



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:30 PM UTC

PDB ID : 2VL7 / pdb_00002vl7
Title : Structure of S. tokodaii Xpd4
Authors : Naismith, J.H.; Johnson, K.A.; Oke, M.; McMahon, S.A.; Liu, L.; White, M.F.; Zawadski, M.; Carter, L.G.
Deposited on : 2008-01-08
Resolution : 2.25 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

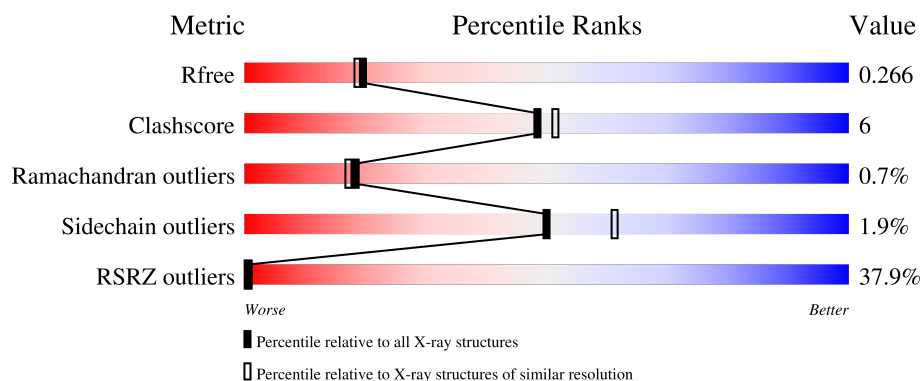
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	540	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3790 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 XPD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3712	2384	629	681	18	0	0	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

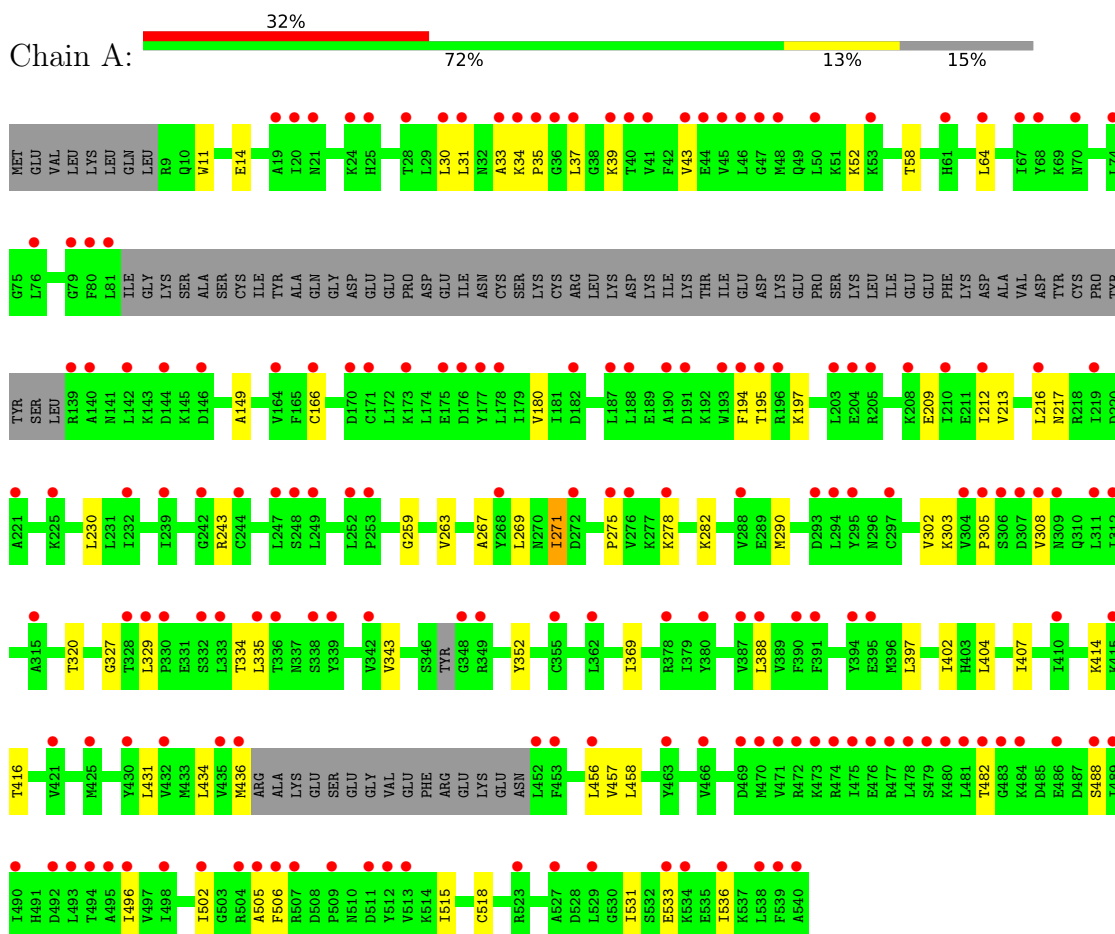
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		

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: XPD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.71Å 100.29Å 62.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.25 29.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.70-2.25) 99.6 (29.70-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.68 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.276 0.230 , 0.266	Depositor DCC
R_{free} test set	1472 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3790	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: PO4

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	0.64	1/3769 (0.0%)	0.81	4/5067 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	ILE	CA-CB	7.44	1.57	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ILE	N-CA-C	6.34	119.93	111.44
1	A	243	ARG	N-CA-C	6.06	117.41	108.86
1	A	496	ILE	CB-CA-C	-6.03	104.17	111.88
1	A	271	ILE	CB-CA-C	5.92	121.81	112.16

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	3712	0	3874	42	0
2	A	5	0	0	0	0
3	A	73	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3790	0	3874	42	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 6.

All (42) 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:43:VAL:HG11	1:A:180:VAL:HG21	1.41	1.02
1:A:456:LEU:HD12	1:A:505:ALA:HB2	1.57	0.85
1:A:290:MET:HE2	1:A:305:PRO:HG3	1.69	0.75
1:A:43:VAL:CG1	1:A:180:VAL:HG21	2.20	0.71
1:A:194:PHE:O	1:A:290:MET:HE1	1.93	0.68
1:A:33:ALA:O	1:A:327:GLY:HA2	1.97	0.65
1:A:290:MET:HE2	1:A:305:PRO:CG	2.27	0.64
1:A:436:MET:HE3	1:A:458:LEU:HD22	1.79	0.63
1:A:533:GLU:HA	1:A:536:ILE:HD12	1.82	0.61
1:A:33:ALA:HB3	1:A:39:LYS:CG	2.32	0.60
1:A:11:TRP:CE3	1:A:343:VAL:HG21	2.37	0.58
1:A:43:VAL:HG11	1:A:180:VAL:CG2	2.26	0.56
1:A:34:LYS:N	1:A:37:LEU:HD12	2.21	0.56
1:A:290:MET:O	1:A:303:LYS:HE2	2.06	0.56
1:A:334:THR:OG1	1:A:482:THR:HG22	2.07	0.55
1:A:334:THR:C	1:A:335:LEU:HD22	2.32	0.55
1:A:35:PRO:HD3	1:A:327:GLY:HA3	1.90	0.54
1:A:33:ALA:HB3	1:A:39:LYS:HG2	1.90	0.54
1:A:404:LEU:HD13	1:A:431:LEU:CD2	2.38	0.53
1:A:269:LEU:HD11	1:A:282:LYS:HD3	1.91	0.53
1:A:30:LEU:HB3	1:A:329:LEU:HD21	1.90	0.52
1:A:31:LEU:C	1:A:329:LEU:HD22	2.34	0.52
1:A:259:GLY:O	1:A:263:VAL:HG23	2.10	0.52
1:A:506:PHE:HE1	1:A:515:ILE:HD11	1.75	0.51
1:A:230:LEU:C	1:A:230:LEU:HD23	2.36	0.51
1:A:11:TRP:HA	1:A:14:GLU:HG2	1.93	0.50
1:A:195:THR:CG2	1:A:302:VAL:HG13	2.45	0.47
1:A:334:THR:O	1:A:335:LEU:HD22	2.16	0.46
1:A:352:TYR:CE1	1:A:531:ILE:HG21	2.50	0.46
1:A:402:ILE:HD11	3:A:2058:HOH:O	2.16	0.45
1:A:456:LEU:HD23	1:A:457:VAL:N	2.32	0.44
1:A:388:LEU:CD2	1:A:434:LEU:HD11	2.48	0.44
1:A:456:LEU:HD23	1:A:456:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:C	1:A:397:LEU:HD23	2.44	0.43
1:A:502:ILE:CG2	1:A:506:PHE:CZ	3.03	0.42
1:A:209:GLU:O	1:A:213:VAL:HG23	2.20	0.42
1:A:212:ILE:HG23	1:A:216:LEU:HD13	2.02	0.42
1:A:197:LYS:HG2	1:A:302:VAL:HG22	2.02	0.42
1:A:64:LEU:HD12	1:A:149:ALA:HB1	2.02	0.41
1:A:217:ASN:ND2	1:A:267:ALA:HB1	2.36	0.41
1:A:52:LYS:NZ	1:A:320:THR:OG1	2.54	0.41
1:A:388:LEU:CD2	1:A:434:LEU:CD1	3.00	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	451/540 (84%)	429 (95%)	19 (4%)	3 (1%)	18 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	414	LYS
1	A	275	PRO

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	420/494 (85%)	412 (98%)	8 (2%)	50 61

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	166	CYS
1	A	271	ILE
1	A	308	VAL
1	A	407	ILE
1	A	416	THR
1	A	488	SER
1	A	518	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	310	GLN
1	A	344	ASN
1	A	368	ASN

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](#)

1 ligand is 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	PO4	A	1541	-	4,4,4	0.94	0	6,6,6	0.58	0

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	459/540 (85%)	1.80	174 (37%) 1 0	55, 64, 81, 92	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	ILE	5.6
1	A	348	GLY	5.3
1	A	40	THR	5.3
1	A	506	PHE	5.0
1	A	452	LEU	4.7
1	A	35	PRO	4.7
1	A	421	VAL	4.6
1	A	61	HIS	4.5
1	A	142	LEU	4.4
1	A	478	LEU	4.2
1	A	475	ILE	4.2
1	A	513	VAL	4.2
1	A	471	VAL	4.0
1	A	64	LEU	4.0
1	A	33	ALA	3.9
1	A	473	LYS	3.9
1	A	37	LEU	3.8
1	A	74	LEU	3.8
1	A	80	PHE	3.7
1	A	489	ILE	3.7
1	A	212	ILE	3.7
1	A	339	TYR	3.7
1	A	205	ARG	3.6
1	A	79	GLY	3.6
1	A	188	LEU	3.6
1	A	330	PRO	3.5
1	A	305	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	3.5
1	A	494	THR	3.4
1	A	221	ALA	3.4
1	A	272	ASP	3.4
1	A	490	ILE	3.3
1	A	512	TYR	3.3
1	A	505	ALA	3.2
1	A	249	LEU	3.2
1	A	275	PRO	3.2
1	A	248	SER	3.2
1	A	294	LEU	3.2
1	A	410	ILE	3.2
1	A	333	LEU	3.2
1	A	146	ASP	3.2
1	A	175	GLU	3.1
1	A	540	ALA	3.1
1	A	276	VAL	3.1
1	A	70	ASN	3.0
1	A	139	ARG	3.0
1	A	171	CYS	3.0
1	A	30	LEU	3.0
1	A	335	LEU	3.0
1	A	178	LEU	3.0
1	A	308	VAL	3.0
1	A	481	LEU	3.0
1	A	306	SER	3.0
1	A	187	LEU	3.0
1	A	34	LYS	3.0
1	A	68	TYR	3.0
1	A	48	MET	3.0
1	A	25	HIS	2.9
1	A	208	LYS	2.9
1	A	394	TYR	2.9
1	A	140	ALA	2.9
1	A	498	ILE	2.9
1	A	493	LEU	2.8
1	A	470	MET	2.8
1	A	67	ILE	2.8
1	A	219	ILE	2.8
1	A	355	CYS	2.8
1	A	47	GLY	2.8
1	A	315	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	2.8
1	A	20	ILE	2.7
1	A	482	THR	2.7
1	A	309	ASN	2.7
1	A	332	SER	2.7
1	A	476	GLU	2.7
1	A	81	LEU	2.7
1	A	216	LEU	2.7
1	A	430	TYR	2.7
1	A	492	ASP	2.7
1	A	511	ASP	2.7
1	A	502	ILE	2.7
1	A	466	VAL	2.7
1	A	469	ASP	2.7
1	A	533	GLU	2.7
1	A	311	LEU	2.7
1	A	329	LEU	2.7
1	A	477	ARG	2.6
1	A	507	ARG	2.6
1	A	425	MET	2.6
1	A	536	ILE	2.6
1	A	293	ASP	2.6
1	A	539	PHE	2.6
1	A	41	VAL	2.6
1	A	268	TYR	2.6
1	A	432	VAL	2.6
1	A	196	ARG	2.6
1	A	342	VAL	2.6
1	A	387	VAL	2.6
1	A	538	LEU	2.5
1	A	21	ASN	2.5
1	A	436	MET	2.5
1	A	415	LYS	2.5
1	A	295	TYR	2.5
1	A	480	LYS	2.5
1	A	456	LEU	2.5
1	A	534	LYS	2.5
1	A	304	VAL	2.5
1	A	46	LEU	2.5
1	A	483	GLY	2.5
1	A	164	VAL	2.4
1	A	328	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	336	THR	2.4
1	A	312	ILE	2.4
1	A	388	LEU	2.4
1	A	253	PRO	2.4
1	A	194	PHE	2.4
1	A	453	PHE	2.4
1	A	496	ILE	2.4
1	A	225	LYS	2.4
1	A	472	ARG	2.4
1	A	44	GLU	2.4
1	A	244	CYS	2.3
1	A	39	LYS	2.3
1	A	195	THR	2.3
1	A	338	SER	2.3
1	A	239	ILE	2.3
1	A	486	GLU	2.3
1	A	24	LYS	2.3
1	A	53	LYS	2.3
1	A	173	LYS	2.3
1	A	474	ARG	2.3
1	A	488	SER	2.3
1	A	288	VAL	2.3
1	A	362	LEU	2.3
1	A	190	ALA	2.3
1	A	484	LYS	2.3
1	A	50	LEU	2.2
1	A	463	TYR	2.2
1	A	45	VAL	2.2
1	A	76	LEU	2.2
1	A	247	LEU	2.2
1	A	495	ALA	2.2
1	A	144	ASP	2.2
1	A	349	ARG	2.2
1	A	28	THR	2.2
1	A	203	LEU	2.2
1	A	176	ASP	2.2
1	A	390	PHE	2.2
1	A	395	GLU	2.2
1	A	297	CYS	2.2
1	A	252	LEU	2.1
1	A	182	ASP	2.1
1	A	435	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	278	LYS	2.1
1	A	378	ARG	2.1
1	A	31	LEU	2.1
1	A	307	ASP	2.1
1	A	193	TRP	2.1
1	A	166	CYS	2.1
1	A	523	ARG	2.1
1	A	177	TYR	2.1
1	A	191	ASP	2.1
1	A	380	TYR	2.1
1	A	509	PRO	2.1
1	A	391	PHE	2.1
1	A	479	SER	2.1
1	A	204	GLU	2.1
1	A	170	ASP	2.1
1	A	527	ALA	2.0
1	A	529	LEU	2.0
1	A	242	GLY	2.0
1	A	19	ALA	2.0
1	A	232	ILE	2.0
1	A	504	ARG	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 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	PO4	A	1541	5/5	0.67	0.14	86,86,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.