



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:32 PM UTC

PDB ID : 4TR2 / pdb_00004tr2
Title : Crystal structure of PvSUB1
Authors : Giganti, D.; Bouillon, A.; Martinez, M.; Weber, P.; Girard-Blanc, C.; Petres, S.; Haouz, A.; Barale, J.C.; Alzari, P.M.
Deposited on : 2014-06-13
Resolution : 2.70 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

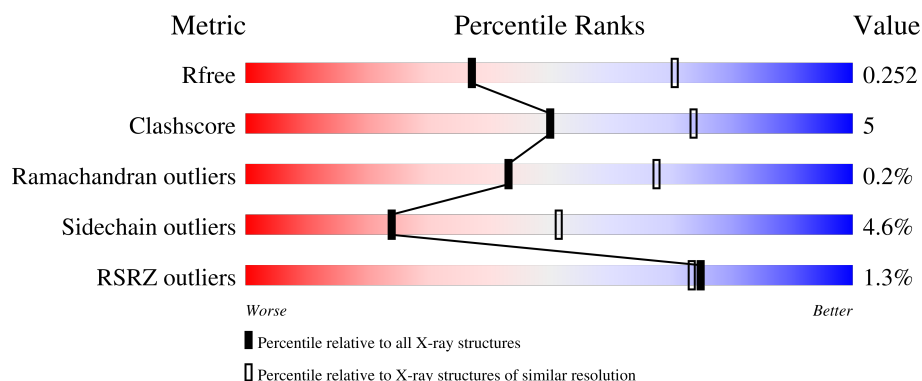
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

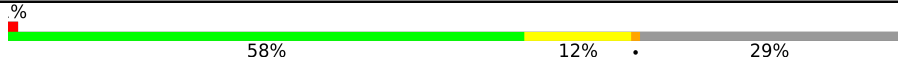
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	663	
1	B	663	

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	807	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7410 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 Subtilisin-like 1 serine protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3674	2295	637	727	15			
1	B	474	Total	C	N	O	S	0	0	0
			3688	2305	639	729	15			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP E6Y8B9
A	-14	LEU	-	expression tag	UNP E6Y8B9
A	-13	LEU	-	expression tag	UNP E6Y8B9
A	-12	VAL	-	expression tag	UNP E6Y8B9
A	-11	ASN	-	expression tag	UNP E6Y8B9
A	-10	GLN	-	expression tag	UNP E6Y8B9
A	-9	SER	-	expression tag	UNP E6Y8B9
A	-8	HIS	-	expression tag	UNP E6Y8B9
A	-7	GLN	-	expression tag	UNP E6Y8B9
A	-6	GLY	-	expression tag	UNP E6Y8B9
A	-5	PHE	-	expression tag	UNP E6Y8B9
A	-4	ASN	-	expression tag	UNP E6Y8B9
A	-3	LYS	-	expression tag	UNP E6Y8B9
A	-2	GLU	-	expression tag	UNP E6Y8B9
A	-1	HIS	-	expression tag	UNP E6Y8B9
A	0	THR	-	expression tag	UNP E6Y8B9
A	1	SER	-	expression tag	UNP E6Y8B9
A	2	LYS	-	expression tag	UNP E6Y8B9
A	3	MET	-	expression tag	UNP E6Y8B9
A	4	VAL	-	expression tag	UNP E6Y8B9
A	5	SER	-	expression tag	UNP E6Y8B9
A	6	ALA	-	expression tag	UNP E6Y8B9
A	7	ILE	-	expression tag	UNP E6Y8B9
A	8	VAL	-	expression tag	UNP E6Y8B9
A	9	LEU	-	expression tag	UNP E6Y8B9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	10	TYR	-	expression tag	UNP E6Y8B9
A	11	VAL	-	expression tag	UNP E6Y8B9
A	12	LEU	-	expression tag	UNP E6Y8B9
A	13	LEU	-	expression tag	UNP E6Y8B9
A	14	ALA	-	expression tag	UNP E6Y8B9
A	15	ALA	-	expression tag	UNP E6Y8B9
A	16	ALA	-	expression tag	UNP E6Y8B9
A	17	ALA	-	expression tag	UNP E6Y8B9
A	18	HIS	-	expression tag	UNP E6Y8B9
A	19	SER	-	expression tag	UNP E6Y8B9
A	20	ALA	-	expression tag	UNP E6Y8B9
A	21	PHE	-	expression tag	UNP E6Y8B9
A	22	ALA	-	expression tag	UNP E6Y8B9
A	23	ALA	-	expression tag	UNP E6Y8B9
A	24	ASP	-	expression tag	UNP E6Y8B9
A	25	PRO	-	expression tag	UNP E6Y8B9
A	631	HIS	-	expression tag	UNP E6Y8B9
A	632	HIS	-	expression tag	UNP E6Y8B9
A	633	HIS	-	expression tag	UNP E6Y8B9
A	634	HIS	-	expression tag	UNP E6Y8B9
A	635	HIS	-	expression tag	UNP E6Y8B9
A	636	HIS	-	expression tag	UNP E6Y8B9
A	637	SER	-	expression tag	UNP E6Y8B9
A	638	SER	-	expression tag	UNP E6Y8B9
A	639	ARG	-	expression tag	UNP E6Y8B9
A	640	ILE	-	expression tag	UNP E6Y8B9
A	641	PRO	-	expression tag	UNP E6Y8B9
A	642	GLU	-	expression tag	UNP E6Y8B9
A	643	ARG	-	expression tag	UNP E6Y8B9
A	644	PRO	-	expression tag	UNP E6Y8B9
A	645	LEU	-	expression tag	UNP E6Y8B9
A	646	GLN	-	expression tag	UNP E6Y8B9
A	647	ILE	-	expression tag	UNP E6Y8B9
B	-15	MET	-	initiating methionine	UNP E6Y8B9
B	-14	LEU	-	expression tag	UNP E6Y8B9
B	-13	LEU	-	expression tag	UNP E6Y8B9
B	-12	VAL	-	expression tag	UNP E6Y8B9
B	-11	ASN	-	expression tag	UNP E6Y8B9
B	-10	GLN	-	expression tag	UNP E6Y8B9
B	-9	SER	-	expression tag	UNP E6Y8B9
B	-8	HIS	-	expression tag	UNP E6Y8B9
B	-7	GLN	-	expression tag	UNP E6Y8B9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP E6Y8B9
B	-5	PHE	-	expression tag	UNP E6Y8B9
B	-4	ASN	-	expression tag	UNP E6Y8B9
B	-3	LYS	-	expression tag	UNP E6Y8B9
B	-2	GLU	-	expression tag	UNP E6Y8B9
B	-1	HIS	-	expression tag	UNP E6Y8B9
B	0	THR	-	expression tag	UNP E6Y8B9
B	1	SER	-	expression tag	UNP E6Y8B9
B	2	LYS	-	expression tag	UNP E6Y8B9
B	3	MET	-	expression tag	UNP E6Y8B9
B	4	VAL	-	expression tag	UNP E6Y8B9
B	5	SER	-	expression tag	UNP E6Y8B9
B	6	ALA	-	expression tag	UNP E6Y8B9
B	7	ILE	-	expression tag	UNP E6Y8B9
B	8	VAL	-	expression tag	UNP E6Y8B9
B	9	LEU	-	expression tag	UNP E6Y8B9
B	10	TYR	-	expression tag	UNP E6Y8B9
B	11	VAL	-	expression tag	UNP E6Y8B9
B	12	LEU	-	expression tag	UNP E6Y8B9
B	13	LEU	-	expression tag	UNP E6Y8B9
B	14	ALA	-	expression tag	UNP E6Y8B9
B	15	ALA	-	expression tag	UNP E6Y8B9
B	16	ALA	-	expression tag	UNP E6Y8B9
B	17	ALA	-	expression tag	UNP E6Y8B9
B	18	HIS	-	expression tag	UNP E6Y8B9
B	19	SER	-	expression tag	UNP E6Y8B9
B	20	ALA	-	expression tag	UNP E6Y8B9
B	21	PHE	-	expression tag	UNP E6Y8B9
B	22	ALA	-	expression tag	UNP E6Y8B9
B	23	ALA	-	expression tag	UNP E6Y8B9
B	24	ASP	-	expression tag	UNP E6Y8B9
B	25	PRO	-	expression tag	UNP E6Y8B9
B	631	HIS	-	expression tag	UNP E6Y8B9
B	632	HIS	-	expression tag	UNP E6Y8B9
B	633	HIS	-	expression tag	UNP E6Y8B9
B	634	HIS	-	expression tag	UNP E6Y8B9
B	635	HIS	-	expression tag	UNP E6Y8B9
B	636	HIS	-	expression tag	UNP E6Y8B9
B	637	SER	-	expression tag	UNP E6Y8B9
B	638	SER	-	expression tag	UNP E6Y8B9
B	639	ARG	-	expression tag	UNP E6Y8B9
B	640	ILE	-	expression tag	UNP E6Y8B9

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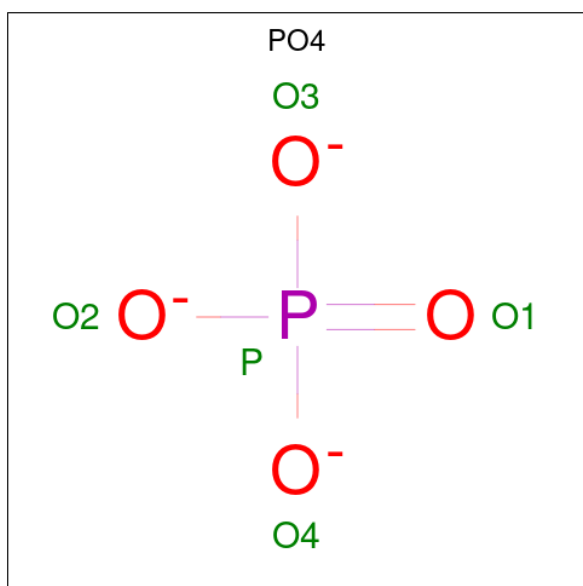
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Chain	Residue	Modelled	Actual	Comment	Reference
B	641	PRO	-	expression tag	UNP E6Y8B9
B	642	GLU	-	expression tag	UNP E6Y8B9
B	643	ARG	-	expression tag	UNP E6Y8B9
B	644	PRO	-	expression tag	UNP E6Y8B9
B	645	LEU	-	expression tag	UNP E6Y8B9
B	646	GLN	-	expression tag	UNP E6Y8B9
B	647	ILE	-	expression tag	UNP E6Y8B9

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Ca 4 4	0	0
2	B	4	Total Ca 4 4	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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

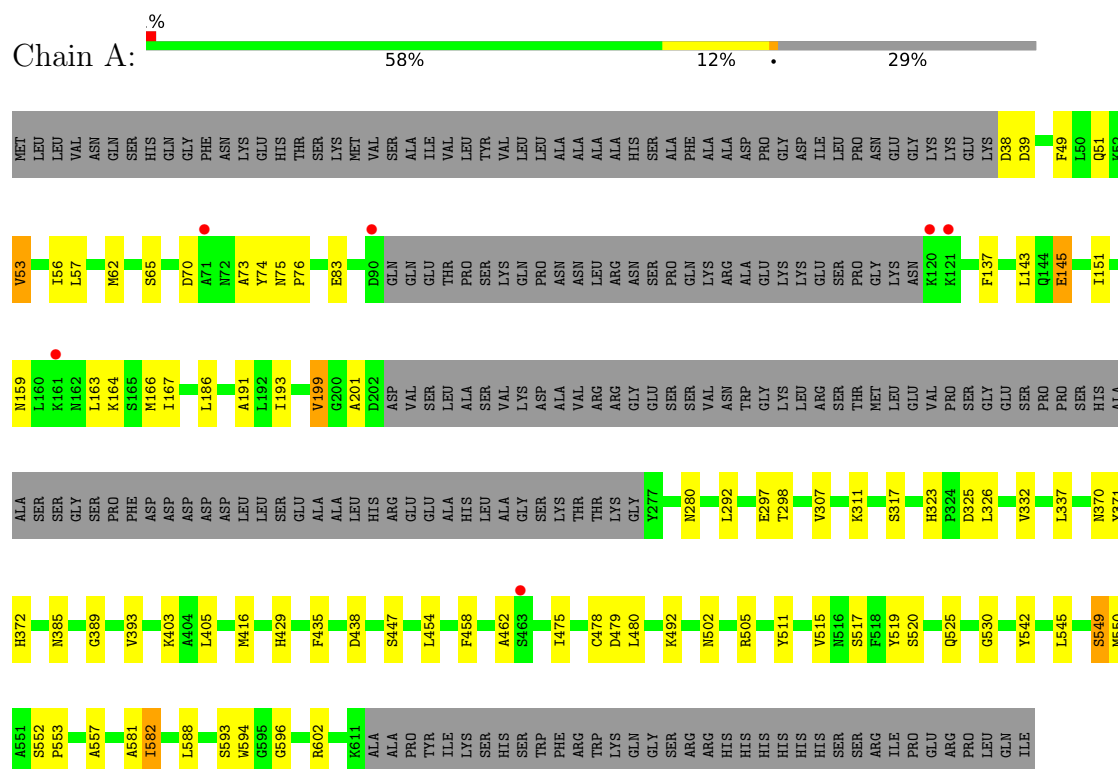
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	8	Total	O	0	0
			8	8		

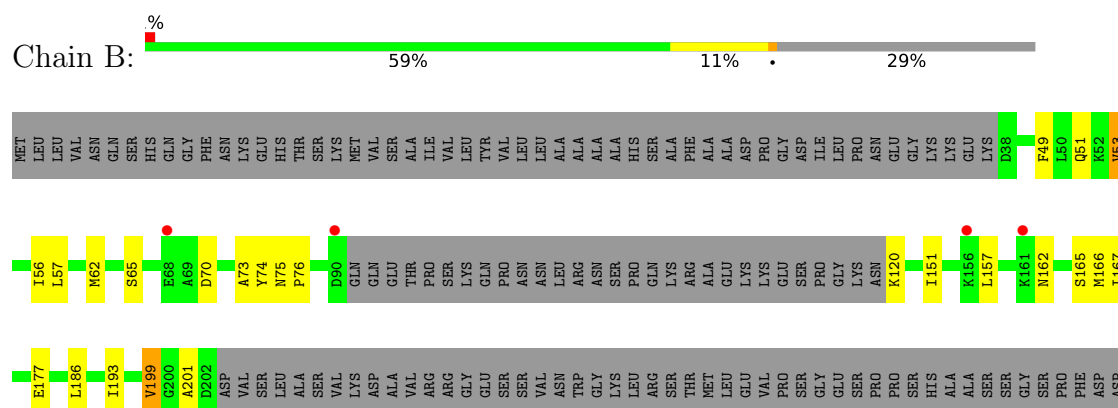
3 Residue-property plots

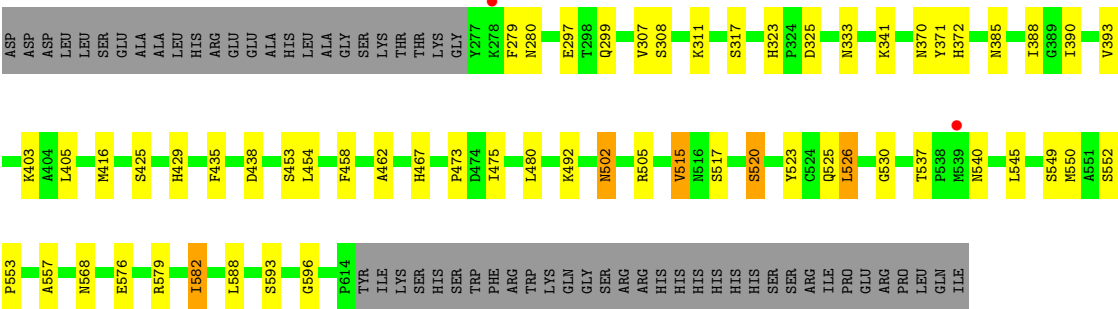
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Subtilisin-like 1 serine protease



- Molecule 1: Subtilisin-like 1 serine protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.00Å 95.00Å 287.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.10 – 2.70 45.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.10-2.70) 99.6 (45.10-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.200 , 0.244 0.212 , 0.252	Depositor DCC
R_{free} test set	1853 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7410	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, CA

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	0.79	0/3732	1.32	11/5051 (0.2%)
1	B	0.80	0/3747	1.34	11/5073 (0.2%)
All	All	0.80	0/7479	1.33	22/10124 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	LEU	N-CA-CB	-6.81	100.80	111.56
1	B	462	ALA	N-CA-C	-6.52	101.30	110.50
1	B	502	ASN	CA-CB-CG	6.43	119.03	112.60
1	A	462	ALA	N-CA-C	-6.07	101.94	110.50
1	B	333	ASN	CA-C-N	5.86	128.79	120.53
1	B	333	ASN	C-N-CA	5.86	128.79	120.53
1	A	39	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	120	LYS	CA-C-N	5.56	130.11	121.26
1	B	120	LYS	C-N-CA	5.56	130.11	121.26
1	B	51	GLN	CA-C-N	5.35	127.45	120.28
1	B	51	GLN	C-N-CA	5.35	127.45	120.28
1	A	145	GLU	CA-C-N	5.31	127.66	120.38
1	A	145	GLU	C-N-CA	5.31	127.66	120.38
1	A	38	ASP	CA-C-N	5.23	128.26	120.31
1	A	38	ASP	C-N-CA	5.23	128.26	120.31
1	A	51	GLN	CA-C-N	5.21	127.25	120.28
1	A	51	GLN	C-N-CA	5.21	127.25	120.28
1	A	458	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	479	ASP	CA-C-N	5.08	127.59	120.28
1	A	479	ASP	C-N-CA	5.08	127.59	120.28
1	B	458	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	582	ILE	N-CA-CB	5.03	117.15	110.26

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	3674	0	3617	43	0
1	B	3688	0	3630	41	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	7	0	0	0	0
4	B	8	0	0	0	0
All	All	7410	0	7247	78	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 5.

All (78) 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:311:LYS:H	1:A:429:HIS:HD2	1.11	0.98
1:B:279:PHE:HZ	1:B:299:GLN:HG3	1.39	0.86
1:B:311:LYS:H	1:B:429:HIS:CD2	1.98	0.81
1:A:454:LEU:HD21	1:B:454:LEU:HD21	1.62	0.80
1:B:279:PHE:CZ	1:B:299:GLN:HG3	2.17	0.79
1:A:311:LYS:H	1:A:429:HIS:CD2	2.01	0.78
1:B:579:ARG:O	1:B:582:ILE:HG13	1.93	0.69
1:A:581:ALA:HA	1:A:602:ARG:HG2	1.80	0.64
1:A:370:ASN:HD22	1:A:372:HIS:H	1.46	0.63
1:B:370:ASN:HD22	1:B:372:HIS:H	1.47	0.62
1:B:525:GLN:HA	1:B:593:SER:HB3	1.84	0.60
1:B:49:PHE:O	1:B:53:VAL:HG23	2.04	0.58
1:A:159:ASN:HA	1:A:166:MET:HG2	1.85	0.58
1:A:525:GLN:HA	1:A:593:SER:HB3	1.86	0.57
1:B:502:ASN:HB3	1:B:517:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:HIS:HD2	1:A:325:ASP:H	1.53	0.56
1:A:49:PHE:O	1:A:53:VAL:HG23	2.05	0.56
1:B:520:SER:HB3	1:B:523:TYR:H	1.69	0.56
1:A:186:LEU:HB3	1:A:193:ILE:HD11	1.88	0.56
1:B:186:LEU:HB3	1:B:193:ILE:HD11	1.88	0.55
1:A:530:GLY:HA2	1:A:550:MET:HB2	1.89	0.55
1:B:530:GLY:HA2	1:B:550:MET:HB2	1.89	0.54
1:A:393:VAL:HB	1:A:557:ALA:CB	2.38	0.53
1:A:199:VAL:HG11	1:A:416:MET:HE3	1.91	0.53
1:B:393:VAL:HB	1:B:557:ALA:CB	2.37	0.53
1:B:57:LEU:HD23	1:B:62:MET:HE3	1.90	0.53
1:A:137:PHE:CD1	1:A:191:ALA:HB2	2.45	0.51
1:B:199:VAL:HG11	1:B:416:MET:HE3	1.91	0.51
1:A:480:LEU:HB2	1:A:520:SER:HB2	1.91	0.51
1:B:74:TYR:HB3	1:B:505:ARG:HB3	1.93	0.50
1:B:162:ASN:HD21	1:B:425:SER:HB3	1.76	0.50
1:A:332:VAL:HG11	1:A:337:LEU:HD22	1.94	0.50
1:B:70:ASP:OD1	1:B:515:VAL:HB	2.12	0.49
1:A:159:ASN:H	1:B:568:ASN:HD22	1.61	0.49
1:A:74:TYR:HB3	1:A:505:ARG:HB3	1.94	0.48
1:A:164:LYS:HE3	1:B:453:SER:O	2.13	0.48
1:B:201:ALA:HB2	1:B:405:LEU:HD13	1.96	0.48
1:B:323:HIS:HD2	1:B:325:ASP:H	1.63	0.47
1:B:323:HIS:CE1	1:B:540:ASN:HA	2.50	0.47
1:A:317:SER:C	1:A:403:LYS:HG3	2.40	0.47
1:A:502:ASN:HB3	1:A:517:SER:HB3	1.96	0.47
1:A:389:GLY:HA3	1:A:542:TYR:CE1	2.50	0.46
1:A:201:ALA:HB2	1:A:405:LEU:HD13	1.97	0.46
1:B:317:SER:C	1:B:403:LYS:HG3	2.41	0.46
1:A:582:ILE:CD1	1:A:594:TRP:HE3	2.28	0.46
1:A:151:ILE:HG12	1:A:186:LEU:HD21	1.97	0.46
1:A:389:GLY:HA3	1:A:542:TYR:CZ	2.51	0.46
1:B:480:LEU:HB2	1:B:520:SER:HB2	1.99	0.45
1:A:588:LEU:HD12	1:A:596:GLY:HA2	1.99	0.44
1:B:199:VAL:HG13	1:B:435:PHE:HB2	1.99	0.44
1:A:163:LEU:HD22	1:A:447:SER:HB2	1.99	0.44
1:A:143:LEU:HB3	1:B:576:GLU:HG2	2.00	0.44
1:B:70:ASP:HB2	1:B:73:ALA:HB2	1.99	0.44
1:B:552:SER:N	1:B:553:PRO:HD2	2.32	0.43
1:A:199:VAL:HG13	1:A:435:PHE:HB2	2.01	0.43
1:A:53:VAL:O	1:A:57:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG12	1:B:186:LEU:HD21	2.00	0.42
1:B:280:ASN:OD1	1:B:385:ASN:HA	2.19	0.42
1:A:280:ASN:OD1	1:A:385:ASN:HA	2.19	0.42
1:A:70:ASP:HB2	1:A:73:ALA:HB2	2.01	0.42
1:A:393:VAL:HB	1:A:557:ALA:HB3	2.01	0.42
1:A:552:SER:N	1:A:553:PRO:HD2	2.34	0.42
1:B:393:VAL:HB	1:B:557:ALA:HB3	2.00	0.42
1:B:157:LEU:HD11	1:B:166:MET:SD	2.59	0.42
1:A:454:LEU:HD21	1:B:454:LEU:CD2	2.42	0.42
1:B:323:HIS:CD2	1:B:325:ASP:H	2.37	0.42
1:A:549:SER:CB	1:A:550:MET:HE2	2.50	0.41
1:B:75:ASN:HD22	1:B:76:PRO:HD2	1.85	0.41
1:A:159:ASN:H	1:B:568:ASN:ND2	2.18	0.41
1:B:549:SER:CB	1:B:550:MET:HE2	2.50	0.41
1:B:53:VAL:O	1:B:57:LEU:HG	2.21	0.41
1:A:62:MET:HE2	1:A:62:MET:HB3	1.83	0.41
1:A:75:ASN:HD22	1:A:76:PRO:HD2	1.86	0.41
1:A:478:CYS:HB2	1:A:519:TYR:CE2	2.56	0.41
1:A:323:HIS:HB3	1:A:326:LEU:HB2	2.03	0.40
1:A:292:LEU:HD13	1:A:511:TYR:CE1	2.57	0.40
1:B:467:HIS:CG	1:B:473:PRO:HB3	2.56	0.40
1:B:588:LEU:HD12	1:B:596:GLY:HA2	2.02	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	465/663 (70%)	446 (96%)	18 (4%)	1 (0%)	43	68
1	B	468/663 (71%)	447 (96%)	20 (4%)	1 (0%)	43	68
All	All	933/1326 (70%)	893 (96%)	38 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	TYR
1	B	371	TYR

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	416/578 (72%)	399 (96%)	17 (4%)	27	56
1	B	416/578 (72%)	395 (95%)	21 (5%)	22	48
All	All	832/1156 (72%)	794 (95%)	38 (5%)	24	51

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	56	ILE
1	A	65	SER
1	A	83	GLU
1	A	145	GLU
1	A	167	ILE
1	A	199	VAL
1	A	297	GLU
1	A	298	THR
1	A	307	VAL
1	A	438	ASP
1	A	475	ILE
1	A	492	LYS
1	A	515	VAL
1	A	545	LEU
1	A	549	SER
1	A	582	ILE
1	B	53	VAL
1	B	56	ILE
1	B	65	SER
1	B	165	SER

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Mol	Chain	Res	Type
1	B	167	ILE
1	B	177	GLU
1	B	199	VAL
1	B	297	GLU
1	B	307	VAL
1	B	308	SER
1	B	341	LYS
1	B	388	ILE
1	B	390	ILE
1	B	438	ASP
1	B	475	ILE
1	B	492	LYS
1	B	515	VAL
1	B	520	SER
1	B	526	LEU
1	B	537	THR
1	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	75	ASN
1	A	86	GLN
1	A	130	ASN
1	A	162	ASN
1	A	285	ASN
1	A	323	HIS
1	A	370	ASN
1	A	429	HIS
1	A	432	ASN
1	A	442	ASN
1	A	494	HIS
1	A	532	ASN
1	A	540	ASN
1	A	541	ASN
1	B	41	HIS
1	B	75	ASN
1	B	162	ASN
1	B	323	HIS
1	B	370	ASN
1	B	427	GLN

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Mol	Chain	Res	Type
1	B	429	HIS
1	B	432	ASN
1	B	442	ASN
1	B	450	HIS
1	B	494	HIS
1	B	532	ASN
1	B	541	ASN
1	B	568	ASN
1	B	605	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](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	805	-	4,4,4	2.16	1 (25%)	6,6,6	0.51	0
3	PO4	A	806	-	4,4,4	2.65	2 (50%)	6,6,6	0.42	0
3	PO4	B	806	-	4,4,4	2.31	3 (75%)	6,6,6	0.51	0
3	PO4	A	807	-	4,4,4	2.14	4 (100%)	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	805	-	4,4,4	1.86	3 (75%)	6,6,6	0.52	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	PO4	P-O1	4.31	1.60	1.50
3	B	806	PO4	P-O1	3.02	1.57	1.50
3	A	805	PO4	P-O1	2.70	1.56	1.50
3	A	807	PO4	P-O1	2.49	1.56	1.50
3	B	805	PO4	P-O2	2.04	1.60	1.54
3	A	807	PO4	P-O4	2.04	1.60	1.54
3	A	806	PO4	P-O4	2.03	1.60	1.54
3	B	806	PO4	P-O2	2.03	1.60	1.54
3	B	805	PO4	P-O4	2.03	1.60	1.54
3	B	806	PO4	P-O4	2.02	1.60	1.54
3	B	805	PO4	P-O3	2.01	1.60	1.54
3	A	807	PO4	P-O3	2.01	1.60	1.54
3	A	807	PO4	P-O2	2.00	1.60	1.54

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	471/663 (71%)	0.04	6 (1%) 75 73	34, 55, 91, 113	0
1	B	474/663 (71%)	0.12	6 (1%) 75 73	37, 59, 89, 119	0
All	All	945/1326 (71%)	0.08	12 (1%) 75 73	34, 58, 90, 119	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	ASP	3.7
1	A	90	ASP	3.2
1	A	463	SER	2.8
1	B	278	LYS	2.8
1	A	121	LYS	2.5
1	B	156	LYS	2.4
1	A	161	LYS	2.3
1	A	120	LYS	2.3
1	B	68	GLU	2.2
1	B	539	MET	2.2
1	B	161	LYS	2.1
1	A	71	ALA	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(Å ²)	Q<0.9
3	PO4	A	807	5/5	0.70	0.15	131,131,132,133	0
3	PO4	A	805	5/5	0.84	0.12	100,100,101,103	0
3	PO4	B	805	5/5	0.88	0.10	86,90,91,94	0
3	PO4	B	806	5/5	0.88	0.13	93,94,96,96	0
3	PO4	A	806	5/5	0.92	0.10	70,73,75,75	0
2	CA	A	804	1/1	0.94	0.07	71,71,71,71	0
2	CA	B	802	1/1	0.98	0.03	66,66,66,66	0
2	CA	A	802	1/1	0.98	0.05	102,102,102,102	0
2	CA	B	801	1/1	0.98	0.05	69,69,69,69	0
2	CA	B	804	1/1	0.99	0.02	60,60,60,60	0
2	CA	A	803	1/1	0.99	0.04	50,50,50,50	0
2	CA	A	801	1/1	0.99	0.03	45,45,45,45	0
2	CA	B	803	1/1	1.00	0.03	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.