



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:16 am GMT

PDB ID : 1A6Q
Title : CRYSTAL STRUCTURE OF THE PROTEIN SERINE/THREONINE
PHOSPHATASE 2C AT 2 Å RESOLUTION
Authors : Das, A.K.; Helps, N.R.; Cohen, P.T.W.; Barford, D.
Deposited on : 1998-02-27
Resolution : 2.00 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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

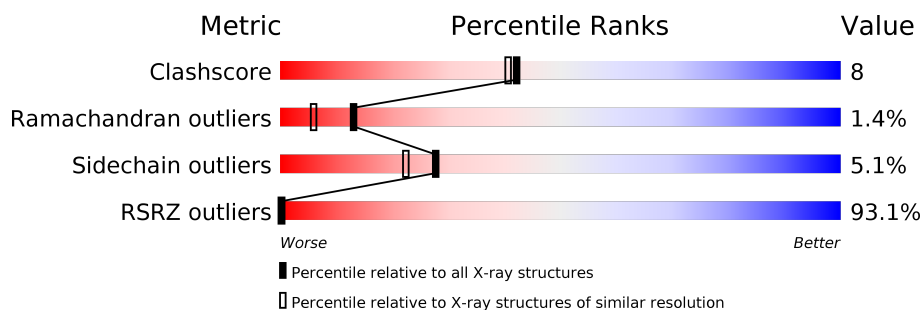
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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. 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	382	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3031 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 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		

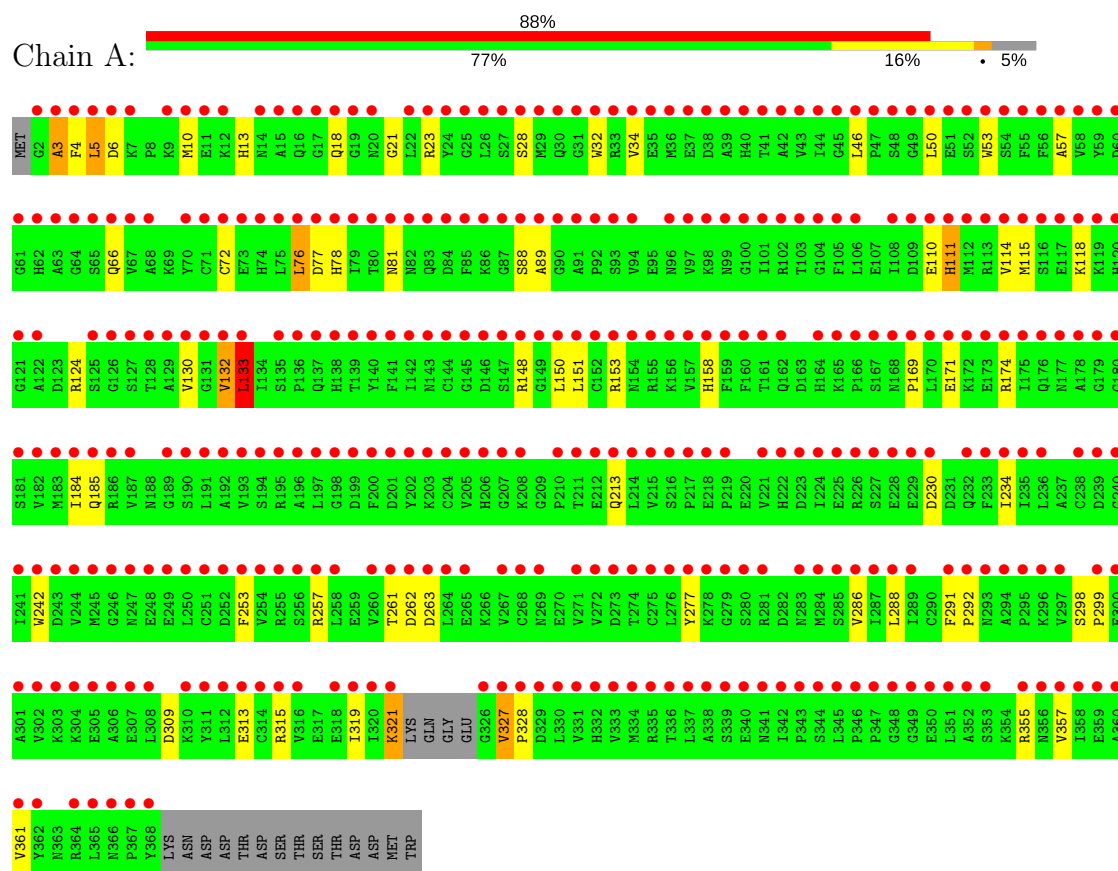
- Molecule 4 is water.

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 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 ($\text{RSRZ} > 2$). 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)	1.87 , 1604.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	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.

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: 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 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	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

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 (44) 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: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:C	1:A:150:LEU:HD12	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:132:VAL:HG11	1:A:234:ILE:HD13	1.96	0.47
1:A:174:ARG:HD2	1:A:213:GLN:O	2.14	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:327:VAL:O	1:A:327:VAL:HG12	2.18	0.43
1:A:5:LEU:HD13	1:A:34:VAL:HA	1.99	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:O	1:A:150:LEU:HD12	2.21	0.41
1:A:253:PHE:O	1:A:257:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:C	1:A:321:LYS:H	2.24	0.41
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 [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	359/382 (94%)	341 (95%)	13 (4%)	5 (1%)	13 6

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 [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	311/329 (94%)	295 (95%)	16 (5%)	28 22

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

Mol	Chain	Res	Type
1	A	5	LEU
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 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 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	3.68	4 (100%)	6,6,6	0.42	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PO4	P-O4	2.21	1.62	1.54
3	A	701	PO4	P-O3	2.99	1.64	1.54
3	A	701	PO4	P-O2	3.24	1.65	1.54
3	A	701	PO4	P-O1	5.46	1.62	1.50

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	363/382 (95%)	5.07	338 (93%) 0 0	10, 22, 46, 81	0

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ALA	24.6
1	A	90	GLY	17.6
1	A	49	GLY	16.9
1	A	39	ALA	14.4
1	A	2	GLY	14.0
1	A	53	TRP	14.0
1	A	38	ASP	13.7
1	A	326	GLY	13.3
1	A	348	GLY	12.6
1	A	297	VAL	12.6
1	A	31	GLY	11.9
1	A	179	GLY	11.8
1	A	204	CYS	11.4
1	A	241	ILE	11.3
1	A	327	VAL	10.3
1	A	85	PHE	10.2
1	A	87	GLY	10.1
1	A	166	PRO	10.0
1	A	205	VAL	9.9
1	A	62	HIS	9.9
1	A	242	TRP	9.8
1	A	14	ASN	9.8
1	A	70	TYR	9.8
1	A	214	LEU	9.7
1	A	157	VAL	9.5
1	A	274	THR	9.2
1	A	159	PHE	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	178	ALA	8.9
1	A	161	THR	8.8
1	A	147	SER	8.7
1	A	277	TYR	8.7
1	A	19	GLY	8.6
1	A	3	ALA	8.5
1	A	253	PHE	8.4
1	A	207	GLY	8.3
1	A	358	ILE	8.3
1	A	264	LEU	8.3
1	A	103	THR	8.3
1	A	368	TYR	8.3
1	A	210	PRO	8.2
1	A	331	VAL	8.1
1	A	267	VAL	8.0
1	A	76	LEU	8.0
1	A	182	VAL	8.0
1	A	229	GLU	7.9
1	A	361	VAL	7.9
1	A	94	VAL	7.8
1	A	226	ARG	7.7
1	A	24	TYR	7.7
1	A	306	ALA	7.7
1	A	75	LEU	7.6
1	A	55	PHE	7.5
1	A	339	SER	7.5
1	A	84	ASP	7.4
1	A	228	GLU	7.4
1	A	79	ILE	7.3
1	A	80	THR	7.3
1	A	43	VAL	7.3
1	A	15	ALA	7.3
1	A	122	ALA	7.2
1	A	193	VAL	7.1
1	A	136	PRO	7.1
1	A	224	ILE	7.1
1	A	198	GLY	7.1
1	A	61	GLY	7.0
1	A	40	HIS	7.0
1	A	52	SER	7.0
1	A	35	GLU	7.0
1	A	316	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLY	6.9
1	A	59	TYR	6.9
1	A	293	ASN	6.9
1	A	320	ILE	6.9
1	A	114	VAL	6.8
1	A	41	THR	6.8
1	A	273	ASP	6.8
1	A	25	GLY	6.8
1	A	32	TRP	6.8
1	A	83	GLN	6.7
1	A	139	THR	6.7
1	A	332	HIS	6.7
1	A	140	TYR	6.6
1	A	63	ALA	6.5
1	A	319	ILE	6.5
1	A	344	SER	6.5
1	A	74	HIS	6.5
1	A	250	LEU	6.5
1	A	206	HIS	6.5
1	A	342	ILE	6.4
1	A	88	SER	6.4
1	A	42	ALA	6.3
1	A	215	VAL	6.3
1	A	254	VAL	6.3
1	A	341	ASN	6.3
1	A	151	LEU	6.2
1	A	314	CYS	6.2
1	A	141	PHE	6.2
1	A	248	GLU	6.2
1	A	180	GLY	6.2
1	A	275	CYS	6.2
1	A	349	GLY	6.2
1	A	155	ARG	6.2
1	A	257	ARG	6.1
1	A	112	MET	6.1
1	A	351	LEU	6.1
1	A	294	ALA	6.1
1	A	162	GLN	6.1
1	A	291	PHE	6.0
1	A	360	ALA	5.9
1	A	312	LEU	5.9
1	A	362	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	5.8
1	A	44	ILE	5.7
1	A	197	LEU	5.7
1	A	172	LYS	5.7
1	A	22	LEU	5.7
1	A	77	ASP	5.6
1	A	154	ASN	5.6
1	A	307	GLU	5.6
1	A	105	PHE	5.6
1	A	34	VAL	5.6
1	A	305	GLU	5.6
1	A	23	ARG	5.5
1	A	54	SER	5.4
1	A	329	ASP	5.4
1	A	251	CYS	5.4
1	A	115	MET	5.3
1	A	213	GLN	5.3
1	A	144	CYS	5.3
1	A	48	SER	5.3
1	A	313	GLU	5.3
1	A	233	PHE	5.3
1	A	30	GLN	5.3
1	A	196	ALA	5.3
1	A	175	ILE	5.2
1	A	211	THR	5.2
1	A	81	ASN	5.2
1	A	149	GLY	5.2
1	A	86	LYS	5.2
1	A	120	HIS	5.2
1	A	129	ALA	5.2
1	A	181	SER	5.2
1	A	308	LEU	5.2
1	A	292	PRO	5.1
1	A	176	GLN	5.1
1	A	50	LEU	5.1
1	A	104	GLY	5.1
1	A	223	ASP	5.1
1	A	46	LEU	5.1
1	A	98	LYS	5.0
1	A	216	SER	5.0
1	A	284	MET	5.0
1	A	311	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	301	ALA	4.9
1	A	20	ASN	4.9
1	A	66	GLN	4.9
1	A	318	GLU	4.9
1	A	4	PHE	4.8
1	A	356	ASN	4.8
1	A	304	LYS	4.8
1	A	97	VAL	4.8
1	A	365	LEU	4.8
1	A	335	ARG	4.8
1	A	67	VAL	4.7
1	A	302	VAL	4.7
1	A	345	LEU	4.7
1	A	168	ASN	4.7
1	A	269	ASN	4.7
1	A	334	MET	4.7
1	A	57	ALA	4.7
1	A	268	CYS	4.7
1	A	343	PRO	4.6
1	A	366	ASN	4.6
1	A	126	GLY	4.6
1	A	350	GLU	4.6
1	A	201	ASP	4.6
1	A	321	LYS	4.5
1	A	127	SER	4.5
1	A	286	VAL	4.5
1	A	246	GLY	4.5
1	A	234	ILE	4.5
1	A	367	PRO	4.5
1	A	202	TYR	4.5
1	A	187	VAL	4.5
1	A	359	GLU	4.5
1	A	194	SER	4.5
1	A	146	ASP	4.5
1	A	7	LYS	4.5
1	A	117	GLU	4.4
1	A	195	ARG	4.4
1	A	116	SER	4.4
1	A	200	PHE	4.3
1	A	346	PRO	4.3
1	A	243	ASP	4.3
1	A	333	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	28	SER	4.3
1	A	296	LYS	4.3
1	A	272	VAL	4.2
1	A	9	LYS	4.2
1	A	299	PRO	4.2
1	A	289	ILE	4.2
1	A	17	GLY	4.1
1	A	353	SER	4.1
1	A	91	ALA	4.1
1	A	167	SER	4.1
1	A	164	HIS	4.1
1	A	285	SER	4.1
1	A	244	VAL	4.1
1	A	102	ARG	4.1
1	A	236	LEU	4.1
1	A	288	LEU	4.1
1	A	118	LYS	4.1
1	A	82	ASN	4.1
1	A	133	LEU	4.0
1	A	11	GLU	4.0
1	A	191	LEU	4.0
1	A	279	GLY	4.0
1	A	352	ALA	4.0
1	A	101	ILE	3.9
1	A	330	LEU	3.9
1	A	300	GLU	3.9
1	A	256	SER	3.9
1	A	56	PHE	3.9
1	A	152	CYS	3.8
1	A	5	LEU	3.8
1	A	338	ALA	3.8
1	A	142	ILE	3.8
1	A	232	GLN	3.8
1	A	217	PRO	3.8
1	A	36	MET	3.8
1	A	121	GLY	3.7
1	A	128	THR	3.7
1	A	12	LYS	3.7
1	A	170	LEU	3.7
1	A	283	ASN	3.7
1	A	208	LYS	3.6
1	A	145	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	3.6
1	A	295	PRO	3.6
1	A	357	VAL	3.6
1	A	6	ASP	3.5
1	A	110	GLU	3.5
1	A	364	ARG	3.5
1	A	99	ASN	3.5
1	A	340	GLU	3.5
1	A	47	PRO	3.5
1	A	158	HIS	3.5
1	A	276	LEU	3.5
1	A	212	GLU	3.5
1	A	235	ILE	3.5
1	A	125	SER	3.5
1	A	203	LYS	3.5
1	A	287	ILE	3.5
1	A	249	GLU	3.4
1	A	177	ASN	3.4
1	A	58	VAL	3.4
1	A	186	ARG	3.4
1	A	199	ASP	3.4
1	A	173	GLU	3.4
1	A	119	LYS	3.3
1	A	238	CYS	3.3
1	A	143	ASN	3.3
1	A	148	ARG	3.3
1	A	92	PRO	3.3
1	A	355	ARG	3.3
1	A	29	MET	3.3
1	A	111	HIS	3.3
1	A	278	LYS	3.2
1	A	60	ASP	3.2
1	A	315	ARG	3.2
1	A	271	VAL	3.2
1	A	156	LYS	3.2
1	A	190	SER	3.1
1	A	137	GLN	3.1
1	A	265	GLU	3.1
1	A	64	GLY	3.1
1	A	303	LYS	3.1
1	A	10	MET	3.1
1	A	225	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLU	3.0
1	A	113	ARG	3.0
1	A	106	LEU	3.0
1	A	240	GLY	3.0
1	A	218	GLU	3.0
1	A	135	SER	3.0
1	A	16	GLN	3.0
1	A	150	LEU	3.0
1	A	71	CYS	3.0
1	A	78	HIS	3.0
1	A	72	CYS	3.0
1	A	219	PRO	3.0
1	A	160	PHE	2.9
1	A	174	ARG	2.9
1	A	230	ASP	2.9
1	A	192	ALA	2.9
1	A	45	GLY	2.9
1	A	131	GLY	2.9
1	A	247	ASN	2.9
1	A	108	ILE	2.9
1	A	153	ARG	2.9
1	A	26	LEU	2.9
1	A	227	SER	2.8
1	A	337	LEU	2.8
1	A	280	SER	2.8
1	A	73	GLU	2.8
1	A	336	THR	2.8
1	A	310	LYS	2.8
1	A	347	PRO	2.8
1	A	68	ALA	2.7
1	A	281	ARG	2.7
1	A	165	LYS	2.7
1	A	260	VAL	2.7
1	A	185	GLN	2.7
1	A	27	SER	2.6
1	A	184	ILE	2.6
1	A	18	GLN	2.6
1	A	33	ARG	2.5
1	A	109	ASP	2.5
1	A	183	MET	2.5
1	A	262	ASP	2.5
1	A	222	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	93	SER	2.4
1	A	169	PRO	2.4
1	A	132	VAL	2.4
1	A	37	GLU	2.4
1	A	171	GLU	2.4
1	A	252	ASP	2.4
1	A	263	ASP	2.3
1	A	239	ASP	2.3
1	A	221	VAL	2.3
1	A	100	GLY	2.3
1	A	138	HIS	2.2
1	A	65	SER	2.2
1	A	245	MET	2.2
1	A	258	LEU	2.1
1	A	261	THR	2.1
1	A	96	ASN	2.1
1	A	328	PRO	2.1

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	701	5/5	0.38	0.49	0.57	37,41,42,45	0
2	MN	A	383	1/1	0.79	0.08	-1.28	34,34,34,34	0
2	MN	A	384	1/1	0.45	0.12	-1.45	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.