



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:54 PM GMT

PDB ID : 1A6Q
Title : CRYSTAL STRUCTURE OF THE PROTEIN SERINE/THREONINE
PHOSPHATASE 2C AT 2 Å RESOLUTION
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Deposited on : 1998-02-27
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

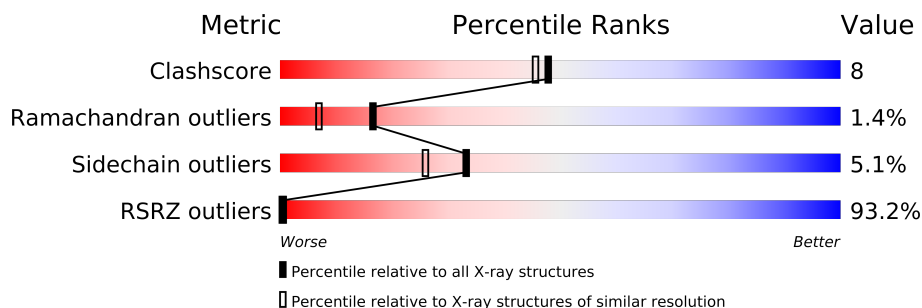
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	382	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	A	701	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3031 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

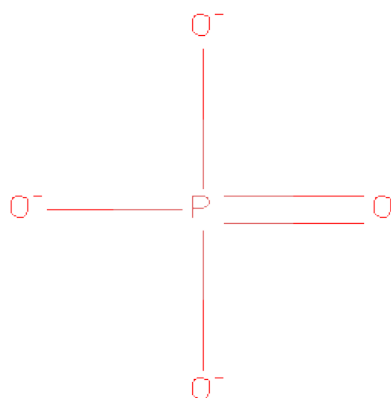
- Molecule 1 is a protein called PHOSPHATASE 2C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2821	1755	500	546	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

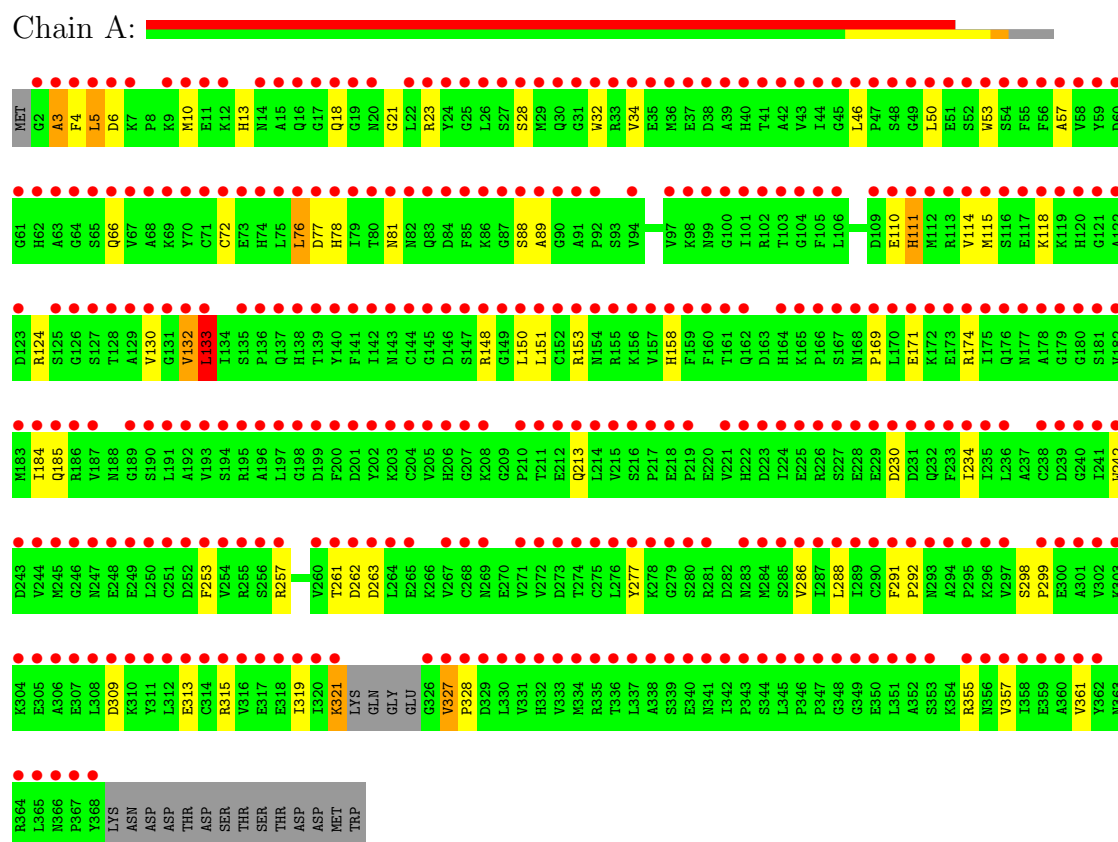
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total 203	O 203	0	0

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 errors 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 ($\text{RSRZ} > 2$). 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: PHOSPHATASE 2C



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.02Å 91.02Å 105.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.00 14.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.00) 95.1 (14.92-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.82	Depositor
R, R_{free}	0.214 , (Not available) 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 260.6	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 33176 reflections	Xtriage
F_o, F_c correlation	0.45	EDS
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MN

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	0.53	0/2876	0.76	1/3883 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	LEU	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2821	0	2746	44	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
4	A	203	0	0	1	0
All	All	3031	0	2746	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:313:GLU:HG2	1:A:361:VAL:HG21	1.55	0.88
1:A:46:LEU:HB2	1:A:50:LEU:HB2	1.65	0.79
1:A:261:THR:HG22	1:A:263:ASP:H	1.47	0.79
1:A:313:GLU:HG2	1:A:361:VAL:CG2	2.18	0.73
1:A:309:ASP:O	1:A:313:GLU:HG3	1.90	0.70
1:A:148:ARG:HB3	1:A:242:TRP:NE1	2.15	0.61
1:A:53:TRP:HD1	1:A:133:LEU:HD22	1.65	0.61
1:A:3:ALA:O	1:A:4:PHE:HB2	2.04	0.58
1:A:13:HIS:HB2	1:A:28:SER:OG	2.05	0.57
1:A:315:ARG:NE	1:A:315:ARG:HA	2.20	0.56
1:A:150:LEU:HD12	1:A:150:LEU:C	2.27	0.55
1:A:4:PHE:HA	1:A:32:TRP:O	2.07	0.54
1:A:77:ASP:O	1:A:81:ASN:HB2	2.08	0.53
1:A:153:ARG:HB3	1:A:158:HIS:HB2	1.89	0.53
1:A:46:LEU:HD22	1:A:76:LEU:HD11	1.90	0.53
1:A:357:VAL:O	1:A:361:VAL:HG23	2.10	0.52
1:A:18:GLN:HG3	1:A:23:ARG:HG2	1.93	0.50
1:A:355:ARG:HG2	1:A:355:ARG:HH11	1.76	0.49
1:A:171:GLU:OE1	1:A:174:ARG:NH2	2.46	0.48
1:A:78:HIS:NE2	1:A:111:HIS:HD2	2.11	0.48
1:A:5:LEU:CD1	1:A:34:VAL:HA	2.44	0.48
1:A:148:ARG:HB3	1:A:242:TRP:CD1	2.49	0.47
1:A:46:LEU:HG	1:A:53:TRP:HB3	1.96	0.47
1:A:174:ARG:HD2	1:A:213:GLN:O	2.14	0.47
1:A:132:VAL:HG11	1:A:234:ILE:HD13	1.96	0.47
1:A:277:TYR:CG	1:A:355:ARG:HD3	2.51	0.46
1:A:327:VAL:HA	1:A:328:PRO:HD2	1.85	0.45
1:A:261:THR:HG22	1:A:262:ASP:N	2.32	0.45
1:A:153:ARG:HG3	1:A:230:ASP:HB3	1.99	0.44
1:A:50:LEU:O	1:A:53:TRP:HB2	2.17	0.44
1:A:5:LEU:HD13	1:A:34:VAL:HA	1.99	0.43
1:A:327:VAL:O	1:A:327:VAL:HG12	2.18	0.43
1:A:110:GLU:O	1:A:114:VAL:HG13	2.17	0.43
1:A:114:VAL:O	1:A:118:LYS:HB2	2.18	0.43
1:A:21:GLY:HA3	4:A:888:HOH:O	2.17	0.43
1:A:298:SER:HA	1:A:299:PRO:HD2	1.88	0.42
1:A:291:PHE:HB3	1:A:292:PRO:HD2	2.02	0.42
1:A:57:ALA:HA	1:A:130:VAL:O	2.20	0.41
1:A:115:MET:HA	1:A:118:LYS:HE2	2.02	0.41
1:A:150:LEU:HD12	1:A:150:LEU:O	2.21	0.41
1:A:319:ILE:C	1:A:321:LYS:H	2.24	0.41
1:A:253:PHE:O	1:A:257:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:319:ILE:C	1:A:321:LYS:N	2.74	0.40
1:A:148:ARG:HB3	1:A:242:TRP:CE2	2.56	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	359/382 (94%)	341 (95%)	13 (4%)	5 (1%)	16 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	88	SER
1	A	184	ILE
1	A	89	ALA
1	A	327	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	311/329 (94%)	295 (95%)	16 (5%)	33 26

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	6	ASP
1	A	10	MET
1	A	66	GLN
1	A	72	CYS
1	A	76	LEU
1	A	111	HIS
1	A	124	ARG
1	A	132	VAL
1	A	133	LEU
1	A	151	LEU
1	A	169	PRO
1	A	185	GLN
1	A	286	VAL
1	A	288	LEU
1	A	321	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	99	ASN
1	A	111	HIS
1	A	138	HIS
1	A	143	ASN
1	A	158	HIS
1	A	177	ASN
1	A	222	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
3	PO4	A	701	-	4,4,4	2.66	3 (75%)	6,6,6	0.31	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
3	PO4	A	701	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PO4	P-O2	3.22	1.65	1.52
3	A	701	PO4	P-O3	3.01	1.64	1.52
3	A	701	PO4	P-O4	2.33	1.62	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	363/382 (95%)	5.33	340 (93%) 0 0	10, 22, 46, 81	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ALA	28.8
1	A	326	GLY	21.1
1	A	49	GLY	19.7
1	A	90	GLY	19.3
1	A	39	ALA	15.4
1	A	38	ASP	15.1
1	A	348	GLY	14.6
1	A	2	GLY	14.6
1	A	31	GLY	14.2
1	A	241	ILE	13.7
1	A	297	VAL	12.8
1	A	179	GLY	12.1
1	A	53	TRP	11.9
1	A	14	ASN	11.7
1	A	166	PRO	11.5
1	A	85	PHE	11.1
1	A	87	GLY	11.0
1	A	84	ASP	10.9
1	A	161	THR	10.8
1	A	62	HIS	10.6
1	A	339	SER	10.6
1	A	293	ASN	10.5
1	A	205	VAL	10.5
1	A	341	ASN	10.4
1	A	178	ALA	10.2
1	A	157	VAL	10.2
1	A	277	TYR	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	229	GLU	9.7
1	A	264	LEU	9.6
1	A	24	TYR	9.6
1	A	358	ILE	9.4
1	A	242	TRP	9.4
1	A	306	ALA	9.3
1	A	204	CYS	9.3
1	A	327	VAL	9.2
1	A	159	PHE	9.2
1	A	361	VAL	9.1
1	A	226	ARG	8.9
1	A	19	GLY	8.9
1	A	368	TYR	8.8
1	A	103	THR	8.8
1	A	151	LEU	8.7
1	A	52	SER	8.6
1	A	147	SER	8.6
1	A	319	ILE	8.4
1	A	253	PHE	8.4
1	A	198	GLY	8.4
1	A	182	VAL	8.4
1	A	3	ALA	8.4
1	A	55	PHE	8.4
1	A	207	GLY	8.3
1	A	274	THR	8.3
1	A	70	TYR	8.3
1	A	320	ILE	8.1
1	A	214	LEU	8.1
1	A	224	ILE	7.9
1	A	75	LEU	7.9
1	A	40	HIS	7.9
1	A	41	THR	7.9
1	A	25	GLY	7.7
1	A	331	VAL	7.6
1	A	250	LEU	7.6
1	A	180	GLY	7.6
1	A	342	ILE	7.5
1	A	273	ASP	7.5
1	A	189	GLY	7.4
1	A	257	ARG	7.4
1	A	267	VAL	7.3
1	A	83	GLN	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	141	PHE	7.1
1	A	94	VAL	7.1
1	A	154	ASN	7.1
1	A	63	ALA	7.0
1	A	32	TRP	7.0
1	A	54	SER	7.0
1	A	35	GLU	7.0
1	A	329	ASP	6.9
1	A	23	ARG	6.8
1	A	136	PRO	6.8
1	A	307	GLU	6.8
1	A	291	PHE	6.8
1	A	312	LEU	6.8
1	A	193	VAL	6.7
1	A	114	VAL	6.7
1	A	228	GLU	6.7
1	A	316	VAL	6.6
1	A	79	ILE	6.6
1	A	210	PRO	6.6
1	A	332	HIS	6.5
1	A	140	TYR	6.5
1	A	15	ALA	6.5
1	A	314	CYS	6.5
1	A	86	LYS	6.4
1	A	112	MET	6.4
1	A	42	ALA	6.4
1	A	351	LEU	6.4
1	A	255	ARG	6.4
1	A	304	LYS	6.4
1	A	61	GLY	6.3
1	A	122	ALA	6.3
1	A	344	SER	6.2
1	A	248	GLU	6.2
1	A	155	ARG	6.2
1	A	146	ASP	6.1
1	A	81	ASN	6.1
1	A	366	ASN	6.1
1	A	80	THR	6.1
1	A	129	ALA	6.1
1	A	215	VAL	6.1
1	A	213	GLN	6.1
1	A	59	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	120	HIS	6.0
1	A	305	GLU	6.0
1	A	50	LEU	6.0
1	A	172	LYS	5.9
1	A	74	HIS	5.9
1	A	34	VAL	5.9
1	A	43	VAL	5.9
1	A	76	LEU	5.9
1	A	162	GLN	5.8
1	A	365	LEU	5.7
1	A	275	CYS	5.7
1	A	287	ILE	5.7
1	A	251	CYS	5.6
1	A	318	GLU	5.6
1	A	349	GLY	5.6
1	A	46	LEU	5.6
1	A	301	ALA	5.5
1	A	181	SER	5.5
1	A	340	GLU	5.5
1	A	176	GLN	5.5
1	A	234	ILE	5.5
1	A	48	SER	5.4
1	A	362	TYR	5.4
1	A	98	LYS	5.3
1	A	346	PRO	5.3
1	A	206	HIS	5.3
1	A	88	SER	5.3
1	A	360	ALA	5.3
1	A	44	ILE	5.2
1	A	284	MET	5.2
1	A	77	ASP	5.2
1	A	216	SER	5.2
1	A	149	GLY	5.1
1	A	139	THR	5.1
1	A	254	VAL	5.1
1	A	292	PRO	5.1
1	A	187	VAL	5.1
1	A	294	ALA	5.1
1	A	313	GLU	5.1
1	A	345	LEU	5.1
1	A	285	SER	5.1
1	A	334	MET	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	168	ASN	5.0
1	A	22	LEU	5.0
1	A	352	ALA	5.0
1	A	308	LEU	5.0
1	A	311	TYR	5.0
1	A	223	ASP	5.0
1	A	105	PHE	5.0
1	A	97	VAL	5.0
1	A	67	VAL	5.0
1	A	116	SER	5.0
1	A	102	ARG	5.0
1	A	4	PHE	4.9
1	A	196	ALA	4.9
1	A	11	GLU	4.8
1	A	30	GLN	4.8
1	A	321	LYS	4.8
1	A	104	GLY	4.8
1	A	175	ILE	4.8
1	A	235	ILE	4.8
1	A	359	GLU	4.7
1	A	17	GLY	4.6
1	A	218	GLU	4.6
1	A	269	ASN	4.6
1	A	240	GLY	4.6
1	A	200	PHE	4.6
1	A	283	ASN	4.6
1	A	7	LYS	4.6
1	A	194	SER	4.6
1	A	115	MET	4.6
1	A	233	PHE	4.6
1	A	236	LEU	4.5
1	A	202	TYR	4.5
1	A	333	VAL	4.5
1	A	335	ARG	4.5
1	A	164	HIS	4.5
1	A	142	ILE	4.5
1	A	211	THR	4.5
1	A	117	GLU	4.5
1	A	20	ASN	4.4
1	A	121	GLY	4.4
1	A	246	GLY	4.4
1	A	268	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	356	ASN	4.4
1	A	148	ARG	4.4
1	A	27	SER	4.3
1	A	244	VAL	4.3
1	A	217	PRO	4.3
1	A	265	GLU	4.3
1	A	9	LYS	4.2
1	A	125	SER	4.2
1	A	197	LEU	4.2
1	A	82	ASN	4.2
1	A	199	ASP	4.2
1	A	302	VAL	4.2
1	A	28	SER	4.2
1	A	144	CYS	4.1
1	A	126	GLY	4.1
1	A	203	LYS	4.1
1	A	201	ASP	4.1
1	A	330	LEU	4.1
1	A	208	LYS	4.1
1	A	289	ILE	4.0
1	A	167	SER	4.0
1	A	256	SER	4.0
1	A	195	ARG	4.0
1	A	118	LYS	4.0
1	A	243	ASP	4.0
1	A	91	ALA	4.0
1	A	353	SER	4.0
1	A	51	GLU	4.0
1	A	192	ALA	4.0
1	A	110	GLU	4.0
1	A	106	LEU	4.0
1	A	158	HIS	3.9
1	A	336	THR	3.9
1	A	10	MET	3.9
1	A	343	PRO	3.9
1	A	232	GLN	3.9
1	A	295	PRO	3.9
1	A	101	ILE	3.8
1	A	127	SER	3.8
1	A	230	ASP	3.8
1	A	47	PRO	3.8
1	A	191	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	367	PRO	3.8
1	A	145	GLY	3.7
1	A	160	PHE	3.7
1	A	143	ASN	3.7
1	A	133	LEU	3.7
1	A	288	LEU	3.6
1	A	66	GLN	3.6
1	A	99	ASN	3.6
1	A	26	LEU	3.6
1	A	173	GLU	3.6
1	A	299	PRO	3.6
1	A	300	GLU	3.5
1	A	56	PHE	3.5
1	A	279	GLY	3.5
1	A	58	VAL	3.5
1	A	186	ARG	3.5
1	A	177	ASN	3.4
1	A	29	MET	3.4
1	A	190	SER	3.4
1	A	57	ALA	3.4
1	A	350	GLU	3.4
1	A	119	LYS	3.4
1	A	364	ARG	3.4
1	A	150	LEU	3.4
1	A	278	LYS	3.4
1	A	152	CYS	3.3
1	A	212	GLU	3.3
1	A	227	SER	3.3
1	A	60	ASP	3.3
1	A	337	LEU	3.3
1	A	5	LEU	3.3
1	A	36	MET	3.3
1	A	338	ALA	3.3
1	A	183	MET	3.3
1	A	281	ARG	3.3
1	A	355	ARG	3.3
1	A	221	VAL	3.2
1	A	272	VAL	3.2
1	A	276	LEU	3.2
1	A	131	GLY	3.2
1	A	239	ASP	3.2
1	A	219	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	238	CYS	3.2
1	A	78	HIS	3.2
1	A	45	GLY	3.2
1	A	286	VAL	3.2
1	A	310	LYS	3.1
1	A	18	GLN	3.1
1	A	111	HIS	3.1
1	A	135	SER	3.1
1	A	249	GLU	3.1
1	A	128	THR	3.1
1	A	303	LYS	3.1
1	A	225	GLU	3.0
1	A	174	ARG	3.0
1	A	68	ALA	3.0
1	A	247	ASN	3.0
1	A	315	ARG	3.0
1	A	137	GLN	3.0
1	A	92	PRO	3.0
1	A	263	ASP	3.0
1	A	16	GLN	3.0
1	A	347	PRO	2.9
1	A	184	ILE	2.9
1	A	170	LEU	2.9
1	A	245	MET	2.9
1	A	222	HIS	2.9
1	A	100	GLY	2.8
1	A	165	LYS	2.8
1	A	113	ARG	2.8
1	A	37	GLU	2.8
1	A	262	ASP	2.8
1	A	64	GLY	2.8
1	A	72	CYS	2.8
1	A	109	ASP	2.7
1	A	280	SER	2.7
1	A	357	VAL	2.7
1	A	156	LYS	2.7
1	A	185	GLN	2.6
1	A	271	VAL	2.6
1	A	12	LYS	2.6
1	A	296	LYS	2.6
1	A	33	ARG	2.6
1	A	130	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	CYS	2.6
1	A	65	SER	2.5
1	A	153	ARG	2.5
1	A	231	ASP	2.4
1	A	132	VAL	2.4
1	A	261	THR	2.4
1	A	252	ASP	2.3
1	A	69	LYS	2.2
1	A	260	VAL	2.2
1	A	6	ASP	2.2
1	A	328	PRO	2.2
1	A	317	GLU	2.1
1	A	290	CYS	2.1
1	A	123	ASP	2.1
1	A	169	PRO	2.1
1	A	309	ASP	2.1
1	A	138	HIS	2.1
1	A	171	GLU	2.0
1	A	73	GLU	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 ⓘ

There are no carbohydrates in this entry.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	701	5/5	0.56	0.77	37,41,42,45	0
2	MN	A	384	1/1	0.17	-1.30	65,65,65,65	0
2	MN	A	383	1/1	0.05	-1.44	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.