



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:53 AM GMT

PDB ID : 2J69
Title : BACTERIAL DYNAMIN-LIKE PROTEIN BDLP
Authors : Low, H.H.; Lowe, J.
Deposited on : 2006-09-26
Resolution : 3.00 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
<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

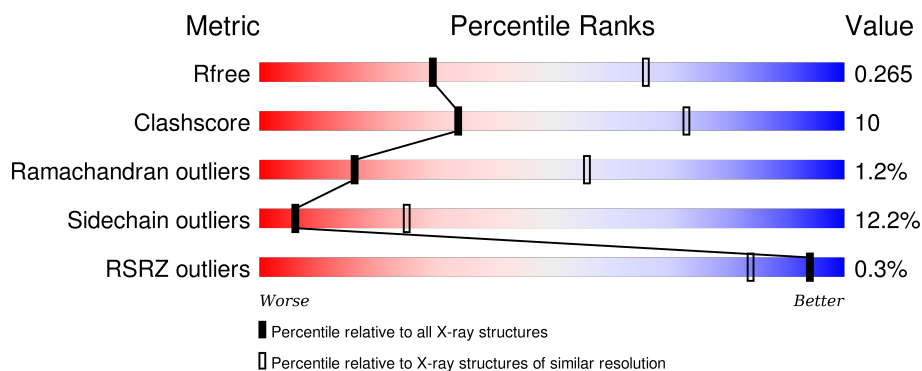
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	695	
1	B	695	
1	C	695	
1	D	695	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21500 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.

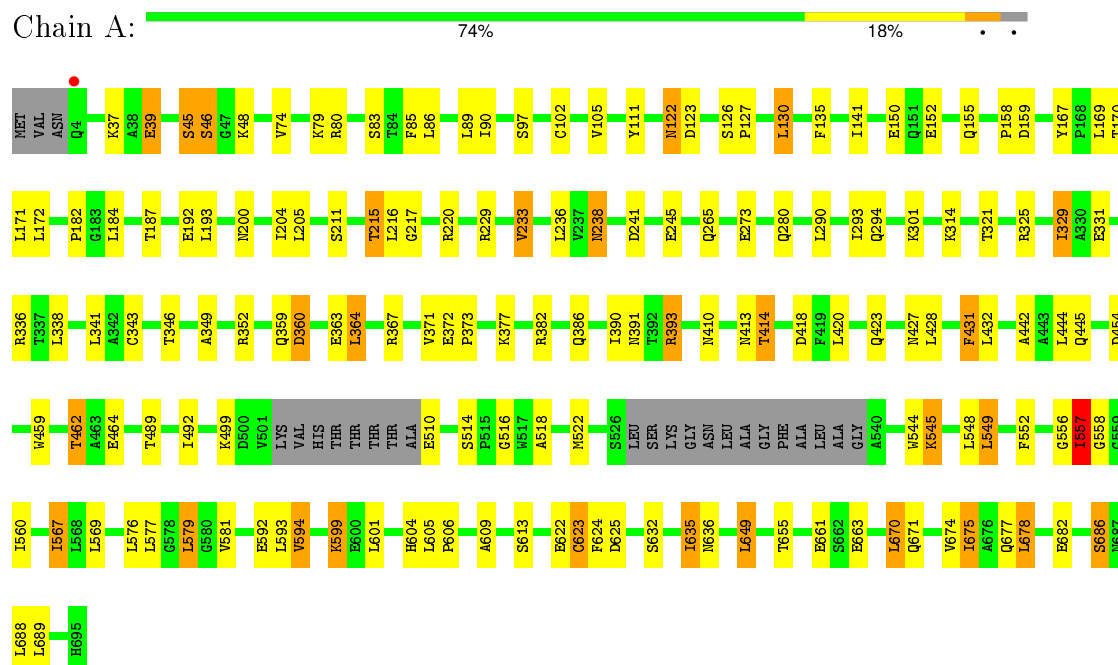
- Molecule 1 is a protein called BACTERIAL DYNAMIN-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			
1	B	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			
1	C	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			
1	D	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			

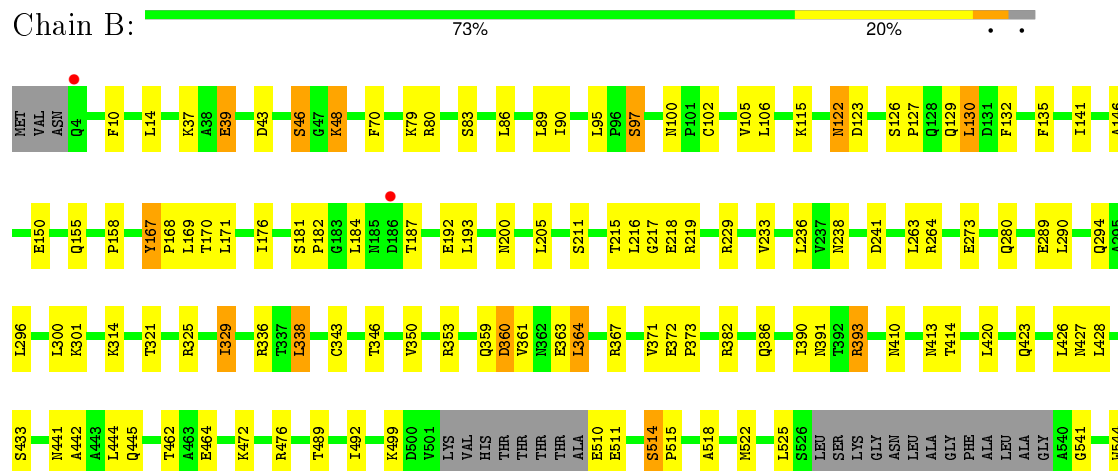
3 Residue-property plots

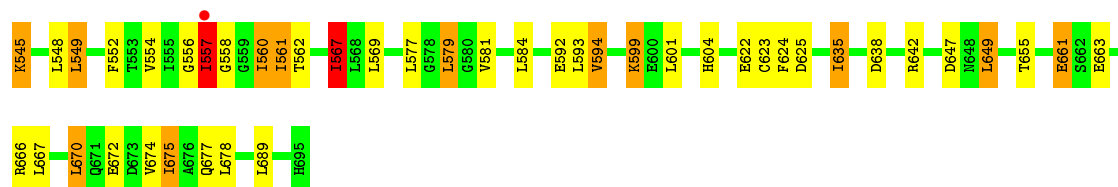
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BACTERIAL DYNAMIN-LIKE PROTEIN



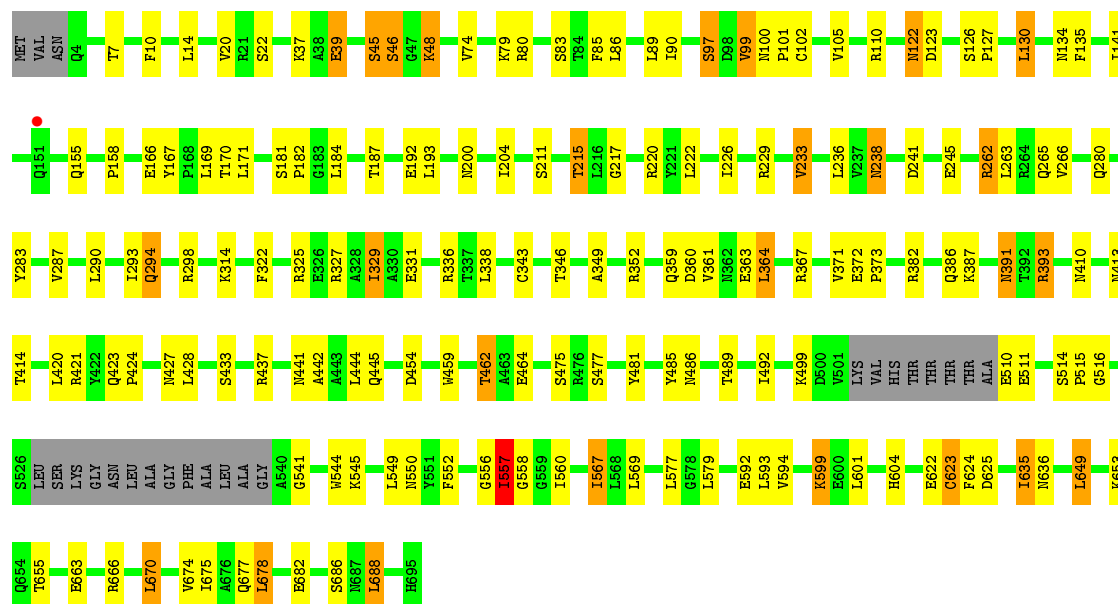
• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN





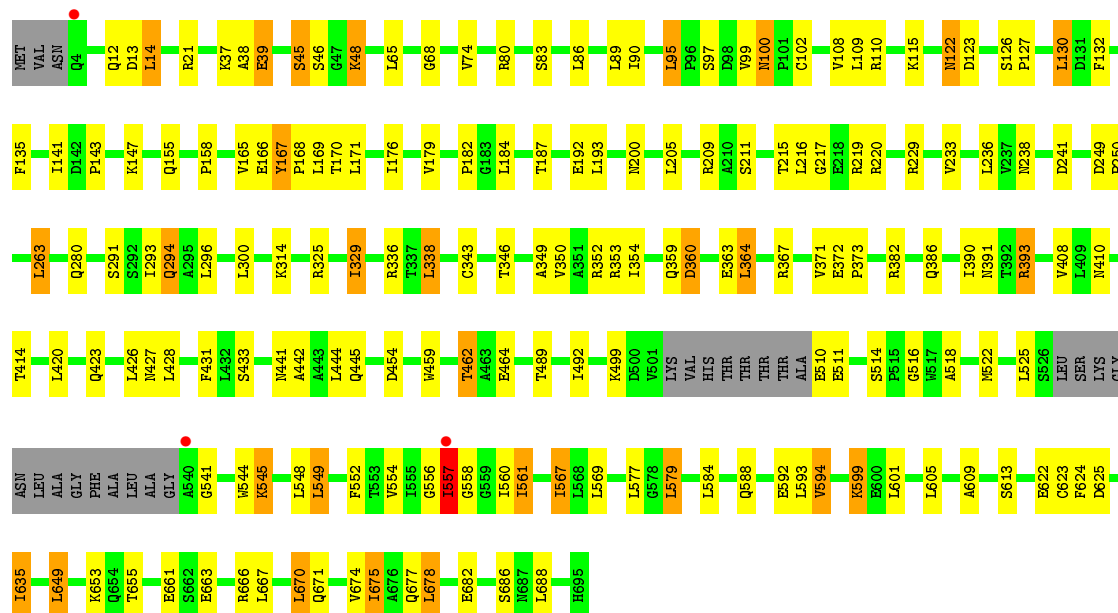
• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

Chain C: 72% 20%



• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

Chain D: 71% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.29 Å 218.60 Å 151.20 Å 90.00° 134.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 34.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.00) 97.0 (34.50-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.281 0.226 , 0.265	Depositor DCC
R_{free} test set	4869 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.1	EDS
Estimated twinning fraction	0.006 for -h,h+2*1,1/2*h+1/2*k 0.009 for -h,-h-2*1,1/2*h-1/2*k 0.004 for -k,-h,-1/2*h+1/2*k-l 0.009 for k,h,-1/2*h-1/2*k-l 0.417 for h+2*1,k,-h-l 0.005 for h+2*1,h,-1/2*h+1/2*k-l 0.007 for k,h+2*1,1/2*h-1/2*k 0.004 for k,-h-2*1,-1/2*h-1/2*k 0.006 for h+2*1,-h,-1/2*h-1/2*k-l 0.459 for -h-2*1,-k,l 0.418 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 96983 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21500	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 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.71	6/5459 (0.1%)	0.71	8/7368 (0.1%)
1	B	0.70	6/5459 (0.1%)	0.71	9/7368 (0.1%)
1	C	0.64	6/5459 (0.1%)	0.67	5/7368 (0.1%)
1	D	0.74	6/5459 (0.1%)	0.68	8/7368 (0.1%)
All	All	0.70	24/21836 (0.1%)	0.69	30/29472 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	557	ILE	CB-CG1	32.69	2.45	1.54
1	A	557	ILE	CB-CG1	29.34	2.36	1.54
1	B	557	ILE	CB-CG1	27.52	2.31	1.54
1	A	567	ILE	CB-CG1	-22.89	0.90	1.54
1	C	557	ILE	CB-CG1	22.48	2.17	1.54
1	D	557	ILE	CB-CG2	17.96	2.08	1.52
1	B	567	ILE	CB-CG1	-17.71	1.04	1.54
1	D	567	ILE	CB-CG1	-17.41	1.05	1.54
1	C	567	ILE	CB-CG1	-16.04	1.09	1.54
1	C	557	ILE	CB-CG2	15.51	2.00	1.52
1	B	557	ILE	CB-CG2	14.84	1.98	1.52
1	B	635	ILE	CB-CG1	-13.86	1.15	1.54
1	A	557	ILE	CB-CG2	11.94	1.89	1.52
1	B	329	ILE	CB-CG1	-11.37	1.22	1.54
1	D	635	ILE	CB-CG1	-10.68	1.24	1.54
1	D	329	ILE	CB-CG1	-10.28	1.25	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	ILE	CB-CG1	-9.30	1.28	1.54
1	C	635	ILE	CB-CG1	-8.75	1.29	1.54
1	A	567	ILE	CB-CG2	7.45	1.75	1.52
1	C	329	ILE	CB-CG1	-7.07	1.34	1.54
1	C	567	ILE	CB-CG2	6.45	1.72	1.52
1	A	329	ILE	CB-CG1	-6.22	1.36	1.54
1	D	567	ILE	CB-CG2	5.81	1.70	1.52
1	B	329	ILE	CB-CG2	5.57	1.70	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	557	ILE	CG1-CB-CG2	-20.40	66.53	111.40
1	B	557	ILE	CG1-CB-CG2	-18.37	70.98	111.40
1	A	557	ILE	CG1-CB-CG2	-18.25	71.25	111.40
1	C	557	ILE	CG1-CB-CG2	-17.13	73.71	111.40
1	B	567	ILE	CG1-CB-CG2	15.15	144.74	111.40
1	A	567	ILE	CG1-CB-CG2	14.87	144.11	111.40
1	A	567	ILE	CA-CB-CG2	-11.99	86.92	110.90
1	C	567	ILE	CA-CB-CG2	-11.61	87.67	110.90
1	B	635	ILE	CG1-CB-CG2	11.58	136.87	111.40
1	D	567	ILE	CG1-CB-CG2	9.97	133.34	111.40
1	B	567	ILE	CA-CB-CG2	-9.68	91.54	110.90
1	D	635	ILE	CG1-CB-CG2	8.93	131.04	111.40
1	D	567	ILE	CA-CB-CG2	-8.39	94.12	110.90
1	B	329	ILE	CA-CB-CG2	-6.97	96.95	110.90
1	A	567	ILE	CA-CB-CG1	6.93	124.16	111.00
1	C	567	ILE	CG1-CB-CG2	6.90	126.57	111.40
1	A	579	LEU	CA-CB-CG	6.61	130.50	115.30
1	A	635	ILE	CA-CB-CG2	-6.50	97.89	110.90
1	A	329	ILE	CA-CB-CG2	-6.47	97.95	110.90
1	C	557	ILE	CB-CG1-CD1	6.35	131.68	113.90
1	B	579	LEU	CA-CB-CG	6.28	129.73	115.30
1	B	557	ILE	CB-CG1-CD1	6.22	131.32	113.90
1	D	579	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	635	ILE	CA-CB-CG1	-6.00	99.59	111.00
1	C	329	ILE	CA-CB-CG2	-5.93	99.04	110.90
1	D	329	ILE	CA-CB-CG2	-5.52	99.87	110.90
1	D	557	ILE	CB-CG1-CD1	5.42	129.08	113.90
1	B	557	ILE	CA-CB-CG2	5.35	121.60	110.90
1	B	216	LEU	CA-CB-CG	5.21	127.30	115.30
1	D	95	LEU	CA-CB-CG	5.08	126.99	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	567	ILE	CB

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	5375	0	5366	125	0
1	B	5375	0	5366	97	0
1	C	5375	0	5366	108	0
1	D	5375	0	5366	108	0
All	All	21500	0	21464	432	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 10.

All (432) 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:567:ILE:CB	1:A:567:ILE:CG2	1.75	1.60
1:D:552:PHE:CD1	1:D:557:ILE:HD12	1.30	1.58
1:A:567:ILE:CD1	1:A:567:ILE:HB	1.21	1.55
1:D:552:PHE:CD1	1:D:557:ILE:CD1	1.92	1.49
1:A:557:ILE:CG2	1:A:557:ILE:CB	1.89	1.47
1:B:552:PHE:CD1	1:B:557:ILE:HD12	1.48	1.46
1:D:552:PHE:CE1	1:D:557:ILE:CD1	1.98	1.43
1:D:552:PHE:CE1	1:D:557:ILE:HD11	1.49	1.42
1:B:552:PHE:CD1	1:B:557:ILE:CD1	2.03	1.42
1:B:557:ILE:CB	1:B:557:ILE:CG2	1.98	1.38
1:C:557:ILE:CG2	1:C:557:ILE:CB	2.00	1.36
1:A:552:PHE:CD1	1:A:557:ILE:HD12	1.60	1.35
1:B:552:PHE:CE1	1:B:557:ILE:HD11	1.62	1.35
1:D:557:ILE:CB	1:D:557:ILE:CG2	2.08	1.31
1:A:552:PHE:CD1	1:A:557:ILE:CD1	2.17	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:PHE:CE1	1:B:557:ILE:CD1	2.14	1.25
1:D:557:ILE:CG2	1:D:560:ILE:HG13	1.66	1.25
1:C:552:PHE:CD1	1:C:557:ILE:HD12	1.73	1.24
1:C:557:ILE:CG1	1:C:557:ILE:CB	2.17	1.23
1:A:567:ILE:CG2	1:A:567:ILE:O	1.87	1.22
1:A:552:PHE:CE1	1:A:557:ILE:HD11	1.75	1.21
1:A:567:ILE:CA	1:A:567:ILE:CG1	2.19	1.20
1:D:557:ILE:HG23	1:D:560:ILE:CG1	1.71	1.20
1:A:557:ILE:HG23	1:A:560:ILE:CG1	1.74	1.17
1:A:552:PHE:CE1	1:A:557:ILE:CD1	2.27	1.17
1:A:567:ILE:CG2	1:A:567:ILE:C	2.11	1.17
1:A:567:ILE:HG22	1:A:567:ILE:C	1.68	1.14
1:C:557:ILE:HG23	1:C:560:ILE:HG13	1.26	1.11
1:C:552:PHE:CD1	1:C:557:ILE:CD1	2.34	1.09
1:A:567:ILE:CG2	1:A:567:ILE:CA	2.28	1.09
1:B:557:ILE:CB	1:B:557:ILE:CG1	2.31	1.09
1:B:557:ILE:HG23	1:B:560:ILE:CG1	1.81	1.09
1:C:567:ILE:HG21	1:C:604:HIS:CE1	1.90	1.07
1:A:557:ILE:CG2	1:A:560:ILE:HG13	1.83	1.06
1:C:552:PHE:CE1	1:C:557:ILE:HD11	1.88	1.06
1:A:567:ILE:HG22	1:A:567:ILE:O	1.54	1.06
1:C:567:ILE:HG22	1:C:567:ILE:O	1.56	1.04
1:C:552:PHE:CE1	1:C:557:ILE:CD1	2.40	1.03
1:A:557:ILE:CB	1:A:557:ILE:CG1	2.36	1.03
1:A:567:ILE:HG23	1:A:567:ILE:O	1.56	1.03
1:A:567:ILE:HG21	1:A:604:HIS:CE1	1.94	1.02
1:A:567:ILE:CB	1:A:567:ILE:HG13	1.52	1.00
1:C:567:ILE:CG2	1:C:567:ILE:O	2.09	1.00
1:A:567:ILE:CB	1:A:567:ILE:HG12	1.52	1.00
1:A:552:PHE:HD1	1:A:557:ILE:CD1	1.73	0.99
1:A:552:PHE:HE1	1:A:557:ILE:HD11	1.24	0.98
1:B:557:ILE:CG2	1:B:560:ILE:HG13	1.94	0.98
1:A:567:ILE:HD12	1:A:567:ILE:HB	1.42	0.98
1:B:552:PHE:HE1	1:B:557:ILE:HD11	1.16	0.98
1:B:557:ILE:HG23	1:B:560:ILE:HG13	0.98	0.98
1:C:557:ILE:HG23	1:C:560:ILE:CG1	1.94	0.97
1:C:567:ILE:CG2	1:C:604:HIS:CE1	2.47	0.97
1:D:552:PHE:HD1	1:D:557:ILE:CD1	1.51	0.96
1:B:552:PHE:HD1	1:B:557:ILE:CD1	1.57	0.96
1:A:39:GLU:HG3	1:A:48:LYS:HG2	1.46	0.95
1:C:39:GLU:HG3	1:C:48:LYS:HG2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:ILE:CB	1:D:557:ILE:CG1	2.45	0.94
1:A:556:GLY:O	1:A:557:ILE:HG13	1.69	0.92
1:A:552:PHE:HD1	1:A:557:ILE:HD12	1.28	0.92
1:D:567:ILE:O	1:D:567:ILE:CG2	2.18	0.92
1:C:557:ILE:HG12	1:C:560:ILE:HG13	1.47	0.92
1:C:552:PHE:HE1	1:C:557:ILE:HD11	1.29	0.91
1:C:552:PHE:HD1	1:C:557:ILE:HD12	1.31	0.90
1:A:567:ILE:CG2	1:A:604:HIS:CE1	2.55	0.90
1:A:567:ILE:CB	1:A:567:ILE:CG1	0.90	0.89
1:A:556:GLY:O	1:A:557:ILE:CG1	2.20	0.89
1:C:557:ILE:CG1	1:C:557:ILE:CG2	2.50	0.89
1:D:557:ILE:CG1	1:D:557:ILE:CG2	2.51	0.89
1:A:567:ILE:CB	1:A:567:ILE:CD1	2.04	0.89
1:B:557:ILE:CG2	1:B:557:ILE:CG1	2.50	0.89
1:A:557:ILE:CG2	1:A:557:ILE:CG1	2.50	0.88
1:B:215:THR:HB	1:B:218:GLU:HG3	1.55	0.87
1:C:567:ILE:CG2	1:C:604:HIS:HE1	1.87	0.86
1:A:567:ILE:CG2	1:A:567:ILE:CG1	2.53	0.85
1:B:552:PHE:HD1	1:B:557:ILE:HD12	1.06	0.85
1:A:557:ILE:HG23	1:A:560:ILE:HG13	0.89	0.84
1:D:552:PHE:CD1	1:D:557:ILE:HD11	1.86	0.84
1:B:552:PHE:CD1	1:B:557:ILE:HD11	1.86	0.83
1:D:567:ILE:HG22	1:D:567:ILE:O	1.78	0.81
1:A:464:GLU:HG2	1:A:544:TRP:HH2	1.46	0.81
1:C:459:TRP:O	1:C:462:THR:HG22	1.80	0.81
1:A:567:ILE:HB	1:A:567:ILE:CG1	0.82	0.81
1:C:567:ILE:HG22	1:C:604:HIS:HE1	1.46	0.80
1:C:557:ILE:CG2	1:C:560:ILE:HG13	2.12	0.79
1:D:552:PHE:HE1	1:D:557:ILE:HD11	1.00	0.78
1:A:459:TRP:O	1:A:462:THR:HG22	1.84	0.78
1:A:245:GLU:HG2	1:C:245:GLU:HG2	1.65	0.77
1:B:46:SER:HB3	1:B:663:GLU:OE2	1.83	0.76
1:D:552:PHE:HE1	1:D:557:ILE:CD1	1.64	0.76
1:A:552:PHE:CD1	1:A:557:ILE:HD11	1.99	0.76
1:B:102:CYS:HB2	1:B:155:GLN:HA	1.68	0.75
1:A:382:ARG:HB2	1:A:635:ILE:HD13	1.66	0.75
1:C:557:ILE:CG1	1:C:560:ILE:HG13	2.15	0.75
1:D:130:LEU:HD13	1:D:135:PHE:HB2	1.70	0.73
1:C:393:ARG:CB	1:C:624:PHE:HB2	2.18	0.73
1:C:557:ILE:HG23	1:C:560:ILE:CB	2.18	0.73
1:C:393:ARG:HB3	1:C:624:PHE:CB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ASN:HD22	1:D:123:ASP:N	1.88	0.72
1:B:122:ASN:HD22	1:B:123:ASP:N	1.86	0.72
1:C:556:GLY:O	1:C:557:ILE:HG13	1.88	0.72
1:C:215:THR:HG22	1:C:217:GLY:H	1.54	0.72
1:A:567:ILE:CG2	1:A:604:HIS:HE1	2.00	0.71
1:A:102:CYS:HB2	1:A:155:GLN:HA	1.73	0.70
1:A:90:ILE:HB	1:A:169:LEU:HD13	1.72	0.70
1:A:557:ILE:H	1:A:558:GLY:HA3	1.56	0.70
1:C:552:PHE:HD1	1:C:557:ILE:CD1	1.87	0.70
1:A:382:ARG:CB	1:A:635:ILE:HD13	2.22	0.70
1:A:46:SER:HB3	1:A:663:GLU:OE2	1.92	0.70
1:C:393:ARG:HB3	1:C:624:PHE:HB2	1.73	0.69
1:D:609:ALA:O	1:D:613:SER:HB2	1.91	0.69
1:D:464:GLU:HG2	1:D:544:TRP:HH2	1.57	0.69
1:B:130:LEU:HD13	1:B:135:PHE:HB2	1.73	0.69
1:D:557:ILE:HG23	1:D:560:ILE:HG13	0.80	0.69
1:C:343:CYS:SG	1:C:674:VAL:HG12	2.33	0.69
1:C:557:ILE:HG12	1:C:560:ILE:CG1	2.20	0.68
1:A:130:LEU:HD13	1:A:135:PHE:HB2	1.74	0.68
1:C:46:SER:HB3	1:C:663:GLU:OE2	1.93	0.68
1:B:552:PHE:HE1	1:B:557:ILE:CD1	1.81	0.68
1:B:556:GLY:O	1:B:557:ILE:CG1	2.42	0.68
1:B:39:GLU:HG3	1:B:48:LYS:HG2	1.75	0.68
1:A:343:CYS:SG	1:A:674:VAL:HG12	2.34	0.68
1:B:556:GLY:O	1:B:557:ILE:HG13	1.93	0.67
1:D:567:ILE:HG23	1:D:567:ILE:O	1.92	0.67
1:D:552:PHE:HD1	1:D:557:ILE:HD12	0.94	0.67
1:A:393:ARG:CB	1:A:624:PHE:HB2	2.24	0.67
1:C:567:ILE:HG23	1:C:567:ILE:O	1.94	0.66
1:B:215:THR:HG22	1:B:217:GLY:H	1.60	0.66
1:B:557:ILE:H	1:B:558:GLY:HA3	1.60	0.66
1:A:557:ILE:HG12	1:A:560:ILE:HG13	1.77	0.66
1:C:122:ASN:HD22	1:C:123:ASP:N	1.94	0.66
1:C:130:LEU:HD13	1:C:135:PHE:HB2	1.76	0.66
1:D:343:CYS:SG	1:D:674:VAL:HG12	2.36	0.65
1:D:557:ILE:N	1:D:558:GLY:HA3	2.11	0.65
1:B:187:THR:HG22	1:B:193:LEU:HD13	1.78	0.65
1:A:122:ASN:HD22	1:A:123:ASP:N	1.93	0.65
1:D:46:SER:HB3	1:D:663:GLU:OE2	1.96	0.65
1:C:552:PHE:CE1	1:C:557:ILE:HD12	2.21	0.65
1:D:557:ILE:HG23	1:D:557:ILE:CG1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:CYS:HB2	1:D:155:GLN:HA	1.78	0.65
1:B:557:ILE:N	1:B:558:GLY:HA3	2.12	0.64
1:B:343:CYS:SG	1:B:674:VAL:HG12	2.37	0.64
1:C:567:ILE:HG22	1:C:604:HIS:CE1	2.26	0.64
1:B:90:ILE:HB	1:B:169:LEU:HD13	1.79	0.63
1:A:518:ALA:O	1:A:522:MET:HG3	1.97	0.63
1:D:423:GLN:HE22	1:D:594:VAL:HG22	1.63	0.63
1:C:102:CYS:HB2	1:C:155:GLN:HA	1.79	0.63
1:A:557:ILE:CG1	1:A:557:ILE:HG23	2.29	0.63
1:D:90:ILE:HB	1:D:169:LEU:HD13	1.80	0.63
1:D:215:THR:HG22	1:D:217:GLY:H	1.64	0.63
1:C:556:GLY:O	1:C:557:ILE:CG1	2.46	0.63
1:B:518:ALA:O	1:B:522:MET:HG3	1.98	0.63
1:A:567:ILE:HG13	1:A:567:ILE:HB	1.36	0.63
1:D:393:ARG:HB3	1:D:624:PHE:CB	2.29	0.62
1:D:359:GLN:O	1:D:360:ASP:HB2	1.98	0.62
1:A:557:ILE:N	1:A:558:GLY:HA3	2.13	0.62
1:A:557:ILE:CG1	1:A:560:ILE:HG13	2.30	0.62
1:A:635:ILE:HG23	1:A:636:ASN:N	2.14	0.62
1:A:74:VAL:HG21	1:A:86:LEU:HD21	1.82	0.61
1:A:215:THR:HG22	1:A:217:GLY:H	1.66	0.61
1:D:518:ALA:O	1:D:522:MET:HG3	1.99	0.61
1:B:464:GLU:HG2	1:B:544:TRP:HH2	1.66	0.60
1:A:382:ARG:HB2	1:A:635:ILE:CD1	2.31	0.60
1:D:423:GLN:CG	1:D:593:LEU:HD12	2.32	0.60
1:A:393:ARG:HB2	1:A:624:PHE:HB2	1.82	0.60
1:C:393:ARG:HB2	1:C:624:PHE:HB2	1.84	0.59
1:D:325:ARG:O	1:D:329:ILE:HD12	2.02	0.59
1:D:393:ARG:HB3	1:D:624:PHE:HB2	1.85	0.59
1:B:661:GLU:HG2	1:C:134:ASN:HD21	1.67	0.59
1:B:382:ARG:HB2	1:B:635:ILE:HG21	1.84	0.58
1:D:187:THR:HG22	1:D:193:LEU:HD13	1.85	0.58
1:B:363:GLU:OE2	1:B:367:ARG:NH2	2.37	0.58
1:C:557:ILE:N	1:C:558:GLY:HA3	2.19	0.57
1:A:393:ARG:HB3	1:A:624:PHE:CB	2.33	0.57
1:C:74:VAL:HG21	1:C:86:LEU:HD21	1.85	0.57
1:B:557:ILE:HG23	1:B:560:ILE:CB	2.33	0.57
1:A:393:ARG:NH2	1:A:625:ASP:OD2	2.37	0.57
1:D:39:GLU:HG3	1:D:48:LYS:HG2	1.87	0.57
1:A:204:ILE:HB	1:A:233:VAL:HB	1.86	0.57
1:A:371:VAL:CG1	1:A:492:ILE:HG12	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:GLU:HG2	1:C:544:TRP:HH2	1.70	0.57
1:D:442:ALA:O	1:D:445:GLN:HB3	2.05	0.57
1:A:442:ALA:O	1:A:445:GLN:HB3	2.06	0.56
1:D:363:GLU:OE2	1:D:367:ARG:NH2	2.39	0.56
1:C:445:GLN:HB2	1:C:569:LEU:HD21	1.86	0.56
1:B:557:ILE:HG12	1:B:560:ILE:HG13	1.88	0.56
1:B:215:THR:O	1:B:219:ARG:HG2	2.06	0.56
1:D:393:ARG:CB	1:D:624:PHE:HB2	2.36	0.56
1:B:423:GLN:HE22	1:B:594:VAL:HG22	1.69	0.56
1:C:325:ARG:O	1:C:329:ILE:HD12	2.05	0.55
1:A:576:LEU:O	1:A:581:VAL:HG22	2.07	0.55
1:D:364:LEU:HD11	1:D:649:LEU:HD13	1.86	0.55
1:D:39:GLU:HG3	1:D:48:LYS:CG	2.37	0.55
1:B:155:GLN:NE2	1:B:158:PRO:HA	2.22	0.55
1:C:442:ALA:O	1:C:445:GLN:HB3	2.07	0.55
1:A:423:GLN:HE22	1:A:594:VAL:HG22	1.71	0.55
1:D:371:VAL:CG1	1:D:492:ILE:HG12	2.37	0.55
1:A:682:GLU:O	1:A:686:SER:HB2	2.06	0.55
1:C:599:LYS:HE2	1:C:599:LYS:HA	1.89	0.55
1:B:371:VAL:HG11	1:B:492:ILE:HG23	1.89	0.54
1:D:372:GLU:N	1:D:373:PRO:HD2	2.22	0.54
1:C:371:VAL:CG1	1:C:492:ILE:HG12	2.37	0.54
1:D:556:GLY:O	1:D:557:ILE:CG1	2.56	0.54
1:D:599:LYS:HE2	1:D:599:LYS:HA	1.90	0.54
1:A:445:GLN:HB2	1:A:569:LEU:HD21	1.90	0.54
1:A:609:ALA:O	1:A:613:SER:HB2	2.08	0.54
1:A:393:ARG:HB3	1:A:624:PHE:HB2	1.88	0.53
1:B:561:ILE:CG2	1:B:562:THR:N	2.72	0.53
1:B:393:ARG:CB	1:B:624:PHE:HB2	2.37	0.53
1:B:359:GLN:O	1:B:360:ASP:HB2	2.08	0.53
1:D:215:THR:O	1:D:219:ARG:HG2	2.09	0.53
1:C:187:THR:HG22	1:C:193:LEU:HD13	1.90	0.53
1:B:39:GLU:HG3	1:B:48:LYS:CG	2.38	0.53
1:C:363:GLU:OE2	1:C:367:ARG:NH2	2.42	0.53
1:B:346:THR:HG21	1:B:670:LEU:HD22	1.91	0.53
1:D:100:ASN:HD22	1:D:102:CYS:H	1.57	0.53
1:C:663:GLU:OE2	1:C:666:ARG:NH2	2.42	0.52
1:B:567:ILE:HD11	1:B:604:HIS:ND1	2.24	0.52
1:C:557:ILE:H	1:C:558:GLY:HA3	1.74	0.52
1:B:393:ARG:HB3	1:B:624:PHE:CB	2.39	0.52
1:D:155:GLN:HE21	1:D:158:PRO:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:ILE:HG12	1:D:560:ILE:HG13	1.92	0.52
1:A:557:ILE:HG12	1:A:560:ILE:CG1	2.40	0.52
1:D:393:ARG:NH2	1:D:625:ASP:OD2	2.40	0.52
1:C:122:ASN:C	1:C:122:ASN:HD22	2.11	0.52
1:A:364:LEU:HD11	1:A:649:LEU:HD13	1.92	0.52
1:D:155:GLN:NE2	1:D:158:PRO:HA	2.25	0.52
1:C:236:LEU:HD22	1:C:290:LEU:HD11	1.92	0.51
1:C:372:GLU:N	1:C:373:PRO:HD2	2.24	0.51
1:D:557:ILE:H	1:D:558:GLY:HA3	1.73	0.51
1:C:39:GLU:CG	1:C:48:LYS:HG2	2.32	0.51
1:D:552:PHE:HD1	1:D:557:ILE:CG1	2.18	0.51
1:C:552:PHE:CD1	1:C:557:ILE:HD11	2.18	0.51
1:B:155:GLN:HE21	1:B:158:PRO:HA	1.75	0.51
1:B:442:ALA:O	1:B:445:GLN:HB3	2.10	0.51
1:A:552:PHE:HE1	1:A:557:ILE:CD1	1.95	0.50
1:B:599:LYS:HA	1:B:599:LYS:HE2	1.92	0.50
1:D:83:SER:OG	1:D:97:SER:HA	2.11	0.50
1:D:556:GLY:O	1:D:557:ILE:HG13	2.11	0.50
1:A:371:VAL:HG12	1:A:371:VAL:O	2.11	0.50
1:B:372:GLU:N	1:B:373:PRO:HD2	2.26	0.50
1:D:671:GLN:O	1:D:675:ILE:HB	2.12	0.50
1:A:321:THR:HA	1:A:325:ARG:HG3	1.94	0.50
1:D:382:ARG:O	1:D:386:GLN:HB2	2.10	0.50
1:A:83:SER:OG	1:A:97:SER:HA	2.11	0.49
1:A:280:GLN:CG	1:B:280:GLN:HE21	2.24	0.49
1:B:581:VAL:HG12	1:B:584:LEU:HD12	1.94	0.49
1:B:325:ARG:O	1:B:329:ILE:HD12	2.12	0.49
1:C:346:THR:HG21	1:C:670:LEU:HD22	1.94	0.49
1:B:83:SER:OG	1:B:97:SER:HA	2.12	0.49
1:D:109:LEU:HD12	1:D:165:VAL:HB	1.93	0.49
1:C:557:ILE:HG23	1:C:560:ILE:HB	1.93	0.49
1:B:329:ILE:HD13	1:B:689:LEU:HD13	1.95	0.49
1:D:678:LEU:HD22	1:D:682:GLU:HG3	1.95	0.49
1:A:372:GLU:N	1:A:373:PRO:HD2	2.27	0.49
1:D:338:LEU:HD23	1:D:525:LEU:HD22	1.93	0.49
1:A:632:SER:O	1:A:635:ILE:HG22	2.13	0.49
1:B:122:ASN:HD22	1:B:122:ASN:C	2.16	0.49
1:C:262:ARG:O	1:C:266:VAL:HG23	2.13	0.49
1:B:557:ILE:CG1	1:B:557:ILE:HG23	2.37	0.49
1:B:382:ARG:O	1:B:386:GLN:HB2	2.13	0.49
1:A:363:GLU:OE2	1:A:367:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ILE:HG22	1:B:562:THR:H	1.79	0.48
1:D:682:GLU:O	1:D:686:SER:HB2	2.13	0.48
1:C:79:LYS:HG2	1:C:99:VAL:HG12	1.94	0.48
1:C:181:SER:HB2	1:C:187:THR:HG21	1.94	0.48
1:D:382:ARG:HB2	1:D:635:ILE:HG21	1.95	0.48
1:B:557:ILE:CG1	1:B:560:ILE:HG13	2.43	0.48
1:A:187:THR:HG22	1:A:193:LEU:HD13	1.95	0.48
1:D:349:ALA:HA	1:D:352:ARG:NH2	2.28	0.48
1:D:459:TRP:O	1:D:462:THR:HG22	2.13	0.48
1:A:382:ARG:O	1:A:386:GLN:HB2	2.13	0.48
1:C:544:TRP:HB2	1:C:623:CYS:SG	2.54	0.48
1:B:393:ARG:HB2	1:B:624:PHE:HB2	1.96	0.48
1:A:346:THR:HG21	1:A:670:LEU:HD22	1.96	0.48
1:C:215:THR:HG22	1:C:217:GLY:N	2.26	0.48
1:A:567:ILE:HG22	1:A:604:HIS:CE1	2.48	0.47
1:D:557:ILE:HG12	1:D:560:ILE:CG1	2.43	0.47
1:A:359:GLN:O	1:A:360:ASP:HB2	2.14	0.47
1:B:638:ASP:O	1:B:642:ARG:HG3	2.14	0.47
1:A:557:ILE:HG23	1:A:560:ILE:CB	2.39	0.47
1:C:83:SER:OG	1:C:97:SER:HA	2.13	0.47
1:A:280:GLN:HG3	1:B:280:GLN:HE21	1.80	0.47
1:D:350:VAL:O	1:D:354:ILE:HG12	2.14	0.47
1:A:349:ALA:HA	1:A:352:ARG:NH2	2.29	0.47
1:C:349:ALA:HA	1:C:352:ARG:NH2	2.29	0.47
1:B:236:LEU:HD22	1:B:290:LEU:HD11	1.97	0.47
1:D:14:LEU:HD21	1:D:176:ILE:HD11	1.97	0.47
1:D:220:ARG:HH11	1:D:454:ASP:CG	2.18	0.47
1:A:329:ILE:HD13	1:A:689:LEU:CD1	2.44	0.46
1:C:486:ASN:HD21	1:C:515:PRO:HD3	1.80	0.46
1:D:350:VAL:HG13	1:D:667:LEU:HB3	1.98	0.46
1:C:155:GLN:NE2	1:C:158:PRO:HA	2.31	0.46
1:C:371:VAL:O	1:C:371:VAL:HG12	2.15	0.46
1:D:346:THR:HG21	1:D:670:LEU:HD22	1.96	0.46
1:D:80:ARG:HD2	1:D:209:ARG:HB2	1.97	0.46
1:A:245:GLU:HG2	1:C:245:GLU:CG	2.42	0.46
1:C:387:LYS:O	1:C:391:ASN:HB2	2.14	0.46
1:C:364:LEU:HD11	1:C:649:LEU:HD13	1.97	0.46
1:A:111:TYR:HB2	1:A:172:LEU:O	2.16	0.46
1:C:393:ARG:HB3	1:C:624:PHE:HB3	1.94	0.46
1:A:390:ILE:O	1:A:393:ARG:HG3	2.16	0.46
1:A:373:PRO:O	1:A:377:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:ILE:CG1	1:D:560:ILE:HG13	2.46	0.45
1:B:393:ARG:NH2	1:B:625:ASP:OD2	2.46	0.45
1:D:215:THR:HG22	1:D:216:LEU:N	2.31	0.45
1:C:382:ARG:O	1:C:386:GLN:HB2	2.17	0.45
1:D:143:PRO:O	1:D:147:LYS:HG2	2.16	0.45
1:D:393:ARG:HB3	1:D:624:PHE:HB3	1.98	0.45
1:C:486:ASN:N	1:C:486:ASN:HD22	2.15	0.45
1:A:605:LEU:N	1:A:606:PRO:HD2	2.32	0.45
1:A:431:PHE:HE1	1:A:577:LEU:HD22	1.82	0.45
1:D:122:ASN:HD22	1:D:122:ASN:C	2.20	0.45
1:B:296:LEU:O	1:B:300:LEU:HB2	2.17	0.45
1:C:294:GLN:O	1:C:298:ARG:HG3	2.16	0.45
1:C:85:PHE:CZ	1:C:236:LEU:HD13	2.52	0.45
1:C:283:TYR:CE1	1:C:287:VAL:HG21	2.52	0.45
1:D:46:SER:HB2	1:D:663:GLU:HG2	1.98	0.45
1:C:181:SER:HB2	1:C:187:THR:CG2	2.46	0.45
1:B:445:GLN:HB2	1:B:569:LEU:HD21	1.98	0.45
1:C:90:ILE:HB	1:C:169:LEU:HD13	1.98	0.45
1:D:122:ASN:HD22	1:D:123:ASP:H	1.65	0.45
1:B:106:LEU:HD13	1:B:193:LEU:HD21	1.99	0.45
1:C:100:ASN:HA	1:C:101:PRO:HD2	1.81	0.44
1:D:423:GLN:HG3	1:D:593:LEU:HD12	1.98	0.44
1:D:74:VAL:HG21	1:D:86:LEU:HD21	1.99	0.44
1:A:382:ARG:CA	1:A:635:ILE:HD13	2.47	0.44
1:B:390:ILE:O	1:B:393:ARG:HG3	2.17	0.44
1:A:79:LYS:O	1:A:80:ARG:HD3	2.17	0.44
1:A:85:PHE:CZ	1:A:236:LEU:HD13	2.53	0.44
1:C:204:ILE:HB	1:C:233:VAL:HB	1.99	0.44
1:D:291:SER:OG	1:D:294:GLN:HB2	2.17	0.44
1:C:557:ILE:CG2	1:C:560:ILE:HB	2.47	0.44
1:A:464:GLU:HG2	1:A:544:TRP:CH2	2.38	0.44
1:C:238:ASN:HA	1:C:238:ASN:HD22	1.59	0.44
1:A:567:ILE:HG13	1:A:567:ILE:N	2.32	0.44
1:C:635:ILE:HG23	1:C:636:ASN:N	2.32	0.44
1:A:241:ASP:N	1:A:241:ASP:OD2	2.43	0.44
1:A:545:LYS:O	1:A:549:LEU:HB2	2.18	0.44
1:D:167:TYR:CD2	1:D:168:PRO:HD2	2.53	0.44
1:B:663:GLU:OE2	1:B:666:ARG:NH2	2.51	0.44
1:B:472:LYS:HE2	1:B:476:ARG:HH12	1.83	0.43
1:C:20:VAL:HG21	1:C:688:LEU:HG	2.00	0.43
1:D:464:GLU:HG2	1:D:544:TRP:CH2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLN:HG3	1:B:130:LEU:N	2.33	0.43
1:D:21:ARG:HG3	1:D:65:LEU:HD22	2.00	0.43
1:B:10:PHE:O	1:B:14:LEU:HB2	2.19	0.43
1:A:341:LEU:HD11	1:A:516:GLY:HA2	2.00	0.43
1:B:146:ALA:O	1:B:150:GLU:HB2	2.18	0.43
1:A:599:LYS:HE2	1:A:599:LYS:HA	2.00	0.43
1:D:220:ARG:NH1	1:D:454:ASP:OD2	2.49	0.43
1:D:390:ILE:O	1:D:393:ARG:HG3	2.19	0.43
1:D:557:ILE:CG2	1:D:560:ILE:CG1	2.58	0.43
1:C:322:PHE:HZ	1:C:327:ARG:HE	1.67	0.43
1:C:86:LEU:HA	1:C:86:LEU:HD23	1.90	0.43
1:A:220:ARG:HH11	1:A:454:ASP:CG	2.22	0.43
1:A:414:THR:HG22	1:A:418:ASP:OD2	2.18	0.43
1:A:382:ARG:HA	1:A:635:ILE:HD13	2.01	0.42
1:B:557:ILE:CG2	1:B:560:ILE:CB	2.97	0.42
1:A:371:VAL:HG13	1:A:492:ILE:HG12	1.99	0.42
1:B:43:ASP:HB3	1:B:48:LYS:HD3	2.01	0.42
1:A:635:ILE:CG2	1:A:636:ASN:N	2.82	0.42
1:A:329:ILE:HG22	1:A:329:ILE:O	2.17	0.42
1:D:86:LEU:HD23	1:D:86:LEU:HA	1.84	0.42
1:D:215:THR:HG22	1:D:217:GLY:N	2.33	0.42
1:A:678:LEU:HD22	1:A:682:GLU:HG3	2.02	0.42
1:A:155:GLN:NE2	1:A:158:PRO:HA	2.35	0.42
1:A:45:SER:HB3	1:A:46:SER:H	1.66	0.42
1:C:46:SER:HB3	1:C:663:GLU:CD	2.40	0.42
1:A:576:LEU:HD22	1:A:581:VAL:HG11	2.01	0.42
1:B:545:LYS:O	1:B:549:LEU:HB2	2.20	0.42
1:C:220:ARG:HH11	1:C:454:ASP:CG	2.22	0.42
1:C:80:ARG:HA	1:C:80:ARG:HD3	1.73	0.42
1:B:393:ARG:HB3	1:B:624:PHE:HB3	2.02	0.42
1:B:638:ASP:OD1	1:B:642:ARG:HD2	2.19	0.42
1:B:364:LEU:HD11	1:B:649:LEU:HD13	2.01	0.42
1:B:672:GLU:O	1:B:675:ILE:HG22	2.20	0.42
1:A:393:ARG:HB3	1:A:624:PHE:HB3	2.00	0.42
1:D:360:ASP:OD1	1:D:653:LYS:HD3	2.20	0.42
1:C:280:GLN:HG2	1:D:280:GLN:HE21	1.85	0.42
1:B:70:PHE:HB2	1:B:176:ILE:HD13	2.01	0.42
1:C:481:TYR:O	1:C:485:TYR:HB2	2.20	0.42
1:B:115:LYS:HB3	1:B:132:PHE:HB2	2.01	0.42
1:D:445:GLN:HB2	1:D:569:LEU:HD21	2.01	0.41
1:C:45:SER:HB3	1:C:46:SER:H	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:GLN:O	1:A:675:ILE:HB	2.20	0.41
1:C:39:GLU:HG3	1:C:48:LYS:CG	2.34	0.41
1:C:682:GLU:O	1:C:686:SER:HB2	2.20	0.41
1:A:544:TRP:HB2	1:A:623:CYS:SG	2.60	0.41
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.94	0.41
1:C:382:ARG:HA	1:C:635:ILE:HD13	2.02	0.41
1:D:408:VAL:O	1:D:605:LEU:HD22	2.20	0.41
1:D:263:LEU:HA	1:D:263:LEU:HD12	1.91	0.41
1:C:393:ARG:NH2	1:C:625:ASP:OD2	2.51	0.41
1:A:215:THR:HG22	1:A:216:LEU:N	2.35	0.41
1:B:393:ARG:HB3	1:B:624:PHE:HB2	1.98	0.41
1:A:236:LEU:HD22	1:A:290:LEU:HD11	2.02	0.41
1:C:222:LEU:HD23	1:C:226:ILE:HD13	2.02	0.41
1:D:38:ALA:O	1:D:666:ARG:NH1	2.53	0.41
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.85	0.41
1:A:557:ILE:CG2	1:A:560:ILE:CB	2.99	0.41
1:D:108:VAL:HG22	1:D:179:VAL:HG13	2.02	0.41
1:D:560:ILE:HG22	1:D:561:ILE:HD13	2.02	0.41
1:D:45:SER:HB3	1:D:46:SER:H	1.67	0.41
1:D:663:GLU:OE2	1:D:666:ARG:NH2	2.54	0.41
1:D:249:ASP:HA	1:D:250:PRO:HD2	1.95	0.41
1:B:79:LYS:O	1:B:80:ARG:HD3	2.21	0.41
1:B:167:TYR:CD2	1:B:168:PRO:HD2	2.56	0.41
1:D:115:LYS:HB3	1:D:132:PHE:HB2	2.02	0.41
1:C:359:GLN:O	1:C:653:LYS:HE3	2.20	0.41
1:A:150:GLU:C	1:A:152:GLU:H	2.24	0.41
1:A:576:LEU:HB3	1:A:581:VAL:HG21	2.03	0.41
1:B:350:VAL:HG13	1:B:667:LEU:HB3	2.03	0.41
1:C:557:ILE:CG1	1:C:557:ILE:HG23	2.45	0.40
1:B:423:GLN:CG	1:B:593:LEU:HD12	2.51	0.40
1:C:678:LEU:HD22	1:C:682:GLU:HG3	2.04	0.40
1:B:338:LEU:HD23	1:B:525:LEU:HD22	2.02	0.40
1:D:296:LEU:O	1:D:300:LEU:HB2	2.22	0.40
1:D:371:VAL:HG11	1:D:492:ILE:HG12	2.02	0.40
1:C:437:ARG:O	1:C:441:ASN:HB2	2.21	0.40
1:D:584:LEU:HB3	1:D:588:GLN:HB2	2.03	0.40
1:B:514:SER:HB2	1:B:515:PRO:HD2	2.03	0.40
1:C:423:GLN:HA	1:C:424:PRO:HD3	1.96	0.40
1:B:264:ARG:HD3	1:B:289:GLU:OE1	2.20	0.40
1:A:238:ASN:HA	1:A:238:ASN:HD22	1.57	0.40
1:D:545:LYS:O	1:D:549:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:HG2	1:B:219:ARG:H	1.67	0.40
1:B:367:ARG:O	1:B:371:VAL:HG23	2.22	0.40
1:C:10:PHE:O	1:C:14:LEU:HB2	2.21	0.40
1:D:110:ARG:O	1:D:166:GLU:HA	2.22	0.40
1:B:181:SER:HB2	1:B:187:THR:CG2	2.52	0.40
1:B:567:ILE:HD11	1:B:604:HIS:CE1	2.57	0.40
1:C:110:ARG:O	1:C:166:GLU:HA	2.21	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	665/695 (96%)	610 (92%)	48 (7%)	7 (1%)	17	58
1	B	665/695 (96%)	612 (92%)	45 (7%)	8 (1%)	16	56
1	C	665/695 (96%)	602 (90%)	54 (8%)	9 (1%)	14	51
1	D	665/695 (96%)	600 (90%)	56 (8%)	9 (1%)	14	51
All	All	2660/2780 (96%)	2424 (91%)	203 (8%)	33 (1%)	16	56

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	LEU
1	A	557	ILE
1	B	428	LEU
1	B	541	GLY
1	B	557	ILE
1	C	428	LEU
1	C	541	GLY
1	C	557	ILE

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Mol	Chain	Res	Type
1	D	360	ASP
1	D	428	LEU
1	D	557	ILE
1	A	360	ASP
1	A	413	ASN
1	B	360	ASP
1	B	413	ASN
1	C	215	THR
1	C	413	ASN
1	D	541	GLY
1	B	182	PRO
1	D	68	GLY
1	A	127	PRO
1	B	127	PRO
1	C	182	PRO
1	D	182	PRO
1	A	215	THR
1	C	360	ASP
1	B	361	VAL
1	D	127	PRO
1	D	561	ILE
1	C	516	GLY
1	A	182	PRO
1	C	127	PRO
1	D	516	GLY

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	584/601 (97%)	518 (89%)	66 (11%)	7	28
1	B	584/601 (97%)	510 (87%)	74 (13%)	5	23
1	C	584/601 (97%)	511 (88%)	73 (12%)	6	24
1	D	584/601 (97%)	511 (88%)	73 (12%)	6	24
All	All	2336/2404 (97%)	2050 (88%)	286 (12%)	6	25

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	39	GLU
1	A	45	SER
1	A	46	SER
1	A	89	LEU
1	A	105	VAL
1	A	122	ASN
1	A	126	SER
1	A	130	LEU
1	A	141	ILE
1	A	159	ASP
1	A	167	TYR
1	A	170	THR
1	A	171	LEU
1	A	184	LEU
1	A	192	GLU
1	A	200	ASN
1	A	205	LEU
1	A	211	SER
1	A	229	ARG
1	A	233	VAL
1	A	238	ASN
1	A	265	GLN
1	A	273	GLU
1	A	293	ILE
1	A	294	GLN
1	A	301	LYS
1	A	314	LYS
1	A	331	GLU
1	A	336	ARG
1	A	338	LEU
1	A	364	LEU
1	A	391	ASN
1	A	393	ARG
1	A	410	ASN
1	A	414	THR
1	A	420	LEU
1	A	427	ASN
1	A	431	PHE
1	A	432	LEU
1	A	444	LEU
1	A	462	THR

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Mol	Chain	Res	Type
1	A	489	THR
1	A	499	LYS
1	A	510	GLU
1	A	514	SER
1	A	545	LYS
1	A	548	LEU
1	A	549	LEU
1	A	579	LEU
1	A	592	GLU
1	A	593	LEU
1	A	594	VAL
1	A	599	LYS
1	A	601	LEU
1	A	622	GLU
1	A	623	CYS
1	A	649	LEU
1	A	655	THR
1	A	661	GLU
1	A	670	LEU
1	A	675	ILE
1	A	677	GLN
1	A	678	LEU
1	A	686	SER
1	A	688	LEU
1	B	37	LYS
1	B	39	GLU
1	B	46	SER
1	B	48	LYS
1	B	89	LEU
1	B	95	LEU
1	B	97	SER
1	B	100	ASN
1	B	105	VAL
1	B	122	ASN
1	B	126	SER
1	B	130	LEU
1	B	141	ILE
1	B	167	TYR
1	B	170	THR
1	B	171	LEU
1	B	184	LEU
1	B	192	GLU

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Mol	Chain	Res	Type
1	B	200	ASN
1	B	205	LEU
1	B	211	SER
1	B	229	ARG
1	B	233	VAL
1	B	238	ASN
1	B	241	ASP
1	B	263	LEU
1	B	273	GLU
1	B	294	GLN
1	B	301	LYS
1	B	314	LYS
1	B	321	THR
1	B	336	ARG
1	B	338	LEU
1	B	353	ARG
1	B	364	LEU
1	B	391	ASN
1	B	393	ARG
1	B	410	ASN
1	B	414	THR
1	B	420	LEU
1	B	426	LEU
1	B	427	ASN
1	B	433	SER
1	B	441	ASN
1	B	444	LEU
1	B	462	THR
1	B	489	THR
1	B	499	LYS
1	B	510	GLU
1	B	511	GLU
1	B	514	SER
1	B	545	LYS
1	B	548	LEU
1	B	549	LEU
1	B	554	VAL
1	B	560	ILE
1	B	561	ILE
1	B	567	ILE
1	B	577	LEU
1	B	579	LEU

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Mol	Chain	Res	Type
1	B	592	GLU
1	B	594	VAL
1	B	599	LYS
1	B	601	LEU
1	B	622	GLU
1	B	623	CYS
1	B	647	ASP
1	B	649	LEU
1	B	655	THR
1	B	661	GLU
1	B	670	LEU
1	B	675	ILE
1	B	677	GLN
1	B	678	LEU
1	C	7	THR
1	C	22	SER
1	C	37	LYS
1	C	39	GLU
1	C	45	SER
1	C	46	SER
1	C	48	LYS
1	C	89	LEU
1	C	97	SER
1	C	99	VAL
1	C	105	VAL
1	C	122	ASN
1	C	126	SER
1	C	130	LEU
1	C	141	ILE
1	C	167	TYR
1	C	170	THR
1	C	171	LEU
1	C	184	LEU
1	C	192	GLU
1	C	200	ASN
1	C	211	SER
1	C	229	ARG
1	C	233	VAL
1	C	238	ASN
1	C	241	ASP
1	C	262	ARG
1	C	263	LEU

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Mol	Chain	Res	Type
1	C	265	GLN
1	C	293	ILE
1	C	294	GLN
1	C	314	LYS
1	C	331	GLU
1	C	336	ARG
1	C	338	LEU
1	C	361	VAL
1	C	364	LEU
1	C	391	ASN
1	C	393	ARG
1	C	410	ASN
1	C	414	THR
1	C	420	LEU
1	C	421	ARG
1	C	427	ASN
1	C	433	SER
1	C	444	LEU
1	C	462	THR
1	C	475	SER
1	C	477	SER
1	C	489	THR
1	C	499	LYS
1	C	510	GLU
1	C	511	GLU
1	C	514	SER
1	C	545	LYS
1	C	549	LEU
1	C	550	ASN
1	C	577	LEU
1	C	579	LEU
1	C	592	GLU
1	C	593	LEU
1	C	594	VAL
1	C	599	LYS
1	C	601	LEU
1	C	622	GLU
1	C	623	CYS
1	C	649	LEU
1	C	655	THR
1	C	670	LEU
1	C	675	ILE

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Mol	Chain	Res	Type
1	C	677	GLN
1	C	678	LEU
1	C	688	LEU
1	D	12	GLN
1	D	13	ASP
1	D	14	LEU
1	D	37	LYS
1	D	39	GLU
1	D	45	SER
1	D	48	LYS
1	D	89	LEU
1	D	95	LEU
1	D	99	VAL
1	D	100	ASN
1	D	122	ASN
1	D	126	SER
1	D	130	LEU
1	D	141	ILE
1	D	167	TYR
1	D	170	THR
1	D	171	LEU
1	D	184	LEU
1	D	192	GLU
1	D	200	ASN
1	D	205	LEU
1	D	211	SER
1	D	229	ARG
1	D	233	VAL
1	D	236	LEU
1	D	238	ASN
1	D	241	ASP
1	D	263	LEU
1	D	293	ILE
1	D	294	GLN
1	D	314	LYS
1	D	336	ARG
1	D	338	LEU
1	D	353	ARG
1	D	364	LEU
1	D	391	ASN
1	D	393	ARG
1	D	410	ASN

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Mol	Chain	Res	Type
1	D	414	THR
1	D	420	LEU
1	D	426	LEU
1	D	427	ASN
1	D	431	PHE
1	D	433	SER
1	D	441	ASN
1	D	444	LEU
1	D	462	THR
1	D	489	THR
1	D	499	LYS
1	D	510	GLU
1	D	511	GLU
1	D	514	SER
1	D	545	LYS
1	D	548	LEU
1	D	549	LEU
1	D	554	VAL
1	D	577	LEU
1	D	579	LEU
1	D	592	GLU
1	D	594	VAL
1	D	599	LYS
1	D	601	LEU
1	D	622	GLU
1	D	623	CYS
1	D	649	LEU
1	D	655	THR
1	D	661	GLU
1	D	670	LEU
1	D	675	ILE
1	D	677	GLN
1	D	678	LEU
1	D	688	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	100	ASN
1	A	122	ASN
1	A	128	GLN

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Mol	Chain	Res	Type
1	A	155	GLN
1	A	191	ASN
1	A	238	ASN
1	A	294	GLN
1	A	362	ASN
1	A	410	ASN
1	A	423	GLN
1	A	450	GLN
1	A	480	GLN
1	A	486	ASN
1	A	550	ASN
1	A	604	HIS
1	A	648	ASN
1	A	654	GLN
1	B	64	ASN
1	B	122	ASN
1	B	128	GLN
1	B	155	GLN
1	B	191	ASN
1	B	238	ASN
1	B	280	GLN
1	B	410	ASN
1	B	450	GLN
1	B	480	GLN
1	B	486	ASN
1	B	550	ASN
1	B	618	ASN
1	B	654	GLN
1	B	659	ASN
1	C	100	ASN
1	C	122	ASN
1	C	134	ASN
1	C	155	GLN
1	C	191	ASN
1	C	238	ASN
1	C	294	GLN
1	C	410	ASN
1	C	423	GLN
1	C	450	GLN
1	C	486	ASN
1	C	550	ASN
1	C	588	GLN

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Mol	Chain	Res	Type
1	C	604	HIS
1	C	614	GLN
1	C	618	ASN
1	C	648	ASN
1	C	654	GLN
1	C	659	ASN
1	D	64	ASN
1	D	100	ASN
1	D	122	ASN
1	D	128	GLN
1	D	155	GLN
1	D	191	ASN
1	D	238	ASN
1	D	280	GLN
1	D	304	GLN
1	D	362	ASN
1	D	410	ASN
1	D	423	GLN
1	D	450	GLN
1	D	486	ASN
1	D	550	ASN
1	D	618	ASN
1	D	652	GLN
1	D	654	GLN
1	D	659	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

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 [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	671/695 (96%)	-0.07	1 (0%) 95 90	35, 59, 84, 104	0
1	B	671/695 (96%)	-0.05	3 (0%) 93 80	35, 59, 84, 104	0
1	C	671/695 (96%)	-0.06	1 (0%) 95 90	35, 59, 84, 104	0
1	D	671/695 (96%)	-0.09	3 (0%) 93 80	35, 59, 84, 104	0
All	All	2684/2780 (96%)	-0.06	8 (0%) 94 84	35, 59, 84, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	GLN	3.5
1	B	4	GLN	3.2
1	D	557	ILE	2.6
1	B	186	ASP	2.3
1	D	540	ALA	2.3
1	B	557	ILE	2.3
1	D	4	GLN	2.3
1	C	151	GLN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.