



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:49 AM GMT

PDB ID : 1QRZ
Title : CATALYTIC DOMAIN OF PLASMINOGEN
Authors : Peisach, E.; Wang, J.; de los Santos, T.; Reich, E.; Ringe, D.
Deposited on : 1999-06-16
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

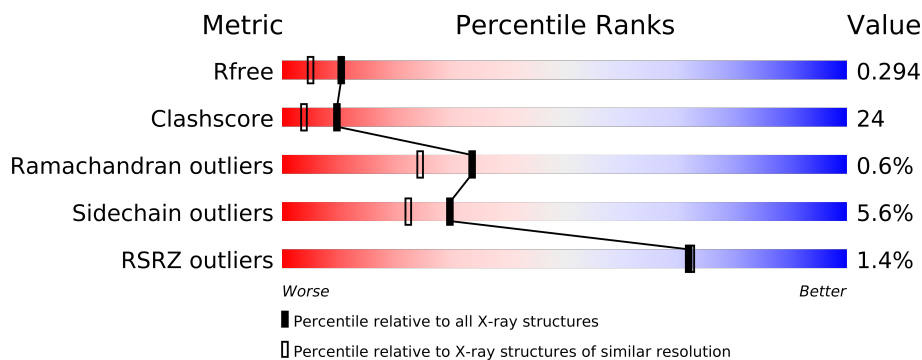
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	246	
1	B	246	
1	C	246	
1	D	246	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8097 atoms, of which 0 are hydrogen and 0 are deuterium.

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	246	Total	C	N	O	S	0	0	0
			1897	1204	336	344	13			
1	B	246	Total	C	N	O	S	0	0	0
			1897	1204	336	344	13			
1	C	246	Total	C	N	O	S	0	0	0
			1897	1204	336	344	13			
1	D	246	Total	C	N	O	S	0	0	0
			1897	1204	336	344	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	585	GLN	MET	ENGINEERED	UNP P00747
A	673	MET	VAL	ENGINEERED	UNP P00747
A	788	LEU	MET	ENGINEERED	UNP P00747
B	585	GLN	MET	ENGINEERED	UNP P00747
B	673	MET	VAL	ENGINEERED	UNP P00747
B	788	LEU	MET	ENGINEERED	UNP P00747
C	585	GLN	MET	ENGINEERED	UNP P00747
C	673	MET	VAL	ENGINEERED	UNP P00747
C	788	LEU	MET	ENGINEERED	UNP P00747
D	585	GLN	MET	ENGINEERED	UNP P00747
D	673	MET	VAL	ENGINEERED	UNP P00747
D	788	LEU	MET	ENGINEERED	UNP P00747

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	119	Total	O	0	0
			119	119		
2	B	134	Total	O	0	0
			134	134		

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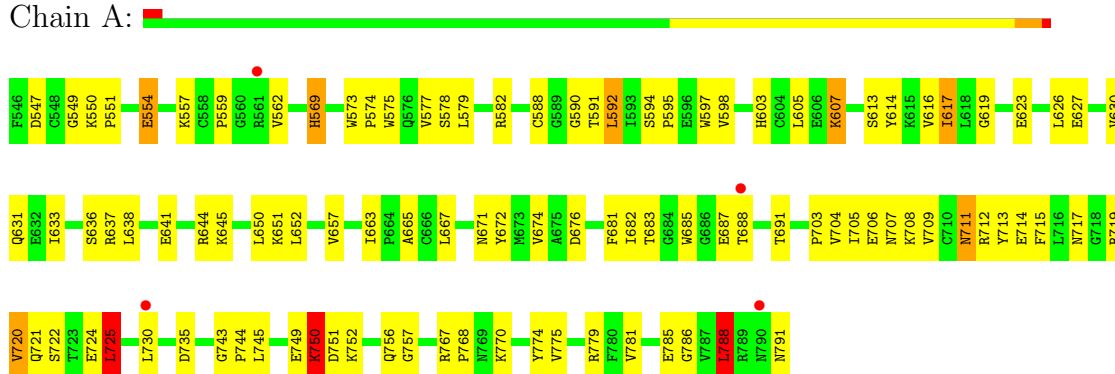
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	164	Total 164	O 164	0	0
2	D	92	Total 92	O 92	0	0

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.

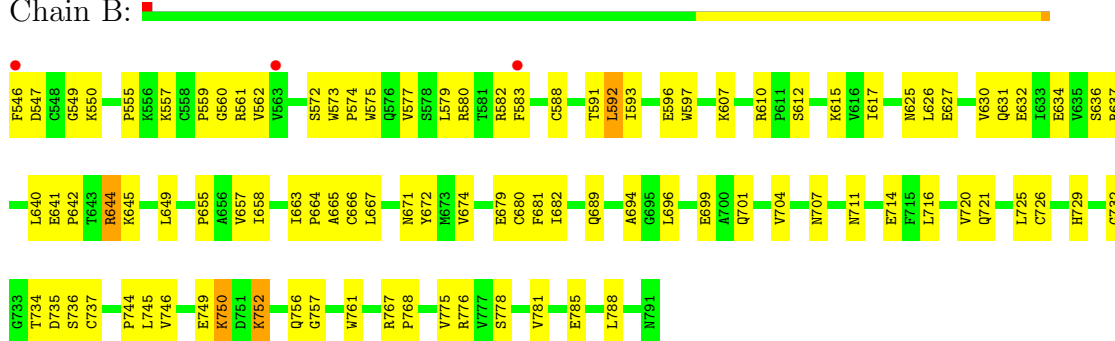
• Molecule 1: PLASMINOGEN

Chain A:



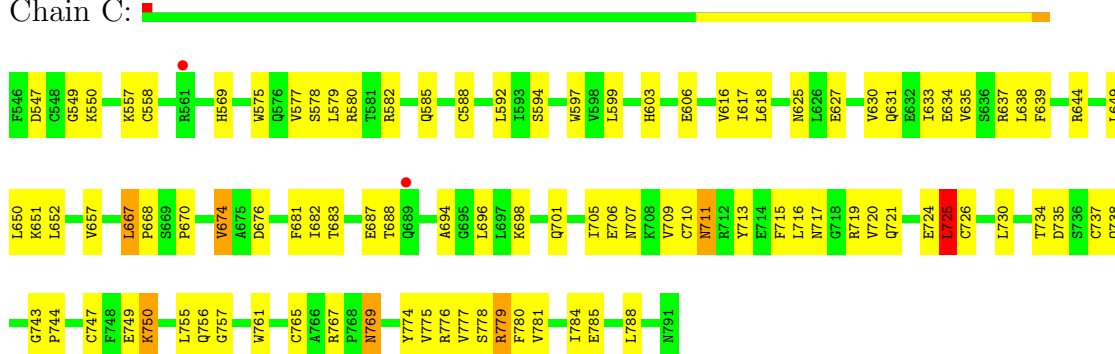
• Molecule 1: PLASMINOGEN

Chain B:



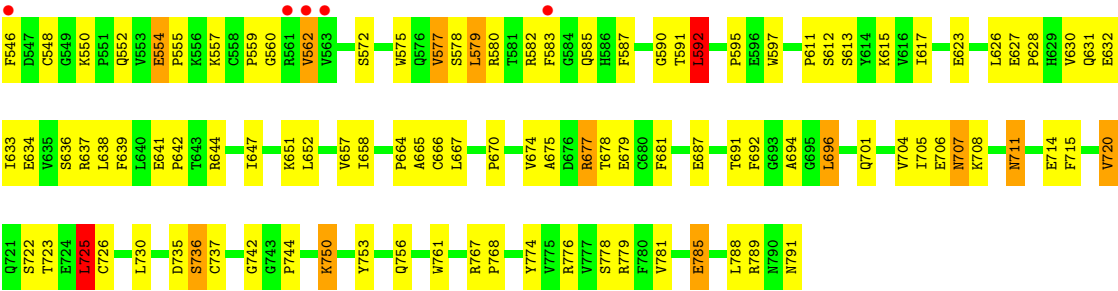
• Molecule 1: PLASMINOGEN

Chain C:



● Molecule 1: PLASMINOGEN

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.66Å 73.58Å 81.36Å 90.00° 108.73° 90.00°	Depositor
Resolution (Å)	35.00 – 2.00 77.33 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.1 (35.00-2.00) 91.6 (77.33-1.97)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 1.97Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.235 , 0.294 0.234 , 0.294	Depositor DCC
R_{free} test set	2869 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 11.0	EDS
Estimated twinning fraction	0.368 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	9 of 63208 reflections (0.014%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8097	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3156e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.70	0/1947	0.87	4/2646 (0.2%)
1	B	0.70	0/1947	0.88	1/2646 (0.0%)
1	C	0.71	0/1947	0.86	1/2646 (0.0%)
1	D	0.69	0/1947	0.88	2/2646 (0.1%)
All	All	0.70	0/7788	0.87	8/10584 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	725	LEU	CA-CB-CG	6.39	130.00	115.30
1	D	592	LEU	CA-CB-CG	6.04	129.18	115.30
1	A	788	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	569	HIS	N-CA-C	-5.32	96.63	111.00
1	B	745	LEU	N-CA-C	-5.21	96.92	111.00
1	D	725	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	725	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	745	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1897	0	1872	97	0
1	B	1897	0	1872	79	0
1	C	1897	0	1872	100	0
1	D	1897	0	1872	97	0
2	A	119	0	0	10	0
2	B	134	0	0	9	0
2	C	164	0	0	13	0
2	D	92	0	0	11	0
All	All	8097	0	7488	366	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (366) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:779:ARG:HH11	1:C:779:ARG:HB3	1.06	1.11
1:D:617:ILE:HD12	1:D:632:GLU:HG2	1.32	1.11
1:A:631:GLN:HE22	1:A:657:VAL:H	1.02	0.97
1:C:779:ARG:NH1	1:C:779:ARG:HB3	1.79	0.95
1:C:631:GLN:HE22	1:C:657:VAL:H	1.01	0.95
1:A:644:ARG:HH22	1:A:721:GLN:HG3	1.28	0.95
1:D:631:GLN:HE22	1:D:657:VAL:H	1.12	0.94
1:C:769:ASN:H	1:C:769:ASN:HD22	1.17	0.90
1:C:644:ARG:HH22	1:C:721:GLN:HG3	1.35	0.88
1:A:578:SER:HB3	1:A:617:ILE:HG12	1.53	0.88
1:A:705:ILE:HG21	1:A:730:LEU:HD21	1.58	0.86
1:A:644:ARG:NH2	1:A:721:GLN:HG3	1.93	0.83
1:B:631:GLN:HE22	1:B:657:VAL:H	1.27	0.83
1:D:617:ILE:CD1	1:D:632:GLU:HG2	2.10	0.82
1:B:644:ARG:HB3	1:B:644:ARG:NH1	1.96	0.81
1:A:631:GLN:NE2	1:A:657:VAL:H	1.76	0.81
1:B:582:ARG:HD3	1:B:612:SER:O	1.82	0.80
1:D:679:GLU:HB3	1:D:701:GLN:HE21	1.44	0.80
1:A:577:VAL:HG12	1:A:590:GLY:C	2.04	0.78
1:D:677:ARG:HB2	1:D:677:ARG:HH11	1.49	0.78
1:C:577:VAL:HG22	1:C:618:LEU:HD21	1.67	0.77
1:A:597:TRP:CZ2	1:A:651:LYS:HD2	2.19	0.77
1:B:644:ARG:HB3	1:B:644:ARG:HH11	1.46	0.76
1:C:706:GLU:HG2	2:C:330:HOH:O	1.83	0.76
1:A:671:ASN:HD22	1:A:779:ARG:HD2	1.50	0.76
1:C:631:GLN:NE2	1:C:657:VAL:H	1.80	0.75
1:A:626:LEU:HB3	1:A:630:VAL:HG21	1.67	0.75
1:D:694:ALA:HA	2:D:143:HOH:O	1.85	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:577:VAL:HG22	1:C:618:LEU:CD2	2.17	0.74
1:B:689:GLN:HA	1:B:689:GLN:OE1	1.87	0.74
1:D:779:ARG:HB3	1:D:779:ARG:NH1	2.02	0.74
1:A:671:ASN:ND2	1:A:779:ARG:HD2	2.02	0.74
1:A:786:GLY:HA3	2:A:27:HOH:O	1.88	0.74
1:A:631:GLN:HE22	1:A:657:VAL:N	1.81	0.73
1:C:577:VAL:HG13	1:C:616:VAL:HG13	1.71	0.73
1:C:769:ASN:N	1:C:769:ASN:HD22	1.85	0.72
1:B:547:ASP:HB2	1:B:550:LYS:HD3	1.70	0.72
1:A:597:TRP:CD1	1:A:788:LEU:HD13	2.25	0.72
1:C:711:ASN:HD21	1:C:720:VAL:H	1.37	0.71
1:C:749:GLU:HG2	1:C:750:LYS:HD3	1.71	0.70
1:B:767:ARG:HB3	1:B:768:PRO:HD2	1.73	0.70
1:B:591:THR:OG1	1:B:744:PRO:HB3	1.91	0.70
1:B:734:THR:HG22	1:B:736:SER:H	1.56	0.69
1:C:603:HIS:O	1:C:606:GLU:HG3	1.93	0.69
1:A:715:PHE:CE1	1:A:730:LEU:HD13	2.28	0.69
1:D:778:SER:O	1:D:781:VAL:HG12	1.92	0.69
1:C:631:GLN:HE22	1:C:657:VAL:N	1.83	0.68
1:B:597:TRP:CD2	1:B:788:LEU:HD22	2.29	0.67
1:D:781:VAL:O	1:D:785:GLU:HG2	1.95	0.67
1:D:674:VAL:HG23	2:D:285:HOH:O	1.94	0.66
1:B:636:SER:O	1:B:637:ARG:HD3	1.94	0.66
1:D:582:ARG:HD3	1:D:613:SER:HA	1.78	0.66
1:A:750:LYS:HG3	1:C:761:TRP:CE3	2.32	0.65
1:B:734:THR:HG22	1:B:736:SER:N	2.12	0.64
1:A:705:ILE:HG22	1:A:709:VAL:HG13	1.80	0.64
1:A:781:VAL:O	1:A:785:GLU:HG2	1.96	0.64
1:B:785:GLU:HG3	2:B:458:HOH:O	1.97	0.64
1:D:559:PRO:HD2	1:D:562:VAL:HG21	1.79	0.64
1:C:725:LEU:HD23	1:C:725:LEU:C	2.19	0.64
1:D:559:PRO:HB2	1:D:562:VAL:HG23	1.79	0.63
1:D:575:TRP:CG	1:D:665:ALA:HB2	2.33	0.63
1:D:705:ILE:HD12	1:D:730:LEU:HD13	1.80	0.63
1:D:631:GLN:NE2	1:D:657:VAL:H	1.91	0.63
1:D:711:ASN:HD21	1:D:720:VAL:H	1.44	0.63
1:A:641:GLU:O	1:A:645:LYS:HA	1.99	0.63
1:C:580:ARG:HD2	1:C:617:ILE:CG1	2.29	0.63
1:B:680:CYS:HB3	1:B:746:VAL:O	1.98	0.63
1:D:595:PRO:HG3	1:D:658:ILE:HD11	1.81	0.63
1:B:597:TRP:CG	1:B:788:LEU:HD22	2.33	0.62
1:C:597:TRP:CD2	1:C:788:LEU:HD22	2.35	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:750:LYS:NZ	1:C:687:GLU:CD	2.54	0.61
1:A:595:PRO:HG2	2:A:150:HOH:O	2.00	0.61
1:B:711:ASN:HD21	1:B:720:VAL:H	1.48	0.61
1:A:743:GLY:HA3	2:A:4:HOH:O	2.00	0.61
1:A:547:ASP:HB2	1:A:550:LYS:HD3	1.81	0.61
1:D:644:ARG:HH11	1:D:723:THR:HG1	1.49	0.61
1:D:725:LEU:HB2	1:D:776:ARG:NH2	2.16	0.61
1:B:711:ASN:HD21	1:B:720:VAL:N	1.98	0.61
1:B:701:GLN:NE2	2:B:495:HOH:O	2.34	0.61
1:A:715:PHE:CZ	1:A:730:LEU:HD13	2.36	0.60
1:D:725:LEU:C	1:D:725:LEU:HD23	2.22	0.60
1:A:708:LYS:HE3	2:B:439:HOH:O	2.02	0.60
1:D:633:ILE:HG21	1:D:652:LEU:HB3	1.84	0.60
1:B:679:GLU:HG3	2:B:311:HOH:O	2.01	0.60
1:A:633:ILE:HG21	1:A:652:LEU:HB3	1.83	0.59
1:C:676:ASP:HB2	1:C:706:GLU:HB2	1.84	0.59
1:A:711:ASN:HD21	1:A:720:VAL:H	1.48	0.59
1:D:677:ARG:HB2	1:D:677:ARG:NH1	2.14	0.59
1:D:651:LYS:HE3	1:D:791:ASN:O	2.02	0.59
1:B:674:VAL:HG23	2:B:64:HOH:O	2.02	0.59
1:D:779:ARG:HB3	1:D:779:ARG:HH11	1.67	0.59
1:B:560:GLY:HA2	1:B:701:GLN:HB3	1.85	0.59
1:C:557:LYS:HG2	1:C:681:PHE:CZ	2.38	0.59
1:A:591:THR:OG1	1:A:744:PRO:HB3	2.03	0.58
1:D:591:THR:OG1	1:D:744:PRO:HB3	2.04	0.58
1:D:687:GLU:HA	2:D:152:HOH:O	2.01	0.58
1:A:713:TYR:HA	1:A:717:ASN:HA	1.84	0.58
1:A:674:VAL:HG11	1:A:704:VAL:HG21	1.84	0.58
1:D:679:GLU:CB	1:D:701:GLN:HE21	2.17	0.58
1:B:615:LYS:NZ	1:B:634:GLU:OE1	2.23	0.58
1:A:603:HIS:ND1	2:A:9:HOH:O	2.33	0.57
1:C:580:ARG:HD2	1:C:617:ILE:HG13	1.85	0.57
1:B:626:LEU:HB3	1:B:630:VAL:HG21	1.86	0.57
1:D:767:ARG:HG2	1:D:767:ARG:HH11	1.69	0.57
1:D:636:SER:O	1:D:637:ARG:HD2	2.05	0.57
1:B:666:CYS:SG	1:B:752:LYS:HD3	2.45	0.57
1:C:633:ILE:HG21	1:C:652:LEU:HB3	1.86	0.57
1:B:707:ASN:HD21	1:B:725:LEU:HA	1.69	0.57
1:D:597:TRP:CD2	1:D:788:LEU:HD22	2.40	0.57
1:D:725:LEU:HB2	1:D:776:ARG:HH21	1.70	0.56
1:C:707:ASN:ND2	2:C:46:HOH:O	2.37	0.56
1:D:735:ASP:HB2	1:D:768:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:725:LEU:C	1:A:725:LEU:HD23	2.25	0.56
1:C:644:ARG:HH22	1:C:721:GLN:CG	2.14	0.56
1:B:734:THR:HG22	1:B:735:ASP:N	2.19	0.56
1:A:592:LEU:HD22	1:A:594:SER:O	2.05	0.56
1:A:651:LYS:NZ	1:A:791:ASN:O	2.39	0.56
1:A:577:VAL:HG12	1:A:590:GLY:O	2.06	0.56
1:D:597:TRP:CG	1:D:788:LEU:HD22	2.41	0.56
1:B:781:VAL:O	1:B:785:GLU:HG2	2.05	0.56
1:C:711:ASN:HD21	1:C:720:VAL:N	2.04	0.56
1:D:776:ARG:HG2	1:D:779:ARG:HG2	1.88	0.56
1:A:749:GLU:HG3	1:A:750:LYS:HD3	1.88	0.55
1:C:582:ARG:HG3	1:C:582:ARG:HH11	1.72	0.55
1:D:705:ILE:CD1	1:D:730:LEU:HD13	2.36	0.55
1:A:706:GLU:O	1:A:709:VAL:HG12	2.07	0.55
1:A:577:VAL:HG11	1:A:598:VAL:HG11	1.89	0.55
1:C:711:ASN:ND2	1:C:720:VAL:HG22	2.21	0.55
1:B:720:VAL:HG21	1:B:726:CYS:SG	2.47	0.55
1:A:617:ILE:CD1	1:A:626:LEU:HD21	2.37	0.55
1:C:769:ASN:ND2	1:C:769:ASN:H	1.96	0.54
1:C:721:GLN:N	1:C:724:GLU:OE1	2.32	0.54
1:B:679:GLU:HB3	1:B:701:GLN:HE21	1.72	0.54
1:A:707:ASN:ND2	2:A:21:HOH:O	2.40	0.54
1:C:682:ILE:HD13	1:C:738:GLN:HB2	1.89	0.54
1:D:711:ASN:HD21	1:D:720:VAL:N	2.05	0.54
1:C:582:ARG:NH1	1:C:582:ARG:HG3	2.22	0.54
1:B:559:PRO:O	1:B:562:VAL:HG23	2.08	0.53
1:A:582:ARG:HH11	1:A:613:SER:HA	1.73	0.53
1:C:707:ASN:HD21	1:C:725:LEU:HA	1.72	0.53
1:C:638:LEU:CD2	1:C:650:LEU:HD22	2.38	0.53
1:A:577:VAL:HG11	1:A:598:VAL:CG1	2.39	0.53
1:B:776:ARG:NH2	2:B:485:HOH:O	2.30	0.53
1:C:747:CYS:HB2	2:C:167:HOH:O	2.07	0.53
1:C:683:THR:OG1	1:C:744:PRO:HG2	2.09	0.53
1:C:696:LEU:N	1:C:696:LEU:HD22	2.24	0.53
1:C:579:LEU:HD11	1:C:650:LEU:HD11	1.90	0.53
1:C:776:ARG:HD2	1:C:779:ARG:HG3	1.91	0.52
1:C:725:LEU:HD22	1:C:774:TYR:HB2	1.91	0.52
1:C:755:LEU:HG	1:C:777:VAL:HG21	1.92	0.52
1:C:637:ARG:HB3	1:C:639:PHE:CE1	2.44	0.52
1:A:579:LEU:HD21	1:A:650:LEU:CD1	2.39	0.52
1:D:789:ARG:CB	1:D:789:ARG:HH11	2.21	0.52
1:D:706:GLU:HG2	2:D:192:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:580:ARG:HD2	1:C:617:ILE:HG12	1.91	0.52
1:A:767:ARG:HB2	1:A:770:LYS:HB2	1.92	0.52
1:B:725:LEU:HB3	1:B:776:ARG:CZ	2.40	0.52
1:C:547:ASP:HB2	1:C:550:LYS:HD3	1.91	0.52
1:C:705:ILE:HG21	1:C:730:LEU:HD21	1.90	0.52
1:D:615:LYS:NZ	1:D:634:GLU:OE1	2.38	0.51
1:D:557:LYS:HE3	1:D:753:TYR:OH	2.10	0.51
1:A:636:SER:O	1:A:637:ARG:HD3	2.10	0.51
1:B:583:PHE:HB2	2:B:396:HOH:O	2.10	0.51
1:D:706:GLU:CG	2:D:192:HOH:O	2.57	0.51
1:B:575:TRP:CG	1:B:665:ALA:HB2	2.45	0.51
1:B:674:VAL:HG11	1:B:704:VAL:HG21	1.92	0.51
1:B:593:ILE:HB	1:B:667:LEU:HD11	1.92	0.51
1:A:577:VAL:CG1	1:A:590:GLY:CA	2.88	0.51
1:A:676:ASP:HB2	1:A:706:GLU:HB2	1.93	0.51
1:B:555:PRO:HA	1:B:572:SER:HB2	1.93	0.51
1:B:627:GLU:O	1:B:630:VAL:HG22	2.10	0.51
1:A:617:ILE:HD12	1:A:626:LEU:CD2	2.41	0.50
1:D:674:VAL:HG11	1:D:704:VAL:HG21	1.92	0.50
1:C:578:SER:HB3	1:C:617:ILE:HB	1.94	0.50
1:C:558:CYS:O	1:C:701:GLN:HB2	2.10	0.50
1:D:583:PHE:N	1:D:583:PHE:CD1	2.79	0.50
1:C:674:VAL:HG22	2:C:95:HOH:O	2.10	0.50
1:D:582:ARG:HG3	1:D:582:ARG:HH11	1.77	0.50
1:A:711:ASN:ND2	1:A:720:VAL:HG13	2.27	0.50
1:B:559:PRO:HD2	1:B:562:VAL:HG21	1.93	0.50
1:C:577:VAL:CG1	1:C:616:VAL:HG13	2.40	0.50
1:C:711:ASN:CG	1:C:720:VAL:HG22	2.32	0.50
1:C:709:VAL:HG21	2:C:441:HOH:O	2.11	0.50
1:D:789:ARG:HB2	1:D:789:ARG:HH11	1.76	0.50
1:B:550:LYS:HB3	2:B:429:HOH:O	2.12	0.49
1:C:737:CYS:HB3	1:C:761:TRP:CD1	2.46	0.49
1:A:575:TRP:CG	1:A:665:ALA:HB2	2.47	0.49
1:D:776:ARG:NH2	2:D:366:HOH:O	2.45	0.49
1:C:696:LEU:O	1:C:698:LYS:HG3	2.13	0.49
1:C:670:PRO:HA	1:C:781:VAL:CG2	2.43	0.49
1:D:674:VAL:HG21	1:D:756:GLN:HB3	1.94	0.49
1:B:644:ARG:CB	1:B:644:ARG:HH11	2.20	0.49
1:D:557:LYS:HA	1:D:681:PHE:CE2	2.47	0.49
1:B:756:GLN:HA	1:B:756:GLN:HE21	1.78	0.49
1:D:785:GLU:O	1:D:789:ARG:HG3	2.13	0.48
1:C:557:LYS:HA	1:C:681:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:779:ARG:NH1	1:C:779:ARG:CB	2.65	0.48
1:B:546:PHE:CD1	1:B:658:ILE:HG22	2.49	0.48
1:A:706:GLU:HG2	2:A:382:HOH:O	2.12	0.48
1:D:694:ALA:O	1:D:696:LEU:HD13	2.14	0.48
1:B:734:THR:CG2	1:B:735:ASP:N	2.76	0.48
1:D:644:ARG:NH1	1:D:723:THR:OG1	2.34	0.48
1:D:579:LEU:HD13	1:D:587:PHE:CZ	2.48	0.48
1:C:592:LEU:CD1	1:C:594:SER:O	2.61	0.48
1:C:780:PHE:HA	2:C:82:HOH:O	2.13	0.48
1:A:682:ILE:HG23	1:A:682:ILE:O	2.14	0.48
1:C:644:ARG:NH2	1:C:721:GLN:HG3	2.18	0.48
1:D:611:PRO:HB3	1:D:638:LEU:HG	1.95	0.48
1:A:756:GLN:HE21	1:A:756:GLN:HA	1.79	0.48
1:D:707:ASN:HD21	1:D:725:LEU:HA	1.79	0.48
1:C:687:GLU:HA	2:C:237:HOH:O	2.13	0.48
1:B:767:ARG:HH11	1:B:767:ARG:HG2	1.79	0.48
1:C:634:GLU:HG2	1:C:635:VAL:O	2.14	0.47
1:D:595:PRO:HG3	1:D:658:ILE:CD1	2.43	0.47
1:A:549:GLY:HA2	1:A:575:TRP:CZ3	2.49	0.47
1:A:719:ARG:HH22	1:D:552:GLN:HA	1.79	0.47
1:D:779:ARG:CB	1:D:779:ARG:HH11	2.28	0.47
1:D:670:PRO:HA	1:D:781:VAL:CG1	2.44	0.47
1:B:694:ALA:O	1:B:696:LEU:HD22	2.14	0.47
1:D:580:ARG:NH2	1:D:623:GLU:O	2.37	0.47
1:C:713:TYR:HD1	1:C:717:ASN:OD1	1.97	0.47
1:A:616:VAL:HG11	1:A:652:LEU:HD21	1.97	0.47
1:D:658:ILE:N	1:D:658:ILE:HD12	2.30	0.47
1:D:637:ARG:HB3	1:D:639:PHE:CE1	2.50	0.47
1:A:707:ASN:HD22	1:A:707:ASN:N	2.13	0.47
1:A:577:VAL:CG1	1:A:590:GLY:HA3	2.45	0.47
1:B:607:LYS:HB2	2:B:506:HOH:O	2.15	0.47
1:D:578:SER:HB3	1:D:617:ILE:HB	1.96	0.47
1:A:597:TRP:CD2	1:A:788:LEU:HD22	2.49	0.47
1:D:737:CYS:HB3	1:D:761:TRP:CD1	2.50	0.47
1:B:596:GLU:CG	1:B:655:PRO:HG3	2.45	0.47
1:C:757:GLY:HA2	1:C:775:VAL:O	2.15	0.47
1:A:750:LYS:HZ1	1:C:687:GLU:CD	2.18	0.46
1:D:735:ASP:O	1:D:736:SER:HB3	2.15	0.46
1:A:554:GLU:HB3	2:A:187:HOH:O	2.14	0.46
1:D:555:PRO:HA	1:D:572:SER:HB2	1.97	0.46
1:A:617:ILE:HD12	1:A:626:LEU:HD21	1.98	0.46
1:C:720:VAL:HG11	1:C:726:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:769:ASN:N	1:C:769:ASN:ND2	2.54	0.46
1:A:605:LEU:HA	1:A:614:TYR:OH	2.15	0.46
1:A:577:VAL:CG2	1:A:616:VAL:HG13	2.46	0.46
1:D:715:PHE:CZ	1:D:730:LEU:HG	2.51	0.46
1:B:557:LYS:HA	1:B:681:PHE:CE2	2.51	0.46
1:A:574:PRO:HB2	1:A:663:ILE:H	1.81	0.46
1:B:714:GLU:H	1:B:714:GLU:CD	2.19	0.46
1:C:644:ARG:HB2	2:C:364:HOH:O	2.15	0.46
1:C:749:GLU:O	1:C:750:LYS:HB2	2.15	0.46
1:C:682:ILE:HD13	1:C:738:GLN:CB	2.46	0.46
1:C:599:LEU:HD23	1:C:755:LEU:HD21	1.97	0.46
1:C:778:SER:O	1:C:781:VAL:HG22	2.16	0.46
1:A:722:SER:C	1:A:724:GLU:H	2.19	0.45
1:B:592:LEU:HD13	1:B:664:PRO:HB3	1.98	0.45
1:B:583:PHE:CD1	1:B:583:PHE:N	2.84	0.45
1:C:734:THR:HG22	1:C:735:ASP:N	2.32	0.45
1:C:743:GLY:HA3	2:C:48:HOH:O	2.15	0.45
1:C:694:ALA:O	1:C:696:LEU:HD22	2.16	0.45
1:B:640:LEU:HD21	1:B:645:LYS:CG	2.47	0.45
1:D:756:GLN:HA	1:D:756:GLN:HE21	1.82	0.45
1:C:637:ARG:HB2	1:C:651:LYS:HB3	1.99	0.45
1:C:756:GLN:NE2	2:C:155:HOH:O	2.48	0.45
1:B:582:ARG:CD	1:B:615:LYS:HE2	2.47	0.45
1:D:696:LEU:N	1:D:696:LEU:CD1	2.80	0.45
1:D:711:ASN:ND2	1:D:720:VAL:HG13	2.32	0.45
1:A:735:ASP:OD1	1:A:768:PRO:HD3	2.17	0.45
1:C:711:ASN:ND2	1:C:720:VAL:H	2.08	0.45
1:C:549:GLY:HA2	1:C:575:TRP:CZ3	2.52	0.44
1:B:711:ASN:ND2	1:B:720:VAL:H	2.14	0.44
1:B:561:ARG:HH22	1:B:732:GLY:HA3	1.82	0.44
1:A:750:LYS:HZ3	1:C:687:GLU:CD	2.18	0.44
1:C:719:ARG:HG3	2:C:142:HOH:O	2.17	0.44
1:B:757:GLY:HA2	1:B:775:VAL:O	2.17	0.44
1:D:548:CYS:C	1:D:666:CYS:SG	2.96	0.44
1:A:705:ILE:CG2	1:A:709:VAL:HG13	2.48	0.44
1:D:560:GLY:HA2	1:D:701:GLN:HB3	1.98	0.44
1:A:683:THR:OG1	1:A:744:PRO:HG2	2.18	0.44
1:C:617:ILE:HG23	1:C:630:VAL:CG1	2.47	0.44
1:B:778:SER:O	1:B:781:VAL:HG12	2.18	0.44
1:D:720:VAL:HG11	1:D:726:CYS:SG	2.58	0.44
1:B:725:LEU:C	1:B:725:LEU:HD12	2.37	0.44
1:D:577:VAL:HG22	1:D:590:GLY:CA	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:675:ALA:O	1:D:678:THR:OG1	2.29	0.44
1:B:574:PRO:HG2	1:B:663:ILE:HB	1.99	0.44
1:A:711:ASN:HD21	1:A:720:VAL:N	2.15	0.43
1:A:682:ILE:HD12	1:A:774:TYR:CE2	2.53	0.43
1:D:554:GLU:OE2	1:D:555:PRO:O	2.35	0.43
1:B:580:ARG:HD2	1:B:617:ILE:CD1	2.48	0.43
1:B:574:PRO:CG	1:B:663:ILE:HB	2.49	0.43
1:C:737:CYS:HB3	1:C:761:TRP:NE1	2.32	0.43
1:D:580:ARG:HG3	1:D:617:ILE:HG12	2.01	0.43
1:D:546:PHE:CD1	1:D:658:ILE:HG22	2.54	0.43
1:C:597:TRP:CZ2	1:C:651:LYS:HD2	2.53	0.43
1:B:671:ASN:O	1:B:672:TYR:C	2.56	0.43
1:C:725:LEU:C	1:C:725:LEU:CD2	2.87	0.43
1:A:547:ASP:HB3	2:A:51:HOH:O	2.19	0.43
1:D:678:THR:HG23	2:D:400:HOH:O	2.18	0.43
1:A:712:ARG:HG2	1:B:632:GLU:HB3	1.99	0.43
1:D:706:GLU:OE2	1:D:708:LYS:HB2	2.18	0.43
1:A:706:GLU:O	1:A:709:VAL:CG1	2.66	0.43
1:D:756:GLN:HA	1:D:756:GLN:NE2	2.33	0.43
1:A:756:GLN:NE2	1:A:756:GLN:HA	2.33	0.43
1:C:627:GLU:HG3	2:C:45:HOH:O	2.18	0.43
1:B:644:ARG:O	1:B:645:LYS:HB2	2.18	0.43
1:D:725:LEU:HD22	1:D:774:TYR:HB2	2.01	0.43
1:D:756:GLN:NE2	2:D:97:HOH:O	2.40	0.43
1:C:668:PRO:HG2	1:C:778:SER:HA	2.01	0.43
1:A:757:GLY:HA2	1:A:775:VAL:O	2.19	0.43
1:D:590:GLY:HA2	1:D:742:GLY:O	2.19	0.42
1:B:749:GLU:HG2	1:B:750:LYS:HG3	2.01	0.42
1:A:619:GLY:HA2	2:A:329:HOH:O	2.19	0.42
1:A:641:GLU:O	1:A:645:LYS:CA	2.66	0.42
1:C:738:GLN:OE1	2:C:502:HOH:O	2.22	0.42
1:C:649:LEU:HD11	1:C:784:ILE:HA	2.00	0.42
1:A:720:VAL:HG23	1:A:724:GLU:HB2	2.01	0.42
1:B:559:PRO:HB2	1:B:562:VAL:HG23	1.99	0.42
1:A:551:PRO:HD3	1:A:575:TRP:CH2	2.55	0.42
1:A:573:TRP:CG	1:A:683:THR:HG21	2.55	0.42
1:C:638:LEU:HD22	1:C:650:LEU:HD22	2.01	0.42
1:B:737:CYS:HB3	1:B:761:TRP:CE2	2.54	0.42
1:D:691:THR:O	1:D:692:PHE:C	2.58	0.42
1:B:549:GLY:HA2	1:B:575:TRP:CZ3	2.55	0.42
1:A:751:ASP:HB3	1:A:752:LYS:HD3	2.01	0.42
1:D:550:LYS:HB3	2:D:252:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:687:GLU:OE2	1:D:750:LYS:HE2	2.20	0.42
1:D:592:LEU:HD13	1:D:664:PRO:HG3	2.01	0.42
1:D:789:ARG:NH1	1:D:789:ARG:HB2	2.34	0.42
1:D:641:GLU:HB2	1:D:647:ILE:HG13	2.01	0.42
1:A:627:GLU:O	1:A:630:VAL:HG22	2.19	0.41
1:A:577:VAL:CG1	1:A:590:GLY:C	2.83	0.41
1:C:674:VAL:HG11	1:C:756:GLN:HG3	2.01	0.41
1:C:625:ASN:N	1:C:625:ASN:ND2	2.69	0.41
1:B:667:LEU:N	1:B:667:LEU:CD1	2.83	0.41
1:A:688:THR:HB	1:A:691:THR:HG21	2.02	0.41
1:A:638:LEU:CD2	1:A:650:LEU:HD22	2.51	0.41
1:D:641:GLU:HA	1:D:642:PRO:HD3	1.84	0.41
1:C:710:CYS:O	1:C:715:PHE:HB2	2.21	0.41
1:A:626:LEU:CB	1:A:630:VAL:HG21	2.44	0.41
1:D:722:SER:O	1:D:776:ARG:HD2	2.20	0.41
1:C:756:GLN:HE21	1:C:756:GLN:HA	1.86	0.41
1:B:580:ARG:HG3	1:B:617:ILE:HD13	2.03	0.41
1:C:667:LEU:HD21	1:C:784:ILE:HG21	2.01	0.41
1:A:559:PRO:HD2	1:A:562:VAL:HG21	2.01	0.41
1:C:765:CYS:HB2	1:C:767:ARG:HH12	1.84	0.41
1:B:641:GLU:HA	1:B:642:PRO:HD3	1.72	0.41
1:B:649:LEU:HA	1:B:649:LEU:HD23	1.96	0.41
1:A:671:ASN:O	1:A:672:TYR:C	2.59	0.41
1:C:716:LEU:O	1:C:719:ARG:HG2	2.21	0.41
1:A:623:GLU:HB2	1:A:685:TRP:CD1	2.56	0.41
1:B:573:TRP:NE1	1:B:699:GLU:OE1	2.50	0.41
1:D:626:LEU:HB3	1:D:630:VAL:HG21	2.03	0.41
1:B:640:LEU:HD21	1:B:645:LYS:HG3	2.01	0.41
1:D:546:PHE:HB3	2:D:302:HOH:O	2.21	0.41
1:A:707:ASN:HD21	1:A:725:LEU:HA	1.86	0.41
1:C:713:TYR:CD1	1:C:717:ASN:OD1	2.73	0.41
1:B:682:ILE:O	1:B:699:GLU:HA	2.21	0.41
1:A:557:LYS:HA	1:A:681:PHE:CE2	2.55	0.41
1:C:580:ARG:HA	1:C:585:GLN:O	2.22	0.40
1:D:714:GLU:H	1:D:714:GLU:CD	2.25	0.40
1:B:582:ARG:HD2	1:B:615:LYS:HE2	2.03	0.40
1:D:627:GLU:HG2	2:D:362:HOH:O	2.20	0.40
1:D:627:GLU:OE1	1:D:628:PRO:HD2	2.22	0.40
1:B:561:ARG:HD2	1:B:729:HIS:CE1	2.57	0.40
1:B:716:LEU:N	1:B:716:LEU:CD2	2.84	0.40
1:A:577:VAL:HG12	1:A:590:GLY:CA	2.52	0.40
1:C:592:LEU:HD11	1:C:594:SER:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:574:PRO:HB2	1:A:663:ILE:N	2.37	0.40
1:A:607:LYS:HB2	2:A:17:HOH:O	2.20	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	244/246 (99%)	232 (95%)	11 (4%)	1 (0%)	43	36
1	B	244/246 (99%)	234 (96%)	9 (4%)	1 (0%)	43	36
1	C	244/246 (99%)	235 (96%)	8 (3%)	1 (0%)	43	36
1	D	244/246 (99%)	229 (94%)	12 (5%)	3 (1%)	19	9
All	All	976/984 (99%)	930 (95%)	40 (4%)	6 (1%)	33	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	562	VAL
1	B	750	LYS
1	C	750	LYS
1	D	736	SER
1	D	750	LYS
1	A	750	LYS

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%)	194 (93%)	14 (7%)	23	16
1	B	208/208 (100%)	199 (96%)	9 (4%)	40	33
1	C	208/208 (100%)	198 (95%)	10 (5%)	35	28
1	D	208/208 (100%)	194 (93%)	14 (7%)	23	16
All	All	832/832 (100%)	785 (94%)	47 (6%)	30	22

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	GLU
1	A	569	HIS
1	A	588	CYS
1	A	592	LEU
1	A	607	LYS
1	A	617	ILE
1	A	667	LEU
1	A	703	PRO
1	A	711	ASN
1	A	714	GLU
1	A	720	VAL
1	A	725	LEU
1	A	750	LYS
1	A	788	LEU
1	B	577	VAL
1	B	579	LEU
1	B	588	CYS
1	B	592	LEU
1	B	610	ARG
1	B	625	ASN
1	B	644	ARG
1	B	721	GLN
1	B	752	LYS
1	C	569	HIS
1	C	588	CYS
1	C	667	LEU
1	C	674	VAL
1	C	688	THR
1	C	711	ASN
1	C	725	LEU
1	C	769	ASN
1	C	779	ARG
1	C	785	GLU

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Mol	Chain	Res	Type
1	D	554	GLU
1	D	577	VAL
1	D	579	LEU
1	D	585	GLN
1	D	592	LEU
1	D	612	SER
1	D	667	LEU
1	D	677	ARG
1	D	696	LEU
1	D	707	ASN
1	D	711	ASN
1	D	720	VAL
1	D	725	LEU
1	D	785	GLU

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

Mol	Chain	Res	Type
1	A	622	GLN
1	A	631	GLN
1	A	671	ASN
1	A	689	GLN
1	A	707	ASN
1	A	711	ASN
1	A	756	GLN
1	B	631	GLN
1	B	701	GLN
1	B	707	ASN
1	B	711	ASN
1	B	721	GLN
1	B	756	GLN
1	B	790	ASN
1	B	791	ASN
1	C	625	ASN
1	C	629	HIS
1	C	631	GLN
1	C	707	ASN
1	C	711	ASN
1	C	756	GLN
1	C	769	ASN
1	D	585	GLN
1	D	622	GLN

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Mol	Chain	Res	Type
1	D	631	GLN
1	D	671	ASN
1	D	701	GLN
1	D	707	ASN
1	D	711	ASN
1	D	756	GLN
1	D	790	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	246/246 (100%)	-0.14	4 (1%) 68 69	4, 16, 40, 54	0
1	B	246/246 (100%)	-0.19	3 (1%) 75 76	3, 16, 40, 56	0
1	C	246/246 (100%)	-0.27	2 (0%) 83 84	3, 14, 34, 56	0
1	D	246/246 (100%)	-0.03	5 (2%) 62 62	4, 20, 44, 55	0
All	All	984/984 (100%)	-0.16	14 (1%) 72 72	3, 17, 40, 56	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	561	ARG	5.1
1	A	561	ARG	3.5
1	B	563	VAL	3.3
1	D	562	VAL	3.0
1	B	583	PHE	2.6
1	A	790	ASN	2.6
1	B	546	PHE	2.5
1	D	546	PHE	2.4
1	C	561	ARG	2.3
1	D	583	PHE	2.3
1	C	689	GLN	2.3
1	A	688	THR	2.2
1	A	730	LEU	2.0
1	D	563	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.