



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:53 PM UTC

PDB ID : 1D0N / pdb_00001d0n
Title : THE CRYSTAL STRUCTURE OF CALCIUM-FREE EQUINE PLASMA GELSOLIN.
Authors : Burtnick, L.D.; Robinson, R.; Li, C.
Deposited on : 1999-09-13
Resolution : 2.50 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

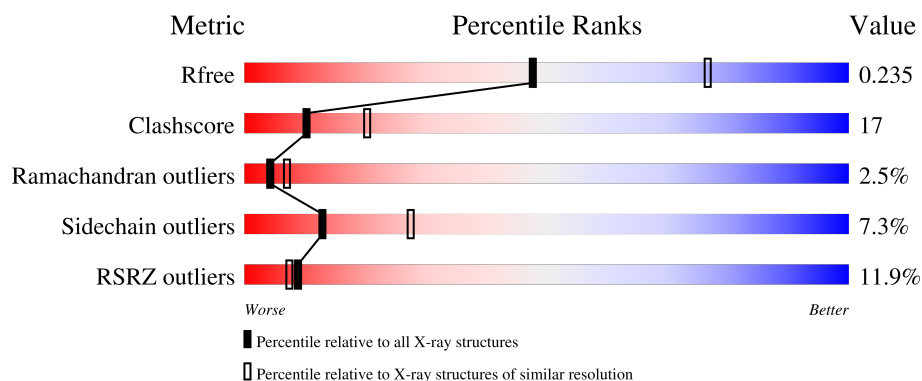
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	729	13% 65% 29% 5%
1	B	729	11% 65% 29% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11666 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 HORSE PLASMA GELSOLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5691	3598	990	1087	16			
1	B	729	Total	C	N	O	S	0	0	0
			5691	3598	990	1087	16			

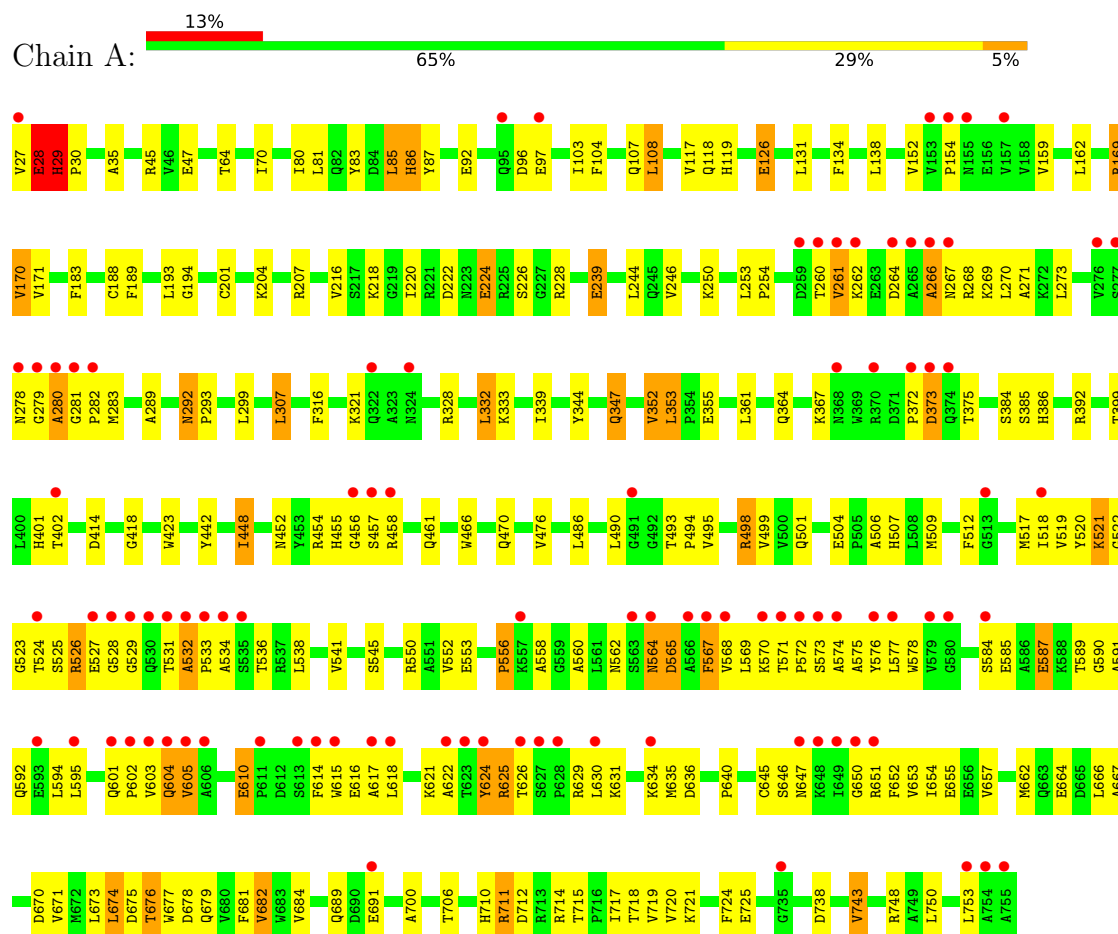
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		
2	B	145	Total	O	0	0
			145	145		

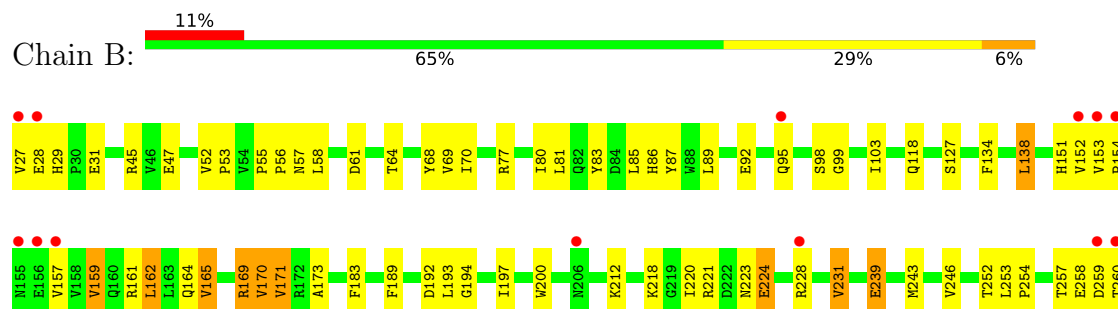
3 Residue-property plots

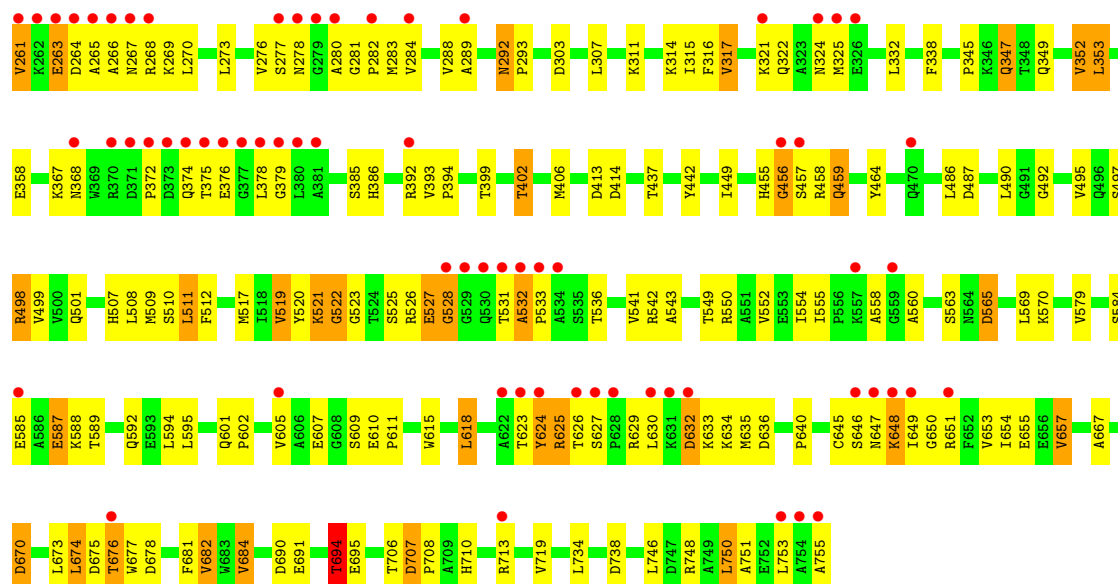
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: HORSE PLASMA GELSOLIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.40Å 169.40Å 154.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.50) 91.7 (20.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.50Å)	Xtriage
Refinement program	CNS, X-PLOR & CNS	Depositor
R, R_{free}	0.205 , 0.238 0.204 , 0.235	Depositor DCC
R_{free} test set	3617 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11666	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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	0.41	0/5825	0.91	14/7894 (0.2%)
1	B	0.44	0/5825	0.93	16/7894 (0.2%)
All	All	0.43	0/11650	0.92	30/15788 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	THR	N-CA-C	-11.10	96.21	110.53
1	A	224	GLU	N-CA-C	-8.40	97.12	110.14
1	B	676	THR	N-CA-C	-7.94	98.05	110.36
1	B	521	LYS	N-CA-C	-7.49	104.28	113.19
1	B	224	GLU	N-CA-C	-6.54	99.55	109.95
1	A	35	ALA	N-CA-C	6.32	119.43	109.96
1	B	495	VAL	N-CA-C	-6.19	99.46	108.87
1	B	678	ASP	N-CA-C	6.07	118.68	111.33
1	A	87	TYR	N-CA-C	-5.90	99.78	109.40
1	B	375	THR	N-CA-C	-5.89	104.93	111.71
1	A	328	ARG	N-CA-C	-5.78	104.35	111.40
1	B	497	SER	N-CA-C	5.50	117.87	108.90
1	A	28	GLU	N-CA-C	5.44	122.38	110.80
1	A	495	VAL	N-CA-C	-5.41	100.79	108.58
1	A	222	ASP	N-CA-C	5.39	117.98	111.40
1	B	171	VAL	N-CA-C	5.38	116.46	108.23
1	B	83	TYR	N-CA-C	5.34	117.60	108.90
1	B	694	THR	N-CA-C	-5.30	106.66	113.23
1	A	29	HIS	CA-C-N	5.25	125.31	119.32
1	A	29	HIS	C-N-CA	5.25	125.31	119.32
1	B	303	ASP	N-CA-C	5.21	116.57	109.18
1	B	602	PRO	N-CA-C	5.18	119.62	111.38
1	A	476	VAL	N-CA-C	-5.13	105.71	110.53
1	A	83	TYR	N-CA-C	5.11	117.39	108.76
1	A	117	VAL	N-CA-C	-5.11	101.22	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	THR	N-CA-C	-5.09	105.82	112.23
1	B	707	ASP	CA-C-N	5.04	124.83	119.28
1	B	707	ASP	C-N-CA	5.04	124.83	119.28
1	B	601	GLN	CA-C-N	5.01	124.91	119.85
1	B	601	GLN	C-N-CA	5.01	124.91	119.85

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	5691	0	5547	198	0
1	B	5691	0	5547	186	0
2	A	139	0	0	7	0
2	B	145	0	0	4	0
All	All	11666	0	11094	384	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 17.

All (384) 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:508:LEU:HG	1:B:517:MET:HE1	1.30	1.08
1:B:118:GLN:HB2	1:B:352:VAL:HG13	1.50	0.93
1:B:579:VAL:HG21	1:B:588:LYS:HE2	1.53	0.90
1:B:29:HIS:HD2	1:B:31:GLU:H	1.20	0.89
1:A:506:ALA:HA	1:A:509:MET:HE3	1.54	0.88
1:A:399:THR:O	1:A:402:THR:HG22	1.77	0.83
1:A:118:GLN:HB2	1:A:352:VAL:HG22	1.59	0.83
1:A:592:GLN:HA	1:A:595:LEU:HD23	1.63	0.81
1:B:558:ALA:HA	1:B:618:LEU:HD23	1.64	0.80
1:B:353:LEU:HD12	1:B:358:GLU:HA	1.64	0.79
1:A:578:TRP:HA	1:A:605:VAL:HG13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASN:HB3	1:A:283:MET:HA	1.67	0.76
1:B:153:VAL:HG12	1:B:157:VAL:HG21	1.69	0.75
1:A:169:ARG:HG3	1:A:655:GLU:OE2	1.88	0.73
1:A:307:LEU:HB3	1:A:316:PHE:HB2	1.71	0.73
1:B:293:PRO:HD3	1:B:710:HIS:ND1	2.03	0.73
1:B:261:VAL:HG13	1:B:263:GLU:HG2	1.70	0.73
1:A:442:TYR:HB3	1:A:523:GLY:O	1.88	0.72
1:A:504:GLU:HG2	1:A:517:MET:HE1	1.71	0.71
1:A:571:THR:HG23	1:A:573:SER:H	1.54	0.71
1:B:267:ASN:O	1:B:268:ARG:HD3	1.91	0.71
1:B:509:MET:HA	1:B:517:MET:HE3	1.72	0.71
1:A:239:GLU:CD	1:A:239:GLU:H	1.99	0.70
1:B:675:ASP:OD1	1:B:676:THR:O	2.10	0.70
1:B:353:LEU:HD23	1:B:353:LEU:N	2.08	0.69
1:A:97:GLU:HG3	2:A:796:HOH:O	1.92	0.68
1:B:64:THR:CG2	1:B:92:GLU:HG2	2.25	0.67
1:A:269:LYS:HB3	1:A:706:THR:O	1.93	0.67
1:A:571:THR:HG22	1:A:574:ALA:O	1.94	0.67
1:A:501:GLN:HE21	1:A:519:VAL:CG1	2.08	0.67
1:B:292:ASN:H	1:B:292:ASN:HD22	1.43	0.67
1:A:647:ASN:ND2	1:A:652:PHE:HD1	1.93	0.67
1:A:455:HIS:O	1:A:457:SER:N	2.28	0.66
1:A:292:ASN:HD22	1:A:292:ASN:H	1.42	0.66
1:A:339:ILE:HG23	1:A:344:TYR:HB2	1.77	0.66
1:A:675:ASP:OD1	1:A:676:THR:O	2.13	0.66
1:B:170:VAL:HA	2:B:799:HOH:O	1.94	0.66
1:B:623:THR:HG22	1:B:624:TYR:H	1.61	0.66
1:A:571:THR:OG1	1:A:572:PRO:HD2	1.95	0.66
1:B:347:GLN:CD	1:B:347:GLN:H	2.02	0.66
1:A:646:SER:HB2	1:A:653:VAL:HG12	1.78	0.65
1:B:317:VAL:HG22	1:B:352:VAL:HB	1.79	0.65
1:A:629:ARG:HG3	1:A:629:ARG:HH11	1.62	0.64
1:A:293:PRO:HD3	1:A:710:HIS:ND1	2.12	0.64
1:A:266:ALA:HB2	1:A:651:ARG:HH11	1.63	0.64
1:A:585:GLU:O	1:A:589:THR:HG22	1.97	0.63
1:B:239:GLU:CD	1:B:239:GLU:H	2.07	0.63
1:B:508:LEU:HG	1:B:517:MET:CE	2.18	0.63
1:A:682:VAL:HG13	1:A:719:VAL:HA	1.80	0.63
1:B:151:HIS:O	1:B:153:VAL:HG23	1.98	0.63
1:A:712:ASP:OD2	1:A:714:ARG:HB2	1.99	0.63
1:B:263:GLU:O	1:B:265:ALA:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ALA:HA	1:B:268:ARG:HE	1.64	0.62
1:B:584:SER:H	1:B:587:GLU:HG2	1.65	0.62
1:A:526:ARG:HG3	1:A:527:GLU:HG2	1.82	0.62
1:B:269:LYS:HB3	1:B:706:THR:O	2.00	0.62
1:A:126:GLU:HG2	1:A:131:LEU:HD21	1.82	0.61
1:B:345:PRO:HB3	1:B:347:GLN:OE1	2.00	0.61
1:A:504:GLU:HG2	1:A:517:MET:CE	2.30	0.61
1:B:676:THR:HG22	1:B:677:TRP:H	1.66	0.61
1:B:630:LEU:O	1:B:634:LYS:HB2	2.01	0.61
1:B:713:ARG:NH2	1:B:713:ARG:HB3	2.16	0.61
1:A:676:THR:HG22	1:A:677:TRP:N	2.16	0.60
1:B:648:LYS:HG2	1:B:649:ILE:HG12	1.83	0.60
1:B:584:SER:H	1:B:587:GLU:CG	2.14	0.60
1:B:623:THR:HG22	1:B:624:TYR:N	2.16	0.60
1:B:588:LYS:O	1:B:592:GLN:HG2	2.02	0.60
1:B:292:ASN:HA	1:B:293:PRO:C	2.27	0.59
1:A:647:ASN:HD21	1:A:652:PHE:HD1	1.48	0.59
1:A:347:GLN:CD	1:A:347:GLN:H	2.09	0.59
1:B:542:ARG:HE	1:B:629:ARG:NH2	2.01	0.59
1:B:29:HIS:CD2	1:B:31:GLU:H	2.12	0.59
1:A:442:TYR:CD2	1:A:525:SER:HB3	2.38	0.59
1:A:575:ALA:HB3	1:A:602:PRO:HA	1.84	0.59
1:A:626:THR:HG22	1:A:626:THR:O	2.02	0.59
1:B:266:ALA:HB2	1:B:651:ARG:HG3	1.85	0.59
1:B:278:ASN:HB3	1:B:283:MET:HA	1.84	0.59
1:B:273:LEU:O	1:B:288:VAL:HG22	2.03	0.59
1:B:321:LYS:HG3	1:B:322:GLN:HG3	1.85	0.59
1:A:267:ASN:O	1:A:268:ARG:HD3	2.03	0.59
1:B:748:ARG:O	1:B:751:ALA:HB3	2.04	0.58
1:B:292:ASN:H	1:B:292:ASN:ND2	2.01	0.58
1:B:153:VAL:CG1	1:B:157:VAL:HG21	2.34	0.58
1:A:260:THR:HG22	1:A:261:VAL:HG23	1.85	0.58
1:B:414:ASP:OD2	1:B:507:HIS:HE1	1.87	0.57
1:A:170:VAL:HA	2:A:849:HOH:O	2.04	0.57
1:A:278:ASN:CB	1:A:283:MET:HA	2.35	0.57
1:A:562:ASN:HB3	1:A:565:ASP:OD1	2.05	0.57
1:A:700:ALA:HB3	1:A:717:ILE:HD13	1.87	0.56
1:A:27:VAL:C	1:A:28:GLU:HG2	2.30	0.56
1:A:45:ARG:HD3	1:A:47:GLU:OE2	2.05	0.56
1:A:64:THR:CG2	1:A:92:GLU:HG2	2.36	0.56
1:A:550:ARG:NH1	1:A:552:VAL:HG21	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:MET:HE1	1:B:338:PHE:HA	1.87	0.56
1:B:394:PRO:O	1:B:406:MET:HE2	2.05	0.56
1:A:414:ASP:OD2	1:A:507:HIS:HE1	1.89	0.56
1:A:753:LEU:HD22	1:A:753:LEU:H	1.71	0.56
1:A:423:TRP:HB2	1:A:448:ILE:HG23	1.88	0.56
1:B:542:ARG:HE	1:B:629:ARG:CZ	2.18	0.56
1:A:401:HIS:HB3	2:A:768:HOH:O	2.05	0.56
1:B:442:TYR:CD2	1:B:525:SER:HB3	2.41	0.56
1:A:509:MET:SD	1:A:550:ARG:HD3	2.46	0.55
1:A:605:VAL:HG21	1:A:610:GLU:HB3	1.88	0.55
1:B:442:TYR:HB3	1:B:523:GLY:O	2.05	0.55
1:A:228:ARG:HB3	1:A:228:ARG:NH1	2.21	0.55
1:A:662:MET:HB3	1:A:664:GLU:OE1	2.06	0.55
1:A:541:VAL:O	1:A:565:ASP:HB2	2.06	0.55
1:B:676:THR:HG22	1:B:677:TRP:N	2.20	0.55
1:B:691:GLU:O	1:B:694:THR:HG22	2.06	0.55
1:A:753:LEU:HD22	1:A:753:LEU:N	2.22	0.55
1:A:466:TRP:HA	1:A:499:VAL:HG13	1.89	0.55
1:B:64:THR:HG22	1:B:92:GLU:HG2	1.89	0.54
1:B:520:TYR:C	1:B:522:GLY:H	2.13	0.54
1:A:662:MET:HE2	1:A:664:GLU:OE1	2.07	0.54
1:A:521:LYS:HB2	1:A:521:LYS:NZ	2.23	0.54
1:B:682:VAL:HG13	1:B:719:VAL:HA	1.88	0.54
1:A:584:SER:H	1:A:587:GLU:CG	2.21	0.54
1:A:682:VAL:HG11	1:A:719:VAL:HG22	1.89	0.54
1:B:512:PHE:HE1	1:B:517:MET:HE2	1.73	0.54
1:A:682:VAL:CG1	1:A:719:VAL:HG22	2.38	0.54
1:B:261:VAL:C	1:B:263:GLU:H	2.16	0.54
1:A:152:VAL:HG22	1:A:154:PRO:HD3	1.90	0.53
1:A:279:GLY:O	1:A:280:ALA:HB2	2.08	0.53
1:A:293:PRO:HD3	1:A:710:HIS:CE1	2.43	0.53
1:A:448:ILE:HD11	1:A:486:LEU:HD23	1.90	0.53
1:B:27:VAL:O	1:B:28:GLU:HB2	2.07	0.53
1:B:455:HIS:O	1:B:456:GLY:C	2.52	0.53
1:B:455:HIS:O	1:B:457:SER:N	2.41	0.53
1:B:647:ASN:HA	1:B:651:ARG:O	2.08	0.53
1:A:458:ARG:HG3	1:A:458:ARG:HH11	1.73	0.53
1:A:646:SER:HB2	1:A:653:VAL:CG1	2.39	0.53
1:A:664:GLU:H	1:A:664:GLU:CD	2.17	0.53
1:B:276:VAL:HG13	1:B:276:VAL:O	2.09	0.52
1:B:706:THR:O	1:B:706:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:SER:HB2	2:B:774:HOH:O	2.09	0.52
1:B:519:VAL:HG13	1:B:552:VAL:HA	1.90	0.52
1:A:527:GLU:HG3	1:A:528:GLY:N	2.25	0.52
1:A:529:GLY:C	1:A:531:THR:H	2.15	0.52
1:B:70:ILE:N	1:B:70:ILE:HD12	2.26	0.51
1:B:80:ILE:HG22	1:B:81:LEU:N	2.25	0.51
1:A:498:ARG:O	1:A:498:ARG:NH1	2.44	0.51
1:A:568:VAL:HG22	1:A:577:LEU:HD12	1.92	0.51
1:B:258:GLU:C	1:B:260:THR:H	2.17	0.51
1:A:418:GLY:HA2	1:A:454:ARG:NH2	2.26	0.51
1:A:601:GLN:HA	1:A:601:GLN:NE2	2.24	0.51
1:B:281:GLY:H	1:B:282:PRO:CD	2.24	0.51
1:A:126:GLU:H	1:A:126:GLU:CD	2.16	0.51
1:A:292:ASN:H	1:A:292:ASN:ND2	2.09	0.51
1:B:392:ARG:HH21	1:B:636:ASP:CG	2.19	0.51
1:A:518:ILE:HD12	1:A:594:LEU:HD13	1.93	0.51
1:A:654:ILE:HG13	1:A:654:ILE:O	2.10	0.51
1:A:527:GLU:HG3	1:A:528:GLY:H	1.75	0.50
1:B:442:TYR:CE2	1:B:525:SER:HB3	2.46	0.50
1:A:281:GLY:H	1:A:282:PRO:HD2	1.76	0.50
1:A:352:VAL:C	1:A:353:LEU:HD23	2.35	0.50
1:B:392:ARG:NH2	1:B:636:ASP:OD1	2.44	0.50
1:A:571:THR:HG23	1:A:573:SER:N	2.25	0.50
1:A:506:ALA:CA	1:A:509:MET:HE3	2.34	0.50
1:B:684:VAL:HG23	1:B:684:VAL:O	2.11	0.50
1:A:80:ILE:HG23	2:A:822:HOH:O	2.11	0.50
1:B:293:PRO:HG2	1:B:367:LYS:HE2	1.93	0.50
1:A:104:PHE:O	1:A:108:LEU:HB2	2.11	0.50
1:B:273:LEU:HB3	1:B:289:ALA:HB3	1.92	0.50
1:B:392:ARG:HG2	1:B:392:ARG:HH11	1.76	0.50
1:B:585:GLU:O	1:B:589:THR:HG22	2.12	0.50
1:A:64:THR:HG22	1:A:92:GLU:HG2	1.93	0.50
1:A:558:ALA:HA	1:A:618:LEU:HD13	1.94	0.50
1:A:392:ARG:NH1	1:A:635:MET:HE2	2.27	0.49
1:A:361:LEU:O	1:A:364:GLN:HG2	2.12	0.49
1:A:743:VAL:CG1	1:A:748:ARG:HH12	2.24	0.49
1:B:231:VAL:HG11	1:B:753:LEU:HD12	1.92	0.49
1:B:646:SER:HB3	1:B:653:VAL:HG13	1.93	0.49
1:A:392:ARG:CZ	1:A:635:MET:HE2	2.42	0.49
1:B:45:ARG:HD3	1:B:47:GLU:CG	2.43	0.49
1:B:95:GLN:CD	1:B:95:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:PHE:CD1	1:A:567:PHE:N	2.80	0.49
1:A:386:HIS:HE1	1:A:640:PRO:O	1.95	0.49
1:A:700:ALA:CB	1:A:717:ILE:HD13	2.41	0.49
1:B:532:ALA:N	1:B:533:PRO:CD	2.76	0.49
1:B:558:ALA:CA	1:B:618:LEU:HD23	2.39	0.49
1:A:270:LEU:HA	1:A:292:ASN:HD21	1.76	0.49
1:B:293:PRO:HD3	1:B:710:HIS:HD1	1.75	0.49
1:A:753:LEU:H	1:A:753:LEU:CD2	2.25	0.49
1:A:526:ARG:O	1:A:527:GLU:C	2.55	0.48
1:B:399:THR:O	1:B:402:THR:HG22	2.13	0.48
1:A:392:ARG:NH2	1:A:636:ASP:OD1	2.46	0.48
1:A:80:ILE:HG22	1:A:81:LEU:N	2.28	0.48
1:B:536:THR:HA	1:B:570:LYS:O	2.13	0.48
1:A:169:ARG:HG3	1:A:655:GLU:CD	2.37	0.48
1:A:493:THR:N	1:A:494:PRO:CD	2.77	0.48
1:A:372:PRO:O	1:A:373:ASP:HB2	2.14	0.48
1:B:197:ILE:O	1:B:231:VAL:HA	2.14	0.48
1:B:267:ASN:HA	1:B:706:THR:CG2	2.44	0.48
1:B:498:ARG:HD2	2:B:800:HOH:O	2.13	0.48
1:A:584:SER:H	1:A:587:GLU:HG2	1.79	0.48
1:A:674:LEU:HB3	1:A:681:PHE:HB2	1.96	0.48
1:B:520:TYR:C	1:B:522:GLY:N	2.69	0.48
1:B:609:SER:O	1:B:611:PRO:HD3	2.14	0.48
1:B:753:LEU:C	1:B:755:ALA:H	2.21	0.48
1:A:498:ARG:HH11	1:A:498:ARG:CG	2.27	0.48
1:A:512:PHE:CE1	1:A:517:MET:HG3	2.49	0.48
1:A:679:GLN:NE2	1:A:718:THR:OG1	2.45	0.48
1:A:601:GLN:HA	1:A:601:GLN:HE21	1.78	0.48
1:B:231:VAL:HG21	1:B:753:LEU:HD12	1.95	0.48
1:B:674:LEU:HB3	1:B:681:PHE:HB2	1.96	0.47
1:A:27:VAL:O	1:A:28:GLU:HG2	2.14	0.47
1:A:615:TRP:HA	1:A:615:TRP:CE3	2.49	0.47
1:B:27:VAL:C	1:B:29:HIS:H	2.22	0.47
1:B:486:LEU:O	1:B:490:LEU:HB2	2.14	0.47
1:A:169:ARG:H	1:A:169:ARG:HG2	1.56	0.47
1:A:575:ALA:O	1:A:603:VAL:HG23	2.15	0.47
1:B:99:GLY:O	1:B:103:ILE:HG13	2.14	0.47
1:A:273:LEU:HB3	1:A:289:ALA:HB3	1.96	0.47
1:A:676:THR:CG2	1:A:677:TRP:N	2.77	0.47
1:B:542:ARG:HH21	1:B:629:ARG:CZ	2.28	0.47
1:B:68:TYR:O	1:B:87:TYR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD22	1:B:98:SER:CB	2.45	0.47
1:B:392:ARG:NH1	1:B:635:MET:HE2	2.30	0.47
1:B:610:GLU:HB2	1:B:615:TRP:NE1	2.29	0.47
1:A:532:ALA:HB3	1:A:533:PRO:CD	2.44	0.47
1:A:224:GLU:C	1:A:226:SER:H	2.23	0.47
1:A:458:ARG:NH2	1:A:738:ASP:OD2	2.48	0.47
1:A:569:LEU:HD21	1:A:617:ALA:HB3	1.96	0.47
1:B:268:ARG:HD2	1:B:311:LYS:HB3	1.97	0.47
1:B:657:VAL:HG22	2:B:813:HOH:O	2.15	0.47
1:A:455:HIS:O	1:A:455:HIS:ND1	2.47	0.47
1:B:541:VAL:O	1:B:565:ASP:HB2	2.15	0.46
1:A:280:ALA:HB1	1:A:333:LYS:HD3	1.96	0.46
1:B:707:ASP:HA	1:B:708:PRO:HD3	1.81	0.46
1:A:504:GLU:CG	1:A:517:MET:HE1	2.42	0.46
1:B:459:GLN:HE21	1:B:459:GLN:HB2	1.53	0.46
1:B:267:ASN:HA	1:B:706:THR:HG21	1.98	0.46
1:B:563:SER:CB	1:B:626:THR:HG23	2.45	0.46
1:A:261:VAL:HG12	1:A:261:VAL:O	2.16	0.46
1:A:629:ARG:HG3	1:A:629:ARG:NH1	2.29	0.46
1:B:258:GLU:O	1:B:258:GLU:HG2	2.15	0.46
1:B:554:ILE:HG22	1:B:555:ILE:N	2.30	0.46
1:B:270:LEU:HA	1:B:292:ASN:HD21	1.80	0.46
1:A:520:TYR:C	1:A:522:GLY:H	2.22	0.46
1:B:543:ALA:HA	1:B:549:THR:HG22	1.98	0.46
1:B:746:LEU:O	1:B:750:LEU:HB2	2.16	0.46
1:B:386:HIS:HE1	1:B:640:PRO:O	1.97	0.46
1:A:188:CYS:HA	1:A:201:CYS:HA	1.98	0.46
1:A:524:THR:OG1	1:A:525:SER:N	2.49	0.46
1:B:558:ALA:C	1:B:560:ALA:H	2.24	0.46
1:A:493:THR:HG23	1:A:724:PHE:CD2	2.51	0.46
1:A:532:ALA:HB3	1:A:533:PRO:HD3	1.97	0.46
1:A:384:SER:HB3	1:A:386:HIS:CD2	2.50	0.45
1:B:171:VAL:HG21	1:B:212:LYS:HB3	1.97	0.45
1:B:347:GLN:CD	1:B:347:GLN:N	2.72	0.45
1:B:607:GLU:OE2	1:B:624:TYR:HE2	1.97	0.45
1:A:624:TYR:HB3	1:A:625:ARG:H	1.40	0.45
1:B:265:ALA:HB1	1:B:268:ARG:HG3	1.98	0.45
1:B:134:PHE:CD1	1:B:138:LEU:HD11	2.51	0.45
1:A:152:VAL:O	1:A:152:VAL:HG13	2.17	0.45
1:B:531:THR:O	1:B:532:ALA:HB3	2.17	0.45
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ILE:C	1:B:651:ARG:H	2.25	0.45
1:B:257:THR:HG22	1:B:259:ASP:H	1.82	0.45
1:A:448:ILE:HD11	1:A:486:LEU:CD2	2.47	0.45
1:B:159:VAL:HG22	1:B:194:GLY:N	2.32	0.45
1:B:527:GLU:O	1:B:528:GLY:C	2.59	0.45
1:A:720:VAL:HG13	1:A:725:GLU:HA	1.99	0.45
1:B:379:GLY:H	1:B:633:LYS:HG2	1.82	0.45
1:A:134:PHE:CD1	1:A:138:LEU:HD11	2.52	0.45
1:A:486:LEU:O	1:A:490:LEU:HB2	2.17	0.45
1:B:324:ASN:HD22	1:B:325:MET:N	2.14	0.45
1:A:616:GLU:C	1:A:618:LEU:H	2.25	0.44
1:B:218:LYS:HB2	1:B:753:LEU:HD21	1.99	0.44
1:A:570:LYS:HD2	1:A:571:THR:H	1.82	0.44
1:A:159:VAL:HG13	1:A:194:GLY:N	2.33	0.44
1:A:458:ARG:HG3	1:A:458:ARG:NH1	2.32	0.44
1:B:413:ASP:O	1:B:414:ASP:HB3	2.16	0.44
1:B:509:MET:HG2	1:B:550:ARG:HB3	1.99	0.44
1:A:584:SER:H	1:A:587:GLU:HG3	1.83	0.44
1:B:69:VAL:C	1:B:70:ILE:HD12	2.43	0.44
1:B:569:LEU:HD22	1:B:618:LEU:HD13	1.99	0.44
1:B:161:ARG:HG3	1:B:192:ASP:HB3	1.98	0.44
1:A:28:GLU:O	1:A:29:HIS:CB	2.64	0.44
1:B:713:ARG:HB3	1:B:713:ARG:HH21	1.82	0.44
1:A:545:SER:HB2	2:A:786:HOH:O	2.18	0.44
1:A:576:TYR:CE2	1:A:614:PHE:HB2	2.53	0.44
1:B:654:ILE:O	1:B:654:ILE:HG13	2.17	0.44
1:A:266:ALA:HA	1:A:652:PHE:O	2.18	0.44
1:B:625:ARG:CZ	1:B:627:SER:HB2	2.48	0.44
1:A:711:ARG:H	1:A:711:ARG:HG2	1.47	0.44
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.87	0.43
1:B:455:HIS:O	1:B:458:ARG:N	2.51	0.43
1:A:70:ILE:HD12	1:A:70:ILE:N	2.33	0.43
1:B:713:ARG:HH21	1:B:713:ARG:CB	2.31	0.43
1:A:262:LYS:O	1:A:262:LYS:HG3	2.18	0.43
1:B:293:PRO:HD3	1:B:710:HIS:CE1	2.53	0.43
1:B:77:ARG:CZ	1:B:378:LEU:HB3	2.48	0.43
1:A:264:ASP:OD1	1:A:651:ARG:HG2	2.18	0.43
1:A:541:VAL:HG21	1:A:591:ALA:HA	2.00	0.43
1:B:169:ARG:HG3	1:B:655:GLU:CD	2.43	0.43
1:B:507:HIS:O	1:B:511:LEU:HD13	2.19	0.43
1:B:684:VAL:O	1:B:684:VAL:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD23	1:A:353:LEU:N	2.33	0.43
1:A:676:THR:HG22	1:A:678:ASP:H	1.84	0.43
1:B:58:LEU:O	1:B:61:ASP:HB2	2.18	0.43
1:A:558:ALA:C	1:A:560:ALA:H	2.25	0.43
1:A:575:ALA:O	1:A:602:PRO:HA	2.19	0.43
1:B:314:LYS:HD3	1:B:349:GLN:HB2	1.99	0.43
1:A:103:ILE:O	1:A:107:GLN:HG3	2.19	0.43
1:A:321:LYS:HG2	1:A:355:GLU:OE2	2.19	0.43
1:B:164:GLN:O	1:B:173:ALA:HA	2.19	0.43
1:B:228:ARG:HB3	1:B:228:ARG:NH1	2.33	0.43
1:B:374:GLN:O	1:B:633:LYS:HE2	2.19	0.43
1:A:603:VAL:O	1:A:604:GLN:C	2.61	0.42
1:B:183:PHE:HA	1:B:189:PHE:CZ	2.54	0.42
1:B:633:LYS:HB2	1:B:633:LYS:NZ	2.34	0.42
1:B:645:CYS:SG	1:B:673:LEU:HG	2.59	0.42
1:B:277:SER:O	1:B:284:VAL:HB	2.19	0.42
1:A:714:ARG:O	1:A:715:THR:C	2.62	0.42
1:B:77:ARG:NH1	1:B:378:LEU:HB3	2.34	0.42
1:B:218:LYS:HE3	1:B:221:ARG:HH22	1.84	0.42
1:B:324:ASN:HD22	1:B:325:MET:H	1.68	0.42
1:A:630:LEU:O	1:A:634:LYS:HB2	2.18	0.42
1:B:57:ASN:O	1:B:223:ASN:HB3	2.20	0.42
1:B:55:PRO:HA	1:B:56:PRO:HD3	1.91	0.42
1:A:207:ARG:HG3	2:A:818:HOH:O	2.18	0.42
1:A:645:CYS:HB2	1:A:671:VAL:O	2.20	0.42
1:A:667:ALA:HB3	1:A:670:ASP:OD2	2.19	0.42
1:A:743:VAL:CG1	1:A:748:ARG:NH1	2.82	0.42
1:A:676:THR:HG21	2:A:856:HOH:O	2.19	0.42
1:B:77:ARG:NH2	1:B:378:LEU:HD13	2.35	0.42
1:B:165:VAL:HG23	1:B:171:VAL:HG13	2.01	0.42
1:A:664:GLU:CD	1:A:664:GLU:N	2.78	0.42
1:A:253:LEU:HA	1:A:254:PRO:HD3	1.81	0.42
1:B:162:LEU:HD11	1:B:183:PHE:CE2	2.55	0.42
1:B:501:GLN:HE22	1:B:521:LYS:HA	1.84	0.42
1:A:29:HIS:HA	1:A:30:PRO:HD2	1.81	0.41
1:A:118:GLN:OE1	1:A:352:VAL:HG21	2.20	0.41
1:A:452:ASN:OD1	1:A:461:GLN:HG2	2.20	0.41
1:A:684:VAL:HG23	1:A:684:VAL:O	2.19	0.41
1:B:161:ARG:CG	1:B:192:ASP:HB3	2.50	0.41
1:B:27:VAL:HG12	1:B:29:HIS:H	1.84	0.41
1:A:250:LYS:NZ	1:A:253:LEU:HG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.93	0.41
1:A:558:ALA:O	1:A:560:ALA:N	2.48	0.41
1:A:645:CYS:SG	1:A:673:LEU:HG	2.61	0.41
1:B:667:ALA:HB3	1:B:670:ASP:HB2	2.02	0.41
1:A:271:ALA:H	1:A:292:ASN:ND2	2.17	0.41
1:B:314:LYS:HD2	1:B:315:ILE:H	1.85	0.41
1:A:562:ASN:OD1	1:A:564:ASN:HB2	2.20	0.41
1:B:626:THR:O	1:B:626:THR:HG22	2.20	0.41
1:A:589:THR:HG23	1:A:590:GLY:N	2.35	0.41
1:A:617:ALA:O	1:A:618:LEU:HD23	2.21	0.41
1:B:220:ILE:O	1:B:224:GLU:HB2	2.20	0.41
1:B:449:ILE:HB	1:B:464:TYR:HB2	2.02	0.41
1:A:85:LEU:O	1:A:119:HIS:N	2.50	0.41
1:A:86:HIS:HA	1:A:119:HIS:O	2.21	0.41
1:A:218:LYS:HB2	1:A:218:LYS:HE3	1.86	0.41
1:A:529:GLY:C	1:A:531:THR:N	2.79	0.41
1:B:138:LEU:HD12	1:B:138:LEU:HA	1.88	0.41
1:B:200:TRP:CD1	1:B:243:MET:HE1	2.55	0.41
1:B:750:LEU:HD12	1:B:750:LEU:HA	1.98	0.41
1:A:239:GLU:CD	1:A:239:GLU:N	2.74	0.41
1:B:458:ARG:NH1	1:B:738:ASP:OD2	2.54	0.41
1:B:487:ASP:OD2	1:B:492:GLY:HA2	2.20	0.41
1:B:490:LEU:HD12	1:B:490:LEU:HA	1.85	0.41
1:B:649:ILE:O	1:B:649:ILE:HG22	2.21	0.41
1:A:498:ARG:HH11	1:A:498:ARG:CB	2.34	0.41
1:A:536:THR:O	1:A:556:PRO:HG2	2.21	0.41
1:A:614:PHE:CD1	1:A:614:PHE:C	2.98	0.41
1:A:152:VAL:C	1:A:154:PRO:HD3	2.46	0.41
1:A:204:LYS:HE2	1:A:204:LYS:HB3	1.92	0.41
1:A:228:ARG:HB3	1:A:228:ARG:CZ	2.50	0.41
1:B:316:PHE:N	1:B:316:PHE:CD2	2.89	0.41
1:B:281:GLY:N	1:B:282:PRO:CD	2.84	0.40
1:B:521:LYS:O	1:B:522:GLY:O	2.40	0.40
1:A:521:LYS:HG2	1:A:553:GLU:CD	2.45	0.40
1:A:689:GLN:HG2	1:A:691:GLU:HG2	2.03	0.40
1:B:374:GLN:C	1:B:376:GLU:N	2.78	0.40
1:A:228:ARG:NH1	1:A:228:ARG:CB	2.82	0.40
1:B:127:SER:HA	1:B:349:GLN:NE2	2.37	0.40
1:B:437:THR:O	1:B:437:THR:HG22	2.21	0.40
1:B:647:ASN:O	1:B:648:LYS:C	2.65	0.40
1:A:520:TYR:C	1:A:522:GLY:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HA	1:B:53:PRO:HD3	1.94	0.40
1:B:253:LEU:HA	1:B:254:PRO:HD3	1.79	0.40
1:B:624:TYR:HB3	1:B:625:ARG:H	1.55	0.40
1:A:216:VAL:O	1:A:220:ILE:HG13	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	727/729 (100%)	653 (90%)	56 (8%)	18 (2%)	4	7
1	B	727/729 (100%)	668 (92%)	41 (6%)	18 (2%)	4	7
All	All	1454/1458 (100%)	1321 (91%)	97 (7%)	36 (2%)	4	7

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ALA
1	A	367	LYS
1	A	373	ASP
1	A	456	GLY
1	A	532	ALA
1	A	624	TYR
1	B	261	VAL
1	B	264	ASP
1	B	522	GLY
1	B	527	GLU
1	B	532	ALA
1	B	625	ARG
1	A	28	GLU
1	A	266	ALA

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Mol	Chain	Res	Type
1	A	534	ALA
1	B	280	ALA
1	B	456	GLY
1	B	632	ASP
1	A	261	VAL
1	A	526	ARG
1	A	621	LYS
1	B	263	GLU
1	B	368	ASN
1	B	526	ARG
1	B	648	LYS
1	A	29	HIS
1	A	631	LYS
1	A	650	GLY
1	B	650	GLY
1	A	556	PRO
1	A	564	ASN
1	A	622	ALA
1	B	152	VAL
1	B	154	PRO
1	B	372	PRO
1	B	528	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	597/597 (100%)	556 (93%)	41 (7%)	14	30
1	B	597/597 (100%)	551 (92%)	46 (8%)	12	25
All	All	1194/1194 (100%)	1107 (93%)	87 (7%)	13	27

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	96	ASP
1	A	108	LEU
1	A	126	GLU
1	A	162	LEU
1	A	169	ARG
1	A	170	VAL
1	A	171	VAL
1	A	193	LEU
1	A	239	GLU
1	A	244	LEU
1	A	246	VAL
1	A	292	ASN
1	A	299	LEU
1	A	307	LEU
1	A	332	LEU
1	A	347	GLN
1	A	352	VAL
1	A	353	LEU
1	A	385	SER
1	A	448	ILE
1	A	470	GLN
1	A	498	ARG
1	A	521	LYS
1	A	538	LEU
1	A	565	ASP
1	A	567	PHE
1	A	587	GLU
1	A	604	GLN
1	A	605	VAL
1	A	610	GLU
1	A	625	ARG
1	A	657	VAL
1	A	666	LEU
1	A	674	LEU
1	A	682	VAL
1	A	711	ARG
1	A	721	LYS
1	A	743	VAL
1	A	750	LEU
1	B	85	LEU
1	B	86	HIS

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Mol	Chain	Res	Type
1	B	138	LEU
1	B	159	VAL
1	B	162	LEU
1	B	165	VAL
1	B	169	ARG
1	B	170	VAL
1	B	193	LEU
1	B	231	VAL
1	B	239	GLU
1	B	246	VAL
1	B	252	THR
1	B	292	ASN
1	B	307	LEU
1	B	317	VAL
1	B	332	LEU
1	B	347	GLN
1	B	352	VAL
1	B	353	LEU
1	B	393	VAL
1	B	402	THR
1	B	459	GLN
1	B	498	ARG
1	B	499	VAL
1	B	510	SER
1	B	511	LEU
1	B	519	VAL
1	B	565	ASP
1	B	587	GLU
1	B	594	LEU
1	B	595	LEU
1	B	605	VAL
1	B	618	LEU
1	B	624	TYR
1	B	632	ASP
1	B	657	VAL
1	B	670	ASP
1	B	674	LEU
1	B	682	VAL
1	B	684	VAL
1	B	690	ASP
1	B	694	THR
1	B	695	GLU

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Mol	Chain	Res	Type
1	B	734	LEU
1	B	750	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	160	GLN
1	A	195	ASN
1	A	196	ASN
1	A	292	ASN
1	A	309	HIS
1	A	322	GLN
1	A	324	ASN
1	A	374	GLN
1	A	386	HIS
1	A	419	GLN
1	A	440	GLN
1	A	459	GLN
1	A	461	GLN
1	A	507	HIS
1	A	540	GLN
1	A	564	ASN
1	A	601	GLN
1	A	647	ASN
1	A	679	GLN
1	A	689	GLN
1	B	29	HIS
1	B	91	ASN
1	B	118	GLN
1	B	155	ASN
1	B	164	GLN
1	B	195	ASN
1	B	206	ASN
1	B	267	ASN
1	B	292	ASN
1	B	322	GLN
1	B	324	ASN
1	B	386	HIS
1	B	440	GLN
1	B	459	GLN
1	B	496	GLN

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Mol	Chain	Res	Type
1	B	507	HIS
1	B	564	ASN
1	B	601	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 [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	729/729 (100%)	0.53	94 (12%) 7 6	14, 40, 98, 100	0
1	B	729/729 (100%)	0.33	79 (10%) 11 9	12, 37, 93, 100	0
All	All	1458/1458 (100%)	0.43	173 (11%) 9 7	12, 38, 96, 100	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	8.6
1	B	457	SER	8.6
1	B	532	ALA	7.9
1	A	532	ALA	7.4
1	B	279	GLY	7.2
1	A	617	ALA	6.7
1	B	531	THR	6.2
1	B	265	ALA	6.2
1	B	624	TYR	6.2
1	B	377	GLY	6.1
1	A	261	VAL	6.0
1	A	260	THR	6.0
1	A	534	ALA	5.8
1	B	378	LEU	5.8
1	A	265	ALA	5.7
1	A	649	ILE	5.6
1	B	260	THR	5.4
1	A	755	ALA	5.3
1	B	261	VAL	5.2
1	A	155	ASN	5.2
1	A	529	GLY	5.2
1	B	280	ALA	4.9
1	A	533	PRO	4.9
1	A	279	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	605	VAL	4.8
1	A	154	PRO	4.7
1	A	457	SER	4.6
1	B	374	GLN	4.5
1	A	624	TYR	4.5
1	A	530	GLN	4.5
1	A	153	VAL	4.4
1	B	630	LEU	4.4
1	A	614	PHE	4.4
1	A	754	ALA	4.3
1	A	650	GLY	4.3
1	B	154	PRO	4.3
1	A	266	ALA	4.3
1	A	627	SER	4.3
1	A	259	ASP	4.2
1	B	379	GLY	4.2
1	B	623	THR	4.1
1	B	157	VAL	4.1
1	B	259	ASP	4.1
1	A	651	ARG	4.1
1	A	513	GLY	4.1
1	A	579	VAL	4.1
1	B	277	SER	4.0
1	A	622	ALA	3.9
1	B	380	LEU	3.9
1	B	27	VAL	3.9
1	A	278	ASN	3.9
1	A	606	ALA	3.9
1	B	267	ASN	3.8
1	A	262	LYS	3.8
1	A	267	ASN	3.8
1	B	533	PRO	3.8
1	B	649	ILE	3.8
1	B	373	ASP	3.7
1	B	153	VAL	3.7
1	B	264	ASP	3.7
1	B	372	PRO	3.7
1	A	531	THR	3.7
1	B	263	GLU	3.6
1	A	574	ALA	3.6
1	B	628	PRO	3.6
1	B	753	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	262	LYS	3.5
1	B	376	GLU	3.5
1	A	691	GLU	3.5
1	A	528	GLY	3.5
1	A	648	LYS	3.4
1	A	264	ASP	3.4
1	B	326	GLU	3.4
1	B	647	ASN	3.4
1	A	282	PRO	3.4
1	B	278	ASN	3.3
1	A	535	SER	3.3
1	B	626	THR	3.3
1	B	266	ALA	3.3
1	A	277	SER	3.3
1	B	155	ASN	3.2
1	A	584	SER	3.2
1	B	648	LYS	3.1
1	A	27	VAL	3.1
1	A	458	ARG	3.1
1	A	630	LEU	3.1
1	A	753	LEU	3.1
1	B	627	SER	3.1
1	B	381	ALA	3.0
1	B	375	THR	3.0
1	A	374	GLN	2.9
1	A	281	GLY	2.9
1	A	571	THR	2.9
1	A	626	THR	2.9
1	A	615	TRP	2.9
1	A	573	SER	2.8
1	B	631	LYS	2.8
1	B	156	GLU	2.8
1	A	568	VAL	2.7
1	A	570	LYS	2.7
1	B	528	GLY	2.7
1	B	282	PRO	2.7
1	A	97	GLU	2.7
1	B	534	ALA	2.7
1	A	577	LEU	2.7
1	A	613	SER	2.7
1	B	152	VAL	2.7
1	B	268	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	646	SER	2.7
1	B	530	GLN	2.7
1	A	373	ASP	2.6
1	A	601	GLN	2.6
1	B	754	ALA	2.6
1	A	628	PRO	2.6
1	A	566	ALA	2.6
1	B	325	MET	2.6
1	A	593	GLU	2.6
1	A	276	VAL	2.6
1	B	755	ALA	2.6
1	B	557	LYS	2.6
1	B	456	GLY	2.5
1	A	564	ASN	2.5
1	A	623	THR	2.5
1	A	324	ASN	2.5
1	A	402	THR	2.5
1	B	28	GLU	2.5
1	B	368	ASN	2.5
1	A	576	TYR	2.4
1	A	567	PHE	2.4
1	A	518	ILE	2.4
1	B	371	ASP	2.4
1	A	595	LEU	2.4
1	B	228	ARG	2.4
1	B	605	VAL	2.4
1	A	280	ALA	2.4
1	A	322	GLN	2.4
1	B	206	ASN	2.4
1	A	456	GLY	2.3
1	A	735	GLY	2.3
1	B	284	VAL	2.3
1	A	611	PRO	2.3
1	A	95	GLN	2.3
1	A	604	GLN	2.3
1	A	527	GLU	2.3
1	A	368	ASN	2.3
1	A	572	PRO	2.3
1	A	602	PRO	2.3
1	B	559	GLY	2.3
1	A	370	ARG	2.3
1	B	370	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	580	GLY	2.2
1	A	157	VAL	2.2
1	B	470	GLN	2.2
1	B	392	ARG	2.2
1	A	634	LYS	2.2
1	B	324	ASN	2.2
1	B	95	GLN	2.2
1	A	491	GLY	2.2
1	A	618	LEU	2.2
1	B	529	GLY	2.2
1	B	713	ARG	2.2
1	A	557	LYS	2.2
1	B	585	GLU	2.1
1	B	622	ALA	2.1
1	A	647	ASN	2.1
1	A	524	THR	2.1
1	A	563	SER	2.1
1	B	632	ASP	2.1
1	A	603	VAL	2.1
1	B	289	ALA	2.0
1	B	676	THR	2.0
1	B	651	ARG	2.0
1	B	321	LYS	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.