



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:24 AM UTC

PDB ID : 2UZX / pdb_00002uzx
Title : Structure of the human receptor tyrosine kinase Met in complex with the
Listeria monocytogenes invasion protein InlB: Crystal form I
Authors : Niemann, H.H.; Jager, V.; Butler, P.J.G.; Van Den Heuvel, J.; Schmidt, S.;
Ferraris, D.; Gherardi, E.; Heinz, D.W.
Deposited on : 2007-05-02
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

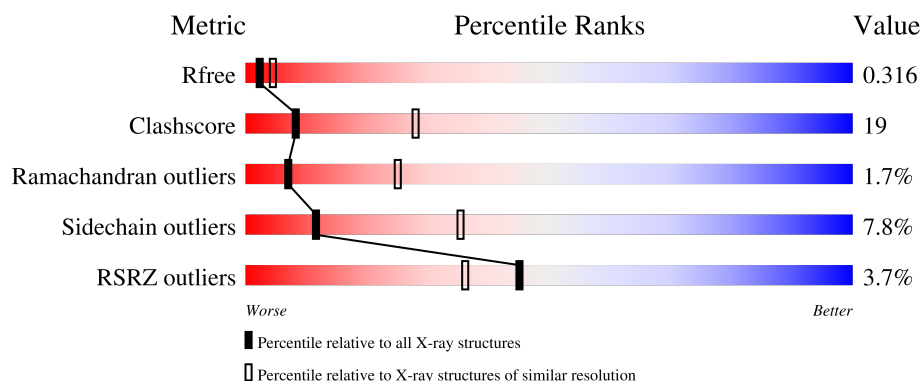
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	289	2% 69% 28% ..
1	C	289	4% 68% 29% ..
2	B	727	2% 43% 27% 5% 25%
2	D	727	5% 43% 27% 5% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13170 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 INTERNALIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2257	1438	379	438	2			
1	C	287	Total	C	N	O	S	0	0	0
			2257	1438	379	438	2			

- Molecule 2 is a protein called HEPATOCYTE GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	547	Total	C	N	O	S	0	0	1
			4328	2757	732	809	30			
2	D	547	Total	C	N	O	S	0	0	1
			4328	2757	732	809	30			

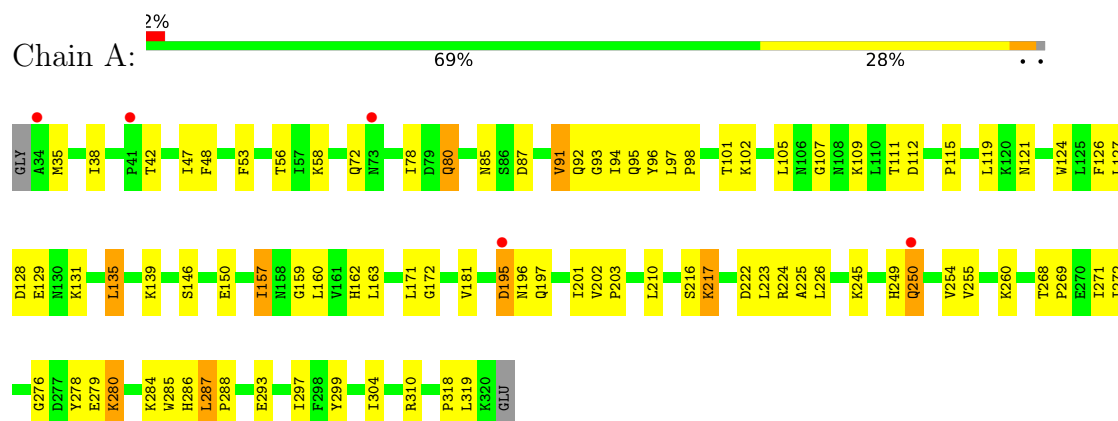
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	CYS	TYR	conflict	UNP P08581
B	344	ALA	GLY	conflict	UNP P08581
D	41	CYS	TYR	conflict	UNP P08581
D	344	ALA	GLY	conflict	UNP P08581

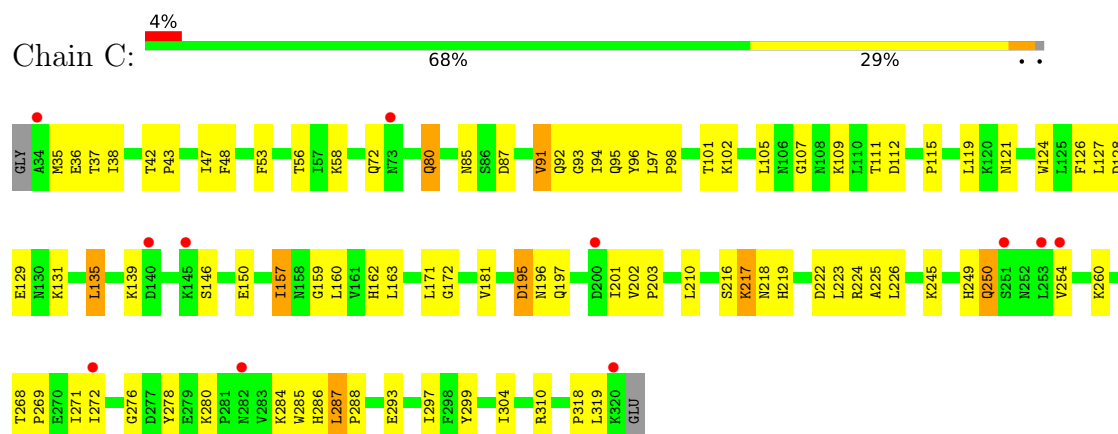
3 Residue-property plots

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.

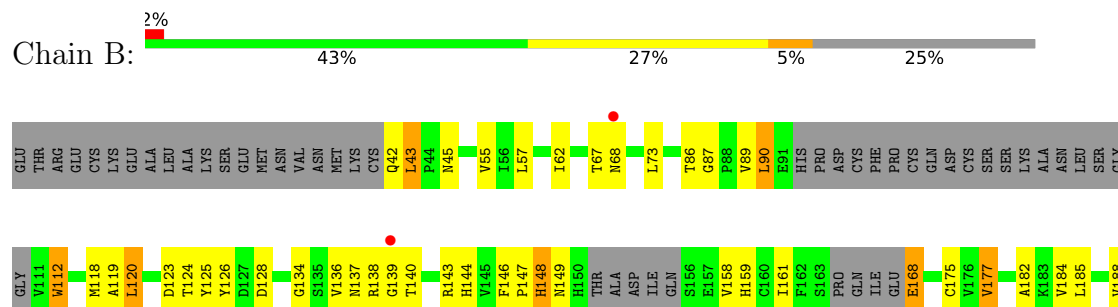
• Molecule 1: INTERNALIN B

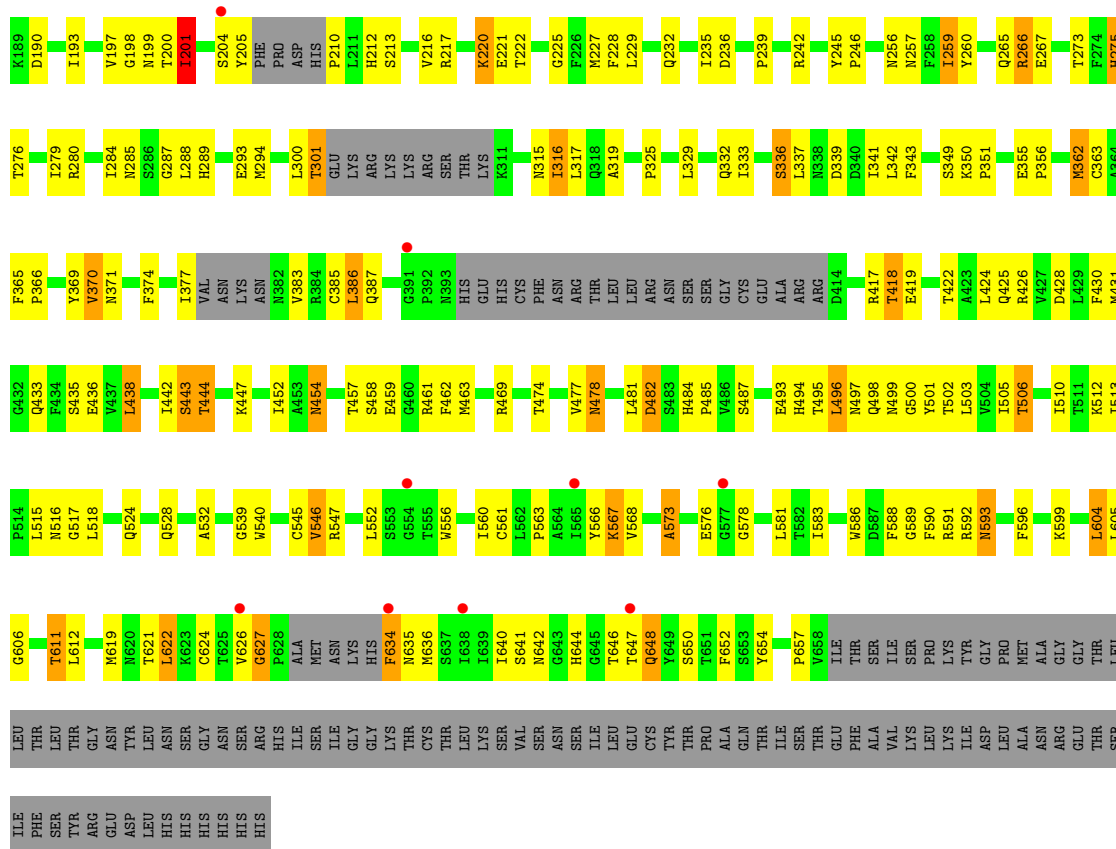


• Molecule 1: INTERNALIN B

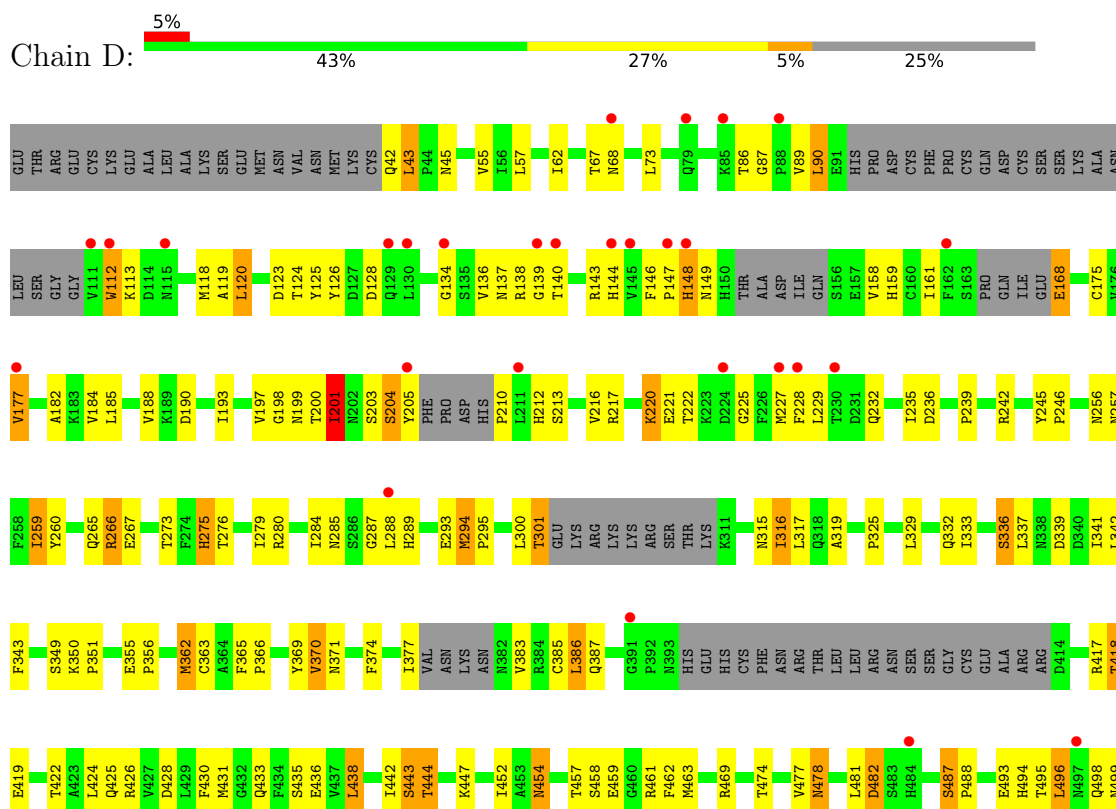


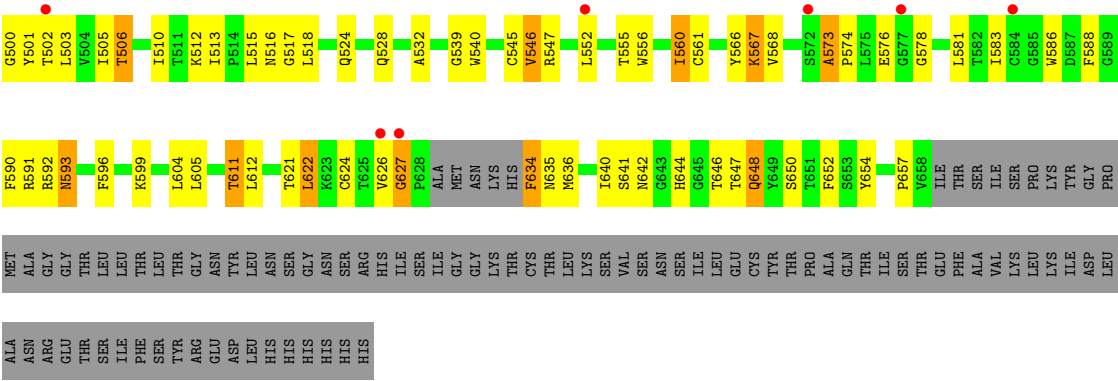
• Molecule 2: HEPATOCYTE GROWTH FACTOR RECEPTOR





• Molecule 2: HEPATOCYTE GROWTH FACTOR RECEPTOR





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.50Å 66.70Å 181.50Å 90.00° 123.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.80) 96.5 (15.00-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.268 , 0.307 0.280 , 0.316	Depositor DCC
R_{free} test set	2482 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13170	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 56.05 % 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 2.8953e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.43	0/2293	0.85	2/3112 (0.1%)
1	C	0.43	0/2293	0.84	2/3112 (0.1%)
2	B	0.46	1/4427 (0.0%)	0.91	16/6001 (0.3%)
2	D	0.46	1/4427 (0.0%)	0.91	16/6001 (0.3%)
All	All	0.45	2/13440 (0.0%)	0.89	36/18226 (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
2	B	0	3
2	D	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	PRO	C-N	-6.62	1.24	1.33
2	D	657	PRO	C-N	-6.24	1.24	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	294	MET	CA-C-N	7.52	127.28	119.76
2	D	294	MET	C-N-CA	7.52	127.28	119.76
2	B	294	MET	CA-C-N	7.52	127.28	119.76
2	B	294	MET	C-N-CA	7.52	127.28	119.76
2	B	201	ILE	N-CA-C	7.08	117.65	107.88
2	D	201	ILE	N-CA-C	7.07	117.64	107.88
2	B	532	ALA	CA-C-N	6.10	126.66	120.38
2	B	532	ALA	C-N-CA	6.10	126.66	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	532	ALA	CA-C-N	6.07	126.63	120.38
2	D	532	ALA	C-N-CA	6.07	126.63	120.38
2	D	112	TRP	N-CA-C	5.68	118.60	110.24
2	B	112	TRP	N-CA-C	5.68	118.59	110.24
2	B	481	LEU	N-CA-C	-5.58	103.27	110.19
2	D	481	LEU	N-CA-C	-5.54	103.32	110.19
2	D	316	ILE	N-CA-C	5.39	115.35	107.37
2	B	316	ILE	N-CA-C	5.36	115.30	107.37
2	D	573	ALA	CA-C-N	5.24	125.52	119.92
2	D	573	ALA	C-N-CA	5.24	125.52	119.92
2	B	573	ALA	CA-C-N	5.22	125.50	119.92
2	B	573	ALA	C-N-CA	5.22	125.50	119.92
2	D	86	THR	N-CA-C	-5.20	107.00	113.19
1	C	245	LYS	CA-C-N	5.19	125.19	119.89
1	C	245	LYS	C-N-CA	5.19	125.19	119.89
1	A	245	LYS	CA-C-N	5.17	125.16	119.89
1	A	245	LYS	C-N-CA	5.17	125.16	119.89
2	B	86	THR	N-CA-C	-5.15	107.06	113.19
2	B	474	THR	CA-C-N	5.13	126.25	119.84
2	B	474	THR	C-N-CA	5.13	126.25	119.84
2	B	190	ASP	N-CA-C	5.11	116.89	110.91
2	D	190	ASP	N-CA-C	5.08	116.86	110.91
2	B	560	ILE	N-CA-C	5.08	115.23	108.11
2	D	177	VAL	N-CA-C	5.08	115.79	108.48
2	B	177	VAL	N-CA-C	5.05	115.75	108.48
2	D	474	THR	CA-C-N	5.03	126.13	119.84
2	D	474	THR	C-N-CA	5.03	126.13	119.84
2	D	560	ILE	N-CA-C	5.01	115.13	108.11

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	168	GLU	Peptide
2	B	210	PRO	Peptide
2	B	627	GLY	Peptide
2	D	168	GLU	Peptide
2	D	210	PRO	Peptide
2	D	627	GLY	Peptide

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	2257	0	2328	73	0
1	C	2257	0	2328	73	0
2	B	4328	0	4212	185	0
2	D	4328	0	4212	180	0
All	All	13170	0	13080	506	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 19.

All (506) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:LEU:HA	2:D:332:GLN:NE2	1.93	0.84
2:D:43:LEU:HD12	2:D:513:ILE:HA	1.61	0.82
2:B:329:LEU:HA	2:B:332:GLN:NE2	1.93	0.82
2:B:43:LEU:HD12	2:B:513:ILE:HA	1.61	0.80
2:B:647:THR:HG22	2:B:648:GLN:H	1.47	0.80
2:D:647:THR:HG22	2:D:648:GLN:H	1.48	0.79
2:B:546:VAL:HG22	2:B:547:ARG:H	1.48	0.78
1:A:157:ILE:HD13	1:A:157:ILE:H	1.49	0.78
2:D:546:VAL:HG22	2:D:547:ARG:H	1.47	0.78
1:C:157:ILE:HD13	1:C:157:ILE:H	1.49	0.76
2:B:329:LEU:HA	2:B:332:GLN:HE21	1.51	0.76
1:A:80:GLN:HB2	1:A:102:LYS:HB2	1.68	0.76
2:B:161:ILE:HG23	2:B:225:GLY:HA2	1.68	0.75
2:B:265:GLN:O	2:B:275:HIS:HB2	1.87	0.75
1:C:80:GLN:HB2	1:C:102:LYS:HB2	1.68	0.75
2:D:561:CYS:H	2:D:644:HIS:HD2	1.32	0.75
2:D:161:ILE:HG23	2:D:225:GLY:HA2	1.68	0.74
2:D:265:GLN:O	2:D:275:HIS:HB2	1.87	0.74
2:B:611:THR:O	2:B:624:CYS:HB2	1.88	0.73
2:D:611:THR:O	2:D:624:CYS:HB2	1.88	0.73
2:B:89:VAL:HB	2:B:136:VAL:HG11	1.71	0.73
1:A:286:HIS:NE2	1:A:288:PRO:HG3	2.03	0.73
1:A:195:ASP:HA	1:A:217:LYS:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:LEU:HG	2:B:626:VAL:HG21	1.71	0.72
1:C:195:ASP:HA	1:C:217:LYS:HB2	1.71	0.72
2:D:329:LEU:HA	2:D:332:GLN:HE21	1.50	0.72
1:C:286:HIS:NE2	1:C:288:PRO:HG3	2.04	0.72
2:D:89:VAL:HB	2:D:136:VAL:HG11	1.71	0.72
2:D:636:MET:HE1	2:D:654:TYR:HD2	1.55	0.72
1:A:85:ASN:O	2:D:496:LEU:HD13	1.90	0.71
2:B:636:MET:HE1	2:B:654:TYR:HD2	1.55	0.71
1:C:135:LEU:HD13	1:C:159:GLY:HA3	1.72	0.71
2:D:581:LEU:HG	2:D:626:VAL:HG21	1.71	0.71
2:B:300:LEU:HD12	2:B:301:THR:H	1.55	0.71
2:B:566:TYR:O	2:B:567:LYS:HB2	1.90	0.71
1:A:135:LEU:HD13	1:A:159:GLY:HA3	1.72	0.71
2:D:300:LEU:HD12	2:D:301:THR:H	1.55	0.70
2:D:566:TYR:O	2:D:567:LYS:HB2	1.90	0.70
2:B:443:SER:HB2	2:B:454:ASN:OD1	1.90	0.70
2:D:443:SER:HB2	2:D:454:ASN:OD1	1.90	0.70
2:B:583:ILE:HD13	2:B:640:ILE:HD11	1.75	0.68
1:C:87:ASP:OD1	1:C:109:LYS:HE3	1.94	0.68
2:D:216:VAL:CG2	2:D:288:LEU:HD11	2.24	0.67
2:D:583:ILE:HD13	2:D:640:ILE:HD11	1.75	0.67
2:B:216:VAL:CG2	2:B:288:LEU:HD11	2.24	0.67
1:A:87:ASP:OD1	1:A:109:LYS:HE3	1.94	0.66
1:C:286:HIS:CD2	1:C:288:PRO:HG3	2.31	0.66
2:D:498:GLN:HG2	2:D:500:GLY:H	1.61	0.66
1:A:286:HIS:CD2	1:A:288:PRO:HG3	2.31	0.65
2:B:498:GLN:HG2	2:B:500:GLY:H	1.61	0.65
1:C:135:LEU:HD21	1:C:157:ILE:HA	1.79	0.65
2:B:590:PHE:CE1	2:B:644:HIS:CE1	2.85	0.65
2:B:636:MET:HE1	2:B:654:TYR:CD2	2.31	0.65
2:D:590:PHE:CE1	2:D:644:HIS:CE1	2.85	0.64
1:A:139:LYS:HE2	1:A:162:HIS:CD2	2.32	0.64
2:B:365:PHE:CE2	2:B:426:ARG:HG2	2.33	0.64
2:D:217:ARG:H	2:D:217:ARG:HD2	1.63	0.64
2:D:636:MET:HE1	2:D:654:TYR:CD2	2.31	0.64
1:A:135:LEU:HD21	1:A:157:ILE:HA	1.79	0.64
1:C:139:LYS:HG2	1:C:162:HIS:CG	2.33	0.64
2:B:43:LEU:HD23	2:B:43:LEU:H	1.63	0.64
1:C:139:LYS:HE2	1:C:162:HIS:CD2	2.32	0.64
2:D:611:THR:C	2:D:624:CYS:HB2	2.24	0.63
2:D:287:GLY:HA2	2:D:289:HIS:NE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:THR:C	2:B:624:CYS:HB2	2.24	0.63
2:D:43:LEU:H	2:D:43:LEU:HD23	1.63	0.63
2:D:148:HIS:CD2	2:D:149:ASN:H	2.17	0.63
2:B:217:ARG:H	2:B:217:ARG:HD2	1.63	0.63
2:B:280:ARG:NH2	2:B:374:PHE:HB3	2.14	0.63
1:A:139:LYS:HG2	1:A:162:HIS:CG	2.33	0.63
1:C:85:ASN:HA	1:C:107:GLY:O	1.99	0.62
2:D:365:PHE:CE2	2:D:426:ARG:HG2	2.33	0.62
1:A:85:ASN:HA	1:A:107:GLY:O	1.99	0.62
2:B:148:HIS:CD2	2:B:149:ASN:H	2.17	0.62
1:C:226:LEU:HD12	1:C:226:LEU:H	1.65	0.62
2:D:626:VAL:HG12	2:D:654:TYR:OH	2.00	0.62
2:B:626:VAL:HG12	2:B:654:TYR:OH	1.99	0.62
2:D:280:ARG:NH2	2:D:374:PHE:HB3	2.14	0.62
2:B:287:GLY:HA2	2:B:289:HIS:NE2	2.13	0.62
2:D:220:LYS:HD3	2:D:225:GLY:O	2.00	0.61
2:B:220:LYS:HD3	2:B:225:GLY:O	2.00	0.61
2:D:605:LEU:HD21	2:D:652:PHE:CE2	2.36	0.61
2:D:634:PHE:HD1	2:D:635:ASN:H	1.49	0.60
2:B:583:ILE:HG21	2:B:640:ILE:HD11	1.84	0.60
2:D:235:ILE:HD12	2:D:417:ARG:HG2	1.83	0.60
1:A:226:LEU:HD12	1:A:226:LEU:H	1.65	0.60
2:B:605:LEU:HD21	2:B:652:PHE:CE2	2.36	0.60
2:B:634:PHE:HD1	2:B:635:ASN:H	1.49	0.60
1:C:139:LYS:HE2	1:C:162:HIS:NE2	2.16	0.60
1:A:139:LYS:HE2	1:A:162:HIS:NE2	2.16	0.60
1:A:249:HIS:HD2	1:A:287:LEU:HD23	1.67	0.59
2:B:612:LEU:HA	2:B:624:CYS:CB	2.32	0.59
2:D:583:ILE:HG21	2:D:640:ILE:HD11	1.84	0.59
2:B:235:ILE:HD12	2:B:417:ARG:HG2	1.83	0.59
2:B:517:GLY:O	2:B:518:LEU:HD13	2.03	0.59
1:C:249:HIS:HD2	1:C:287:LEU:HD23	1.67	0.58
2:B:430:PHE:HB3	2:B:433:GLN:HB3	1.85	0.58
2:B:216:VAL:HG21	2:B:288:LEU:HD11	1.85	0.58
2:D:517:GLY:O	2:D:518:LEU:HD13	2.03	0.58
2:D:430:PHE:HB3	2:D:433:GLN:HB3	1.84	0.58
2:D:578:GLY:HA2	2:D:627:GLY:H	1.67	0.58
2:D:612:LEU:HA	2:D:624:CYS:CB	2.32	0.58
2:B:578:GLY:HA2	2:B:627:GLY:H	1.67	0.58
2:D:125:TYR:CE1	2:D:188:VAL:HG11	2.38	0.58
2:B:497:ASN:HD22	2:D:555:THR:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:VAL:HG21	2:D:288:LEU:HD11	1.85	0.58
2:D:634:PHE:HB3	2:D:636:MET:HE2	1.86	0.58
2:B:125:TYR:CE1	2:B:188:VAL:HG11	2.38	0.57
2:B:287:GLY:HA2	2:B:289:HIS:CE1	2.39	0.57
2:B:634:PHE:HB3	2:B:636:MET:HE2	1.86	0.57
2:D:287:GLY:HA2	2:D:289:HIS:CE1	2.39	0.57
1:A:224:ARG:HH21	1:A:260:LYS:CD	2.18	0.57
2:B:561:CYS:H	2:B:644:HIS:HD2	1.53	0.57
2:B:216:VAL:HB	2:B:288:LEU:HD11	1.86	0.57
1:A:201:ILE:HG13	1:A:225:ALA:HB3	1.87	0.56
2:B:539:GLY:HA3	2:B:556:TRP:NE1	2.20	0.56
1:C:224:ARG:HH21	1:C:260:LYS:CD	2.18	0.56
2:D:539:GLY:HA3	2:D:556:TRP:NE1	2.19	0.56
2:D:220:LYS:HG3	2:D:227:MET:HE2	1.88	0.56
2:D:266:ARG:O	2:D:266:ARG:HG2	2.05	0.56
2:B:266:ARG:O	2:B:266:ARG:HG2	2.05	0.56
2:D:216:VAL:HB	2:D:288:LEU:HD11	1.86	0.56
2:D:200:THR:O	2:D:201:ILE:HG23	2.07	0.55
2:B:220:LYS:HG3	2:B:227:MET:HE2	1.88	0.55
2:D:229:LEU:HD22	2:D:285:ASN:HB3	1.89	0.55
1:C:201:ILE:HG13	1:C:225:ALA:HB3	1.88	0.55
1:A:101:THR:HG22	1:A:121:ASN:O	2.07	0.55
1:A:285:TRP:HB3	1:A:287:LEU:HD13	1.89	0.55
2:B:287:GLY:CA	2:B:289:HIS:NE2	2.69	0.55
1:C:101:THR:HG22	1:C:121:ASN:O	2.07	0.55
2:D:287:GLY:CA	2:D:289:HIS:NE2	2.70	0.54
2:D:583:ILE:HG21	2:D:640:ILE:CD1	2.37	0.54
2:B:592:ARG:HD3	2:B:593:ASN:H	1.73	0.54
2:B:144:HIS:ND1	2:B:158:VAL:HG22	2.22	0.54
2:B:200:THR:O	2:B:201:ILE:HG23	2.07	0.54
1:C:285:TRP:HB3	1:C:287:LEU:HD13	1.89	0.54
1:A:48:PHE:HA	1:A:92:GLN:O	2.08	0.54
2:B:260:TYR:HA	2:B:279:ILE:O	2.08	0.54
2:B:499:ASN:O	2:B:515:LEU:HB2	2.08	0.54
2:B:647:THR:HG22	2:B:648:GLN:N	2.20	0.54
2:D:118:MET:CB	2:D:177:VAL:HG11	2.38	0.54
2:B:125:TYR:HE1	1:C:43:PRO:HD3	1.73	0.54
2:B:284:ILE:O	2:B:285:ASN:HB2	2.08	0.54
2:B:457:THR:HG22	2:B:458:SER:N	2.22	0.54
2:B:583:ILE:HG21	2:B:640:ILE:CD1	2.37	0.54
2:D:198:GLY:HA2	2:D:213:SER:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:592:ARG:HD3	2:D:593:ASN:H	1.73	0.54
2:D:260:TYR:HA	2:D:279:ILE:O	2.08	0.53
2:D:457:THR:HG22	2:D:458:SER:N	2.22	0.53
2:B:229:LEU:HD22	2:B:285:ASN:HB3	1.89	0.53
1:C:48:PHE:HA	1:C:92:GLN:O	2.08	0.53
2:D:463:MET:HB3	2:D:478:ASN:HA	1.89	0.53
1:C:318:PRO:O	1:C:319:LEU:HD23	2.09	0.53
2:D:144:HIS:ND1	2:D:158:VAL:HG22	2.22	0.53
2:B:198:GLY:HA2	2:B:213:SER:O	2.08	0.53
2:B:362:MET:O	2:B:428:ASP:HA	2.08	0.53
2:B:591:ARG:HB2	2:B:596:PHE:CZ	2.43	0.53
2:D:499:ASN:O	2:D:515:LEU:HB2	2.07	0.53
2:B:118:MET:CB	2:B:177:VAL:HG11	2.38	0.53
2:D:316:ILE:O	2:D:316:ILE:HG22	2.09	0.53
1:C:286:HIS:O	1:C:288:PRO:HD3	2.09	0.53
2:D:591:ARG:HB2	2:D:596:PHE:CZ	2.43	0.53
2:D:216:VAL:CB	2:D:288:LEU:HD11	2.39	0.53
2:D:362:MET:O	2:D:428:ASP:HA	2.08	0.53
2:D:424:LEU:HD23	2:D:425:GLN:N	2.24	0.53
2:B:424:LEU:HD23	2:B:425:GLN:N	2.25	0.52
1:A:318:PRO:O	1:A:319:LEU:HD23	2.09	0.52
2:B:463:MET:HB3	2:B:478:ASN:HA	1.90	0.52
2:D:284:ILE:O	2:D:285:ASN:HB2	2.08	0.52
2:B:216:VAL:CB	2:B:288:LEU:HD11	2.39	0.52
1:C:285:TRP:HB3	1:C:287:LEU:CD1	2.39	0.52
2:D:138:ARG:HH22	2:D:205:TYR:C	2.17	0.52
2:D:647:THR:HG22	2:D:648:GLN:N	2.20	0.52
1:A:285:TRP:HB3	1:A:287:LEU:CD1	2.39	0.52
2:B:482:ASP:OD1	2:B:506:THR:HB	2.09	0.52
2:B:539:GLY:HA3	2:B:556:TRP:CE2	2.44	0.52
1:A:58:LYS:HD2	1:A:58:LYS:C	2.35	0.52
1:C:58:LYS:HD2	1:C:58:LYS:C	2.35	0.52
2:D:482:ASP:OD1	2:D:506:THR:HB	2.09	0.52
2:D:539:GLY:HA3	2:D:556:TRP:CE2	2.44	0.52
1:A:297:ILE:HD12	1:A:297:ILE:N	2.25	0.52
2:B:452:ILE:N	2:B:452:ILE:HD12	2.25	0.52
2:B:612:LEU:HA	2:B:624:CYS:HB3	1.91	0.52
1:C:128:ASP:OD2	1:C:150:GLU:N	2.32	0.52
2:B:43:LEU:HD11	2:B:513:ILE:HG12	1.92	0.52
1:C:299:TYR:OH	1:C:310:ARG:HD2	2.10	0.52
2:B:498:GLN:HE21	2:B:500:GLY:HA2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:ILE:N	2:D:452:ILE:HD12	2.25	0.52
2:D:612:LEU:HA	2:D:624:CYS:HB3	1.91	0.52
2:D:612:LEU:HD23	2:D:624:CYS:HB3	1.93	0.51
1:A:128:ASP:OD2	1:A:150:GLU:N	2.32	0.51
2:B:300:LEU:HD12	2:B:301:THR:N	2.25	0.51
2:B:385:CYS:O	2:B:386:LEU:C	2.53	0.51
2:D:216:VAL:HG23	2:D:288:LEU:HD21	1.92	0.51
2:D:317:LEU:HD11	2:D:319:ALA:O	2.11	0.51
1:C:297:ILE:HD12	1:C:297:ILE:N	2.25	0.51
2:D:540:TRP:CZ3	2:D:545:CYS:HB2	2.45	0.51
1:A:286:HIS:O	1:A:288:PRO:HD3	2.09	0.51
2:B:612:LEU:HD23	2:B:624:CYS:HB3	1.92	0.51
1:C:157:ILE:HG12	1:C:181:VAL:HG11	1.93	0.51
2:B:138:ARG:HH22	2:B:205:TYR:C	2.17	0.51
2:B:342:LEU:HB3	2:B:365:PHE:HB2	1.93	0.51
1:A:97:LEU:O	1:A:119:LEU:HD22	2.11	0.51
2:B:287:GLY:HA3	2:B:289:HIS:CD2	2.45	0.51
2:D:287:GLY:HA3	2:D:289:HIS:CD2	2.45	0.51
2:B:317:LEU:HD11	2:B:319:ALA:O	2.11	0.51
1:A:299:TYR:OH	1:A:310:ARG:HD2	2.10	0.51
2:B:239:PRO:HG3	2:B:242:ARG:NH2	2.26	0.51
2:D:276:THR:HG21	2:D:317:LEU:HB2	1.93	0.51
1:A:139:LYS:HG2	1:A:162:HIS:CD2	2.46	0.50
2:B:288:LEU:HD12	2:B:288:LEU:N	2.26	0.50
2:B:316:ILE:HG22	2:B:316:ILE:O	2.09	0.50
1:C:97:LEU:O	1:C:119:LEU:HD22	2.11	0.50
2:D:288:LEU:HD12	2:D:288:LEU:N	2.27	0.50
2:D:316:ILE:HD13	2:D:349:SER:HB3	1.92	0.50
2:B:143:ARG:HB2	2:B:159:HIS:HB2	1.93	0.50
2:B:216:VAL:HG23	2:B:288:LEU:HD21	1.92	0.50
2:B:454:ASN:HB2	2:B:462:PHE:CZ	2.46	0.50
2:B:563:PRO:HG3	2:B:642:ASN:ND2	2.26	0.50
2:B:316:ILE:HD13	2:B:349:SER:HB3	1.92	0.50
2:D:454:ASN:HB2	2:D:462:PHE:CZ	2.46	0.50
1:A:157:ILE:HG12	1:A:181:VAL:HG11	1.93	0.50
2:D:573:ALA:HB3	2:D:652:PHE:CZ	2.46	0.50
2:B:540:TRP:CZ3	2:B:545:CYS:HB2	2.45	0.50
1:C:124:TRP:CD1	1:C:146:SER:HB3	2.46	0.50
2:D:239:PRO:HG3	2:D:242:ARG:NH2	2.27	0.50
2:D:342:LEU:HB3	2:D:365:PHE:HB2	1.93	0.50
2:D:385:CYS:O	2:D:386:LEU:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:495:THR:O	2:D:498:GLN:HB3	2.12	0.50
1:A:254:VAL:HG22	1:A:284:LYS:HG2	1.94	0.50
2:B:276:THR:HG21	2:B:317:LEU:HB2	1.93	0.50
1:C:272:ILE:HG21	1:C:276:GLY:HA3	1.93	0.50
1:A:272:ILE:HG21	1:A:276:GLY:HA3	1.94	0.50
2:B:454:ASN:HB2	2:B:462:PHE:CE1	2.47	0.50
1:C:268:THR:HG22	1:C:278:TYR:HE2	1.77	0.50
2:D:447:LYS:HE3	2:D:516:ASN:OD1	2.12	0.50
2:D:498:GLN:HE21	2:D:500:GLY:HA2	1.75	0.50
2:B:495:THR:O	2:B:498:GLN:HB3	2.12	0.49
2:B:573:ALA:HB3	2:B:652:PHE:CZ	2.46	0.49
1:A:224:ARG:NH2	1:A:260:LYS:HD2	2.28	0.49
2:D:43:LEU:HD11	2:D:513:ILE:HG12	1.92	0.49
1:C:139:LYS:HG2	1:C:162:HIS:CD2	2.46	0.49
2:D:185:LEU:HD12	2:D:259:ILE:HG23	1.94	0.49
2:B:185:LEU:HD12	2:B:259:ILE:HG23	1.94	0.49
2:B:447:LYS:HE3	2:B:516:ASN:OD1	2.12	0.49
1:C:254:VAL:HG22	1:C:284:LYS:HG2	1.94	0.49
2:D:143:ARG:HB2	2:D:159:HIS:HB2	1.93	0.49
2:D:184:VAL:HG22	2:D:197:VAL:HG22	1.95	0.49
1:C:38:ILE:HG12	1:C:72:GLN:OE1	2.13	0.49
1:C:111:THR:HG22	1:C:131:LYS:HB2	1.94	0.49
2:D:279:ILE:HG13	2:D:293:GLU:HG2	1.95	0.49
1:A:38:ILE:HG12	1:A:72:GLN:OE1	2.13	0.49
2:D:217:ARG:HB3	2:D:228:PHE:CE2	2.48	0.49
1:A:124:TRP:CD1	1:A:146:SER:HB3	2.46	0.49
1:A:202:VAL:N	1:A:203:PRO:CD	2.76	0.49
2:D:560:ILE:HA	2:D:644:HIS:CD2	2.48	0.49
2:D:438:LEU:HB3	2:D:458:SER:HB3	1.95	0.49
2:D:454:ASN:HB2	2:D:462:PHE:CE1	2.47	0.49
2:B:457:THR:HG22	2:B:459:GLU:N	2.27	0.49
2:D:188:VAL:HG22	2:D:193:ILE:HG12	1.95	0.49
2:B:188:VAL:HG22	2:B:193:ILE:HG12	1.95	0.48
2:D:199:ASN:HB2	2:D:212:HIS:O	2.13	0.48
2:B:217:ARG:HB3	2:B:228:PHE:CE2	2.48	0.48
2:B:438:LEU:HB3	2:B:458:SER:HB3	1.94	0.48
2:D:43:LEU:HD12	2:D:512:LYS:O	2.13	0.48
1:A:268:THR:HG22	1:A:278:TYR:HE2	1.77	0.48
2:B:43:LEU:HD12	2:B:512:LYS:O	2.13	0.48
2:D:457:THR:HG22	2:D:459:GLU:N	2.27	0.48
2:B:418:THR:OG1	2:B:419:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ARG:NH2	1:C:260:LYS:HD2	2.28	0.48
1:C:202:VAL:N	1:C:203:PRO:CD	2.76	0.48
1:A:111:THR:HG22	1:A:131:LYS:HB2	1.95	0.48
2:B:279:ILE:HG13	2:B:293:GLU:HG2	1.95	0.48
2:B:184:VAL:HG22	2:B:197:VAL:HG22	1.95	0.48
2:B:199:ASN:HB2	2:B:212:HIS:O	2.13	0.48
2:B:325:PRO:HG3	2:B:341:ILE:HG13	1.96	0.48
1:C:124:TRP:HB3	1:C:126:PHE:HE1	1.79	0.48
1:A:95:GLN:H	1:A:95:GLN:CD	2.22	0.47
1:A:201:ILE:HG13	1:A:225:ALA:CB	2.44	0.47
2:B:546:VAL:HG22	2:B:547:ARG:N	2.25	0.47
2:B:220:LYS:HD2	2:B:227:MET:HG2	1.96	0.47
2:B:493:GLU:HB2	2:B:501:TYR:CZ	2.49	0.47
2:D:220:LYS:HD2	2:D:227:MET:HG2	1.96	0.47
1:A:157:ILE:HB	1:A:160:LEU:HD12	1.97	0.47
1:C:95:GLN:H	1:C:95:GLN:CD	2.22	0.47
2:D:300:LEU:HD12	2:D:301:THR:N	2.25	0.47
2:D:493:GLU:HB2	2:D:501:TYR:CZ	2.49	0.47
1:A:157:ILE:H	1:A:157:ILE:CD1	2.25	0.47
2:B:232:GLN:HB3	2:B:417:ARG:HH22	1.80	0.47
1:C:111:THR:HG22	1:C:131:LYS:CB	2.44	0.47
1:C:157:ILE:HB	1:C:160:LEU:HD12	1.97	0.47
2:D:325:PRO:HG3	2:D:341:ILE:HG13	1.96	0.47
2:D:546:VAL:HG22	2:D:547:ARG:N	2.25	0.47
2:B:581:LEU:HG	2:B:626:VAL:CG2	2.44	0.47
2:D:350:LYS:HB3	2:D:351:PRO:HD2	1.96	0.47
1:A:111:THR:HG22	1:A:131:LYS:CB	2.44	0.47
1:A:124:TRP:HB3	1:A:126:PHE:HE1	1.79	0.47
2:B:137:ASN:HB2	2:B:140:THR:HG22	1.97	0.47
2:B:498:GLN:HG2	2:B:499:ASN:N	2.30	0.47
2:D:113:LYS:HB3	2:D:113:LYS:HE3	1.53	0.47
1:C:150:GLU:HG2	1:C:172:GLY:N	2.30	0.47
2:B:217:ARG:HG3	2:B:217:ARG:HH11	1.80	0.46
2:B:148:HIS:CD2	2:B:149:ASN:N	2.83	0.46
1:C:171:LEU:HD23	1:C:171:LEU:HA	1.78	0.46
2:D:498:GLN:HG2	2:D:499:ASN:N	2.30	0.46
2:B:161:ILE:HD12	2:B:161:ILE:N	2.30	0.46
2:B:540:TRP:HZ3	2:B:545:CYS:HB2	1.81	0.46
2:D:62:ILE:HB	2:D:73:LEU:HB2	1.97	0.46
2:D:213:SER:OG	2:D:236:ASP:HA	2.15	0.46
1:C:38:ILE:HD11	1:C:72:GLN:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:461:ARG:HE	2:D:461:ARG:HB3	1.59	0.46
2:B:568:VAL:CG1	2:B:581:LEU:HD22	2.45	0.46
2:D:147:PRO:O	2:D:148:HIS:CB	2.63	0.46
2:D:239:PRO:HA	2:D:242:ARG:NE	2.30	0.46
2:D:245:TYR:HA	2:D:246:PRO:HD3	1.61	0.46
2:B:147:PRO:O	2:B:148:HIS:CB	2.63	0.46
1:C:201:ILE:HG13	1:C:225:ALA:CB	2.45	0.46
2:D:43:LEU:CD1	2:D:513:ILE:HA	2.40	0.46
2:D:137:ASN:HB2	2:D:140:THR:HG22	1.97	0.46
2:D:232:GLN:HB3	2:D:417:ARG:HH22	1.80	0.46
1:A:38:ILE:HD11	1:A:72:GLN:N	2.31	0.46
2:B:220:LYS:HB2	2:B:222:THR:HG22	1.98	0.46
2:B:239:PRO:HA	2:B:242:ARG:NE	2.30	0.46
2:D:568:VAL:CG1	2:D:581:LEU:HD22	2.45	0.46
2:D:641:SER:HB2	2:D:646:THR:HG22	1.98	0.46
1:A:150:GLU:HG2	1:A:172:GLY:N	2.30	0.46
2:B:213:SER:OG	2:B:236:ASP:HA	2.15	0.46
2:D:463:MET:HB2	2:D:477:VAL:O	2.16	0.46
2:D:581:LEU:HG	2:D:626:VAL:CG2	2.44	0.46
2:B:350:LYS:HB3	2:B:351:PRO:HD2	1.96	0.45
2:D:217:ARG:O	2:D:217:ARG:HG2	2.16	0.45
1:C:216:SER:C	1:C:217:LYS:HG2	2.41	0.45
1:A:249:HIS:CD2	1:A:287:LEU:HD23	2.50	0.45
2:D:161:ILE:N	2:D:161:ILE:HD12	2.31	0.45
2:B:62:ILE:HB	2:B:73:LEU:HB2	1.97	0.45
2:B:377:ILE:O	2:B:377:ILE:HD12	2.17	0.45
2:B:417:ARG:HD2	2:B:417:ARG:N	2.32	0.45
2:B:641:SER:HB2	2:B:646:THR:HG22	1.98	0.45
2:B:642:ASN:OD1	2:B:644:HIS:HB2	2.16	0.45
2:B:457:THR:HG22	2:B:459:GLU:H	1.82	0.45
2:B:329:LEU:CD1	2:B:333:ILE:HD13	2.47	0.45
1:A:96:TYR:O	1:A:98:PRO:HD3	2.17	0.45
2:B:256:ASN:O	2:B:257:ASN:HB2	2.17	0.45
2:B:370:VAL:HG12	2:B:371:ASN:N	2.32	0.45
2:B:590:PHE:CE1	2:B:644:HIS:ND1	2.85	0.45
2:D:418:THR:OG1	2:D:419:GLU:N	2.47	0.45
2:D:457:THR:CG2	2:D:458:SER:N	2.80	0.45
2:D:503:LEU:HB3	2:D:510:ILE:HD11	1.99	0.45
2:D:540:TRP:HZ3	2:D:545:CYS:HB2	1.81	0.45
2:D:590:PHE:CE1	2:D:644:HIS:ND1	2.85	0.45
2:D:561:CYS:H	2:D:644:HIS:CD2	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LEU:CD1	2:B:513:ILE:HA	2.40	0.45
2:B:605:LEU:HD22	2:B:626:VAL:HG13	1.99	0.45
1:C:272:ILE:CG2	1:C:276:GLY:HA3	2.47	0.45
2:D:220:LYS:HB2	2:D:222:THR:HG22	1.98	0.45
2:D:256:ASN:O	2:D:257:ASN:HB2	2.17	0.45
2:D:417:ARG:N	2:D:417:ARG:HD2	2.31	0.45
2:B:457:THR:CG2	2:B:458:SER:N	2.80	0.45
2:B:463:MET:HB2	2:B:477:VAL:O	2.17	0.45
2:D:329:LEU:CD1	2:D:333:ILE:HD13	2.47	0.45
1:A:216:SER:C	1:A:217:LYS:HG2	2.41	0.44
1:A:272:ILE:CG2	1:A:276:GLY:HA3	2.47	0.44
1:A:128:ASP:O	1:A:129:GLU:HB2	2.18	0.44
2:D:148:HIS:CD2	2:D:149:ASN:N	2.83	0.44
2:D:642:ASN:OD1	2:D:644:HIS:HB2	2.16	0.44
2:B:182:ALA:HA	2:B:198:GLY:O	2.17	0.44
2:B:161:ILE:CG2	2:B:225:GLY:HA2	2.44	0.44
2:B:496:LEU:HD13	1:C:85:ASN:O	2.17	0.44
2:B:503:LEU:HB3	2:B:510:ILE:HD11	1.99	0.44
2:B:217:ARG:O	2:B:217:ARG:HG2	2.16	0.44
1:C:201:ILE:CD1	1:C:226:LEU:HD11	2.47	0.44
2:D:217:ARG:HG3	2:D:217:ARG:HH11	1.81	0.44
1:A:201:ILE:CD1	1:A:226:LEU:HD11	2.47	0.44
1:C:96:TYR:O	1:C:98:PRO:HD3	2.17	0.44
2:D:605:LEU:HD22	2:D:626:VAL:HG13	1.99	0.44
2:B:284:ILE:HD13	2:B:289:HIS:HD2	1.83	0.44
2:D:137:ASN:HB2	2:D:140:THR:CG2	2.48	0.44
2:D:366:PRO:O	2:D:369:TYR:HB3	2.17	0.44
2:D:457:THR:HG22	2:D:459:GLU:H	1.81	0.44
2:D:67:THR:O	2:D:68:ASN:HB2	2.18	0.44
2:D:329:LEU:HD13	2:D:333:ILE:HD13	2.00	0.44
2:B:90:LEU:HD23	2:B:90:LEU:H	1.83	0.43
1:C:35:MET:HE3	1:C:35:MET:HA	2.00	0.43
1:C:105:LEU:HB2	1:C:127:LEU:HD23	2.00	0.43
1:C:157:ILE:H	1:C:157:ILE:CD1	2.25	0.43
2:D:377:ILE:O	2:D:377:ILE:HD12	2.17	0.43
1:A:286:HIS:C	1:A:288:PRO:HD3	2.44	0.43
2:B:67:THR:O	2:B:68:ASN:HB2	2.18	0.43
2:B:461:ARG:HE	2:B:461:ARG:HB3	1.60	0.43
1:C:249:HIS:CD2	1:C:287:LEU:HD23	2.50	0.43
2:D:284:ILE:HD13	2:D:289:HIS:HD2	1.83	0.43
1:A:269:PRO:HD2	1:A:278:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:VAL:CG2	2:B:505:ILE:HD11	2.49	0.43
2:B:566:TYR:HB2	2:B:586:TRP:CZ3	2.53	0.43
1:C:42:THR:HB	1:C:47:ILE:HD11	2.00	0.43
2:D:370:VAL:HG12	2:D:371:ASN:N	2.32	0.43
2:D:566:TYR:HB2	2:D:586:TRP:CZ3	2.53	0.43
2:B:329:LEU:HD13	2:B:333:ILE:HD13	2.00	0.43
2:B:366:PRO:O	2:B:369:TYR:HB3	2.17	0.43
1:C:250:GLN:HE21	1:C:250:GLN:HB2	1.67	0.43
2:D:146:PHE:HA	2:D:147:PRO:HD3	1.79	0.43
1:A:196:ASN:HB3	1:A:197:GLN:H	1.58	0.43
2:B:284:ILE:H	2:B:287:GLY:H	1.66	0.43
2:D:182:ALA:HA	2:D:198:GLY:O	2.17	0.43
2:B:245:TYR:HA	2:B:246:PRO:HD3	1.61	0.43
1:C:269:PRO:HD2	1:C:278:TYR:CD2	2.54	0.43
2:D:500:GLY:HA3	2:D:515:LEU:HD12	2.01	0.43
1:A:105:LEU:HB2	1:A:127:LEU:HD23	2.00	0.43
2:B:43:LEU:H	2:B:43:LEU:CD2	2.31	0.43
1:C:128:ASP:O	1:C:129:GLU:HB2	2.17	0.43
2:D:55:VAL:CG2	2:D:505:ILE:HD11	2.48	0.43
2:D:138:ARG:NH1	2:D:205:TYR:O	2.52	0.43
2:B:588:PHE:CD2	2:B:622:LEU:HD13	2.54	0.43
2:B:566:TYR:O	2:B:566:TYR:CG	2.72	0.42
2:D:138:ARG:HG3	2:D:175:CYS:HB3	2.01	0.42
2:D:343:PHE:CE1	2:D:444:THR:HG21	2.54	0.42
2:B:125:TYR:CE1	1:C:43:PRO:HD3	2.54	0.42
2:B:137:ASN:HB2	2:B:140:THR:CG2	2.48	0.42
1:C:223:LEU:HB3	1:C:226:LEU:HD13	2.00	0.42
2:D:430:PHE:O	2:D:431:MET:C	2.62	0.42
2:B:315:ASN:C	2:B:316:ILE:HD12	2.44	0.42
1:C:112:ASP:OD1	1:C:112:ASP:C	2.62	0.42
1:C:157:ILE:HB	1:C:160:LEU:CD1	2.49	0.42
1:A:42:THR:HB	1:A:47:ILE:HD11	2.00	0.42
1:A:223:LEU:HB3	1:A:226:LEU:HD13	2.00	0.42
2:D:315:ASN:C	2:D:316:ILE:HD12	2.44	0.42
2:D:494:HIS:HB2	2:D:515:LEU:CD1	2.49	0.42
2:D:636:MET:HE3	2:D:636:MET:HB2	1.85	0.42
1:A:112:ASP:OD1	1:A:112:ASP:C	2.62	0.42
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.84	0.42
2:B:138:ARG:NH1	2:B:205:TYR:O	2.52	0.42
2:B:500:GLY:HA3	2:B:515:LEU:HD12	2.01	0.42
2:B:567:LYS:HA	2:B:567:LYS:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:LEU:HD23	2:D:90:LEU:H	1.84	0.42
1:A:94:ILE:HG22	1:A:115:PRO:HB3	2.01	0.42
2:B:343:PHE:CE1	2:B:444:THR:HG21	2.54	0.42
2:D:119:ALA:O	2:D:120:LEU:HD13	2.20	0.42
2:D:294:MET:HA	2:D:295:PRO:HD3	1.74	0.42
2:D:566:TYR:O	2:D:566:TYR:CG	2.72	0.42
1:A:157:ILE:HD13	1:A:157:ILE:N	2.26	0.42
2:D:284:ILE:HB	2:D:289:HIS:CD2	2.55	0.42
1:A:53:PHE:O	1:A:56:THR:HB	2.19	0.42
2:B:484:HIS:HA	2:B:485:PRO:HD3	1.94	0.42
1:C:53:PHE:O	1:C:56:THR:HB	2.19	0.42
1:C:196:ASN:HB3	1:C:197:GLN:H	1.57	0.42
1:C:286:HIS:C	1:C:288:PRO:HD3	2.44	0.42
1:A:35:MET:HE3	1:A:35:MET:HA	2.00	0.42
1:A:157:ILE:HB	1:A:160:LEU:CD1	2.49	0.42
2:B:119:ALA:O	2:B:120:LEU:HD13	2.20	0.42
2:B:355:GLU:HA	2:B:356:PRO:HD3	1.85	0.42
1:C:94:ILE:HG22	1:C:115:PRO:HB3	2.02	0.42
2:D:355:GLU:HA	2:D:356:PRO:HD3	1.85	0.42
1:A:48:PHE:CE1	1:A:93:GLY:O	2.73	0.41
2:B:494:HIS:HB2	2:B:515:LEU:CD1	2.49	0.41
2:B:636:MET:HE3	2:B:636:MET:HB2	1.85	0.41
2:D:43:LEU:H	2:D:43:LEU:CD2	2.31	0.41
2:B:138:ARG:HG3	2:B:175:CYS:HB3	2.01	0.41
2:B:267:GLU:HA	2:B:275:HIS:ND1	2.35	0.41
2:B:350:LYS:HB3	2:B:351:PRO:CD	2.50	0.41
2:D:284:ILE:H	2:D:287:GLY:H	1.67	0.41
2:B:293:GLU:CD	2:B:386:LEU:HD11	2.46	0.41
2:B:325:PRO:HD3	2:B:339:ASP:O	2.20	0.41
1:C:218:ASN:HB3	1:C:219:HIS:H	1.71	0.41
2:D:524:GLN:HB2	2:D:528:GLN:HE22	1.86	0.41
2:B:627:GLY:HA2	2:B:654:TYR:OH	2.21	0.41
2:D:588:PHE:CD2	2:D:622:LEU:HD13	2.54	0.41
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.78	0.41
1:A:268:THR:HA	1:A:269:PRO:HD3	1.86	0.41
2:D:134:GLY:O	2:D:139:GLY:HA2	2.20	0.41
2:D:293:GLU:CD	2:D:386:LEU:HD11	2.46	0.41
1:C:268:THR:HA	1:C:269:PRO:HD3	1.86	0.41
2:D:284:ILE:H	2:D:287:GLY:HA3	1.86	0.41
2:B:124:THR:HG22	2:B:128:ASP:HA	2.03	0.41
2:B:336:SER:O	2:B:339:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:PHE:O	2:B:431:MET:C	2.62	0.41
2:D:336:SER:O	2:D:339:ASP:HB2	2.21	0.41
2:D:647:THR:CG2	2:D:648:GLN:H	2.26	0.41
2:B:284:ILE:HB	2:B:289:HIS:CD2	2.55	0.41
2:B:612:LEU:HA	2:B:624:CYS:HB2	2.03	0.41
2:D:203:SER:O	2:D:204:SER:HB3	2.20	0.41
2:D:487:SER:HA	2:D:488:PRO:HD3	1.85	0.41
2:B:134:GLY:O	2:B:139:GLY:HA2	2.21	0.41
2:B:647:THR:CG2	2:B:648:GLN:H	2.26	0.41
1:C:48:PHE:CE1	1:C:93:GLY:O	2.73	0.41
2:D:573:ALA:HA	2:D:574:PRO:HD3	1.82	0.41
2:D:634:PHE:CB	2:D:636:MET:HE2	2.51	0.41
1:A:224:ARG:NH2	1:A:260:LYS:CD	2.84	0.41
2:B:146:PHE:HA	2:B:147:PRO:HD3	1.79	0.41
2:B:229:LEU:CD2	2:B:285:ASN:HB3	2.51	0.41
2:D:612:LEU:HA	2:D:624:CYS:HB2	2.03	0.41
1:A:279:GLU:O	1:A:280:LYS:C	2.64	0.40
2:B:634:PHE:CB	2:B:636:MET:HE2	2.51	0.40
2:D:124:THR:HG22	2:D:128:ASP:HA	2.03	0.40
2:D:267:GLU:HA	2:D:275:HIS:ND1	2.35	0.40
1:A:250:GLN:HE21	1:A:250:GLN:HB2	1.68	0.40
1:A:255:VAL:HB	1:A:285:TRP:HZ3	1.86	0.40
2:D:325:PRO:HD3	2:D:339:ASP:O	2.21	0.40
2:B:515:LEU:HD23	2:B:515:LEU:HA	1.84	0.40
2:B:524:GLN:HB2	2:B:528:GLN:HE22	1.86	0.40
2:B:605:LEU:HD12	2:B:605:LEU:HA	1.93	0.40
1:C:36:GLU:O	1:C:37:THR:HB	2.22	0.40
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.84	0.40
1:C:226:LEU:HD12	1:C:226:LEU:N	2.34	0.40
1:A:78:ILE:HD12	1:A:97:LEU:HD21	2.04	0.40
2:B:589:GLY:HA3	2:B:619:MET:HE1	2.03	0.40
2:B:604:LEU:HD12	2:B:606:GLY:O	2.22	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	285/289 (99%)	253 (89%)	30 (10%)	2 (1%)	18	47
1	C	285/289 (99%)	252 (88%)	31 (11%)	2 (1%)	18	47
2	B	529/727 (73%)	450 (85%)	67 (13%)	12 (2%)	5	18
2	D	529/727 (73%)	451 (85%)	66 (12%)	12 (2%)	5	18
All	All	1628/2032 (80%)	1406 (86%)	194 (12%)	28 (2%)	7	25

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	148	HIS
2	D	148	HIS
2	B	87	GLY
2	B	386	LEU
2	B	552	LEU
2	D	87	GLY
2	D	386	LEU
2	D	552	LEU
2	B	204	SER
2	B	478	ASN
2	B	546	VAL
2	B	567	LYS
2	D	204	SER
2	D	478	ASN
2	D	546	VAL
2	D	567	LYS
2	B	266	ARG
2	B	482	ASP
2	B	593	ASN
2	D	266	ARG
2	D	482	ASP
2	D	593	ASN
1	A	280	LYS
1	C	280	LYS
2	B	126	TYR
2	D	126	TYR
1	A	91	VAL
1	C	91	VAL

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	264/265 (100%)	251 (95%)	13 (5%)	22	55
1	C	264/265 (100%)	251 (95%)	13 (5%)	22	55
2	B	493/654 (75%)	447 (91%)	46 (9%)	8	27
2	D	493/654 (75%)	447 (91%)	46 (9%)	8	27
All	All	1514/1838 (82%)	1396 (92%)	118 (8%)	11	35

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	91	VAL
1	A	135	LEU
1	A	157	ILE
1	A	163	LEU
1	A	195	ASP
1	A	217	LYS
1	A	222	ASP
1	A	250	GLN
1	A	271	ILE
1	A	287	LEU
1	A	293	GLU
1	A	304	ILE
2	B	42	GLN
2	B	43	LEU
2	B	45	ASN
2	B	57	LEU
2	B	90	LEU
2	B	112	TRP
2	B	120	LEU
2	B	123	ASP
2	B	168	GLU
2	B	201	ILE
2	B	220	LYS

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Mol	Chain	Res	Type
2	B	221	GLU
2	B	259	ILE
2	B	273	THR
2	B	275	HIS
2	B	301	THR
2	B	336	SER
2	B	337	LEU
2	B	362	MET
2	B	363	CYS
2	B	370	VAL
2	B	383	VAL
2	B	387	GLN
2	B	418	THR
2	B	422	THR
2	B	435	SER
2	B	436	GLU
2	B	438	LEU
2	B	442	ILE
2	B	443	SER
2	B	444	THR
2	B	454	ASN
2	B	469	ARG
2	B	487	SER
2	B	496	LEU
2	B	502	THR
2	B	506	THR
2	B	576	GLU
2	B	599	LYS
2	B	604	LEU
2	B	611	THR
2	B	621	THR
2	B	622	LEU
2	B	634	PHE
2	B	648	GLN
2	B	650	SER
1	C	80	GLN
1	C	91	VAL
1	C	135	LEU
1	C	157	ILE
1	C	163	LEU
1	C	195	ASP
1	C	217	LYS

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Mol	Chain	Res	Type
1	C	222	ASP
1	C	250	GLN
1	C	271	ILE
1	C	287	LEU
1	C	293	GLU
1	C	304	ILE
2	D	42	GLN
2	D	43	LEU
2	D	45	ASN
2	D	57	LEU
2	D	90	LEU
2	D	112	TRP
2	D	120	LEU
2	D	123	ASP
2	D	168	GLU
2	D	201	ILE
2	D	220	LYS
2	D	221	GLU
2	D	259	ILE
2	D	273	THR
2	D	275	HIS
2	D	301	THR
2	D	336	SER
2	D	337	LEU
2	D	362	MET
2	D	363	CYS
2	D	370	VAL
2	D	383	VAL
2	D	387	GLN
2	D	418	THR
2	D	422	THR
2	D	435	SER
2	D	436	GLU
2	D	438	LEU
2	D	442	ILE
2	D	443	SER
2	D	444	THR
2	D	454	ASN
2	D	469	ARG
2	D	487	SER
2	D	496	LEU
2	D	502	THR

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Mol	Chain	Res	Type
2	D	506	THR
2	D	576	GLU
2	D	599	LYS
2	D	604	LEU
2	D	611	THR
2	D	621	THR
2	D	622	LEU
2	D	634	PHE
2	D	648	GLN
2	D	650	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	249	HIS
1	A	250	GLN
2	B	45	ASN
2	B	60	HIS
2	B	129	GLN
2	B	137	ASN
2	B	148	HIS
2	B	265	GLN
2	B	285	ASN
2	B	289	HIS
2	B	332	GLN
2	B	498	GLN
2	B	542	HIS
2	B	594	ASN
2	B	644	HIS
1	C	212	ASN
1	C	249	HIS
1	C	250	GLN
2	D	45	ASN
2	D	129	GLN
2	D	137	ASN
2	D	148	HIS
2	D	265	GLN
2	D	285	ASN
2	D	289	HIS
2	D	332	GLN
2	D	498	GLN

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Mol	Chain	Res	Type
2	D	542	HIS
2	D	594	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	287/289 (99%)	0.14	5 (1%) 69 60	29, 55, 82, 116	0
1	C	287/289 (99%)	0.18	11 (3%) 44 35	36, 60, 91, 111	0
2	B	547/727 (75%)	0.09	11 (2%) 65 56	17, 55, 95, 119	0
2	D	547/727 (75%)	0.58	35 (6%) 25 18	43, 74, 117, 155	0
All	All	1668/2032 (82%)	0.27	62 (3%) 45 36	17, 62, 103, 155	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	134	GLY	5.9
2	D	111	VAL	5.1
1	A	73	ASN	5.0
2	D	577	GLY	4.9
1	C	34	ALA	4.0
1	C	200	ASP	3.7
2	B	139	GLY	3.5
2	B	577	GLY	3.4
1	C	254	VAL	3.4
1	C	253	LEU	3.1
2	D	162	PHE	3.0
1	C	251	SER	3.0
2	D	552	LEU	2.9
2	B	68	ASN	2.9
2	D	140	THR	2.9
2	D	484	HIS	2.9
1	C	320	LYS	2.9
1	A	41	PRO	2.8
1	C	272	ILE	2.8
2	D	227	MET	2.7
2	D	144	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	88	PRO	2.6
2	D	211	LEU	2.6
2	D	391	GLY	2.6
2	B	626	VAL	2.5
2	D	228	PHE	2.5
2	D	79	GLN	2.5
2	D	502	THR	2.5
2	B	554	GLY	2.5
2	D	626	VAL	2.5
2	D	148	HIS	2.5
1	C	73	ASN	2.5
2	D	177	VAL	2.4
2	D	627	GLY	2.4
1	A	34	ALA	2.4
1	A	195	ASP	2.4
2	D	112	TRP	2.4
2	B	634	PHE	2.3
2	D	115	ASN	2.2
1	A	250	GLN	2.2
1	C	145	LYS	2.2
2	D	85	LYS	2.2
2	D	572	SER	2.2
2	D	147	PRO	2.2
2	B	204	SER	2.2
2	D	497	ASN	2.2
2	D	145	VAL	2.2
2	D	139	GLY	2.2
2	D	205	TYR	2.2
2	D	230	THR	2.1
2	D	288	LEU	2.1
2	B	638	ILE	2.1
2	D	224	ASP	2.1
2	B	647	THR	2.1
2	D	130	LEU	2.1
2	D	584	CYS	2.0
2	D	68	ASN	2.0
1	C	140	ASP	2.0
2	D	129	GLN	2.0
1	C	282	ASN	2.0
2	B	391	GLY	2.0
2	B	565	ILE	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 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.