



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:19 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

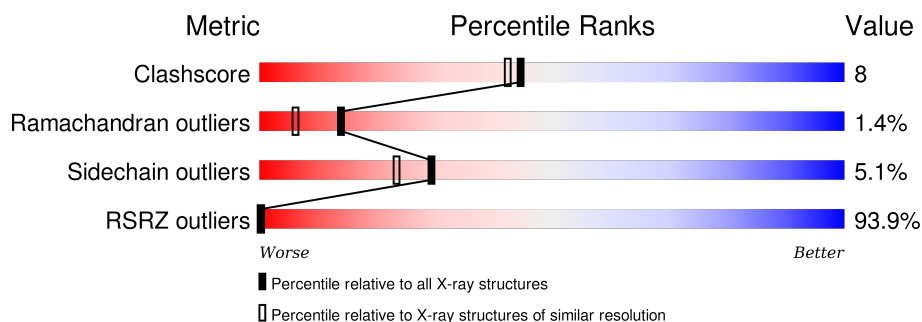
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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

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)	2.24 , 1757.4	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:O	1:A:257:ARG:HG2	2.21	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%)	14	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%)	29	23

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	2.89	4 (100%)	6,6,6	0.27	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-O1	2.26	1.62	1.52
3	A	701	PO4	P-O4	2.44	1.62	1.53
3	A	701	PO4	P-O3	3.21	1.64	1.53
3	A	701	PO4	P-O2	3.45	1.65	1.53

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

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%)	5.28	341 (93%) 0 0	10, 22, 46, 81	0

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ALA	24.7
1	A	90	GLY	18.1
1	A	49	GLY	17.3
1	A	2	GLY	14.9
1	A	39	ALA	14.8
1	A	53	TRP	14.4
1	A	38	ASP	14.2
1	A	326	GLY	13.4
1	A	297	VAL	13.4
1	A	348	GLY	13.0
1	A	179	GLY	12.4
1	A	31	GLY	12.3
1	A	241	ILE	11.8
1	A	204	CYS	11.7
1	A	85	PHE	10.7
1	A	327	VAL	10.6
1	A	205	VAL	10.5
1	A	87	GLY	10.5
1	A	166	PRO	10.3
1	A	157	VAL	10.2
1	A	62	HIS	10.1
1	A	242	TRP	10.1
1	A	14	ASN	10.0
1	A	214	LEU	9.9
1	A	70	TYR	9.8
1	A	159	PHE	9.5
1	A	274	THR	9.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	161	THR	9.3
1	A	178	ALA	9.3
1	A	147	SER	9.0
1	A	19	GLY	9.0
1	A	3	ALA	9.0
1	A	253	PHE	8.9
1	A	277	TYR	8.9
1	A	358	ILE	8.8
1	A	264	LEU	8.8
1	A	207	GLY	8.7
1	A	331	VAL	8.6
1	A	103	THR	8.6
1	A	210	PRO	8.5
1	A	368	TYR	8.5
1	A	267	VAL	8.4
1	A	361	VAL	8.4
1	A	182	VAL	8.3
1	A	94	VAL	8.2
1	A	76	LEU	8.2
1	A	229	GLU	8.2
1	A	306	ALA	8.0
1	A	24	TYR	7.9
1	A	75	LEU	7.8
1	A	55	PHE	7.8
1	A	43	VAL	7.8
1	A	226	ARG	7.8
1	A	15	ALA	7.8
1	A	84	ASP	7.7
1	A	79	ILE	7.6
1	A	80	THR	7.6
1	A	228	GLU	7.6
1	A	339	SER	7.6
1	A	122	ALA	7.6
1	A	193	VAL	7.6
1	A	224	ILE	7.5
1	A	136	PRO	7.4
1	A	316	VAL	7.4
1	A	114	VAL	7.3
1	A	320	ILE	7.3
1	A	198	GLY	7.3
1	A	40	HIS	7.3
1	A	293	ASN	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	61	GLY	7.2
1	A	52	SER	7.2
1	A	35	GLU	7.1
1	A	41	THR	7.1
1	A	25	GLY	7.1
1	A	59	TYR	7.1
1	A	189	GLY	7.1
1	A	273	ASP	7.1
1	A	32	TRP	7.0
1	A	83	GLN	6.9
1	A	344	SER	6.9
1	A	139	THR	6.9
1	A	140	TYR	6.9
1	A	332	HIS	6.9
1	A	250	LEU	6.8
1	A	319	ILE	6.8
1	A	74	HIS	6.8
1	A	63	ALA	6.8
1	A	342	ILE	6.7
1	A	206	HIS	6.7
1	A	42	ALA	6.7
1	A	215	VAL	6.6
1	A	141	PHE	6.6
1	A	341	ASN	6.6
1	A	88	SER	6.5
1	A	151	LEU	6.5
1	A	254	VAL	6.5
1	A	180	GLY	6.5
1	A	155	ARG	6.4
1	A	314	CYS	6.4
1	A	351	LEU	6.4
1	A	257	ARG	6.4
1	A	275	CYS	6.4
1	A	248	GLU	6.3
1	A	294	ALA	6.3
1	A	360	ALA	6.3
1	A	112	MET	6.3
1	A	349	GLY	6.3
1	A	162	GLN	6.3
1	A	291	PHE	6.1
1	A	312	LEU	6.1
1	A	44	ILE	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	6.1
1	A	362	TYR	6.1
1	A	34	VAL	6.0
1	A	154	ASN	5.9
1	A	197	LEU	5.9
1	A	172	LYS	5.9
1	A	22	LEU	5.9
1	A	77	ASP	5.8
1	A	105	PHE	5.8
1	A	307	GLU	5.8
1	A	23	ARG	5.8
1	A	305	GLU	5.7
1	A	329	ASP	5.7
1	A	175	ILE	5.6
1	A	54	SER	5.6
1	A	233	PHE	5.5
1	A	251	CYS	5.5
1	A	48	SER	5.5
1	A	144	CYS	5.5
1	A	86	LYS	5.5
1	A	115	MET	5.4
1	A	196	ALA	5.4
1	A	149	GLY	5.4
1	A	308	LEU	5.4
1	A	81	ASN	5.4
1	A	129	ALA	5.4
1	A	181	SER	5.4
1	A	30	GLN	5.4
1	A	213	GLN	5.4
1	A	223	ASP	5.4
1	A	211	THR	5.4
1	A	50	LEU	5.4
1	A	104	GLY	5.3
1	A	313	GLU	5.3
1	A	120	HIS	5.3
1	A	176	GLN	5.2
1	A	301	ALA	5.2
1	A	292	PRO	5.2
1	A	97	VAL	5.2
1	A	46	LEU	5.2
1	A	216	SER	5.2
1	A	57	ALA	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	98	LYS	5.2
1	A	284	MET	5.1
1	A	67	VAL	5.1
1	A	302	VAL	5.1
1	A	4	PHE	5.1
1	A	311	TYR	5.1
1	A	20	ASN	5.1
1	A	304	LYS	5.1
1	A	356	ASN	5.0
1	A	365	LEU	5.0
1	A	318	GLU	5.0
1	A	66	GLN	4.9
1	A	234	ILE	4.9
1	A	268	CYS	4.9
1	A	187	VAL	4.8
1	A	345	LEU	4.8
1	A	201	ASP	4.8
1	A	246	GLY	4.8
1	A	335	ARG	4.8
1	A	334	MET	4.8
1	A	126	GLY	4.8
1	A	127	SER	4.8
1	A	168	ASN	4.8
1	A	343	PRO	4.8
1	A	366	ASN	4.8
1	A	269	ASN	4.8
1	A	286	VAL	4.7
1	A	202	TYR	4.7
1	A	359	GLU	4.7
1	A	194	SER	4.7
1	A	367	PRO	4.7
1	A	321	LYS	4.7
1	A	146	ASP	4.6
1	A	350	GLU	4.6
1	A	116	SER	4.6
1	A	333	VAL	4.6
1	A	195	ARG	4.6
1	A	200	PHE	4.5
1	A	243	ASP	4.5
1	A	117	GLU	4.5
1	A	7	LYS	4.5
1	A	91	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	272	VAL	4.5
1	A	289	ILE	4.5
1	A	28	SER	4.5
1	A	346	PRO	4.5
1	A	244	VAL	4.4
1	A	296	LYS	4.4
1	A	299	PRO	4.4
1	A	9	LYS	4.3
1	A	353	SER	4.3
1	A	102	ARG	4.3
1	A	82	ASN	4.3
1	A	236	LEU	4.3
1	A	288	LEU	4.3
1	A	167	SER	4.3
1	A	164	HIS	4.3
1	A	17	GLY	4.2
1	A	118	LYS	4.2
1	A	352	ALA	4.2
1	A	285	SER	4.2
1	A	133	LEU	4.2
1	A	279	GLY	4.2
1	A	191	LEU	4.2
1	A	101	ILE	4.1
1	A	11	GLU	4.1
1	A	56	PHE	4.1
1	A	142	ILE	4.1
1	A	256	SER	4.1
1	A	330	LEU	4.1
1	A	232	GLN	4.0
1	A	152	CYS	4.0
1	A	5	LEU	4.0
1	A	300	GLU	3.9
1	A	121	GLY	3.9
1	A	338	ALA	3.9
1	A	170	LEU	3.9
1	A	283	ASN	3.8
1	A	357	VAL	3.8
1	A	128	THR	3.8
1	A	145	GLY	3.8
1	A	36	MET	3.8
1	A	208	LYS	3.8
1	A	217	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	3.8
1	A	287	ILE	3.8
1	A	12	LYS	3.7
1	A	295	PRO	3.7
1	A	158	HIS	3.7
1	A	47	PRO	3.7
1	A	276	LEU	3.7
1	A	58	VAL	3.7
1	A	235	ILE	3.7
1	A	99	ASN	3.6
1	A	110	GLU	3.6
1	A	340	GLU	3.6
1	A	125	SER	3.6
1	A	212	GLU	3.6
1	A	364	ARG	3.6
1	A	6	ASP	3.6
1	A	203	LYS	3.6
1	A	177	ASN	3.5
1	A	119	LYS	3.5
1	A	173	GLU	3.5
1	A	249	GLU	3.5
1	A	238	CYS	3.5
1	A	186	ARG	3.5
1	A	271	VAL	3.4
1	A	199	ASP	3.4
1	A	143	ASN	3.4
1	A	111	HIS	3.4
1	A	29	MET	3.4
1	A	355	ARG	3.4
1	A	92	PRO	3.4
1	A	148	ARG	3.4
1	A	60	ASP	3.3
1	A	315	ARG	3.3
1	A	137	GLN	3.3
1	A	64	GLY	3.3
1	A	156	LYS	3.2
1	A	278	LYS	3.2
1	A	303	LYS	3.2
1	A	190	SER	3.2
1	A	225	GLU	3.2
1	A	265	GLU	3.2
1	A	240	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	10	MET	3.2
1	A	106	LEU	3.2
1	A	135	SER	3.2
1	A	218	GLU	3.2
1	A	150	LEU	3.2
1	A	71	CYS	3.1
1	A	113	ARG	3.1
1	A	51	GLU	3.1
1	A	16	GLN	3.1
1	A	230	ASP	3.1
1	A	72	CYS	3.1
1	A	160	PHE	3.1
1	A	247	ASN	3.1
1	A	131	GLY	3.1
1	A	219	PRO	3.1
1	A	45	GLY	3.1
1	A	78	HIS	3.1
1	A	108	ILE	3.1
1	A	192	ALA	3.0
1	A	26	LEU	3.0
1	A	174	ARG	3.0
1	A	227	SER	3.0
1	A	337	LEU	3.0
1	A	336	THR	3.0
1	A	153	ARG	3.0
1	A	68	ALA	3.0
1	A	280	SER	2.9
1	A	73	GLU	2.9
1	A	310	LYS	2.9
1	A	347	PRO	2.9
1	A	281	ARG	2.8
1	A	260	VAL	2.8
1	A	185	GLN	2.8
1	A	184	ILE	2.8
1	A	165	LYS	2.7
1	A	27	SER	2.7
1	A	33	ARG	2.6
1	A	109	ASP	2.6
1	A	18	GLN	2.6
1	A	262	ASP	2.6
1	A	132	VAL	2.6
1	A	37	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	93	SER	2.5
1	A	222	HIS	2.5
1	A	169	PRO	2.5
1	A	221	VAL	2.5
1	A	183	MET	2.5
1	A	100	GLY	2.5
1	A	252	ASP	2.5
1	A	239	ASP	2.5
1	A	263	ASP	2.4
1	A	171	GLU	2.4
1	A	65	SER	2.3
1	A	138	HIS	2.3
1	A	245	MET	2.3
1	A	261	THR	2.2
1	A	258	LEU	2.2
1	A	328	PRO	2.2
1	A	96	ASN	2.1
1	A	134	ILE	2.1
1	A	21	GLY	2.0
1	A	317	GLU	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. 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	0.39	0.48	0.53	37,41,42,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	A	383	1/1	0.79	0.08	-1.29	34,34,34,34	0
2	MN	A	384	1/1	0.44	0.12	-1.45	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.