



Full wwPDB EM Validation Report ⓘ

May 3, 2026 – 12:38 AM JST

PDB ID : 9UNO / pdb_00009uno
EMDB ID : EMD-64358
Title : native NMDA receptor-GluN1/N2A in the inactive state
Authors : Yu, J.; Xu, R.S.; Ge, J.P.
Deposited on : 2025-04-24
Resolution : 3.55 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

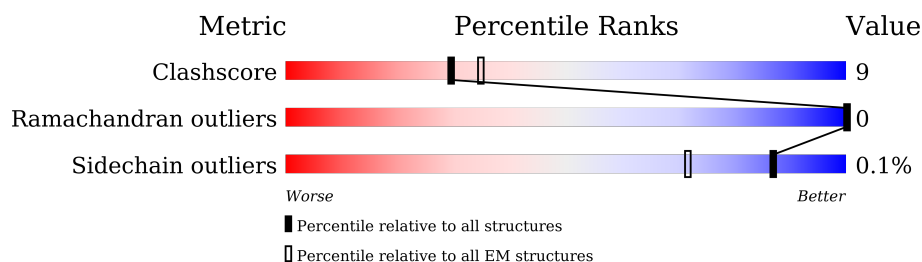
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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	813	
1	C	813	
2	B	809	
2	D	809	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22941 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.

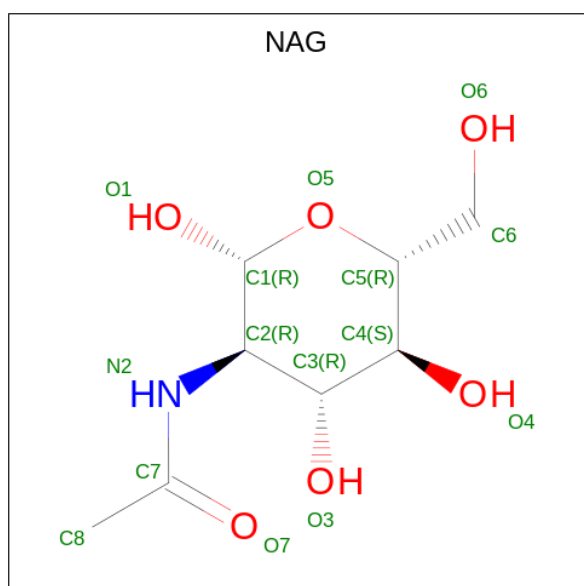
- Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	786	Total	C	N	O	S	0	0
			5722	3670	980	1042	30		
1	C	786	Total	C	N	O	S	0	0
			5658	3627	976	1027	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	789	Total	C	N	O	S	0	0
			5586	3615	916	1021	34		
2	D	779	Total	C	N	O	S	0	0
			5627	3651	934	1010	32		

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



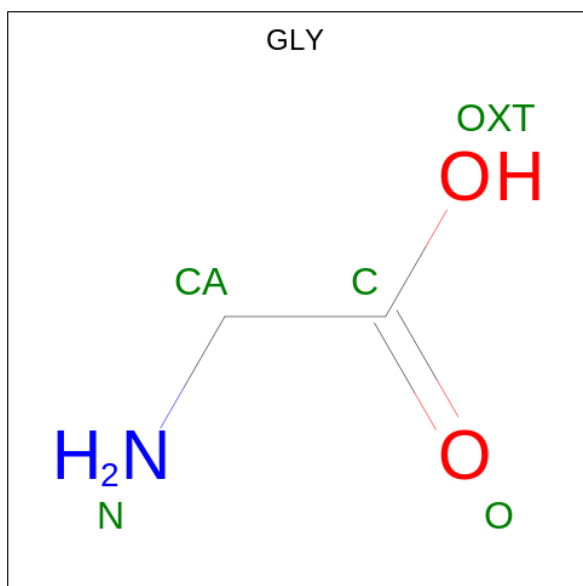
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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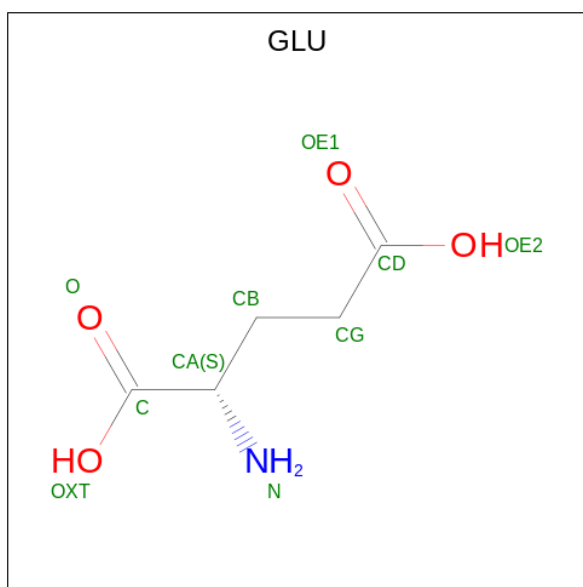
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			14	8	1	5	

- 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: $C_5H_9NO_4$).

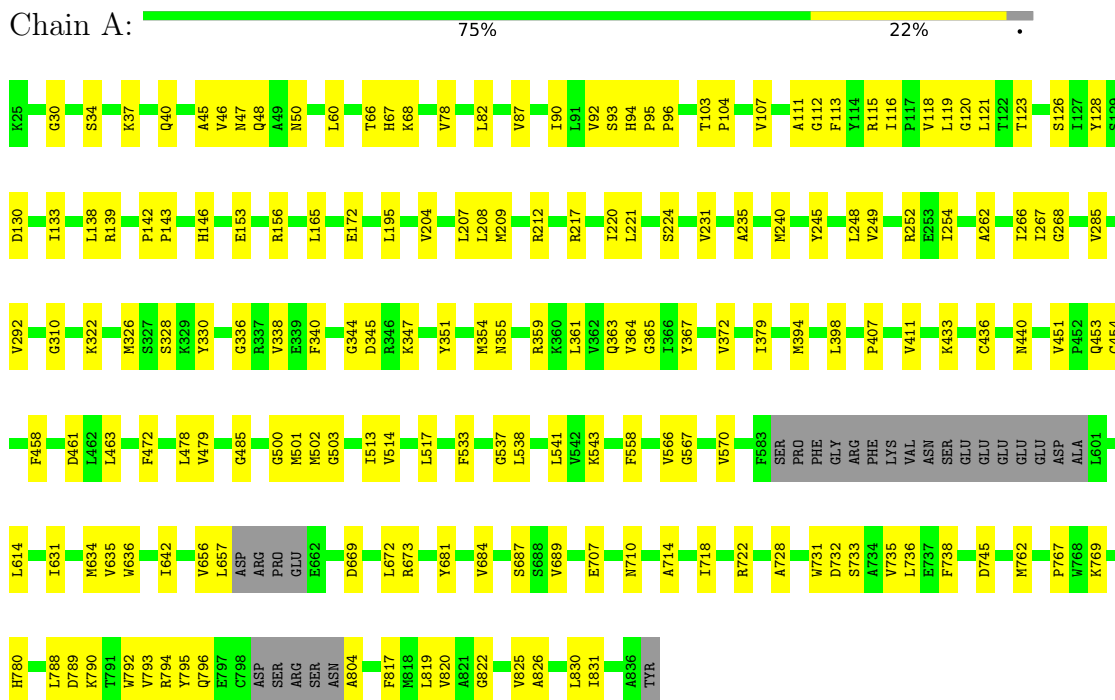


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			9	5	1	3	
5	D	1	Total	C	N	O	0
			9	5	1	3	

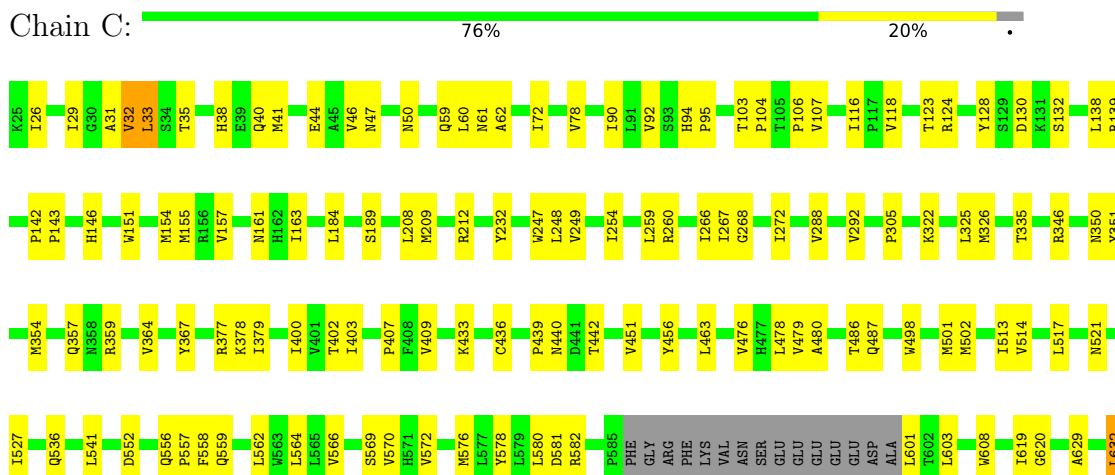
3 Residue-property plots

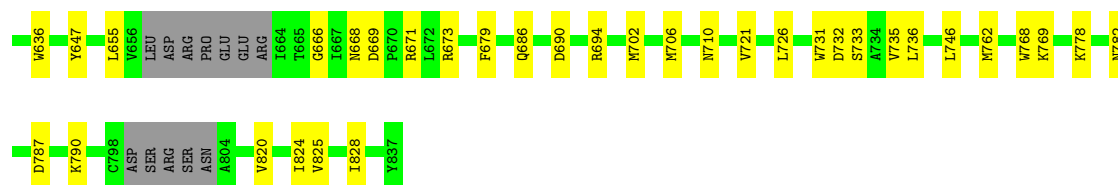
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



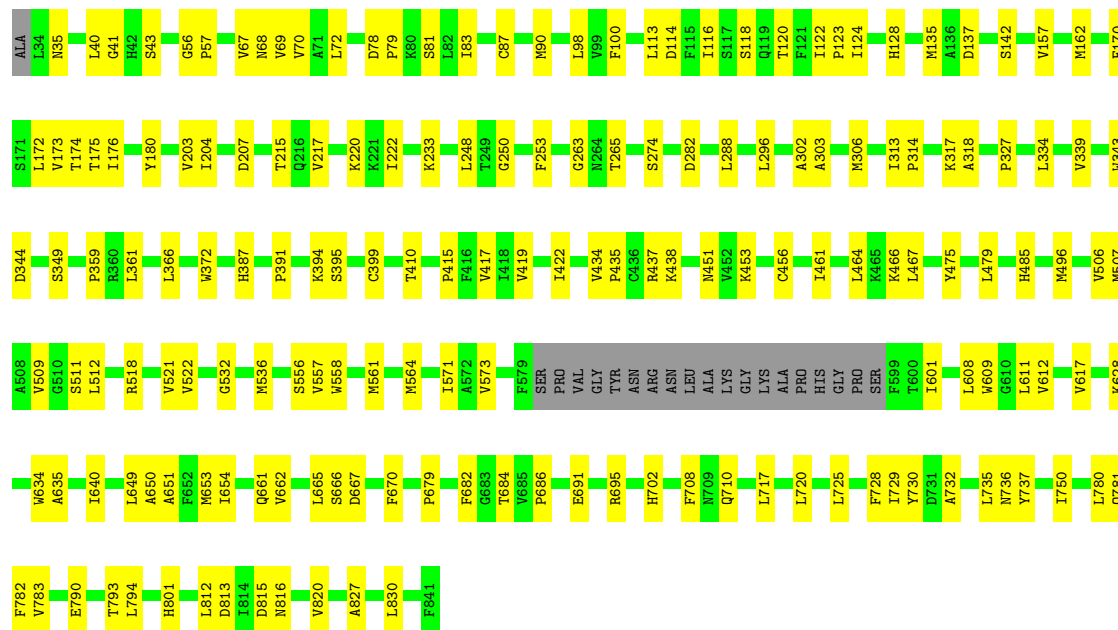
- Molecule 1: Glutamate receptor ionotropic, NMDA 1





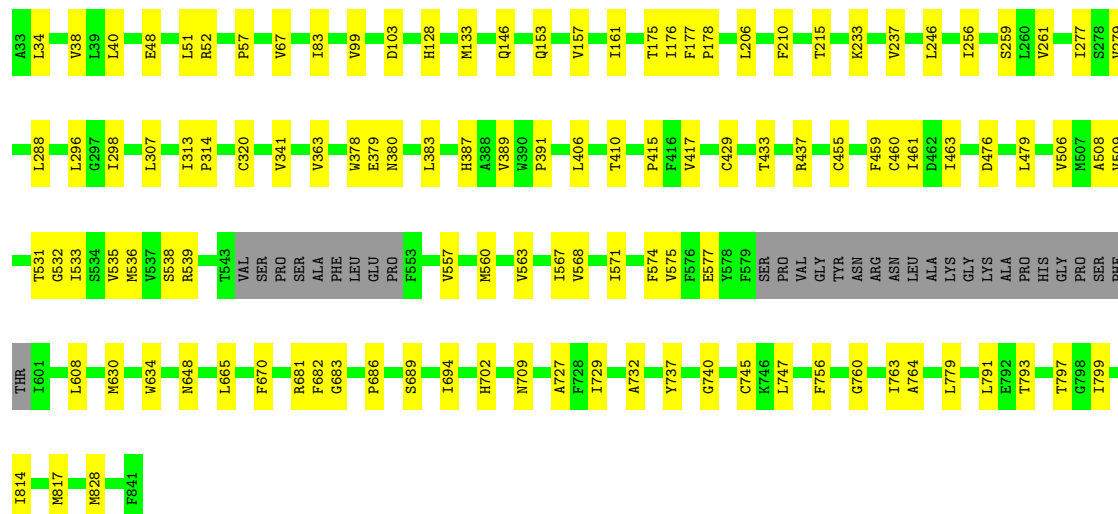
- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B: 76% 21% .



- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain D: 82% 14% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	0.12	0/5848	0.29	0/7999
1	C	0.23	0/5785	0.37	0/7923
2	B	0.11	0/5711	0.28	0/7841
2	D	0.11	0/5756	0.26	0/7887
All	All	0.15	0/23100	0.30	0/31650

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	5722	0	5386	116	0
1	C	5658	0	5254	115	0
2	B	5586	0	5117	119	0
2	D	5627	0	5226	78	0
3	A	112	0	104	0	0
3	B	42	0	39	1	0
3	C	112	0	104	1	0
3	D	56	0	52	1	0
4	A	4	0	2	0	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	2	0
5	D	9	0	5	1	0
All	All	22941	0	21296	405	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 (405) 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:A:195:LEU:HB3	1:A:207:LEU:HD12	1.60	0.84
2:B:662:VAL:HB	2:B:750:ILE:HG12	1.65	0.79
1:C:407:PRO:HG2	1:C:735:VAL:HA	1.68	0.76
2:B:57:PRO:HD3	2:B:296:LEU:HD13	1.68	0.76
1:A:831:ILE:HD11	2:D:575:VAL:HG22	1.69	0.75
2:B:564:MET:HE1	2:B:634:TRP:HE1	1.50	0.75
1:C:479:VAL:HG21	1:C:501:MET:HG2	1.69	0.73
1:A:762:MET:HE1	1:A:769:LYS:HA	1.71	0.73
2:D:535:VAL:HG12	2:D:729:ILE:HG12	1.70	0.72
1:A:463:LEU:HB2	1:A:514:VAL:HG11	1.71	0.72
2:B:649:LEU:HG	2:B:653:MET:HE1	1.71	0.70
2:B:506:VAL:HG13	2:B:507:MET:HG3	1.74	0.70
2:B:730:TYR:HH	5:B:904:GLU:N	1.88	0.70
1:C:155:MET:HE1	1:C:184:LEU:HD21	1.74	0.69
2:D:298:ILE:HG12	2:D:341:VAL:HG11	1.75	0.69
1:A:398:LEU:HD12	1:A:472:PHE:HE1	1.59	0.68
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.76	0.68
1:A:340:PHE:H	1:A:347:LYS:HZ2	1.40	0.67
1:C:26:ILE:HG22	1:C:59:GLN:HB2	1.77	0.66
1:C:463:LEU:HB2	1:C:514:VAL:HG11	1.78	0.66
1:A:394:MET:HE1	1:A:767:PRO:HG3	1.75	0.66
2:D:206:LEU:HD22	2:D:215:THR:HG23	1.77	0.66
1:C:254:ILE:HD12	1:C:354:MET:HE3	1.78	0.66
2:D:417:VAL:HG13	2:D:461:ILE:HD11	1.78	0.65
2:D:686:PRO:HB3	2:D:709:ASN:HD21	1.60	0.65
1:C:580:LEU:HD11	1:C:629:ALA:HB2	1.78	0.65
1:C:673:ARG:HA	1:C:702:MET:HE1	1.79	0.65
2:B:651:ALA:HB2	1:C:655:LEU:HD13	1.77	0.65
2:B:35:ASN:ND2	2:B:68:ASN:OD1	2.30	0.65
1:C:254:ILE:HD13	1:C:268:GLY:HA3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:VAL:HG12	2:D:363:VAL:HG22	1.78	0.64
1:A:94:HIS:HA	1:A:103:THR:HG21	1.79	0.64
2:B:114:ASP:HB2	2:B:135:MET:HE1	1.79	0.64
1:A:363:GLN:NE2	1:A:365:GLY:O	2.31	0.63
2:B:90:MET:HE1	2:B:318:ALA:H	1.63	0.63
1:A:93:SER:HB3	1:A:121:LEU:HD12	1.79	0.63
2:D:539:ARG:NH2	2:D:745:CYS:O	2.32	0.63
1:C:558:PHE:HE2	1:C:647:TYR:HB2	1.65	0.62
1:A:90:ILE:HB	1:A:118:VAL:HG12	1.80	0.62
2:D:557:VAL:HA	2:D:560:MET:HE2	1.81	0.62
1:A:78:VAL:HG11	1:A:107:VAL:HG22	1.80	0.62
1:C:72:ILE:HD13	2:D:320:CYS:HB2	1.80	0.62
2:B:162:MET:HE1	2:B:170:PHE:HB3	1.82	0.62
2:B:684:THR:HG22	2:B:729:ILE:HB	1.82	0.61
1:A:681:TYR:HB3	1:A:728:ALA:HB3	1.82	0.61
1:C:357:GLN:NE2	1:C:378:LYS:O	2.33	0.61
1:C:541:LEU:HB2	1:C:736:LEU:HD13	1.83	0.61
1:A:440:ASN:HB2	1:A:451:VAL:HB	1.83	0.60
1:A:60:LEU:HD21	1:A:292:VAL:HG21	1.83	0.60
1:A:235:ALA:HB1	1:A:240:MET:HB2	1.83	0.60
2:D:567:ILE:O	2:D:571:ILE:HG13	2.02	0.60
1:C:322:LYS:O	1:C:326:MET:HG2	2.02	0.60
2:D:379:GLU:HG2	2:D:380:ASN:H	1.67	0.60
1:A:463:LEU:HD13	1:A:514:VAL:HG21	1.84	0.60
1:C:78:VAL:HG11	1:C:107:VAL:HG22	1.84	0.59
1:A:500:GLY:O	1:A:503:GLY:N	2.35	0.59
1:A:310:GLY:N	2:B:78:ASP:OD2	2.30	0.59
2:B:79:PRO:O	2:B:83:ILE:HG12	2.03	0.59
2:B:306:MET:HE1	2:B:314:PRO:HD3	1.83	0.59
2:D:568:VAL:HG23	2:D:608:LEU:HD13	1.85	0.59
2:B:306:MET:HE1	2:B:313:ILE:HA	1.85	0.59
1:C:90:ILE:HB	1:C:118:VAL:HG12	1.85	0.58
1:C:541:LEU:HD21	1:C:746:LEU:HB3	1.84	0.58
1:A:133:ILE:HD11	2:B:137:ASP:H	1.69	0.58
1:A:209:MET:HG2	1:A:212:ARG:HH21	1.68	0.58
2:B:686:PRO:HD2	3:B:902:NAG:H82	1.84	0.58
1:A:411:VAL:HG11	1:A:478:LEU:HD21	1.85	0.58
2:B:394:LYS:N	2:B:399:CYS:SG	2.71	0.58
1:A:338:VAL:HG22	1:A:347:LYS:HZ1	1.69	0.58
2:B:410:THR:HG23	2:B:479:LEU:HD23	1.86	0.58
1:A:139:ARG:NH1	1:A:345:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:ALA:HB1	2:B:334:LEU:HD22	1.87	0.57
2:B:666:SER:H	2:B:670:PHE:HD1	1.53	0.57
1:C:824:ILE:HG13	1:C:825:VAL:N	2.20	0.57
1:A:351:TYR:HB2	1:A:367:TYR:HB3	1.86	0.57
1:A:407:PRO:HG3	1:A:735:VAL:HA	1.87	0.56
1:A:543:LYS:NZ	1:A:722:ARG:O	2.38	0.56
1:A:634:MET:HE1	2:B:617:VAL:HG11	1.87	0.56
2:B:438:LYS:HB2	2:B:479:LEU:HD12	1.88	0.56
1:A:126:SER:N	1:A:172:GLU:OE1	2.38	0.56
1:C:260:ARG:O	1:C:359:ARG:NH2	2.39	0.56
2:B:220:LYS:HE2	2:D:246:LEU:HD22	1.87	0.56
2:B:437:ARG:HD2	2:B:451:ASN:HB3	1.86	0.56
1:A:461:ASP:OD2	1:A:792:TRP:NE1	2.33	0.56
1:C:357:GLN:OE1	1:C:377:ARG:NH2	2.39	0.55
1:A:570:VAL:HG11	1:A:614:LEU:HD22	1.87	0.55
2:B:628:LYS:HE2	1:C:608:TRP:NE1	2.21	0.55
1:C:566:VAL:O	1:C:570:VAL:HG23	2.07	0.55
1:C:581:ASP:OD2	1:C:601:LEU:N	2.40	0.55
1:C:72:ILE:HD11	2:D:83:ILE:HG23	1.88	0.55
2:B:536:MET:HB3	2:B:728:PHE:HB3	1.88	0.55
1:C:61:ASN:OD1	3:C:901:NAG:N2	2.40	0.55
1:C:132:SER:HB3	2:D:178:PRO:HB2	1.90	0.54
1:C:559:GLN:H	1:C:562:LEU:HD12	1.71	0.54
1:A:673:ARG:O	1:A:673:ARG:NH1	2.37	0.54
2:B:485:HIS:NE2	2:B:511:SER:OG	2.40	0.54
2:D:175:THR:HG22	2:D:176:ILE:H	1.72	0.54
1:A:204:VAL:HG11	1:A:231:VAL:HG12	1.89	0.54
1:C:486:THR:HG21	1:C:686:GLN:HG2	1.88	0.54
1:C:732:ASP:OD2	4:C:909:GLY:N	2.41	0.54
1:C:570:VAL:HG22	1:C:636:TRP:HZ2	1.73	0.54
2:B:556:SER:OG	2:B:557:VAL:N	2.36	0.54
1:C:576:MET:HE2	2:D:828:MET:SD	2.47	0.53
2:B:496:MET:HE2	2:B:512:LEU:HD11	1.90	0.53
2:B:736:ASN:O	2:B:801:HIS:NE2	2.39	0.53
2:D:740:GLY:O	2:D:799:ILE:N	2.41	0.53
2:D:34:LEU:HB2	2:D:67:VAL:HG22	1.90	0.53
2:D:763:ILE:HD13	2:D:779:LEU:HD11	1.91	0.53
2:D:814:ILE:HG13	2:D:817:MET:H	1.74	0.53
2:B:650:ALA:O	2:B:654:ILE:HG12	2.08	0.53
1:A:208:LEU:HD12	1:A:240:MET:HG3	1.91	0.53
2:B:628:LYS:HE2	1:C:608:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:532:GLY:O	2:D:732:ALA:N	2.41	0.53
1:A:30:GLY:HA3	1:A:82:LEU:HD12	1.91	0.53
2:B:684:THR:OG1	2:B:691:GLU:OE2	2.27	0.53
1:C:436:CYS:HA	1:C:476:VAL:HG23	1.91	0.53
1:A:322:LYS:O	1:A:326:MET:HG2	2.09	0.53
1:C:50:ASN:HB3	1:C:60:LEU:HD12	1.91	0.53
1:C:402:THR:HG21	1:C:409:VAL:HG11	1.91	0.53
1:C:536:GLN:HB2	1:C:733:SER:HB3	1.89	0.53
1:C:578:TYR:CZ	1:C:582:ARG:HD2	2.44	0.53
1:A:642:ILE:HG21	2:B:820:VAL:HG11	1.91	0.53
2:B:339:VAL:O	2:B:349:SER:OG	2.24	0.53
2:B:558:TRP:O	2:B:561:MET:HG3	2.09	0.53
1:C:668:ASN:OD1	1:C:673:ARG:NH2	2.41	0.53
2:D:683:GLY:O	2:D:729:ILE:N	2.41	0.53
1:A:254:ILE:HD13	1:A:268:GLY:HA3	1.90	0.52
1:A:249:VAL:HG21	1:A:266:ILE:HD11	1.91	0.52
1:C:498:TRP:HE1	1:C:502:MET:CB	2.23	0.52
1:A:153:GLU:OE2	1:A:372:VAL:N	2.43	0.52
1:A:707:GLU:HA	1:A:710:ASN:OD1	2.10	0.52
2:B:662:VAL:O	2:B:667:ASP:HB3	2.10	0.52
2:B:790:GLU:O	2:B:794:LEU:HG	2.08	0.52
1:C:124:ARG:NH1	1:C:142:PRO:O	2.43	0.52
1:C:248:LEU:HA	1:C:267:ILE:HG22	1.92	0.52
1:C:272:ILE:HG12	1:C:350:ASN:HB2	1.91	0.52
2:D:793:THR:O	2:D:797:THR:OG1	2.26	0.52
2:D:298:ILE:HG23	2:D:341:VAL:HG21	1.91	0.52
2:B:682:PHE:O	2:B:708:PHE:HB2	2.10	0.52
2:B:233:LYS:HD2	2:B:263:GLY:HA3	1.92	0.51
2:B:665:LEU:HA	2:B:670:PHE:CE1	2.44	0.51
1:C:463:LEU:HD13	1:C:514:VAL:HG21	1.92	0.51
2:B:464:LEU:HD13	2:B:509:VAL:HG11	1.93	0.51
1:C:116:ILE:HD11	1:C:305:PRO:HD2	1.91	0.51
1:A:364:VAL:HG21	1:A:379:ILE:HD12	1.93	0.51
2:B:57:PRO:HB2	2:B:67:VAL:HG11	1.92	0.51
1:C:400:ILE:HG23	1:C:514:VAL:H	1.74	0.51
1:A:128:TYR:HB2	1:A:139:ARG:NH2	2.26	0.51
2:B:417:VAL:HG13	2:B:461:ILE:HD11	1.92	0.51
1:A:436:CYS:O	1:A:453:GLN:N	2.40	0.51
2:B:274:SER:HA	2:B:366:LEU:HD22	1.93	0.51
2:B:695:ARG:HA	2:B:702:HIS:HB2	1.93	0.51
1:C:104:PRO:HB2	1:C:128:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:ALA:HB3	2:D:764:ALA:HB3	1.92	0.51
2:B:217:VAL:HA	2:B:220:LYS:HD2	1.92	0.50
2:B:813:ASP:H	2:B:816:ASN:HD21	1.58	0.50
1:A:45:ALA:HB1	1:A:285:VAL:HG21	1.94	0.50
1:C:40:GLN:O	1:C:44:GLU:HG2	2.11	0.50
1:A:120:GLY:N	1:A:138:LEU:O	2.39	0.50
2:D:694:ILE:HG22	2:D:702:HIS:HB2	1.92	0.50
2:B:318:ALA:HB2	2:B:327:PRO:HG3	1.93	0.50
2:D:153:GLN:O	2:D:157:VAL:HG23	2.11	0.50
2:D:681:ARG:O	2:D:727:ALA:N	2.45	0.50
1:A:804:ALA:O	2:D:648:ASN:ND2	2.45	0.50
2:B:174:THR:HB	2:B:180:TYR:HB2	1.93	0.50
2:D:560:MET:HA	2:D:563:VAL:HG22	1.94	0.50
1:A:262:ALA:O	1:A:359:ARG:NH1	2.45	0.50
2:B:571:ILE:HG21	1:C:820:VAL:HG13	1.93	0.50
2:D:433:THR:HB	2:D:455:CYS:HB3	1.94	0.50
1:C:61:ASN:OD1	1:C:62:ALA:N	2.45	0.49
1:C:570:VAL:HG22	1:C:636:TRP:CZ2	2.47	0.49
2:B:422:ILE:HD11	2:B:453:LYS:HG2	1.93	0.49
2:B:611:LEU:HD23	2:B:635:ALA:HB2	1.94	0.49
2:D:157:VAL:HG22	2:D:378:TRP:CE3	2.47	0.49
1:C:154:MET:HA	1:C:157:VAL:HG12	1.93	0.49
1:C:576:MET:HE1	1:C:632:LEU:HD22	1.94	0.49
1:A:220:ILE:HG13	1:A:248:LEU:HB2	1.95	0.49
2:B:435:PRO:HB3	2:B:453:LYS:HE3	1.95	0.49
1:C:47:ASN:HA	1:C:50:ASN:HD21	1.77	0.49
1:C:351:TYR:HB2	1:C:367:TYR:HB3	1.95	0.49
2:D:38:VAL:HG22	2:D:99:VAL:HB	1.94	0.49
1:A:669:ASP:HB3	1:A:672:LEU:HB2	1.94	0.49
1:C:762:MET:HE1	1:C:768:TRP:O	2.13	0.49
2:D:307:LEU:HD21	2:D:313:ILE:HD12	1.95	0.49
2:D:459:PHE:CE2	2:D:791:LEU:HB3	2.48	0.49
2:D:538:SER:HA	2:D:747:LEU:HA	1.95	0.49
1:A:533:PHE:HA	1:A:780:HIS:NE2	2.28	0.48
1:A:634:MET:SD	2:B:609:TRP:HB3	2.53	0.48
2:B:40:LEU:HD23	2:B:41:GLY:O	2.13	0.48
2:B:780:LEU:HA	2:B:783:VAL:HG12	1.95	0.48
1:A:221:LEU:HD11	1:A:231:VAL:HG21	1.94	0.48
1:C:364:VAL:HG21	1:C:379:ILE:HD13	1.94	0.48
2:D:571:ILE:HG21	2:D:630:MET:HE3	1.95	0.48
2:B:518:ARG:NH2	5:B:904:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:VAL:HG21	2:B:601:ILE:HG13	1.94	0.48
2:B:612:VAL:HG23	2:B:634:TRP:CH2	2.48	0.48
1:A:130:ASP:OD1	1:A:130:ASP:N	2.43	0.48
1:C:46:VAL:O	1:C:50:ASN:ND2	2.47	0.48
1:A:570:VAL:HG12	1:A:636:TRP:CH2	2.49	0.48
2:B:265:THR:HG1	2:B:372:TRP:CD1	2.31	0.48
1:C:130:ASP:OD1	1:C:130:ASP:N	2.46	0.47
2:D:533:ILE:HG23	2:D:756:PHE:HB3	1.95	0.47
2:B:120:THR:HB	2:B:122:ILE:HG22	1.96	0.47
2:B:207:ASP:H	2:B:215:THR:HG22	1.78	0.47
2:B:665:LEU:HG	2:B:670:PHE:CD1	2.49	0.47
1:C:721:VAL:HA	1:C:726:LEU:O	2.14	0.47
1:A:684:VAL:HG13	1:A:687:SER:HB3	1.97	0.47
2:D:665:LEU:HA	2:D:670:PHE:HD2	1.79	0.47
1:A:817:PHE:HA	1:A:820:VAL:HG12	1.95	0.47
2:B:274:SER:HB2	2:B:395:SER:HA	1.97	0.47
1:C:94:HIS:CG	1:C:95:PRO:HD2	2.50	0.47
1:A:635:VAL:HG11	2:B:827:ALA:HB2	1.97	0.47
1:A:656:VAL:HG13	1:A:657:LEU:HG	1.96	0.47
1:A:82:LEU:HD23	1:A:82:LEU:H	1.80	0.47
2:B:172:LEU:HB2	2:B:203:VAL:HG23	1.96	0.47
2:B:612:VAL:HG23	2:B:634:TRP:HH2	1.80	0.47
1:C:138:LEU:HD22	1:C:325:LEU:HB3	1.97	0.47
2:D:686:PRO:HG2	3:D:904:NAG:H82	1.97	0.47
2:B:100:PHE:CD2	2:B:113:LEU:HD11	2.50	0.47
2:B:118:SER:HB3	2:B:142:SER:HB3	1.96	0.47
2:B:415:PRO:HG3	2:B:737:TYR:CG	2.50	0.47
1:A:47:ASN:HA	1:A:50:ASN:HD21	1.79	0.46
1:A:330:TYR:HD1	1:A:336:GLY:HA2	1.81	0.46
1:C:402:THR:HB	1:C:478:LEU:HD23	1.96	0.46
1:C:433:LYS:HG2	1:C:456:TYR:HB3	1.97	0.46
1:C:820:VAL:O	1:C:824:ILE:HG12	2.16	0.46
2:B:98:LEU:HD23	2:B:124:ILE:HG12	1.98	0.46
1:A:139:ARG:N	1:A:344:GLY:O	2.37	0.46
2:B:521:VAL:HG13	2:B:522:VAL:HG13	1.97	0.46
2:B:665:LEU:HD23	2:B:666:SER:N	2.31	0.46
1:A:165:LEU:O	1:A:195:LEU:N	2.43	0.46
1:C:124:ARG:HA	1:C:139:ARG:NH2	2.31	0.46
1:A:113:PHE:CE2	2:B:79:PRO:HD3	2.51	0.46
2:B:87:CYS:HA	2:B:90:MET:HG2	1.98	0.46
1:C:249:VAL:HG21	1:C:266:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:ND2	1:A:379:ILE:HG13	2.31	0.46
1:A:795:TYR:HB3	1:A:796:GLN:H	1.57	0.46
1:A:822:GLY:HA2	1:A:825:VAL:HG12	1.98	0.46
2:B:717:LEU:HA	2:B:720:LEU:HD12	1.96	0.46
1:A:354:MET:HB3	1:A:361:LEU:HD22	1.98	0.46
1:A:398:LEU:HD12	1:A:472:PHE:CE1	2.45	0.46
1:C:143:PRO:HD2	1:C:146:HIS:ND1	2.30	0.45
1:A:34:SER:HB2	1:A:96:PRO:HD3	1.99	0.45
2:B:70:VAL:HG12	2:B:72:LEU:HG	1.99	0.45
1:A:111:ALA:HB1	1:A:116:ILE:HB	1.98	0.45
1:A:112:GLY:O	1:A:115:ARG:NH1	2.40	0.45
2:B:790:GLU:O	2:B:793:THR:OG1	2.27	0.45
1:C:762:MET:HE1	1:C:769:LYS:HA	1.98	0.45
2:D:574:PHE:HA	2:D:577:GLU:HG2	1.98	0.45
2:B:781:GLN:OE1	1:C:521:ASN:ND2	2.49	0.45
1:C:161:ASN:HB3	1:C:189:SER:HB2	1.97	0.45
1:C:608:TRP:CZ3	1:C:619:ILE:HD13	2.51	0.45
1:A:458:PHE:CE2	1:A:788:LEU:HB3	2.52	0.45
1:C:439:PRO:HB2	1:C:442:THR:HB	1.98	0.45
1:C:487:GLN:HG2	1:C:498:TRP:CZ3	2.51	0.45
2:D:161:ILE:HD13	2:D:383:LEU:HD21	1.98	0.45
1:A:123:THR:O	1:A:139:ARG:NE	2.50	0.45
1:C:29:ILE:HD13	1:C:288:VAL:HG11	1.98	0.45
2:D:256:ILE:HG12	2:D:277:ILE:HB	1.99	0.45
1:A:566:VAL:O	1:A:570:VAL:HG13	2.16	0.45
1:C:671:ARG:NH1	1:C:679:PHE:HA	2.32	0.45
1:A:37:LYS:HA	1:A:40:GLN:NE2	2.32	0.45
2:B:157:VAL:HG21	2:B:361:LEU:HD13	1.99	0.45
1:A:819:LEU:HD11	2:D:634:TRP:CE3	2.52	0.44
2:D:48:GLU:H	2:D:51:LEU:HD12	1.81	0.44
1:C:208:LEU:O	1:C:212:ARG:HG3	2.18	0.44
1:C:103:THR:O	1:C:106:PRO:HD2	2.17	0.44
1:C:439:PRO:HG2	1:C:480:ALA:HA	1.99	0.44
1:A:541:LEU:HD22	1:A:736:LEU:HD22	1.98	0.44
1:C:124:ARG:HA	1:C:139:ARG:HH21	1.82	0.44
1:C:403:ILE:HB	1:C:501:MET:SD	2.57	0.44
1:A:153:GLU:HA	1:A:156:ARG:HG2	2.00	0.44
1:C:731:TRP:CG	1:C:732:ASP:H	2.36	0.44
1:C:778:LYS:O	1:C:782:ASN:HB2	2.17	0.44
2:D:389:VAL:HG11	2:D:437:ARG:HD3	1.99	0.44
2:B:56:GLY:HA3	2:B:69:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ILE:HD12	2:B:116:ILE:HD11	2.00	0.44
1:C:31:ALA:HB1	1:C:33:LEU:HD13	2.00	0.44
1:C:824:ILE:O	1:C:828:ILE:HG12	2.18	0.44
2:D:536:MET:SD	2:D:747:LEU:HD13	2.57	0.44
1:A:558:PHE:HE1	2:B:812:LEU:HD12	1.82	0.44
2:B:303:ALA:HA	2:B:306:MET:HG2	2.00	0.44
2:D:103:ASP:OD1	2:D:128:HIS:NE2	2.50	0.43
1:A:217:ARG:HA	1:A:217:ARG:HD3	1.87	0.43
1:A:485:GLY:HA3	1:A:502:MET:HG2	2.00	0.43
1:A:513:ILE:HG21	1:A:517:LEU:HD22	2.00	0.43
2:B:359:PRO:HG2	2:B:361:LEU:HD12	2.00	0.43
1:A:104:PRO:HG2	1:A:128:TYR:CZ	2.53	0.43
1:A:267:ILE:HG12	1:A:379:ILE:HD11	2.00	0.43
2:B:661:GLN:HG3	2:B:679:PRO:HD3	2.00	0.43
2:D:437:ARG:NH1	2:D:476:ASP:O	2.50	0.43
2:D:682:PHE:HA	2:D:727:ALA:HB3	2.00	0.43
1:A:82:LEU:HB2	1:A:87:VAL:HG11	2.00	0.43
2:B:464:LEU:HD12	2:B:467:LEU:HD11	2.00	0.43
2:D:57:PRO:HD3	2:D:296:LEU:HB3	1.99	0.43
1:A:537:GLY:O	1:A:733:SER:N	2.47	0.43
2:D:460:CYS:O	2:D:463:ILE:HG22	2.18	0.43
2:D:379:GLU:HG2	2:D:380:ASN:N	2.31	0.43
1:C:32:VAL:HG11	1:C:107:VAL:HG21	1.99	0.43
2:D:133:MET:O	2:D:146:GLN:NE2	2.51	0.43
2:D:233:LYS:O	2:D:237:VAL:HG13	2.18	0.43
2:B:434:VAL:HG11	2:B:475:TYR:HE2	1.84	0.43
2:B:710:GLN:CD	2:B:725:LEU:HD11	2.44	0.43
2:D:210:PHE:HA	2:D:215:THR:HG21	2.00	0.43
1:A:570:VAL:HG12	1:A:636:TRP:CZ2	2.54	0.42
2:B:343:TRP:CE3	2:B:344:ASP:HB2	2.54	0.42
2:B:466:LYS:HB3	2:B:782:PHE:CZ	2.54	0.42
2:D:40:LEU:HD22	2:D:52:ARG:HD3	2.01	0.42
2:B:122:ILE:HD12	2:B:123:PRO:HD2	2.01	0.42
1:A:92:VAL:HG21	1:A:104:PRO:HA	2.01	0.42
2:D:379:GLU:CG	2:D:380:ASN:H	2.32	0.42
2:D:387:HIS:NE2	2:D:391:PRO:HD3	2.35	0.42
2:D:463:ILE:HD12	2:D:463:ILE:HA	1.92	0.42
2:D:531:THR:HG22	2:D:760:GLY:HA2	2.00	0.42
1:A:328:SER:O	1:A:338:VAL:HG23	2.19	0.42
2:B:175:THR:OG1	2:B:176:ILE:N	2.52	0.42
1:A:46:VAL:O	1:A:50:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD23	1:A:138:LEU:HB2	2.01	0.42
1:A:567:GLY:O	1:A:570:VAL:HG22	2.19	0.42
1:A:790:LYS:HA	1:A:794:ARG:HG3	2.02	0.42
2:B:536:MET:HG2	2:B:720:LEU:HD13	2.02	0.42
2:B:813:ASP:H	2:B:816:ASN:ND2	2.18	0.42
1:C:92:VAL:HG11	1:C:104:PRO:HA	2.00	0.42
1:C:254:ILE:O	1:C:259:LEU:HB2	2.19	0.42
1:A:224:SER:HA	1:A:252:ARG:HH11	1.84	0.42
2:D:415:PRO:HG3	2:D:737:TYR:CG	2.55	0.42
1:A:631:ILE:HG21	2:B:830:LEU:HD22	2.02	0.42
2:B:536:MET:HB2	2:B:735:LEU:HD13	2.01	0.42
1:C:513:ILE:HG21	1:C:517:LEU:HD22	2.01	0.42
2:D:233:LYS:NZ	2:D:261:VAL:O	2.41	0.42
2:D:410:THR:O	2:D:479:LEU:HA	2.19	0.42
1:C:104:PRO:HG3	1:C:123:THR:HG21	2.02	0.42
1:C:232:TYR:OH	1:C:249:VAL:HG11	2.19	0.42
1:C:564:LEU:HD23	1:C:564:LEU:HA	1.90	0.42
1:C:619:ILE:HG23	1:C:620:GLY:N	2.34	0.42
2:D:40:LEU:HD11	2:D:288:LEU:HD13	2.01	0.42
2:B:248:LEU:HD12	2:B:248:LEU:HA	1.92	0.42
1:C:706:MET:O	1:C:710:ASN:N	2.53	0.42
1:A:789:ASP:OD1	1:A:793:VAL:HB	2.20	0.42
2:B:43:SER:HG	2:B:128:HIS:CE1	2.38	0.42
1:C:556:GLN:N	1:C:557:PRO:HD2	2.35	0.42
2:D:406:LEU:HD22	2:D:506:VAL:HG11	2.02	0.42
2:B:78:ASP:HB2	2:B:81:SER:HB3	2.02	0.41
1:C:527:ILE:HB	1:C:762:MET:O	2.20	0.41
1:A:826:ALA:O	1:A:830:LEU:HD23	2.20	0.41
2:B:250:GLY:H	2:B:253:PHE:HB2	1.85	0.41
1:C:666:GLY:N	1:C:669:ASP:OD2	2.40	0.41
1:C:686:GLN:N	1:C:690:ASP:OD2	2.50	0.41
2:D:689:SER:HB3	5:D:905:GLU:OE1	2.20	0.41
1:A:543:LYS:HD2	1:A:722:ARG:HA	2.03	0.41
2:B:532:GLY:O	2:B:732:ALA:N	2.53	0.41
2:B:649:LEU:HD12	2:B:649:LEU:HA	1.92	0.41
2:B:173:VAL:HG23	2:B:173:VAL:O	2.19	0.41
2:B:725:LEU:HD23	2:B:725:LEU:HA	1.94	0.41
1:C:155:MET:SD	1:C:163:ILE:HD13	2.60	0.41
1:A:95:PRO:HD3	1:A:103:THR:HB	2.03	0.41
1:C:38:HIS:HA	1:C:41:MET:HG2	2.03	0.41
1:C:209:MET:HE1	1:C:212:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ASN:HB2	1:C:451:VAL:HB	2.01	0.41
1:C:578:TYR:CE2	1:C:603:LEU:HB3	2.56	0.41
2:B:419:VAL:HG12	2:B:456:CYS:HB3	2.03	0.41
1:C:247:TRP:HB3	1:C:266:ILE:HG13	2.02	0.41
1:C:569:SER:HA	1:C:572:VAL:HG12	2.02	0.41
2:D:571:ILE:O	2:D:575:VAL:HG23	2.21	0.41
1:A:142:PRO:HA	1:A:143:PRO:HD3	1.93	0.41
1:C:552:ASP:OD1	1:C:552:ASP:N	2.53	0.41
2:D:259:SER:HB3	2:D:279:VAL:O	2.21	0.41
1:A:66:THR:OG1	1:A:67:HIS:N	2.54	0.41
1:A:217:ARG:NH1	1:A:245:TYR:OH	2.54	0.41
1:A:221:LEU:HD11	1:A:231:VAL:CG2	2.51	0.41
1:A:221:LEU:HD22	1:A:249:VAL:HG13	2.03	0.41
1:A:433:LYS:HD2	1:A:454:CYS:SG	2.61	0.41
1:A:731:TRP:CG	1:A:732:ASP:H	2.39	0.41
2:B:204:ILE:HD12	2:B:222:ILE:HD11	2.03	0.41
2:B:282:ASP:N	2:B:282:ASP:OD1	2.54	0.41
1:C:690:ASP:O	1:C:694:ARG:HG2	2.21	0.41
1:A:45:ALA:O	1:A:48:GLN:HG3	2.21	0.41
2:B:815:ASP:OD1	2:B:815:ASP:N	2.54	0.41
1:C:151:TRP:CZ3	1:C:248:LEU:HB3	2.57	0.41
1:C:335:THR:HG22	1:C:346:ARG:NH1	2.35	0.41
1:A:538:LEU:HD11	1:A:689:VAL:HG22	2.02	0.40
1:C:35:THR:HG22	1:C:38:HIS:ND1	2.36	0.40
2:D:177:PHE:CD1	2:D:178:PRO:HD2	2.56	0.40
1:A:68:LYS:HE3	1:A:68:LYS:HB3	1.86	0.40
1:A:479:VAL:HG21	1:A:501:MET:HG2	2.03	0.40
2:B:317:LYS:HD2	2:B:317:LYS:HA	1.90	0.40
2:B:387:HIS:CE1	2:B:391:PRO:HG3	2.56	0.40
2:B:518:ARG:HA	2:B:521:VAL:HG12	2.03	0.40
1:C:60:LEU:HD21	1:C:292:VAL:HG21	2.03	0.40
2:D:175:THR:HG22	2:D:176:ILE:N	2.35	0.40
2:D:429:CYS:HB3	2:D:433:THR:OG1	2.21	0.40
2:D:568:VAL:HG21	2:D:634:TRP:CE3	2.57	0.40
1:A:714:ALA:O	1:A:718:ILE:HG12	2.22	0.40
2:B:608:LEU:O	2:B:634:TRP:HH2	2.04	0.40
2:B:640:ILE:HD12	1:C:647:TYR:OH	2.21	0.40
1:C:576:MET:CE	1:C:632:LEU:HD22	2.51	0.40
1:C:787:ASP:HA	1:C:790:LYS:HE2	2.02	0.40
2:D:313:ILE:HD12	2:D:314:PRO:HD2	2.03	0.40
2:D:460:CYS:HB3	2:D:509:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HD2	1:A:146:HIS:ND1	2.35	0.40
1:A:407:PRO:HB3	1:A:738:PHE:CG	2.57	0.40
2:B:40:LEU:HD21	2:B:288:LEU:HD21	2.02	0.40
2:D:288:LEU:HD23	2:D:288:LEU:HA	1.91	0.40
1:A:543:LYS:HE3	1:A:745:ASP:OD2	2.21	0.40
2:B:601:ILE:H	2:B:601:ILE:HD12	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	778/813 (96%)	743 (96%)	35 (4%)	0	100	100
1	C	778/813 (96%)	747 (96%)	31 (4%)	0	100	100
2	B	785/809 (97%)	753 (96%)	32 (4%)	0	100	100
2	D	773/809 (96%)	746 (96%)	27 (4%)	0	100	100
All	All	3114/3244 (96%)	2989 (96%)	125 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	560/701 (80%)	560 (100%)	0	100	100
1	C	541/701 (77%)	538 (99%)	3 (1%)	78	79
2	B	529/707 (75%)	529 (100%)	0	100	100
2	D	540/707 (76%)	540 (100%)	0	100	100
All	All	2170/2816 (77%)	2167 (100%)	3 (0%)	87	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	VAL
1	C	33	LEU
1	C	632	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	47	ASN
1	A	50	ASN
1	A	375	ASN
2	B	96	HIS
2	B	146	GLN
2	B	358	HIS
2	B	693	ASN
2	B	702	HIS
1	C	50	ASN
1	C	290	GLN
1	C	404	HIS
1	C	453	GLN
1	C	520	ASN
1	C	709	HIS
2	D	44	HIS
2	D	201	GLN
2	D	614	ASN
2	D	736	ASN

5.3.3 RNA ⓘ

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](#)

27 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	C	904	1	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	C	902	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	901	1	14,14,15	0.17	0	17,19,21	0.41	0
3	NAG	B	901	2	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	C	906	1	14,14,15	0.25	0	17,19,21	0.37	0
3	NAG	C	901	1	14,14,15	0.32	0	17,19,21	0.41	0
4	GLY	C	909	-	3,3,4	0.61	0	0,2,4	-	-
3	NAG	D	901	2	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	A	907	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	903	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	D	902	2	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	C	905	1	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	D	904	2	14,14,15	0.17	0	17,19,21	0.38	0
3	NAG	A	902	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	D	903	2	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	A	906	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	C	908	1	14,14,15	0.23	0	17,19,21	0.43	0
5	GLU	B	904	-	7,8,9	0.86	0	4,9,11	1.01	0
3	NAG	A	905	1	14,14,15	0.30	0	17,19,21	0.38	0
3	NAG	B	903	2	14,14,15	0.23	0	17,19,21	0.42	0
5	GLU	D	905	-	7,8,9	0.83	0	4,9,11	1.10	0
3	NAG	B	902	2	14,14,15	0.18	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	907	1	14,14,15	0.20	0	17,19,21	0.42	0
4	GLY	A	909	-	3,3,4	0.61	0	0,2,4	-	-
3	NAG	A	904	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	C	903	1	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	A	908	1	14,14,15	0.24	0	17,19,21	0.50	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	C	904	1	-	2/6/23/26	0/1/1/1
3	NAG	C	902	1	-	2/6/23/26	0/1/1/1
3	NAG	A	901	1	-	4/6/23/26	0/1/1/1
3	NAG	B	901	2	-	2/6/23/26	0/1/1/1
3	NAG	C	906	1	-	0/6/23/26	0/1/1/1
3	NAG	C	901	1	-	2/6/23/26	0/1/1/1
4	GLY	C	909	-	-	0/0/1/2	-
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	903	1	-	2/6/23/26	0/1/1/1
3	NAG	D	902	2	-	2/6/23/26	0/1/1/1
3	NAG	C	905	1	-	1/6/23/26	0/1/1/1
3	NAG	D	904	2	-	2/6/23/26	0/1/1/1
3	NAG	A	902	1	-	0/6/23/26	0/1/1/1
3	NAG	D	903	2	-	2/6/23/26	0/1/1/1
3	NAG	A	906	1	-	2/6/23/26	0/1/1/1
3	NAG	C	908	1	-	0/6/23/26	0/1/1/1
5	GLU	B	904	-	-	3/6/7/9	-
3	NAG	A	905	1	-	2/6/23/26	0/1/1/1
3	NAG	B	903	2	-	0/6/23/26	0/1/1/1
5	GLU	D	905	-	-	1/6/7/9	-
3	NAG	B	902	2	-	2/6/23/26	0/1/1/1
3	NAG	C	907	1	-	0/6/23/26	0/1/1/1
4	GLY	A	909	-	-	0/0/1/2	-
3	NAG	A	904	1	-	2/6/23/26	0/1/1/1
3	NAG	C	903	1	-	2/6/23/26	0/1/1/1
3	NAG	A	908	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 (41) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	B	902	NAG	O5-C5-C6-O6
5	B	904	GLU	OE1-CD-CG-CB
5	B	904	GLU	OE2-CD-CG-CB
5	D	905	GLU	CA-CB-CG-CD

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	NAG	1	0
4	C	909	GLY	1	0
3	D	904	NAG	1	0
5	B	904	GLU	2	0
5	D	905	GLU	1	0
3	B	902	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.