2.3
1	A	1820[A]	GLN	2.3
1	B	1958	GLN	2.3
1	B	1923	GLN	2.2
1	A	1750	ASP	2.2
1	A	1753	PRO	2.2
1	A	1951[A]	CYS	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(Å ²)	Q<0.9
2	CL	B	810	1/1	0.68	0.11	67,67,67,67	0
2	CL	A	802	1/1	0.69	0.14	74,74,74,74	0
2	CL	B	804	1/1	0.73	0.21	77,77,77,77	0
4	EDO	B	737	4/4	0.79	0.19	41,43,50,64	4
2	CL	B	808	1/1	0.81	0.10	77,77,77,77	0
2	CL	A	803	1/1	0.83	0.10	54,54,54,54	0
4	EDO	A	729	4/4	0.84	0.24	42,44,50,65	4
2	CL	B	809	1/1	0.85	0.12	61,61,61,61	0
2	CL	B	801	1/1	0.86	0.14	57,57,57,57	0
2	CL	A	807	1/1	0.87	0.22	67,67,67,67	0
2	CL	B	805	1/1	0.87	0.18	74,74,74,74	0
3	NA	A	811	1/1	0.91	0.10	38,38,38,38	0
4	EDO	A	726	4/4	0.91	0.20	28,37,41,42	4
4	EDO	B	728	4/4	0.93	0.15	22,33,36,41	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	725	4/4	0.96	0.37	26,30,33,67	4
4	EDO	B	734	4/4	0.96	0.15	14,21,22,37	4
4	EDO	B	741	4/4	0.96	0.20	18,24,28,33	4
4	EDO	A	722	4/4	0.97	0.18	18,19,25,39	4

6.5 Other polymers [i](#)

There are no such residues in this entry.