



Full wwPDB EM Validation Report ⓘ

May 3, 2026 – 12:53 AM JST

PDB ID : 9UN3 / pdb_00009un3
EMDB ID : EMD-64338
Title : native NMDA receptor-GluN1/N2B in the open state
Authors : Yu, J.; Xu, R.S.; Ge, J.P.
Deposited on : 2025-04-23
Resolution : 3.37 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

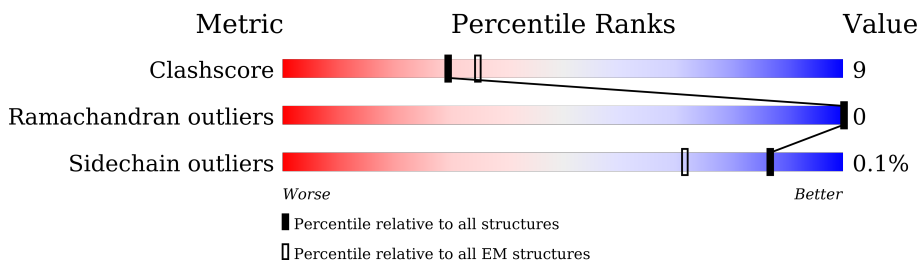
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.37 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	817	77% 22% .
1	C	817	76% 22% .
2	B	817	78% 19% .
2	D	817	77% 21% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24220 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

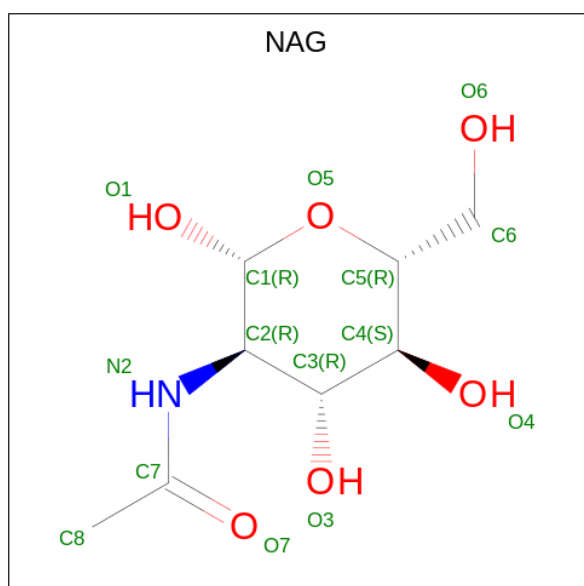
- Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	805	Total	C	N	O	S	0	0
			6007	3848	1036	1088	35		
1	C	805	Total	C	N	O	S	0	0
			5978	3837	1029	1079	33		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	798	Total	C	N	O	S	0	0
			5944	3852	974	1077	41		
2	D	799	Total	C	N	O	S	0	0
			5929	3844	962	1082	41		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



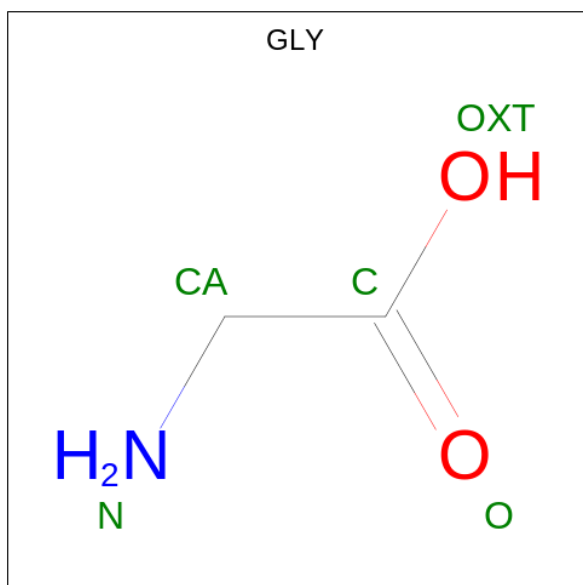
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

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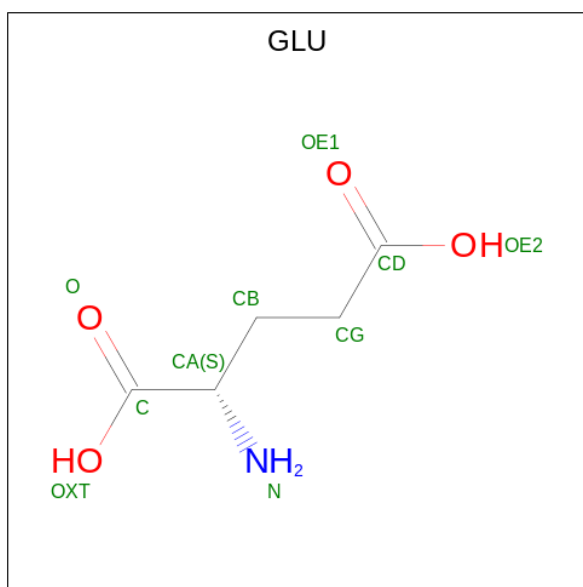
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).

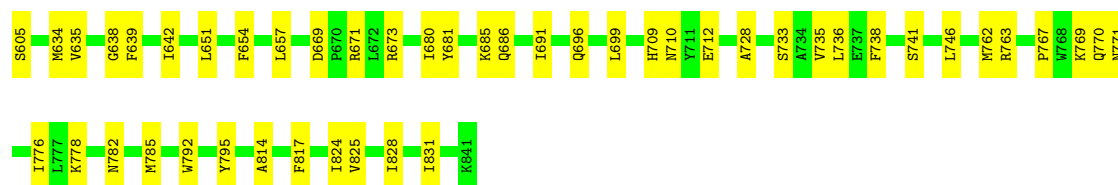


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			4	2	1	1	
4	C	1	Total	C	N	O	0
			4	2	1	1	

- Molecule 5 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).

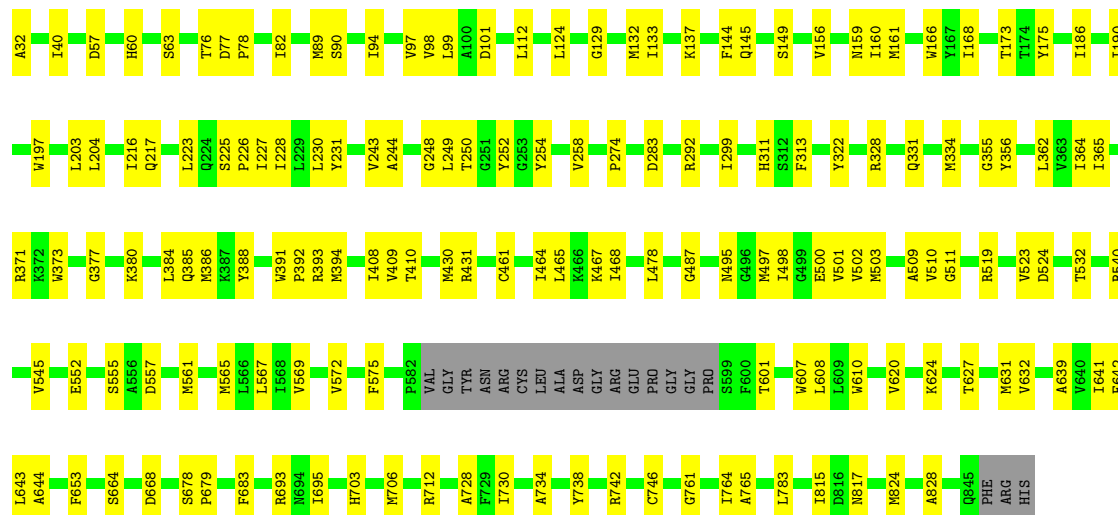


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			9	5	1	3	
5	D	1	Total	C	N	O	0
			9	5	1	3	



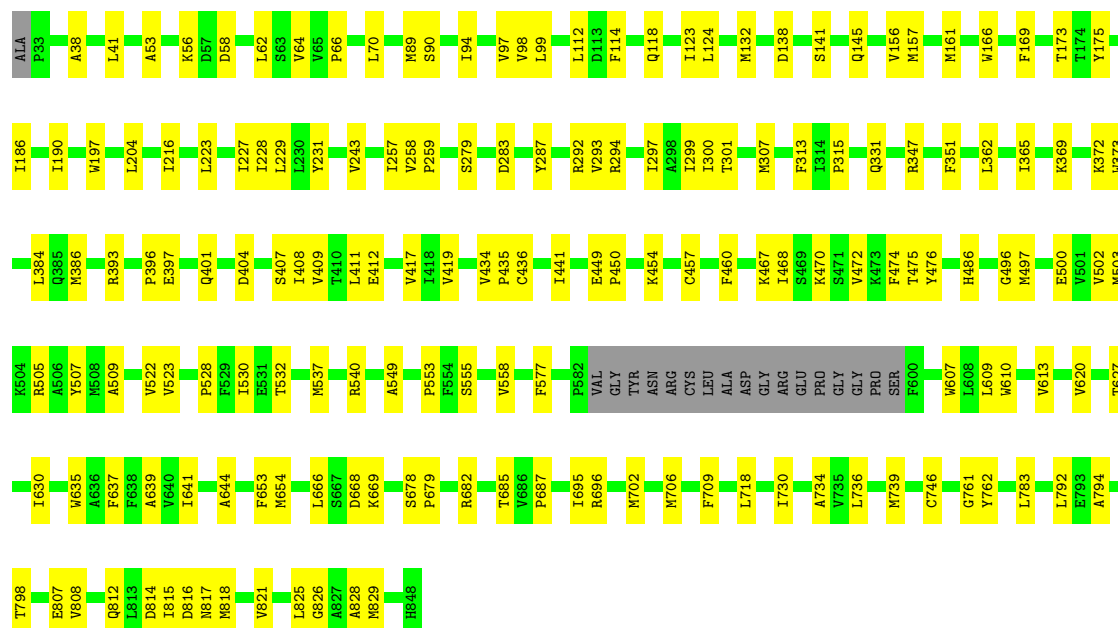
- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain B: 78% 19% .



- Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D: 77% 21% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/6144	0.40	0/8378
1	C	0.24	0/6117	0.37	0/8351
2	B	0.13	0/6084	0.27	0/8299
2	D	0.24	0/6063	0.35	0/8268
All	All	0.22	0/24408	0.35	0/33296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6007	0	5757	119	0
1	C	5978	0	5706	121	0
2	B	5944	0	5649	105	0
2	D	5929	0	5632	117	0
3	A	112	0	104	0	0
3	B	56	0	52	0	0
3	C	98	0	91	1	0
3	D	70	0	65	1	0
4	A	4	0	2	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	2	1	0
5	B	9	0	5	1	0
5	D	9	0	5	0	0
All	All	24220	0	23070	434	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 9.

All (434) 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:441:ILE:HA	2:D:449:GLU:HA	1.32	1.10
1:A:295:LEU:HG	1:A:301:ILE:HG13	1.61	0.81
2:B:631:MET:HE1	1:C:824:ILE:HG12	1.67	0.76
1:A:218:VAL:HG12	1:A:246:VAL:HB	1.66	0.76
2:B:98:VAL:HG12	2:B:124:LEU:HB2	1.68	0.75
1:A:467:ALA:HA	1:A:472:PHE:HB2	1.69	0.75
2:D:696:ARG:HB2	2:D:702:MET:HG3	1.68	0.74
1:C:125:MET:O	1:C:139:ARG:NH2	2.21	0.73
1:A:816:VAL:HA	1:A:819:LEU:HD12	1.70	0.73
1:C:354:MET:HE3	1:C:361:LEU:HB3	1.72	0.72
1:C:685:LYS:HB3	1:C:710:ASN:HB3	1.72	0.71
2:B:430:MET:SD	2:B:431:ARG:N	2.66	0.69
2:D:528:PRO:HB3	2:D:761:GLY:HA3	1.75	0.68
2:B:465:LEU:HD22	2:B:510:VAL:HG21	1.76	0.68
1:C:305:PRO:HB3	1:C:311:ASN:HD22	1.57	0.68
1:C:437:THR:HA	1:C:452:PRO:HA	1.76	0.67
1:A:518:THR:HG1	4:A:909:GLY:N	1.93	0.66
1:C:92:VAL:HG21	1:C:104:PRO:HA	1.77	0.66
2:D:90:SER:HA	2:D:94:ILE:HG22	1.78	0.65
1:A:341:ASN:ND2	1:A:345:ASP:OD1	2.29	0.65
1:C:407:PRO:HG3	1:C:735:VAL:HA	1.78	0.65
1:A:312:THR:HG21	2:B:76:THR:HB	1.80	0.64
2:B:252:TYR:OH	2:B:393:ARG:NH2	2.31	0.64
2:D:441:ILE:HA	2:D:449:GLU:CA	2.20	0.64
2:D:502:VAL:HG13	2:D:503:MET:HE2	1.79	0.64
1:A:129:SER:OG	1:A:139:ARG:NH2	2.31	0.64
1:A:681:TYR:HB3	1:A:728:ALA:HB3	1.79	0.64
2:D:156:VAL:HG21	2:D:362:LEU:HD12	1.79	0.64
2:B:99:LEU:HD23	2:B:112:LEU:HD11	1.78	0.64
1:A:78:VAL:HG11	1:A:107:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ILE:HD13	1:C:350:ASN:HB3	1.79	0.63
1:C:94:HIS:HA	1:C:103:THR:HG21	1.81	0.63
2:B:230:LEU:HB3	2:B:258:VAL:HG12	1.81	0.63
1:C:562:LEU:HD21	2:D:818:MET:HG3	1.81	0.62
1:A:635:VAL:HG21	2:B:828:ALA:HB1	1.80	0.62
1:C:635:VAL:HG21	2:D:828:ALA:HB1	1.81	0.62
2:D:369:LYS:HE3	2:D:372:LYS:HD3	1.81	0.62
2:B:664:SER:N	2:B:668:ASP:OD2	2.33	0.61
1:C:169:ASP:HB2	1:C:199:PRO:HD3	1.81	0.61
1:C:501:MET:HE1	1:C:515:ALA:HB3	1.82	0.61
1:C:104:PRO:HG2	1:C:128:TYR:CZ	2.35	0.61
2:D:132:MET:O	2:D:145:GLN:NE2	2.33	0.61
1:A:693:PHE:CG	1:A:706:MET:HE1	2.36	0.61
1:C:91:LEU:HD13	1:C:119:LEU:HB2	1.82	0.61
1:C:505:LEU:HA	1:C:510:ALA:HB3	1.82	0.61
1:A:762:MET:HE1	1:A:769:LYS:HA	1.83	0.60
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.83	0.60
1:A:305:PRO:HD3	1:A:315:TRP:HB3	1.82	0.60
1:A:291:ALA:HB1	1:A:324:VAL:HG23	1.84	0.60
2:D:114:PHE:O	2:D:118:GLN:NE2	2.34	0.60
2:B:132:MET:O	2:B:145:GLN:NE2	2.35	0.60
1:A:634:MET:SD	2:B:610:TRP:HB3	2.42	0.59
2:D:814:ASP:H	2:D:817:ASN:HD22	1.50	0.59
2:B:695:ILE:HG22	2:B:703:HIS:HB2	1.84	0.59
1:C:167:VAL:HG21	1:C:177:GLN:HB2	1.84	0.59
2:B:644:ALA:HB3	1:C:651:LEU:HD23	1.84	0.59
2:B:608:LEU:HA	2:B:620:VAL:HG21	1.85	0.59
2:D:434:VAL:HG21	2:D:476:TYR:HE2	1.68	0.59
1:C:463:LEU:HB2	1:C:514:VAL:HG11	1.85	0.58
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.85	0.58
1:C:239:ASN:HB3	3:C:903:NAG:HN2	1.69	0.58
1:A:125:MET:O	1:A:139:ARG:NH1	2.37	0.57
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.87	0.57
1:C:556:GLN:HB3	1:C:654:PHE:HB3	1.87	0.57
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.86	0.57
1:A:315:TRP:CE3	1:A:317:THR:HG23	2.39	0.57
1:C:438:GLY:HA3	1:C:478:LEU:HD12	1.85	0.57
2:D:435:PRO:HB3	2:D:454:LYS:HE3	1.84	0.57
1:A:536:GLN:NE2	1:A:756:SER:O	2.38	0.57
1:C:486:THR:HG22	1:C:691:ILE:HD11	1.87	0.57
2:B:607:TRP:HD1	2:B:620:VAL:HG23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:HIS:HA	1:A:41:MET:HG3	1.87	0.56
2:B:76:THR:HG22	2:B:77:ASP:H	1.70	0.56
1:C:92:VAL:HG12	1:C:120:GLY:HA2	1.88	0.56
2:D:223:LEU:HD13	2:D:228:ILE:HG12	1.87	0.56
2:D:549:ALA:HB1	2:D:654:MET:HA	1.87	0.56
2:B:175:TYR:HE1	2:B:204:LEU:HG	1.71	0.56
1:C:559:GLN:OE1	1:C:562:LEU:HB2	2.06	0.56
1:C:654:PHE:HE2	2:D:812:GLN:HG2	1.70	0.56
1:C:436:CYS:O	1:C:477:HIS:HA	2.05	0.56
1:A:602:THR:HG23	1:A:605:SER:H	1.71	0.56
1:C:825:VAL:O	1:C:828:ILE:HG22	2.06	0.56
1:C:86:GLN:HG2	1:C:306:ARG:HA	1.88	0.56
1:C:533:PHE:HB2	1:C:785:MET:HE1	1.87	0.56
1:A:436:CYS:HB3	1:A:476:VAL:HG13	1.87	0.56
2:D:540:ARG:NH2	2:D:746:CYS:O	2.39	0.56
1:C:79:CYS:HA	1:C:83:ILE:HD13	1.87	0.55
2:D:384:LEU:HD13	2:D:386:MET:HE1	1.89	0.55
1:C:673:ARG:NH1	1:C:673:ARG:O	2.38	0.55
1:A:675:PRO:HG3	1:A:701:THR:HB	1.88	0.55
2:B:540:ARG:NH1	2:B:746:CYS:O	2.39	0.55
2:B:410:THR:HA	2:B:497:MET:HE3	1.88	0.55
2:D:826:GLY:HA2	2:D:829:MET:HE3	1.87	0.55
2:B:311:HIS:CE1	2:B:334:MET:HE2	2.42	0.55
1:C:499:ASN:ND2	1:C:686:GLN:OE1	2.40	0.55
2:D:807:GLU:HG2	2:D:808:VAL:H	1.72	0.55
1:C:415:MET:HG2	1:C:417:ASP:H	1.71	0.54
1:C:559:GLN:HE22	2:D:815:ILE:HG13	1.73	0.54
1:A:407:PRO:HG3	1:A:735:VAL:HA	1.89	0.54
1:A:513:ILE:HG21	1:A:517:LEU:HD22	1.89	0.54
1:A:685:LYS:HB3	1:A:710:ASN:HB3	1.89	0.54
1:A:813:MET:O	1:A:816:VAL:HG22	2.08	0.54
1:A:830:LEU:HD21	2:D:630:ILE:HD12	1.90	0.54
1:C:128:TYR:HB2	1:C:139:ARG:NH2	2.22	0.54
2:D:294:ARG:HH22	2:D:347:ARG:HH22	1.56	0.54
2:D:98:VAL:HG22	2:D:124:LEU:HD12	1.89	0.54
2:D:216:ILE:HG22	2:D:243:VAL:HG11	1.89	0.54
2:D:99:LEU:HD13	2:D:112:LEU:HD21	1.88	0.53
1:A:147:GLN:NE2	1:A:251:GLU:HG3	2.23	0.53
1:C:436:CYS:HB3	1:C:478:LEU:HG	1.90	0.53
1:C:561:THR:HB	2:D:815:ILE:HD11	1.90	0.53
2:D:537:MET:HB2	2:D:736:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:HA	1:C:252:ARG:HD3	1.90	0.53
1:C:513:ILE:HG21	1:C:517:LEU:HD22	1.90	0.53
1:C:559:GLN:NE2	2:D:815:ILE:HG13	2.24	0.53
2:D:706:MET:HE1	2:D:730:ILE:HD12	1.91	0.53
2:B:502:VAL:HG12	2:B:503:MET:HE2	1.91	0.53
1:C:511:ASP:OD1	1:C:763:ARG:NH2	2.42	0.53
1:A:470:MET:HE1	1:A:772:VAL:HG22	1.89	0.53
1:A:544:LYS:H	1:A:746:LEU:HA	1.74	0.53
1:C:543:LYS:HA	1:C:746:LEU:HD13	1.91	0.53
1:A:562:LEU:HD23	2:B:815:ILE:HD13	1.91	0.53
2:D:393:ARG:HE	2:D:396:PRO:HG2	1.73	0.53
2:D:38:ALA:HB2	2:D:89:MET:HE2	1.90	0.52
2:B:57:ASP:O	2:B:60:HIS:ND1	2.42	0.52
1:C:195:LEU:HB3	1:C:207:LEU:HD13	1.91	0.52
1:C:537:GLY:O	1:C:733:SER:N	2.37	0.52
2:D:190:ILE:HD12	2:D:197:TRP:CG	2.45	0.52
1:A:115:ARG:HG3	1:A:314:ILE:HD12	1.91	0.52
1:A:249:VAL:HB	1:A:253:GLU:HB2	1.90	0.52
1:A:543:LYS:O	1:A:663:ARG:NH2	2.43	0.52
1:C:461:ASP:OD2	1:C:792:TRP:NE1	2.41	0.52
2:B:706:MET:HE1	2:B:730:ILE:HD12	1.91	0.51
1:C:117:PRO:HG2	1:C:321:PHE:HD2	1.74	0.51
2:B:642:PHE:HD2	2:B:643:LEU:HD22	1.76	0.51
1:A:35:THR:OG1	1:A:38:HIS:HB2	2.10	0.51
1:A:46:VAL:HG21	1:A:62:ALA:HB2	1.92	0.51
2:D:687:PRO:HG2	3:D:903:NAG:H61	1.92	0.51
2:D:229:LEU:HD23	2:D:257:ILE:HB	1.93	0.51
2:D:522:VAL:HG12	2:D:523:VAL:HG13	1.93	0.51
2:B:408:ILE:HB	2:B:478:LEU:HD23	1.91	0.51
2:D:825:LEU:HG	2:D:829:MET:HE2	1.93	0.51
1:A:680:ILE:HD11	1:A:709:HIS:CG	2.46	0.51
2:D:138:ASP:HB2	2:D:141:SER:HB3	1.92	0.51
2:B:190:ILE:HD12	2:B:197:TRP:CG	2.46	0.50
2:D:530:ILE:HG22	2:D:762:TYR:HB2	1.93	0.50
1:A:558:PHE:CD2	1:A:562:LEU:HD13	2.47	0.50
1:C:93:SER:HA	1:C:121:LEU:HB2	1.93	0.50
1:A:518:THR:OG1	4:A:909:GLY:N	2.45	0.50
2:B:464:ILE:O	2:B:468:ILE:HG12	2.11	0.50
1:A:44:GLU:HA	1:A:47:ASN:ND2	2.25	0.50
1:A:573:VAL:O	1:A:577:LEU:HD23	2.10	0.50
2:B:627:THR:HG21	1:C:831:ILE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:TYR:HA	2:B:394:MET:HE1	1.93	0.50
2:D:53:ALA:HA	2:D:56:LYS:HD2	1.93	0.50
2:D:62:LEU:HB3	2:D:64:VAL:HG12	1.93	0.50
2:D:166:TRP:HB3	2:D:227:ILE:HG13	1.94	0.50
2:D:307:MET:HG2	2:D:313:PHE:O	2.11	0.50
2:B:94:ILE:HD11	2:B:97:VAL:HG22	1.94	0.49
1:C:680:ILE:HD11	1:C:709:HIS:CG	2.46	0.49
2:B:738:TYR:OH	2:B:742:ARG:NH2	2.36	0.49
1:A:152:PHE:HA	1:A:155:MET:HE2	1.94	0.49
1:C:67:HIS:HA	1:C:74:MET:HE1	1.94	0.49
1:C:681:TYR:HB3	1:C:728:ALA:HB3	1.94	0.49
2:D:175:TYR:HE1	2:D:204:LEU:HB3	1.77	0.49
1:A:33:LEU:HD11	1:A:38:HIS:HB3	1.95	0.49
1:A:357:GLN:HG3	1:A:380:ILE:HD12	1.93	0.49
1:A:699:LEU:HB3	1:A:702:MET:HB2	1.94	0.49
2:B:216:ILE:HG22	2:B:243:VAL:HG11	1.95	0.49
1:A:27:VAL:HB	1:A:60:LEU:HG	1.94	0.49
2:B:32:ALA:N	2:B:63:SER:O	2.46	0.49
2:B:156:VAL:HG21	2:B:362:LEU:HD12	1.94	0.49
2:D:190:ILE:HG23	2:D:197:TRP:HB2	1.95	0.49
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.95	0.49
1:A:331:ALA:HA	1:A:337:ARG:HA	1.94	0.49
1:A:433:LYS:HB3	1:A:456:TYR:HB3	1.94	0.49
2:B:223:LEU:HD13	2:B:228:ILE:HD13	1.93	0.49
2:B:365:ILE:HG21	2:B:373:TRP:HB3	1.95	0.49
2:B:377:GLY:HA2	2:B:386:MET:HA	1.95	0.49
1:C:533:PHE:HB3	1:C:776:ILE:HD13	1.94	0.49
1:A:415:MET:HG2	1:A:417:ASP:H	1.78	0.48
2:D:678:SER:OG	2:D:679:PRO:HD3	2.13	0.48
1:A:745:ASP:OD1	1:A:745:ASP:N	2.43	0.48
2:D:497:MET:HB3	2:D:509:ALA:HB1	1.95	0.48
2:D:666:LEU:HD11	2:D:695:ILE:HD11	1.94	0.48
2:B:532:THR:H	2:B:761:GLY:HA2	1.77	0.48
1:C:83:ILE:HA	1:C:87:VAL:HG12	1.96	0.48
1:C:354:MET:CE	1:C:361:LEU:HB3	2.43	0.48
2:D:685:THR:OG1	2:D:730:ILE:O	2.31	0.48
2:B:129:GLY:HA2	2:B:132:MET:HE1	1.96	0.48
2:D:365:ILE:HG21	2:D:373:TRP:HB3	1.96	0.48
2:B:78:PRO:O	2:B:82:ILE:HG13	2.13	0.48
1:A:542:VAL:HB	1:A:663:ARG:HH21	1.79	0.48
1:A:651:LEU:HD21	2:D:641:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:MET:HE2	1:C:513:ILE:HG23	1.96	0.48
2:B:311:HIS:HB3	2:B:313:PHE:CE2	2.47	0.48
1:C:778:LYS:O	1:C:782:ASN:ND2	2.46	0.48
2:B:101:ASP:HB2	2:B:129:GLY:H	1.78	0.48
1:A:34:SER:OG	1:A:67:HIS:HB2	2.14	0.47
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.95	0.47
2:B:186:ILE:O	2:B:190:ILE:HG12	2.13	0.47
1:C:139:ARG:HD3	1:C:141:VAL:O	2.15	0.47
1:C:197:PHE:HZ	1:C:223:ALA:HB2	1.80	0.47
1:C:30:GLY:HA3	1:C:82:LEU:HD12	1.96	0.47
2:D:468:ILE:O	2:D:472:VAL:HG22	2.15	0.47
2:D:668:ASP:OD1	2:D:669:LYS:N	2.47	0.47
1:A:744:CYS:HB3	1:A:798:CYS:HB3	1.50	0.47
2:D:315:PRO:HG3	2:D:331:GLN:HB3	1.96	0.47
1:A:326:MET:SD	1:A:344:GLY:HA2	2.54	0.47
1:A:656:VAL:HG13	1:A:658:ASP:H	1.78	0.47
1:A:664:ILE:HG22	1:A:666:GLY:H	1.79	0.47
2:B:133:ILE:HD13	2:B:145:GLN:HB2	1.96	0.47
1:C:112:GLY:O	1:C:115:ARG:NH1	2.47	0.47
2:D:682:ARG:HG2	2:D:709:PHE:HE2	1.79	0.47
2:D:467:LYS:HD3	2:D:783:LEU:HD11	1.97	0.47
2:B:190:ILE:HG23	2:B:197:TRP:HB2	1.97	0.47
1:C:638:GLY:O	1:C:642:ILE:HG12	2.15	0.47
2:B:328:ARG:HB2	2:B:331:GLN:HG2	1.96	0.46
2:B:567:LEU:HD21	2:B:610:TRP:NE1	2.29	0.46
2:D:112:LEU:HD22	2:D:123:ILE:HG21	1.97	0.46
2:D:287:TYR:CE2	2:D:292:ARG:HG2	2.50	0.46
1:A:614:LEU:HA	1:A:640:ALA:HB1	1.98	0.46
1:A:647:TYR:HE2	1:A:651:LEU:HD22	1.80	0.46
1:A:44:GLU:HA	1:A:47:ASN:HD21	1.80	0.46
1:C:814:ALA:HA	1:C:817:PHE:CD2	2.51	0.46
2:D:637:PHE:O	2:D:641:ILE:HG12	2.15	0.46
1:A:154:MET:HA	1:A:157:VAL:HG22	1.97	0.46
1:A:206:ALA:O	1:A:209:MET:HB2	2.16	0.46
2:B:467:LYS:HD3	2:B:783:LEU:HD11	1.98	0.46
2:D:409:VAL:HG21	2:D:500:GLU:HG3	1.96	0.46
2:B:712:ARG:HH11	2:B:712:ARG:HG2	1.81	0.46
2:D:97:VAL:O	2:D:123:ILE:HA	2.15	0.46
2:B:244:ALA:HB1	2:B:249:LEU:HB2	1.98	0.46
1:C:639:PHE:HD1	2:D:821:VAL:HG22	1.80	0.46
2:D:393:ARG:NE	2:D:396:PRO:HG2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:CE2	1:A:62:ALA:HB1	2.50	0.46
1:A:512:MET:HG2	1:A:514:VAL:HG23	1.97	0.46
1:A:664:ILE:HD12	1:A:672:LEU:HB2	1.98	0.46
2:B:137:LYS:HZ2	2:B:355:GLY:HA3	1.81	0.46
2:B:524:ASP:N	2:B:524:ASP:OD1	2.46	0.46
2:D:816:ASP:OD1	2:D:817:ASN:N	2.49	0.46
2:B:283:ASP:O	2:B:292:ARG:NH2	2.49	0.46
1:C:217:ARG:HA	1:C:217:ARG:HD3	1.81	0.46
1:C:559:GLN:NE2	1:C:561:THR:OG1	2.46	0.46
2:D:412:GLU:HA	2:D:417:VAL:HB	1.97	0.46
1:C:551:LEU:HD12	1:C:551:LEU:H	1.82	0.45
2:D:99:LEU:HD22	2:D:112:LEU:HD11	1.99	0.45
1:A:558:PHE:O	1:A:563:TRP:NE1	2.49	0.45
2:B:90:SER:HA	2:B:94:ILE:HG21	1.98	0.45
2:B:380:LYS:HG2	2:B:385:GLN:HE22	1.81	0.45
2:B:501:VAL:HG13	2:B:523:VAL:HG11	1.98	0.45
2:B:693:ARG:HA	2:B:693:ARG:HD2	1.78	0.45
1:C:741:SER:OG	1:C:795:TYR:O	2.25	0.45
2:B:124:LEU:HD23	2:B:144:PHE:HB2	1.98	0.45
1:C:70:ASN:OD1	1:C:73:GLN:HB2	2.16	0.45
2:D:397:GLU:HA	2:D:401:GLN:H	1.82	0.45
1:A:114:TYR:HB3	1:A:305:PRO:HG2	1.98	0.45
1:A:541:LEU:HD22	1:A:736:LEU:HD22	1.98	0.45
2:D:407:SER:O	2:D:507:TYR:N	2.49	0.45
1:A:91:LEU:HD13	1:A:121:LEU:HD11	1.98	0.45
2:B:250:THR:HG23	2:B:274:PRO:HB3	1.98	0.45
1:C:205:THR:HA	1:C:208:LEU:HB2	1.98	0.45
1:C:407:PRO:HB3	1:C:738:PHE:CD2	2.52	0.45
1:C:414:THR:OG1	1:C:419:THR:O	2.28	0.45
1:C:463:LEU:HD13	1:C:514:VAL:HG21	1.99	0.45
2:D:460:PHE:CE1	2:D:792:LEU:HB3	2.52	0.45
1:A:165:LEU:HD22	1:A:180:LEU:HD23	1.97	0.45
1:C:165:LEU:HB3	1:C:194:VAL:HG12	1.98	0.45
2:B:217:GLN:HG2	2:B:243:VAL:HG13	1.98	0.45
2:D:186:ILE:O	2:D:190:ILE:HG12	2.16	0.45
1:A:651:LEU:HD23	2:D:644:ALA:HB3	1.98	0.45
2:B:40:ILE:HB	2:B:99:LEU:HD13	1.99	0.45
1:C:37:LYS:O	1:C:40:GLN:HG2	2.17	0.45
1:C:696:GLN:HB3	1:C:699:LEU:HD23	1.99	0.45
2:D:157:MET:HE1	2:D:259:PRO:HD3	1.98	0.45
1:A:816:VAL:HG11	2:D:641:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:HD23	1:C:93:SER:HB2	1.99	0.45
2:D:814:ASP:H	2:D:817:ASN:ND2	2.15	0.45
1:A:558:PHE:HD2	1:A:562:LEU:HD13	1.82	0.44
2:B:608:LEU:HD21	2:B:632:VAL:HG21	1.99	0.44
1:C:28:ASN:ND2	1:C:85:SER:O	2.32	0.44
1:C:148:SER:HA	1:C:151:TRP:CE3	2.52	0.44
2:D:161:MET:HE1	2:D:169:PHE:CB	2.47	0.44
1:A:810:PHE:HA	2:D:558:VAL:HG21	1.98	0.44
1:C:814:ALA:HA	1:C:817:PHE:HD2	1.83	0.44
2:D:56:LYS:HG3	2:D:58:ASP:H	1.83	0.44
2:D:161:MET:HE1	2:D:169:PHE:HB3	1.99	0.44
1:A:664:ILE:HG21	1:A:672:LEU:HD22	1.99	0.44
2:B:391:TRP:CE3	2:B:392:PRO:HD2	2.53	0.44
2:B:510:VAL:HG12	2:B:764:ILE:HG12	1.98	0.44
1:C:357:GLN:N	1:C:360:LYS:O	2.49	0.44
1:A:316:LYS:O	1:A:319:PRO:HD2	2.18	0.44
1:A:648:THR:HG22	2:D:644:ALA:HB2	1.99	0.44
2:B:166:TRP:HB3	2:B:227:ILE:HG13	1.99	0.44
1:C:634:MET:SD	2:D:610:TRP:HB3	2.57	0.44
1:A:290:GLN:O	1:A:294:GLU:HG2	2.17	0.44
1:A:558:PHE:HB2	1:A:563:TRP:CE2	2.52	0.44
2:B:498:ILE:HA	2:B:501:VAL:HG12	1.99	0.44
1:C:602:THR:HG23	1:C:605:SER:H	1.81	0.44
1:C:685:LYS:HE2	1:C:712:GLU:HA	1.99	0.44
2:D:502:VAL:HG13	2:D:503:MET:CE	2.46	0.44
1:A:722:ARG:NH1	1:A:745:ASP:OD2	2.51	0.44
1:A:808:LEU:HD13	2:D:555:SER:HB3	1.99	0.44
2:B:380:LYS:HD3	2:B:380:LYS:HA	1.82	0.44
2:B:409:VAL:HG21	2:B:500:GLU:HG3	2.00	0.44
2:D:467:LYS:HG2	2:D:470:LYS:HZ2	1.83	0.44
1:A:67:HIS:HA	1:A:74:MET:HE1	2.00	0.44
1:A:86:GLN:HG2	1:A:304:PRO:HG2	2.00	0.44
2:D:449:GLU:N	2:D:450:PRO:HD3	2.32	0.44
2:D:794:ALA:HA	2:D:798:THR:HG23	2.00	0.44
1:A:124:ARG:HH21	1:A:142:PRO:HG2	1.82	0.44
1:C:394:MET:HE1	1:C:767:PRO:HG2	2.00	0.44
1:C:481:ASP:HB3	1:C:500:GLY:HA2	1.99	0.44
2:B:371:ARG:HD3	2:B:371:ARG:HA	1.80	0.43
2:B:519:ARG:NH2	5:B:905:GLU:OE1	2.48	0.43
2:D:293:VAL:O	2:D:297:ILE:HG12	2.18	0.43
2:B:555:SER:OG	2:B:557:ASP:OD1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:PRO:HD3	1:C:735:VAL:HG13	2.00	0.43
2:D:718:LEU:HD21	2:D:739:MET:HB3	2.00	0.43
1:A:789:ASP:O	1:A:794:ARG:HG2	2.19	0.43
2:B:641:ILE:HG23	1:C:651:LEU:HD21	2.00	0.43
2:B:124:LEU:HD13	2:B:299:ILE:HD11	2.01	0.43
2:B:461:CYS:HA	2:B:464:ILE:HG22	2.00	0.43
1:C:45:ALA:HB1	1:C:285:VAL:HG11	2.00	0.43
1:C:634:MET:HE2	1:C:634:MET:HB2	1.92	0.43
1:C:654:PHE:CE2	2:D:812:GLN:HG2	2.52	0.43
2:D:112:LEU:HD23	2:D:112:LEU:HA	1.91	0.43
1:A:167:VAL:HG13	1:A:196:GLN:HG3	1.99	0.43
2:B:532:THR:HG22	2:B:734:ALA:HB2	2.00	0.43
1:C:669:ASP:OD1	1:C:671:ARG:NE	2.42	0.43
2:D:299:ILE:HD12	2:D:351:PHE:HE2	1.83	0.43
1:C:657:LEU:HD23	1:C:657:LEU:H	1.83	0.43
1:A:32:VAL:HA	1:A:65:VAL:O	2.18	0.43
1:A:315:TRP:H	1:A:315:TRP:CD1	2.36	0.43
2:B:244:ALA:O	2:B:248:GLY:N	2.39	0.43
2:B:624:LYS:HE3	2:B:624:LYS:HB2	1.91	0.43
1:C:523:ARG:HH22	4:C:908:GLY:N	2.17	0.43
1:A:463:LEU:HB2	1:A:514:VAL:HG11	2.00	0.43
1:A:680:ILE:HG22	1:A:727:HIS:CE1	2.54	0.43
1:C:425:THR:HG23	1:C:427:ASN:H	1.84	0.43
1:C:541:LEU:HB2	1:C:736:LEU:HD13	2.00	0.43
2:D:66:PRO:HB3	2:D:301:THR:HG21	1.99	0.43
2:B:824:MET:HE2	2:B:824:MET:HB3	1.95	0.42
1:C:217:ARG:NH1	1:C:245:TYR:OH	2.52	0.42
1:C:770:GLN:HG2	1:C:771:ASN:N	2.34	0.42
2:D:486:HIS:O	2:D:496:GLY:HA3	2.18	0.42
1:A:274:GLY:HA2	1:A:280:HIS:HE1	1.84	0.42
2:B:642:PHE:CD2	2:B:643:LEU:HD22	2.54	0.42
2:D:408:ILE:HD13	2:D:476:TYR:HB2	2.01	0.42
2:B:497:MET:HE1	2:B:511:GLY:HA3	2.01	0.42
2:D:555:SER:H	2:D:558:VAL:HB	1.84	0.42
1:A:626:SER:O	1:A:630:ARG:HG3	2.20	0.42
1:A:434:VAL:HG11	1:A:474:TYR:HE1	1.84	0.42
2:B:226:PRO:HA	2:B:254:TYR:HD1	1.84	0.42
1:C:330:TYR:HB3	1:C:338:VAL:HB	2.00	0.42
1:C:368:ASN:OD1	1:C:369:GLY:N	2.53	0.42
2:D:404:ASP:O	2:D:475:THR:N	2.53	0.42
1:A:697:VAL:O	2:B:430:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:569:VAL:HA	2:B:572:VAL:HG22	2.01	0.42
2:B:575:PHE:HE2	2:B:601:THR:HA	1.84	0.42
1:C:79:CYS:O	1:C:308:CYS:HB2	2.20	0.42
1:C:178:LYS:O	1:C:181:GLU:HG3	2.19	0.42
1:C:490:VAL:HB	1:C:493:SER:HB3	2.02	0.42
2:D:53:ALA:O	2:D:56:LYS:HG2	2.20	0.42
1:A:73:GLN:HG3	2:B:322:TYR:CE1	2.55	0.42
1:A:786:GLU:OE2	1:A:786:GLU:N	2.53	0.42
2:B:168:ILE:HG22	2:B:225:SER:HB2	2.02	0.42
1:C:118:VAL:O	1:C:138:LEU:N	2.53	0.42
2:D:283:ASP:O	2:D:292:ARG:NH2	2.51	0.42
1:A:155:MET:HE1	1:A:184:LEU:HD21	2.02	0.41
2:B:149:SER:HB3	2:B:356:TYR:CG	2.55	0.41
1:C:407:PRO:HG2	1:C:408:PHE:HD1	1.85	0.41
1:C:563:TRP:O	1:C:566:VAL:HG22	2.19	0.41
2:D:500:GLU:OE2	2:D:505:ARG:NH1	2.52	0.41
2:D:807:GLU:HG2	2:D:808:VAL:N	2.33	0.41
1:A:197:PHE:HB3	1:A:207:LEU:HD12	2.02	0.41
2:D:41:LEU:HD12	2:D:70:LEU:HD21	2.02	0.41
1:A:696:GLN:HG3	1:A:699:LEU:HD12	2.03	0.41
1:C:407:PRO:HG2	1:C:408:PHE:CD1	2.55	0.41
2:D:609:LEU:HD22	2:D:635:TRP:CD1	2.55	0.41
1:A:138:LEU:HD11	1:A:322:LYS:HG3	2.01	0.41
1:A:320:LEU:HD13	1:A:323:ARG:HH21	1.85	0.41
2:B:160:ILE:HD11	2:B:364:ILE:HG12	2.03	0.41
2:D:112:LEU:HD22	2:D:123:ILE:HD13	2.03	0.41
2:D:607:TRP:CD1	2:D:620:VAL:HG12	2.56	0.41
2:B:161:MET:HE3	2:B:197:TRP:CZ3	2.55	0.41
2:D:124:LEU:HD11	2:D:300:ILE:HG12	2.03	0.41
2:D:472:VAL:HG23	2:D:474:PHE:HD1	1.85	0.41
1:C:567:GLY:O	1:C:570:VAL:HG12	2.20	0.41
2:D:577:PHE:HB3	2:D:627:THR:HG23	2.03	0.41
1:A:93:SER:OG	1:A:94:HIS:N	2.54	0.41
1:A:459:CYS:HB3	1:A:514:VAL:HG12	2.03	0.41
1:A:632:LEU:HA	1:A:632:LEU:HD12	1.76	0.41
2:B:545:VAL:HG11	2:B:817:ASN:HA	2.02	0.41
1:C:208:LEU:HB3	1:C:238:LEU:HD12	2.03	0.41
1:A:30:GLY:HA2	1:A:63:THR:O	2.21	0.41
1:A:326:MET:HE2	1:A:326:MET:HB2	1.91	0.41
1:A:577:LEU:HD22	1:A:632:LEU:HD23	2.03	0.41
1:C:38:HIS:HA	1:C:41:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ILE:HD13	1:C:512:MET:HB3	2.03	0.41
1:C:762:MET:HE1	1:C:769:LYS:HA	2.03	0.41
2:D:258:VAL:O	2:D:279:SER:HA	2.21	0.41
2:D:532:THR:HG22	2:D:734:ALA:HB2	2.03	0.41
2:D:613:VAL:HA	2:D:639:ALA:HB1	2.03	0.41
1:A:608:TRP:HH2	2:D:630:ILE:HG13	1.86	0.41
2:B:487:GLY:HA2	2:B:495:ASN:O	2.21	0.41
2:B:678:SER:HB3	2:B:679:PRO:HD3	2.04	0.41
1:C:217:ARG:HE	1:C:393:GLN:HG3	1.86	0.41
1:C:232:TYR:OH	1:C:249:VAL:HG11	2.21	0.41
2:D:411:LEU:N	2:D:497:MET:HE2	2.35	0.41
1:A:537:GLY:O	1:A:733:SER:N	2.49	0.40
1:A:644:VAL:O	1:A:648:THR:HG23	2.21	0.40
2:B:203:LEU:HD23	2:B:203:LEU:HA	1.90	0.40
1:C:405:GLN:HG3	1:C:407:PRO:HD2	2.03	0.40
2:B:552:GLU:HG2	2:B:653:PHE:CD1	2.57	0.40
2:B:561:MET:O	2:B:565:MET:HB3	2.21	0.40
1:C:407:PRO:HB3	1:C:738:PHE:CG	2.57	0.40
2:D:553:PRO:HG3	2:D:653:PHE:HD2	1.86	0.40
1:A:103:THR:OG1	1:A:104:PRO:HD3	2.21	0.40
1:A:635:VAL:HG21	2:B:828:ALA:CB	2.51	0.40
2:B:388:TYR:CG	2:B:392:PRO:HD3	2.56	0.40
2:B:683:PHE:HB3	2:B:728:ALA:HB3	2.03	0.40
1:A:232:TYR:OH	1:A:249:VAL:HG11	2.21	0.40
2:B:159:ASN:HB3	2:B:384:LEU:HD11	2.02	0.40
1:C:124:ARG:NH1	1:C:271:LEU:HD22	2.36	0.40
1:C:144:TYR:O	1:C:147:GLN:HB2	2.21	0.40
2:D:434:VAL:O	2:D:436:CYS:SG	2.80	0.40
1:A:55:SER:OG	1:A:56:TRP:N	2.55	0.40
1:A:603:LEU:HD12	1:A:604:SER:N	2.36	0.40
1:A:721:VAL:HA	1:A:726:LEU:O	2.22	0.40
2:B:89:MET:HB3	2:B:94:ILE:HD12	2.03	0.40
2:B:639:ALA:O	2:B:643:LEU:HD23	2.20	0.40
1:C:550:THR:O	1:C:553:SER:HB2	2.22	0.40
2:D:419:VAL:HG22	2:D:457:CYS:HB3	2.04	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 PDB entries followed by that with respect to all EM entries.

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	801/817 (98%)	775 (97%)	26 (3%)	0	100	100
1	C	801/817 (98%)	771 (96%)	30 (4%)	0	100	100
2	B	794/817 (97%)	769 (97%)	25 (3%)	0	100	100
2	D	795/817 (97%)	757 (95%)	38 (5%)	0	100	100
All	All	3191/3268 (98%)	3072 (96%)	119 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	606/705 (86%)	605 (100%)	1 (0%)	87	85
1	C	598/705 (85%)	597 (100%)	1 (0%)	87	85
2	B	600/713 (84%)	600 (100%)	0	100	100
2	D	597/713 (84%)	597 (100%)	0	100	100
All	All	2401/2836 (85%)	2399 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	THR
1	C	562	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	393	GLN
1	A	449	HIS
1	A	521	ASN
1	A	525	GLN
1	A	696	GLN
2	B	159	ASN
2	B	385	GLN
2	B	662	GLN
1	C	47	ASN
1	C	86	GLN
1	C	101	HIS
1	C	162	HIS
1	C	196	GLN
1	C	290	GLN
1	C	311	ASN
1	C	405	GLN
1	C	556	GLN
1	C	742	GLN
1	C	780	HIS
2	D	153	GLN
2	D	159	ASN
2	D	516	ASN
2	D	662	GLN
2	D	775	GLN
2	D	782	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	D	901	2	14,14,15	0.28	0	17,19,21	0.36	0
3	NAG	A	907	1	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	A	908	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	C	902	1	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	A	905	1	14,14,15	0.25	0	17,19,21	0.42	0
4	GLY	A	909	-	3,3,4	0.60	0	0,2,4	-	-
5	GLU	B	905	-	7,8,9	0.86	0	4,9,11	0.99	0
3	NAG	D	904	2	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	A	903	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	B	901	2	14,14,15	0.24	0	17,19,21	0.37	0
4	GLY	C	908	-	3,3,4	0.60	0	0,2,4	-	-
3	NAG	C	905	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	C	903	1	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	D	903	2	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	D	905	2	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	A	906	1	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	B	902	2	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	A	902	1	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	B	904	2	14,14,15	0.44	0	17,19,21	0.41	0
3	NAG	C	906	1	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	B	903	2	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	A	904	1	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	C	904	1	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	C	907	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	A	901	1	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	D	902	2	14,14,15	0.19	0	17,19,21	0.42	0
5	GLU	D	906	-	7,8,9	0.84	0	4,9,11	1.01	0
3	NAG	C	901	1	14,14,15	0.28	0	17,19,21	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	901	2	-	2/6/23/26	0/1/1/1
3	NAG	A	907	1	-	2/6/23/26	0/1/1/1
3	NAG	A	908	1	-	2/6/23/26	0/1/1/1
3	NAG	C	902	1	-	4/6/23/26	0/1/1/1
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	GLY	A	909	-	-	0/0/1/2	-
5	GLU	B	905	-	-	2/6/7/9	-
3	NAG	D	904	2	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	3/6/23/26	0/1/1/1
3	NAG	B	901	2	-	2/6/23/26	0/1/1/1
4	GLY	C	908	-	-	0/0/1/2	-
3	NAG	C	905	1	-	2/6/23/26	0/1/1/1
3	NAG	C	903	1	-	2/6/23/26	0/1/1/1
3	NAG	D	903	2	-	2/6/23/26	0/1/1/1
3	NAG	D	905	2	-	2/6/23/26	0/1/1/1
3	NAG	A	906	1	-	2/6/23/26	0/1/1/1
3	NAG	B	902	2	-	2/6/23/26	0/1/1/1
3	NAG	A	902	1	-	0/6/23/26	0/1/1/1
3	NAG	B	904	2	-	0/6/23/26	0/1/1/1
3	NAG	C	906	1	-	2/6/23/26	0/1/1/1
3	NAG	B	903	2	-	2/6/23/26	0/1/1/1
3	NAG	A	904	1	-	1/6/23/26	0/1/1/1
3	NAG	C	904	1	-	3/6/23/26	0/1/1/1
3	NAG	C	907	1	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	2/6/23/26	0/1/1/1
3	NAG	D	902	2	-	4/6/23/26	0/1/1/1
5	GLU	D	906	-	-	1/6/7/9	-
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	906	GLU	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	D	905	NAG	C4-C5-C6-O6
3	B	903	NAG	O5-C5-C6-O6
3	D	902	NAG	C4-C5-C6-O6
3	A	908	NAG	O5-C5-C6-O6
3	C	907	NAG	O5-C5-C6-O6
3	D	905	NAG	O5-C5-C6-O6
3	C	902	NAG	O5-C5-C6-O6
3	C	901	NAG	O5-C5-C6-O6
3	D	902	NAG	O5-C5-C6-O6
3	C	906	NAG	O5-C5-C6-O6
3	A	908	NAG	C4-C5-C6-O6
3	B	903	NAG	C4-C5-C6-O6
3	B	902	NAG	O5-C5-C6-O6
3	A	907	NAG	O5-C5-C6-O6
3	B	901	NAG	O5-C5-C6-O6
3	D	903	NAG	O5-C5-C6-O6
3	C	907	NAG	C4-C5-C6-O6
3	C	901	NAG	C4-C5-C6-O6
3	C	902	NAG	C4-C5-C6-O6
3	C	906	NAG	C4-C5-C6-O6
3	A	901	NAG	O5-C5-C6-O6
3	A	907	NAG	C4-C5-C6-O6
3	B	902	NAG	C4-C5-C6-O6
3	A	903	NAG	C8-C7-N2-C2
3	A	903	NAG	O7-C7-N2-C2
3	C	902	NAG	C8-C7-N2-C2
3	C	902	NAG	O7-C7-N2-C2
3	C	904	NAG	C8-C7-N2-C2
3	C	904	NAG	O7-C7-N2-C2
3	D	902	NAG	C8-C7-N2-C2
3	D	902	NAG	O7-C7-N2-C2
3	D	901	NAG	O5-C5-C6-O6
3	B	901	NAG	C4-C5-C6-O6
3	D	903	NAG	C4-C5-C6-O6
3	C	905	NAG	O5-C5-C6-O6
3	C	903	NAG	C4-C5-C6-O6
3	D	901	NAG	C4-C5-C6-O6
3	A	903	NAG	O5-C5-C6-O6
3	C	903	NAG	O5-C5-C6-O6
3	A	901	NAG	C4-C5-C6-O6
3	A	904	NAG	O5-C5-C6-O6
3	A	906	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	905	NAG	C4-C5-C6-O6
3	C	904	NAG	O5-C5-C6-O6
5	B	905	GLU	OE1-CD-CG-CB
5	B	905	GLU	OE2-CD-CG-CB
3	A	906	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	909	GLY	2	0
5	B	905	GLU	1	0
4	C	908	GLY	1	0
3	C	903	NAG	1	0
3	D	903	NAG	1	0

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.