



Full wwPDB EM Validation Report ⓘ

May 3, 2026 – 12:49 AM JST

PDB ID : 9UN2 / pdb_00009un2
EMDB ID : EMD-64337
Title : native NMDAR receptor-GluN1/N2B in the inactive state
Authors : Yu, J.; Xu, R.S.; Ge, J.P.
Deposited on : 2025-04-23
Resolution : 4.30 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

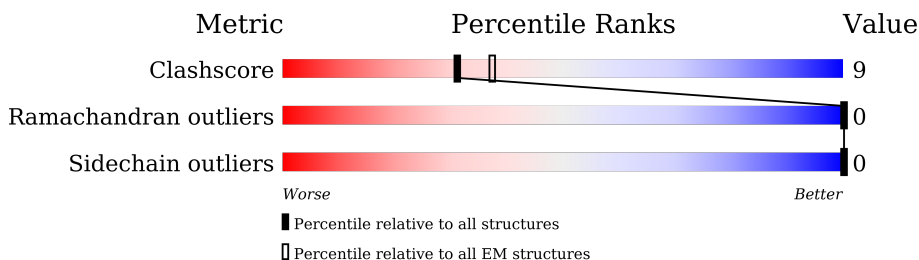
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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)	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	819	
1	C	819	
2	B	809	
2	D	809	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21861 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.

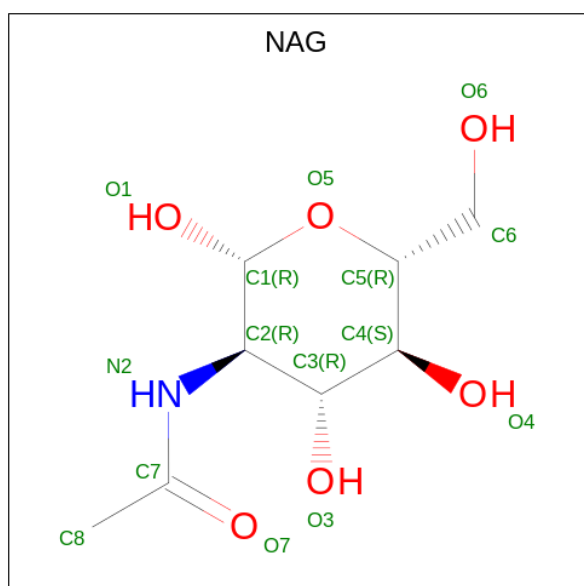
- Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			5480	3512	919	1022	27		
1	C	789	Total	C	N	O	S	0	0
			5528	3552	931	1014	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	779	Total	C	N	O	S	0	0
			5211	3352	867	959	33		
2	D	791	Total	C	N	O	S	0	0
			5404	3494	884	990	36		

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

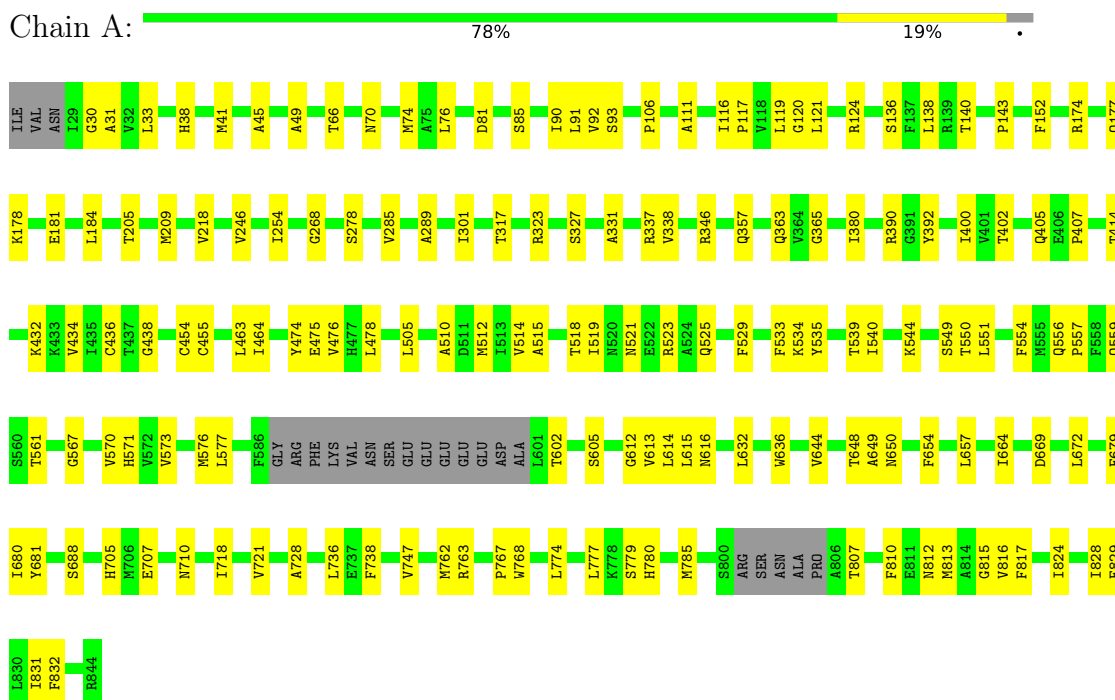


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3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

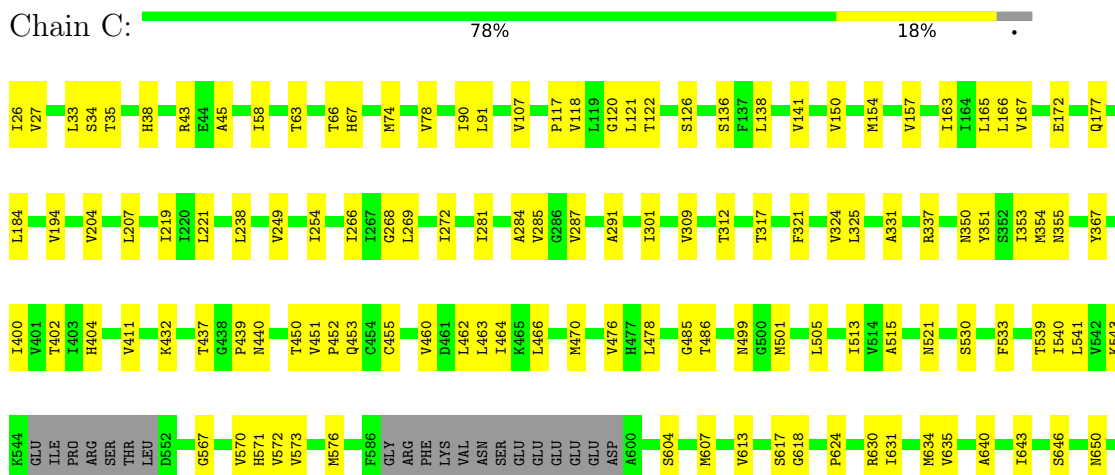
3 Residue-property plots

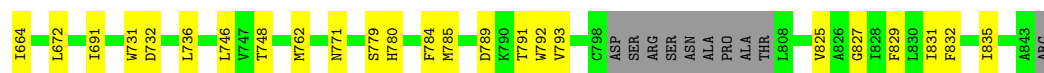
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Glutamate receptor ionotropic, NMDA 1



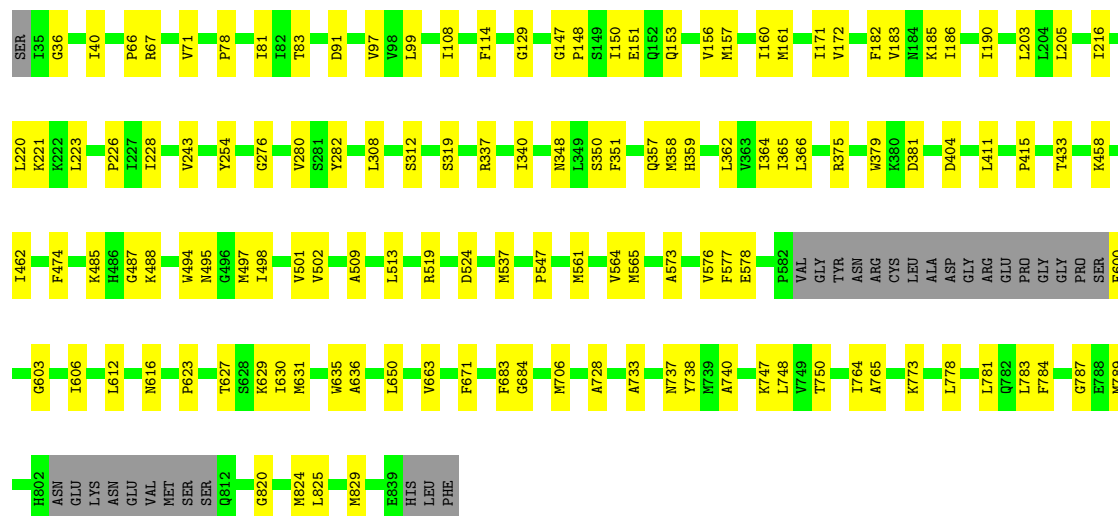
- Molecule 1: Glutamate receptor ionotropic, NMDA 1





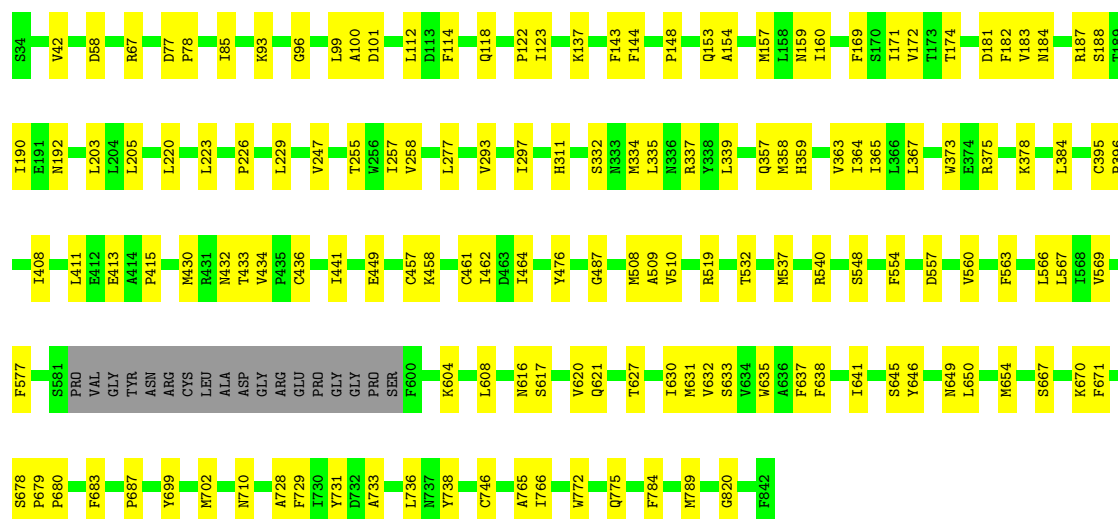
• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain B: 80% 16% .



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B

Chain D: 79% 18% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53147	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	0.09	0/5593	0.25	0/7690
1	C	0.10	0/5647	0.27	0/7746
2	B	0.10	0/5301	0.28	0/7280
2	D	0.10	0/5506	0.28	0/7553
All	All	0.10	0/22047	0.27	0/30269

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	5480	0	4908	102	0
1	C	5528	0	5044	93	0
2	B	5211	0	4600	91	0
2	D	5404	0	4837	99	0
3	A	84	0	78	1	0
3	C	112	0	104	1	0
3	D	42	0	39	0	0
All	All	21861	0	19610	364	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 (364) 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:C:791:THR:HG22	1:C:792:TRP:H	1.42	0.84
1:A:405:GLN:HG3	1:A:407:PRO:HD2	1.66	0.78
1:A:540:ILE:HD11	1:A:728:ALA:HB1	1.69	0.75
1:C:67:HIS:HA	1:C:74:MET:HE2	1.71	0.73
2:D:114:PHE:O	2:D:118:GLN:NE2	2.24	0.71
2:D:509:ALA:HB3	2:D:765:ALA:HB3	1.74	0.68
1:C:45:ALA:HB1	1:C:285:VAL:HG11	1.76	0.67
2:B:494:TRP:HB3	2:B:498:ILE:HG23	1.76	0.67
1:A:573:VAL:HA	1:A:576:MET:HE2	1.78	0.66
2:D:174:THR:HG22	2:D:205:LEU:HB2	1.78	0.66
2:B:781:LEU:HA	2:B:784:PHE:HD2	1.62	0.65
1:A:824:ILE:HA	1:A:828:ILE:HG22	1.79	0.65
2:D:537:MET:HB3	2:D:729:PHE:HB3	1.79	0.65
2:B:612:LEU:HD21	2:B:636:ALA:HA	1.78	0.65
2:D:784:PHE:HA	2:D:789:MET:HE1	1.77	0.65
1:A:117:PRO:HA	1:A:136:SER:HB2	1.79	0.64
1:C:470:MET:HE1	1:C:771:ASN:HB3	1.78	0.64
2:D:137:LYS:NZ	2:D:143:PHE:O	2.30	0.64
1:C:402:THR:HA	1:C:515:ALA:HB2	1.79	0.64
2:D:334:MET:SD	2:D:337:ARG:NH2	2.70	0.64
1:C:291:ALA:HB1	1:C:324:VAL:HG23	1.79	0.63
1:C:439:PRO:HD2	1:C:478:LEU:HB3	1.80	0.63
1:C:34:SER:OG	1:C:67:HIS:ND1	2.32	0.62
2:B:205:LEU:HD22	2:B:216:ILE:HG12	1.80	0.62
1:A:810:PHE:HA	1:A:813:MET:HB3	1.82	0.62
1:A:30:GLY:HA3	1:A:90:ILE:HG13	1.80	0.61
1:C:117:PRO:HA	1:C:136:SER:HB2	1.82	0.61
1:A:463:LEU:HB2	1:A:514:VAL:HG21	1.83	0.61
1:A:31:ALA:HA	1:A:92:VAL:HB	1.83	0.60
2:D:159:ASN:HD21	2:D:384:LEU:HD22	1.66	0.60
1:A:93:SER:H	1:A:121:LEU:HD23	1.65	0.60
2:B:172:VAL:HA	2:B:203:LEU:HB3	1.83	0.60
2:B:631:MET:HE1	1:C:825:VAL:HG22	1.83	0.60
2:B:40:ILE:HA	2:B:71:VAL:HB	1.83	0.60
1:A:140:THR:O	1:A:346:ARG:NE	2.32	0.60
1:C:309:VAL:HA	2:D:78:PRO:HB3	1.84	0.60
2:B:153:GLN:O	2:B:157:MET:HE3	2.02	0.59
2:B:684:GLY:HA2	2:B:706:MET:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:THR:HG23	2:D:77:ASP:HA	1.84	0.59
2:D:99:LEU:HD13	2:D:112:LEU:HD21	1.83	0.59
2:D:332:SER:HB2	2:D:335:LEU:HB3	1.84	0.59
2:D:220:LEU:HD23	2:D:223:LEU:HD12	1.83	0.59
1:A:567:GLY:O	1:A:571:HIS:ND1	2.34	0.58
1:A:76:LEU:HD11	2:B:83:THR:HG21	1.85	0.58
1:A:91:LEU:HB2	1:A:119:LEU:HB3	1.86	0.58
1:A:363:GLN:NE2	1:A:365:GLY:O	2.36	0.58
1:C:166:LEU:HB2	1:C:219:ILE:HD11	1.85	0.58
2:D:99:LEU:HD22	2:D:112:LEU:HD11	1.85	0.58
2:B:411:LEU:HD11	2:B:485:LYS:HA	1.84	0.58
1:C:117:PRO:HG2	1:C:321:PHE:HB3	1.85	0.58
1:C:301:ILE:HD11	1:C:317:THR:HA	1.86	0.58
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.85	0.58
1:A:817:PHE:HE1	2:D:566:LEU:HD22	1.69	0.57
1:A:436:CYS:SG	1:A:455:CYS:N	2.76	0.57
2:D:432:ASN:OD1	2:D:433:THR:N	2.37	0.57
1:C:26:ILE:HG23	1:C:27:VAL:HG23	1.86	0.57
1:C:604:SER:HA	1:C:607:MET:HE2	1.87	0.57
2:B:561:MET:HA	2:B:564:VAL:HG22	1.87	0.57
2:B:151:GLU:HA	2:B:185:LYS:HD3	1.86	0.57
2:D:67:ARG:NH2	2:D:93:LYS:O	2.38	0.57
2:B:733:ALA:O	2:B:737:ASN:ND2	2.38	0.57
1:C:437:THR:HA	1:C:452:PRO:HA	1.86	0.57
1:C:67:HIS:HA	1:C:74:MET:CE	2.36	0.56
1:A:331:ALA:HA	1:A:337:ARG:HA	1.87	0.56
2:D:461:CYS:HB2	2:D:510:VAL:HG12	1.86	0.56
1:A:829:PHE:HA	1:A:832:PHE:HD2	1.69	0.56
2:B:561:MET:O	2:B:565:MET:HG3	2.06	0.56
2:B:524:ASP:HB2	2:B:773:LYS:HE2	1.86	0.56
1:C:163:ILE:HD11	1:C:184:LEU:HD11	1.86	0.56
2:B:365:ILE:HA	2:B:375:ARG:HA	1.87	0.55
2:B:778:LEU:HD23	2:B:781:LEU:HD21	1.88	0.55
2:D:157:MET:HE2	2:D:257:ILE:HG12	1.89	0.55
1:A:218:VAL:HG12	1:A:246:VAL:HB	1.88	0.55
2:B:186:ILE:O	2:B:190:ILE:HG12	2.06	0.55
1:A:45:ALA:HB1	1:A:285:VAL:HG21	1.87	0.55
2:B:157:MET:HA	2:B:160:ILE:HD12	1.88	0.55
1:C:533:PHE:HA	1:C:780:HIS:HE1	1.71	0.55
2:B:308:LEU:HD12	2:B:312:SER:HA	1.88	0.55
2:B:433:THR:HG22	2:B:458:LYS:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:HG12	1:C:455:CYS:HB3	1.89	0.55
1:C:539:THR:HG23	1:C:736:LEU:HD12	1.89	0.55
1:C:779:SER:HB2	1:C:785:MET:HE1	1.88	0.55
1:C:613:VAL:O	2:D:616:ASN:ND2	2.40	0.55
2:B:379:TRP:NE1	2:B:381:ASP:O	2.40	0.54
2:D:277:LEU:HB3	2:D:367:LEU:HD12	1.89	0.54
1:C:404:HIS:CG	1:C:411:VAL:HG22	2.42	0.54
2:B:282:TYR:OH	2:B:357:GLN:NE2	2.40	0.54
1:C:78:VAL:HG21	1:C:107:VAL:HG22	1.90	0.54
1:C:432:LYS:HD3	1:C:792:TRP:HH2	1.72	0.54
2:B:404:ASP:HB2	2:B:474:PHE:HA	1.88	0.54
2:D:434:VAL:HG11	2:D:476:TYR:HE2	1.73	0.54
2:B:537:MET:HE1	2:B:750:THR:HA	1.88	0.54
1:C:272:ILE:HD13	1:C:350:ASN:HB3	1.88	0.53
1:C:541:LEU:HD12	1:C:748:THR:HB	1.90	0.53
1:A:518:THR:O	1:A:523:ARG:NH1	2.40	0.53
1:A:70:ASN:HA	1:A:74:MET:HE1	1.91	0.53
1:A:38:HIS:HA	1:A:41:MET:HG2	1.90	0.53
1:A:402:THR:HA	1:A:515:ALA:HB2	1.90	0.53
1:A:649:ALA:HB3	2:B:650:LEU:HD22	1.90	0.53
1:C:640:ALA:HA	1:C:643:ILE:HG12	1.91	0.53
1:C:827:GLY:O	1:C:831:ILE:HG12	2.09	0.52
2:D:408:ILE:HG13	2:D:508:MET:HB2	1.91	0.52
1:C:126:SER:N	1:C:172:GLU:OE1	2.38	0.52
1:C:167:VAL:HG21	1:C:177:GLN:HB3	1.92	0.52
1:C:331:ALA:HA	1:C:337:ARG:HA	1.92	0.52
1:A:432:LYS:HD2	1:A:464:ILE:HG21	1.91	0.52
2:D:645:SER:O	2:D:649:ASN:ND2	2.42	0.52
2:B:182:PHE:HA	2:B:185:LYS:HE3	1.92	0.52
2:B:276:GLY:HA2	2:B:366:LEU:HD21	1.92	0.51
2:D:441:ILE:HA	2:D:449:GLU:HA	1.91	0.51
1:A:505:LEU:O	1:A:763:ARG:NH1	2.44	0.51
1:A:549:SER:O	1:A:812:ASN:ND2	2.44	0.51
2:B:226:PRO:HA	2:B:254:TYR:HD1	1.75	0.51
2:B:498:ILE:O	2:B:502:VAL:HG23	2.11	0.51
1:C:567:GLY:O	1:C:571:HIS:ND1	2.38	0.51
1:C:541:LEU:HD21	1:C:746:LEU:HD12	1.93	0.51
1:A:534:LYS:NZ	1:A:535:TYR:O	2.43	0.51
1:C:90:ILE:HB	1:C:118:VAL:HG22	1.91	0.51
1:C:238:LEU:HA	3:C:903:NAG:H82	1.93	0.51
2:B:36:GLY:HA3	2:B:66:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:NH1	1:A:327:SER:HB3	2.26	0.50
2:B:547:PRO:HB3	2:B:820:GLY:H	1.76	0.50
2:D:699:TYR:HB2	2:D:702:MET:SD	2.51	0.50
1:C:439:PRO:HA	1:C:450:THR:HA	1.93	0.50
2:D:160:ILE:HD11	2:D:364:ILE:HG21	1.92	0.50
1:C:120:GLY:N	1:C:138:LEU:O	2.33	0.50
1:C:505:LEU:HD13	1:C:513:ILE:HG13	1.93	0.50
1:A:301:ILE:HA	1:A:317:THR:HG21	1.94	0.50
1:C:541:LEU:HB2	1:C:736:LEU:HD13	1.92	0.50
2:D:646:TYR:HA	2:D:649:ASN:HD21	1.75	0.50
1:A:602:THR:HG23	1:A:605:SER:H	1.75	0.50
2:B:280:VAL:HG12	2:B:364:ILE:HG12	1.94	0.50
1:A:205:THR:HG22	1:A:209:MET:HE3	1.93	0.50
1:A:523:ARG:HH12	1:A:688:SER:HB3	1.76	0.50
1:A:533:PHE:O	1:A:780:HIS:NE2	2.43	0.50
2:B:337:ARG:HA	2:B:340:ILE:HG12	1.92	0.50
2:B:683:PHE:HB3	2:B:728:ALA:HB3	1.94	0.50
1:C:779:SER:HB3	1:C:784:PHE:HB3	1.92	0.50
1:A:613:VAL:O	2:B:616:ASN:ND2	2.43	0.49
2:D:226:PRO:O	2:D:255:THR:OG1	2.27	0.49
1:A:519:ILE:HG23	1:A:529:PHE:HD2	1.76	0.49
1:A:551:LEU:HB3	1:A:815:GLY:HA3	1.94	0.49
1:C:618:GLY:N	2:D:617:SER:OG	2.44	0.49
2:D:258:VAL:HB	2:D:277:LEU:HD11	1.93	0.49
1:A:707:GLU:HA	1:A:710:ASN:ND2	2.28	0.49
1:C:269:LEU:HG	1:C:353:ILE:HA	1.94	0.49
1:C:351:TYR:HB2	1:C:367:TYR:HB3	1.94	0.49
1:C:91:LEU:HB3	1:C:121:LEU:HD11	1.94	0.49
2:D:537:MET:N	2:D:729:PHE:O	2.34	0.49
2:B:820:GLY:O	2:B:824:MET:HG2	2.12	0.49
1:A:407:PRO:HB3	1:A:738:PHE:CG	2.47	0.49
1:C:400:ILE:HB	1:C:476:VAL:HA	1.94	0.49
2:B:350:SER:HB3	2:B:358:MET:HE1	1.95	0.49
2:B:509:ALA:HB3	2:B:765:ALA:HB3	1.95	0.48
2:D:563:PHE:HA	2:D:567:LEU:HG	1.95	0.48
2:B:221:LYS:HG2	2:D:247:VAL:O	2.14	0.48
1:C:440:ASN:HB2	1:C:451:VAL:HB	1.96	0.48
1:C:486:THR:HG22	1:C:691:ILE:HD11	1.94	0.48
2:D:566:LEU:HA	2:D:569:VAL:HG12	1.95	0.48
2:B:156:VAL:HG22	2:B:379:TRP:CD2	2.49	0.48
2:B:223:LEU:HD21	2:B:228:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:829:PHE:HA	1:C:832:PHE:HD2	1.78	0.48
1:A:414:THR:HG22	1:A:454:CYS:HB2	1.95	0.48
1:A:779:SER:HB2	1:A:785:MET:HE3	1.95	0.48
2:D:183:VAL:O	2:D:187:ARG:HG2	2.13	0.48
2:B:359:HIS:HB3	2:B:381:ASP:HA	1.95	0.48
1:C:540:ILE:O	1:C:748:THR:OG1	2.25	0.48
1:C:791:THR:HG22	1:C:792:TRP:N	2.20	0.48
1:C:572:VAL:O	1:C:576:MET:HG3	2.14	0.48
1:C:664:ILE:HG21	1:C:672:LEU:HG	1.96	0.48
2:D:683:PHE:CZ	2:D:702:MET:HB2	2.49	0.48
2:B:97:VAL:HG13	2:B:99:LEU:HD23	1.96	0.48
2:B:340:ILE:O	2:B:350:SER:OG	2.28	0.48
1:A:824:ILE:HD11	2:D:631:MET:HG2	1.94	0.48
2:D:608:LEU:HB3	2:D:620:VAL:HG21	1.96	0.48
1:A:550:THR:O	1:A:812:ASN:ND2	2.47	0.47
2:B:524:ASP:N	2:B:524:ASP:OD1	2.46	0.47
1:A:400:ILE:HB	1:A:476:VAL:HA	1.96	0.47
2:B:150:ILE:HG23	2:B:185:LYS:NZ	2.28	0.47
2:D:311:HIS:NE2	2:D:334:MET:HE3	2.29	0.47
1:A:832:PHE:HD1	2:D:627:THR:HB	1.80	0.47
2:B:91:ASP:HA	2:B:319:SER:HA	1.95	0.47
2:B:781:LEU:HD13	1:C:521:ASN:HA	1.97	0.47
2:D:683:PHE:HZ	2:D:702:MET:HB2	1.80	0.47
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.97	0.47
2:D:181:ASP:HA	2:D:184:ASN:ND2	2.29	0.47
1:A:828:ILE:HG23	1:A:832:PHE:CE2	2.49	0.47
2:D:42:VAL:N	2:D:100:ALA:O	2.44	0.47
2:D:687:PRO:HB3	2:D:710:ASN:HD22	1.79	0.47
1:A:438:GLY:HA3	1:A:478:LEU:HD12	1.96	0.47
1:A:539:THR:HG23	1:A:736:LEU:HD12	1.96	0.47
2:B:488:LYS:N	2:B:495:ASN:OD1	2.43	0.47
2:B:537:MET:HE2	2:B:537:MET:HA	1.97	0.47
2:B:578:GLU:HB3	2:B:600:PHE:CE2	2.50	0.47
1:C:354:MET:HE3	1:C:355:ASN:N	2.30	0.47
1:C:789:ASP:HA	1:C:793:VAL:HB	1.97	0.47
1:A:559:GLN:HG2	1:A:561:THR:H	1.79	0.47
1:A:664:ILE:HD11	1:A:679:PHE:HZ	1.79	0.47
1:A:832:PHE:CD1	2:D:627:THR:HB	2.49	0.47
2:D:604:LYS:HB3	2:D:621:GLN:HE22	1.79	0.47
1:A:92:VAL:HA	1:A:121:LEU:HD21	1.96	0.47
1:A:120:GLY:N	1:A:138:LEU:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ILE:HB	2:B:129:GLY:HA3	1.97	0.47
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.97	0.47
2:D:365:ILE:HA	2:D:375:ARG:HA	1.96	0.47
1:A:556:GLN:HG3	1:A:557:PRO:HD3	1.96	0.46
2:B:498:ILE:HG12	2:B:519:ARG:HG2	1.97	0.46
1:C:150:VAL:HG21	1:C:269:LEU:HD22	1.97	0.46
2:D:537:MET:O	2:D:729:PHE:N	2.44	0.46
1:A:178:LYS:O	1:A:181:GLU:HG3	2.16	0.46
1:A:323:ARG:HH12	1:A:327:SER:HB3	1.79	0.46
2:B:487:GLY:HA3	2:B:498:ILE:HG22	1.97	0.46
1:C:249:VAL:HG21	1:C:266:ILE:HD12	1.98	0.46
1:A:521:ASN:OD1	1:A:525:GLN:NE2	2.49	0.46
1:A:577:LEU:HG	1:A:632:LEU:HD22	1.98	0.46
2:D:458:LYS:C	2:D:462:ILE:HD13	2.40	0.46
2:D:537:MET:HB2	2:D:736:LEU:HD13	1.98	0.46
1:A:106:PRO:HG3	2:B:114:PHE:CZ	2.51	0.46
2:D:144:PHE:HE2	2:D:339:LEU:HD13	1.81	0.46
2:D:411:LEU:HG	2:D:413:GLU:H	1.81	0.46
1:A:570:VAL:HG21	1:A:614:LEU:HD11	1.97	0.46
1:C:501:MET:HB3	1:C:513:ILE:HD13	1.98	0.46
1:A:338:VAL:HG22	1:A:346:ARG:HH12	1.81	0.45
2:D:461:CYS:HA	2:D:464:ILE:HG12	1.98	0.45
2:B:157:MET:O	2:B:161:MET:HG2	2.16	0.45
1:A:81:ASP:O	1:A:85:SER:OG	2.28	0.45
2:B:78:PRO:HD2	2:B:81:ILE:HB	1.98	0.45
2:B:497:MET:HE2	2:B:513:LEU:HD11	1.98	0.45
1:A:174:ARG:O	1:A:177:GLN:HG3	2.16	0.45
1:C:631:ILE:O	1:C:634:MET:HG3	2.17	0.45
2:D:357:GLN:HG2	2:D:359:HIS:H	1.80	0.45
1:A:615:LEU:HD22	2:D:637:PHE:HB2	1.98	0.45
1:A:615:LEU:HD13	2:D:633:SER:O	2.17	0.45
2:D:430:MET:HB2	2:D:433:THR:HG22	1.98	0.45
2:B:220:LEU:HD12	2:B:243:VAL:HG12	1.99	0.45
2:B:458:LYS:C	2:B:462:ILE:HD13	2.42	0.45
2:B:627:THR:HB	1:C:835:ILE:HD12	1.98	0.45
1:C:731:TRP:CG	1:C:732:ASP:H	2.34	0.45
1:A:91:LEU:HD12	1:A:92:VAL:HG23	1.99	0.45
1:A:612:GLY:O	1:A:616:ASN:N	2.50	0.45
1:C:91:LEU:HD11	1:C:284:ALA:HB1	1.98	0.45
1:A:390:ARG:NE	1:A:392:TYR:O	2.50	0.45
2:B:498:ILE:HA	2:B:501:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:ALA:O	2:B:764:ILE:HG13	2.17	0.45
1:C:165:LEU:HB3	1:C:194:VAL:HA	1.99	0.45
2:D:42:VAL:HB	2:D:101:ASP:HA	1.99	0.45
2:D:58:ASP:N	2:D:58:ASP:OD1	2.50	0.45
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.99	0.44
2:D:671:PHE:HZ	2:D:678:SER:H	1.65	0.44
1:C:26:ILE:HD12	1:C:58:ILE:HG12	1.99	0.44
2:B:623:PRO:O	2:B:629:LYS:NZ	2.49	0.44
1:C:35:THR:OG1	1:C:38:HIS:HB2	2.17	0.44
1:C:43:ARG:HD3	1:C:63:THR:HG21	1.99	0.44
2:D:154:ALA:HB2	2:D:182:PHE:HE1	1.82	0.44
2:D:171:ILE:HD13	2:D:229:LEU:HD12	2.00	0.44
1:A:681:TYR:HB3	1:A:728:ALA:HB3	1.99	0.44
1:A:774:LEU:HD23	1:A:777:LEU:HD21	1.99	0.44
1:A:718:ILE:HA	1:A:721:VAL:HG22	1.99	0.44
2:B:348:ASN:HB3	2:B:359:HIS:HD2	1.82	0.44
1:C:204:VAL:HG12	1:C:207:LEU:HB2	2.00	0.44
1:A:66:THR:OG1	1:A:74:MET:SD	2.75	0.44
2:D:188:SER:O	2:D:192:ASN:ND2	2.51	0.44
2:D:415:PRO:HG3	2:D:738:TYR:CD2	2.53	0.44
1:A:828:ILE:HG23	1:A:832:PHE:HE2	1.83	0.44
1:A:832:PHE:HE1	2:D:630:ILE:HG13	1.83	0.44
2:D:687:PRO:HD3	2:D:710:ASN:HB2	1.99	0.44
1:A:767:PRO:HB2	1:A:768:TRP:CD1	2.53	0.43
2:D:683:PHE:HB3	2:D:728:ALA:HB3	2.00	0.43
1:A:828:ILE:HD12	1:A:831:ILE:HG13	2.00	0.43
2:D:577:PHE:HE2	2:D:631:MET:HG3	1.84	0.43
2:B:147:GLY:N	2:B:148:PRO:CD	2.81	0.43
2:D:358:MET:SD	2:D:358:MET:N	2.79	0.43
2:D:772:TRP:HA	2:D:775:GLN:NE2	2.33	0.43
1:A:554:PHE:HB2	1:A:813:MET:HE1	1.99	0.43
1:A:644:VAL:O	1:A:648:THR:HG23	2.19	0.43
2:B:358:MET:HG2	2:B:359:HIS:CD2	2.53	0.43
2:B:740:ALA:HA	2:B:748:LEU:HB2	2.01	0.43
2:D:632:VAL:HA	2:D:635:TRP:HB3	2.00	0.43
1:A:807:THR:HA	2:D:554:PHE:H	1.84	0.43
2:D:650:LEU:O	2:D:654:MET:HG2	2.18	0.43
2:D:679:PRO:N	2:D:680:PRO:HD2	2.33	0.43
1:A:124:ARG:HA	1:A:143:PRO:HA	2.00	0.43
2:B:783:LEU:O	2:B:787:GLY:N	2.50	0.43
2:D:557:ASP:HA	2:D:560:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HB1	1:A:289:ALA:HB2	2.00	0.43
1:C:432:LYS:NZ	1:C:464:ILE:HD12	2.34	0.43
1:C:624:PRO:HG2	1:C:630:ARG:HA	1.99	0.43
2:B:308:LEU:HA	2:B:312:SER:HA	2.00	0.43
2:D:112:LEU:HD22	2:D:123:ILE:HG21	2.00	0.43
2:D:766:ILE:HG23	2:D:766:ILE:O	2.19	0.43
1:A:278:SER:HB2	3:A:903:NAG:H62	2.01	0.42
2:D:365:ILE:HG21	2:D:373:TRP:HB3	2.00	0.42
2:D:548:SER:HA	2:D:820:GLY:HA3	2.01	0.42
2:B:415:PRO:HB3	2:B:738:TYR:CD2	2.54	0.42
1:C:33:LEU:HD21	1:C:281:ILE:HD11	2.01	0.42
1:C:268:GLY:O	1:C:354:MET:N	2.40	0.42
1:C:268:GLY:C	1:C:269:LEU:HD12	2.44	0.42
2:B:171:ILE:HG21	2:B:183:VAL:HG12	2.00	0.42
2:B:182:PHE:O	2:B:185:LYS:HG2	2.19	0.42
1:C:570:VAL:HA	1:C:573:VAL:HG22	2.01	0.42
2:D:395:CYS:HA	2:D:396:PRO:HD3	1.89	0.42
1:A:205:THR:O	1:A:209:MET:HG2	2.19	0.42
2:B:216:ILE:HG22	2:B:243:VAL:HG11	2.01	0.42
2:B:627:THR:HA	2:B:630:ILE:HG12	2.00	0.42
1:C:460:VAL:O	1:C:463:LEU:HG	2.19	0.42
2:D:148:PRO:HG2	2:D:153:GLN:HE21	1.84	0.42
1:A:650:ASN:C	1:A:650:ASN:HD22	2.27	0.42
1:C:631:ILE:O	1:C:635:VAL:HG23	2.19	0.42
2:D:363:VAL:HA	2:D:378:LYS:HA	2.01	0.42
2:D:413:GLU:OE2	2:D:731:TYR:OH	2.35	0.42
1:A:510:ALA:O	1:A:763:ARG:NH2	2.53	0.42
1:A:680:ILE:HD12	1:A:705:HIS:NE2	2.35	0.42
2:B:351:PHE:HA	2:B:357:GLN:HA	2.00	0.42
1:A:400:ILE:N	1:A:475:GLU:O	2.47	0.42
2:B:783:LEU:C	2:B:789:MET:HE1	2.45	0.42
2:D:96:GLY:HA2	2:D:122:PRO:HG2	2.02	0.42
1:A:357:GLN:HG2	1:A:380:ILE:HB	2.01	0.42
2:B:223:LEU:HD11	2:B:228:ILE:HD12	2.01	0.42
1:C:122:THR:HA	1:C:141:VAL:HG11	2.02	0.42
2:D:487:GLY:O	2:D:519:ARG:NH2	2.53	0.42
2:D:638:PHE:HA	2:D:641:ILE:HG22	2.02	0.42
1:A:254:ILE:HD12	1:A:268:GLY:HA3	2.01	0.42
1:C:530:SER:HB3	1:C:762:MET:HE1	2.01	0.42
2:D:169:PHE:HZ	2:D:190:ILE:HG13	1.85	0.42
2:D:172:VAL:HG22	2:D:203:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ALA:HB1	2:B:577:PHE:CE1	2.55	0.41
1:C:617:SER:N	2:D:617:SER:OG	2.52	0.41
2:D:181:ASP:HA	2:D:184:ASN:HD21	1.83	0.41
1:A:654:PHE:HA	1:A:657:LEU:HG	2.03	0.41
1:A:669:ASP:HB3	1:A:672:LEU:HB2	2.02	0.41
2:B:203:LEU:HG	2:B:205:LEU:HG	2.02	0.41
1:C:437:THR:HA	1:C:453:GLN:H	1.84	0.41
2:D:293:VAL:O	2:D:297:ILE:HG12	2.20	0.41
1:A:33:LEU:HD21	1:A:38:HIS:HB2	2.03	0.41
2:B:663:VAL:HG22	2:B:671:PHE:HE1	1.85	0.41
1:C:462:LEU:O	1:C:466:LEU:HD23	2.20	0.41
1:C:485:GLY:HA2	1:C:499:ASN:O	2.21	0.41
2:B:603:GLY:HA2	2:B:606:ILE:HG12	2.02	0.41
1:C:154:MET:HA	1:C:157:VAL:HG22	2.03	0.41
2:B:36:GLY:HA2	2:B:67:ARG:HD3	2.03	0.41
2:B:612:LEU:HD22	2:B:635:TRP:CE3	2.56	0.41
2:B:747:LYS:HB2	2:B:747:LYS:HE2	1.83	0.41
1:C:138:LEU:HG	1:C:325:LEU:HD23	2.00	0.41
1:C:646:SER:O	1:C:650:ASN:ND2	2.54	0.41
1:C:287:VAL:HG13	1:C:325:LEU:HD11	2.02	0.41
1:A:813:MET:HE3	1:A:816:VAL:HG23	2.03	0.41
2:D:667:SER:HB2	2:D:670:LYS:HB2	2.02	0.41
1:A:512:MET:HE1	1:A:762:MET:SD	2.60	0.41
2:B:573:ALA:HA	2:B:576:VAL:HG12	2.03	0.41
1:C:34:SER:HA	1:C:66:THR:HA	2.03	0.41
1:C:543:LYS:HA	1:C:746:LEU:HD13	2.03	0.41
1:A:152:PHE:HE1	1:A:184:LEU:HD23	1.86	0.40
1:A:570:VAL:HG11	1:A:614:LEU:HD11	2.04	0.40
2:B:825:LEU:O	2:B:829:MET:HG2	2.21	0.40
1:C:254:ILE:HD11	1:C:268:GLY:HA3	2.03	0.40
1:A:434:VAL:HG11	1:A:474:TYR:HE2	1.86	0.40
1:A:614:LEU:HD21	1:A:636:TRP:HZ2	1.87	0.40
2:D:408:ILE:HG13	2:D:508:MET:CB	2.51	0.40
2:D:508:MET:HE3	2:D:509:ALA:H	1.87	0.40
2:D:532:THR:O	2:D:733:ALA:HB3	2.21	0.40
2:D:540:ARG:NH1	2:D:746:CYS:O	2.55	0.40
1:A:544:LYS:HA	1:A:747:VAL:HG12	2.04	0.40
2:D:85:ILE:HD13	2:D:85:ILE:HA	1.94	0.40
2:D:436:CYS:SG	2:D:457:CYS:N	2.94	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	791/819 (97%)	769 (97%)	22 (3%)	0	100	100
1	C	781/819 (95%)	758 (97%)	23 (3%)	0	100	100
2	B	773/809 (96%)	747 (97%)	26 (3%)	0	100	100
2	D	787/809 (97%)	758 (96%)	29 (4%)	0	100	100
All	All	3132/3256 (96%)	3032 (97%)	100 (3%)	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	494/706 (70%)	494 (100%)	0	100	100
1	C	515/706 (73%)	515 (100%)	0	100	100
2	B	441/706 (62%)	441 (100%)	0	100	100
2	D	477/706 (68%)	477 (100%)	0	100	100
All	All	1927/2824 (68%)	1927 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	47	ASN
1	A	453	GLN
1	A	742	GLN
2	B	145	GLN
2	B	159	ASN
2	B	224	GLN
2	B	348	ASN
2	B	359	HIS
2	B	432	ASN
2	B	615	ASN
2	B	662	GLN
2	B	775	GLN
1	C	38	HIS
1	C	101	HIS
1	C	257	ASN
1	C	363	GLN
1	C	521	ASN
1	C	556	GLN
1	C	705	HIS
1	C	780	HIS
2	D	118	GLN
2	D	159	ASN
2	D	192	ASN
2	D	615	ASN
2	D	649	ASN
2	D	672	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

17 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	A	906	1	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	A	901	1	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	C	901	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	903	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	C	908	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	902	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	902	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	A	905	1	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	C	904	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	D	903	2	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	D	901	2	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	906	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	C	907	1	14,14,15	0.27	0	17,19,21	0.37	0
3	NAG	D	902	2	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	C	903	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	904	1	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	C	905	1	14,14,15	0.23	0	17,19,21	0.42	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	A	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	901	1	-	2/6/23/26	0/1/1/1
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1
3	NAG	A	903	1	-	2/6/23/26	0/1/1/1
3	NAG	C	908	1	-	2/6/23/26	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	NAG	C	904	1	-	4/6/23/26	0/1/1/1
3	NAG	D	903	2	-	2/6/23/26	0/1/1/1
3	NAG	D	901	2	-	2/6/23/26	0/1/1/1
3	NAG	C	906	1	-	2/6/23/26	0/1/1/1
3	NAG	C	907	1	-	0/6/23/26	0/1/1/1
3	NAG	D	902	2	-	3/6/23/26	0/1/1/1
3	NAG	C	903	1	-	2/6/23/26	0/1/1/1
3	NAG	A	904	1	-	2/6/23/26	0/1/1/1
3	NAG	C	905	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 (33) torsion outliers are listed below:

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

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	NAG	1	0
3	C	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.