



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:59 PM EDT

PDB ID : 3V65 / pdb_00003v65
Title : Crystal structure of agrin and LRP4 complex
Authors : Zong, Y.; Jin, R.
Deposited on : 2011-12-18
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

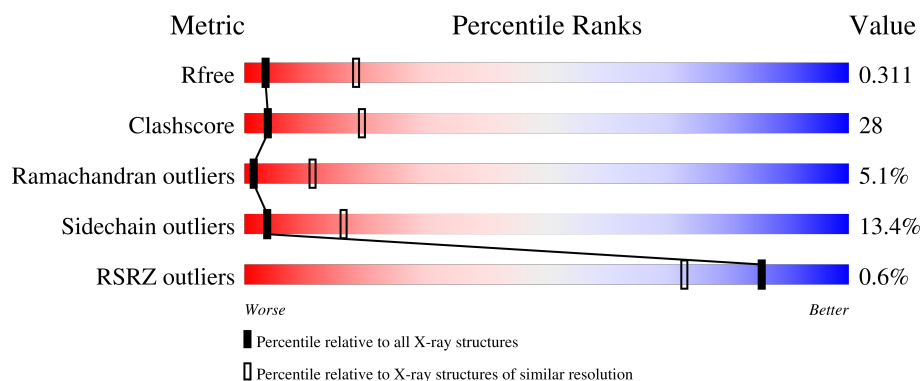
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	191	% 57% 36% 7%
1	C	191	45% 43% 11% .
2	B	386	38% 40% 6% . 15%
2	D	386	% 43% 42% 12% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8566 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 Agrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1470	927	263	277	3			
1	C	191	Total	C	N	O	S	0	0	0
			1470	927	263	277	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1758	ALA	-	expression tag	UNP P25304
C	1758	ALA	-	expression tag	UNP P25304

- Molecule 2 is a protein called Low-density lipoprotein receptor-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2639	1657	489	478	15			
2	D	377	Total	C	N	O	S	0	0	0
			2985	1854	557	551	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	738	GLN	-	expression tag	UNP Q9QYP1
D	738	GLN	-	expression tag	UNP Q9QYP1

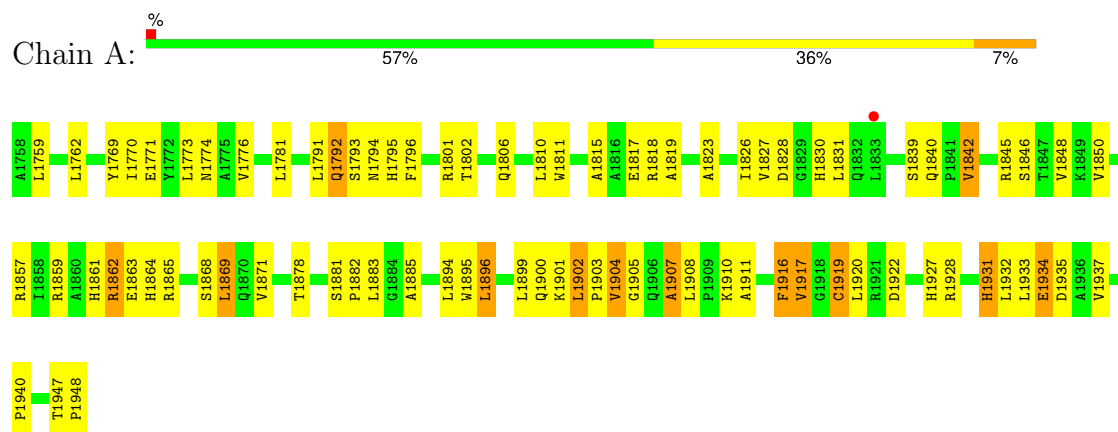
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

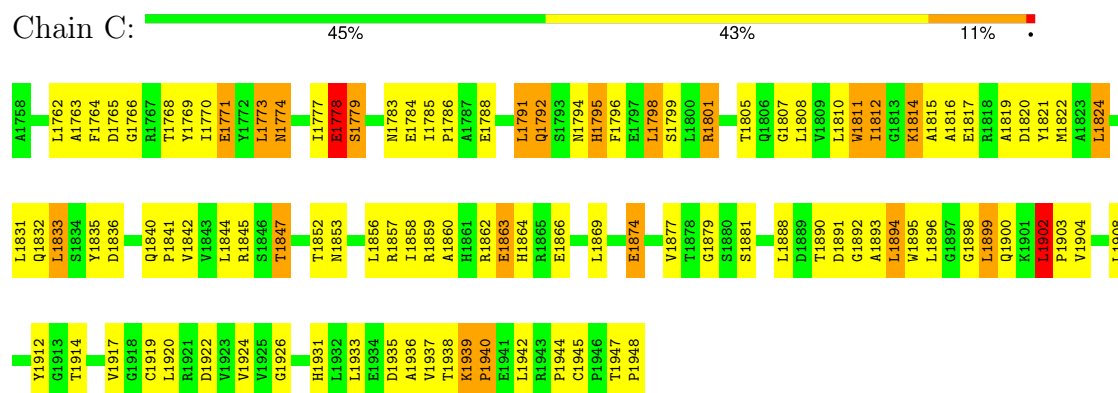
3 Residue-property plots

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.

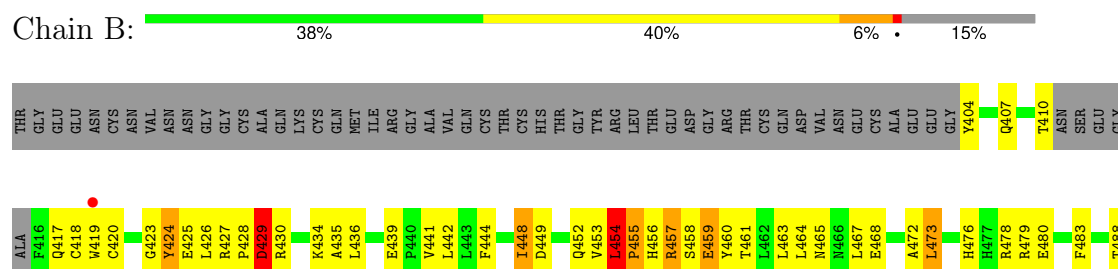
• Molecule 1: Agrin

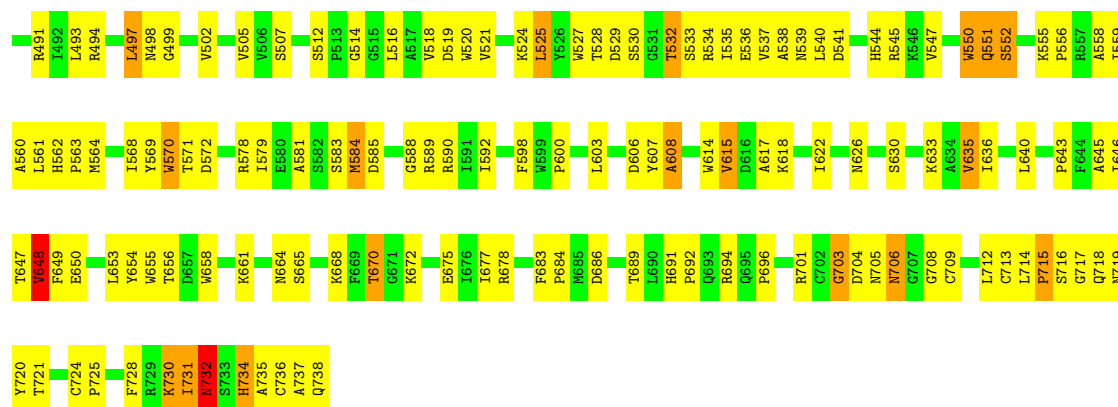


• Molecule 1: Agrin

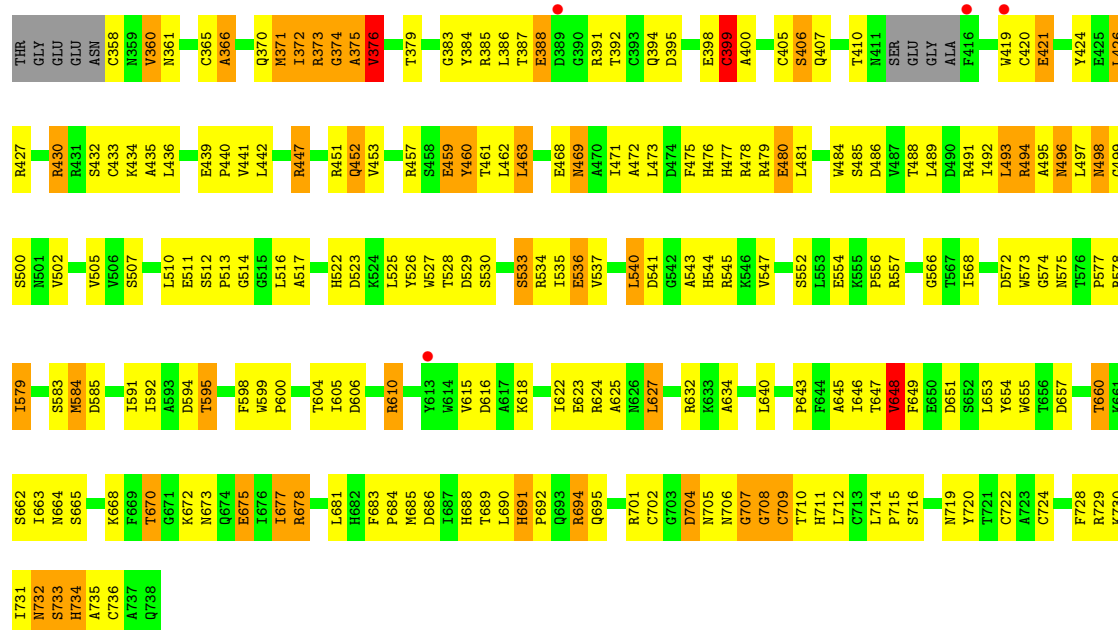
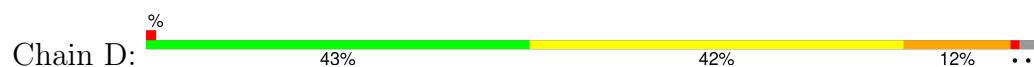


• Molecule 2: Low-density lipoprotein receptor-related protein 4





• Molecule 2: Low-density lipoprotein receptor-related protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.72Å 110.23Å 158.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.30 60.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (60.00-3.30) 94.6 (60.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.297 0.242 , 0.311	Depositor DCC
R_{free} test set	1101 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	104.1	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8566	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.68	0/1499	0.93	5/2041 (0.2%)
1	C	0.71	0/1499	0.92	2/2041 (0.1%)
2	B	0.80	0/2711	0.98	11/3684 (0.3%)
2	D	0.79	0/3059	0.96	6/4152 (0.1%)
All	All	0.76	0/8768	0.96	24/11918 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	454	LEU	CA-C-N	7.50	129.22	119.84
2	B	454	LEU	C-N-CA	7.50	129.22	119.84
2	B	734	HIS	N-CA-C	-7.21	105.66	114.75
1	A	1904	VAL	N-CA-C	6.97	118.69	109.21
2	B	465	ASN	N-CA-C	6.70	121.20	111.02
2	B	724	CYS	CA-C-N	6.29	127.70	119.84
2	B	724	CYS	C-N-CA	6.29	127.70	119.84
2	D	707	GLY	N-CA-C	-6.12	105.37	112.83
2	B	550	TRP	N-CA-C	-6.07	107.70	114.62
2	D	648	VAL	CB-CA-C	-5.99	102.63	111.19
2	B	648	VAL	CB-CA-C	-5.95	102.82	111.68
1	A	1910	LYS	N-CA-C	5.78	117.58	111.28
1	C	1770	ILE	N-CA-C	5.73	116.25	107.77
2	D	691	HIS	CA-C-N	5.71	125.83	119.32
2	D	691	HIS	C-N-CA	5.71	125.83	119.32
2	B	570	TRP	N-CA-C	5.60	116.77	108.60
2	B	439	GLU	CA-C-N	-5.58	114.18	119.76
2	B	439	GLU	C-N-CA	-5.58	114.18	119.76
1	A	1908	LEU	N-CA-C	5.55	118.34	110.24
2	D	439	GLU	CA-C-N	5.44	125.34	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	439	GLU	C-N-CA	5.44	125.34	119.85
1	A	1908	LEU	CA-C-N	5.36	125.27	119.85
1	A	1908	LEU	C-N-CA	5.36	125.27	119.85
1	C	1764	PHE	N-CA-C	5.34	117.31	109.24

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	1470	0	1474	66	0
1	C	1470	0	1474	91	0
2	B	2639	0	2536	146	1
2	D	2985	0	2844	186	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
All	All	8566	0	8328	481	1

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 28.

All (481) 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:694:ARG:HG2	2:D:694:ARG:HH11	1.01	1.15
1:C:1773:LEU:H	1:C:1937:VAL:HG21	1.11	1.11
2:D:579:ILE:HG22	2:D:592:ILE:HB	1.30	1.07
2:D:453:VAL:HG12	2:D:460:TYR:HB2	1.11	1.06
2:D:705:ASN:OD1	2:D:708:GLY:HA3	1.59	1.03
1:C:1773:LEU:N	1:C:1937:VAL:HG21	1.75	1.01
2:B:622:ILE:HD13	2:B:636:ILE:HD12	1.45	0.95
2:B:476:HIS:ND1	2:B:479:ARG:HB2	1.81	0.94
2:B:691:HIS:ND1	2:B:692:PRO:HD2	1.84	0.93
2:B:468:GLU:HG3	2:B:488:THR:OG1	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:440:PRO:HG3	2:D:649:PHE:CE2	2.05	0.91
1:C:1769:TYR:HB3	1:C:1898:GLY:O	1.72	0.90
1:C:1763:ALA:HB1	1:C:1945:CYS:SG	2.11	0.89
2:D:610:ARG:HG3	2:D:610:ARG:HH11	1.39	0.88
2:B:532:THR:HG23	2:B:534:ARG:HE	1.37	0.88
1:C:1933:LEU:HA	1:C:1936:ALA:HB2	1.57	0.86
1:C:1768:THR:HG23	1:C:1940:PRO:HG2	1.58	0.86
2:B:524:LYS:HE2	2:B:712:LEU:HD22	1.58	0.86
2:D:528:THR:HG22	2:D:535:ILE:HG12	1.57	0.85
2:D:441:VAL:HG21	2:D:452:GLN:HG3	1.59	0.84
1:C:1794:ASN:O	1:C:1795:HIS:HB2	1.77	0.84
2:D:672:LYS:O	2:D:673:ASN:HB2	1.77	0.84
2:D:406:SER:HB3	2:D:432:SER:HA	1.62	0.81
2:D:694:ARG:HG2	2:D:694:ARG:NH1	1.79	0.81
2:D:705:ASN:OD1	2:D:708:GLY:CA	2.29	0.81
2:B:410:THR:HB	2:B:417:GLN:HE22	1.46	0.81
2:B:472:ALA:HB2	2:B:514:GLY:O	1.81	0.81
2:D:453:VAL:HG12	2:D:460:TYR:CB	2.04	0.80
2:B:407:GLN:HE21	2:B:608:ALA:HB1	1.46	0.80
2:B:716:SER:HB3	2:B:721:THR:HG23	1.65	0.79
2:B:537:VAL:HG22	2:B:538:ALA:H	1.49	0.77
1:C:1798:LEU:HD11	1:C:1920:LEU:HD23	1.66	0.77
2:B:658:TRP:O	2:B:661:LYS:HD3	1.85	0.77
2:D:711:HIS:CD2	2:D:736:CYS:HB2	2.20	0.77
2:D:663:ILE:HD12	2:D:681:LEU:HD11	1.66	0.77
1:C:1763:ALA:CB	1:C:1945:CYS:SG	2.73	0.76
2:D:610:ARG:HH11	2:D:610:ARG:CG	1.98	0.76
2:D:424:TYR:HB3	2:D:433:CYS:HB3	1.68	0.76
2:B:579:ILE:HD13	2:B:614:TRP:CD2	2.19	0.76
2:D:370:GLN:C	2:D:372:ILE:H	1.94	0.75
2:D:584:MET:HB2	2:D:715:PRO:O	1.86	0.75
2:D:716:SER:H	2:D:720:TYR:HA	1.51	0.75
1:A:1795:HIS:ND1	1:A:1861:HIS:HD2	1.84	0.74
2:B:603:LEU:HD12	2:B:614:TRP:HB3	1.69	0.74
2:B:656:THR:HB	2:B:684:PRO:HB2	1.69	0.74
1:A:1902:LEU:H	1:A:1903:PRO:HD3	1.52	0.74
1:C:1801:ARG:HD3	1:C:1853:ASN:HA	1.68	0.74
1:A:1771:GLU:HB2	1:A:1895:TRP:CE2	2.23	0.74
2:B:622:ILE:HD11	2:B:640:LEU:HD21	1.70	0.73
2:B:635:VAL:HG11	2:B:668:LYS:O	1.87	0.73
2:D:480:GLU:HA	2:D:497:LEU:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1812:ILE:HG22	1:C:1822:MET:HG2	1.71	0.73
2:B:460:TYR:HA	2:B:678:ARG:HH12	1.53	0.72
1:A:1792:GLN:OE1	1:A:1864:HIS:NE2	2.22	0.72
1:C:1774:ASN:H	1:C:1893:ALA:HA	1.55	0.71
1:A:1842:VAL:HG13	1:A:1882:PRO:HD3	1.72	0.71
2:D:523:ASP:HB3	2:D:540:LEU:HD22	1.73	0.71
1:C:1774:ASN:HB3	1:C:1892:GLY:C	2.14	0.70
2:D:615:VAL:HG22	2:D:622:ILE:HG12	1.73	0.70
2:B:708:GLY:HA2	2:B:713:CYS:SG	2.31	0.70
2:D:566:GLY:C	2:D:584:MET:HG2	2.17	0.70
2:B:528:THR:HG22	2:B:535:ILE:HG12	1.73	0.70
2:B:468:GLU:CG	2:B:488:THR:OG1	2.39	0.69
1:A:1826:ILE:HD11	1:A:1916:PHE:HE2	1.56	0.69
2:D:398:GLU:O	2:D:399:CYS:HB2	1.92	0.69
2:D:694:ARG:HH11	2:D:694:ARG:CG	1.93	0.69
2:D:469:ASN:HB2	2:D:488:THR:HG23	1.73	0.69
2:B:532:THR:HG23	2:B:534:ARG:NE	2.08	0.69
2:D:469:ASN:CB	2:D:488:THR:HG23	2.23	0.69
2:D:657:ASP:HB3	2:D:660:THR:HG23	1.75	0.68
1:C:1812:ILE:HG13	1:C:1894:LEU:HB3	1.75	0.68
2:D:358:CYS:SG	2:D:371:MET:N	2.67	0.68
2:B:524:LYS:NZ	2:B:713:CYS:O	2.27	0.68
2:D:468:GLU:HG3	2:D:489:LEU:HD21	1.75	0.67
2:D:527:TRP:NE1	2:D:536:GLU:HG3	2.10	0.67
2:D:575:ASN:O	2:D:577:PRO:HD3	1.95	0.67
1:C:1812:ILE:CG2	1:C:1822:MET:HG2	2.25	0.67
2:D:554:GLU:HB2	2:D:574:GLY:HA3	1.75	0.67
2:D:598:PHE:HB3	2:D:618:LYS:HB3	1.75	0.66
2:B:731:ILE:O	2:B:732:ASN:HB2	1.95	0.66
2:B:537:VAL:HG22	2:B:538:ALA:N	2.10	0.66
1:C:1814:LYS:HE3	1:C:1891:ASP:HB3	1.77	0.66
1:C:1844:LEU:HD21	1:C:1879:GLY:HA3	1.78	0.66
1:A:1902:LEU:O	1:A:1904:VAL:HG13	1.95	0.66
1:A:1817:GLU:HG3	1:A:1905:GLY:HA2	1.78	0.65
1:A:1818:ARG:O	1:A:1818:ARG:HD3	1.97	0.65
2:D:358:CYS:N	2:D:361:ASN:HB2	2.10	0.65
2:D:498:ASN:HB3	2:D:500:SER:OG	1.96	0.65
2:D:653:LEU:O	2:D:665:SER:HA	1.96	0.65
2:B:454:LEU:HD13	2:B:457:ARG:NH2	2.12	0.65
2:D:405:CYS:O	2:D:406:SER:C	2.39	0.65
2:D:447:ARG:HH21	1:C:1786:PRO:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1861:HIS:CE1	1:A:1863:GLU:HG2	2.32	0.64
1:C:1815:ALA:HB1	1:C:1904:VAL:HG11	1.79	0.64
1:A:1831:LEU:HG	1:A:1850:VAL:HG11	1.78	0.64
2:D:420:CYS:H	2:D:426:LEU:HD23	1.61	0.64
2:D:627:LEU:H	2:D:627:LEU:HD23	1.63	0.64
1:C:1771:GLU:HB3	1:C:1895:TRP:CE2	2.32	0.64
1:C:1824:LEU:HD11	1:C:1831:LEU:HD13	1.81	0.63
1:A:1792:GLN:OE1	1:C:1864:HIS:NE2	2.32	0.63
2:D:516:LEU:HD22	2:D:525:LEU:HD11	1.80	0.63
2:D:573:TRP:HB3	2:D:600:PRO:HD2	1.81	0.63
1:A:1801:ARG:HH22	1:A:1947:THR:HA	1.64	0.63
2:B:646:ILE:HD11	2:B:653:LEU:HD22	1.81	0.63
1:C:1902:LEU:N	1:C:1903:PRO:HD2	2.14	0.63
2:B:448:ILE:O	2:B:467:LEU:HB2	1.99	0.63
2:D:701:ARG:NH1	2:D:719:ASN:O	2.32	0.63
2:D:366:ALA:HB2	2:D:391:ARG:O	1.98	0.62
2:D:681:LEU:HB2	2:D:684:PRO:HG3	1.80	0.62
2:B:407:GLN:NE2	2:B:608:ALA:HB1	2.12	0.62
2:D:579:ILE:HG22	2:D:592:ILE:CB	2.19	0.62
1:A:1861:HIS:HE1	1:A:1863:GLU:HG2	1.63	0.62
2:D:536:GLU:HB3	2:D:547:VAL:HA	1.82	0.62
2:D:610:ARG:C	2:D:627:LEU:HD21	2.24	0.62
2:D:704:ASP:OD1	2:D:704:ASP:N	2.32	0.62
1:A:1770:ILE:O	1:A:1895:TRP:HA	2.00	0.61
2:D:452:GLN:HE22	2:D:463:LEU:HD22	1.65	0.61
1:C:1857:ARG:HH22	1:C:1922:ASP:HB3	1.65	0.61
1:A:1811:TRP:CE3	1:A:1823:ALA:HB2	2.35	0.61
2:D:491:ARG:HD3	2:D:507:SER:HA	1.83	0.61
1:C:1771:GLU:HB3	1:C:1895:TRP:NE1	2.16	0.61
2:D:605:ILE:O	2:D:694:ARG:NH2	2.30	0.61
1:A:1902:LEU:N	1:A:1903:PRO:HD3	2.16	0.60
2:B:423:GLY:C	2:B:424:TYR:HD2	2.09	0.60
1:C:1771:GLU:HB3	1:C:1895:TRP:CD1	2.36	0.60
1:C:1824:LEU:HD11	1:C:1831:LEU:CD1	2.31	0.60
2:B:703:GLY:O	2:B:705:ASN:N	2.33	0.60
2:D:530:SER:HA	2:D:556:PRO:HD2	1.83	0.60
1:C:1816:ALA:HB3	1:C:1819:ALA:HB2	1.83	0.60
1:C:1807:GLY:HA2	1:C:1914:THR:OG1	2.01	0.60
2:B:454:LEU:HD13	2:B:457:ARG:HH21	1.66	0.60
2:B:560:ALA:HB3	2:B:569:TYR:HB2	1.83	0.60
2:D:405:CYS:O	2:D:407:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:LEU:N	2:D:627:LEU:CD2	2.64	0.60
2:B:713:CYS:HB2	2:B:720:TYR:HD1	1.67	0.60
2:B:606:ASP:HB2	2:B:648:VAL:HG21	1.82	0.60
2:D:420:CYS:H	2:D:426:LEU:CD2	2.14	0.60
1:C:1779:SER:HB3	1:C:1784:GLU:O	2.02	0.59
2:B:455:PRO:O	2:B:677:ILE:HG12	2.03	0.59
2:D:374:GLY:O	2:D:375:ALA:HB2	2.01	0.59
1:C:1794:ASN:O	1:C:1795:HIS:CB	2.50	0.59
2:D:663:ILE:HD12	2:D:681:LEU:CD1	2.32	0.59
2:B:442:LEU:HB2	2:B:453:VAL:HG23	1.84	0.59
2:B:689:THR:HB	2:B:694:ARG:HG3	1.85	0.59
2:D:606:ASP:OD2	2:D:668:LYS:HE3	2.02	0.59
1:C:1811:TRP:CD1	1:C:1811:TRP:C	2.81	0.59
1:A:1794:ASN:OD1	1:A:1862:ARG:NH1	2.35	0.59
1:A:1857:ARG:HH12	1:A:1922:ASP:HB2	1.68	0.59
2:D:584:MET:HG3	2:D:715:PRO:HG2	1.83	0.59
2:D:716:SER:N	2:D:720:TYR:HA	2.16	0.59
1:C:1766:GLY:HA3	1:C:1917:VAL:HG13	1.83	0.59
1:C:1794:ASN:OD1	1:C:1862:ARG:NH1	2.36	0.59
1:A:1795:HIS:ND1	1:A:1861:HIS:CD2	2.71	0.58
2:B:452:GLN:HB2	2:B:461:THR:HB	1.86	0.58
2:D:544:HIS:HB3	2:D:712:LEU:HD21	1.83	0.58
2:D:594:ASP:OD2	2:D:594:ASP:N	2.35	0.58
2:B:713:CYS:HB2	2:B:720:TYR:CD1	2.37	0.58
2:D:370:GLN:C	2:D:372:ILE:N	2.61	0.58
2:D:689:THR:HB	2:D:694:ARG:HD2	1.86	0.58
2:B:665:SER:HB3	2:B:677:ILE:CD1	2.34	0.58
2:B:423:GLY:C	2:B:436:LEU:HG	2.29	0.57
2:D:655:TRP:CE2	2:D:664:ASN:HB2	2.39	0.57
1:C:1773:LEU:HB2	1:C:1937:VAL:CG2	2.34	0.57
2:D:440:PRO:HG3	2:D:649:PHE:HE2	1.64	0.57
2:D:598:PHE:CD2	2:D:618:LYS:HG2	2.40	0.57
1:A:1815:ALA:C	1:A:1904:VAL:HG11	2.29	0.57
2:B:521:VAL:HB	2:B:563:PRO:HB3	1.86	0.57
2:B:701:ARG:HG3	2:B:715:PRO:HB3	1.85	0.56
1:C:1792:GLN:HA	1:C:1862:ARG:NH2	2.19	0.56
2:B:460:TYR:HA	2:B:678:ARG:NH1	2.20	0.56
2:B:588:GLY:O	2:B:590:ARG:NH1	2.37	0.56
2:D:427:ARG:NE	2:D:434:LYS:HB2	2.20	0.56
2:D:453:VAL:CG1	2:D:460:TYR:HB2	2.07	0.56
2:B:491:ARG:HD3	2:B:507:SER:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:ARG:O	2:B:429:ASP:N	2.38	0.56
2:B:463:LEU:HD23	2:B:464:LEU:HG	1.87	0.56
2:B:529:ASP:HB3	2:B:532:THR:HB	1.88	0.56
2:D:447:ARG:NH2	1:C:1786:PRO:HB2	2.20	0.56
1:C:1824:LEU:HD22	1:C:1833:LEU:HB2	1.86	0.56
1:C:1773:LEU:HB2	1:C:1937:VAL:HG21	1.87	0.56
1:C:1791:LEU:HD11	1:C:1890:THR:HB	1.86	0.56
1:A:1818:ARG:HH22	1:A:1907:ALA:HB1	1.71	0.55
1:C:1810:LEU:HD12	1:C:1896:LEU:HD13	1.87	0.55
2:B:569:TYR:HB3	2:B:603:LEU:HD21	1.88	0.55
2:D:365:CYS:O	2:D:365:CYS:SG	2.65	0.55
2:D:491:ARG:CD	2:D:507:SER:HA	2.37	0.55
1:C:1853:ASN:ND2	1:C:1948:PRO:HB3	2.22	0.55
1:C:1908:LEU:HB3	1:C:1912:TYR:HB2	1.89	0.55
1:C:1832:GLN:HB3	1:C:1845:ARG:HG3	1.88	0.55
2:B:562:HIS:CE1	2:B:564:MET:HE2	2.42	0.55
2:D:484:TRP:CE2	2:D:493:LEU:HD12	2.42	0.55
1:C:1795:HIS:CD2	1:C:1796:PHE:H	2.24	0.55
2:B:670:THR:HB	2:B:672:LYS:H	1.72	0.55
2:D:662:SER:HA	2:D:681:LEU:HD12	1.89	0.54
2:D:610:ARG:HG3	2:D:610:ARG:NH1	2.15	0.54
2:D:419:TRP:CZ3	2:D:421:GLU:HG2	2.43	0.54
1:A:1817:GLU:HG3	1:A:1905:GLY:CA	2.37	0.53
2:B:670:THR:HG21	2:B:672:LYS:HD2	1.89	0.53
2:B:734:HIS:CE1	2:B:735:ALA:HB2	2.43	0.53
2:D:384:TYR:O	2:D:386:LEU:N	2.41	0.53
2:D:469:ASN:HB2	2:D:488:THR:CG2	2.38	0.53
2:B:556:PRO:HA	2:B:571:THR:O	2.09	0.53
2:D:370:GLN:O	2:D:372:ILE:N	2.39	0.53
1:C:1902:LEU:H	1:C:1903:PRO:HD2	1.73	0.53
2:B:622:ILE:CD1	2:B:640:LEU:HD21	2.38	0.53
1:A:1801:ARG:NH1	1:A:1948:PRO:HD3	2.24	0.53
2:B:537:VAL:CG2	2:B:538:ALA:H	2.17	0.53
2:B:559:ILE:HD11	2:B:568:ILE:HD11	1.89	0.53
2:D:484:TRP:CZ2	2:D:493:LEU:HD13	2.44	0.53
2:B:649:PHE:CZ	2:B:691:HIS:CD2	2.96	0.53
1:C:1947:THR:OG1	1:C:1948:PRO:HD2	2.08	0.53
2:B:533:SER:C	2:B:534:ARG:HG3	2.33	0.53
2:D:568:ILE:HD11	2:D:584:MET:HA	1.90	0.53
2:D:534:ARG:HD2	2:D:547:VAL:CG1	2.39	0.53
2:B:423:GLY:C	2:B:424:TYR:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:598:PHE:HB3	2:B:618:LYS:HB3	1.91	0.52
2:D:578:ARG:HD2	2:D:591:ILE:HD12	1.90	0.52
1:A:1894:LEU:HD23	1:A:1895:TRP:N	2.25	0.52
1:A:1894:LEU:HD23	1:A:1894:LEU:C	2.35	0.52
2:D:517:ALA:HB3	2:D:526:TYR:HB2	1.90	0.52
2:B:731:ILE:HD12	2:B:737:ALA:HB3	1.90	0.52
2:D:371:MET:O	2:D:371:MET:HG2	2.10	0.52
2:D:677:ILE:HG22	2:D:678:ARG:N	2.25	0.52
1:A:1899:LEU:HB3	1:A:1902:LEU:HB2	1.92	0.52
2:B:418:CYS:HB2	2:B:430:ARG:O	2.09	0.52
1:C:1778:GLU:OE1	1:C:1778:GLU:N	2.43	0.52
1:A:1928:ARG:NH1	1:A:1935:ASP:OD2	2.42	0.52
2:B:472:ALA:HA	2:B:686:ASP:HB2	1.91	0.52
2:D:469:ASN:HD22	2:D:471:ILE:HD11	1.75	0.52
2:D:627:LEU:H	2:D:627:LEU:CD2	2.23	0.52
1:C:1857:ARG:HG2	1:C:1859:ARG:HH12	1.75	0.52
2:D:724:CYS:HB3	2:D:728:PHE:HB2	1.92	0.51
2:D:372:ILE:HG22	2:D:373:ARG:H	1.75	0.51
2:D:526:TYR:CD2	2:D:537:VAL:HB	2.46	0.51
1:C:1821:TYR:CE2	1:C:1836:ASP:HB3	2.46	0.51
2:B:525:LEU:HD23	2:B:525:LEU:C	2.36	0.51
2:B:730:LYS:O	2:B:731:ILE:HB	2.10	0.51
2:B:728:PHE:HA	2:B:738:GLN:HA	1.92	0.51
2:D:732:ASN:O	2:D:734:HIS:N	2.44	0.51
1:C:1792:GLN:HG3	1:C:1864:HIS:NE2	2.26	0.51
1:C:1902:LEU:N	1:C:1903:PRO:CD	2.74	0.51
2:D:557:ARG:NH1	2:D:557:ARG:HG3	2.26	0.51
2:D:441:VAL:HG23	2:D:453:VAL:O	2.11	0.50
2:D:710:THR:OG1	2:D:735:ALA:HA	2.10	0.50
1:C:1832:GLN:HA	1:C:1845:ARG:HA	1.92	0.50
2:B:665:SER:HB3	2:B:677:ILE:HD11	1.93	0.50
2:D:622:ILE:HG13	2:D:640:LEU:HD11	1.92	0.50
2:B:648:VAL:HG23	2:B:694:ARG:NH1	2.27	0.50
2:D:522:HIS:CE1	2:D:715:PRO:HG3	2.47	0.50
1:A:1902:LEU:N	1:A:1903:PRO:CD	2.73	0.50
2:D:654:TYR:CD2	2:D:665:SER:HB3	2.47	0.50
1:A:1927:HIS:CE1	1:C:1795:HIS:HB3	2.47	0.50
1:A:1931:HIS:HB3	1:A:1934:GLU:HG2	1.94	0.50
2:B:564:MET:SD	2:B:564:MET:N	2.83	0.50
2:B:579:ILE:HD13	2:B:614:TRP:CE3	2.46	0.50
2:D:468:GLU:HB2	2:D:486:ASP:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1812:ILE:CD1	1:C:1894:LEU:HG	2.41	0.50
1:A:1771:GLU:HB2	1:A:1895:TRP:CZ2	2.46	0.49
1:A:1846:SER:OG	1:A:1848:VAL:HB	2.11	0.49
2:D:386:LEU:HD22	2:D:388:GLU:OE2	2.13	0.49
2:D:710:THR:OG1	2:D:734:HIS:O	2.26	0.49
2:B:579:ILE:HG22	2:B:592:ILE:HB	1.94	0.49
2:B:561:LEU:HB3	2:B:584:MET:HE2	1.94	0.49
1:C:1812:ILE:HD12	1:C:1894:LEU:HG	1.93	0.49
2:B:718:GLN:N	2:B:718:GLN:CD	2.71	0.49
2:D:420:CYS:HB3	2:D:424:TYR:HB2	1.95	0.49
2:D:645:ALA:O	2:D:655:TRP:HA	2.13	0.49
2:B:559:ILE:HA	2:B:569:TYR:O	2.12	0.49
2:D:572:ASP:O	2:D:577:PRO:HA	2.13	0.49
2:D:624:ARG:O	2:D:632:ARG:HA	2.13	0.49
1:C:1902:LEU:H	1:C:1903:PRO:CD	2.25	0.49
1:A:1846:SER:CB	1:A:1871:VAL:HG21	2.42	0.49
1:C:1773:LEU:HD22	1:C:1893:ALA:HB2	1.94	0.49
2:B:561:LEU:CD2	2:B:568:ILE:HG13	2.43	0.48
1:C:1808:LEU:HD13	1:C:1912:TYR:HD2	1.78	0.48
2:D:670:THR:C	2:D:672:LYS:H	2.21	0.48
2:B:536:GLU:HG2	2:B:547:VAL:HA	1.95	0.48
2:B:538:ALA:HB2	2:B:545:ARG:HG2	1.93	0.48
2:B:649:PHE:CZ	2:B:691:HIS:HD2	2.31	0.48
2:B:649:PHE:HZ	2:B:691:HIS:CD2	2.30	0.48
1:A:1793:SER:HA	1:A:1862:ARG:O	2.13	0.48
2:B:569:TYR:CD2	2:B:581:ALA:HB2	2.48	0.48
2:D:516:LEU:HA	2:D:516:LEU:HD23	1.37	0.48
1:C:1774:ASN:HD22	1:C:1892:GLY:HA2	1.79	0.48
2:B:527:TRP:CZ2	2:B:536:GLU:HB2	2.49	0.48
2:D:615:VAL:HG11	2:D:643:PRO:HB2	1.96	0.48
1:A:1846:SER:HB2	1:A:1871:VAL:CG2	2.44	0.48
1:C:1796:PHE:HB3	1:C:1924:VAL:O	2.13	0.48
2:B:617:ALA:HA	2:B:643:PRO:HD2	1.94	0.48
1:A:1865:ARG:HG2	1:A:1881:SER:OG	2.14	0.48
2:D:387:THR:O	2:D:388:GLU:C	2.57	0.48
2:B:647:THR:HG22	2:B:654:TYR:HB2	1.96	0.47
2:B:456:HIS:CE1	2:B:675:GLU:OE2	2.67	0.47
2:D:469:ASN:ND2	2:D:471:ILE:HD11	2.29	0.47
2:B:670:THR:HG21	2:B:672:LYS:CD	2.43	0.47
1:A:1840:GLN:HB2	1:A:1882:PRO:HG2	1.97	0.47
2:D:496:ASN:O	2:D:499:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:715:PRO:HA	2:D:720:TYR:HA	1.95	0.47
1:A:1810:LEU:HD23	1:A:1811:TRP:N	2.29	0.47
1:C:1763:ALA:HB3	1:C:1945:CYS:N	2.30	0.47
1:A:1846:SER:C	1:A:1848:VAL:H	2.22	0.47
2:B:476:HIS:ND1	2:B:478:ARG:O	2.48	0.47
2:D:447:ARG:HD2	2:D:685:MET:HE3	1.97	0.47
2:D:647:THR:CG2	2:D:654:TYR:HB2	2.45	0.47
1:C:1815:ALA:HB1	1:C:1904:VAL:CG1	2.45	0.47
2:B:476:HIS:CD2	2:B:520:TRP:HA	2.50	0.47
1:C:1765:ASP:HB2	1:C:1768:THR:OG1	2.15	0.47
1:C:1795:HIS:CD2	1:C:1796:PHE:N	2.83	0.47
2:D:374:GLY:O	2:D:375:ALA:CB	2.63	0.46
2:D:492:ILE:HG13	2:D:510:LEU:CD1	2.45	0.46
1:A:1919:CYS:O	1:A:1920:LEU:HD12	2.15	0.46
2:B:544:HIS:ND1	2:B:712:LEU:HG	2.30	0.46
1:A:1818:ARG:O	1:A:1819:ALA:C	2.58	0.46
2:D:557:ARG:HG3	2:D:557:ARG:HH11	1.81	0.46
2:D:651:ASP:HA	2:D:668:LYS:HD3	1.97	0.46
1:C:1766:GLY:C	1:C:1768:THR:H	2.24	0.46
2:D:471:ILE:HD12	2:D:685:MET:HG3	1.98	0.46
2:D:475:PHE:CE1	2:D:695:GLN:NE2	2.84	0.46
1:A:1830:HIS:HB2	1:A:1845:ARG:NH2	2.30	0.46
2:D:533:SER:OG	2:D:554:GLU:O	2.34	0.46
2:B:585:ASP:OD2	2:B:716:SER:HB2	2.15	0.46
2:B:731:ILE:O	2:B:732:ASN:CB	2.63	0.46
2:D:471:ILE:HG13	1:C:1785:ILE:HG21	1.97	0.46
1:A:1796:PHE:C	1:A:1796:PHE:CD2	2.94	0.46
1:A:1806:GLN:NE2	1:A:1828:ASP:H	2.14	0.46
2:B:457:ARG:HB3	2:B:459:GLU:H	1.81	0.46
1:C:1763:ALA:H	1:C:1944:PRO:HA	1.80	0.46
1:A:1818:ARG:HA	1:A:1818:ARG:NH1	2.30	0.45
2:D:388:GLU:CD	2:D:388:GLU:H	2.23	0.45
2:D:472:ALA:HB2	2:D:514:GLY:O	2.16	0.45
2:D:485:SER:HA	2:D:492:ILE:HA	1.98	0.45
2:D:599:TRP:O	2:D:616:ASP:HA	2.17	0.45
2:D:702:CYS:O	2:D:707:GLY:HA3	2.16	0.45
1:A:1827:VAL:HG22	1:A:1911:ALA:HB3	1.99	0.45
2:B:530:SER:HA	2:B:556:PRO:HD2	1.99	0.45
2:B:615:VAL:HG22	2:B:622:ILE:HG13	1.98	0.45
2:D:457:ARG:C	2:D:459:GLU:H	2.24	0.45
2:B:600:PRO:HA	2:B:615:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:452:GLN:HE22	2:D:463:LEU:CD2	2.30	0.45
2:D:471:ILE:CD1	2:D:685:MET:HG3	2.47	0.45
2:D:604:THR:HG23	2:D:648:VAL:HG22	1.98	0.45
2:B:434:LYS:HG2	2:B:435:ALA:N	2.32	0.45
2:D:657:ASP:HB3	2:D:660:THR:CG2	2.46	0.45
2:D:554:GLU:CB	2:D:574:GLY:HA3	2.45	0.45
2:D:691:HIS:CG	2:D:692:PRO:HD2	2.52	0.45
2:D:583:SER:O	2:D:585:ASP:N	2.49	0.44
2:B:555:LYS:N	2:B:572:ASP:OD2	2.50	0.44
2:D:394:GLN:HB3	2:D:395:ASP:H	1.58	0.44
2:D:665:SER:OG	2:D:675:GLU:HB3	2.17	0.44
1:A:1883:LEU:HD23	2:D:534:ARG:NH1	2.32	0.44
2:B:585:ASP:HA	2:B:714:LEU:HD13	1.99	0.44
2:D:494:ARG:HH21	2:D:541:ASP:HA	1.82	0.44
1:C:1857:ARG:HG2	1:C:1859:ARG:NH1	2.32	0.44
2:B:483:PHE:CD1	2:B:518:VAL:HG21	2.53	0.44
2:B:532:THR:O	2:B:534:ARG:HG3	2.18	0.44
2:D:476:HIS:HB3	2:D:481:LEU:HB2	1.99	0.44
2:B:708:GLY:CA	2:B:713:CYS:SG	3.03	0.44
2:D:575:ASN:C	2:D:577:PRO:HD3	2.43	0.44
2:B:552:SER:HB2	2:B:589:ARG:NH2	2.33	0.44
2:D:681:LEU:H	2:D:681:LEU:HG	1.66	0.44
2:B:404:TYR:N	2:B:404:TYR:CD2	2.86	0.44
2:B:731:ILE:O	2:B:731:ILE:HG22	2.18	0.44
2:D:375:ALA:C	2:D:376:VAL:HG23	2.43	0.44
2:D:722:CYS:HB2	2:D:733:SER:O	2.17	0.43
1:A:1801:ARG:NH2	1:A:1947:THR:HA	2.32	0.43
2:D:624:ARG:HG2	2:D:625:ALA:N	2.33	0.43
1:C:1853:ASN:HD22	1:C:1948:PRO:HB3	1.82	0.43
2:B:622:ILE:HD12	2:B:640:LEU:HD11	2.00	0.43
2:B:706:ASN:O	2:B:708:GLY:N	2.49	0.43
1:C:1779:SER:O	1:C:1783:ASN:N	2.31	0.43
1:C:1792:GLN:HG3	1:C:1864:HIS:CE1	2.54	0.43
1:C:1799:SER:HA	1:C:1857:ARG:HA	2.00	0.43
2:B:519:ASP:HB2	2:B:561:LEU:HD13	2.01	0.43
1:C:1773:LEU:H	1:C:1937:VAL:CG2	2.02	0.43
1:A:1773:LEU:HG	1:A:1937:VAL:HG21	2.00	0.43
2:B:552:SER:HB3	2:B:578:ARG:HH12	1.83	0.43
2:D:485:SER:HB2	2:D:513:PRO:HB2	1.99	0.43
2:D:728:PHE:N	2:D:728:PHE:CD2	2.86	0.43
1:A:1802:THR:OG1	1:A:1917:VAL:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:ARG:HH22	1:A:1907:ALA:CB	2.31	0.43
2:D:494:ARG:NH2	2:D:541:ASP:HA	2.34	0.43
2:D:566:GLY:CA	2:D:584:MET:HG2	2.49	0.43
1:A:1931:HIS:O	1:A:1935:ASP:HB2	2.19	0.43
2:B:424:TYR:CD2	2:B:424:TYR:N	2.87	0.43
2:B:453:VAL:HG11	2:B:678:ARG:HD3	1.99	0.43
1:A:1859:ARG:O	1:A:1869:LEU:HA	2.19	0.43
2:B:560:ALA:O	2:B:569:TYR:N	2.48	0.43
2:B:626:ASN:HB2	2:B:630:SER:O	2.19	0.43
2:D:494:ARG:HB3	2:D:505:VAL:CG2	2.48	0.43
2:D:625:ALA:HB2	2:D:632:ARG:HB2	2.01	0.43
1:C:1836:ASP:HB2	1:C:1841:PRO:HB3	2.01	0.43
2:B:615:VAL:HG13	2:B:643:PRO:HG2	2.00	0.43
2:B:703:GLY:C	2:B:705:ASN:N	2.77	0.43
2:D:388:GLU:CD	2:D:388:GLU:N	2.77	0.43
2:D:715:PRO:HA	2:D:720:TYR:CB	2.49	0.43
1:A:1839:SER:H	1:A:1885:ALA:CB	2.32	0.42
2:B:454:LEU:HA	2:B:455:PRO:HD2	1.70	0.42
2:B:583:SER:O	2:B:585:ASP:N	2.52	0.42
2:B:607:TYR:CD2	2:B:696:PRO:HG3	2.54	0.42
2:D:407:GLN:HG3	2:D:420:CYS:HA	2.01	0.42
2:D:424:TYR:CD1	2:D:435:ALA:HA	2.54	0.42
1:C:1821:TYR:HE2	1:C:1836:ASP:HB3	1.83	0.42
1:A:1781:LEU:HD23	1:A:1781:LEU:HA	1.86	0.42
2:B:521:VAL:HG21	2:B:563:PRO:HB2	2.01	0.42
2:B:534:ARG:HG2	2:B:550:TRP:HA	2.01	0.42
2:B:537:VAL:CG2	2:B:538:ALA:N	2.77	0.42
2:B:653:LEU:O	2:B:665:SER:HA	2.20	0.42
2:D:492:ILE:HG23	2:D:516:LEU:HD11	2.01	0.42
2:B:654:TYR:CD2	2:B:677:ILE:CD1	3.02	0.42
2:B:655:TRP:CE2	2:B:664:ASN:HB2	2.54	0.42
2:B:429:ASP:OD1	2:B:430:ARG:N	2.53	0.42
2:D:441:VAL:CG2	2:D:452:GLN:HG3	2.42	0.42
2:D:492:ILE:HG13	2:D:510:LEU:HD11	2.02	0.42
2:D:646:ILE:HD12	2:D:655:TRP:HB3	2.00	0.42
2:D:388:GLU:N	2:D:388:GLU:OE1	2.53	0.42
2:D:477:HIS:C	2:D:479:ARG:H	2.27	0.42
2:D:655:TRP:NE1	2:D:664:ASN:HB2	2.35	0.42
1:C:1847:THR:HG23	1:C:1874:GLU:HG3	2.02	0.42
1:C:1895:TRP:CZ3	1:C:1899:LEU:HG	2.55	0.42
1:A:1817:GLU:C	1:A:1819:ALA:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:705:ASN:HA	2:D:708:GLY:H	1.85	0.41
1:A:1865:ARG:HD2	1:A:1883:LEU:HA	2.02	0.41
2:B:444:PHE:C	2:B:473:LEU:HD21	2.45	0.41
2:B:476:HIS:CE1	2:B:479:ARG:HB2	2.50	0.41
1:A:1762:LEU:HD12	1:A:1932:LEU:HD22	2.03	0.41
1:A:1801:ARG:CZ	1:A:1948:PRO:HD3	2.50	0.41
2:B:420:CYS:SG	2:B:426:LEU:N	2.93	0.41
2:D:371:MET:HE3	2:D:376:VAL:HG22	2.02	0.41
2:D:462:LEU:HD23	2:D:463:LEU:N	2.34	0.41
2:D:512:SER:O	2:D:529:ASP:HA	2.20	0.41
2:B:539:ASN:HB3	2:B:541:ASP:OD2	2.21	0.41
2:D:728:PHE:N	2:D:728:PHE:HD2	2.18	0.41
2:D:595:THR:O	2:D:632:ARG:NH2	2.42	0.41
2:D:647:THR:HG22	2:D:654:TYR:HB2	2.02	0.41
1:C:1796:PHE:CZ	1:C:1860:ALA:HB3	2.55	0.41
1:C:1939:LYS:HA	1:C:1940:PRO:HD3	1.84	0.41
1:A:1769:TYR:CD2	1:A:1900:GLN:HB2	2.55	0.41
1:A:1896:LEU:HD12	1:A:1896:LEU:HA	1.88	0.41
2:B:527:TRP:CE2	2:B:536:GLU:HB2	2.56	0.41
2:B:532:THR:CG2	2:B:534:ARG:HB2	2.50	0.41
2:B:649:PHE:CE2	2:B:650:GLU:HG3	2.56	0.41
2:D:714:LEU:HA	2:D:715:PRO:HD2	1.95	0.41
2:D:719:ASN:HB3	2:D:720:TYR:H	1.60	0.41
1:C:1899:LEU:CD2	1:C:1900:GLN:H	2.33	0.41
1:C:1931:HIS:HB2	1:C:1935:ASP:OD2	2.21	0.41
2:B:478:ARG:C	2:B:480:GLU:H	2.27	0.41
2:D:623:GLU:HA	2:D:634:ALA:HA	2.01	0.41
2:B:550:TRP:CZ3	2:B:551:GLN:HG2	2.56	0.41
2:D:534:ARG:HD2	2:D:547:VAL:HG13	2.02	0.41
2:B:525:LEU:CD2	2:B:527:TRP:HE3	2.33	0.41
2:B:716:SER:CB	2:B:721:THR:HG23	2.43	0.41
2:D:511:GLU:N	2:D:529:ASP:OD2	2.44	0.41
1:C:1812:ILE:HG13	1:C:1894:LEU:CB	2.49	0.41
1:C:1822:MET:CB	1:C:1835:TYR:HB3	2.51	0.41
1:A:1868:SER:HB2	1:A:1878:THR:HG22	2.02	0.41
1:C:1822:MET:HB2	1:C:1835:TYR:HB3	2.02	0.41
1:A:1857:ARG:NH1	1:A:1922:ASP:HB2	2.34	0.40
2:B:497:LEU:C	2:B:499:GLY:N	2.79	0.40
2:D:484:TRP:CZ2	2:D:493:LEU:CD1	3.04	0.40
2:D:495:ALA:HB2	2:D:502:VAL:HG12	2.02	0.40
2:D:645:ALA:CB	2:D:686:ASP:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1927:HIS:HE1	1:C:1926:GLY:O	2.04	0.40
2:B:483:PHE:CD2	2:B:494:ARG:HB3	2.56	0.40
1:C:1801:ARG:HD2	1:C:1801:ARG:C	2.46	0.40
1:C:1810:LEU:HD21	1:C:1812:ILE:HD12	2.02	0.40
2:B:555:LYS:O	2:B:572:ASP:HA	2.21	0.40
2:B:661:LYS:HA	2:B:661:LYS:HD2	1.89	0.40
2:D:360:VAL:HG13	2:D:361:ASN:ND2	2.36	0.40
2:D:372:ILE:O	2:D:374:GLY:N	2.54	0.40
2:B:525:LEU:CD2	2:B:527:TRP:CE3	3.04	0.40
2:B:558:ALA:O	2:B:570:TRP:HA	2.21	0.40
2:D:391:ARG:HD2	2:D:391:ARG:N	2.37	0.40
2:D:707:GLY:C	2:D:709:CYS:N	2.79	0.40
1:C:1791:LEU:CD1	1:C:1888:LEU:HD23	2.52	0.40
1:C:1844:LEU:HD22	1:C:1877:VAL:HG12	2.02	0.40
1:A:1792:GLN:HG3	1:C:1863:GLU:OE2	2.22	0.40
2:B:424:TYR:HD2	2:B:424:TYR:N	2.19	0.40
2:B:476:HIS:ND1	2:B:479:ARG:CB	2.68	0.40
2:B:645:ALA:O	2:B:655:TRP:HB2	2.21	0.40
2:D:398:GLU:O	2:D:399:CYS:CB	2.66	0.40
2:D:578:ARG:HD2	2:D:591:ILE:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:TRP:CH2	2:D:543:ALA:CB[4_455]	2.15	0.05

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	189/191 (99%)	165 (87%)	18 (10%)	6 (3%)	3 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	189/191 (99%)	150 (79%)	31 (16%)	8 (4%)	2	14
2	B	326/386 (84%)	262 (80%)	46 (14%)	18 (6%)	1	10
2	D	373/386 (97%)	295 (79%)	55 (15%)	23 (6%)	1	9
All	All	1077/1154 (93%)	872 (81%)	150 (14%)	55 (5%)	1	11

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1774	ASN
1	A	1940	PRO
2	B	704	ASP
2	B	706	ASN
2	B	731	ILE
2	D	360	VAL
2	D	375	ALA
2	D	385	ARG
2	D	388	GLU
2	D	399	CYS
2	D	406	SER
2	D	584	MET
1	C	1795	HIS
2	B	429	ASP
2	B	703	GLY
2	B	717	GLY
2	B	732	ASN
2	D	430	ARG
2	D	708	GLY
1	C	1778	GLU
1	C	1852	THR
1	A	1916	PHE
2	B	428	PRO
2	B	552	SER
2	B	584	MET
2	B	719	ASN
2	B	730	LYS
2	D	373	ARG
2	D	709	CYS
1	C	1774	ASN
1	C	1820	ASP
1	C	1940	PRO
2	B	455	PRO

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Mol	Chain	Res	Type
2	B	459	GLU
2	B	498	ASN
2	D	376	VAL
2	D	447	ARG
2	D	683	PHE
2	D	733	SER
1	A	1902	LEU
1	A	1917	VAL
2	B	608	ALA
2	B	715	PRO
2	B	725	PRO
2	D	366	ALA
2	D	371	MET
2	D	372	ILE
2	D	374	GLY
2	D	400	ALA
2	D	478	ARG
1	C	1840	GLN
1	C	1902	LEU
1	A	1907	ALA
2	D	383	GLY
2	D	677	ILE

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	156/156 (100%)	143 (92%)	13 (8%)	10	34
1	C	156/156 (100%)	122 (78%)	34 (22%)	1	5
2	B	283/327 (86%)	254 (90%)	29 (10%)	7	26
2	D	321/327 (98%)	274 (85%)	47 (15%)	3	14
All	All	916/966 (95%)	793 (87%)	123 (13%)	4	16

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1759	LEU
1	A	1776	VAL
1	A	1791	LEU
1	A	1792	GLN
1	A	1842	VAL
1	A	1862	ARG
1	A	1869	LEU
1	A	1896	LEU
1	A	1901	LYS
1	A	1919	CYS
1	A	1931	HIS
1	A	1933	LEU
1	A	1934	GLU
2	B	424	TYR
2	B	425	GLU
2	B	429	ASP
2	B	441	VAL
2	B	448	ILE
2	B	449	ASP
2	B	454	LEU
2	B	457	ARG
2	B	458	SER
2	B	473	LEU
2	B	493	LEU
2	B	497	LEU
2	B	502	VAL
2	B	505	VAL
2	B	512	SER
2	B	516	LEU
2	B	525	LEU
2	B	532	THR
2	B	540	LEU
2	B	551	GLN
2	B	615	VAL
2	B	633	LYS
2	B	635	VAL
2	B	648	VAL
2	B	670	THR
2	B	683	PHE
2	B	709	CYS
2	B	732	ASN
2	B	736	CYS
2	D	376	VAL

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Mol	Chain	Res	Type
2	D	379	THR
2	D	392	THR
2	D	399	CYS
2	D	410	THR
2	D	421	GLU
2	D	426	LEU
2	D	430	ARG
2	D	436	LEU
2	D	442	LEU
2	D	451	ARG
2	D	452	GLN
2	D	459	GLU
2	D	460	TYR
2	D	461	THR
2	D	463	LEU
2	D	469	ASN
2	D	473	LEU
2	D	480	GLU
2	D	493	LEU
2	D	494	ARG
2	D	496	ASN
2	D	498	ASN
2	D	533	SER
2	D	536	GLU
2	D	540	LEU
2	D	545	ARG
2	D	552	SER
2	D	579	ILE
2	D	595	THR
2	D	610	ARG
2	D	627	LEU
2	D	648	VAL
2	D	660	THR
2	D	670	THR
2	D	675	GLU
2	D	678	ARG
2	D	688	HIS
2	D	690	LEU
2	D	694	ARG
2	D	704	ASP
2	D	706	ASN
2	D	729	ARG

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Mol	Chain	Res	Type
2	D	730	LYS
2	D	731	ILE
2	D	732	ASN
2	D	734	HIS
1	C	1762	LEU
1	C	1771	GLU
1	C	1773	LEU
1	C	1777	ILE
1	C	1778	GLU
1	C	1779	SER
1	C	1788	GLU
1	C	1791	LEU
1	C	1792	GLN
1	C	1798	LEU
1	C	1801	ARG
1	C	1805	THR
1	C	1811	TRP
1	C	1812	ILE
1	C	1814	LYS
1	C	1817	GLU
1	C	1824	LEU
1	C	1833	LEU
1	C	1842	VAL
1	C	1847	THR
1	C	1856	LEU
1	C	1858	ILE
1	C	1863	GLU
1	C	1866	GLU
1	C	1869	LEU
1	C	1874	GLU
1	C	1881	SER
1	C	1894	LEU
1	C	1899	LEU
1	C	1902	LEU
1	C	1919	CYS
1	C	1938	THR
1	C	1939	LYS
1	C	1942	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1774	ASN
1	A	1832	GLN
1	A	1861	HIS
1	A	1927	HIS
2	B	407	GLN
2	B	551	GLN
2	B	626	ASN
2	B	642	HIS
2	B	691	HIS
2	B	711	HIS
2	D	361	ASN
2	D	452	GLN
2	D	469	ASN
2	D	477	HIS
2	D	498	ASN
2	D	562	HIS
2	D	674	GLN
2	D	711	HIS
2	D	718	GLN
2	D	719	ASN
1	C	1774	ASN
1	C	1927	HIS

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/191 (100%)	-0.35	1 (0%) 87 76	48, 78, 138, 167	0
1	C	191/191 (100%)	-0.25	0 100 100	35, 121, 178, 240	0
2	B	330/386 (85%)	-0.38	1 (0%) 90 82	34, 66, 125, 169	0
2	D	377/386 (97%)	-0.43	4 (1%) 78 60	30, 65, 139, 240	0
All	All	1089/1154 (94%)	-0.37	6 (0%) 85 73	30, 75, 152, 240	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	419	TRP	4.0
2	D	419	TRP	3.2
2	D	416	PHE	2.7
2	D	613	TYR	2.7
2	D	389	ASP	2.3
1	A	1833	LEU	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	2001	1/1	0.82	0.14	143,143,143,143	0
3	CA	A	2001	1/1	0.87	0.20	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.