



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 1DDJ / pdb_00001ddj
Title : CRYSTAL STRUCTURE OF HUMAN PLASMINOGEN CATALYTIC DO-
MAIN
Authors : Wang, X.; Terzyan, S.; Tang, J.; Loy, J.; Lin, X.; Zhang, X.
Deposited on : 1999-11-10
Resolution : 2.00 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

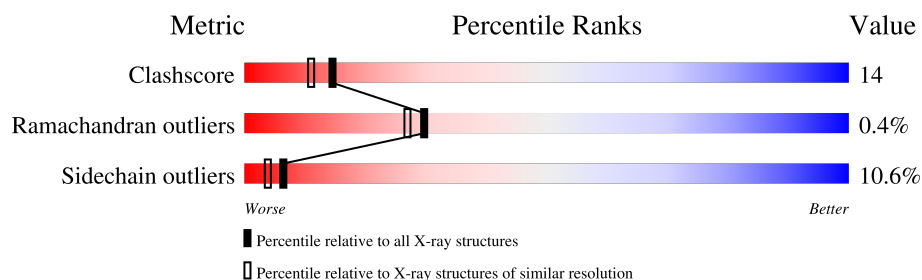
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	
1	C	247	
1	D	247	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8341 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	247	Total	C	N	O	S	0	0	0
			1900	1206	336	344	14			
1	B	247	Total	C	N	O	S	0	0	0
			1900	1206	336	344	14			
1	C	247	Total	C	N	O	S	0	0	0
			1900	1206	336	344	14			
1	D	247	Total	C	N	O	S	0	0	0
			1900	1206	336	344	14			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

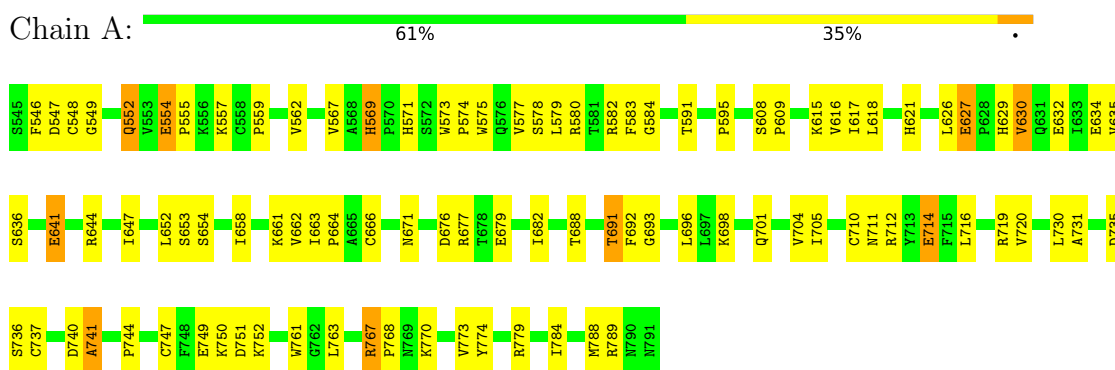
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	176	Total	O	0	0
			176	176		
2	B	218	Total	O	0	0
			218	218		
2	C	165	Total	O	0	0
			165	165		
2	D	182	Total	O	0	0
			182	182		

3 Residue-property plots

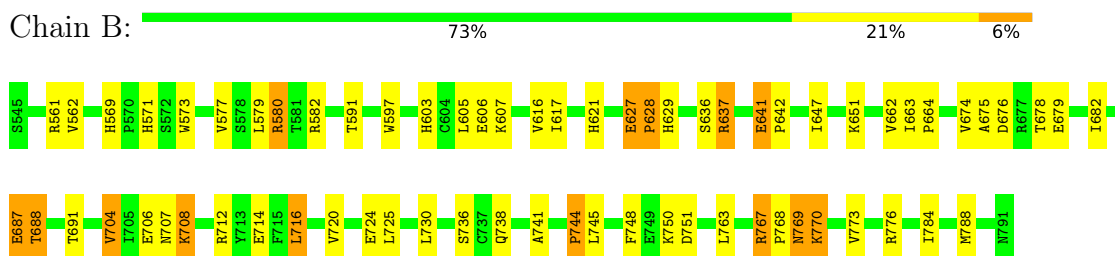
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

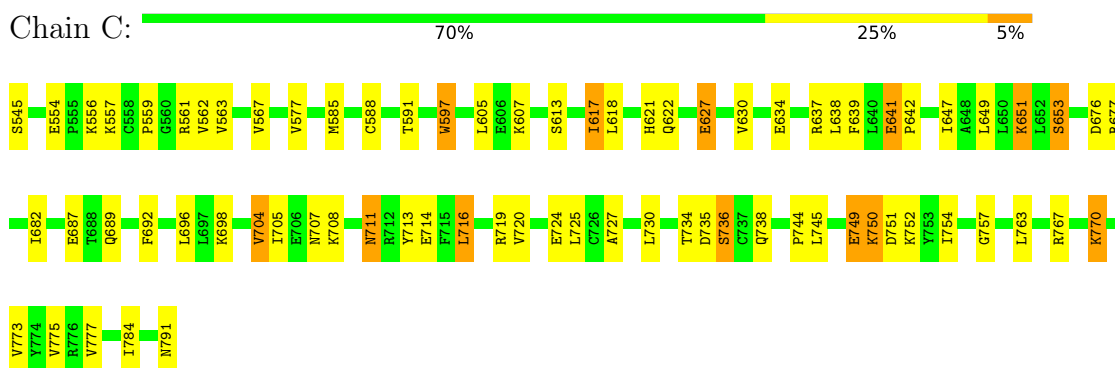
• Molecule 1: PLASMINOGEN



• Molecule 1: PLASMINOGEN

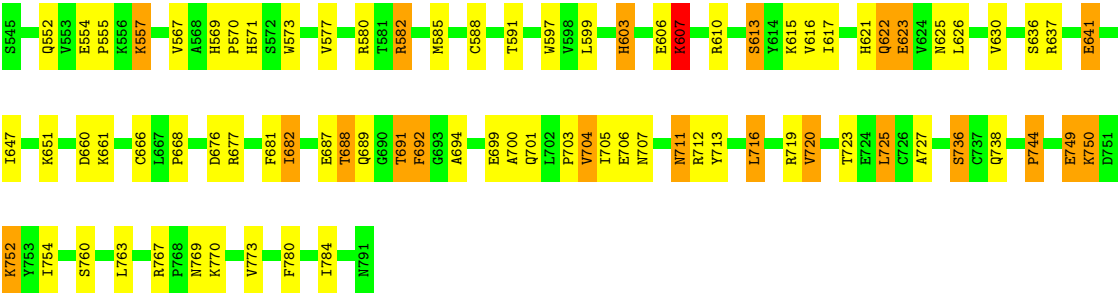


• Molecule 1: PLASMINOGEN



• Molecule 1: PLASMINOGEN

Chain D: 67% 24% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.49Å 46.16Å 126.65Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	82.1 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8341	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.44	0/1950	0.99	8/2650 (0.3%)
1	B	0.46	0/1950	1.00	14/2650 (0.5%)
1	C	0.44	0/1950	0.95	8/2650 (0.3%)
1	D	0.45	0/1950	0.96	11/2650 (0.4%)
All	All	0.45	0/7800	0.98	41/10600 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	HIS	N-CA-C	-9.15	104.19	114.62
1	A	573	TRP	CA-C-N	8.97	128.71	119.56
1	A	573	TRP	C-N-CA	8.97	128.71	119.56
1	B	569	HIS	N-CA-C	-8.65	98.75	109.65
1	D	641	GLU	CA-C-N	7.57	127.95	119.32
1	D	641	GLU	C-N-CA	7.57	127.95	119.32
1	B	738	GLN	N-CA-C	7.14	119.96	110.53
1	D	567	VAL	N-CA-C	-7.11	100.42	109.30
1	B	768	PRO	N-CA-C	-6.99	105.12	113.86
1	D	738	GLN	N-CA-C	6.77	119.26	110.53
1	B	641	GLU	CA-C-N	6.53	126.22	119.82
1	B	641	GLU	C-N-CA	6.53	126.22	119.82
1	C	713	TYR	N-CA-C	6.49	118.94	111.02
1	C	641	GLU	CA-C-N	6.41	126.09	119.56
1	C	641	GLU	C-N-CA	6.41	126.09	119.56
1	C	642	PRO	N-CA-C	6.41	122.17	113.84
1	B	621	HIS	N-CA-C	-6.29	104.82	113.18
1	D	623	GLU	N-CA-C	6.23	120.08	112.23
1	C	567	VAL	N-CA-C	-6.21	100.76	109.21
1	D	569	HIS	N-CA-C	-6.17	101.87	109.65
1	D	607	LYS	N-CA-C	6.08	118.70	111.71
1	B	642	PRO	N-CA-C	6.06	121.80	113.98
1	A	567	VAL	N-CA-C	-5.80	101.23	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	675	ALA	N-CA-C	5.69	117.88	110.43
1	B	745	LEU	N-CA-C	-5.68	97.90	108.02
1	B	741	ALA	N-CA-C	-5.62	102.71	110.35
1	C	736	SER	N-CA-C	5.55	118.12	109.52
1	C	777	VAL	N-CA-C	5.54	116.94	110.62
1	A	569	HIS	N-CA-C	-5.53	102.81	109.83
1	A	741	ALA	N-CA-C	-5.49	102.27	110.23
1	A	641	GLU	CA-C-N	5.45	125.11	119.56
1	A	641	GLU	C-N-CA	5.45	125.11	119.56
1	B	744	PRO	N-CA-C	5.38	119.75	111.57
1	D	736	SER	N-CA-C	5.32	117.16	108.76
1	D	573	TRP	CA-C-N	5.21	124.92	119.82
1	D	573	TRP	C-N-CA	5.21	124.92	119.82
1	B	573	TRP	CA-C-N	5.20	124.87	119.56
1	B	573	TRP	C-N-CA	5.20	124.87	119.56
1	C	597	TRP	N-CA-C	5.18	117.85	109.40
1	D	744	PRO	N-CA-C	5.03	119.21	111.57
1	B	682	ILE	N-CA-C	-5.02	101.25	108.53

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	1900	0	1876	73	0
1	B	1900	0	1876	42	0
1	C	1900	0	1876	44	0
1	D	1900	0	1876	57	0
2	A	176	0	0	7	0
2	B	218	0	0	2	0
2	C	165	0	0	4	0
2	D	182	0	0	2	0
All	All	8341	0	7504	211	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 14.

All (211) 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:B:627:GLU:HG3	1:B:628:PRO:HD2	1.42	0.99
1:D:580:ARG:HG3	1:D:617:ILE:HD13	1.46	0.95
1:C:711:ASN:HD21	1:C:720:VAL:H	1.16	0.93
1:A:627:GLU:HG3	1:A:629:HIS:CE1	2.09	0.87
1:B:580:ARG:HG3	1:B:617:ILE:HD13	1.57	0.85
1:A:711:ASN:HD21	1:A:720:VAL:H	1.23	0.83
1:D:711:ASN:HD21	1:D:720:VAL:H	1.28	0.82
1:A:627:GLU:HG3	1:A:629:HIS:HE1	1.47	0.79
1:D:711:ASN:ND2	1:D:720:VAL:HG13	1.96	0.79
1:B:627:GLU:CG	1:B:628:PRO:HD2	2.13	0.79
1:A:671:ASN:HD22	1:A:779:ARG:HD3	1.49	0.78
1:D:780:PHE:O	1:D:784:ILE:HG12	1.84	0.78
1:C:734:THR:HG22	1:C:736:SER:H	1.50	0.77
1:A:580:ARG:HG3	1:A:617:ILE:HD13	1.66	0.77
1:D:688:THR:O	1:D:694:ALA:HB1	1.83	0.77
1:B:577:VAL:HG13	1:B:616:VAL:HG13	1.67	0.76
1:A:546:PHE:HB2	1:A:658:ILE:HG21	1.70	0.73
1:B:603:HIS:HA	1:B:606:GLU:HG3	1.70	0.73
1:A:591:THR:OG1	1:A:744:PRO:HB3	1.90	0.72
1:C:677:ARG:HH11	1:C:677:ARG:HG2	1.55	0.71
1:D:622:GLN:HG2	1:D:625:ASN:O	1.92	0.70
1:D:707:ASN:HD21	1:D:725:LEU:HA	1.57	0.69
1:D:767:ARG:HB2	1:D:770:LYS:HB2	1.74	0.68
1:C:708:LYS:HG3	2:C:810:HOH:O	1.93	0.68
1:D:691:THR:HG22	1:D:692:PHE:H	1.60	0.67
1:A:627:GLU:HG2	1:A:630:VAL:HG23	1.76	0.67
1:A:671:ASN:HD22	1:A:779:ARG:HH11	1.44	0.65
1:D:603:HIS:O	1:D:606:GLU:HG2	1.97	0.65
1:C:749:GLU:HG2	2:C:900:HOH:O	1.97	0.64
1:C:577:VAL:HG22	1:C:618:LEU:CD2	2.28	0.63
1:D:676:ASP:HB2	1:D:706:GLU:HG3	1.81	0.63
1:A:696:LEU:O	1:A:698:LYS:HE3	1.97	0.63
1:A:677:ARG:HG2	1:A:677:ARG:HH11	1.64	0.62
1:B:767:ARG:HB2	1:B:770:LYS:H	1.64	0.62
1:A:789:ARG:HG2	1:A:789:ARG:O	1.98	0.62
1:C:725:LEU:HD12	1:C:725:LEU:C	2.24	0.62
1:C:734:THR:HG22	1:C:736:SER:N	2.14	0.61
1:C:677:ARG:HG2	1:C:677:ARG:NH1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:GLU:CD	1:A:701:GLN:HE21	2.09	0.61
1:C:641:GLU:HB2	1:C:647:ILE:HG23	1.82	0.60
1:D:597:TRP:CZ2	1:D:651:LYS:HD2	2.35	0.60
1:A:580:ARG:HB2	1:A:615:LYS:HG3	1.84	0.60
1:B:597:TRP:CZ2	1:B:651:LYS:HG3	2.36	0.60
1:D:603:HIS:O	1:D:606:GLU:CG	2.49	0.60
1:A:571:HIS:HD2	2:A:807:HOH:O	1.85	0.60
1:A:784:ILE:HG22	1:A:788:MET:HE2	1.83	0.60
1:C:627:GLU:HG2	1:C:630:VAL:HG23	1.83	0.59
1:D:599:LEU:HD13	1:D:784:ILE:HD12	1.85	0.59
1:A:629:HIS:NE2	1:A:661:LYS:HD3	2.17	0.59
1:A:714:GLU:HG3	1:B:730:LEU:HB2	1.83	0.59
1:D:711:ASN:HD21	1:D:720:VAL:HG13	1.66	0.58
1:A:559:PRO:HG2	1:A:562:VAL:CG2	2.33	0.58
1:B:580:ARG:CG	1:B:617:ILE:HD13	2.30	0.58
1:B:627:GLU:HG3	1:B:628:PRO:CD	2.26	0.58
1:C:556:LYS:O	1:C:557:LYS:HB2	2.04	0.57
1:C:770:LYS:HE2	2:C:815:HOH:O	2.03	0.57
1:A:677:ARG:HG2	2:A:929:HOH:O	2.04	0.57
1:A:617:ILE:CD1	1:A:632:GLU:HG2	2.35	0.56
1:A:747:CYS:HB2	2:A:874:HOH:O	2.04	0.56
1:D:725:LEU:C	1:D:725:LEU:HD12	2.31	0.55
1:C:724:GLU:HG2	1:C:763:LEU:HD13	1.89	0.55
1:A:719:ARG:HD2	2:A:897:HOH:O	2.07	0.54
1:A:779:ARG:HD2	2:A:935:HOH:O	2.07	0.54
1:D:705:ILE:O	1:D:706:GLU:C	2.51	0.54
1:D:591:THR:OG1	1:D:744:PRO:HB3	2.07	0.54
1:A:626:LEU:HD13	1:A:630:VAL:HG11	1.90	0.54
1:C:734:THR:HG22	1:C:735:ASP:N	2.23	0.53
1:A:671:ASN:ND2	1:A:779:ARG:HD3	2.22	0.53
1:A:559:PRO:HG2	1:A:562:VAL:HG23	1.91	0.53
1:B:687:GLU:O	1:B:688:THR:HB	2.09	0.53
1:B:688:THR:HG23	1:B:688:THR:O	2.08	0.53
1:B:577:VAL:CG1	1:B:616:VAL:HG13	2.36	0.53
1:B:716:LEU:HD21	1:B:773:VAL:HG21	1.92	0.52
1:D:580:ARG:NH2	1:D:626:LEU:HD21	2.25	0.52
1:B:607:LYS:HD3	1:B:607:LYS:H	1.74	0.52
1:A:641:GLU:HB2	1:A:647:ILE:HG23	1.92	0.52
1:C:707:ASN:HD21	1:C:725:LEU:HA	1.75	0.51
1:A:574:PRO:HG2	1:A:575:TRP:CE3	2.46	0.51
1:A:712:ARG:NH2	1:B:676:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:VAL:HG22	1:A:618:LEU:CD2	2.41	0.51
1:B:707:ASN:HD21	1:B:725:LEU:HA	1.75	0.51
1:D:570:PRO:HG3	1:D:621:HIS:CD2	2.45	0.51
1:A:682:ILE:HD12	1:A:774:TYR:CE2	2.45	0.51
1:B:636:SER:O	1:B:637:ARG:HG2	2.10	0.51
1:C:750:LYS:HG2	1:C:751:ASP:N	2.25	0.51
1:A:671:ASN:ND2	1:A:779:ARG:HH11	2.06	0.51
1:B:784:ILE:HG22	1:B:788:MET:HE2	1.92	0.50
1:D:725:LEU:HD12	1:D:725:LEU:O	2.11	0.50
1:D:641:GLU:HB2	1:D:647:ILE:HG22	1.93	0.50
1:C:676:ASP:OD2	1:D:712:ARG:NH2	2.44	0.50
1:D:713:TYR:CD2	1:D:713:TYR:C	2.89	0.50
1:C:597:TRP:CZ2	1:C:651:LYS:HG3	2.46	0.50
1:B:724:GLU:HG2	1:B:763:LEU:HD13	1.94	0.50
1:D:552:GLN:HG3	1:D:660:ASP:HB2	1.93	0.50
1:A:579:LEU:HD23	1:A:616:VAL:HG12	1.93	0.50
1:C:627:GLU:H	1:C:627:GLU:CD	2.18	0.49
1:B:788:MET:HE1	2:B:858:HOH:O	2.13	0.49
1:D:682:ILE:HG22	1:D:700:ALA:HB3	1.95	0.49
1:A:636:SER:HB3	1:A:653:SER:HA	1.95	0.49
1:D:719:ARG:HD2	2:D:947:HOH:O	2.11	0.49
1:A:577:VAL:HG12	1:A:578:SER:N	2.27	0.48
1:C:627:GLU:HG2	1:C:630:VAL:CG2	2.43	0.48
1:D:711:ASN:ND2	1:D:720:VAL:CG1	2.72	0.48
1:D:580:ARG:HH22	1:D:626:LEU:HD21	1.78	0.48
1:D:610:ARG:O	1:D:613:SER:HB2	2.13	0.48
1:D:767:ARG:HD2	1:D:770:LYS:HG3	1.95	0.48
1:B:603:HIS:HA	1:B:606:GLU:CG	2.42	0.48
1:D:704:VAL:HA	1:D:727:ALA:HA	1.96	0.48
1:A:546:PHE:HB2	1:A:658:ILE:CG2	2.41	0.48
1:B:607:LYS:HD3	1:B:607:LYS:N	2.28	0.48
1:B:676:ASP:CG	1:B:706:GLU:HG2	2.38	0.48
1:C:621:HIS:CD2	1:C:696:LEU:HD12	2.49	0.48
1:D:571:HIS:CG	1:D:661:LYS:HD3	2.49	0.48
1:C:637:ARG:HB3	1:C:639:PHE:CE1	2.49	0.48
1:D:763:LEU:HB3	1:D:773:VAL:HB	1.96	0.47
1:C:577:VAL:HG22	1:C:618:LEU:HD23	1.96	0.47
1:A:644:ARG:HB3	1:A:644:ARG:CZ	2.43	0.47
1:B:571:HIS:HD2	2:B:809:HOH:O	1.96	0.47
1:C:682:ILE:HB	1:C:745:LEU:HD23	1.96	0.47
1:A:677:ARG:HG2	1:A:677:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:LEU:O	1:C:698:LYS:HD3	2.13	0.47
1:A:617:ILE:HD11	1:A:632:GLU:HG2	1.97	0.46
1:A:693:GLY:HA2	1:A:696:LEU:HD12	1.96	0.46
1:D:749:GLU:HG3	1:D:754:ILE:HD11	1.97	0.46
1:C:705:ILE:HD13	1:C:730:LEU:HD21	1.97	0.46
1:C:682:ILE:HD13	1:C:738:GLN:HB2	1.96	0.46
1:D:666:CYS:SG	1:D:752:LYS:HD3	2.55	0.46
1:A:731:ALA:HB1	1:B:769:ASN:HD21	1.80	0.46
1:A:582:ARG:HG3	1:A:583:PHE:N	2.30	0.46
1:C:563:VAL:O	1:C:734:THR:OG1	2.34	0.46
1:C:591:THR:OG1	1:C:744:PRO:HB3	2.15	0.46
1:D:557:LYS:HG3	1:D:681:PHE:CZ	2.51	0.46
1:A:735:ASP:O	1:A:736:SER:HB3	2.16	0.46
1:A:737:CYS:HB3	1:A:761:TRP:CD1	2.50	0.45
1:D:571:HIS:HA	2:D:810:HOH:O	2.15	0.45
1:D:582:ARG:O	1:D:582:ARG:HG3	2.15	0.45
1:A:584:GLY:HA2	1:A:615:LYS:CE	2.46	0.45
1:D:711:ASN:HD21	1:D:720:VAL:CG1	2.29	0.45
1:A:749:GLU:HB3	2:A:910:HOH:O	2.16	0.45
1:D:571:HIS:ND1	1:D:661:LYS:HD3	2.31	0.45
1:C:719:ARG:HD2	2:C:897:HOH:O	2.16	0.45
1:D:580:ARG:CG	1:D:617:ILE:HD13	2.32	0.45
1:D:681:PHE:CE2	1:D:701:GLN:HB2	2.51	0.45
1:A:682:ILE:HD12	1:A:774:TYR:HE2	1.81	0.45
1:B:662:VAL:C	1:B:663:ILE:HG13	2.41	0.45
1:A:562:VAL:O	1:A:562:VAL:HG12	2.17	0.45
1:C:696:LEU:HD22	1:C:696:LEU:N	2.31	0.44
1:D:554:GLU:OE1	1:D:555:PRO:HD2	2.17	0.44
1:A:627:GLU:CD	1:A:627:GLU:H	2.24	0.44
1:B:580:ARG:CD	1:B:617:ILE:HD13	2.47	0.44
1:C:559:PRO:HD2	1:C:562:VAL:HG21	1.99	0.44
1:C:634:GLU:O	1:C:653:SER:HB3	2.17	0.44
1:D:703:PRO:O	1:D:727:ALA:HA	2.16	0.44
1:A:634:GLU:HG3	1:A:635:VAL:N	2.31	0.44
1:B:636:SER:C	1:B:637:ARG:HG2	2.42	0.44
1:B:688:THR:O	1:B:688:THR:CG2	2.66	0.44
1:B:641:GLU:HB2	1:B:647:ILE:HG23	2.00	0.44
1:A:580:ARG:NH2	2:A:841:HOH:O	2.50	0.44
1:B:716:LEU:CD2	1:B:773:VAL:HG21	2.48	0.44
1:A:552:GLN:OE1	1:A:552:GLN:HA	2.17	0.44
1:A:577:VAL:CG1	1:A:578:SER:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:749:GLU:HG3	1:D:754:ILE:CD1	2.48	0.43
1:D:636:SER:C	1:D:637:ARG:HG2	2.44	0.43
1:D:716:LEU:HD11	1:D:773:VAL:HG21	1.99	0.43
1:C:649:LEU:HD11	1:C:784:ILE:HG23	2.00	0.43
1:D:622:GLN:HG2	1:D:625:ASN:C	2.44	0.43
1:A:579:LEU:HD23	1:A:579:LEU:HA	1.77	0.43
1:B:591:THR:OG1	1:B:744:PRO:HB3	2.19	0.43
1:A:705:ILE:HD13	1:A:730:LEU:HD21	2.00	0.43
1:D:676:ASP:O	1:D:677:ARG:HB2	2.18	0.43
1:C:716:LEU:CD2	1:C:773:VAL:HG21	2.49	0.43
1:A:608:SER:HA	1:A:609:PRO:HD3	1.83	0.43
1:B:725:LEU:HD22	1:B:776:ARG:HA	2.00	0.43
1:A:663:ILE:HA	1:A:664:PRO:HD3	1.88	0.43
1:A:751:ASP:OD2	1:A:751:ASP:N	2.52	0.42
1:A:662:VAL:C	1:A:663:ILE:HG13	2.44	0.42
1:D:668:PRO:HB3	1:D:754:ILE:HG21	2.02	0.42
1:D:750:LYS:HD3	1:D:750:LYS:HA	1.78	0.42
1:A:584:GLY:HA2	1:A:615:LYS:HE3	2.00	0.42
1:A:763:LEU:HB3	1:A:773:VAL:HB	2.01	0.42
1:C:705:ILE:HD13	1:C:730:LEU:CD2	2.50	0.42
1:C:757:GLY:HA2	1:C:775:VAL:O	2.20	0.42
1:B:597:TRP:CE2	1:B:651:LYS:HG3	2.54	0.42
1:D:676:ASP:CB	1:D:706:GLU:HG3	2.49	0.42
1:C:676:ASP:O	1:C:677:ARG:HB2	2.18	0.42
1:D:760:SER:HB3	1:D:763:LEU:HD12	2.02	0.42
1:C:559:PRO:HB2	1:C:562:VAL:HG23	2.02	0.41
1:D:577:VAL:HG13	1:D:616:VAL:HG13	2.01	0.41
1:B:663:ILE:HA	1:B:664:PRO:HD3	1.97	0.41
1:A:559:PRO:HG2	1:A:562:VAL:HG21	2.01	0.41
1:A:554:GLU:HA	1:A:555:PRO:HD3	1.85	0.41
1:B:716:LEU:HD22	1:B:720:VAL:CG2	2.50	0.41
1:C:704:VAL:HA	1:C:727:ALA:HA	2.03	0.41
1:B:748:PHE:CZ	1:B:751:ASP:HA	2.55	0.41
1:A:595:PRO:O	1:A:652:LEU:HD12	2.20	0.41
1:A:710:CYS:O	1:A:716:LEU:HB2	2.21	0.41
1:C:605:LEU:HD13	1:C:638:LEU:HD22	2.01	0.41
1:B:561:ARG:HG3	1:B:562:VAL:N	2.36	0.41
1:B:678:THR:HB	1:B:704:VAL:HG13	2.03	0.41
1:C:617:ILE:HG23	1:C:630:VAL:CG1	2.51	0.41
1:D:725:LEU:C	1:D:725:LEU:CD1	2.94	0.41
1:A:666:CYS:SG	1:A:752:LYS:HD2	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:GLY:HA2	1:A:575:TRP:CZ3	2.56	0.40
1:A:548:CYS:C	1:A:666:CYS:SG	3.04	0.40
1:A:676:ASP:OD1	1:B:712:ARG:NH2	2.54	0.40
1:A:767:ARG:O	1:A:768:PRO:C	2.65	0.40
1:B:708:LYS:HB3	1:B:708:LYS:HE2	1.82	0.40
1:D:607:LYS:HB2	1:D:607:LYS:HE3	1.72	0.40
1:A:554:GLU:O	1:A:569:HIS:HD2	2.04	0.40
1:A:740:ASP:O	1:A:741:ALA:C	2.63	0.40
1:C:651:LYS:CE	1:C:791:ASN:OXT	2.69	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	245/247 (99%)	232 (95%)	12 (5%)	1 (0%)	30	27
1	B	245/247 (99%)	228 (93%)	14 (6%)	3 (1%)	10	6
1	C	245/247 (99%)	227 (93%)	18 (7%)	0	100	100
1	D	245/247 (99%)	227 (93%)	18 (7%)	0	100	100
All	All	980/988 (99%)	914 (93%)	62 (6%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	691	THR
1	B	688	THR
1	B	629	HIS
1	B	628	PRO

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	208/208 (100%)	193 (93%)	15 (7%)	13	10
1	B	208/208 (100%)	189 (91%)	19 (9%)	9	6
1	C	208/208 (100%)	183 (88%)	25 (12%)	5	3
1	D	208/208 (100%)	179 (86%)	29 (14%)	3	2
All	All	832/832 (100%)	744 (89%)	88 (11%)	6	4

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	ASP
1	A	552	GLN
1	A	554	GLU
1	A	557	LYS
1	A	627	GLU
1	A	630	VAL
1	A	654	SER
1	A	688	THR
1	A	691	THR
1	A	692	PHE
1	A	704	VAL
1	A	714	GLU
1	A	750	LYS
1	A	767	ARG
1	A	770	LYS
1	B	579	LEU
1	B	580	ARG
1	B	582	ARG
1	B	605	LEU
1	B	627	GLU
1	B	637	ARG
1	B	674	VAL
1	B	679	GLU
1	B	687	GLU

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Mol	Chain	Res	Type
1	B	691	THR
1	B	704	VAL
1	B	708	LYS
1	B	714	GLU
1	B	716	LEU
1	B	736	SER
1	B	750	LYS
1	B	767	ARG
1	B	769	ASN
1	B	770	LYS
1	C	545	SER
1	C	554	GLU
1	C	561	ARG
1	C	585	MET
1	C	588	CYS
1	C	607	LYS
1	C	613	SER
1	C	617	ILE
1	C	622	GLN
1	C	627	GLU
1	C	651	LYS
1	C	653	SER
1	C	687	GLU
1	C	689	GLN
1	C	692	PHE
1	C	704	VAL
1	C	711	ASN
1	C	714	GLU
1	C	716	LEU
1	C	749	GLU
1	C	750	LYS
1	C	752	LYS
1	C	754	ILE
1	C	767	ARG
1	C	770	LYS
1	D	557	LYS
1	D	582	ARG
1	D	585	MET
1	D	588	CYS
1	D	603	HIS
1	D	607	LYS
1	D	613	SER

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Mol	Chain	Res	Type
1	D	615	LYS
1	D	622	GLN
1	D	623	GLU
1	D	630	VAL
1	D	682	ILE
1	D	687	GLU
1	D	688	THR
1	D	689	GLN
1	D	691	THR
1	D	692	PHE
1	D	699	GLU
1	D	704	VAL
1	D	711	ASN
1	D	716	LEU
1	D	720	VAL
1	D	723	THR
1	D	725	LEU
1	D	736	SER
1	D	749	GLU
1	D	750	LYS
1	D	752	LYS
1	D	769	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	HIS
1	A	571	HIS
1	A	622	GLN
1	A	671	ASN
1	A	701	GLN
1	A	707	ASN
1	A	711	ASN
1	A	721	GLN
1	A	791	ASN
1	B	552	GLN
1	B	707	ASN
1	B	717	ASN
1	B	738	GLN
1	B	769	ASN
1	C	571	HIS
1	C	671	ASN

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Mol	Chain	Res	Type
1	C	707	ASN
1	C	711	ASN
1	C	721	GLN
1	C	729	HIS
1	C	756	GLN
1	C	790	ASN
1	D	552	GLN
1	D	569	HIS
1	D	571	HIS
1	D	576	GLN
1	D	707	ASN
1	D	711	ASN
1	D	717	ASN
1	D	721	GLN
1	D	756	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](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.