



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 AM UTC

PDB ID : 4NWF / pdb_00004nwf
Title : Crystal structure of the tyrosine phosphatase SHP-2 with N308D mutation
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Deposited on : 2013-12-06
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

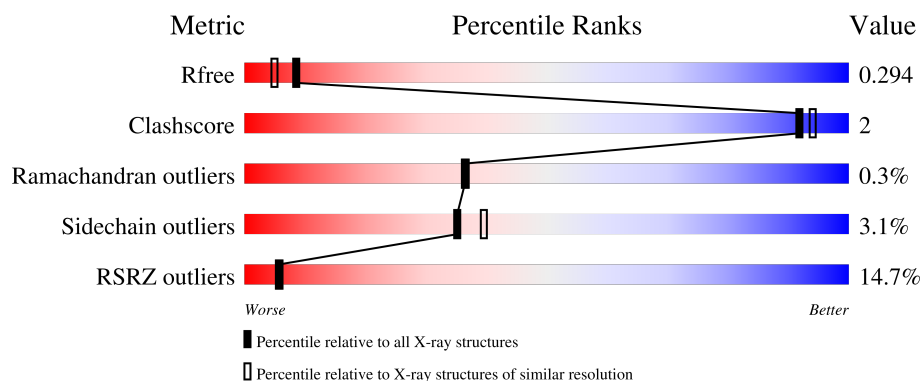
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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 $\leq 5\%$. 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	539	15% 82% 9% 9%
1	B	539	12% 85% 7% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8689 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 Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	1	0
			3975	2501	708	748	18			
1	B	496	Total	C	N	O	S	0	2	0
			4025	2529	716	761	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	ASP	ASN	engineered mutation	UNP Q06124
A	?	-	GLN	deletion	UNP Q06124
A	?	-	ALA	deletion	UNP Q06124
A	?	-	LEU	deletion	UNP Q06124
A	?	-	LEU	deletion	UNP Q06124
B	308	ASP	ASN	engineered mutation	UNP Q06124
B	?	-	GLN	deletion	UNP Q06124
B	?	-	ALA	deletion	UNP Q06124
B	?	-	LEU	deletion	UNP Q06124
B	?	-	LEU	deletion	UNP Q06124

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

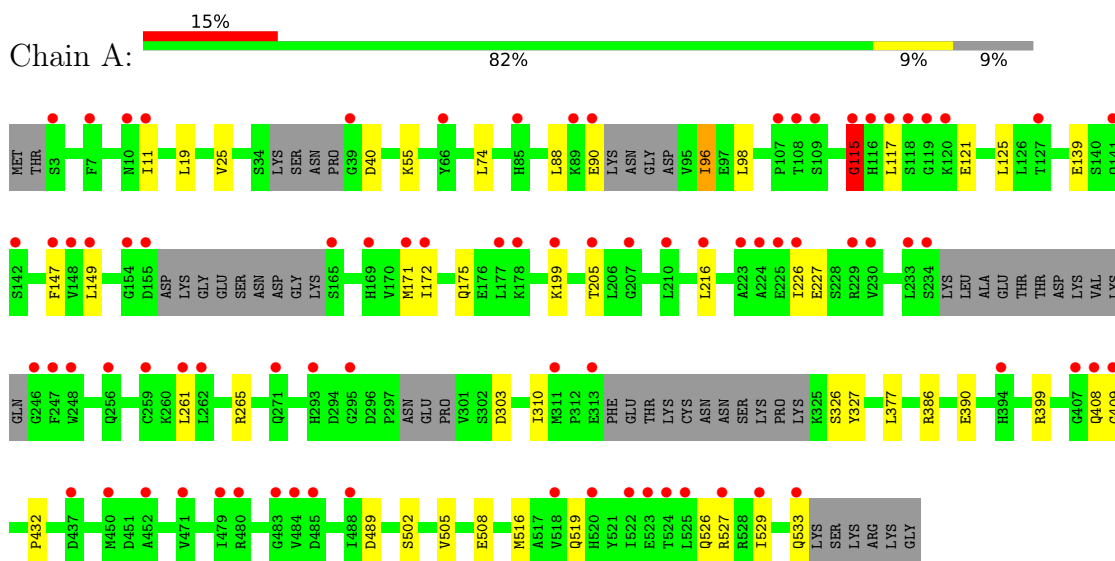
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	326	Total	O	0	0
			326	326		
4	B	329	Total	O	0	0
			329	329		

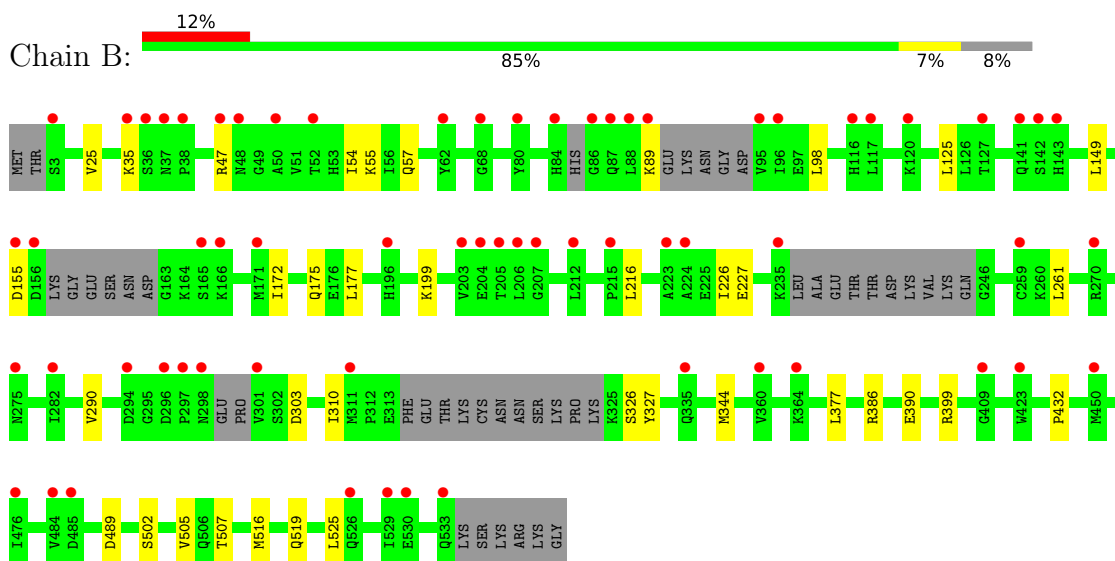
3 Residue-property plots

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: Tyrosine-protein phosphatase non-receptor type 11



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.28Å 55.88Å 91.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 99.8 (20.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.09Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.266 , 0.309 0.260 , 0.294	Depositor DCC
R_{free} test set	954 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8689	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8214e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, GOL

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	0.72	0/4058	1.18	8/5471 (0.1%)
1	B	0.72	0/4107	1.18	7/5536 (0.1%)
All	All	0.72	0/8165	1.18	15/11007 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	GLY	N-CA-C	6.04	121.46	113.37
1	B	507	THR	CA-C-N	6.02	128.34	120.28
1	B	507	THR	C-N-CA	6.02	128.34	120.28
1	B	35	LYS	CA-C-N	5.63	127.76	120.44
1	B	35	LYS	C-N-CA	5.63	127.76	120.44
1	A	489	ASP	CA-C-N	5.42	124.67	120.33
1	A	489	ASP	C-N-CA	5.42	124.67	120.33
1	B	303	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	115	GLY	CA-C-N	5.38	128.24	120.38
1	A	115	GLY	C-N-CA	5.38	128.24	120.38
1	A	303	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	489	ASP	CA-C-N	5.28	124.55	120.33
1	B	489	ASP	C-N-CA	5.28	124.55	120.33
1	A	265	ARG	CA-C-N	5.20	127.25	120.28
1	A	265	ARG	C-N-CA	5.20	127.25	120.28

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	3975	0	3895	15	0
1	B	4025	0	3944	13	0
2	A	16	0	24	0	0
2	B	12	0	18	0	0
3	A	6	0	8	0	0
4	A	326	0	0	0	0
4	B	329	0	0	0	0
All	All	8689	0	7889	26	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 2.

All (26) 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:A:432:PRO:HG3	1:A:516:MET:HG2	1.89	0.55
1:B:432:PRO:HG3	1:B:516:MET:HG2	1.90	0.53
1:B:390:GLU:HG2	1:B:399:ARG:HG2	1.90	0.53
1:A:390:GLU:HG2	1:A:399:ARG:HG2	1.90	0.53
1:B:432:PRO:HD3	1:B:516:MET:HE2	1.91	0.53
1:A:149:LEU:HB2	1:A:172:ILE:HD11	1.97	0.47
1:A:25:VAL:HG11	1:B:175:GLN:HB3	1.97	0.46
1:A:526:GLN:HA	1:A:529:ILE:HD12	1.98	0.45
1:B:55:LYS:HE3	1:B:57:GLN:HB3	1.99	0.45
1:B:149:LEU:HB2	1:B:172:ILE:HD11	1.98	0.45
1:A:88:LEU:HD23	1:A:96:ILE:HB	1.98	0.44
1:A:175:GLN:HB3	1:B:25:VAL:HG11	1.99	0.44
1:A:377:LEU:HD13	1:A:386:ARG:HB2	2.00	0.44
1:A:117:LEU:HD22	1:A:121:GLU:HB3	1.99	0.44
1:A:310:ILE:HB	1:A:327:TYR:HB2	2.00	0.43
1:B:310:ILE:HB	1:B:327:TYR:HB2	2.01	0.43
1:B:377:LEU:HD13	1:B:386:ARG:HB2	2.00	0.43
1:A:11:ILE:HD11	1:A:19:LEU:HD12	2.01	0.43
1:B:125:LEU:HB3	1:B:216:LEU:HD21	2.01	0.43
1:A:139:GLU:HG2	1:A:147:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:HG3	1:B:519:GLN:HE21	1.84	0.42
1:A:125:LEU:HB3	1:A:216:LEU:HD21	2.01	0.42
1:A:115:GLY:HA2	1:A:139:GLU:HG3	2.02	0.41
1:B:54:ILE:HG12	1:B:89:LYS:HD3	2.03	0.41
1:B:290:VAL:HG11	1:B:344:MET:HG3	2.04	0.40
1:A:227:GLU:HG3	1:A:519:GLN:HE21	1.85	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	476/539 (88%)	467 (98%)	7 (2%)	2 (0%)	30	28
1	B	484/539 (90%)	475 (98%)	8 (2%)	1 (0%)	43	44
All	All	960/1078 (89%)	942 (98%)	15 (2%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	A	505	VAL
1	B	505	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	436/480 (91%)	419 (96%)	17 (4%)	28	31
1	B	442/480 (92%)	432 (98%)	10 (2%)	44	51
All	All	878/960 (92%)	851 (97%)	27 (3%)	35	39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	55	LYS
1	A	74	LEU
1	A	90	GLU
1	A	96	ILE
1	A	98	LEU
1	A	171	MET
1	A	199	LYS
1	A	205	THR
1	A	226	ILE
1	A	261	LEU
1	A	326	SER
1	A	408	GLN
1	A	502	SER
1	A	508	GLU
1	A	527	ARG
1	A	533	GLN
1	B	47	ARG
1	B	98	LEU
1	B	155	ASP
1	B	177	LEU
1	B	199	LYS
1	B	226	ILE
1	B	261	LEU
1	B	326	SER
1	B	502	SER
1	B	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	196	HIS
1	A	211	GLN

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	271	GLN
1	A	293	HIS
1	A	446	GLN
1	A	519	GLN
1	B	37	ASN
1	B	211	GLN
1	B	256	GLN
1	B	275	ASN
1	B	298	ASN
1	B	519	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
2	EDO	A	604	-	3,3,3	0.54	0	2,2,2	0.29	0
2	EDO	B	601	-	3,3,3	0.51	0	2,2,2	0.32	0
3	GOL	A	602	-	5,5,5	0.07	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	602	-	3,3,3	0.55	0	2,2,2	0.26	0
2	EDO	A	601	-	3,3,3	0.52	0	2,2,2	0.36	0
2	EDO	A	605	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	603	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	B	603	-	3,3,3	0.51	0	2,2,2	0.36	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
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
3	GOL	A	602	-	-	0/4/4/4	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	605	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-

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 [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	489/539 (90%)	1.01	80 (16%) 4 4	16, 37, 65, 106	1 (0%)
1	B	496/539 (92%)	0.96	65 (13%) 7 7	16, 36, 67, 100	2 (0%)
All	All	985/1078 (91%)	0.98	145 (14%) 6 6	16, 37, 66, 106	3 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	HIS	5.4
1	A	409	GLY	5.3
1	B	533	GLN	5.2
1	A	85[A]	HIS	4.7
1	B	89	LYS	4.6
1	A	223	ALA	4.6
1	A	533	GLN	4.5
1	A	108	THR	4.5
1	A	11	ILE	4.5
1	A	177	LEU	4.5
1	B	298	ASN	4.2
1	B	48	ASN	4.1
1	B	86	GLY	4.0
1	A	248	TRP	3.9
1	B	84	HIS	3.9
1	A	165	SER	3.8
1	A	234	SER	3.7
1	B	206	LEU	3.7
1	A	484	VAL	3.7
1	A	230	VAL	3.7
1	B	409	GLY	3.6
1	A	226	ILE	3.6
1	A	527	ARG	3.5
1	B	223	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	224	ALA	3.4
1	B	36	SER	3.4
1	B	87	GLN	3.4
1	A	450	MET	3.3
1	B	142	SER	3.3
1	A	407	GLY	3.3
1	B	207	GLY	3.3
1	B	301	VAL	3.3
1	A	522	ILE	3.3
1	A	10	ASN	3.2
1	B	141	GLN	3.2
1	A	119	GLY	3.2
1	B	88	LEU	3.2
1	A	116	HIS	3.1
1	A	524	THR	3.1
1	B	166	LYS	3.1
1	B	96	ILE	3.1
1	B	204	GLU	3.1
1	B	296	ASP	3.0
1	A	117	LEU	3.0
1	A	313	GLU	3.0
1	B	38	PRO	3.0
1	A	311	MET	3.0
1	B	530	GLU	2.9
1	B	484	VAL	2.9
1	A	141	GLN	2.9
1	A	90	GLU	2.9
1	A	171	MET	2.9
1	A	293	HIS	2.9
1	B	205	THR	2.9
1	B	95	VAL	2.8
1	A	488	ILE	2.8
1	B	224	ALA	2.8
1	B	165	SER	2.8
1	A	437	ASP	2.8
1	A	154	GLY	2.8
1	A	120	LYS	2.8
1	B	529	ILE	2.8
1	B	171	MET	2.8
1	A	149	LEU	2.7
1	B	364	LYS	2.7
1	B	37	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	148	VAL	2.7
1	A	118	SER	2.7
1	B	485	ASP	2.7
1	A	210	LEU	2.6
1	A	216	LEU	2.6
1	B	143	HIS	2.6
1	A	256	GLN	2.6
1	A	233	LEU	2.6
1	B	212	LEU	2.6
1	B	215	PRO	2.6
1	A	66	TYR	2.6
1	B	450	MET	2.6
1	A	485	ASP	2.6
1	A	207	GLY	2.5
1	B	120	LYS	2.5
1	A	246	GLY	2.5
1	B	35	LYS	2.5
1	A	3	SER	2.5
1	A	39	GLY	2.5
1	B	47	ARG	2.5
1	B	335	GLN	2.5
1	A	89	LYS	2.5
1	A	479	ILE	2.5
1	B	476	ILE	2.5
1	A	155	ASP	2.4
1	A	178	LYS	2.4
1	A	115	GLY	2.4
1	A	480	ARG	2.4
1	B	235	LYS	2.4
1	B	62	TYR	2.4
1	B	526	GLN	2.4
1	A	247	PHE	2.4
1	B	156	ASP	2.3
1	A	127	THR	2.3
1	B	127	THR	2.3
1	A	259	CYS	2.3
1	A	525	LEU	2.3
1	B	52	THR	2.3
1	A	523	GLU	2.2
1	A	529	ILE	2.2
1	B	282	ILE	2.2
1	A	205	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	155	ASP	2.2
1	B	50	ALA	2.2
1	A	225	GLU	2.2
1	A	408	GLN	2.2
1	B	423	TRP	2.2
1	B	68	GLY	2.2
1	B	117	LEU	2.2
1	A	7	PHE	2.2
1	A	471	VAL	2.1
1	B	196	HIS	2.1
1	A	452	ALA	2.1
1	B	259[A]	CYS	2.1
1	B	275	ASN	2.1
1	A	295	GLY	2.1
1	A	394	HIS	2.1
1	A	271	GLN	2.1
1	B	297	PRO	2.1
1	A	169	HIS	2.1
1	B	360	VAL	2.1
1	A	109	SER	2.1
1	A	261	LEU	2.1
1	A	262	LEU	2.1
1	B	3	SER	2.1
1	A	107	PRO	2.1
1	B	80	TYR	2.1
1	A	483	GLY	2.1
1	A	142	SER	2.1
1	B	311	MET	2.0
1	B	270	ARG	2.0
1	A	172	ILE	2.0
1	A	147	PHE	2.0
1	A	518	VAL	2.0
1	B	203	VAL	2.0
1	B	294	ASP	2.0
1	A	229	ARG	2.0
1	A	520	HIS	2.0
1	A	199	LYS	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	EDO	B	602	4/4	0.57	0.22	51,51,51,52	0
2	EDO	A	601	4/4	0.60	0.20	55,55,55,55	0
3	GOL	A	602	6/6	0.60	0.17	52,53,53,53	0
2	EDO	B	603	4/4	0.61	0.18	54,54,55,55	0
2	EDO	A	605	4/4	0.71	0.19	46,46,46,48	0
2	EDO	A	603	4/4	0.74	0.17	61,62,62,63	0
2	EDO	B	601	4/4	0.79	0.13	52,52,53,53	0
2	EDO	A	604	4/4	0.82	0.15	38,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.