



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:03 PM EST

PDB ID : 5JP1
Title : Structure of Xanthomonas campestris effector protein XopD bound to tomato SUMO
Authors : Pruneda, J.N.; Komander, D.
Deposited on : 2016-05-03
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

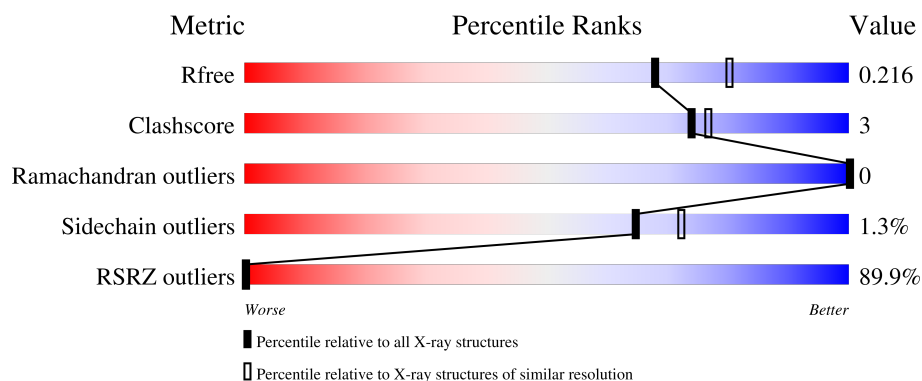
1 Overall quality at a glance

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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	220	<div> <div>80%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
2	B	96	<div> <div>74%</div> <div>74%</div> <div>7%</div> <div>19%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2398 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 Xanthomonas outer protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	1	0
			1540	964	278	293	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLY	-	expression tag	UNP Q3BYJ5
A	297	PRO	-	expression tag	UNP Q3BYJ5

- Molecule 2 is a protein called Small ubiquitin-related modifier.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	2	0
			637	394	115	121	7			

There is a discrepancy between the modelled and reference sequences:

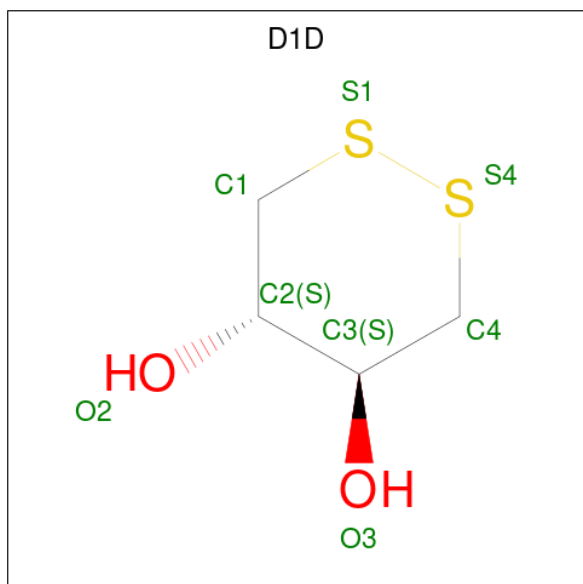
Chain	Residue	Modelled	Actual	Comment	Reference
B	96	AYE	-	expression tag	UNP Q9SMD1

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula: C₄H₈O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

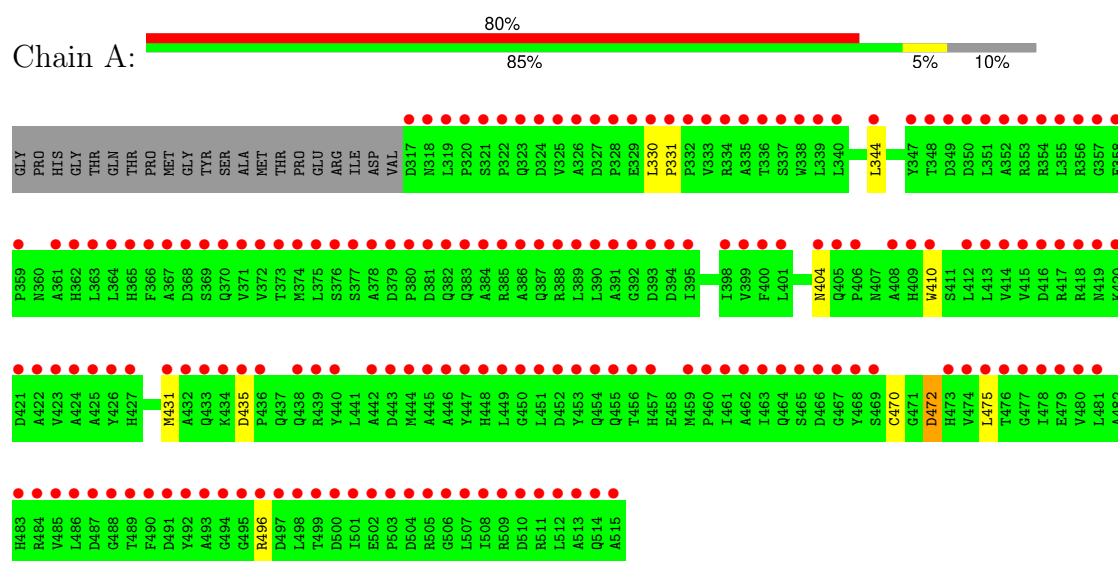
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	148	Total 148	O 148	0	0
5	B	51	Total 51	O 51	0	0

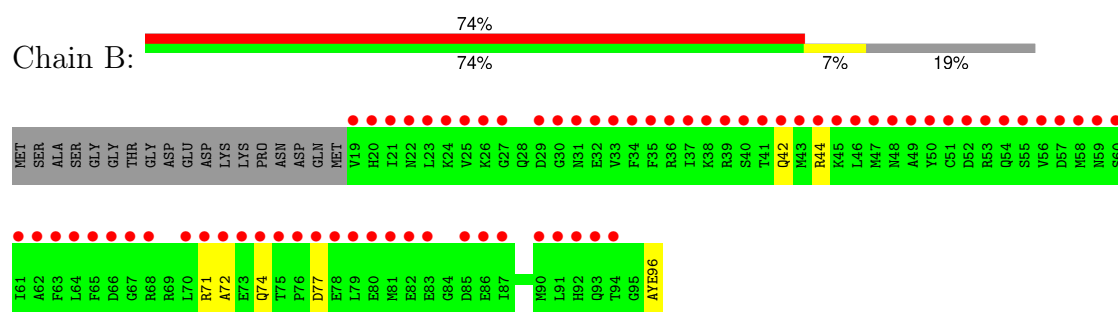
3 Residue-property plots

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. 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. 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: Xanthomonas outer protein D



• Molecule 2: Small ubiquitin-related modifier



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	119.10Å 119.10Å 50.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.55 – 2.10 59.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (59.55-2.10) 97.9 (59.55-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.181 , 0.217 0.184 , 0.216	Depositor DCC
R_{free} test set	1281 reflections (5.43%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.62	EDS
Total number of atoms	2398	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: MLI, D1D, AYE

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	0.28	0/1580	0.44	0/2159
2	B	0.33	0/646	0.49	0/862
All	All	0.29	0/2226	0.45	0/3021

There are no bond length outliers.

There are no bond angle outliers.

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	1540	0	1463	6	0
2	B	637	0	626	5	0
3	A	7	0	2	0	0
3	B	7	0	2	0	0
4	A	8	0	6	3	0
5	A	148	0	0	0	0
5	B	51	0	0	0	0
All	All	2398	0	2099	13	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 3.

All (13) 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)
4:A:602:D1D:C2	4:A:602:D1D:C3	1.75	1.60
2:B:71:ARG:H	2:B:74:GLN:HE21	1.37	0.73
2:B:71:ARG:H	2:B:74:GLN:NE2	1.96	0.64
4:A:602:D1D:C2	4:A:602:D1D:O3	2.44	0.60
2:B:44:ARG:HB3	2:B:72:ALA:HB1	1.84	0.58
1:A:431:MET:HE1	1:A:435:ASP:HB2	1.88	0.56
2:B:42:GLN:OE1	2:B:44:ARG:NH1	2.40	0.53
4:A:602:D1D:C3	4:A:602:D1D:O2	2.44	0.51
1:A:404:ASN:HB2	1:A:410:TRP:CZ3	2.47	0.49
1:A:472:ASP:OD1	1:A:472:ASP:N	2.51	0.44
1:A:330:LEU:HD12	1:A:331:PRO:HD2	2.01	0.42
1:A:344:LEU:HG	1:A:475:LEU:HD21	2.02	0.42
1:A:470:CYS:HB3	2:B:96:AYE:H3A	1.70	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	198/220 (90%)	191 (96%)	7 (4%)	0	100	100
2	B	77/96 (80%)	77 (100%)	0	0	100	100
All	All	275/316 (87%)	268 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	157/182 (86%)	155 (99%)	2 (1%)	65	72
2	B	69/82 (84%)	68 (99%)	1 (1%)	62	70
All	All	226/264 (86%)	223 (99%)	3 (1%)	65	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ASP
1	A	496	ARG
2	B	77	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
2	B	48	ASN
2	B	74	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](#)

3 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	$\# Z > 2$
4	D1D	A	602	-	8,8,8	10.69	8 (100%)	6,10,10	1.09	0
3	MLI	B	101	-	6,6,6	1.33	0	7,7,7	1.29	0
3	MLI	A	601	-	6,6,6	1.32	0	7,7,7	1.30	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
4	D1D	A	602	-	-	-	0/1/1/1
3	MLI	B	101	-	-	0/4/4/4	-
3	MLI	A	601	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	D1D	C3-C2	15.47	1.75	1.52
4	A	602	D1D	C4-S4	-14.56	1.64	1.82
4	A	602	D1D	C1-S1	-14.53	1.64	1.82
4	A	602	D1D	O2-C2	-9.08	1.24	1.43
4	A	602	D1D	O3-C3	-9.08	1.24	1.43
4	A	602	D1D	C1-C2	6.27	1.64	1.52
4	A	602	D1D	C4-C3	6.23	1.64	1.52
4	A	602	D1D	S4-S1	-2.86	1.76	2.02

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	D1D	3	0

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

Warning: The R factor obtained from EDS is 0.4348, which does not match the depositor's R factor of 0.1813. Please interpret the results in this section carefully.

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	199/220 (90%)	4.04	177 (88%) 0 0	10, 25, 49, 81	1 (0%)
2	B	77/96 (80%)	4.32	71 (92%) 0 0	13, 33, 56, 57	2 (2%)
All	All	276/316 (87%)	4.12	248 (89%) 0 0	10, 28, 52, 81	3 (1%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	ASP	13.3
1	A	488	GLY	11.6
1	A	318	ASN	11.6
1	A	513	ALA	10.2
1	A	515	ALA	10.0
2	B	56	VAL	9.7
1	A	434	LYS	9.2
2	B	19	VAL	9.2
1	A	421	ASP	9.0
1	A	514	GLN	8.1
1	A	319	LEU	7.8
2	B	30	GLY	7.6
2	B	55	SER	7.4
2	B	57	ASP	7.3
1	A	493	ALA	7.2
2	B	42	GLN	7.1
1	A	507	LEU	7.0
1	A	380	PRO	7.0
1	A	511	ARG	6.9
1	A	332	PRO	6.8
2	B	20	HIS	6.8
1	A	492	TYR	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	490	PHE	6.7
1	A	356	ARG	6.5
2	B	86	GLU	6.5
1	A	322	PRO	6.5
1	A	377	SER	6.5
2	B	53	ARG	6.5
1	A	329	GLU	6.4
1	A	379	ASP	6.4
1	A	432	ALA	6.4
2	B	29	ASP	6.4
2	B	83	GLU	6.3
1	A	486	LEU	6.3
1	A	321	SER	6.2
1	A	497	ASP	6.2
1	A	390	LEU	6.1
2	B	59	ASN	6.0
2	B	33	VAL	6.0
2	B	70	LEU	6.0
2	B	35	PHE	5.9
1	A	496	ARG	5.9
2	B	82	GLU	5.9
1	A	419	ASN	5.8
1	A	394	ASP	5.8
1	A	353	ARG	5.8
1	A	325	VAL	5.8
1	A	326	ALA	5.8
1	A	334	ARG	5.7
1	A	451	LEU	5.7
1	A	355	LEU	5.7
1	A	455	GLN	5.6
1	A	436	PRO	5.6
1	A	363	LEU	5.5
1	A	422	ALA	5.5
1	A	464	GLN	5.5
1	A	378	ALA	5.5
1	A	510	ASP	5.5
1	A	467	GLY	5.4
2	B	39	ARG	5.4
2	B	52	ASP	5.4
1	A	468	TYR	5.4
2	B	74	GLN	5.4
1	A	480	VAL	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	359	PRO	5.2
1	A	450	GLY	5.2
1	A	435	ASP	5.2
1	A	463	ILE	5.2
1	A	331	PRO	5.2
2	B	87	ILE	5.2
2	B	58	MET	5.2
1	A	433	GLN	5.1
1	A	328	PRO	5.1
1	A	393	ASP	5.0
2	B	54	GLN	5.0
2	B	77	ASP	5.0
1	A	361	ALA	5.0
1	A	374	MET	4.9
1	A	398	ILE	4.9
2	B	41	THR	4.9
2	B	48	ASN	4.9
1	A	423	VAL	4.9
1	A	381	ASP	4.9
2	B	71	ARG	4.9
1	A	499	THR	4.9
1	A	357	GLY	4.8
1	A	384	ALA	4.8
2	B	40	SER	4.8
2	B	23	LEU	4.7
1	A	388	ARG	4.7
1	A	489	THR	4.7
2	B	63	PHE	4.6
1	A	348	THR	4.5
1	A	456	THR	4.5
1	A	485	VAL	4.5
1	A	509	ARG	4.4
1	A	461	ILE	4.4
1	A	391	ALA	4.4
1	A	447	TYR	4.4
1	A	324	ASP	4.4
1	A	327	ASP	4.4
2	B	51	CYS	4.4
1	A	491	ASP	4.4
2	B	27	GLY	4.3
2	B	80	GLU	4.3
1	A	323	GLN	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	4.3
2	B	37	ILE	4.2
1	A	366	PHE	4.2
1	A	333	VAL	4.2
2	B	61[A]	ILE	4.2
1	A	420	LYS	4.2
1	A	376	SER	4.1
1	A	465	SER	4.1
1	A	364	LEU	4.1
1	A	320	PRO	4.1
1	A	440	TYR	4.1
1	A	330	LEU	4.1
1	A	389	LEU	4.1
1	A	481	LEU	4.1
2	B	31	ASN	4.1
2	B	24	LYS	4.0
2	B	45	LYS	4.0
2	B	85	ASP	4.0
1	A	454	GLN	4.0
1	A	506	GLY	4.0
1	A	449	LEU	4.0
2	B	32	GLU	4.0
2	B	44	ARG	4.0
1	A	500	ASP	3.9
1	A	494	GLY	3.9
1	A	351	LEU	3.9
1	A	417	ARG	3.9
1	A	462	ALA	3.9
1	A	479	GLU	3.9
2	B	73	GLU	3.8
2	B	68	ARG	3.8
1	A	466	ASP	3.8
2	B	66	ASP	3.8
2	B	78	GLU	3.8
1	A	427	HIS	3.8
1	A	512	LEU	3.8
1	A	439	ARG	3.8
1	A	418	ARG	3.8
1	A	426	TYR	3.8
1	A	338	TRP	3.8
2	B	94	THR	3.7
1	A	387	GLN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	72	ALA	3.7
2	B	75	THR	3.7
2	B	93	GLN	3.7
1	A	498	LEU	3.7
2	B	92	HIS	3.6
1	A	340	LEU	3.6
1	A	373	THR	3.6
2	B	47[A]	MET	3.6
2	B	79	LEU	3.6
1	A	460	PRO	3.6
1	A	372	VAL	3.6
2	B	21	ILE	3.5
1	A	483	HIS	3.5
1	A	386	ALA	3.5
1	A	473	HIS	3.5
1	A	444	MET	3.5
1	A	416	ASP	3.5
1	A	508	ILE	3.4
2	B	49	ALA	3.4
2	B	65	PHE	3.4
1	A	431	MET	3.4
2	B	91	LEU	3.4
1	A	424	ALA	3.4
1	A	457	HIS	3.4
1	A	392	GLY	3.4
1	A	477	GLY	3.4
2	B	34	PHE	3.3
1	A	344	LEU	3.3
1	A	408	ALA	3.3
1	A	349	ASP	3.3
2	B	36	ARG	3.3
2	B	22	ASN	3.3
1	A	448	HIS	3.3
1	A	410	TRP	3.2
2	B	50	TYR	3.2
2	B	46	LEU	3.1
2	B	43	MET	3.1
1	A	382	GLN	3.1
2	B	76	PRO	3.1
1	A	354	ARG	3.1
1	A	453	TYR	3.1
1	A	504	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	476	THR	3.1
1	A	443	ASP	3.0
1	A	469	SER	3.0
1	A	365	HIS	3.0
2	B	81	MET	3.0
2	B	38	LYS	3.0
1	A	385	ARG	3.0
1	A	425	ALA	2.9
1	A	339	LEU	2.9
2	B	62	ALA	2.9
1	A	362	HIS	2.9
1	A	375	LEU	2.9
2	B	64	LEU	2.9
1	A	459	MET	2.8
1	A	474	VAL	2.8
1	A	495	GLY	2.8
1	A	367	ALA	2.7
2	B	60	SER	2.8
1	A	452	ASP	2.7
1	A	413	LEU	2.7
1	A	371	VAL	2.7
1	A	478	ILE	2.7
2	B	26	LYS	2.6
1	A	337	SER	2.6
1	A	412	LEU	2.6
1	A	383	GLN	2.6
1	A	400	PHE	2.4
1	A	395	ILE	2.4
1	A	505	ARG	2.4
1	A	445	ALA	2.4
1	A	350	ASP	2.4
1	A	438	GLN	2.4
1	A	442	ALA	2.4
1	A	446	ALA	2.4
1	A	415	VAL	2.4
1	A	370	GLN	2.4
1	A	501	ILE	2.4
1	A	502	GLU	2.3
1	A	484	ARG	2.3
1	A	475	LEU	2.3
1	A	405	GLN	2.3
1	A	368	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	358	GLU	2.3
1	A	347	TYR	2.3
1	A	406	PRO	2.2
1	A	336	THR	2.2
1	A	399	VAL	2.2
1	A	404	ASN	2.2
1	A	503	PRO	2.2
1	A	414	VAL	2.2
2	B	90	MET	2.2
1	A	369	SER	2.1
2	B	25	VAL	2.1
1	A	409	HIS	2.1
1	A	352	ALA	2.1
2	B	67	GLY	2.1
1	A	487	ASP	2.0
1	A	401[A]	LEU	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 monosaccharides 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(Å ²)	Q<0.9
3	MLI	A	601	7/7	0.47	0.40	69,70,71,71	0
4	D1D	A	602	8/8	0.58	0.29	64,65,67,67	8
3	MLI	B	101	7/7	0.65	0.29	25,27,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.