



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 06:47 AM EDT

PDB ID : 1L4Z  
Title : X-RAY CRYSTAL STRUCTURE OF THE COMPLEX OF MICROPLASMINOGEN WITH ALPHA DOMAIN OF STREPTOKINASE IN THE PRESENCE CADMIUM IONS  
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Deposited on : 2002-03-06  
Resolution : 2.80 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

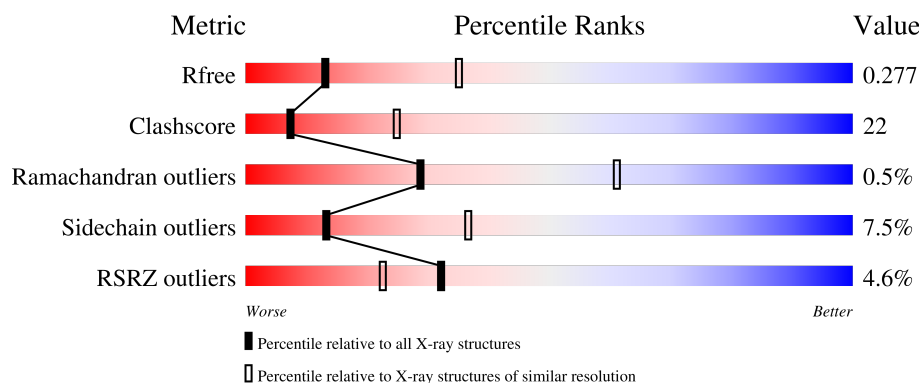
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	248	<div> <div>4%</div> <div>62%</div> <div>37%</div> <div>.</div> </div>
2	B	136	<div> <div>5%</div> <div>53%</div> <div>32%</div> <div>7%</div> <div>8%</div> </div>

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	CD	B	202	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2958 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 Plasminogen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	2	0	0
			1907	1211	337	345	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	ALA	SER	engineered mutation	UNP P00747

- Molecule 2 is a protein called Streptokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	15	0	0
			975	615	165	193	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P00779
B	6	ALA	TRP	engineered mutation	UNP P00779
B	?	-	HIS	deletion	UNP P00779
B	?	-	GLY	deletion	UNP P00779
B	?	-	GLY	deletion	UNP P00779
B	?	-	LYS	deletion	UNP P00779
B	?	-	THR	deletion	UNP P00779
B	?	-	GLU	deletion	UNP P00779
B	?	-	GLN	deletion	UNP P00779
B	?	-	GLY	deletion	UNP P00779
B	?	-	LEU	deletion	UNP P00779
B	?	-	SER	deletion	UNP P00779
B	?	-	PRO	deletion	UNP P00779
B	?	-	LYS	deletion	UNP P00779

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

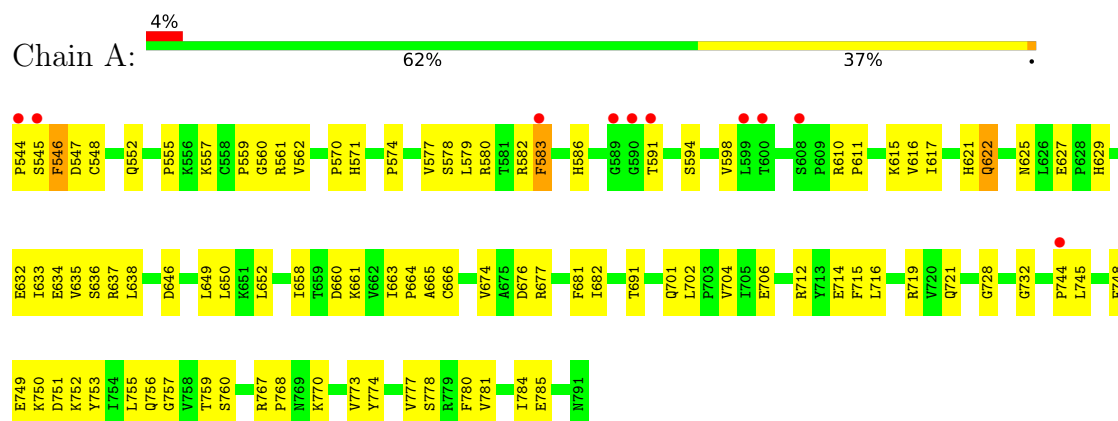
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total 45	O 45	0	0
4	B	25	Total 25	O 25	0	0

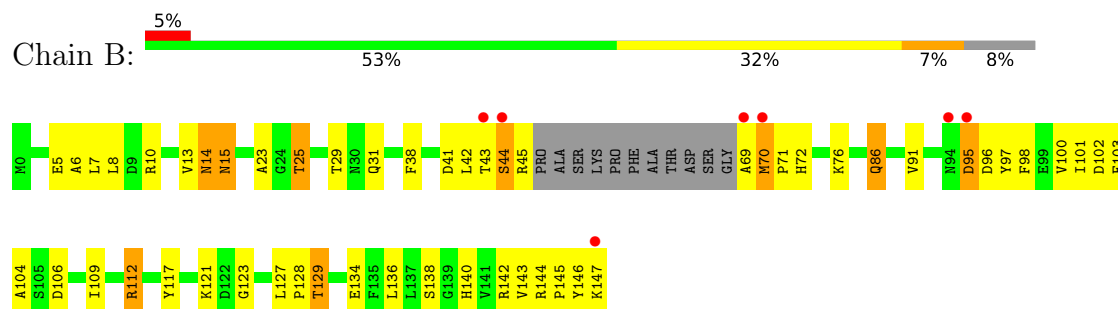
### 3 Residue-property plots [i](#)

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: Plasminogen



#### • Molecule 2: Streptokinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.40Å 118.40Å 134.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.00-2.80) 96.6 (24.72-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.77 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.220 , 0.262 0.237 , 0.277	Depositor DCC
$R_{free}$ test set	967 reflections (5.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CD

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	0.54	0/1958	0.76	0/2661
2	B	0.56	1/991 (0.1%)	0.74	0/1342
All	All	0.55	1/2949 (0.0%)	0.75	0/4003

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GLU	CD-OE2	-5.98	1.19	1.25

There are no bond angle outliers.

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	1907	0	1884	71	0
2	B	975	0	967	57	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
4	A	45	0	0	5	0
4	B	25	0	0	4	0
All	All	2958	0	2851	127	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 22.

All (127) 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)
2:B:45:ARG:HA	2:B:72:HIS:HB2	1.45	0.98
2:B:45:ARG:HB2	2:B:129:THR:HG23	1.47	0.95
1:A:580:ARG:HD3	1:A:617:ILE:HD13	1.50	0.90
1:A:755:LEU:CD2	1:A:777:VAL:HG21	2.05	0.87
2:B:45:ARG:CA	2:B:72:HIS:HB2	2.05	0.85
2:B:10:ARG:HD3	2:B:134:GLU:OE2	1.82	0.80
2:B:25:THR:HG21	4:B:207:HOH:O	1.85	0.75
1:A:580:ARG:HG2	1:A:586:HIS:HA	1.69	0.74
1:A:544:PRO:HA	1:A:547:ASP:OD1	1.88	0.74
2:B:8:LEU:HA	2:B:112:ARG:HH11	1.53	0.74
2:B:8:LEU:HA	2:B:112:ARG:NH1	2.03	0.73
1:A:755:LEU:HD22	1:A:777:VAL:HG21	1.71	0.73
1:A:615:LYS:HD3	1:A:632:GLU:OE1	1.88	0.72
2:B:45:ARG:HA	2:B:72:HIS:CB	2.19	0.72
1:A:591:THR:OG1	1:A:744:PRO:HB3	1.90	0.71
2:B:45:ARG:HD3	2:B:129:THR:OG1	1.91	0.71
2:B:43:THR:OG1	2:B:69:ALA:HB3	1.91	0.69
2:B:42:LEU:O	2:B:43:THR:HG23	1.93	0.67
2:B:42:LEU:HA	2:B:70:MET:O	1.96	0.65
1:A:666:CYS:SG	1:A:752:LYS:HD2	2.37	0.65
1:A:580:ARG:HD3	1:A:617:ILE:CD1	2.23	0.65
1:A:570:PRO:HA	1:A:621:HIS:CD2	2.32	0.64
2:B:72:HIS:CE1	2:B:129:THR:HA	2.31	0.64
2:B:43:THR:O	2:B:44:SER:HB2	1.98	0.64
1:A:578:SER:HB3	1:A:617:ILE:HB	1.79	0.63
2:B:44:SER:O	2:B:45:ARG:HB2	1.96	0.63
1:A:760:SER:HB3	1:A:773:VAL:O	1.98	0.63
2:B:98:PHE:CE1	2:B:145:PRO:HG3	2.35	0.62
1:A:748:PHE:HB2	1:A:753:TYR:CE1	2.34	0.62
2:B:91:VAL:HG21	2:B:97:TYR:CD1	2.35	0.62
1:A:580:ARG:CD	1:A:617:ILE:HD13	2.26	0.61
2:B:7:LEU:HD22	2:B:7:LEU:H	1.66	0.61
1:A:577:VAL:HG13	1:A:616:VAL:HG13	1.83	0.60
2:B:13:VAL:HG12	2:B:14:ASN:H	1.67	0.60
2:B:98:PHE:HE1	2:B:145:PRO:HG3	1.66	0.59
2:B:13:VAL:HG12	2:B:14:ASN:N	2.20	0.57
1:A:676:ASP:O	1:A:677:ARG:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:SER:O	1:A:546:PHE:HB2	2.05	0.56
1:A:748:PHE:CZ	1:A:751:ASP:HA	2.41	0.56
2:B:101:ILE:HG12	2:B:144:ARG:NH1	2.21	0.56
1:A:633:ILE:HG21	1:A:652:LEU:HB3	1.89	0.55
2:B:8:LEU:H	2:B:8:LEU:HD23	1.72	0.55
1:A:582:ARG:HG3	1:A:583:PHE:N	2.22	0.55
1:A:627:GLU:OE1	1:A:629:HIS:CE1	2.60	0.54
2:B:100:VAL:HA	2:B:143:VAL:HG12	1.90	0.54
2:B:45:ARG:N	2:B:72:HIS:HB2	2.22	0.54
1:A:546:PHE:CE1	1:A:552:GLN:HG3	2.42	0.54
2:B:44:SER:O	2:B:45:ARG:CB	2.56	0.54
1:A:757:GLY:HA2	1:A:777:VAL:HG23	1.88	0.53
1:A:780:PHE:O	1:A:784:ILE:HG13	2.08	0.53
2:B:45:ARG:HB2	2:B:129:THR:CG2	2.30	0.53
1:A:610:ARG:HH11	1:A:610:ARG:HG3	1.73	0.52
2:B:97:TYR:HA	4:B:208:HOH:O	2.10	0.52
2:B:13:VAL:HG12	2:B:15:ASN:H	1.75	0.51
1:A:627:GLU:HG3	4:A:47:HOH:O	2.09	0.51
2:B:102:ASP:OD1	2:B:103:PHE:N	2.44	0.51
2:B:101:ILE:O	2:B:102:ASP:HB2	2.11	0.51
2:B:104:ALA:C	2:B:106:ASP:H	2.14	0.50
1:A:616:VAL:C	1:A:617:ILE:HD12	2.33	0.50
1:A:555:PRO:O	1:A:557:LYS:HG3	2.12	0.49
1:A:622:GLN:HB3	1:A:625:ASN:O	2.13	0.49
2:B:44:SER:HB3	2:B:71:PRO:HB3	1.94	0.49
1:A:781:VAL:O	1:A:785:GLU:HG2	2.12	0.49
1:A:634:GLU:HG2	1:A:635:VAL:N	2.28	0.49
1:A:561:ARG:HD3	1:A:732:GLY:O	2.13	0.48
1:A:715:PHE:O	1:A:770:LYS:HE3	2.14	0.48
1:A:745:LEU:C	1:A:745:LEU:HD23	2.33	0.48
1:A:629:HIS:NE2	1:A:661:LYS:HD3	2.29	0.48
1:A:649:LEU:HD11	1:A:784:ILE:HG23	1.95	0.48
1:A:774:TYR:N	1:A:774:TYR:CD1	2.80	0.48
2:B:7:LEU:HD23	4:B:216:HOH:O	2.13	0.48
2:B:72:HIS:ND1	2:B:129:THR:HA	2.29	0.47
1:A:598:VAL:HB	1:A:650:LEU:HB2	1.97	0.47
1:A:629:HIS:CD2	1:A:661:LYS:HD3	2.49	0.47
1:A:755:LEU:HD21	1:A:777:VAL:HG21	1.93	0.47
2:B:101:ILE:HG12	2:B:144:ARG:HH12	1.79	0.47
1:A:559:PRO:HG2	1:A:562:VAL:CG2	2.44	0.47
2:B:45:ARG:CB	2:B:129:THR:HG23	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:ALA:C	2:B:106:ASP:N	2.67	0.46
1:A:574:PRO:HG3	4:A:80:HOH:O	2.16	0.46
2:B:72:HIS:ND1	2:B:128:PRO:O	2.46	0.46
1:A:702:LEU:HD22	1:A:728:GLY:HA2	1.98	0.45
1:A:615:LYS:HD2	1:A:617:ILE:HD11	1.98	0.45
1:A:681:PHE:CE1	1:A:701:GLN:HB2	2.52	0.45
1:A:559:PRO:HG2	1:A:562:VAL:HG21	1.99	0.45
1:A:759:THR:HA	1:A:774:TYR:CD2	2.52	0.45
2:B:15:ASN:HD22	2:B:15:ASN:HA	1.63	0.44
2:B:7:LEU:HD21	2:B:136:LEU:HB2	2.00	0.44
2:B:91:VAL:HG21	2:B:97:TYR:HD1	1.80	0.44
2:B:121:LYS:C	2:B:123:GLY:H	2.21	0.44
1:A:756:GLN:HA	1:A:756:GLN:OE1	2.17	0.44
2:B:72:HIS:HB3	2:B:127:LEU:O	2.18	0.43
2:B:95:ASP:N	2:B:95:ASP:OD1	2.51	0.43
2:B:23:ALA:O	2:B:140:HIS:HA	2.18	0.43
1:A:546:PHE:HE1	1:A:552:GLN:HG3	1.82	0.43
1:A:570:PRO:HA	1:A:621:HIS:HD2	1.80	0.43
2:B:109:ILE:HA	2:B:136:LEU:O	2.19	0.43
1:A:716:LEU:HA	1:A:716:LEU:HD23	1.67	0.43
1:A:767:ARG:HB3	1:A:768:PRO:CD	2.49	0.42
1:A:610:ARG:HG3	1:A:610:ARG:NH1	2.33	0.42
1:A:611:PRO:HB3	1:A:638:LEU:HG	2.01	0.42
2:B:38:PHE:CD1	2:B:86:GLN:HG2	2.54	0.42
1:A:611:PRO:HG3	1:A:636:SER:O	2.20	0.42
1:A:682:ILE:O	1:A:682:ILE:HG13	2.19	0.42
1:A:571:HIS:CD2	1:A:661:LYS:HE3	2.55	0.42
2:B:70:MET:HA	2:B:71:PRO:HD3	1.85	0.42
2:B:45:ARG:O	2:B:45:ARG:HG2	2.19	0.42
1:A:574:PRO:HB2	1:A:663:ILE:H	1.85	0.42
1:A:712:ARG:HD2	4:A:70:HOH:O	2.19	0.42
1:A:646:ASP:HB2	4:A:12:HOH:O	2.20	0.41
2:B:29:THR:OG1	2:B:31:GLN:HG2	2.20	0.41
1:A:658:ILE:HD12	1:A:664:PRO:HD3	2.03	0.41
1:A:691:THR:HG23	2:B:117:TYR:O	2.21	0.41
2:B:45:ARG:HD3	2:B:129:THR:CG2	2.51	0.41
1:A:611:PRO:CG	1:A:636:SER:O	2.69	0.41
1:A:548:CYS:HB2	1:A:665:ALA:C	2.41	0.41
1:A:560:GLY:O	1:A:561:ARG:HB2	2.21	0.41
1:A:719:ARG:HD3	4:A:52:HOH:O	2.21	0.41
2:B:76:LYS:HE2	2:B:102:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:HIS:CG	1:A:661:LYS:HG2	2.56	0.41
1:A:674:VAL:HG21	1:A:756:GLN:HG3	2.03	0.41
1:A:778:SER:HA	1:A:781:VAL:HG23	2.03	0.40
2:B:142:ARG:HD3	4:B:209:HOH:O	2.20	0.40
1:A:676:ASP:HB2	1:A:706:GLU:HB2	2.03	0.40
1:A:616:VAL:O	1:A:617:ILE:HD12	2.22	0.40
2:B:6:ALA:HB1	2:B:8:LEU:CD2	2.52	0.40
2:B:101:ILE:HD11	2:B:144:ARG:HB3	2.03	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	246/248 (99%)	225 (92%)	20 (8%)	1 (0%)	34	66
2	B	121/136 (89%)	111 (92%)	9 (7%)	1 (1%)	19	49
All	All	367/384 (96%)	336 (92%)	29 (8%)	2 (0%)	29	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	44	SER
1	A	546	PHE

### 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	209/209 (100%)	198 (95%)	11 (5%)	22	54
2	B	109/117 (93%)	96 (88%)	13 (12%)	5	16
All	All	318/326 (98%)	294 (92%)	24 (8%)	13	37

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	579	LEU
1	A	583	PHE
1	A	594	SER
1	A	622	GLN
1	A	637	ARG
1	A	660	ASP
1	A	704	VAL
1	A	714	GLU
1	A	721	GLN
1	A	749	GLU
1	A	750	LYS
2	B	14	ASN
2	B	15	ASN
2	B	25	THR
2	B	41	ASP
2	B	70	MET
2	B	86	GLN
2	B	95	ASP
2	B	96	ASP
2	B	112	ARG
2	B	129	THR
2	B	138	SER
2	B	146	TYR
2	B	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	HIS
1	A	701	GLN
1	A	729	HIS
1	A	790	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
2	B	15	ASN
2	B	86	GLN
2	B	90	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 monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	248/248 (100%)	0.06	10 (4%) 38 28	34, 47, 70, 79	12 (4%)
2	B	125/136 (91%)	0.10	7 (5%) 24 16	37, 53, 72, 89	10 (8%)
All	All	373/384 (97%)	0.07	17 (4%) 32 22	34, 49, 72, 89	22 (5%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	69	ALA	4.5
2	B	44	SER	4.3
1	A	545	SER	3.7
1	A	591	THR	3.6
1	A	590	GLY	3.4
2	B	70	MET	2.9
1	A	744	PRO	2.9
1	A	589	GLY	2.8
1	A	600	THR	2.7
2	B	147	LYS	2.6
2	B	43	THR	2.5
1	A	544	PRO	2.4
2	B	94	ASN	2.4
2	B	95	ASP	2.1
1	A	583	PHE	2.0
1	A	608	SER	2.0
1	A	599	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, 95<sup>th</sup> 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
3	CD	B	202	1/1	0.39	0.82	62,62,62,62	0
3	CD	A	106	1/1	0.94	0.11	68,68,68,68	1
3	CD	A	103	1/1	0.96	0.04	74,74,74,74	1
3	CD	A	105	1/1	0.96	0.06	74,74,74,74	1
3	CD	A	104	1/1	0.98	0.04	76,76,76,76	0
3	CD	B	201	1/1	1.00	0.07	49,49,49,49	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.