



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:37 AM UTC

PDB ID : 1LOW / pdb_00001low
Title : Aspartyl-tRNA synthetase-1 from space-grown crystals
Authors : Ng, J.D.; Sauter, C.; Lorber, B.; Kirkland, N.; Arnez, J.; Giege, R.
Deposited on : 2002-02-14
Resolution : 2.01 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

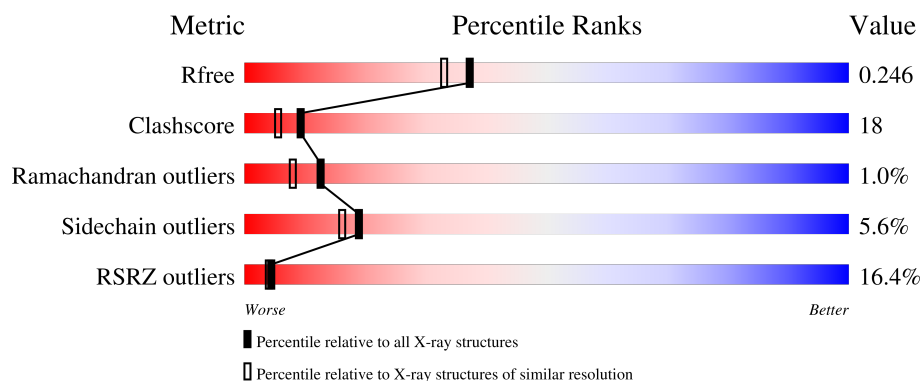
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	580	17% 64% 31% ..
1	B	580	16% 66% 30% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9521 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 Aspartyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4667	2980	840	836	11			
1	B	580	Total	C	N	O	S	0	0	0
			4667	2980	840	836	11			

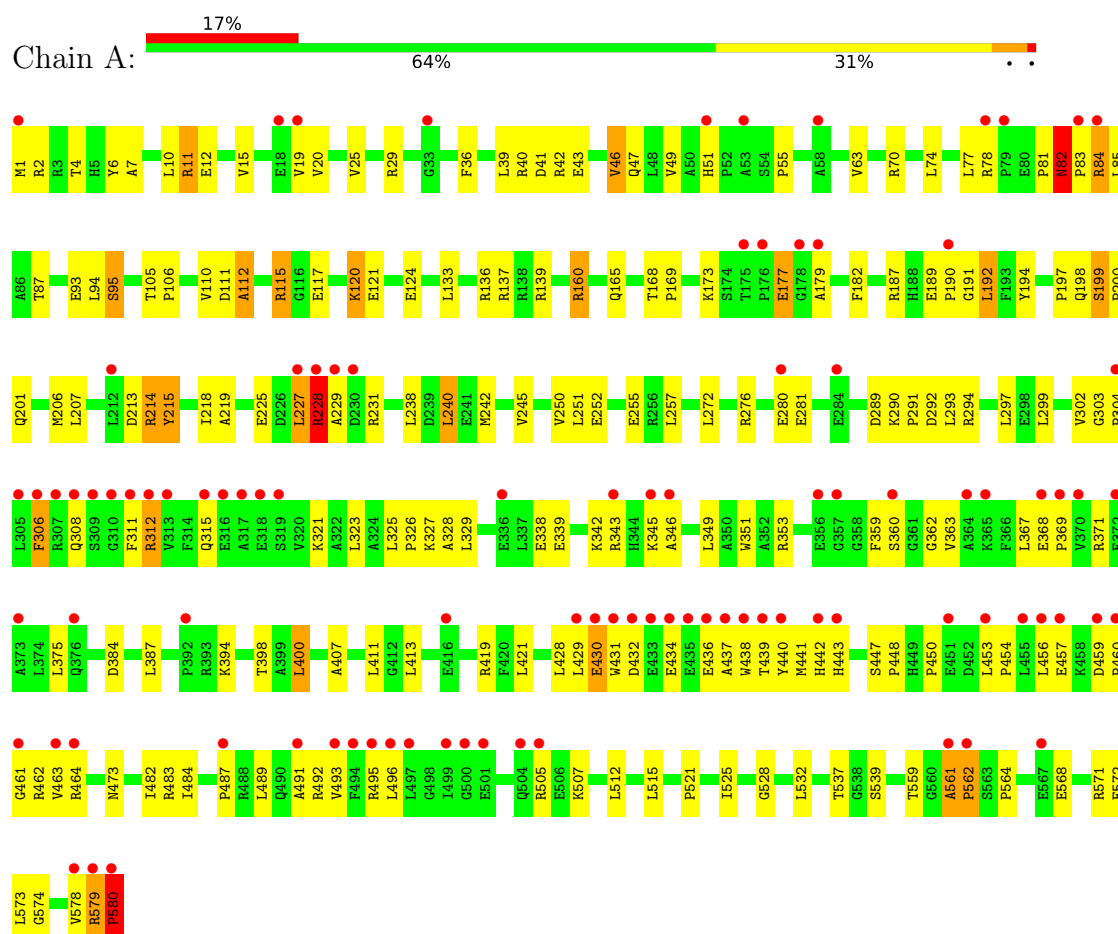
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	109	Total	O	0	0
			109	109		

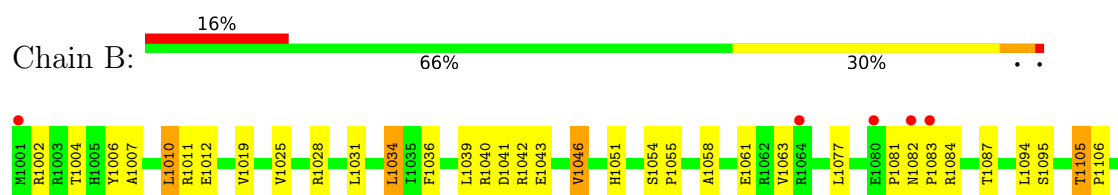
3 Residue-property plots

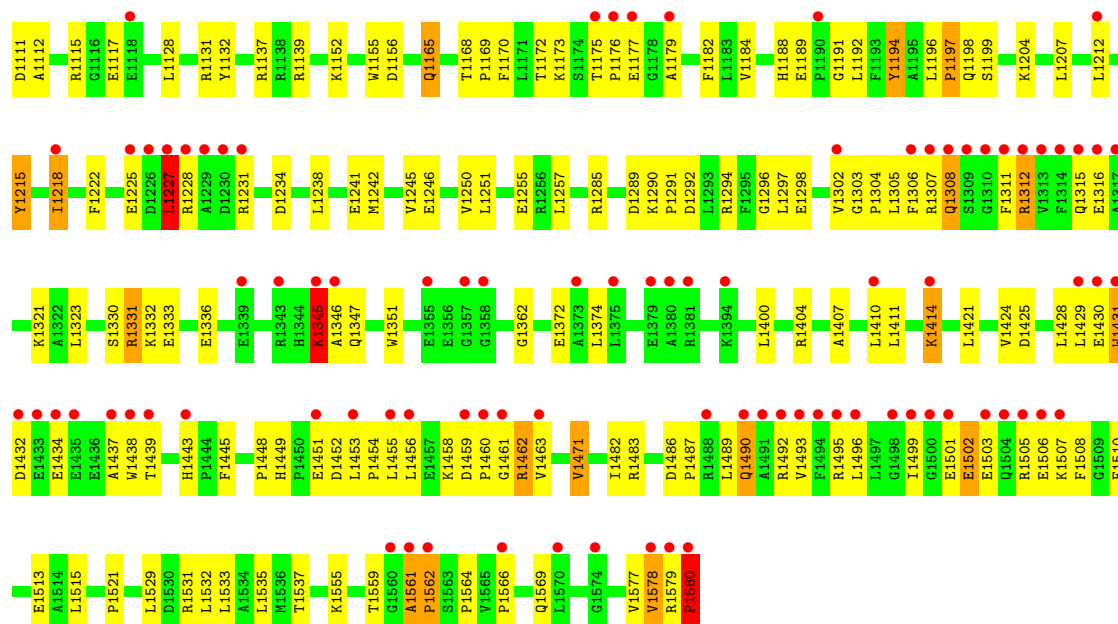
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Aspartyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.02Å 156.10Å 177.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.98 – 2.01 11.98 – 2.01	Depositor EDS
% Data completeness (in resolution range)	70.7 (11.98-2.01) 70.6 (11.98-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.246 0.217 , 0.246	Depositor DCC
R_{free} test set	2438 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.49	0/4779	1.02	31/6467 (0.5%)
1	B	0.53	0/4779	1.31	34/6467 (0.5%)
All	All	0.51	0/9558	1.17	65/12934 (0.5%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1561	ALA	CA-C-N	47.86	179.67	119.84
1	B	1561	ALA	C-N-CA	47.86	179.67	119.84
1	B	1561	ALA	C-N-CD	-12.63	73.21	125.00
1	A	561	ALA	CA-C-N	10.97	153.34	127.00
1	A	561	ALA	C-N-CA	10.97	153.34	127.00
1	A	561	ALA	C-N-CD	-9.71	99.25	120.60
1	A	218	ILE	N-CA-C	-7.92	95.04	107.15
1	A	580	PRO	N-CA-C	7.86	131.74	112.10
1	A	580	PRO	CA-N-CD	-7.29	101.80	112.00
1	A	579	ARG	C-N-CD	-7.23	95.35	125.00
1	B	1105	THR	CA-C-N	7.06	124.74	119.66
1	B	1105	THR	C-N-CA	7.06	124.74	119.66
1	A	238	LEU	N-CA-C	-6.90	97.98	108.96
1	B	1238	LEU	N-CA-C	-6.87	98.04	108.96
1	B	1111	ASP	N-CA-C	6.84	121.86	112.90
1	A	194	TYR	N-CA-C	-6.82	99.86	110.42
1	A	434	GLU	N-CA-C	6.73	121.65	113.17
1	B	1095	SER	N-CA-C	-6.72	105.64	114.31
1	B	1482	ILE	N-CA-C	-6.71	100.08	109.21
1	A	182	PHE	N-CA-C	-6.58	98.90	109.96
1	B	1182	PHE	N-CA-C	-6.29	99.39	109.96
1	B	1006	TYR	N-CA-C	-6.28	100.28	110.20
1	B	1434	GLU	N-CA-C	6.24	121.06	113.38
1	B	1194	TYR	N-CA-C	-6.16	100.87	110.42
1	B	1437	ALA	N-CA-C	6.12	118.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	N-CA-C	-6.10	105.37	114.64
1	A	111	ASP	N-CA-C	5.97	120.72	112.90
1	B	1521	PRO	N-CA-C	-5.92	101.90	111.19
1	A	482	ILE	N-CA-C	-5.91	101.17	109.21
1	B	1218	ILE	N-CA-C	-5.88	96.85	106.32
1	A	95	SER	N-CA-C	-5.87	106.46	113.97
1	A	580	PRO	CA-CB-CG	-5.79	93.51	104.50
1	B	1580	PRO	CA-CB-CG	-5.76	93.55	104.50
1	A	112	ALA	N-CA-C	5.74	117.21	111.07
1	B	1112	ALA	N-CA-C	5.71	117.18	111.07
1	A	306	PHE	N-CA-C	5.68	121.11	113.72
1	A	133	LEU	N-CA-C	-5.67	106.50	113.41
1	B	1228	ARG	N-CA-C	-5.61	106.11	114.64
1	A	437	ALA	N-CA-C	5.59	118.38	110.50
1	B	1316	GLU	N-CA-C	-5.54	105.78	112.54
1	B	1306	PHE	N-CA-C	5.53	120.90	113.72
1	A	528	GLY	N-CA-C	-5.52	100.10	113.18
1	A	94	LEU	N-CA-C	5.51	118.44	110.28
1	A	197	PRO	N-CA-C	5.38	118.93	110.80
1	A	82	ASN	CA-C-N	5.38	126.56	119.84
1	A	82	ASN	C-N-CA	5.38	126.56	119.84
1	A	187	ARG	N-CA-C	5.35	117.53	111.11
1	B	1346	ALA	N-CA-C	-5.32	100.73	109.40
1	B	1212	LEU	N-CA-C	-5.32	98.63	107.99
1	B	1197	PRO	N-CA-C	5.32	118.83	110.80
1	B	1196	LEU	N-CA-C	-5.30	102.51	110.24
1	B	1082	ASN	CA-C-N	5.28	126.43	119.84
1	B	1082	ASN	C-N-CA	5.28	126.43	119.84
1	B	1094	LEU	N-CA-C	5.26	118.06	110.28
1	B	1308	GLN	N-CA-C	-5.24	99.64	110.80
1	A	6	TYR	N-CA-C	-5.22	101.95	110.20
1	B	1580	PRO	CA-N-CD	-5.19	104.74	112.00
1	A	521	PRO	N-CA-C	-5.15	103.11	111.14
1	A	177	GLU	N-CA-C	5.14	117.20	109.23
1	A	346	ALA	N-CA-C	-5.14	101.02	109.40
1	B	1227	LEU	N-CA-C	5.14	117.99	109.46
1	B	1502	GLU	N-CA-C	-5.13	107.57	113.88
1	B	1177	GLU	N-CA-C	5.11	117.15	109.23
1	B	1246	GLU	N-CA-C	-5.04	102.73	110.14
1	A	219	ALA	N-CA-C	5.02	117.99	109.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4667	0	4679	193	0
1	B	4667	0	4676	173	0
2	A	78	0	0	1	0
2	B	109	0	0	3	0
All	All	9521	0	9355	339	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 18.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1307:ARG:HD3	1:B:1315:GLN:HG2	1.27	1.15
1:A:579:ARG:HB3	1:A:580:PRO:HD2	1.31	1.13
1:A:574:GLY:HA3	1:B:1580:PRO:HG3	1.30	1.13
1:A:306:PHE:HB3	1:A:315:GLN:HE22	1.19	1.04
1:A:160:ARG:HH11	1:A:160:ARG:HB3	1.23	1.03
1:B:1428:LEU:HD22	1:B:1448:PRO:HB3	1.47	0.96
1:B:1302:VAL:HG23	1:B:1305:LEU:HD12	1.48	0.95
1:B:1296:GLY:O	1:B:1404:ARG:NH1	1.99	0.95
1:A:574:GLY:CA	1:B:1580:PRO:HG3	1.96	0.94
1:B:1430:GLU:HG2	1:B:1431:TRP:H	1.38	0.88
1:A:120:LYS:H	1:A:120:LYS:HD3	1.36	0.87
1:B:1579:ARG:O	1:B:1580:PRO:HB3	1.75	0.86
1:B:1218:ILE:O	1:B:1218:ILE:HG13	1.74	0.85
1:B:1172:THR:HG22	1:B:1173:LYS:H	1.41	0.84
1:A:2:ARG:NH2	1:B:1245:VAL:HG12	1.93	0.84
1:B:1424:VAL:HG12	1:B:1425:ASP:H	1.43	0.84
1:A:115:ARG:HH11	1:A:115:ARG:HB2	1.42	0.83
1:B:1424:VAL:HG12	1:B:1425:ASP:N	1.94	0.83
1:A:292:ASP:OD1	1:A:294:ARG:HD3	1.80	0.80
1:A:179:ALA:HB3	1:A:198:GLN:OE1	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ARG:CB	1:A:580:PRO:HD2	2.01	0.78
1:A:428:LEU:HD22	1:A:448:PRO:HB3	1.66	0.78
1:A:110:VAL:HG13	1:A:137:ARG:HG2	1.65	0.78
1:B:1297:LEU:HB2	1:B:1404:ARG:NH1	1.99	0.78
1:A:306:PHE:HB3	1:A:315:GLN:NE2	1.99	0.77
1:A:240:LEU:HD21	1:A:242:MET:HE2	1.66	0.77
1:A:411:LEU:HB2	1:A:413:LEU:HD13	1.67	0.76
1:A:190:PRO:HD3	1:B:1580:PRO:HD2	1.68	0.76
1:B:1242:MET:CE	1:B:1250:VAL:HG22	2.16	0.76
1:A:84:ARG:HE	1:A:84:ARG:HA	1.50	0.75
1:A:227:LEU:HD12	1:A:231:ARG:CB	2.17	0.74
1:A:173:LYS:HB2	1:B:1561:ALA:HB2	1.70	0.74
1:A:227:LEU:HD12	1:A:231:ARG:HB3	1.69	0.73
1:B:1179:ALA:HB3	1:B:1198:GLN:OE1	1.88	0.73
1:A:4:THR:OG1	1:A:19:VAL:HG23	1.87	0.73
1:A:120:LYS:HD3	1:A:120:LYS:N	2.03	0.73
1:B:1137:ARG:HH22	1:B:1139:ARG:NH2	1.87	0.72
1:B:1242:MET:HE2	1:B:1250:VAL:HG22	1.70	0.72
1:A:561:ALA:HB2	1:B:1173:LYS:HB2	1.71	0.72
1:B:1566:PRO:HG2	1:B:1569:GLN:HB2	1.72	0.71
1:B:1297:LEU:HB2	1:B:1404:ARG:HH11	1.54	0.71
1:A:251:LEU:O	1:A:255:GLU:HG3	1.89	0.71
1:B:1307:ARG:HD3	1:B:1315:GLN:CG	2.16	0.71
1:B:1011:ARG:HG3	1:B:1011:ARG:HH11	1.57	0.70
1:A:579:ARG:O	1:A:580:PRO:HB2	1.90	0.70
1:A:82:ASN:HD22	1:A:82:ASN:C	2.00	0.69
1:A:306:PHE:CB	1:A:315:GLN:HE22	2.01	0.69
1:B:1455:LEU:HD23	1:B:1458:LYS:HE3	1.72	0.69
1:A:190:PRO:HB3	1:B:1580:PRO:CD	2.23	0.69
1:A:448:PRO:HD2	1:A:484:ILE:HD11	1.73	0.69
1:A:574:GLY:HA3	1:B:1580:PRO:CG	2.18	0.69
1:B:1430:GLU:HG2	1:B:1431:TRP:N	2.08	0.69
1:B:1307:ARG:HB2	1:B:1315:GLN:OE1	1.93	0.69
1:A:160:ARG:HB3	1:A:160:ARG:NH1	2.04	0.68
1:A:55:PRO:HG2	1:A:95:SER:O	1.94	0.68
1:A:572:GLU:O	1:B:1580:PRO:HB2	1.94	0.67
1:B:1449:HIS:ND1	1:B:1451:GLU:HG2	2.09	0.67
1:A:190:PRO:HB3	1:B:1580:PRO:HD3	1.76	0.67
1:A:432:ASP:HB3	1:A:438:TRP:HA	1.77	0.67
1:B:1155:TRP:CH2	1:B:1165:GLN:HG3	2.30	0.67
1:A:303:GLY:N	1:A:304:PRO:HD2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:GLU:HG3	1:B:1227:LEU:HB2	1.77	0.66
1:B:1012:GLU:HG3	1:B:1077:LEU:HD21	1.77	0.66
1:B:1432:ASP:CG	1:B:1438:TRP:HA	2.20	0.65
1:B:1430:GLU:CG	1:B:1431:TRP:H	2.09	0.65
1:A:110:VAL:HG13	1:A:137:ARG:CG	2.27	0.65
1:A:487:PRO:HG3	1:A:515:LEU:HB3	1.80	0.64
1:B:1058:ALA:O	1:B:1061:GLU:HG2	1.98	0.64
1:A:25:VAL:HG21	1:A:63:VAL:HG11	1.80	0.64
1:A:112:ALA:HA	1:A:115:ARG:NH1	2.13	0.64
1:A:110:VAL:HG11	1:A:136:ARG:HB2	1.79	0.64
1:B:1155:TRP:CZ2	1:B:1165:GLN:HG3	2.31	0.64
1:A:206:MET:HE2	1:B:1132:TYR:CD2	2.33	0.64
1:A:229:ALA:HB3	1:A:231:ARG:NH1	2.13	0.64
1:A:110:VAL:HG12	1:A:110:VAL:O	1.95	0.64
1:B:1115:ARG:HB3	1:B:1117:GLU:HG3	1.79	0.64
1:B:1424:VAL:CG1	1:B:1425:ASP:H	2.10	0.64
1:A:447:SER:HA	1:A:484:ILE:HD11	1.79	0.63
1:B:1004:THR:OG1	1:B:1019:VAL:HG23	1.98	0.62
1:B:1168:THR:HG23	1:B:1169:PRO:HD2	1.81	0.62
1:B:1292:ASP:OD2	1:B:1294:ARG:HD3	1.99	0.62
1:A:112:ALA:HA	1:A:115:ARG:HH12	1.65	0.62
1:B:1432:ASP:CB	1:B:1438:TRP:HA	2.30	0.62
1:A:489:LEU:O	1:A:489:LEU:HD23	2.00	0.62
1:B:1449:HIS:CE1	1:B:1451:GLU:HG2	2.35	0.62
1:A:299:LEU:HD22	1:A:400:LEU:HD13	1.81	0.62
1:A:456:LEU:O	1:A:496:LEU:HD21	2.00	0.61
1:A:574:GLY:N	1:B:1580:PRO:HG3	2.14	0.61
1:B:1331:ARG:HG2	1:B:1331:ARG:HH11	1.64	0.61
1:A:228:ARG:H	1:A:228:ARG:HD3	1.64	0.61
1:B:1302:VAL:CG2	1:B:1305:LEU:HD12	2.26	0.61
1:B:1025:VAL:HG21	1:B:1063:VAL:HG11	1.83	0.61
1:A:368:GLU:N	1:A:369:PRO:HD2	2.16	0.61
1:B:1231:ARG:HH11	1:B:1531:ARG:HH21	1.48	0.61
1:A:432:ASP:CB	1:A:438:TRP:HA	2.31	0.60
1:A:505:ARG:O	1:A:505:ARG:HG2	2.01	0.60
1:B:1578:VAL:HG12	1:B:1579:ARG:N	2.17	0.60
1:A:84:ARG:HA	1:A:84:ARG:NE	2.16	0.60
1:A:225:GLU:O	1:A:227:LEU:HD22	2.00	0.60
1:A:562:PRO:HD3	1:B:1194:TYR:CE1	2.37	0.60
1:B:1031:LEU:HD22	1:B:1036:PHE:CE1	2.37	0.59
1:B:1489:LEU:HD23	1:B:1489:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:HD12	1:A:489:LEU:HD22	1.83	0.59
1:B:1137:ARG:HH22	1:B:1139:ARG:HH21	1.49	0.59
1:B:1529:LEU:O	1:B:1533:LEU:HD23	2.02	0.59
1:A:4:THR:HG1	1:A:19:VAL:HG23	1.68	0.59
1:B:1499:ILE:HG23	1:B:1503:GLU:OE1	2.03	0.59
1:A:228:ARG:HD3	1:A:228:ARG:N	2.18	0.59
1:B:1432:ASP:HB3	1:B:1438:TRP:HA	1.84	0.59
1:B:1579:ARG:O	1:B:1580:PRO:CB	2.44	0.58
1:B:1456:LEU:O	1:B:1460:PRO:HG3	2.03	0.58
1:A:343:ARG:HE	1:A:343:ARG:HA	1.68	0.58
1:A:25:VAL:HG21	1:A:63:VAL:CG1	2.33	0.58
1:A:115:ARG:HH11	1:A:115:ARG:CB	2.15	0.58
1:B:1034:LEU:HD12	1:B:1036:PHE:CE1	2.39	0.58
1:A:371:ARG:O	1:A:375:LEU:HD13	2.03	0.58
1:B:1336:GLU:OE2	1:B:1410:LEU:HD21	2.04	0.58
1:A:462:ARG:O	1:A:462:ARG:HG3	2.02	0.58
1:A:7:ALA:O	1:A:46:VAL:HG22	2.04	0.58
1:B:1007:ALA:HB1	1:B:1046:VAL:HG22	1.86	0.58
1:B:1430:GLU:HB3	1:B:1439:THR:HG23	1.86	0.58
1:A:7:ALA:O	1:A:46:VAL:CG2	2.52	0.57
1:A:463:VAL:HG23	1:A:463:VAL:O	2.04	0.57
1:A:7:ALA:HB1	1:A:46:VAL:HG23	1.86	0.57
1:A:173:LYS:HB2	1:B:1559:THR:CG2	2.35	0.57
1:A:579:ARG:O	1:A:580:PRO:CB	2.52	0.57
1:B:1555:LYS:HG2	1:B:1562:PRO:HG3	1.86	0.57
1:A:430:GLU:HG2	1:A:441:MET:HB2	1.86	0.57
1:B:1455:LEU:HD13	1:B:1462:ARG:HE	1.70	0.57
1:A:81:PRO:O	1:A:83:PRO:HD3	2.05	0.57
1:A:430:GLU:OE1	1:A:441:MET:HE3	2.05	0.57
1:A:173:LYS:HB2	1:B:1559:THR:HG22	1.86	0.56
1:B:1204:LYS:HD2	1:B:1241:GLU:HB2	1.87	0.56
1:B:1242:MET:HE1	1:B:1250:VAL:HA	1.87	0.56
1:B:1438:TRP:CD1	1:B:1438:TRP:H	2.24	0.56
1:B:1007:ALA:O	1:B:1046:VAL:HG13	2.06	0.56
1:B:1251:LEU:O	1:B:1255:GLU:HG3	2.05	0.56
1:B:1225:GLU:HB2	1:B:1227:LEU:HD23	1.88	0.56
1:B:1443:HIS:HE1	1:B:1445:PHE:CD1	2.24	0.56
1:A:12:GLU:HG3	1:A:77:LEU:HD21	1.88	0.55
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.70	0.55
1:A:339:GLU:O	1:A:343:ARG:HG2	2.06	0.55
1:B:1566:PRO:HG2	1:B:1569:GLN:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TRP:HD1	1:A:431:TRP:O	1.90	0.54
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.73	0.54
1:B:1345:LYS:HB2	1:B:1345:LYS:NZ	2.21	0.54
1:B:1503:GLU:O	1:B:1507:LYS:HG2	2.07	0.54
1:A:160:ARG:HH11	1:A:160:ARG:CB	2.08	0.54
1:A:177:GLU:HB2	1:A:507:LYS:NZ	2.23	0.54
1:A:431:TRP:O	1:A:431:TRP:CD1	2.61	0.54
1:A:537:THR:HG23	1:A:539:SER:OG	2.07	0.54
1:B:1004:THR:HG1	1:B:1019:VAL:HG23	1.72	0.54
1:A:2:ARG:HH22	1:B:1245:VAL:HG12	1.69	0.54
1:B:1455:LEU:HD13	1:B:1462:ARG:NE	2.23	0.54
1:B:1039:LEU:HD13	1:B:1040:ARG:N	2.23	0.53
1:A:82:ASN:C	1:A:82:ASN:ND2	2.66	0.53
1:A:12:GLU:O	1:A:15:VAL:HG23	2.08	0.53
1:A:39:LEU:HD13	1:A:40:ARG:N	2.23	0.53
1:A:349:LEU:HD11	1:A:387:LEU:HD12	1.90	0.53
1:B:1421:LEU:HG	1:B:1471:VAL:HG13	1.90	0.53
1:A:49:VAL:HG13	1:A:93:GLU:HA	1.90	0.53
1:A:115:ARG:NH1	1:A:117:GLU:CD	2.67	0.53
1:A:227:LEU:HD12	1:A:231:ARG:HB2	1.88	0.53
1:A:359:PHE:CE1	1:A:371:ARG:HG3	2.43	0.53
1:A:189:GLU:HB3	1:A:192:LEU:HD22	1.91	0.53
1:A:430:GLU:HG2	1:A:441:MET:CB	2.39	0.53
1:A:290:LYS:N	1:A:291:PRO:HD3	2.23	0.53
1:B:1507:LYS:HG3	1:B:1508:PHE:CD2	2.44	0.52
1:A:564:PRO:HA	1:B:1191:GLY:O	2.09	0.52
1:B:1152:LYS:HE2	1:B:1156:ASP:OD1	2.08	0.52
1:A:343:ARG:HA	1:A:343:ARG:NE	2.25	0.52
1:A:492:ARG:HA	1:A:495:ARG:HD2	1.92	0.52
1:A:215:TYR:C	1:A:215:TYR:CD2	2.87	0.52
1:A:439:THR:HG22	1:A:440:TYR:N	2.23	0.52
1:A:453:LEU:N	1:A:454:PRO:HD2	2.24	0.52
1:A:363:VAL:HG22	1:A:363:VAL:O	2.10	0.52
1:A:559:THR:HG23	1:B:1510:PHE:CE2	2.45	0.51
1:A:10:LEU:HD22	1:A:46:VAL:HG11	1.93	0.51
1:A:492:ARG:HA	1:A:495:ARG:CD	2.39	0.51
1:B:1424:VAL:CG1	1:B:1425:ASP:N	2.64	0.51
1:B:1456:LEU:O	1:B:1496:LEU:HD11	2.11	0.51
1:A:456:LEU:HG	1:A:496:LEU:HD21	1.93	0.51
1:A:489:LEU:HD23	1:A:489:LEU:C	2.35	0.51
1:A:573:LEU:C	1:B:1580:PRO:HG3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1492:ARG:O	1:B:1495:ARG:HB2	2.11	0.51
1:A:191:GLY:O	1:B:1564:PRO:HA	2.10	0.51
1:A:302:VAL:C	1:A:304:PRO:HD2	2.35	0.51
1:B:1302:VAL:HG22	1:B:1302:VAL:O	2.10	0.50
1:B:1311:PHE:O	1:B:1312:ARG:C	2.54	0.50
1:B:1459:ASP:OD1	1:B:1462:ARG:HD2	2.11	0.50
1:A:227:LEU:H	1:A:227:LEU:CD2	2.25	0.50
1:B:1042:ARG:HD3	1:B:1043:GLU:OE1	2.10	0.50
1:A:568:GLU:OE2	1:A:568:GLU:N	2.44	0.50
1:B:1025:VAL:HG21	1:B:1063:VAL:CG1	2.40	0.50
1:B:1242:MET:HE3	1:B:1245:VAL:HG11	1.93	0.50
1:A:110:VAL:HG11	1:A:136:ARG:CB	2.42	0.50
1:B:1081:PRO:O	1:B:1083:PRO:HD3	2.10	0.50
1:B:1010:LEU:HD23	1:B:1046:VAL:HG11	1.93	0.50
1:B:1218:ILE:HG12	2:B:19:HOH:O	2.12	0.50
1:B:1010:LEU:O	1:B:1087:THR:HG22	2.12	0.50
1:B:1189:GLU:HB2	1:B:1192:LEU:HD22	1.94	0.50
1:A:447:SER:HA	1:A:484:ILE:CD1	2.41	0.50
1:B:1007:ALA:O	1:B:1046:VAL:CG1	2.60	0.50
1:B:1321:LYS:CB	1:B:1400:LEU:HD12	2.41	0.50
1:A:311:PHE:O	1:A:312:ARG:C	2.55	0.49
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.77	0.49
1:A:245:VAL:HG12	1:B:1002:ARG:NH2	2.26	0.49
1:A:432:ASP:CG	1:A:438:TRP:HA	2.38	0.49
1:B:1332:LYS:O	1:B:1332:LYS:HD3	2.12	0.49
1:B:1537:THR:O	1:B:1537:THR:CG2	2.61	0.49
1:A:190:PRO:CD	1:B:1580:PRO:HD2	2.40	0.49
1:A:242:MET:HE1	1:A:250:VAL:HA	1.94	0.49
1:B:1011:ARG:HH11	1:B:1011:ARG:CG	2.20	0.49
1:A:579:ARG:NH1	1:A:579:ARG:HB2	2.28	0.48
1:B:1285:ARG:HD2	1:B:1298:GLU:OE1	2.14	0.48
1:A:84:ARG:C	1:A:85:LEU:HD22	2.37	0.48
1:B:1489:LEU:HD23	1:B:1489:LEU:C	2.39	0.48
1:A:11:ARG:HH21	1:A:87:THR:HG22	1.78	0.48
1:A:227:LEU:HD23	1:A:227:LEU:O	2.14	0.48
1:A:120:LYS:H	1:A:120:LYS:CD	2.10	0.48
1:B:1222:PHE:CD2	1:B:1234:ASP:HB3	2.49	0.48
1:B:1290:LYS:N	1:B:1291:PRO:HD3	2.28	0.47
1:A:407:ALA:O	1:A:411:LEU:HG	2.14	0.47
1:B:1297:LEU:HB3	1:B:1323:LEU:HD11	1.95	0.47
1:B:1040:ARG:HG2	1:B:1041:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1531:ARG:O	1:B:1535:LEU:HD23	2.14	0.47
1:A:177:GLU:HB2	1:A:507:LYS:HZ2	1.80	0.47
1:A:297:LEU:HB3	1:A:323:LEU:HD11	1.97	0.47
1:A:561:ALA:HB2	1:B:1173:LYS:CB	2.43	0.47
1:B:1002:ARG:HA	2:B:31:HOH:O	2.13	0.47
1:B:1225:GLU:CG	1:B:1227:LEU:HD23	2.45	0.47
1:A:338:GLU:HG2	1:A:342:LYS:HE2	1.97	0.47
1:B:1296:GLY:C	1:B:1404:ARG:HH12	2.17	0.47
1:B:1489:LEU:HD23	1:B:1493:VAL:HG23	1.97	0.47
1:B:1492:ARG:HA	1:B:1495:ARG:HD2	1.96	0.47
1:A:325:LEU:HD12	1:A:329:LEU:HD11	1.95	0.46
1:A:168:THR:HG23	1:A:169:PRO:HD2	1.97	0.46
1:A:49:VAL:HG22	1:A:51:HIS:CD2	2.50	0.46
1:A:326:PRO:HA	1:A:384:ASP:OD1	2.15	0.46
1:B:1537:THR:O	1:B:1537:THR:HG22	2.14	0.46
1:B:1414:LYS:HE3	1:B:1414:LYS:H	1.79	0.46
1:A:242:MET:HE3	1:A:250:VAL:HG22	1.98	0.46
1:A:438:TRP:CH2	1:A:460:PRO:HG2	2.50	0.46
1:A:115:ARG:HB2	1:A:115:ARG:NH1	2.22	0.46
1:B:1453:LEU:N	1:B:1454:PRO:HD2	2.30	0.46
1:A:240:LEU:HD22	1:A:525:ILE:HG22	1.98	0.46
1:A:42:ARG:HG3	1:A:43:GLU:N	2.31	0.46
1:A:1:MET:SD	1:A:70:ARG:NH1	2.89	0.45
1:A:289:ASP:C	1:A:291:PRO:HD3	2.41	0.45
1:B:1292:ASP:OD2	1:B:1294:ARG:CD	2.64	0.45
1:A:351:TRP:O	1:A:362:GLY:HA3	2.17	0.45
1:B:1011:ARG:CG	1:B:1011:ARG:NH1	2.77	0.45
1:A:39:LEU:HD13	1:A:39:LEU:C	2.42	0.45
1:B:1184:VAL:HB	1:B:1194:TYR:HB2	1.99	0.45
1:A:294:ARG:HD2	1:A:473:ASN:CG	2.42	0.45
1:A:303:GLY:N	1:A:304:PRO:CD	2.78	0.45
1:A:19:VAL:HG22	1:A:20:VAL:N	2.32	0.45
1:A:83:PRO:O	1:A:84:ARG:HB2	2.17	0.45
1:A:110:VAL:O	1:A:110:VAL:CG1	2.65	0.45
1:A:537:THR:CG2	1:A:539:SER:OG	2.65	0.45
1:A:559:THR:O	1:B:1173:LYS:HD2	2.17	0.44
1:A:190:PRO:HB2	1:B:1577:VAL:CG1	2.48	0.44
1:A:559:THR:HG22	1:B:1173:LYS:HD2	2.00	0.44
1:A:7:ALA:HB2	1:A:39:LEU:HD12	2.00	0.44
1:B:1502:GLU:O	1:B:1506:GLU:HG3	2.17	0.44
1:A:492:ARG:O	1:A:495:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1321:LYS:HB2	1:B:1400:LEU:HD12	1.98	0.44
1:B:1421:LEU:HG	1:B:1471:VAL:CG1	2.47	0.44
1:A:2:ARG:HA	2:A:617:HOH:O	2.16	0.44
1:B:1505:ARG:HG2	1:B:1505:ARG:HH11	1.81	0.44
1:A:213:ASP:OD1	1:A:214:ARG:HD3	2.17	0.44
1:B:1330:SER:OG	1:B:1333:GLU:HG3	2.17	0.44
1:A:450:PRO:O	1:A:453:LEU:HB2	2.18	0.44
1:A:429:LEU:HD13	1:A:438:TRP:CB	2.47	0.43
1:B:1486:ASP:HA	1:B:1487:PRO:HD3	1.89	0.43
1:A:349:LEU:HD13	1:A:349:LEU:C	2.43	0.43
1:A:321:LYS:HB2	1:A:400:LEU:HD12	2.00	0.43
1:A:489:LEU:HD23	1:A:493:VAL:HG23	2.00	0.43
1:B:1555:LYS:HG2	1:B:1562:PRO:CG	2.47	0.43
1:A:387:LEU:N	1:A:387:LEU:HD22	2.34	0.43
1:B:1168:THR:HG23	1:B:1169:PRO:CD	2.48	0.43
1:A:229:ALA:HB3	1:A:231:ARG:HH12	1.79	0.43
1:B:1289:ASP:C	1:B:1291:PRO:HD3	2.43	0.43
1:B:1459:ASP:C	1:B:1461:GLY:H	2.26	0.43
1:B:1501:GLU:O	1:B:1505:ARG:HG3	2.19	0.43
1:A:173:LYS:CB	1:B:1559:THR:CG2	2.97	0.43
1:A:40:ARG:HG2	1:A:41:ASP:N	2.34	0.43
1:B:1175:THR:HG23	1:B:1176:PRO:HD2	2.00	0.43
1:A:1:MET:N	1:A:1:MET:HE2	2.33	0.42
1:A:36:PHE:CD1	1:A:36:PHE:N	2.87	0.42
1:A:189:GLU:CB	1:A:192:LEU:HD22	2.48	0.42
1:B:1172:THR:HG22	1:B:1173:LYS:N	2.21	0.42
1:B:1227:LEU:HB3	1:B:1231:ARG:HB2	2.00	0.42
1:B:1307:ARG:HD2	1:B:1307:ARG:HA	1.73	0.42
1:A:227:LEU:HB2	1:A:231:ARG:HB2	2.01	0.42
1:A:457:GLU:OE1	1:A:492:ARG:NH2	2.52	0.42
1:B:1452:ASP:HB3	1:B:1463:VAL:HG13	2.01	0.42
1:A:280:GLU:HG3	1:A:281:GLU:N	2.34	0.42
1:A:367:LEU:C	1:A:369:PRO:HD2	2.44	0.42
1:B:1002:ARG:HD3	2:B:31:HOH:O	2.19	0.42
1:B:1170:PHE:O	1:B:1197:PRO:HD3	2.19	0.42
1:A:368:GLU:N	1:A:369:PRO:CD	2.82	0.42
1:A:47:GLN:NE2	1:A:78:ARG:NH2	2.66	0.42
1:B:1042:ARG:CD	1:B:1043:GLU:OE1	2.68	0.42
1:B:1487:PRO:HG3	1:B:1515:LEU:HB3	2.02	0.42
1:A:459:ASP:C	1:A:461:GLY:H	2.27	0.42
1:A:491:ALA:O	1:A:495:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:ARG:NH1	1:B:1061:GLU:O	2.49	0.42
1:B:1407:ALA:O	1:B:1411:LEU:HG	2.19	0.42
1:A:327:LYS:HG2	1:A:328:ALA:N	2.35	0.42
1:A:7:ALA:CB	1:A:39:LEU:HD12	2.49	0.41
1:A:137:ARG:HH22	1:A:139:ARG:NH2	2.18	0.41
1:A:293:LEU:O	1:A:419:ARG:NH1	2.53	0.41
1:B:1105:THR:HA	1:B:1106:PRO:HD3	1.82	0.41
1:A:121:GLU:OE2	1:A:139:ARG:NH2	2.53	0.41
1:B:1428:LEU:CD2	1:B:1448:PRO:HB3	2.35	0.41
1:B:1456:LEU:HG	1:B:1496:LEU:HD11	2.01	0.41
1:A:394:LYS:O	1:A:398:THR:HG23	2.20	0.41
1:B:1004:THR:OG1	1:B:1019:VAL:CG2	2.66	0.41
1:B:1490:GLN:OE1	1:B:1490:GLN:O	2.38	0.41
1:A:448:PRO:CD	1:A:484:ILE:HD11	2.46	0.41
1:A:353:ARG:HB2	1:A:360:SER:OG	2.20	0.41
1:B:1351:TRP:O	1:B:1362:GLY:HA3	2.20	0.41
1:B:1430:GLU:CG	1:B:1431:TRP:N	2.74	0.41
1:A:105:THR:HA	1:A:106:PRO:HD3	1.91	0.41
1:A:487:PRO:HG3	1:A:515:LEU:CB	2.50	0.41
1:B:1347:GLN:OE1	1:B:1347:GLN:HA	2.21	0.41
1:B:1429:LEU:HD13	1:B:1438:TRP:HB2	2.03	0.41
1:B:1188:HIS:O	1:B:1189:GLU:HG3	2.21	0.41
1:B:1303:GLY:N	1:B:1304:PRO:CD	2.84	0.41
1:A:442:HIS:HB2	1:A:443:HIS:H	1.71	0.40
1:A:579:ARG:HB2	1:A:579:ARG:CZ	2.50	0.40
1:B:1054:SER:HA	1:B:1055:PRO:HD3	1.92	0.40
1:B:1331:ARG:HH11	1:B:1331:ARG:CG	2.33	0.40
1:A:443:HIS:HE2	1:A:483:ARG:HH11	1.70	0.40
1:B:1215:TYR:CD2	1:B:1215:TYR:C	2.99	0.40
1:A:571:ARG:HD2	1:A:571:ARG:HA	1.87	0.40
1:A:199:SER:HA	1:A:200:PRO:HD3	1.89	0.40
1:B:1189:GLU:CB	1:B:1192:LEU:HD22	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	578/580 (100%)	537 (93%)	35 (6%)	6 (1%)	12	8
1	B	578/580 (100%)	538 (93%)	34 (6%)	6 (1%)	12	8
All	All	1156/1160 (100%)	1075 (93%)	69 (6%)	12 (1%)	12	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	312	ARG
1	B	1084	ARG
1	B	1312	ARG
1	B	1562	PRO
1	A	308	GLN
1	B	1308	GLN
1	A	345	LYS
1	A	562	PRO
1	B	1345	LYS
1	B	1578	VAL
1	A	578	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	483/483 (100%)	454 (94%)	29 (6%)	17	14
1	B	483/483 (100%)	458 (95%)	25 (5%)	21	18
All	All	966/966 (100%)	912 (94%)	54 (6%)	19	16

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	46	VAL
1	A	74	LEU
1	A	82	ASN
1	A	115	ARG
1	A	120	LYS
1	A	124	GLU
1	A	160	ARG
1	A	165	GLN
1	A	192	LEU
1	A	199	SER
1	A	201	GLN
1	A	207	LEU
1	A	214	ARG
1	A	215	TYR
1	A	227	LEU
1	A	228	ARG
1	A	240	LEU
1	A	252	GLU
1	A	257	LEU
1	A	272	LEU
1	A	400	LEU
1	A	421	LEU
1	A	430	GLU
1	A	436	GLU
1	A	464	ARG
1	A	512	LEU
1	A	532	LEU
1	A	580	PRO
1	B	1010	LEU
1	B	1034	LEU
1	B	1046	VAL
1	B	1051	HIS
1	B	1128	LEU
1	B	1131	ARG
1	B	1165	GLN
1	B	1199	SER
1	B	1207	LEU
1	B	1215	TYR
1	B	1227	LEU
1	B	1257	LEU
1	B	1331	ARG
1	B	1345	LYS

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Mol	Chain	Res	Type
1	B	1372	GLU
1	B	1374	LEU
1	B	1414	LYS
1	B	1431	TRP
1	B	1462	ARG
1	B	1471	VAL
1	B	1483	ARG
1	B	1490	GLN
1	B	1513	GLU
1	B	1532	LEU
1	B	1580	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	82	ASN
1	A	143	ASN
1	A	205	GLN
1	A	315	GLN
1	A	376	GLN
1	B	1047	GLN
1	B	1143	ASN
1	B	1376	GLN
1	B	1504	GLN
1	B	1569	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	580/580 (100%)	0.69	97 (16%)  	14, 38, 91, 139	0
1	B	580/580 (100%)	0.56	93 (16%)  	14, 33, 90, 136	0
All	All	1160/1160 (100%)	0.62	190 (16%)  	14, 35, 91, 139	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1580	PRO	12.8
1	A	227	LEU	7.2
1	B	1309	SER	7.2
1	B	1437	ALA	6.9
1	A	580	PRO	6.8
1	B	1310	GLY	6.7
1	B	1317	ALA	6.4
1	A	431	TRP	6.0
1	B	1434	GLU	5.9
1	B	1307	ARG	5.9
1	B	1315	GLN	5.8
1	A	437	ALA	5.7
1	B	1578	VAL	5.6
1	A	561	ALA	5.5
1	B	1561	ALA	5.3
1	B	1439	THR	5.3
1	A	439	THR	5.2
1	B	1432	ASP	5.2
1	A	438	TRP	5.2
1	A	357	GLY	5.1
1	B	1227	LEU	5.1
1	A	317	ALA	5.0
1	B	1083	PRO	5.0
1	A	176	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	1438	TRP	5.0
1	B	1346	ALA	4.9
1	B	1229	ALA	4.8
1	B	1431	TRP	4.8
1	A	578	VAL	4.8
1	A	494	PHE	4.6
1	A	461	GLY	4.6
1	B	1579	ARG	4.5
1	B	1433	GLU	4.5
1	A	456	LEU	4.4
1	B	1496	LEU	4.4
1	A	319	SER	4.4
1	A	315	GLN	4.4
1	A	1	MET	4.3
1	A	499	ILE	4.3
1	A	436	GLU	4.2
1	B	1435	GLU	4.2
1	B	1491	ALA	4.2
1	A	434	GLU	4.1
1	B	1176	PRO	4.0
1	B	1500	GLY	4.0
1	A	453	LEU	4.0
1	B	1175	THR	4.0
1	A	443	HIS	4.0
1	B	1498	GLY	4.0
1	B	1231	ARG	3.9
1	A	497	LEU	3.9
1	A	579	ARG	3.9
1	B	1504	GLN	3.8
1	A	562	PRO	3.8
1	A	370	VAL	3.8
1	B	1358	GLY	3.7
1	B	1082	ASN	3.7
1	A	309	SER	3.7
1	A	311	PHE	3.7
1	A	175	THR	3.6
1	A	84	ARG	3.6
1	A	493	VAL	3.6
1	B	1177	GLU	3.6
1	B	1001	MET	3.5
1	A	229	ALA	3.4
1	A	491	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	307	ARG	3.4
1	B	1451	GLU	3.4
1	B	1562	PRO	3.4
1	B	1218	ILE	3.4
1	B	1316	GLU	3.4
1	B	1311	PHE	3.4
1	A	304	PRO	3.3
1	B	1312	ARG	3.3
1	B	1459	ASP	3.3
1	A	501	GLU	3.3
1	A	432	ASP	3.3
1	B	1230	ASP	3.3
1	A	308	GLN	3.2
1	B	1460	PRO	3.2
1	B	1345	LYS	3.2
1	A	429	LEU	3.2
1	B	1308	GLN	3.2
1	A	33	GLY	3.1
1	B	1429	LEU	3.1
1	B	1461	GLY	3.1
1	A	230	ASP	3.1
1	A	280	GLU	3.1
1	B	1225	GLU	3.1
1	B	1506	GLU	3.0
1	A	305	LEU	3.0
1	A	310	GLY	3.0
1	A	504	GLN	3.0
1	B	1313	VAL	3.0
1	A	316	GLU	2.9
1	A	464	ARG	2.9
1	A	178	GLY	2.9
1	A	313	VAL	2.9
1	A	372	GLU	2.9
1	B	1373	ALA	2.9
1	A	496	LEU	2.9
1	A	79	PRO	2.9
1	B	1339	GLU	2.9
1	B	1574	GLY	2.9
1	A	212	LEU	2.8
1	A	19	VAL	2.8
1	B	1456	LEU	2.8
1	B	1495	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	440	TYR	2.8
1	B	1302	VAL	2.8
1	B	1490	GLN	2.8
1	A	284	GLU	2.8
1	B	1455	LEU	2.8
1	A	460	PRO	2.8
1	A	457	GLU	2.7
1	B	1212	LEU	2.7
1	A	416	GLU	2.7
1	A	430	GLU	2.7
1	B	1507	LYS	2.7
1	A	312	ARG	2.7
1	A	495	ARG	2.7
1	B	1492	ARG	2.7
1	A	364	ALA	2.6
1	A	368	GLU	2.6
1	A	455	LEU	2.6
1	A	369	PRO	2.6
1	B	1566	PRO	2.6
1	B	1118	GLU	2.6
1	B	1306	PHE	2.6
1	A	343	ARG	2.6
1	B	1381	ARG	2.6
1	B	1357	GLY	2.6
1	A	373	ALA	2.6
1	A	459	ASP	2.6
1	A	51	HIS	2.6
1	A	346	ALA	2.6
1	B	1488	ARG	2.6
1	B	1505	ARG	2.6
1	B	1430	GLU	2.5
1	B	1501	GLU	2.5
1	B	1503	GLU	2.5
1	B	1494	PHE	2.5
1	A	376	GLN	2.5
1	A	463	VAL	2.5
1	A	336	GLU	2.4
1	B	1179	ALA	2.4
1	A	18	GLU	2.4
1	A	318	GLU	2.4
1	B	1493	VAL	2.4
1	B	1190	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	306	PHE	2.4
1	B	1499	ILE	2.4
1	A	228	ARG	2.4
1	A	345	LYS	2.4
1	B	1380	ALA	2.4
1	A	500	GLY	2.4
1	A	442	HIS	2.4
1	B	1410	LEU	2.3
1	A	505	ARG	2.3
1	A	360	SER	2.3
1	A	53	ALA	2.3
1	B	1379	GLU	2.3
1	B	1463	VAL	2.3
1	B	1560	GLY	2.3
1	A	365	LYS	2.3
1	B	1394	LYS	2.3
1	B	1355	GLU	2.2
1	A	83	PRO	2.2
1	A	392	PRO	2.2
1	B	1570	LEU	2.2
1	B	1228	ARG	2.2
1	A	435	GLU	2.2
1	B	1443	HIS	2.2
1	A	487	PRO	2.2
1	B	1314	PHE	2.2
1	B	1375	LEU	2.2
1	A	78	ARG	2.2
1	B	1226	ASP	2.2
1	A	356	GLU	2.1
1	A	179	ALA	2.1
1	B	1343	ARG	2.1
1	A	451	GLU	2.1
1	A	58	ALA	2.1
1	B	1414	LYS	2.1
1	B	1453	LEU	2.1
1	A	567	GLU	2.1
1	B	1080	GLU	2.1
1	A	433	GLU	2.0
1	B	1064	ARG	2.0
1	A	190	PRO	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.