



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:33 PM GMT

PDB ID : 4TR2
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
<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

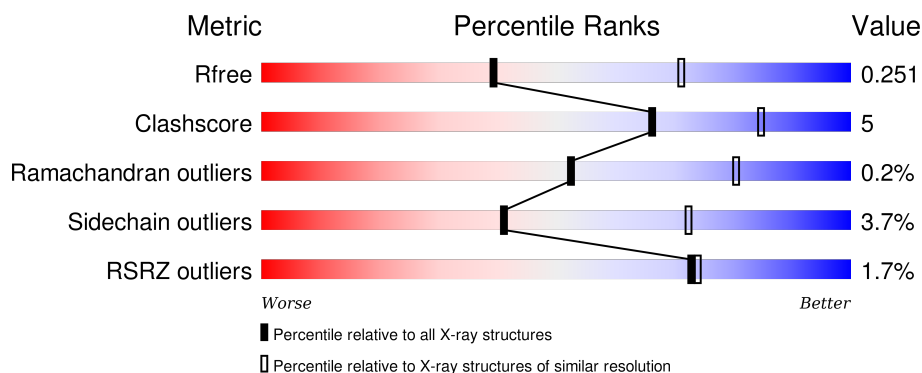
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 60%, grey 29%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 60% 11% 29% </div> </div>
1	B	663	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 61%, grey 29%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 61% 10% 29% </div> </div>

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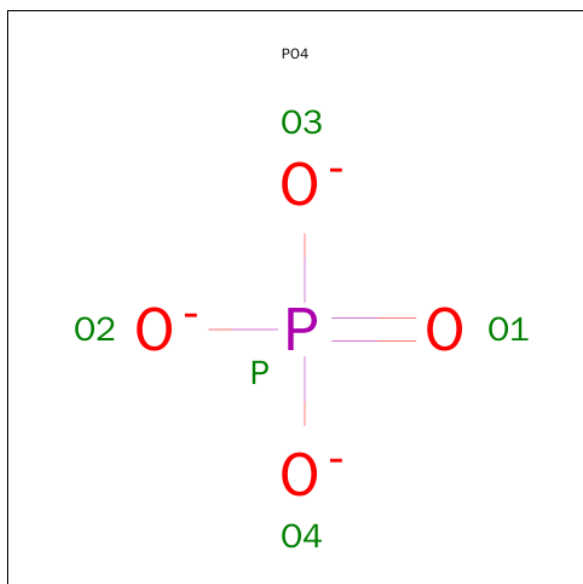
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Chain	Residue	Modelled	Actual	Comment	Reference
B	641	PRO	-	expression tag	UNP E6Y8B9
B	642	GLU	-	expression tag	UNP E6Y8B9
B	643	ARG	-	expression tag	UNP E6Y8B9
B	644	PRO	-	expression tag	UNP E6Y8B9
B	645	LEU	-	expression tag	UNP E6Y8B9
B	646	GLN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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: 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		

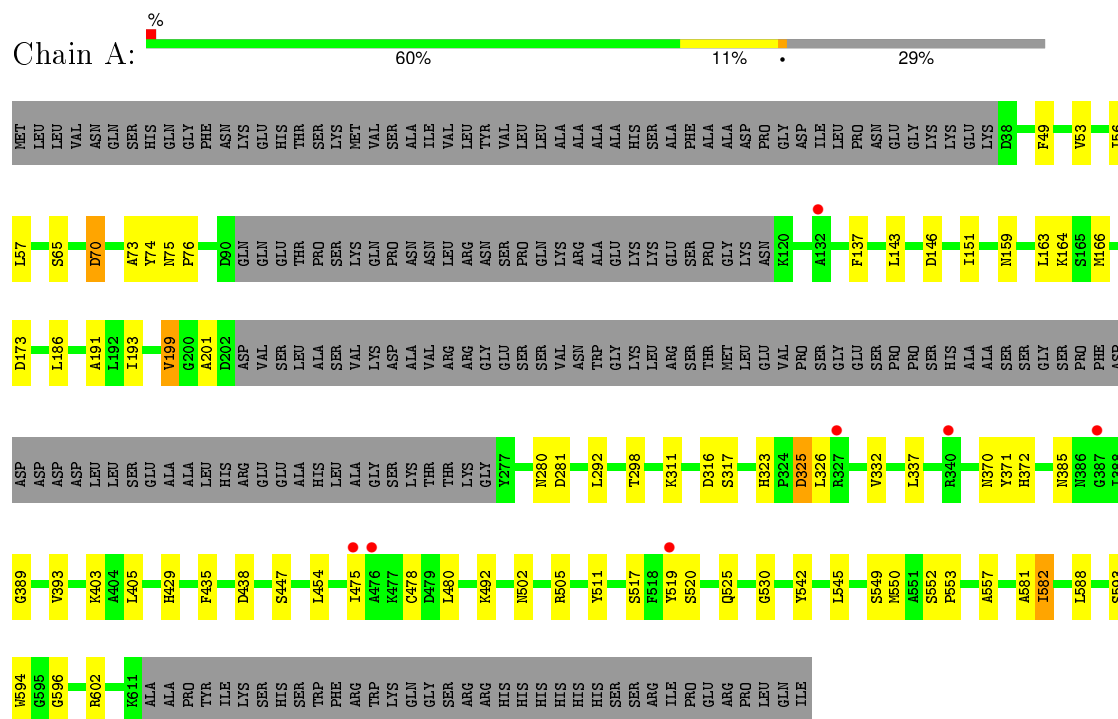
- Molecule 4 is water.

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

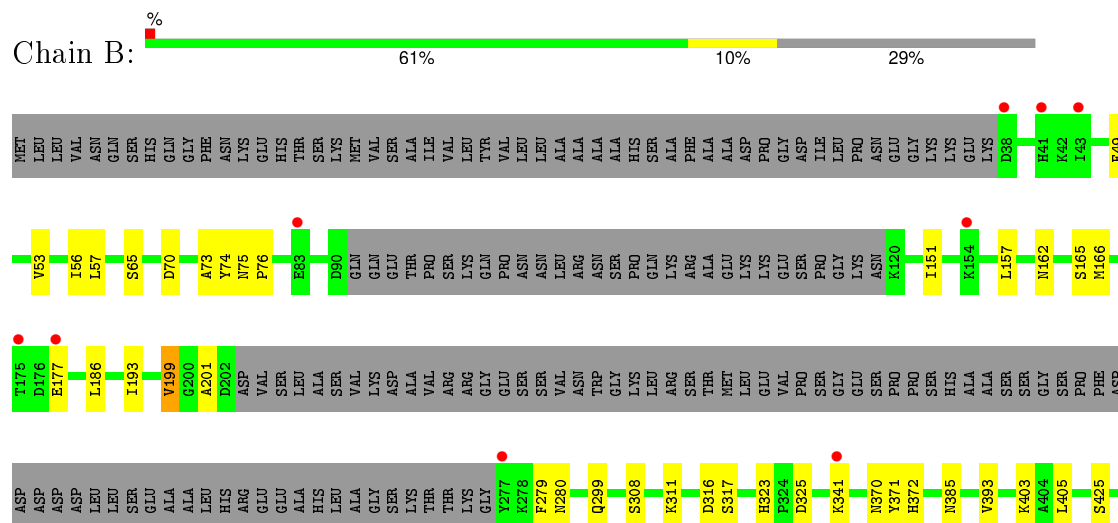
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



H429	
F435	
D438	
S453	
L454	
H467	
P473	
D474	
L475	
L480	
K492	
N502	
R505	
V515	
N516	
S517	
S520	
Y523	
C524	
Q525	
L526	
G530	
N540	
L545	
S549	
M550	
A551	
S552	
P553	
A557	
N568	
E576	
R579	
I582	
L588	
S593	

G596
P614
TYR
ILE
LYS
SER
HIS
SER
TRP
PHE
ARG
TRP
LYS
GLN
GLY
SER
ARG
ARG
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
ARG
ILE
PRO
GLU
ARG
PRO
LEU
GLN
ILE

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.00 Å 95.00 Å 287.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.10 – 2.70 43.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.10-2.70) 99.6 (43.71-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.69 Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.200 , 0.244 0.212 , 0.251	Depositor DCC
R_{free} test set	1853 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37100 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/3732	0.68	0/5051
1	B	0.47	0/3747	0.68	0/5073
All	All	0.47	0/7479	0.68	0/10124

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	3674	0	3617	40	0
1	B	3688	0	3630	38	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	72	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 (72) 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
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:B:393:VAL:HB	1:B:557:ALA:CB	2.37	0.53
1:A:137:PHE:CD1	1:A:191:ALA:HB2	2.45	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: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:A:582:ILE:CD1	1:A:594:TRP:HE3	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:199:VAL:HG13	1:B:435:PHE:HB2	1.99	0.44
1:A:588:LEU:HD12	1:A:596:GLY:HA2	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
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:317:SER:C	1:A:403:LYS:HG3	2.40	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: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:317:SER:C	1:B:403:LYS:HG3	2.41	0.41
1:B:53:VAL:O	1:B:57:LEU:HG	2.21	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:588:LEU:HD12	1:B:596:GLY:HA2	2.02	0.40
1:B:467:HIS:CG	1:B:473:PRO:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	52	80
1	B	468/663 (71%)	447 (96%)	20 (4%)	1 (0%)	52	80
All	All	933/1326 (70%)	893 (96%)	38 (4%)	2 (0%)	52	80

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%)	400 (96%)	16 (4%)	40	71
1	B	416/578 (72%)	401 (96%)	15 (4%)	42	73
All	All	832/1156 (72%)	801 (96%)	31 (4%)	41	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ILE
1	A	65	SER
1	A	70	ASP
1	A	146	ASP
1	A	173	ASP
1	A	199	VAL
1	A	281	ASP
1	A	298	THR
1	A	316	ASP
1	A	325	ASP

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Mol	Chain	Res	Type
1	A	438	ASP
1	A	475	ILE
1	A	492	LYS
1	A	545	LEU
1	A	549	SER
1	A	582	ILE
1	B	56	ILE
1	B	65	SER
1	B	165	SER
1	B	177	GLU
1	B	199	VAL
1	B	308	SER
1	B	316	ASP
1	B	341	LYS
1	B	438	ASP
1	B	475	ILE
1	B	492	LYS
1	B	520	SER
1	B	526	LEU
1	B	545	LEU
1	B	549	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	162	ASN
1	A	299	GLN
1	A	305	ASN
1	A	323	HIS
1	A	370	ASN
1	A	429	HIS
1	A	532	ASN
1	A	540	ASN
1	B	41	HIS
1	B	75	ASN
1	B	162	ASN
1	B	305	ASN
1	B	323	HIS
1	B	370	ASN
1	B	427	GLN
1	B	429	HIS

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Mol	Chain	Res	Type
1	B	450	HIS
1	B	494	HIS
1	B	532	ASN
1	B	540	ASN
1	B	568	ASN
1	B	605	ASN

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 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	1.74	0	6,6,6	0.27	0
3	PO4	A	806	-	4,4,4	1.81	0	6,6,6	0.26	0
3	PO4	A	807	-	4,4,4	1.77	0	6,6,6	0.27	0
3	PO4	B	805	-	4,4,4	1.73	0	6,6,6	0.28	0
3	PO4	B	806	-	4,4,4	1.81	0	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	805	-	-	0/0/0/0	0/0/0/0
3	PO4	A	806	-	-	0/0/0/0	0/0/0/0
3	PO4	A	807	-	-	0/0/0/0	0/0/0/0
3	PO4	B	805	-	-	0/0/0/0	0/0/0/0
3	PO4	B	806	-	-	0/0/0/0	0/0/0/0

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 ⓘ

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 [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%)	0.02	7 (1%)	76 76	34, 55, 91, 113	0
1	B	474/663 (71%)	0.08	9 (1%)	70 70	37, 59, 89, 119	0
All	All	945/1326 (71%)	0.05	16 (1%)	73 74	34, 58, 90, 119	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	154	LYS	3.4
1	B	177	GLU	3.3
1	B	38	ASP	3.1
1	A	340	ARG	2.9
1	B	341	LYS	2.9
1	A	132	ALA	2.6
1	B	43	ILE	2.6
1	B	83	GLU	2.6
1	B	277	TYR	2.5
1	A	387	GLY	2.5
1	A	519	TYR	2.4
1	A	327	ARG	2.4
1	B	41	HIS	2.3
1	A	476	ALA	2.2
1	A	475	ILE	2.1
1	B	175	THR	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	806	5/5	0.96	0.16	1.75	70,73,75,75	0
3	PO4	A	807	5/5	0.78	0.23	1.14	131,131,132,133	0
3	PO4	B	806	5/5	0.95	0.18	0.13	93,94,96,96	0
2	CA	B	804	1/1	0.98	0.04	-1.48	60,60,60,60	0
2	CA	B	803	1/1	0.99	0.06	-1.84	44,44,44,44	0
2	CA	A	804	1/1	0.92	0.06	-1.85	71,71,71,71	0
2	CA	B	802	1/1	0.94	0.07	-2.50	66,66,66,66	0
2	CA	A	803	1/1	0.98	0.05	-2.53	50,50,50,50	0
2	CA	B	801	1/1	0.98	0.09	-2.59	69,69,69,69	0
2	CA	A	802	1/1	0.91	0.08	-3.09	102,102,102,102	0
2	CA	A	801	1/1	0.99	0.04	-3.21	45,45,45,45	0
3	PO4	B	805	5/5	0.96	0.16	-	86,90,91,94	0
3	PO4	A	805	5/5	0.94	0.10	-	100,100,101,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.