



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:02 AM UTC

PDB ID : 2J69 / pdb_00002j69
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

<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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

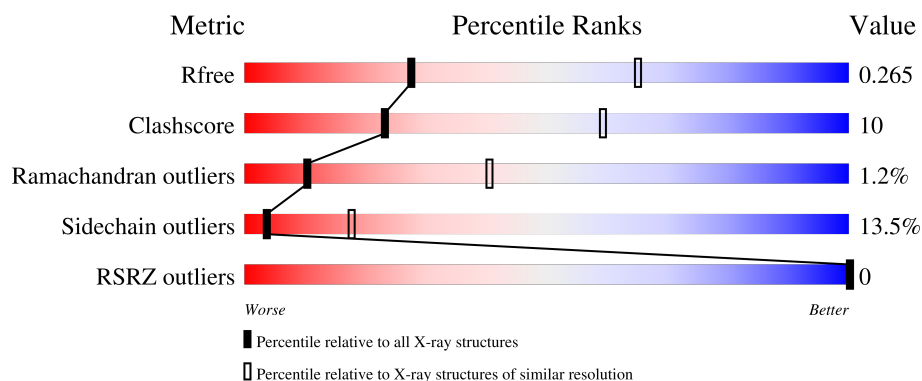
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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.

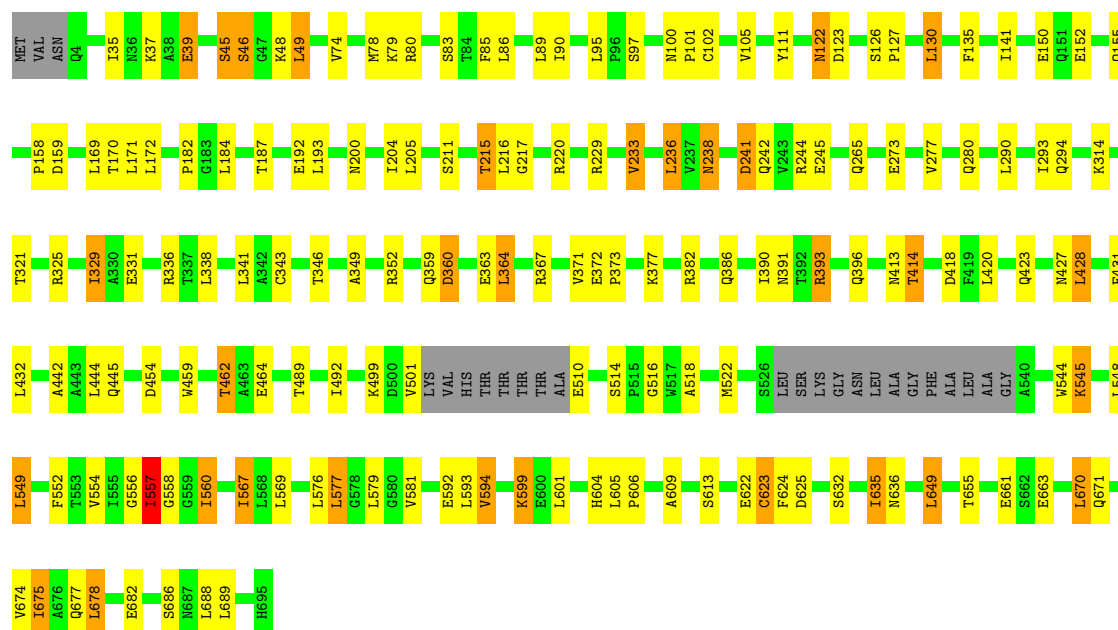
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			
1	B	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			
1	C	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			
1	D	671	Total	C	N	O	S	0	0	0
			5375	3385	941	1037	12			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

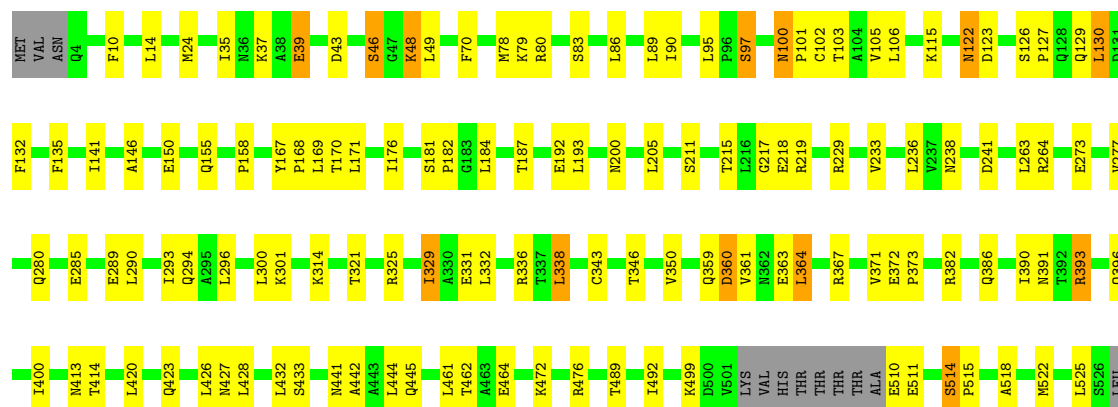
• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

Chain A: 



• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

Chain B: 





● Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

S514	P373	L236	S126	ME1
P515	R352	V237	P127	VAL
G516	Q356	D241	L130	Q4
S517	I390	D249	D131	Q12
A518	R393	P250	F132	D13
M522	R396	L263	F135	L14
L525	Q396	R264	I141	R21
S526	I400	Q265	D142	M24
LEU	V408	Q280	P143	I36
SER	LYS	S291	K147	N36
GLY	ASN	I293	Q155	K37
LEU	T414	I294	E158	A38
LEU	L420	A295	P168	E39
GLY	Q423	L296	P165	S45
PHE	L426	L300	E166	S46
ALA	L427	L300	P167	G47
LEU	L428	K314	L169	K48
ALA	L433	T321	L171	L49
GLY	N441	R325	I176	L65
ALA	A442	I329	V179	G68
LEU	A443	A330	P182	V74
LEU	Q445	E331	G183	M78
S552	D454	L332	L184	K79
T553	W459	R336	S83	R80
V554	T460	I337	T187	S83
S556	L461	L338	E192	L86
L557	T462	C343	L193	L89
S558	K463	T346	N200	I90
S559	A464	A349	L205	L95
L560	T489	V350	R209	P96
S561	I492	A351	A210	S97
L568	K499	R352	S211	D98
L569	D500	I354	T215	V99
S570	LYS	Q359	L216	N100
L577	VAL	D360	G217	P101
S578	HIS	E363	E218	C102
L579	THR	L364	R219	T103
L584	THR	R367	R220	V108
Q588	THR	R367	R229	L109
S592	ALA	V371	V233	R110
L593	E510	P370		K115
S594	F511			N122
				D122



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.29Å 218.60Å 151.20Å 90.00° 134.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.00) 96.9 (50.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.281 0.225 , 0.265	Depositor DCC
R_{free} test set	4869 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
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
F_o, F_c correlation	0.96	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.93	6/5459 (0.1%)	0.98	13/7368 (0.2%)
1	B	0.91	6/5459 (0.1%)	0.99	15/7368 (0.2%)
1	C	0.81	6/5459 (0.1%)	0.97	14/7368 (0.2%)
1	D	0.96	6/5459 (0.1%)	0.97	13/7368 (0.2%)
All	All	0.90	24/21836 (0.1%)	0.98	55/29472 (0.2%)

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	46.07	2.45	1.53
1	A	557	ILE	CB-CG1	41.37	2.36	1.53
1	B	557	ILE	CB-CG1	38.83	2.31	1.53
1	C	557	ILE	CB-CG1	31.77	2.17	1.53
1	A	567	ILE	CB-CG1	-31.75	0.90	1.53
1	B	567	ILE	CB-CG1	-24.50	1.04	1.53
1	D	567	ILE	CB-CG1	-24.07	1.05	1.53
1	C	567	ILE	CB-CG1	-22.16	1.09	1.53
1	B	635	ILE	CB-CG1	-19.11	1.15	1.53
1	D	557	ILE	CB-CG2	16.97	2.08	1.52
1	B	329	ILE	CB-CG1	-15.62	1.22	1.53
1	C	557	ILE	CB-CG2	14.66	2.00	1.52
1	D	635	ILE	CB-CG1	-14.65	1.24	1.53
1	D	329	ILE	CB-CG1	-14.10	1.25	1.53
1	B	557	ILE	CB-CG2	14.03	1.98	1.52
1	A	635	ILE	CB-CG1	-12.72	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	635	ILE	CB-CG1	-11.95	1.29	1.53
1	A	557	ILE	CB-CG2	11.31	1.89	1.52
1	C	329	ILE	CB-CG1	-9.59	1.34	1.53
1	A	329	ILE	CB-CG1	-8.41	1.36	1.53
1	A	567	ILE	CB-CG2	7.08	1.75	1.52
1	C	567	ILE	CB-CG2	6.15	1.72	1.52
1	D	567	ILE	CB-CG2	5.55	1.70	1.52
1	B	329	ILE	CB-CG2	5.33	1.70	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	557	ILE	CG1-CB-CG2	-14.72	66.53	110.70
1	A	567	ILE	CA-CB-CG2	-13.87	86.92	110.50
1	C	567	ILE	CA-CB-CG2	-13.43	87.67	110.50
1	B	557	ILE	CG1-CB-CG2	-13.24	70.98	110.70
1	A	557	ILE	CG1-CB-CG2	-13.15	71.25	110.70
1	C	557	ILE	CG1-CB-CG2	-12.33	73.71	110.70
1	B	567	ILE	CG1-CB-CG2	11.35	144.74	110.70
1	B	567	ILE	CA-CB-CG2	-11.15	91.54	110.50
1	A	567	ILE	CG1-CB-CG2	11.14	144.11	110.70
1	B	103	THR	N-CA-C	-9.98	103.24	114.62
1	D	567	ILE	CA-CB-CG2	-9.63	94.12	110.50
1	C	103	THR	N-CA-C	-8.95	103.47	114.75
1	B	635	ILE	CG1-CB-CG2	8.72	136.87	110.70
1	C	557	ILE	CB-CG1-CD1	8.52	131.68	113.80
1	B	557	ILE	CB-CG1-CD1	8.34	131.32	113.80
1	A	567	ILE	CA-CB-CG1	8.10	124.16	110.40
1	B	329	ILE	CA-CB-CG2	-7.97	96.95	110.50
1	D	567	ILE	CG1-CB-CG2	7.55	133.34	110.70
1	A	635	ILE	CA-CB-CG2	-7.42	97.89	110.50
1	A	329	ILE	CA-CB-CG2	-7.38	97.95	110.50
1	D	557	ILE	CB-CG1-CD1	7.28	129.08	113.80
1	D	49	LEU	N-CA-C	-7.03	100.08	110.48
1	D	635	ILE	CG1-CB-CG2	6.78	131.04	110.70
1	C	329	ILE	CA-CB-CG2	-6.74	99.04	110.50
1	A	557	ILE	CB-CG1-CD1	6.71	127.89	113.80
1	B	557	ILE	CA-CB-CG2	6.53	121.60	110.50
1	D	570	GLY	CA-C-N	6.46	126.97	119.47
1	D	570	GLY	C-N-CA	6.46	126.97	119.47
1	B	49	LEU	N-CA-C	-6.38	100.11	110.20
1	A	635	ILE	CA-CB-CG1	-6.36	99.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	LEU	N-CA-C	-6.35	101.55	110.50
1	D	103	THR	N-CA-C	-6.31	104.79	113.18
1	D	329	ILE	CA-CB-CG2	-6.25	99.87	110.50
1	C	100	ASN	CA-C-N	6.23	127.63	119.84
1	C	100	ASN	C-N-CA	6.23	127.63	119.84
1	B	100	ASN	CA-C-N	6.21	126.39	119.32
1	B	100	ASN	C-N-CA	6.21	126.39	119.32
1	C	570	GLY	CA-C-N	6.18	127.57	119.84
1	C	570	GLY	C-N-CA	6.18	127.57	119.84
1	C	557	ILE	CA-CB-CG2	5.91	120.55	110.50
1	C	567	ILE	CB-CG1-CD1	-5.74	101.75	113.80
1	C	557	ILE	CA-CB-CG1	5.70	120.10	110.40
1	D	567	ILE	CA-CB-CG1	5.64	119.99	110.40
1	A	635	ILE	CB-CG1-CD1	-5.46	102.34	113.80
1	B	567	ILE	CB-CG1-CD1	-5.44	102.37	113.80
1	A	557	ILE	CA-CB-CG2	5.41	119.70	110.50
1	D	100	ASN	CA-C-N	5.33	126.50	119.84
1	D	100	ASN	C-N-CA	5.33	126.50	119.84
1	B	570	GLY	CA-C-N	5.31	126.48	119.84
1	B	570	GLY	C-N-CA	5.31	126.48	119.84
1	C	567	ILE	CG1-CB-CG2	5.29	126.57	110.70
1	A	49	LEU	N-CA-C	-5.26	101.89	110.20
1	A	100	ASN	CA-C-N	5.19	125.49	119.47
1	A	100	ASN	C-N-CA	5.19	125.49	119.47
1	B	557	ILE	CA-CB-CG1	5.18	119.21	110.40

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	128	0
1	B	5375	0	5366	100	0
1	C	5375	0	5366	111	0
1	D	5375	0	5366	111	0
All	All	21500	0	21464	444	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 (444) 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:HB	1:A:567:ILE:CD1	1.21	1.55
1:D:552:PHE:CD1	1:D:557:ILE:CD1	1.92	1.49
1:A:557:ILE:CB	1:A:557:ILE:CG2	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:CG2	1:B:557:ILE:CB	1.98	1.38
1:C:557:ILE:CB	1:C:557:ILE:CG2	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:CG2	1:D:557:ILE:CB	2.08	1.31
1:A:552:PHE:CD1	1:A:557:ILE:CD1	2.17	1.28
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:CB	1:C:557:ILE:CG1	2.17	1.23
1:A:567:ILE:CG2	1:A:567:ILE:O	1.87	1.22
1:A:567:ILE:CG2	1:A:567:ILE:C	2.11	1.22
1:A:552:PHE:CE1	1:A:557:ILE:HD11	1.75	1.21
1:A:567:ILE:CG1	1:A:567:ILE:CA	2.19	1.20
1:D:557:ILE:HG23	1:D:560:ILE:CG1	1.71	1.20
1:A:567:ILE:C	1:A:567:ILE:HG22	1.68	1.18
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:A:567:ILE:HG23	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:A:567:ILE:O	1:A:567:ILE:HG22	1.54	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:C:567:ILE:O	1:C:567:ILE:CG2	2.09	0.98
1:C:567:ILE:O	1:C:567:ILE:HG22	1.56	0.98
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:HB	1:A:567:ILE:HD12	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
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:CG2	1:D:567:ILE:O	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:CG2	1:C:557:ILE:CG1	2.50	0.89
1:D:557:ILE:CG2	1:D:557:ILE:CG1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:D:567:ILE:HG22	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
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:A:382:ARG:CB	1:A:635:ILE:HD13	2.22	0.70
1:C:552:PHE:HD1	1:C:557:ILE:CD1	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:130:LEU:HD13	1:A:135:PHE:HB2	1.74	0.68
1:C:557:ILE:HG12	1:C:560:ILE:CG1	2.20	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:O	1:D:567:ILE:HG23	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:O	1:C:567:ILE:HG23	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:A:122:ASN:HD22	1:A:123:ASP:N	1.93	0.65
1:B:187:THR:HG22	1:B:193:LEU:HD13	1.78	0.65
1:D:557:ILE:N	1:D:558:GLY:HA3	2.11	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:102:CYS:HB2	1:D:155:GLN:HA	1.78	0.65
1:D:557:ILE:HG23	1:D:557:ILE:CG1	2.27	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:A:518:ALA:O	1:A:522:MET:HG3	1.97	0.63
1:B:90:ILE:HB	1:B:169:LEU:HD13	1.79	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:HG23	1:A:557:ILE:CG1	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:HB	1:A:567:ILE:HG13	1.36	0.63
1:D:359:GLN:O	1:D:360:ASP:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:ARG:HB3	1:D:624:PHE:CB	2.29	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:B:78:MET:HE3	1:B:101:PRO:HA	1.85	0.59
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:B:661:GLU:HG2	1:C:134:ASN:HD21	1.67	0.59
1:D:393:ARG:HB3	1:D:624:PHE:HB2	1.85	0.59
1:C:24:MET:HE2	1:C:332:LEU:HD22	1.84	0.58
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:B:24:MET:HE2	1:B:332:LEU:HD22	1.86	0.57
1:A:393:ARG:HB3	1:A:624:PHE:CB	2.33	0.57
1:C:557:ILE:N	1:C:558:GLY:HA3	2.19	0.57
1:C:74:VAL:HG21	1:C:86:LEU:HD21	1.85	0.57
1:A:393:ARG:NH2	1:A:625:ASP:OD2	2.37	0.57
1:B:557:ILE:HG23	1:B:560:ILE:CB	2.33	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
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:C:122:ASN:HD22	1:C:122:ASN:C	2.11	0.56
1:A:442:ALA:O	1:A:445:GLN:HB3	2.06	0.56
1:C:445:GLN:HB2	1:C:569:LEU:HD21	1.86	0.56
1:D:363:GLU:OE2	1:D:367:ARG:NH2	2.39	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:B:423:GLN:HE22	1:B:594:VAL:HG22	1.69	0.56
1:D:393:ARG:CB	1:D:624:PHE:HB2	2.36	0.56
1:A:576:LEU:O	1:A:581:VAL:HG22	2.07	0.55
1:C:325:ARG:O	1:C:329:ILE:HD12	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:423:GLN:HE22	1:A:594:VAL:HG22	1.71	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: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:HA	1:D:599:LYS:HE2	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:B:122:ASN:HD22	1:B:122:ASN:C	2.16	0.54
1:A:393:ARG:HB3	1:A:624:PHE:HB2	1.88	0.53
1:B:359:GLN:O	1:B:360:ASP:HB2	2.08	0.53
1:B:393:ARG:CB	1:B:624:PHE:HB2	2.37	0.53
1:C:187:THR:HG22	1:C:193:LEU:HD13	1.90	0.53
1:D:215:THR:O	1:D:219:ARG:HG2	2.09	0.53
1:B:561:ILE:CG2	1:B:562:THR:N	2.72	0.53
1:B:39:GLU:HG3	1:B:48:LYS:CG	2.38	0.53
1:B:346:THR:HG21	1:B:670:LEU:HD22	1.91	0.53
1:C:363:GLU:OE2	1:C:367:ARG:NH2	2.42	0.53
1:D:100:ASN:HD22	1:D:102:CYS:H	1.57	0.53
1:B:567:ILE:HD11	1:B:604:HIS:ND1	2.24	0.52
1:C:663:GLU:OE2	1:C:666:ARG:NH2	2.42	0.52
1:C:557:ILE:H	1:C:558:GLY:HA3	1.74	0.52
1:D:24:MET:HE2	1:D:332:LEU:HD22	1.92	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
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: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:D:220:ARG:HH11	1:D:454:ASP:CG	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:CG	1:C:48:LYS:HG2	2.32	0.51
1:C:552:PHE:CD1	1:C:557:ILE:HD11	2.18	0.51
1:D:552:PHE:HD1	1:D:557:ILE:CG1	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:HE2	1:B:599:LYS:HA	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:D:122:ASN:HD22	1:D:122:ASN:C	2.20	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:325:ARG:O	1:B:329:ILE:HD12	2.12	0.49
1:B:581:VAL:HG12	1:B:584:LEU:HD12	1.94	0.49
1:B:83:SER:OG	1:B:97:SER:HA	2.12	0.49
1:C:346:THR:HG21	1:C:670:LEU:HD22	1.94	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:A:372:GLU:N	1:A:373:PRO:HD2	2.27	0.49
1:B:329:ILE:HD13	1:B:689:LEU:HD13	1.95	0.49
1:D:338:LEU:HD23	1:D:525:LEU:HD22	1.93	0.49
1:D:678:LEU:HD22	1:D:682:GLU:HG3	1.95	0.49
1:A:632:SER:O	1:A:635:ILE:HG22	2.13	0.49
1:C:262:ARG:O	1:C:266:VAL:HG23	2.13	0.49
1:A:363:GLU:OE2	1:A:367:ARG:NH2	2.46	0.49
1:B:382:ARG:O	1:B:386:GLN:HB2	2.13	0.49
1:B:557:ILE:CG1	1:B:557:ILE:HG23	2.37	0.49
1:B:561:ILE:HG22	1:B:562:THR:H	1.79	0.48
1:C:79:LYS:HG2	1:C:99:VAL:HG12	1.94	0.48
1:D:682:GLU:O	1:D:686:SER:HB2	2.13	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:A:187:THR:HG22	1:A:193:LEU:HD13	1.95	0.48
1:B:557:ILE:CG1	1:B:560:ILE:HG13	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG21	1:A:670:LEU:HD22	1.96	0.48
1:A:382:ARG:O	1:A:386:GLN:HB2	2.13	0.48
1:B:393:ARG:HB2	1:B:624:PHE:HB2	1.96	0.48
1:C:544:TRP:HB2	1:C:623:CYS:SG	2.54	0.48
1:C:215:THR:HG22	1:C:217:GLY:N	2.26	0.48
1:C:220:ARG:HH11	1:C:454:ASP:CG	2.22	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:220:ARG:HH11	1:A:454:ASP:CG	2.22	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:A:349:ALA:HA	1:A:352:ARG:NH2	2.29	0.47
1:D:350:VAL:O	1:D:354:ILE:HG12	2.14	0.47
1:B:236:LEU:HD22	1:B:290:LEU:HD11	1.97	0.47
1:C:349:ALA:HA	1:C:352:ARG:NH2	2.29	0.47
1:C:46:SER:HB3	1:C:663:GLU:CD	2.40	0.47
1:D:14:LEU:HD21	1:D:176:ILE:HD11	1.97	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:A:78:MET:HE3	1:A:101:PRO:HA	1.97	0.46
1:C:155:GLN:NE2	1:C:158:PRO:HA	2.31	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:371:VAL:HG12	1:C:371:VAL:O	2.15	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:A:373:PRO:O	1:A:377:LYS:HG3	2.16	0.46
1:A:390:ILE:O	1:A:393:ARG:HG3	2.16	0.46
1:C:393:ARG:HB3	1:C:624:PHE:HB3	1.94	0.46
1:B:393:ARG:NH2	1:B:625:ASP:OD2	2.46	0.45
1:D:557:ILE:CG1	1:D:560:ILE:HG13	2.46	0.45
1:C:382:ARG:O	1:C:386:GLN:HB2	2.17	0.45
1:A:150:GLU:C	1:A:152:GLU:H	2.24	0.45
1:D:143:PRO:O	1:D:147:LYS:HG2	2.16	0.45
1:A:431:PHE:HE1	1:A:577:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:N	1:A:606:PRO:HD2	2.32	0.45
1:C:486:ASN:N	1:C:486:ASN:HD22	2.15	0.45
1:D:393:ARG:HB3	1:D:624:PHE:HB3	1.98	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: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:C:181:SER:HB2	1:C:187:THR:CG2	2.46	0.45
1:D:46:SER:HB2	1:D:663:GLU:HG2	1.98	0.45
1:B:106:LEU:HD13	1:B:193:LEU:HD21	1.99	0.45
1:D:122:ASN:HD22	1:D:123:ASP:H	1.65	0.45
1:C:100:ASN:HA	1:C:101:PRO:HD2	1.81	0.44
1:D:74:VAL:HG21	1:D:86:LEU:HD21	1.99	0.44
1:D:423:GLN:HG3	1:D:593:LEU:HD12	1.98	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: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:C:204:ILE:HB	1:C:233:VAL:HB	1.99	0.44
1:D:215:THR:HG22	1:D:216:LEU:N	2.31	0.44
1:D:291:SER:OG	1:D:294:GLN:HB2	2.17	0.44
1:A:464:GLU:HG2	1:A:544:TRP:CH2	2.38	0.44
1:C:557:ILE:CG2	1:C:560:ILE:HB	2.47	0.44
1:C:238:ASN:HD22	1:C:238:ASN:HA	1.59	0.44
1:A:241:ASP:OD2	1:A:241:ASP:N	2.43	0.44
1:A:242:GLN:C	1:A:244:ARG:N	2.73	0.44
1:A:567:ILE:HG13	1:A:567:ILE:N	2.32	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:C:197:TYR:O	1:C:198:VAL:C	2.61	0.43
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:D:464:GLU:HG2	1:D:544:TRP:CH2	2.45	0.43
1:A:341:LEU:HD11	1:A:516:GLY:HA2	2.00	0.43
1:B:10:PHE:O	1:B:14:LEU:HB2	2.19	0.43
1:B:146:ALA:O	1:B:150:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LYS:HE2	1:A:599:LYS:HA	2.00	0.43
1:C:635:ILE:HG23	1:C:636:ASN:N	2.32	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:C:322:PHE:HZ	1:C:327:ARG:HE	1.67	0.43
1:D:557:ILE:CG2	1:D:560:ILE:CG1	2.58	0.43
1:A:414:THR:HG22	1:A:418:ASP:OD2	2.18	0.43
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.90	0.43
1:A:382:ARG:HA	1:A:635:ILE:HD13	2.01	0.42
1:A:371:VAL:HG13	1:A:492:ILE:HG12	1.99	0.42
1:B:557:ILE:CG2	1:B:560:ILE:CB	2.97	0.42
1:B:43:ASP:HB3	1:B:48:LYS:HD3	2.01	0.42
1:A:329:ILE:O	1:A:329:ILE:HG22	2.17	0.42
1:A:635:ILE:CG2	1:A:636:ASN:N	2.82	0.42
1:D:86:LEU:HD23	1:D:86:LEU:HA	1.84	0.42
1:A:678:LEU:HD22	1:A:682:GLU:HG3	2.02	0.42
1:D:215:THR:HG22	1:D:217:GLY:N	2.33	0.42
1:A:45:SER:HB3	1:A:46:SER:H	1.66	0.42
1:A:155:GLN:NE2	1:A:158:PRO:HA	2.35	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:80:ARG:HA	1:C:80:ARG:HD3	1.73	0.42
1:B:46:SER:HB3	1:B:663:GLU:CD	2.44	0.42
1:B:364:LEU:HD11	1:B:649:LEU:HD13	2.01	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:672:GLU:O	1:B:675:ILE:HG22	2.20	0.42
1:C:122:ASN:C	1:C:122:ASN:ND2	2.78	0.42
1:A:393:ARG:HB3	1:A:624:PHE:HB3	2.00	0.42
1:B:70:PHE:HB2	1:B:176:ILE:HD13	2.01	0.42
1:B:115:LYS:HB3	1:B:132:PHE:HB2	2.01	0.42
1:C:280:GLN:HG2	1:D:280:GLN:HE21	1.85	0.42
1:C:481:TYR:O	1:C:485:TYR:HB2	2.20	0.42
1:D:360:ASP:OD1	1:D:653:LYS:HD3	2.20	0.42
1:D:445:GLN:HB2	1:D:569:LEU:HD21	2.01	0.41
1:A:671:GLN:O	1:A:675:ILE:HB	2.20	0.41
1:C:45:SER:HB3	1:C:46:SER:H	1.60	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:86:LEU:HD23	1:A:86:LEU:HA	1.94	0.41
1:A:544:TRP:HB2	1:A:623:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ARG:HA	1:C:635:ILE:HD13	2.02	0.41
1:D:263:LEU:HD12	1:D:263:LEU:HA	1.91	0.41
1:D:408:VAL:O	1:D:605:LEU:HD22	2.20	0.41
1:A:122:ASN:HD22	1:A:122:ASN:C	2.24	0.41
1:C:393:ARG:NH2	1:C:625:ASP:OD2	2.51	0.41
1:A:236:LEU:HD22	1:A:290:LEU:HD11	2.02	0.41
1:B:393:ARG:HB3	1:B:624:PHE:HB2	1.98	0.41
1:C:222:LEU:HD23	1:C:226:ILE:HD13	2.02	0.41
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.85	0.41
1:D:38:ALA:O	1:D:666:ARG:NH1	2.53	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: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:C:359:GLN:O	1:C:653:LYS:HE3	2.20	0.41
1:D:45:SER:HB3	1:D:46:SER:H	1.67	0.41
1:D:115:LYS:HB3	1:D:132:PHE:HB2	2.02	0.41
1:D:249:ASP:HA	1:D:250:PRO:HD2	1.95	0.41
1:D:560:ILE:HG22	1:D:561:ILE:HD13	2.02	0.41
1:D:663:GLU:OE2	1:D:666:ARG:NH2	2.54	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:D:78:MET:HE3	1:D:101:PRO:HA	2.02	0.41
1:D:220:ARG:NH1	1:D:454:ASP:CG	2.80	0.41
1:B:338:LEU:HD23	1:B:525:LEU:HD22	2.02	0.40
1:B:423:GLN:CG	1:B:593:LEU:HD12	2.51	0.40
1:C:557:ILE:CG1	1:C:557:ILE:HG23	2.45	0.40
1:C:678:LEU:HD22	1:C:682:GLU:HG3	2.04	0.40
1:D:296:LEU:O	1:D:300:LEU:HB2	2.22	0.40
1:A:215:THR:HG22	1:A:216:LEU:N	2.35	0.40
1:B:514:SER:HB2	1:B:515:PRO:HD2	2.03	0.40
1:C:437:ARG:O	1:C:441:ASN:HB2	2.21	0.40
1:D:371:VAL:HG11	1:D:492:ILE:HG12	2.02	0.40
1:D:584:LEU:HB3	1:D:588:GLN:HB2	2.03	0.40
1:A:238:ASN:HD22	1:A:238:ASN:HA	1.57	0.40
1:B:264:ARG:HD3	1:B:289:GLU:OE1	2.20	0.40
1:C:423:GLN:HA	1:C:424:PRO:HD3	1.96	0.40
1:D:545:LYS:O	1:D:549:LEU:HB2	2.20	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	11	43
1	B	665/695 (96%)	612 (92%)	45 (7%)	8 (1%)	10	40
1	C	665/695 (96%)	602 (90%)	54 (8%)	9 (1%)	9	36
1	D	665/695 (96%)	600 (90%)	56 (8%)	9 (1%)	9	36
All	All	2660/2780 (96%)	2424 (91%)	203 (8%)	33 (1%)	10	40

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
1	D	360	ASP
1	D	428	LEU
1	D	557	ILE

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Mol	Chain	Res	Type
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%)	511 (88%)	73 (12%)	4	20
1	B	584/601 (97%)	503 (86%)	81 (14%)	3	17
1	C	584/601 (97%)	498 (85%)	86 (15%)	3	15
1	D	584/601 (97%)	509 (87%)	75 (13%)	4	19
All	All	2336/2404 (97%)	2021 (86%)	315 (14%)	4	18

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	37	LYS
1	A	39	GLU
1	A	45	SER
1	A	46	SER
1	A	49	LEU
1	A	89	LEU
1	A	95	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	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	236	LEU
1	A	238	ASN
1	A	241	ASP
1	A	265	GLN
1	A	273	GLU
1	A	277	VAL
1	A	293	ILE
1	A	294	GLN
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	396	GLN
1	A	414	THR
1	A	420	LEU
1	A	427	ASN
1	A	428	LEU

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Mol	Chain	Res	Type
1	A	432	LEU
1	A	444	LEU
1	A	462	THR
1	A	489	THR
1	A	499	LYS
1	A	501	VAL
1	A	510	GLU
1	A	514	SER
1	A	545	LYS
1	A	548	LEU
1	A	549	LEU
1	A	554	VAL
1	A	560	ILE
1	A	577	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	688	LEU
1	B	35	ILE
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

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Mol	Chain	Res	Type
1	B	130	LEU
1	B	141	ILE
1	B	170	THR
1	B	171	LEU
1	B	184	LEU
1	B	192	GLU
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	277	VAL
1	B	285	GLU
1	B	293	ILE
1	B	294	GLN
1	B	301	LYS
1	B	314	LYS
1	B	321	THR
1	B	331	GLU
1	B	336	ARG
1	B	338	LEU
1	B	364	LEU
1	B	391	ASN
1	B	393	ARG
1	B	396	GLN
1	B	400	ILE
1	B	414	THR
1	B	420	LEU
1	B	426	LEU
1	B	427	ASN
1	B	432	LEU
1	B	433	SER
1	B	441	ASN
1	B	444	LEU
1	B	461	LEU
1	B	462	THR
1	B	489	THR
1	B	499	LYS

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Mol	Chain	Res	Type
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
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	B	688	LEU
1	C	7	THR
1	C	14	LEU
1	C	35	ILE
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

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Mol	Chain	Res	Type
1	C	141	ILE
1	C	154	LYS
1	C	159	ASP
1	C	170	THR
1	C	171	LEU
1	C	184	LEU
1	C	192	GLU
1	C	193	LEU
1	C	200	ASN
1	C	205	LEU
1	C	211	SER
1	C	229	ARG
1	C	233	VAL
1	C	236	LEU
1	C	238	ASN
1	C	241	ASP
1	C	262	ARG
1	C	263	LEU
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	396	GLN
1	C	400	ILE
1	C	414	THR
1	C	420	LEU
1	C	421	ARG
1	C	427	ASN
1	C	428	LEU
1	C	432	LEU
1	C	433	SER
1	C	441	ASN
1	C	444	LEU
1	C	462	THR
1	C	475	SER

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Mol	Chain	Res	Type
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	548	LEU
1	C	549	LEU
1	C	554	VAL
1	C	560	ILE
1	C	577	LEU
1	C	579	LEU
1	C	592	GLU
1	C	593	LEU
1	C	594	VAL
1	C	598	LYS
1	C	599	LYS
1	C	601	LEU
1	C	622	GLU
1	C	623	CYS
1	C	649	LEU
1	C	651	LYS
1	C	655	THR
1	C	670	LEU
1	C	675	ILE
1	C	677	GLN
1	C	678	LEU
1	C	688	LEU
1	D	12	GLN
1	D	14	LEU
1	D	35	ILE
1	D	37	LYS
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

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Mol	Chain	Res	Type
1	D	141	ILE
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	216	LEU
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	265	GLN
1	D	293	ILE
1	D	294	GLN
1	D	314	LYS
1	D	321	THR
1	D	331	GLU
1	D	336	ARG
1	D	338	LEU
1	D	364	LEU
1	D	393	ARG
1	D	396	GLN
1	D	400	ILE
1	D	414	THR
1	D	420	LEU
1	D	426	LEU
1	D	427	ASN
1	D	433	SER
1	D	441	ASN
1	D	444	LEU
1	D	461	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

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Mol	Chain	Res	Type
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	593	LEU
1	D	594	VAL
1	D	599	LYS
1	D	601	LEU
1	D	622	GLU
1	D	649	LEU
1	D	655	THR
1	D	661	GLU
1	D	670	LEU
1	D	674	VAL
1	D	675	ILE
1	D	677	GLN
1	D	678	LEU
1	D	688	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	120	HIS
1	A	122	ASN
1	A	128	GLN
1	A	155	GLN
1	A	185	ASN
1	A	191	ASN
1	A	238	ASN
1	A	261	ASN
1	A	268	ASN
1	A	294	GLN
1	A	362	ASN
1	A	396	GLN
1	A	423	GLN
1	A	450	GLN
1	A	480	GLN
1	A	486	ASN
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	604	HIS
1	A	618	ASN
1	A	648	ASN
1	A	652	GLN
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	242	GLN
1	B	268	ASN
1	B	280	GLN
1	B	345	HIS
1	B	410	ASN
1	B	480	GLN
1	B	486	ASN
1	B	550	ASN
1	B	618	ASN
1	B	652	GLN
1	B	654	GLN
1	B	659	ASN
1	B	677	GLN
1	C	64	ASN
1	C	122	ASN
1	C	134	ASN
1	C	155	GLN
1	C	191	ASN
1	C	212	GLN
1	C	238	ASN
1	C	242	GLN
1	C	268	ASN
1	C	280	GLN
1	C	334	GLN
1	C	362	ASN
1	C	396	GLN
1	C	423	GLN
1	C	450	GLN
1	C	480	GLN
1	C	486	ASN
1	C	550	ASN

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Mol	Chain	Res	Type
1	C	604	HIS
1	C	652	GLN
1	C	654	GLN
1	C	659	ASN
1	C	677	GLN
1	C	687	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	242	GLN
1	D	280	GLN
1	D	304	GLN
1	D	345	HIS
1	D	362	ASN
1	D	410	ASN
1	D	486	ASN
1	D	550	ASN
1	D	607	GLN
1	D	618	ASN
1	D	652	GLN
1	D	654	GLN
1	D	659	ASN
1	D	687	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 oligosaccharides 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%)	-1.37	0 100 100	35, 59, 84, 104	0
1	B	671/695 (96%)	-1.35	0 100 100	35, 59, 84, 104	0
1	C	671/695 (96%)	-1.37	0 100 100	35, 59, 84, 104	0
1	D	671/695 (96%)	-1.38	0 100 100	35, 59, 84, 104	0
All	All	2684/2780 (96%)	-1.37	0 100 100	35, 59, 84, 104	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.