WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 07:23 AM EDT

PDB ID : 1L7E

Title : Crystal Structure of R. rubrum Transhydrogenase Domain I with Bound NADH

Authors : Prasad, G.S.; Wahlberg, M.; Sridhar, V.; Yamaguchi, M.; Hatefi, Y.; Stout, C.D.

Deposited on : 2002-03-14

Resolution : 1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

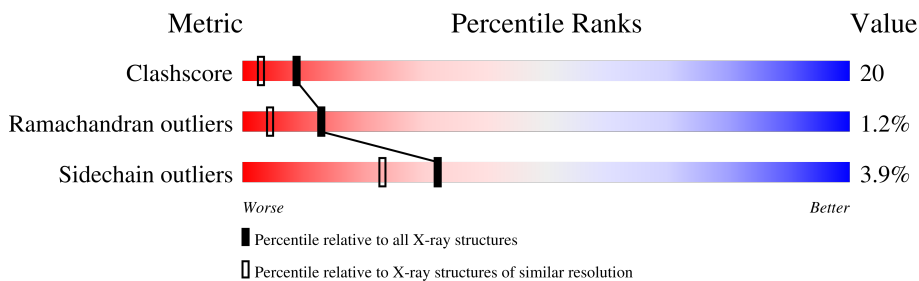|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Clashscore		20
Ramachandran outliers		1.2%
Sidechain outliers		3.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	384	60% 34% • • •
1	B	384	63% 28% • 7%
1	C	384	59% 30% • 8%
1	D	384	62% 32% • •

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2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11327 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called nicotinamide nucleotide Transhydrogenase, subunit alpha 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2736	1727	472	520	17			
1	B	357	Total	C	N	O	S	0	0	0
			2618	1655	456	491	16			
1	C	353	Total	C	N	O	S	0	0	0
			2586	1636	448	486	16			
1	D	367	Total	C	N	O	S	0	0	0
			2692	1701	467	507	17			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).
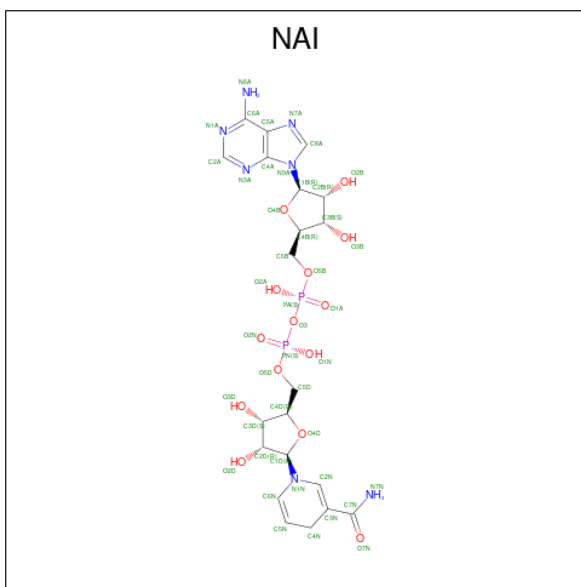
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	136	Total O 136 136	0	0
3	B	136	Total O 136 136	0	0
3	C	158	Total O 158 158	0	0
3	D	177	Total O 177 177	0	0

3 Residue-property plots ⓘ

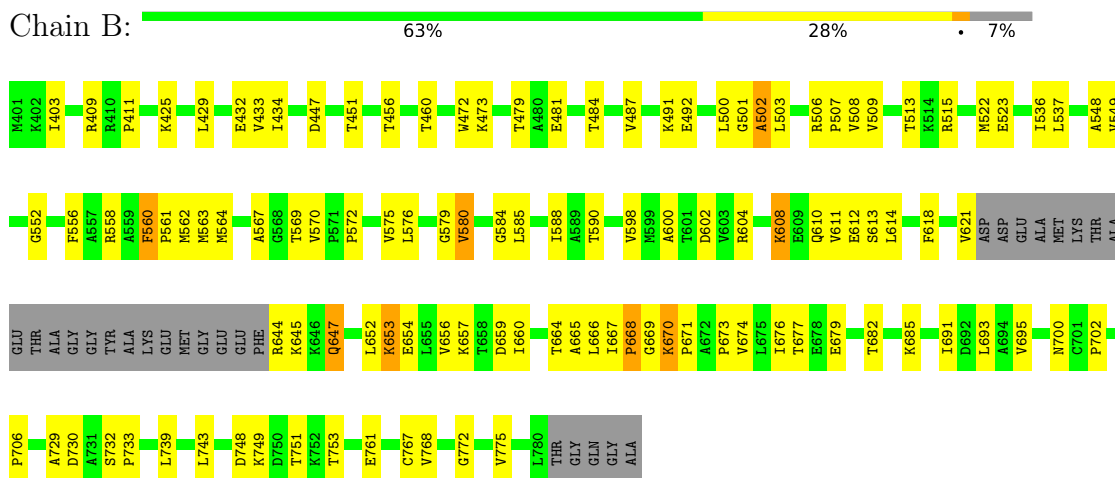These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

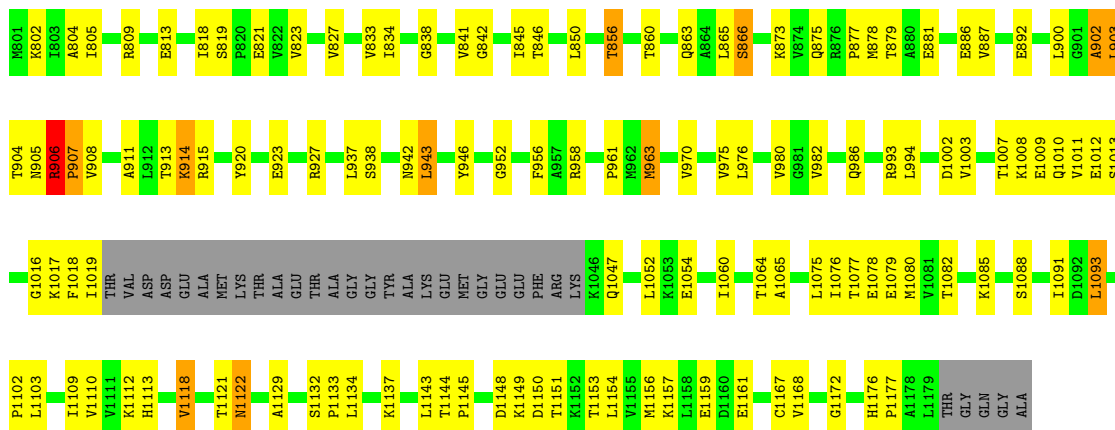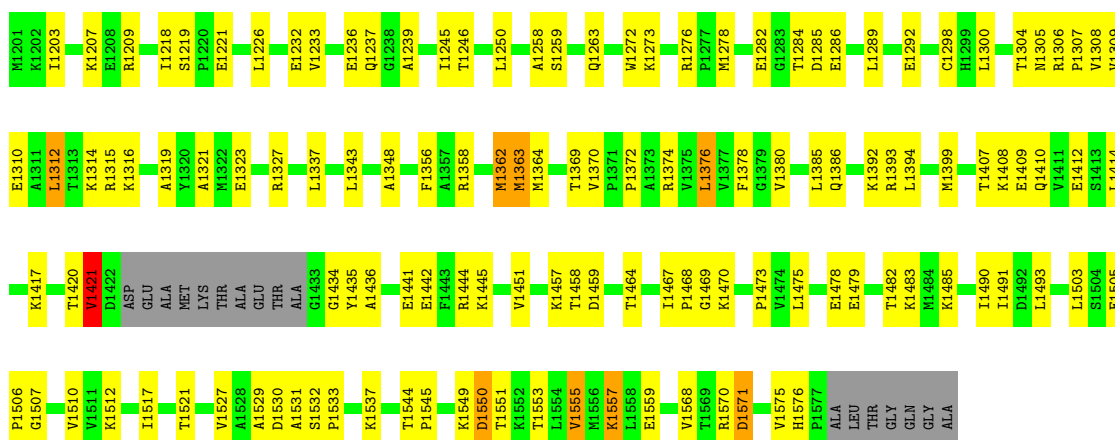• Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1

Chain A:

• Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1

Chain B:

• Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1

Chain C:

M801 K802 I803 A804 I805 R809 E813 I818 S819 P820 E821 V822 V823 V827 V833 I834 G838 V841 G842 I845 T846 L850 T856 T860 Q863 A864 L865 S866 K873 V874 Q875 R876 P877 M878 T879 A880 E881 E886 V887 E892 L900 G901 A902 L903

T904 N905 A906 P907 V908 A911 L912 T913 K914 R915 Y920 E923 R927 L937 S938 N942 L943 Y946 G952 F956 A957 R958 P961 M962 M963 V970 V975 L976 V980 G981 V982 Q986 R993 L994 D1002 V1003 T1007 K1008 E1009 Q1010 V1011 E1012 S1013

G1016 K1017 F1018 I1019 THR VAL ASP ASP GLU ALA MET LYS THR ALA GLU THR ALA GLY GLY TYR ALA LYS GLU MET GLY GLU PHE ARG LYS K1046 Q1047 L1052 K1053 E1054 I1060 T1064 A1065 L1075 I1076 T1077 E1078 E1079 M1080 V1081 T1082 K1085 S1088 I1091 D1092 L1093

P1102 L1103 I1109 V1110 V1111 K1112 H1113 V1118 T1121 N1122 A1129 S1132 P1133 L1134 K1137 L1143 T1144 P1145 D1148 K1149 D1150 T1151 K1152 T1153 L1154 V1155 M1156 K1157 L1158 E1159 D1160 E1161 C1167 V1168 G1172 H1176 P1177 A1178 L1179 THR GLN GLY ALA

• Molecule 1: nicotinamide nucleotide Transhydrogenase, subunit alpha 1

Chain D:

62%   32%   • •

M1201 K1202 I1203 K1207 E1208 R1209 I1218 S1219 P1220 E1221 L1226 E1232 V1233 E1236 Q1237 G1238 A1239 I1245 T1246 L1250 A1258 S1259 Q1263 W1272 K1273 R1276 P1277 M1278 E1282 G1283 T1284 D1285 E1286 L1289 E1292 C1298 H1299 L1300 T1304 N1305 R1306 P1307 V1308 V1309

E1310 A1311 L1312 T1313 K1314 R1315 K1316 A1319 Y1320 A1321 M1322 E1323 R1327 L1337 L1343 A1348 F1356 A1357 R1358 M1362 M1363 M1364 T1369 V1370 P1371 P1372 A1373 R1374 V1375 L1376 V1377 F1378 G1379 V1380 L1385 Q1386 K1392 R1393 L1394 M1399 T1407 K1408 E1409 Q1410 V1411 E1412 S1413 L1414

K1417 T1420 V1421 D1422 GLU ALA MET LYS THR ALA GLU THR ALA G1433 G1434 Y1435 A1436 E1441 E1442 F1443 R1444 K1445 V1451 K1457 T1458 D1459 T1464 I1467 P1468 G1469 K1470 P1473 V1474 L1475 E1478 E1479 T1482 K1483 M1484 K1485 I1490 I1491 D1492 L1493 L1503 S1504 E1505

P1506 G1507 V1510 V1511 K1512 I1517 T1521 V1527 A1528 A1529 D1530 A1531 S1532 P1533 K1537 T1544 P1545 K1549 D1550 T1551 K1552 T1553 L1554 V1555 M1556 K1557 L1558 E1559 V1568 T1569 R1570 D1571 V1575 H1576 P1577 ALA LEU THR GLY GLN GLY ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.14Å 116.68Å 92.60Å 90.00° 106.28° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11327	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

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: NAI

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	0.40	0/2772	0.74	7/3756 (0.2%)
1	B	0.34	0/2652	0.63	1/3596 (0.0%)
1	C	0.36	0/2620	0.64	0/3554
1	D	0.36	0/2727	0.63	0/3694
All	All	0.37	0/10771	0.66	8/14600 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	233	GLY	C-N-CA	9.19	141.61	122.30
1	A	234	GLY	C-N-CA	7.52	140.50	121.70
1	A	241	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	A	231	THR	N-CA-CB	5.92	121.56	110.30
1	A	235	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	351	THR	N-CA-C	-5.53	96.08	111.00
1	B	432	GLU	N-CA-C	-5.45	96.30	111.00
1	A	245	LYS	CB-CA-C	5.29	120.99	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	231	THR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	GLY	Mainchain
1	A	241	GLU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2736	0	2857	121	0
1	B	2618	0	2752	115	0
1	C	2586	0	2717	118	0
1	D	2692	0	2819	100	0
2	A	44	0	27	1	0
2	D	44	0	27	1	0
3	A	136	0	0	2	0
3	B	136	0	0	6	0
3	C	158	0	0	1	0
3	D	177	0	0	6	0
All	All	11327	0	11199	444	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 20.

All (444) 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:1077:THR:H	1:C:1080:MET:HE3	0.98	1.08
1:D:1557:LYS:H	1:D:1557:LYS:HD2	1.30	0.97
1:C:906:ARG:H	1:C:907:PRO:HD2	1.30	0.96
1:B:748:ASP:O	1:B:749:LYS:HG2	1.66	0.95
1:A:163:MET:HB2	1:A:170:VAL:HG12	1.49	0.94
1:B:564:MET:HG3	1:B:569:THR:HG22	1.49	0.94
1:C:1110:VAL:HG11	1:C:1112:LYS:HE2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1077:THR:N	1:C:1080:MET:HE3	1.84	0.92
1:C:834:ILE:HG12	1:C:856:THR:CG2	2.08	0.84
1:B:585:LEU:HG	1:B:614:LEU:HD11	1.58	0.83
1:A:131:ALA:HA	1:A:134:MET:HE2	1.60	0.83
1:C:1157:LYS:HB3	1:C:1159:GLU:OE2	1.79	0.83
1:B:500:LEU:C	1:B:502:ALA:H	1.82	0.83
1:D:1245:ILE:CG2	1:D:1250:LEU:HD11	2.09	0.82
1:C:1078:GLU:HB2	1:C:1103:LEU:HD11	1.62	0.81
1:B:552:GLY:CA	1:B:691:ILE:HD11	2.11	0.81
1:A:129:SER:HA	1:A:132:GLN:HE21	1.46	0.80
1:D:1434:GLY:HA3	1:D:1468:PRO:HG2	1.64	0.80
1:B:674:VAL:HG13	1:B:702:PRO:HD3	1.65	0.79
1:D:1286:GLU:HA	1:D:1289:LEU:HD23	1.62	0.79
1:C:845:ILE:HG22	1:C:850:LEU:HD21	1.63	0.79
1:D:1510:VAL:HG22	1:D:1517:ILE:HB	1.63	0.79
1:C:906:ARG:N	1:C:907:PRO:HD2	1.98	0.79
1:B:664:THR:HG22	1:B:693:LEU:HD12	1.65	0.79
1:A:284:MET:HE3	1:A:315:VAL:HG11	1.64	0.78
1:C:1110:VAL:CG1	1:C:1112:LYS:HE2	2.13	0.78
1:A:129:SER:HA	1:A:132:GLN:NE2	1.96	0.78
1:B:409:ARG:HD3	1:B:484:THR:HG21	1.66	0.77
1:C:879:THR:HG23	1:C:908:VAL:HG22	1.66	0.77
1:C:911:ALA:HA	1:C:914:LYS:HD2	1.65	0.77
1:C:834:ILE:HG12	1:C:856:THR:HG23	1.65	0.77
1:A:284:MET:HE1	1:A:290:ILE:HD11	1.65	0.76
1:D:1306:ARG:O	1:D:1309:VAL:HG22	1.85	0.76
1:A:267:ILE:HG21	1:A:270:LYS:HD2	1.66	0.76
1:A:131:ALA:HA	1:A:134:MET:CE	2.16	0.76
1:D:1245:ILE:HG22	1:D:1250:LEU:HD11	1.67	0.75
1:D:1292:GLU:HG3	1:D:1315:ARG:O	1.85	0.75
1:D:1420:THR:O	1:D:1421:VAL:HG13	1.87	0.74
1:B:536:ILE:HG13	1:B:537:LEU:HD12	1.68	0.74
1:B:548:ALA:O	1:B:691:ILE:HD13	1.87	0.74
1:A:264:THR:HG22	1:A:293:LEU:HD12	1.69	0.73
1:C:906:ARG:H	1:C:907:PRO:CD	2.01	0.73
1:B:564:MET:HG3	1:B:569:THR:CG2	2.17	0.73
1:D:1258:ALA:HA	1:D:1263:GLN:HE21	1.54	0.73
1:C:905:ASN:O	1:C:906:ARG:HB3	1.89	0.73
1:B:677:THR:HG23	3:B:908:HOH:O	1.87	0.72
1:C:1019:ILE:HG21	1:C:1054:GLU:HG3	1.72	0.72
1:B:665:ALA:HB3	1:B:700:ASN:ND2	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:GLU:O	1:B:682:THR:HG22	1.90	0.72
1:D:1259:SER:H	1:D:1263:GLN:NE2	1.87	0.71
1:C:905:ASN:HB3	1:C:907:PRO:HD2	1.72	0.71
1:D:1308:VAL:O	1:D:1312:LEU:HD22	1.90	0.71
1:A:62:ALA:HA	1:A:89:LEU:HD12	1.71	0.70
1:A:222:ASP:O	1:A:223:ASP:HB2	1.91	0.70
1:A:240:GLY:O	1:A:244:ARG:HB2	1.90	0.70
1:C:802:LYS:NZ	1:C:834:ILE:HD12	2.08	0.69
1:C:911:ALA:HA	1:C:914:LYS:CD	2.22	0.69
1:A:163:MET:HB2	1:A:170:VAL:CG1	2.23	0.69
1:C:906:ARG:N	1:C:907:PRO:CD	2.55	0.68
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.59	0.67
1:B:666:LEU:O	1:B:668:PRO:HD3	1.94	0.67
1:B:501:GLY:O	1:B:503:LEU:N	2.28	0.67
1:A:235:TYR:CD2	1:A:268:PRO:HG3	2.29	0.67
1:D:1203:ILE:HD11	1:D:1272:TRP:CD2	2.29	0.66
1:D:1305:ASN:O	1:D:1308:VAL:HG12	1.95	0.66
1:A:278:GLU:O	1:A:282:THR:HG23	1.94	0.66
1:D:1549:LYS:HG2	3:D:592:HOH:O	1.94	0.65
1:B:600:ALA:HB3	1:B:611:VAL:HG11	1.78	0.65
1:A:23:VAL:HG11	1:A:55:ALA:HB2	1.79	0.65
1:A:237:LYS:HE2	1:A:238:GLU:H	1.61	0.65
1:B:506:ARG:HB3	1:B:507:PRO:HD3	1.77	0.64
1:D:1421:VAL:HA	3:D:332:HOH:O	1.98	0.64
1:B:556:PHE:CE2	1:B:558:ARG:HB2	2.31	0.64
1:C:1129:ALA:HB3	1:D:1358:ARG:HG3	1.79	0.64
1:B:500:LEU:O	1:B:502:ALA:N	2.30	0.64
1:B:500:LEU:C	1:B:502:ALA:N	2.51	0.64
1:B:523:GLU:HA	1:B:537:LEU:HD11	1.78	0.64
1:B:409:ARG:CD	1:B:484:THR:HG21	2.27	0.64
1:B:600:ALA:HB3	1:B:611:VAL:CG1	2.28	0.63
1:B:653:LYS:HE3	1:B:657:LYS:HZ1	1.62	0.63
1:C:1077:THR:H	1:C:1080:MET:CE	1.92	0.63
1:C:1009:GLU:O	1:C:1013:SER:HB2	1.99	0.63
1:C:923:GLU:HB2	1:C:937:LEU:HD11	1.81	0.62
1:D:1559:GLU:H	1:D:1559:GLU:CD	2.02	0.62
1:B:552:GLY:HA2	1:B:691:ILE:HD11	1.81	0.62
1:D:1306:ARG:N	1:D:1307:PRO:HD2	2.14	0.62
1:C:1076:ILE:O	1:C:1102:PRO:HD2	1.99	0.61
1:A:274:VAL:HG13	1:A:302:PRO:HD3	1.81	0.61
1:A:174:ARG:NH1	1:A:197:VAL:HG11	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MET:HE3	1:A:84:THR:HB	1.83	0.61
1:C:1168:VAL:HA	1:C:1176:HIS:HB2	1.83	0.61
1:A:221:VAL:HG21	1:A:243:PHE:CE1	2.36	0.61
1:B:673:PRO:O	1:B:700:ASN:HA	2.01	0.61
1:B:666:LEU:HD23	1:B:666:LEU:H	1.66	0.60
1:A:158:ARG:HG3	1:B:729:ALA:HB3	1.81	0.60
1:B:608:LYS:HG2	1:B:618:PHE:CG	2.36	0.60
1:C:980:VAL:O	1:C:980:VAL:HG12	2.01	0.60
1:A:284:MET:CE	1:A:290:ILE:HD11	2.31	0.60
1:D:1532:SER:HB2	1:D:1533:PRO:HD3	1.83	0.60
1:B:669:GLY:O	1:B:670:LYS:HB2	2.01	0.60
1:A:267:ILE:CG2	1:A:270:LYS:HD2	2.30	0.60
1:D:1356:PHE:CZ	1:D:1459:ASP:HB3	2.37	0.60
1:C:845:ILE:HG22	1:C:850:LEU:CD2	2.32	0.60
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.17	0.59
1:B:644:ARG:HH11	1:B:644:ARG:HG3	1.67	0.59
1:C:900:LEU:HD23	1:C:1168:VAL:HG21	1.84	0.59
1:C:1143:LEU:HD11	1:C:1154:LEU:HD11	1.84	0.59
1:B:732:SER:HB2	1:B:733:PRO:HD3	1.84	0.59
1:D:1464:THR:HG22	1:D:1493:LEU:HD12	1.85	0.59
1:A:207:THR:HA	1:A:210:GLN:HE21	1.66	0.59
1:C:920:TYR:OH	1:C:1156:MET:HG2	2.01	0.58
1:B:604:ARG:HH11	1:B:604:ARG:HB2	1.68	0.58
1:B:667:ILE:HG13	1:B:667:ILE:O	2.03	0.58
1:C:1144:THR:HB	1:C:1145:PRO:HD3	1.84	0.58
1:D:1479:GLU:OE2	1:D:1483:LYS:HE3	2.02	0.58
1:D:1575:VAL:HG23	1:D:1576:HIS:N	2.18	0.58
1:C:1012:GLU:HA	1:C:1016:GLY:O	2.04	0.58
1:C:1151:THR:O	1:C:1153:THR:HG23	2.04	0.58
1:D:1410:GLN:O	1:D:1414:LEU:HD13	2.03	0.58
1:A:115:ARG:HG2	1:A:115:ARG:HH21	1.69	0.58
1:B:665:ALA:HB3	1:B:700:ASN:HD21	1.69	0.58
1:C:1091:ILE:HD13	1:C:1118:VAL:HG13	1.86	0.58
1:A:265:ALA:CB	1:A:275:LEU:HD11	2.34	0.58
1:D:1246:THR:O	1:D:1250:LEU:HD13	2.03	0.58
1:C:1109:ILE:HG12	1:C:1118:VAL:HB	1.85	0.57
1:C:900:LEU:CD2	1:C:1168:VAL:HG21	2.34	0.57
1:B:751:THR:O	1:B:753:THR:HG23	2.04	0.57
1:C:873:LYS:NZ	1:C:873:LYS:HB3	2.19	0.57
1:A:374:ILE:HG22	1:A:377:PRO:HD3	1.86	0.57
1:C:975:VAL:HG22	1:C:1060:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1278:MET:HA	1:D:1282:GLU:OE2	2.05	0.57
1:D:1399:MET:HG3	1:D:1417:LYS:HG3	1.86	0.57
1:D:1386:GLN:HE22	1:D:1393:ARG:NH1	2.03	0.57
1:C:1132:SER:HB2	1:C:1133:PRO:HD3	1.87	0.57
1:D:1399:MET:SD	1:D:1417:LYS:HD2	2.45	0.56
1:A:222:ASP:O	1:A:223:ASP:CB	2.52	0.56
1:B:653:LYS:HE2	1:B:654:GLU:OE2	2.06	0.56
1:B:670:LYS:HD3	1:B:671:PRO:HD2	1.87	0.56
1:C:823:VAL:O	1:C:827:VAL:HG23	2.06	0.56
1:C:927:ARG:HB3	1:C:927:ARG:NH1	2.21	0.56
1:B:500:LEU:HD23	1:B:768:VAL:HG21	1.86	0.56
1:A:87:VAL:HG12	1:A:115:ARG:HD3	1.87	0.56
1:C:834:ILE:HG12	1:C:856:THR:HG21	1.87	0.56
1:B:522:MET:HE2	1:B:739:LEU:HD23	1.87	0.55
1:C:903:LEU:O	1:C:903:LEU:HG	2.05	0.55
1:A:310:VAL:HG12	1:A:312:LYS:HG2	1.89	0.55
1:B:645:LYS:C	1:B:647:GLN:H	2.10	0.55
1:A:36:GLU:OE2	1:A:61:ALA:HB2	2.07	0.55
1:B:447:ASP:O	1:B:451:THR:HG23	2.07	0.55
1:A:110:GLU:O	1:A:114:LYS:HG3	2.07	0.55
1:A:3:ILE:CG2	1:A:33:VAL:HG22	2.36	0.55
1:C:802:LYS:HZ3	1:C:834:ILE:HD12	1.71	0.55
1:C:961:PRO:HG2	1:C:963:MET:HE3	1.88	0.55
1:B:537:LEU:HD13	3:B:875:HOH:O	2.07	0.55
1:A:284:MET:CE	1:A:315:VAL:HG11	2.37	0.54
1:B:676:ILE:O	1:B:702:PRO:HD2	2.08	0.54
1:D:1555:VAL:HG22	1:D:1555:VAL:O	2.05	0.54
1:A:142:ASN:HD21	1:A:186:GLN:HE21	1.54	0.54
1:A:204:ARG:HD3	2:A:701:NAI:O2B	2.07	0.54
1:B:433:VAL:C	1:B:434:ILE:HD12	2.28	0.54
1:C:958:ARG:HG3	1:D:1529:ALA:HB3	1.88	0.54
1:A:18:ILE:HG13	1:A:19:SER:N	2.23	0.54
1:B:653:LYS:O	1:B:656:VAL:HG12	2.07	0.54
1:C:887:VAL:HG12	1:C:915:ARG:HD3	1.89	0.54
1:B:473:LYS:NZ	1:B:473:LYS:HB3	2.23	0.54
1:D:1386:GLN:HE22	1:D:1393:ARG:HH12	1.55	0.54
1:B:604:ARG:HB2	1:B:604:ARG:NH1	2.22	0.54
1:C:1151:THR:HG23	1:C:1153:THR:OG1	2.08	0.54
1:D:1276:ARG:CZ	1:D:1305:ASN:ND2	2.71	0.53
1:B:584:GLY:O	1:B:588:ILE:HG13	2.09	0.53
1:A:58:ALA:HB3	1:A:64:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1441:GLU:OE1	1:D:1445:LYS:NZ	2.42	0.53
1:A:86:GLU:HA	1:A:89:LEU:HD23	1.91	0.53
1:D:1407:THR:HA	1:D:1410:GLN:HE21	1.73	0.53
1:D:1551:THR:O	1:D:1553:THR:HG23	2.08	0.53
1:B:685:LYS:HG2	3:B:897:HOH:O	2.08	0.53
1:C:878:MET:HB2	1:C:886:GLU:HG3	1.91	0.53
1:C:1011:VAL:HG21	1:C:1018:PHE:HD2	1.72	0.53
1:D:1364:MET:HA	1:D:1369:THR:HG22	1.90	0.53
1:B:522:MET:CE	1:B:739:LEU:HD23	2.39	0.53
1:B:552:GLY:HA3	1:B:691:ILE:HD11	1.89	0.53
1:D:1376:LEU:HD11	1:D:1451:VAL:HG13	1.91	0.53
1:C:833:VAL:O	1:C:856:THR:HG22	2.09	0.53
1:B:563:MET:HB2	1:B:570:VAL:HB	1.90	0.52
1:A:265:ALA:C	1:A:266:LEU:HD12	2.30	0.52
1:B:608:LYS:HE2	1:B:612:GLU:OE1	2.09	0.52
1:A:105:ASN:O	1:A:108:VAL:HG12	2.09	0.52
1:B:572:PRO:HG3	1:C:1177:PRO:HD3	1.92	0.52
1:C:846:THR:O	1:C:850:LEU:CD2	2.58	0.52
1:C:892:GLU:HG2	1:C:915:ARG:O	2.10	0.52
1:B:523:GLU:HA	1:B:537:LEU:CD1	2.39	0.52
1:D:1570:ARG:HD3	3:D:254:HOH:O	2.09	0.52
1:D:1503:LEU:HD22	1:D:1512:LYS:HD2	1.92	0.52
1:A:143:LEU:HD11	1:A:334:LEU:HD12	1.90	0.51
1:A:199:MET:HG2	1:A:254:GLU:HG2	1.92	0.51
1:D:1285:ASP:O	1:D:1289:LEU:HD22	2.10	0.51
1:A:237:LYS:HE2	1:A:238:GLU:N	2.25	0.51
1:C:902:ALA:C	1:C:904:THR:H	2.12	0.51
1:A:192:LYS:HE3	1:A:196:ALA:O	2.10	0.51
1:A:170:VAL:HG21	1:B:730:ASP:OD1	2.10	0.51
1:C:1007:THR:O	1:C:1011:VAL:HG23	2.10	0.51
1:D:1203:ILE:CG2	1:D:1233:VAL:HG22	2.40	0.51
1:B:653:LYS:HG3	1:B:654:GLU:N	2.24	0.51
1:B:500:LEU:CD2	1:B:768:VAL:HG21	2.41	0.51
1:C:943:LEU:HD21	1:C:1134:LEU:HD12	1.93	0.51
1:C:1008:LYS:HE2	1:C:1012:GLU:OE2	2.11	0.51
1:D:1362:MET:HA	1:D:1370:VAL:O	2.11	0.51
1:D:1321:ALA:HB1	1:D:1323:GLU:OE2	2.10	0.51
1:A:346:HIS:ND1	1:A:357:LYS:HG2	2.26	0.51
1:B:523:GLU:CA	1:B:537:LEU:HD11	2.40	0.51
1:D:1527:VAL:HG12	1:D:1530:ASP:HB2	1.93	0.51
1:C:958:ARG:HG2	1:D:1530:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG11	1:A:239:MET:HG3	1.93	0.50
1:A:344:THR:HB	1:A:345:PRO:HD3	1.92	0.50
1:D:1408:LYS:O	1:D:1412:GLU:HG3	2.12	0.50
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.76	0.50
1:A:221:VAL:HG21	1:A:243:PHE:HE1	1.76	0.50
1:B:409:ARG:NE	1:B:484:THR:HG21	2.27	0.50
1:B:563:MET:O	1:B:569:THR:HA	2.12	0.50
1:C:1078:GLU:O	1:C:1082:THR:HG23	2.12	0.50
1:D:1306:ARG:O	1:D:1310:GLU:HG3	2.09	0.50
1:A:170:VAL:O	1:A:170:VAL:HG13	2.11	0.50
1:B:503:LEU:HA	3:B:886:HOH:O	2.11	0.50
1:D:1568:VAL:HA	1:D:1576:HIS:HB2	1.94	0.50
1:A:162:MET:HB2	1:A:172:PRO:HD3	1.92	0.49
1:A:282:THR:HG22	1:A:313:HIS:CE1	2.47	0.49
1:C:813:GLU:OE2	1:C:1122:ASN:ND2	2.42	0.49
1:D:1245:ILE:HG22	1:D:1250:LEU:CD1	2.39	0.49
1:D:1407:THR:HA	1:D:1410:GLN:NE2	2.27	0.49
1:A:352:LYS:O	1:A:352:LYS:HG3	2.12	0.49
1:B:612:GLU:HB3	1:C:906:ARG:HD2	1.94	0.49
1:B:644:ARG:HG3	1:B:644:ARG:NH1	2.28	0.49
1:C:846:THR:O	1:C:850:LEU:HD22	2.12	0.49
1:C:1143:LEU:CD1	1:C:1154:LEU:HD11	2.41	0.49
1:B:743:LEU:C	1:B:743:LEU:HD23	2.33	0.49
1:A:348:ASP:O	1:A:352:LYS:HA	2.13	0.49
1:B:434:ILE:HG13	1:B:456:THR:OG1	2.12	0.49
1:B:610:GLN:O	1:B:613:SER:HB3	2.13	0.49
1:A:221:VAL:HG23	1:A:222:ASP:N	2.28	0.49
1:D:1544:THR:HB	1:D:1545:PRO:HD3	1.95	0.49
1:A:72:TRP:CG	1:A:339:LEU:HD13	2.48	0.49
1:B:523:GLU:HB2	1:B:537:LEU:HD11	1.95	0.49
1:C:994:LEU:HG	1:D:1394:LEU:HD21	1.94	0.49
1:A:238:GLU:OE2	1:A:270:LYS:HD3	2.13	0.49
1:A:184:GLY:O	1:A:188:ILE:HG13	2.13	0.48
1:C:1085:LYS:HG2	1:C:1088:SER:OG	2.14	0.48
1:A:278:GLU:HG3	1:A:303:LEU:HD11	1.95	0.48
1:B:537:LEU:HD12	1:B:537:LEU:N	2.28	0.48
1:A:90:ILE:HG21	1:A:117:ILE:HD13	1.95	0.48
1:B:580:VAL:HG12	1:B:580:VAL:O	2.12	0.48
1:C:802:LYS:HZ2	1:C:834:ILE:HD12	1.78	0.48
1:A:115:ARG:HG2	1:A:115:ARG:NH2	2.29	0.48
1:A:176:LEU:HG	1:A:178:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:GLY:O	1:B:584:GLY:HA3	2.14	0.48
1:A:134:MET:CE	1:A:362:THR:HG21	2.44	0.48
1:B:549:VAL:HG21	1:B:590:THR:HB	1.95	0.48
1:C:1091:ILE:HD13	1:C:1118:VAL:CG1	2.43	0.48
1:C:1078:GLU:HG3	1:C:1103:LEU:HD21	1.95	0.48
1:A:203:VAL:HG12	1:A:243:PHE:CZ	2.48	0.48
1:A:21:GLU:HA	1:A:24:LYS:HZ2	1.79	0.47
1:D:1304:THR:O	1:D:1304:THR:HG22	2.13	0.47
1:B:561:PRO:HG2	1:B:563:MET:CE	2.45	0.47
1:C:920:TYR:CE1	1:C:1167:CYS:HB2	2.49	0.47
1:C:1064:THR:HG22	1:C:1093:LEU:HD22	1.95	0.47
1:D:1470:LYS:HE2	1:D:1470:LYS:HA	1.95	0.47
1:A:376:HIS:O	1:A:376:HIS:CD2	2.67	0.47
1:B:411:PRO:HG2	3:B:905:HOH:O	2.14	0.47
1:C:865:LEU:O	1:C:866:SER:C	2.53	0.47
1:D:1221:GLU:HB2	3:D:164:HOH:O	2.15	0.47
1:D:1327:ARG:HH22	1:D:1435:TYR:CB	2.27	0.47
1:A:76:ARG:HE	1:A:105:ASN:ND2	2.12	0.47
1:B:508:VAL:HG13	1:B:509:VAL:N	2.30	0.47
1:B:695:VAL:HG22	1:B:706:PRO:HG3	1.97	0.47
1:D:1363:MET:O	1:D:1369:THR:HA	2.15	0.47
1:B:564:MET:HA	1:B:569:THR:HG22	1.97	0.47
1:C:805:ILE:N	1:C:805:ILE:HD12	2.29	0.47
1:C:821:GLU:OE2	1:C:1137:LYS:HE2	2.15	0.46
1:A:265:ALA:HB2	1:A:275:LEU:HD11	1.96	0.46
1:B:644:ARG:O	1:B:644:ARG:HG2	2.15	0.46
1:C:993:ARG:HG2	1:C:993:ARG:HH21	1.80	0.46
1:D:1203:ILE:HG21	1:D:1226:LEU:HD13	1.97	0.46
1:D:1436:ALA:HB2	2:D:702:NAI:O2B	2.15	0.46
1:D:1300:LEU:HD11	1:D:1319:ALA:HB1	1.97	0.46
1:A:180:VAL:HG12	1:A:180:VAL:O	2.15	0.46
1:B:653:LYS:HD2	1:B:657:LYS:HE2	1.96	0.46
1:B:537:LEU:CD1	1:B:537:LEU:N	2.79	0.46
1:B:556:PHE:CZ	1:B:659:ASP:HB3	2.51	0.46
1:B:652:LEU:HD13	1:B:652:LEU:O	2.15	0.46
1:C:881:GLU:CD	1:C:881:GLU:H	2.18	0.46
1:A:23:VAL:CG1	1:A:55:ALA:HB2	2.46	0.46
1:A:310:VAL:CG1	1:A:312:LYS:HG2	2.46	0.46
1:B:604:ARG:NH1	1:B:604:ARG:CB	2.79	0.46
1:A:47:ASP:HB3	1:A:57:ILE:HG13	1.98	0.46
1:B:575:VAL:HG22	1:B:660:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1386:GLN:NE2	1:D:1393:ARG:NH1	2.64	0.46
1:C:952:GLY:HA2	1:C:1091:ILE:HD11	1.97	0.46
1:C:1010:GLN:O	1:C:1013:SER:HB3	2.16	0.46
1:C:1082:THR:HG22	1:C:1113:HIS:CD2	2.51	0.46
1:C:1159:GLU:CD	1:C:1159:GLU:H	2.18	0.46
1:A:268:PRO:HA	3:A:786:HOH:O	2.15	0.45
1:A:375:VAL:O	1:A:376:HIS:CD2	2.69	0.45
1:C:904:THR:O	1:C:904:THR:HG22	2.16	0.45
1:A:276:ILE:O	1:A:302:PRO:HD2	2.16	0.45
1:B:767:CYS:O	1:B:775:VAL:HG23	2.16	0.45
1:C:877:PRO:HA	1:C:886:GLU:OE1	2.16	0.45
1:D:1306:ARG:N	1:D:1307:PRO:CD	2.79	0.45
1:C:838:GLY:O	1:C:841:VAL:HG22	2.16	0.45
1:C:911:ALA:CA	1:C:914:LYS:HD2	2.41	0.45
1:A:163:MET:CB	1:A:170:VAL:HG12	2.33	0.45
1:A:221:VAL:HG23	1:A:222:ASP:H	1.82	0.45
1:B:425:LYS:O	1:B:429:LEU:HG	2.16	0.45
1:B:679:GLU:O	1:B:682:THR:CG2	2.62	0.45
1:B:556:PHE:CZ	1:B:558:ARG:HB2	2.51	0.45
1:A:85:ASP:O	1:A:89:LEU:CD2	2.65	0.45
1:A:85:ASP:OD1	1:A:88:ALA:HB2	2.17	0.45
1:B:563:MET:O	1:B:570:VAL:N	2.38	0.45
1:C:818:ILE:HG13	1:C:819:SER:N	2.31	0.45
1:C:1143:LEU:HD11	1:C:1154:LEU:HD21	1.99	0.45
1:A:188:ILE:HG23	1:A:198:VAL:HG11	1.99	0.45
1:A:275:LEU:HG	1:A:300:ASN:HB3	1.99	0.45
1:B:523:GLU:CB	1:B:537:LEU:HD11	2.47	0.45
1:A:263:THR:HB	1:A:300:ASN:OD1	2.17	0.45
1:D:1490:ILE:HD12	1:D:1517:ILE:HD13	1.97	0.45
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.52	0.45
1:B:479:THR:OG1	1:B:481:GLU:HB2	2.17	0.45
1:C:813:GLU:OE2	1:C:875:GLN:NE2	2.43	0.45
1:C:920:TYR:CZ	1:C:1156:MET:HG2	2.51	0.45
1:C:1017:LYS:HD2	1:C:1017:LYS:N	2.32	0.45
1:D:1362:MET:HB2	1:D:1372:PRO:HD3	1.98	0.45
1:D:1507:GLY:N	1:D:1521:THR:HG23	2.32	0.44
1:A:265:ALA:O	1:A:266:LEU:HD12	2.18	0.44
1:C:927:ARG:CB	1:C:927:ARG:HH11	2.29	0.44
1:A:90:ILE:CG2	1:A:117:ILE:HD13	2.47	0.44
1:B:513:THR:HG23	1:B:772:GLY:O	2.17	0.44
1:C:804:ALA:HA	1:C:834:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:ALA:O	1:C:904:THR:N	2.44	0.44
1:B:434:ILE:HD12	1:B:434:ILE:N	2.33	0.44
1:C:956:PHE:CE2	1:C:958:ARG:HB2	2.52	0.44
1:D:1444:ARG:HD3	3:D:282:HOH:O	2.17	0.44
1:A:375:VAL:O	1:A:376:HIS:CG	2.71	0.44
1:D:1363:MET:HB2	1:D:1370:VAL:CG2	2.47	0.44
1:B:487:VAL:HG12	1:B:515:ARG:HD3	1.99	0.44
1:A:85:ASP:O	1:A:89:LEU:HD23	2.18	0.43
1:C:923:GLU:HA	1:C:937:LEU:CD1	2.48	0.43
1:D:1258:ALA:CA	1:D:1263:GLN:HE21	2.27	0.43
1:D:1570:ARG:O	1:D:1571:ASP:HB2	2.17	0.43
1:A:124:LEU:O	1:A:125:MET:C	2.57	0.43
1:A:221:VAL:HG11	1:A:247:GLN:HA	2.00	0.43
1:A:376:HIS:CD2	1:A:376:HIS:C	2.92	0.43
1:C:841:VAL:HG23	1:C:842:GLY:N	2.33	0.43
1:C:942:ASN:O	1:C:986:GLN:HG2	2.18	0.43
1:D:1250:LEU:CD1	1:D:1250:LEU:N	2.81	0.43
1:A:310:VAL:HG11	3:A:765:HOH:O	2.18	0.43
1:C:927:ARG:NH1	1:C:927:ARG:CB	2.81	0.43
1:A:161:PRO:HB3	1:A:194:LEU:O	2.17	0.43
1:A:281:VAL:HG22	1:A:284:MET:HE1	2.00	0.43
1:A:359:GLU:OE1	1:A:359:GLU:N	2.45	0.43
1:A:136:ILE:O	1:A:140:GLN:HG2	2.19	0.43
1:B:666:LEU:O	1:B:666:LEU:HG	2.19	0.43
1:B:768:VAL:C	1:B:775:VAL:HG22	2.39	0.43
1:B:472:TRP:CG	1:B:739:LEU:HD13	2.53	0.43
1:B:588:ILE:HG23	1:B:598:VAL:HG11	1.99	0.43
1:D:1207:LYS:HG3	1:D:1239:ALA:HA	2.00	0.43
1:B:645:LYS:C	1:B:647:GLN:N	2.72	0.43
1:C:834:ILE:HA	1:C:856:THR:HG23	1.99	0.43
1:C:993:ARG:HG2	1:C:993:ARG:NH2	2.34	0.43
1:C:1002:ASP:OD1	1:C:1003:VAL:N	2.51	0.43
1:A:348:ASP:C	1:A:351:THR:O	2.57	0.43
1:A:265:ALA:HB3	1:A:275:LEU:HD11	2.00	0.42
1:D:1203:ILE:HD11	1:D:1272:TRP:CG	2.55	0.42
1:D:1203:ILE:HG22	1:D:1232:GLU:O	2.19	0.42
1:D:1374:ARG:HD3	1:D:1457:LYS:O	2.19	0.42
1:B:536:ILE:HG13	1:B:537:LEU:CD1	2.44	0.42
1:C:1065:ALA:CB	1:C:1075:LEU:HD11	2.50	0.42
1:C:1161:GLU:OE2	1:C:1161:GLU:CA	2.67	0.42
1:A:18:ILE:HG13	1:A:19:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LEU:CD1	1:B:537:LEU:H	2.31	0.42
1:C:943:LEU:CD2	1:C:1134:LEU:HD12	2.49	0.42
1:D:1273:LYS:HG2	1:D:1298:CYS:HB3	2.00	0.42
1:A:375:VAL:O	1:A:375:VAL:HG23	2.19	0.42
1:C:860:THR:OG1	1:C:863:GLN:HG3	2.19	0.42
1:C:946:TYR:HB2	1:D:1363:MET:HE3	2.01	0.42
1:D:1316:LYS:HB3	1:D:1316:LYS:HE2	1.81	0.42
1:D:1385:LEU:HD23	1:D:1385:LEU:HA	1.89	0.42
1:B:560:PHE:N	1:B:561:PRO:HD2	2.35	0.42
1:B:669:GLY:O	1:B:670:LYS:CB	2.67	0.42
1:D:1510:VAL:CG2	1:D:1517:ILE:HB	2.43	0.42
1:A:156:PHE:CZ	1:A:158:ARG:HB2	2.55	0.42
1:D:1378:PHE:HB3	1:D:1475:LEU:HD13	2.01	0.42
1:A:337:LYS:HE3	1:B:567:ALA:O	2.20	0.42
1:B:491:LYS:HG2	1:B:492:GLU:N	2.34	0.42
1:C:1168:VAL:HA	1:C:1176:HIS:CB	2.50	0.42
1:D:1343:LEU:CD1	1:D:1531:ALA:HA	2.50	0.42
1:D:1356:PHE:CE2	1:D:1358:ARG:HB2	2.55	0.42
1:D:1392:LYS:HD2	1:D:1392:LYS:HA	1.84	0.42
1:A:3:ILE:HD11	1:A:72:TRP:CE2	2.55	0.42
1:D:1380:VAL:O	1:D:1380:VAL:HG12	2.20	0.42
1:C:913:THR:O	1:C:1172:GLY:HA2	2.20	0.41
1:D:1478:GLU:O	1:D:1482:THR:HG23	2.19	0.41
1:D:1209:ARG:NH1	1:D:1236:GLU:OE2	2.53	0.41
1:A:23:VAL:O	1:A:27:VAL:HG23	2.20	0.41
1:A:106:ARG:HD2	1:A:106:ARG:O	2.20	0.41
1:C:845:ILE:CG2	1:C:850:LEU:HD21	2.43	0.41
1:D:1348:ALA:HB1	1:D:1491:ILE:HG21	2.02	0.41
1:D:1537:LYS:HD2	3:D:215:HOH:O	2.20	0.41
1:C:923:GLU:HA	1:C:937:LEU:HD13	2.01	0.41
1:D:1467:ILE:HG13	1:D:1473:PRO:HD3	2.02	0.41
1:A:208:LYS:HA	1:A:218:PHE:CD1	2.55	0.41
1:A:178:PHE:HB3	1:A:275:LEU:HD12	2.02	0.41
1:A:323:VAL:N	1:A:324:PRO:CD	2.84	0.41
1:C:1148:ASP:HB3	1:C:1151:THR:HG22	2.01	0.41
1:D:1305:ASN:C	1:D:1307:PRO:HD2	2.41	0.41
1:C:1112:LYS:HE3	3:C:325:HOH:O	2.20	0.41
1:C:1149:LYS:H	1:C:1149:LYS:HG2	1.51	0.41
1:A:19:SER:O	1:A:23:VAL:HG23	2.21	0.41
1:B:761:GLU:HB2	3:B:852:HOH:O	2.20	0.41
1:D:1218:ILE:HG13	1:D:1219:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1490:ILE:HD12	1:D:1517:ILE:CD1	2.51	0.41
1:D:1575:VAL:HG23	1:D:1576:HIS:H	1.84	0.41
1:A:126:PRO:HG2	1:A:361:GLU:O	2.20	0.41
1:A:170:VAL:CG1	1:A:170:VAL:O	2.69	0.41
1:A:264:THR:O	1:A:266:LEU:HD13	2.21	0.41
1:A:348:ASP:O	1:A:351:THR:O	2.38	0.41
1:B:564:MET:CE	1:B:569:THR:HG21	2.51	0.41
1:B:621:VAL:CB	1:B:647:GLN:HA	2.51	0.41
1:D:1575:VAL:CG2	1:D:1576:HIS:N	2.84	0.41
1:B:562:MET:HA	1:B:570:VAL:O	2.20	0.41
1:C:905:ASN:HB3	1:C:906:ARG:H	1.48	0.41
1:A:332:SER:HB2	1:A:333:PRO:HD3	2.03	0.40
1:C:818:ILE:HG13	1:C:819:SER:H	1.86	0.40
1:D:1505:GLU:HA	1:D:1506:PRO:HD3	1.96	0.40
1:A:4:ALA:HB3	1:A:65:LEU:HD23	2.04	0.40
1:B:403:ILE:O	1:B:403:ILE:HG23	2.21	0.40
1:B:767:CYS:O	1:B:775:VAL:CG2	2.70	0.40
1:B:670:LYS:HD3	1:B:671:PRO:CD	2.51	0.40
1:D:1327:ARG:NH2	1:D:1435:TYR:CB	2.84	0.40
1:D:1469:GLY:O	1:D:1470:LYS:HE3	2.21	0.40
1:A:376:HIS:O	1:A:376:HIS:CG	2.73	0.40
1:C:938:SER:HB2	1:C:982:VAL:HG21	2.02	0.40
1:A:79:THR:OG1	1:A:82:GLU:HG3	2.22	0.40
1:B:580:VAL:HG23	1:B:602:ASP:HB2	2.02	0.40
1:C:980:VAL:HG11	1:C:1007:THR:HB	2.03	0.40
1:C:1161:GLU:OE2	1:C:1161:GLU:HA	2.21	0.40
1:D:1458:THR:O	1:D:1485:LYS:NZ	2.54	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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/384 (96%)	344 (94%)	21 (6%)	3 (1%)	19	9
1	B	353/384 (92%)	327 (93%)	21 (6%)	5 (1%)	11	3
1	C	349/384 (91%)	324 (93%)	18 (5%)	7 (2%)	7	1
1	D	363/384 (94%)	344 (95%)	17 (5%)	2 (1%)	25	15
All	All	1433/1536 (93%)	1339 (93%)	77 (5%)	17 (1%)	13	4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	376	HIS
1	B	502	ALA
1	C	866	SER
1	C	906	ARG
1	D	1421	VAL
1	D	1550	ASP
1	B	670	LYS
1	C	1121	THR
1	B	668	PRO
1	C	903	LEU
1	C	902	ALA
1	C	1122	ASN
1	A	233	GLY
1	B	460	THR
1	B	580	VAL
1	C	907	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/296 (98%)	279 (96%)	10 (4%)	36	27
1	B	277/296 (94%)	272 (98%)	5 (2%)	59	55
1	C	274/296 (93%)	260 (95%)	14 (5%)	24	14

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	284/296 (96%)	269 (95%)	15 (5%)	22	13
All	All	1124/1184 (95%)	1080 (96%)	44 (4%)	32	23

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	63	GLN
1	A	81	GLU
1	A	127	ARG
1	A	164	MET
1	A	224	GLU
1	A	231	THR
1	A	237	LYS
1	A	351	THR
1	A	376	HIS
1	B	560	PHE
1	B	576	LEU
1	B	608	LYS
1	B	647	GLN
1	B	653	LYS
1	C	809	ARG
1	C	856	THR
1	C	906	ARG
1	C	914	LYS
1	C	943	LEU
1	C	963	MET
1	C	970	VAL
1	C	976	LEU
1	C	1047	GLN
1	C	1052	LEU
1	C	1079	GLU
1	C	1093	LEU
1	C	1118	VAL
1	C	1150	ASP
1	D	1237	GLN
1	D	1284	THR
1	D	1312	LEU
1	D	1314	LYS
1	D	1337	LEU
1	D	1362	MET
1	D	1363	MET

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Mol	Chain	Res	Type
1	D	1376	LEU
1	D	1409	GLU
1	D	1421	VAL
1	D	1442	GLU
1	D	1550	ASP
1	D	1555	VAL
1	D	1557	LYS
1	D	1571	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	105	ASN
1	A	132	GLN
1	A	142	ASN
1	A	210	GLN
1	A	313	HIS
1	A	320	HIS
1	A	376	HIS
1	B	437	GLN
1	B	542	ASN
1	B	586	GLN
1	B	647	GLN
1	B	720	HIS
1	C	867	GLN
1	C	899	HIS
1	C	1047	GLN
1	C	1100	ASN
1	C	1120	HIS
1	D	1263	GLN
1	D	1305	ASN
1	D	1386	GLN
1	D	1410	GLN
1	D	1520	HIS

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
2	NAI	D	702	-	42,48,48	2.48	15 (35%)	47,73,73	1.96	10 (21%)
2	NAI	A	701	-	42,48,48	2.53	14 (33%)	47,73,73	1.90	9 (19%)

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
2	NAI	D	702	-	-	12/25/72/72	0/5/5/5
2	NAI	A	701	-	-	10/25/72/72	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAI	C2A-N3A	7.33	1.43	1.32
2	D	702	NAI	C2A-N3A	7.25	1.43	1.32
2	A	701	NAI	C4A-N3A	6.93	1.45	1.35
2	D	702	NAI	C7N-C3N	6.60	1.62	1.48
2	D	702	NAI	C4A-N3A	6.50	1.44	1.35
2	A	701	NAI	C7N-C3N	6.42	1.62	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	NAI	O4D-C4D	3.86	1.53	1.45
2	A	701	NAI	C6N-C5N	3.77	1.40	1.33
2	D	702	NAI	C6N-C5N	3.61	1.39	1.33
2	A	701	NAI	O4D-C4D	3.45	1.52	1.45
2	A	701	NAI	O4B-C1B	-3.30	1.36	1.41
2	A	701	NAI	C4N-C3N	-3.18	1.43	1.49
2	D	702	NAI	C4N-C3N	-2.98	1.44	1.49
2	D	702	NAI	C7N-N7N	2.84	1.40	1.33
2	D	702	NAI	C6A-C5A	2.78	1.53	1.43
2	D	702	NAI	O4B-C1B	-2.77	1.37	1.41
2	A	701	NAI	C7N-N7N	2.69	1.40	1.33
2	D	702	NAI	PN-O1N	-2.68	1.42	1.55
2	A	701	NAI	PN-O1N	-2.63	1.43	1.55
2	D	702	NAI	C3B-C4B	2.58	1.59	1.53
2	A	701	NAI	O2B-C2B	-2.54	1.37	1.43
2	D	702	NAI	O2B-C2B	-2.50	1.37	1.43
2	A	701	NAI	C3B-C4B	2.50	1.59	1.53
2	A	701	NAI	C6A-C5A	2.49	1.52	1.43
2	A	701	NAI	O3D-C3D	-2.40	1.37	1.43
2	D	702	NAI	C3D-C4D	2.39	1.59	1.53
2	A	701	NAI	C3D-C4D	2.38	1.59	1.53
2	D	702	NAI	O3B-C3B	2.27	1.48	1.43
2	D	702	NAI	O3D-C3D	-2.21	1.37	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	NAI	C3N-C2N-N1N	-6.35	114.03	123.10
2	A	701	NAI	C3N-C2N-N1N	-6.33	114.06	123.10
2	D	702	NAI	C2A-N1A-C6A	4.60	126.62	118.75
2	A	701	NAI	N3A-C2A-N1A	-4.59	121.51	128.68
2	A	701	NAI	C2A-N1A-C6A	4.52	126.49	118.75
2	D	702	NAI	N3A-C2A-N1A	-4.49	121.66	128.68
2	D	702	NAI	C5A-C6A-N6A	3.89	126.27	120.35
2	A	701	NAI	C5A-C6A-N6A	3.57	125.78	120.35
2	D	702	NAI	C5A-C6A-N1A	-3.31	112.84	120.35
2	A	701	NAI	C5A-C6A-N1A	-3.12	113.28	120.35
2	D	702	NAI	C3B-C2B-C1B	-3.01	96.45	100.98
2	A	701	NAI	O4B-C1B-C2B	3.00	111.31	106.93
2	D	702	NAI	O3D-C3D-C4D	-2.70	103.23	111.05
2	D	702	NAI	C1D-N1N-C6N	-2.65	115.13	120.83
2	A	701	NAI	O3D-C3D-C4D	-2.63	103.46	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	NAI	C1D-N1N-C6N	-2.59	115.25	120.83
2	D	702	NAI	O4D-C4D-C3D	-2.53	100.10	105.11
2	A	701	NAI	O4D-C4D-C3D	-2.48	100.20	105.11
2	D	702	NAI	O2B-C2B-C1B	2.05	118.44	110.85

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NAI	C5D-O5D-PN-O1N
2	A	701	NAI	O4D-C4D-C5D-O5D
2	A	701	NAI	C3D-C4D-C5D-O5D
2	D	702	NAI	O4B-C4B-C5B-O5B
2	D	702	NAI	C5D-O5D-PN-O1N
2	D	702	NAI	O4D-C4D-C5D-O5D
2	D	702	NAI	C3D-C4D-C5D-O5D
2	A	701	NAI	O4D-C1D-N1N-C2N
2	D	702	NAI	O4D-C1D-N1N-C2N
2	A	701	NAI	O4B-C4B-C5B-O5B
2	A	701	NAI	PN-O3-PA-O5B
2	D	702	NAI	PN-O3-PA-O5B
2	A	701	NAI	C5D-O5D-PN-O3
2	D	702	NAI	C5D-O5D-PN-O3
2	A	701	NAI	PA-O3-PN-O1N
2	D	702	NAI	PA-O3-PN-O1N
2	A	701	NAI	C5D-O5D-PN-O2N
2	D	702	NAI	C5D-O5D-PN-O2N
2	D	702	NAI	C3B-C4B-C5B-O5B
2	A	701	NAI	PA-O3-PN-O2N
2	D	702	NAI	PA-O3-PN-O2N
2	D	702	NAI	C5B-O5B-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	NAI	1	0
2	A	701	NAI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAI D 702

Ligand NAI A 701

Bond lengths

Bond angles

Torsions

Rings
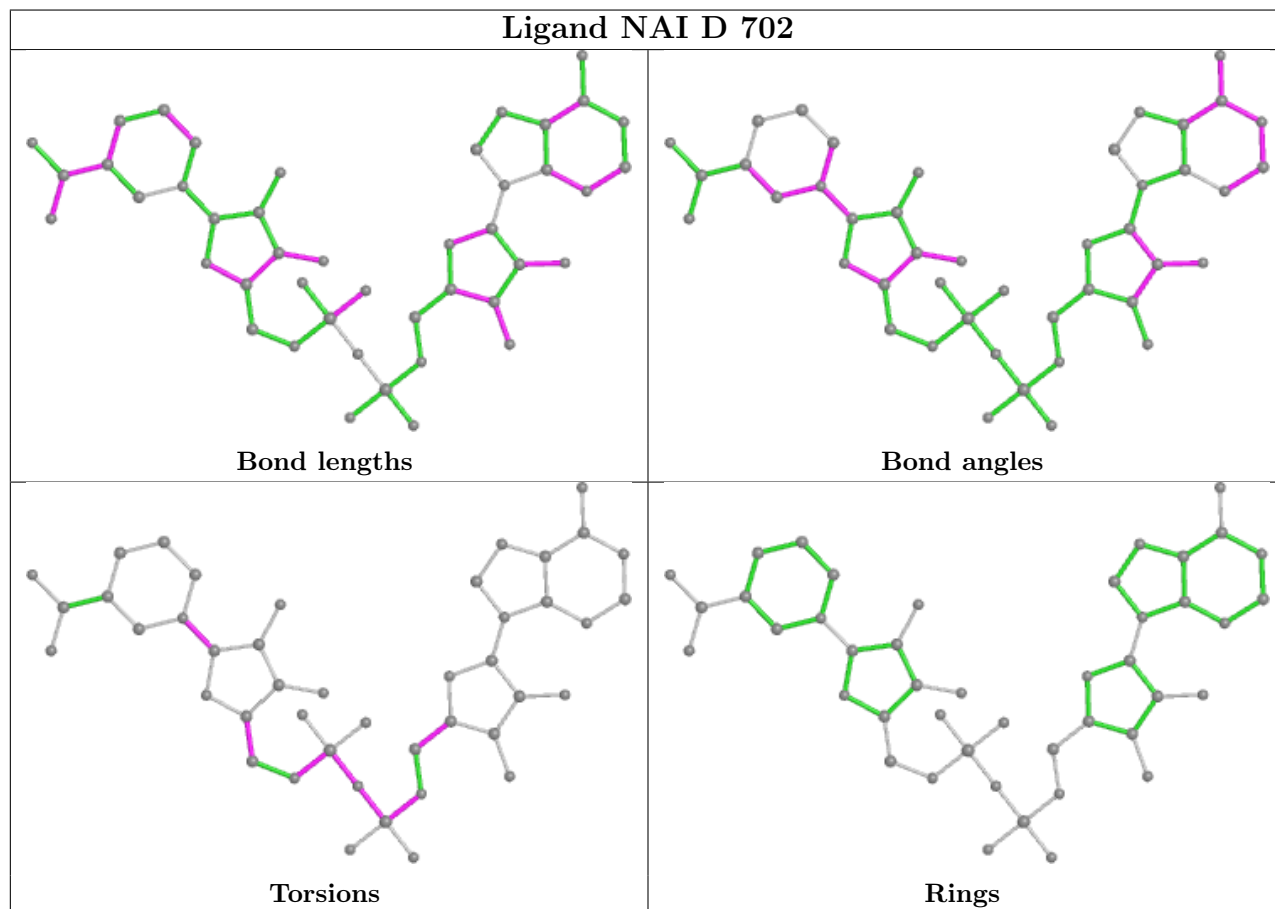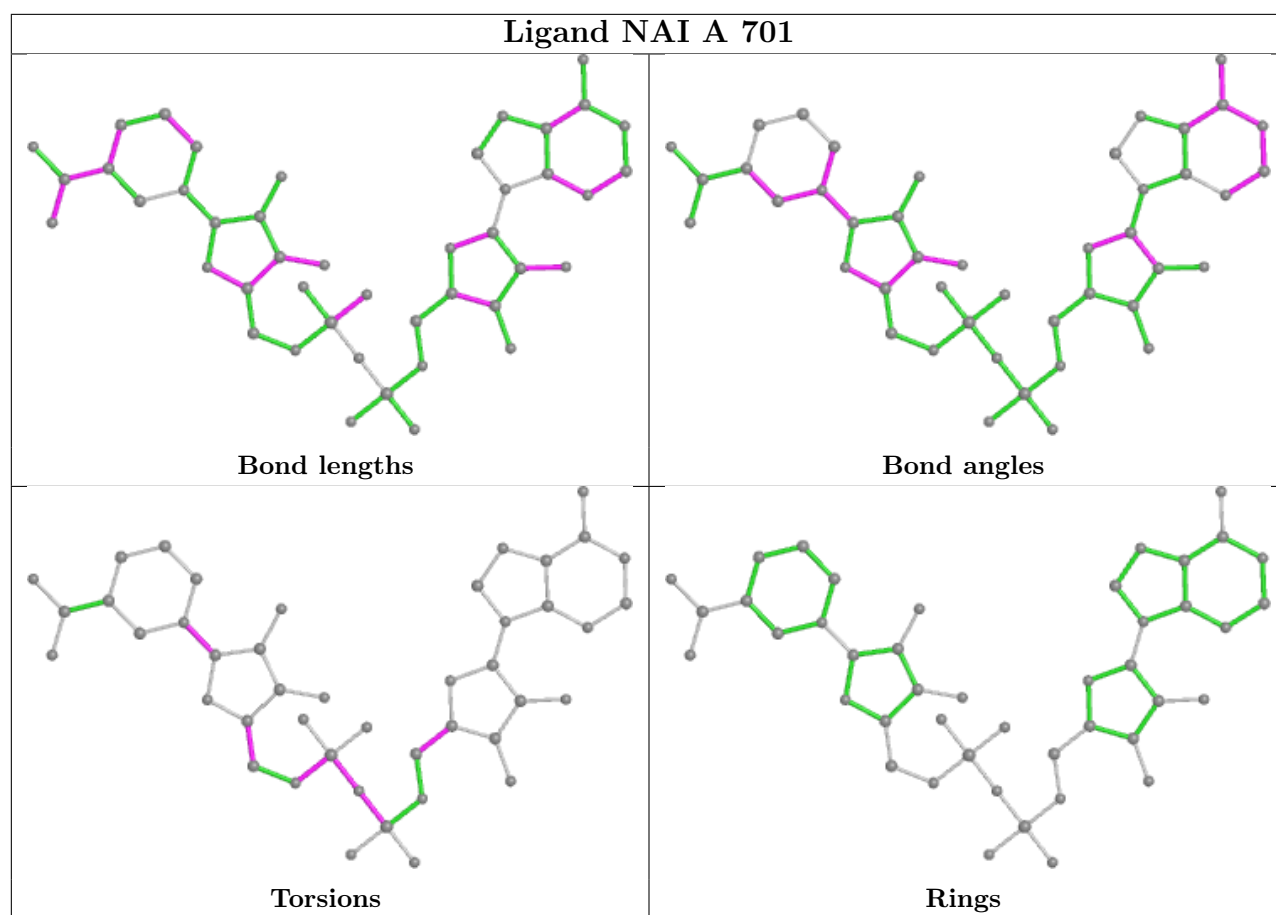
5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.