



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 3B8H / pdb_00003b8h
Title : Structure of the eEF2-ExoA(E546A)-NAD⁺ complex
Authors : Jorgensen, R.; Merrill, A.R.
Deposited on : 2007-11-01
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

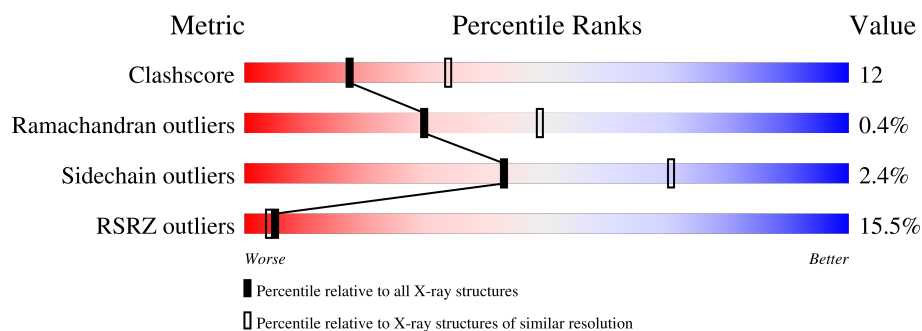
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	842	2% 70% 26% ..
1	C	842	11% 70% 26% ..
1	E	842	43% 60% 37% ..
2	B	207	% 86% 14% .
2	D	207	% 85% 14% .
2	F	207	% 86% 14% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24719 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			
1	E	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			

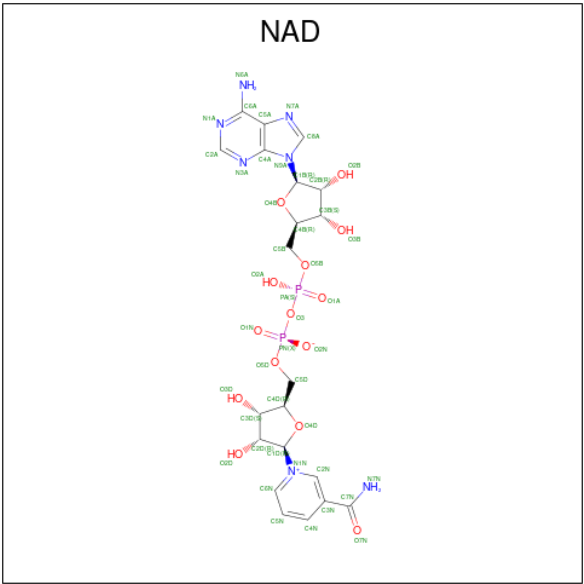
- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	1	0
			1592	1004	286	302			
2	D	207	Total	C	N	O	0	0	0
			1584	999	283	302			
2	F	207	Total	C	N	O	0	0	0
			1584	999	283	302			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	399	ALA	-	expression tag	UNP P11439
B	407	VAL	ILE	SEE REMARK 999	UNP P11439
B	515	SER	GLY	SEE REMARK 999	UNP P11439
B	546	ALA	GLU	engineered mutation	UNP P11439
D	399	ALA	-	expression tag	UNP P11439
D	407	VAL	ILE	SEE REMARK 999	UNP P11439
D	515	SER	GLY	SEE REMARK 999	UNP P11439
D	546	ALA	GLU	engineered mutation	UNP P11439
F	399	ALA	-	expression tag	UNP P11439
F	407	VAL	ILE	SEE REMARK 999	UNP P11439
F	515	SER	GLY	SEE REMARK 999	UNP P11439
F	546	ALA	GLU	engineered mutation	UNP P11439

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

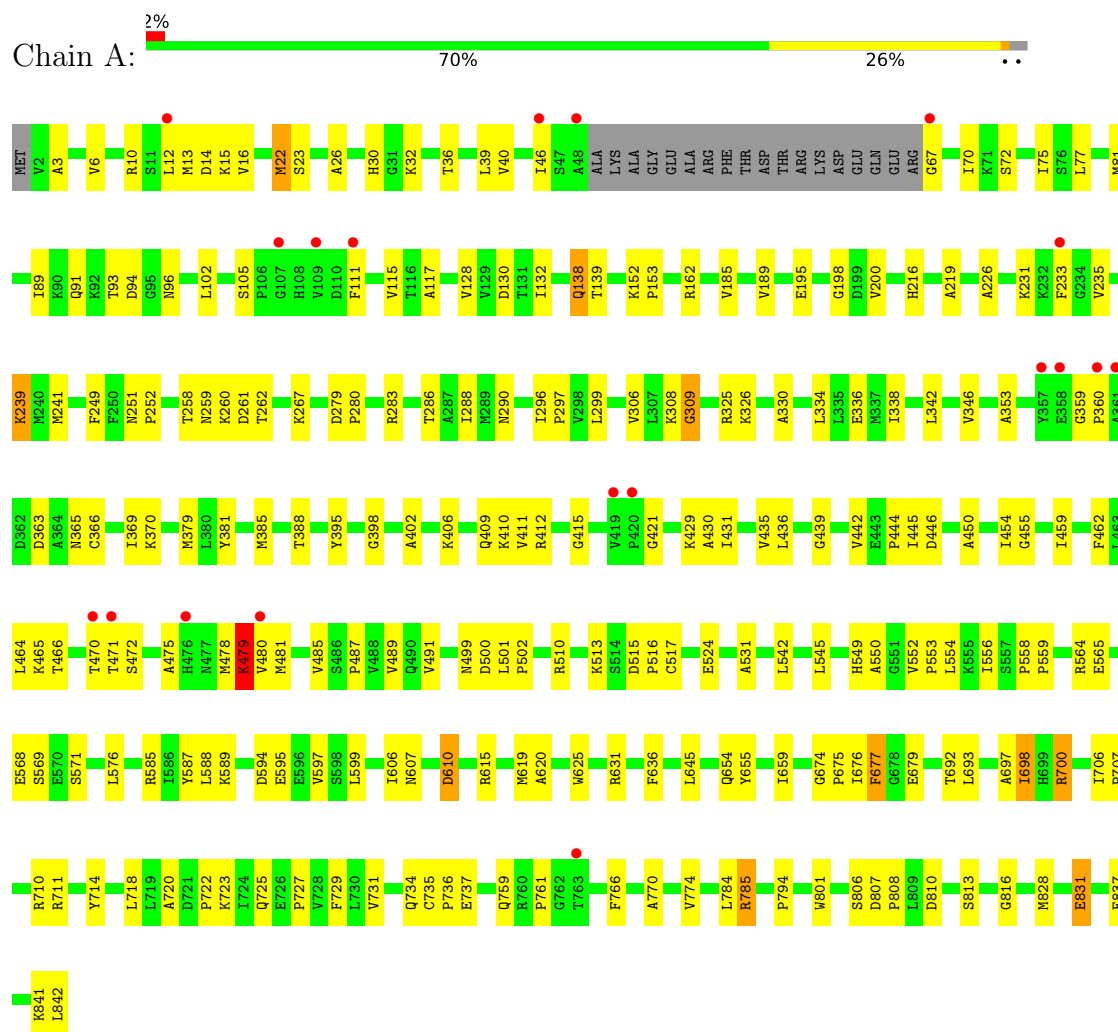
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	116	Total	O	0	0
			116	116		
4	C	77	Total	O	0	0
			77	77		
4	D	142	Total	O	0	0
			142	142		
4	E	60	Total	O	0	0
			60	60		
4	F	88	Total	O	0	0
			88	88		

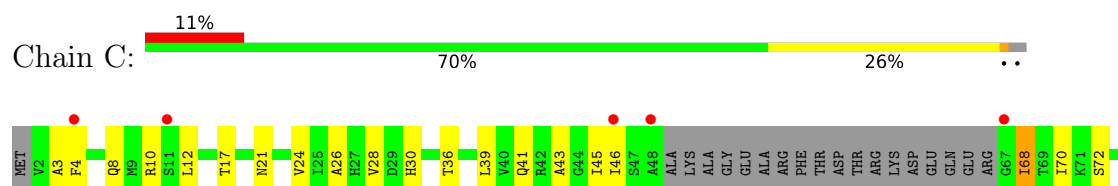
3 Residue-property plots [i](#)

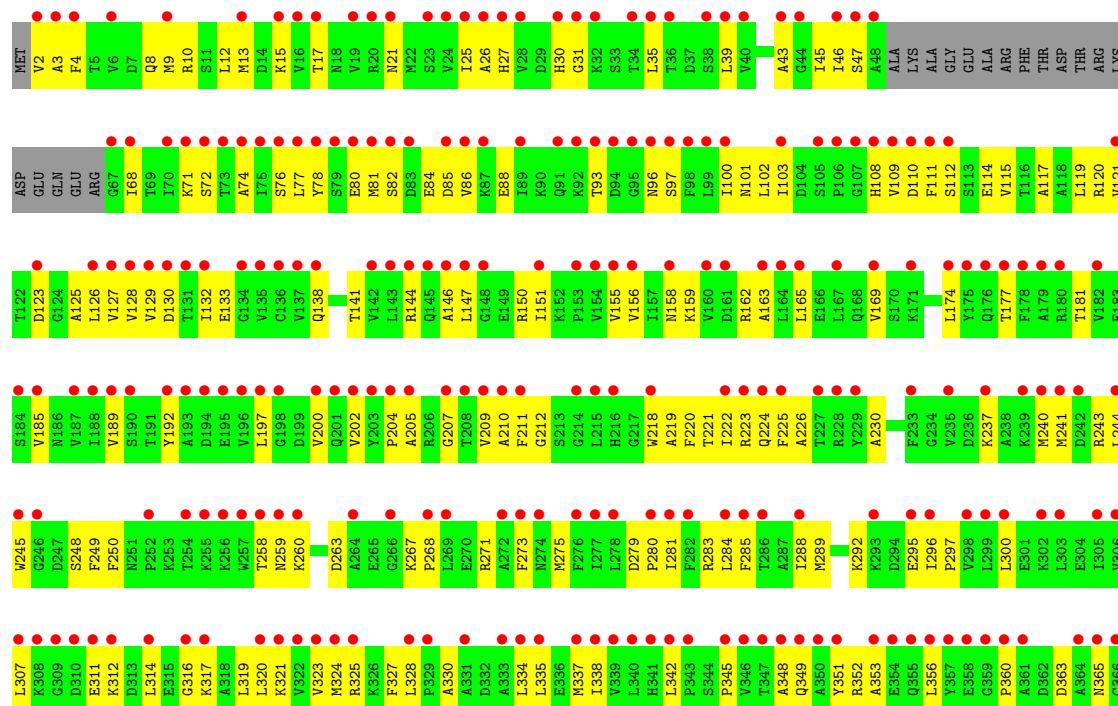
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

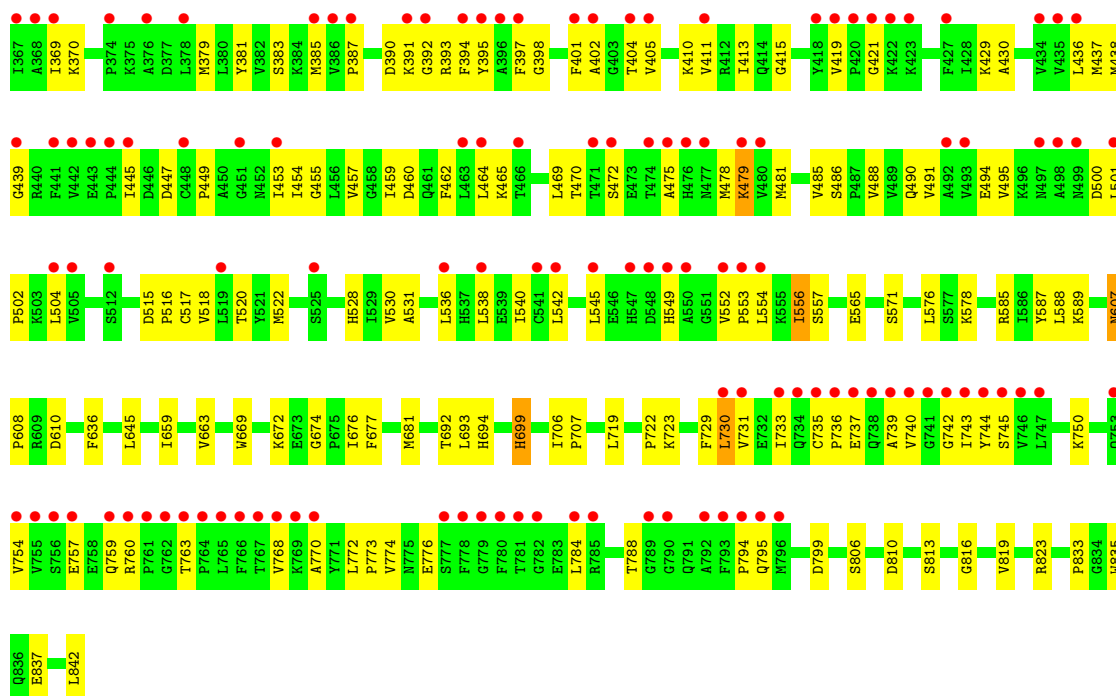
• Molecule 1: Elongation factor 2



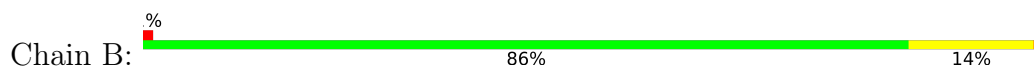
• Molecule 1: Elongation factor 2



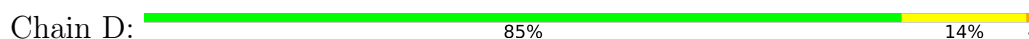




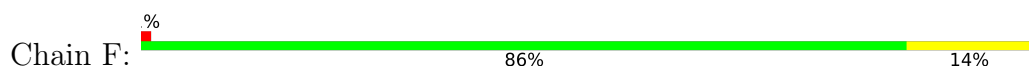
- Molecule 2: Exotoxin A



- Molecule 2: Exotoxin A



- Molecule 2: Exotoxin A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	329.44Å 68.16Å 191.63Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	24.99 – 2.50 24.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.99-2.50) 99.5 (24.99-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24719	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9175e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.27	0/6517	0.73	7/8823 (0.1%)
1	C	0.27	0/6517	0.74	9/8823 (0.1%)
1	E	0.26	0/6517	0.71	6/8823 (0.1%)
2	B	0.28	0/1634	0.71	0/2225
2	D	0.29	0/1623	0.74	2/2211 (0.1%)
2	F	0.28	0/1623	0.71	0/2211
All	All	0.27	0/24431	0.73	24/33116 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	ASN	CB-CA-C	7.34	118.34	109.31
1	E	674	GLY	CA-C-N	6.25	125.87	119.56
1	E	674	GLY	C-N-CA	6.25	125.87	119.56
1	A	674	GLY	CA-C-N	5.87	125.97	119.87
1	A	674	GLY	C-N-CA	5.87	125.97	119.87
2	D	489	ALA	N-CA-C	-5.66	105.64	112.54
2	D	438	GLY	N-CA-C	5.64	118.40	110.38
1	C	415	GLY	CA-C-N	5.53	125.88	119.47
1	C	415	GLY	C-N-CA	5.53	125.88	119.47
1	C	251	ASN	CA-C-N	5.49	125.32	119.28
1	C	251	ASN	C-N-CA	5.49	125.32	119.28
1	C	448	CYS	CA-C-N	5.36	125.34	120.03
1	C	448	CYS	C-N-CA	5.36	125.34	120.03
1	A	415	GLY	CA-C-N	5.33	124.51	118.97
1	A	415	GLY	C-N-CA	5.33	124.51	118.97
1	C	607	ASN	CA-C-N	5.31	125.12	119.28
1	C	607	ASN	C-N-CA	5.31	125.12	119.28
1	E	607	ASN	CA-C-N	5.16	124.95	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	607	ASN	C-N-CA	5.16	124.95	119.28
1	A	359	GLY	CA-C-N	5.04	124.95	119.76
1	A	359	GLY	C-N-CA	5.04	124.95	119.76
1	A	67	GLY	N-CA-C	-5.00	98.79	113.30
1	E	415	GLY	CA-C-N	5.00	124.17	118.97
1	E	415	GLY	C-N-CA	5.00	124.17	118.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	6472	152	0
1	C	6415	0	6488	158	0
1	E	6415	0	6488	243	0
2	B	1592	0	1554	20	0
2	D	1584	0	1541	16	0
2	F	1584	0	1541	19	0
3	B	44	0	26	1	0
3	D	44	0	26	1	0
3	F	44	0	26	2	0
4	A	109	0	0	2	0
4	B	116	0	0	1	0
4	C	77	0	0	0	0
4	D	142	0	0	2	0
4	E	60	0	0	1	0
4	F	88	0	0	0	0
All	All	24719	0	24162	601	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 12.

All (601) 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:785:ARG:HG2	1:A:785:ARG:HH11	1.18	1.02
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.44	0.98
1:C:404:THR:HG22	1:C:449:PRO:HA	1.48	0.95
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.54	0.89
1:C:694:HIS:CE1	1:C:699:DDE:HD2	2.09	0.88
1:E:391:LYS:HG3	1:E:392:GLY:H	1.38	0.88
1:C:759:GLN:HG2	1:C:760:ARG:H	1.43	0.84
2:B:490:ARG:HH22	2:B:492[B]:ARG:HH21	1.19	0.84
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.60	0.84
1:A:258:THR:HG22	1:A:260:LYS:H	1.43	0.83
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.58	0.82
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.61	0.82
1:C:132:ILE:HD12	1:C:132:ILE:H	1.46	0.81
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.64	0.79
1:E:404:THR:HG22	1:E:449:PRO:HA	1.64	0.79
1:A:470:THR:HG22	1:A:472:SER:H	1.47	0.78
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.66	0.78
1:E:556:ILE:HG22	1:E:557:SER:H	1.50	0.76
1:A:785:ARG:HH11	1:A:785:ARG:CG	1.99	0.75
1:A:568:GLU:HG3	1:A:723:LYS:HD2	1.69	0.73
2:B:490:ARG:HH22	2:B:492[B]:ARG:NH2	1.87	0.72
1:A:470:THR:HG21	1:A:475:ALA:HB3	1.69	0.72
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.72	0.71
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.26	0.70
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.73	0.70
1:E:141:THR:HA	1:E:144:ARG:HH11	1.57	0.69
1:C:823:ARG:HA	1:C:828:MET:HE3	1.73	0.69
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.75	0.69
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.74	0.68
1:C:699:DDE:HAC2	1:C:699:DDE:NAD	2.08	0.68
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.28	0.68
1:C:529:ILE:HG22	1:C:530:VAL:H	1.58	0.68
1:C:465:LYS:HE3	1:C:517:CYS:SG	2.34	0.68
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.74	0.67
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.75	0.67
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.76	0.67
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.76	0.67
1:C:68:ILE:HG12	1:C:390:ASP:HB2	1.77	0.66
1:C:70:ILE:HG22	1:C:388:THR:HG22	1.77	0.66
1:A:810:ASP:O	1:A:816:GLY:HA3	1.96	0.66
1:C:379:MET:HB3	1:C:478:MET:HE2	1.78	0.65
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.79	0.65
1:C:70:ILE:O	1:C:440:ARG:HG2	1.97	0.64
1:C:324:MET:HE2	1:C:324:MET:HA	1.77	0.64
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.78	0.64
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.79	0.64
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.79	0.64
2:F:490:ARG:HD3	2:F:492:ARG:HD3	1.79	0.63
1:E:324:MET:HE2	1:E:324:MET:HA	1.80	0.63
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.81	0.63
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.80	0.63
2:F:517:THR:HG23	2:F:547:GLU:HA	1.79	0.63
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.78	0.63
1:C:275:MET:HE2	1:C:276:PHE:CZ	2.34	0.63
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.34	0.63
1:C:396:ALA:HB3	1:C:456:LEU:HB2	1.81	0.62
1:E:240:MET:HE3	1:E:240:MET:HA	1.80	0.62
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.64	0.62
1:A:283:ARG:HB3	1:A:299:LEU:HD21	1.82	0.62
1:A:381:TYR:O	1:A:398:GLY:HA3	1.98	0.62
1:C:419:VAL:HG12	1:C:421:GLY:H	1.65	0.62
1:A:697:ALA:HA	1:A:700:ARG:HD2	1.81	0.62
1:A:81:MET:HE1	1:A:336:GLU:HA	1.82	0.62
1:E:26:ALA:CB	1:E:128:VAL:HB	2.30	0.62
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.82	0.61
1:C:251:ASN:HB2	1:C:269:LEU:HD22	1.82	0.61
1:E:207:GLY:O	1:E:337:MET:HG2	1.99	0.61
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.81	0.61
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.82	0.61
1:C:374:PRO:O	1:C:404:THR:HG23	1.98	0.61
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.83	0.61
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.82	0.61
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.31	0.61
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.82	0.61
1:A:10:ARG:HH22	1:A:446:ASP:HB2	1.66	0.60
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.82	0.60
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.83	0.60
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.82	0.60
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.82	0.60
2:B:460:GLN:HG3	2:B:462:LEU:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLU:HG3	1:A:723:LYS:HG3	1.83	0.59
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.84	0.59
1:E:522:MET:HE2	1:E:528:HIS:NE2	2.18	0.59
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.85	0.59
1:A:606:ILE:HD12	1:A:619:MET:HG2	1.82	0.59
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.42	0.59
1:C:106:PRO:HG3	1:C:114:GLU:HB3	1.84	0.59
2:D:488:ASP:HB2	2:D:490:ARG:H	1.67	0.59
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.84	0.59
2:B:490:ARG:NH2	2:B:492[B]:ARG:HH21	1.97	0.58
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.85	0.58
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.85	0.58
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.38	0.58
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.85	0.58
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.84	0.58
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.44	0.58
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.69	0.58
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.85	0.58
1:E:321:LYS:O	1:E:325:ARG:HG3	2.02	0.58
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.84	0.58
2:D:598:PRO:HG2	2:D:600:TYR:CE1	2.38	0.58
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.84	0.58
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.69	0.58
1:E:391:LYS:HG3	1:E:392:GLY:N	2.16	0.58
1:E:9:MET:O	1:E:13:MET:HG3	2.03	0.58
1:C:772:LEU:HD23	1:C:796:MET:HE1	1.84	0.57
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.86	0.57
1:A:785:ARG:HG2	1:A:785:ARG:NH1	1.99	0.57
1:C:759:GLN:HG2	1:C:760:ARG:N	2.16	0.57
1:C:308:LYS:HE2	1:C:326:LYS:NZ	2.20	0.57
1:C:379:MET:HE3	1:C:478:MET:HE2	1.87	0.57
1:C:585:ARG:HB2	1:C:692:THR:OG1	2.05	0.57
1:E:150:ARG:HB3	1:E:351:TYR:HE1	1.69	0.57
1:A:138:GLN:HG3	1:A:139:THR:N	2.20	0.56
1:A:568:GLU:HG3	1:A:723:LYS:CD	2.35	0.56
1:E:349:GLN:O	1:E:370:LYS:HA	2.05	0.56
2:D:432:ARG:HD2	4:D:802:HOH:O	2.05	0.56
2:D:460:GLN:HG3	2:D:462:LEU:HD11	1.88	0.56
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.88	0.56
1:E:478:MET:O	1:E:479:LYS:C	2.48	0.56
1:C:496:LYS:H	1:C:554:LEU:HD22	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:MET:HG2	1:E:465:LYS:HA	1.87	0.56
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.86	0.56
1:A:111:PHE:O	1:A:115:VAL:HG23	2.06	0.56
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.88	0.56
1:A:81:MET:O	1:A:96:ASN:HB3	2.05	0.56
1:A:198:GLY:O	1:A:200:VAL:HG23	2.06	0.56
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.87	0.56
1:C:314:LEU:HD22	1:C:318:ALA:HB1	1.87	0.56
1:C:529:ILE:HG22	1:C:530:VAL:N	2.21	0.56
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.88	0.56
1:A:10:ARG:NH2	1:A:446:ASP:H	2.04	0.55
1:A:569:SER:O	1:A:720:ALA:HB1	2.06	0.55
1:C:17:THR:HB	1:C:92:LYS:O	2.06	0.55
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.88	0.55
1:E:365:ASN:O	1:E:369:ILE:HG12	2.06	0.55
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.88	0.55
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.89	0.55
1:A:388:THR:HG21	1:A:395:TYR:CG	2.41	0.55
1:C:240:MET:HE3	1:C:244:LEU:HD21	1.87	0.55
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.87	0.55
1:C:83:ASP:O	1:C:86:VAL:HG12	2.06	0.55
1:C:511:LEU:HG	1:C:518:VAL:HG11	1.88	0.55
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.89	0.55
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.89	0.55
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.41	0.55
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.88	0.55
1:E:784:LEU:HD12	4:E:850:HOH:O	2.07	0.55
1:A:16:VAL:HG21	1:A:450:ALA:O	2.07	0.54
1:E:80:GLU:O	1:E:81:MET:HE2	2.07	0.54
1:E:226:ALA:O	1:E:230:ALA:HB2	2.07	0.54
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.07	0.54
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.43	0.54
1:E:381:TYR:O	1:E:398:GLY:HA3	2.07	0.54
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.89	0.54
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.90	0.54
1:C:279:ASP:O	1:C:283:ARG:HG2	2.07	0.54
1:E:296:ILE:O	1:E:300:LEU:HD13	2.08	0.54
1:A:654:GLN:HG2	1:A:655:TYR:CE1	2.43	0.54
1:A:258:THR:HG22	1:A:260:LYS:N	2.19	0.53
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.08	0.53
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:522:MET:HB2	2:F:490:ARG:NH2	2.23	0.53
1:A:365:ASN:O	1:A:369:ILE:HG13	2.09	0.53
1:E:810:ASP:O	1:E:816:GLY:HA3	2.08	0.53
1:A:117:ALA:HA	1:A:481:MET:SD	2.49	0.53
1:E:806:SER:HB2	1:E:813:SER:HB2	1.91	0.53
1:A:737:GLU:HB2	1:A:766:PHE:HE2	1.74	0.53
1:E:722:PRO:O	1:E:723:LYS:HD2	2.09	0.53
1:E:74:ALA:HA	1:E:102:LEU:O	2.09	0.53
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.90	0.53
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.89	0.53
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.90	0.53
1:A:200:VAL:HG12	1:A:200:VAL:O	2.07	0.53
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.44	0.53
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.39	0.53
1:C:183:GLU:O	1:C:187:VAL:HG23	2.09	0.53
1:E:21:ASN:HB2	1:E:123:ASP:OD1	2.09	0.53
2:B:470:TYR:CD2	3:B:700:NAD:H2D	2.44	0.52
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.90	0.52
1:A:478:MET:O	1:A:479:LYS:C	2.52	0.52
1:A:806:SER:HB2	1:A:813:SER:HB2	1.91	0.52
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.90	0.52
1:E:538:LEU:O	1:E:542:LEU:HG	2.09	0.52
1:A:338:ILE:O	1:A:342:LEU:HB2	2.08	0.52
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.92	0.52
1:C:43:ALA:HB1	1:C:78:TYR:O	2.09	0.52
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.90	0.52
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.44	0.52
2:F:517:THR:CG2	2:F:547:GLU:HA	2.40	0.52
1:C:81:MET:HE1	1:C:336:GLU:HA	1.92	0.52
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.75	0.52
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.92	0.52
1:E:129:VAL:HG12	1:E:130:ASP:N	2.25	0.52
1:C:810:ASP:O	1:C:816:GLY:HA3	2.09	0.52
1:A:40:VAL:HG22	1:A:75:ILE:HG21	1.90	0.51
1:A:675:PRO:HD3	1:A:714:TYR:CD1	2.45	0.51
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.92	0.51
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.45	0.51
1:E:419:VAL:HG12	1:E:421:GLY:H	1.75	0.51
1:C:274:ASN:HA	1:C:278:LEU:HB2	1.93	0.51
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.91	0.51
1:A:466:THR:HG21	1:A:481:MET:HE3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.93	0.51
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.93	0.51
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.40	0.51
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.46	0.51
1:E:391:LYS:CG	1:E:392:GLY:H	2.18	0.51
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.92	0.51
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.74	0.51
1:C:501:LEU:C	1:C:501:LEU:HD23	2.36	0.51
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.93	0.51
1:C:736:PRO:O	1:C:740:VAL:HG23	2.11	0.51
1:E:25:ILE:HG13	1:E:125:ALA:HB1	1.93	0.51
1:E:750:LYS:HD2	1:E:776:GLU:O	2.11	0.51
1:E:165:LEU:HD23	1:E:317:LYS:HE2	1.93	0.50
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.93	0.50
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.26	0.50
1:E:410:LYS:HA	1:E:430:ALA:HA	1.94	0.50
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.47	0.50
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.93	0.50
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.41	0.50
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.92	0.50
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.36	0.50
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.94	0.50
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.94	0.50
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.94	0.50
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.47	0.49
1:C:72:SER:HA	1:C:439:GLY:O	2.12	0.49
1:C:759:GLN:CG	1:C:760:ARG:H	2.12	0.49
1:C:524:GLU:HA	1:C:524:GLU:OE1	2.11	0.49
1:C:546:GLU:HA	1:C:550:ALA:HB3	1.92	0.49
1:E:108:HIS:O	1:E:111:PHE:HD2	1.95	0.49
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.94	0.49
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.93	0.49
1:C:8:GLN:O	1:C:12:LEU:HB2	2.12	0.49
1:E:82:SER:O	1:E:86:VAL:HG23	2.12	0.49
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.47	0.49
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.78	0.49
1:E:123:ASP:OD1	1:E:123:ASP:N	2.44	0.49
1:E:608:PRO:HA	1:E:636:PHE:CE2	2.47	0.49
1:A:22:MET:HG2	1:A:23:SER:N	2.26	0.49
1:A:30:HIS:NE2	1:A:130:ASP:HB2	2.27	0.49
1:E:699:DDE:HAB2	1:E:699:DDE:HAT2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:MET:HE1	1:E:316:GLY:C	2.38	0.49
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.94	0.49
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.95	0.49
1:A:93:THR:HG22	1:A:94:ASP:H	1.78	0.49
1:C:589:LYS:HD2	1:C:689:LEU:HD11	1.95	0.49
1:E:397:PHE:CD1	1:E:437:MET:HG3	2.47	0.49
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.94	0.49
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.48	0.49
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.47	0.49
1:E:117:ALA:HA	1:E:481:MET:SD	2.53	0.49
1:E:222:ILE:HD13	1:E:245:TRP:HB2	1.94	0.49
1:E:556:ILE:HG22	1:E:557:SER:N	2.24	0.49
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.95	0.49
1:C:321:LYS:O	1:C:325:ARG:HG3	2.12	0.48
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.43	0.48
1:C:826:HIS:HB2	1:C:828:MET:HE2	1.96	0.48
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.95	0.48
1:E:289:MET:HE3	1:E:320:LEU:HB2	1.94	0.48
1:E:459:ILE:O	1:E:459:ILE:HG22	2.12	0.48
1:C:30:HIS:CE1	1:C:130:ASP:HB2	2.48	0.48
1:A:72:SER:HA	1:A:439:GLY:O	2.13	0.48
1:A:828:MET:HE2	2:B:576:ARG:HE	1.78	0.48
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.28	0.48
1:E:163:ALA:O	1:E:169:VAL:HG12	2.14	0.48
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.96	0.48
1:E:588:LEU:C	1:E:588:LEU:HD12	2.38	0.48
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.94	0.48
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.94	0.48
1:A:510:ARG:HD2	1:A:549:HIS:HA	1.96	0.48
1:E:454:ILE:HG13	1:E:455:GLY:N	2.28	0.48
1:E:181:THR:O	1:E:185:VAL:HG23	2.14	0.48
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.49	0.48
1:C:3:ALA:HA	1:C:46:ILE:O	2.14	0.48
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.96	0.48
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.96	0.47
1:C:237:LYS:O	1:C:241:MET:HG2	2.14	0.47
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.29	0.47
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.96	0.47
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.47
1:A:588:LEU:HD12	1:A:588:LEU:C	2.39	0.47
1:A:785:ARG:CG	1:A:785:ARG:NH1	2.66	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.14	0.47
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.29	0.47
1:E:659:ILE:O	1:E:663:VAL:HG23	2.14	0.47
1:A:216:HIS:O	1:A:325:ARG:HG3	2.14	0.47
1:C:494:GLU:O	1:C:554:LEU:HB3	2.15	0.47
1:E:132:ILE:HD12	1:E:132:ILE:N	2.29	0.47
1:A:93:THR:HG22	1:A:94:ASP:N	2.29	0.47
1:A:479:LYS:HE3	1:A:479:LYS:HA	1.96	0.47
1:A:722:PRO:O	1:A:723:LYS:HG2	2.15	0.47
1:A:831:GLU:CD	1:A:831:GLU:H	2.21	0.47
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.47
1:C:627:VAL:O	1:C:631:ARG:HG3	2.14	0.47
1:E:223:ARG:HG3	1:E:241:MET:SD	2.54	0.47
1:E:369:ILE:HD12	1:E:401:PHE:HB3	1.96	0.47
1:A:406:LYS:HB2	1:A:409:GLN:HB2	1.96	0.47
1:A:501:LEU:N	1:A:502:PRO:HD2	2.29	0.47
1:A:568:GLU:HG3	1:A:723:LYS:CG	2.44	0.47
1:C:588:LEU:C	1:C:588:LEU:HD12	2.40	0.47
1:E:10:ARG:NH2	1:E:449:PRO:HD3	2.29	0.47
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.96	0.47
1:E:218:TRP:HB3	1:E:324:MET:HB3	1.96	0.47
1:E:279:ASP:O	1:E:283:ARG:HG2	2.14	0.47
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.95	0.47
1:A:607:ASN:O	1:A:615:ARG:HD3	2.15	0.47
2:B:516:LEU:O	2:B:545:PRO:HD2	2.14	0.47
1:E:731:VAL:HG12	1:E:770:ALA:O	2.15	0.47
1:A:286:THR:O	1:A:290:ASN:HB2	2.15	0.47
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.50	0.47
1:C:296:ILE:N	1:C:297:PRO:HD2	2.29	0.47
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.97	0.47
1:E:80:GLU:HA	1:E:96:ASN:O	2.14	0.47
1:C:498:ALA:HA	1:C:501:LEU:HB2	1.97	0.47
1:E:250:PHE:HB3	1:E:275:MET:HE1	1.95	0.47
1:E:772:LEU:HD12	1:E:773:PRO:HD2	1.96	0.47
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.97	0.46
1:C:108:HIS:ND1	1:C:109:VAL:N	2.64	0.46
1:C:401:PHE:HB2	1:C:478:MET:HE1	1.96	0.46
1:E:225:PHE:CE2	1:E:328:LEU:HD11	2.50	0.46
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.97	0.46
1:C:251:ASN:C	1:C:251:ASN:ND2	2.73	0.46
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.97	0.46
1:E:185:VAL:O	1:E:189:VAL:HG23	2.16	0.46
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.50	0.46
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.96	0.46
1:C:491:VAL:HG13	1:C:538:LEU:HD21	1.98	0.46
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.51	0.46
1:E:244:LEU:O	1:E:273:PHE:HB2	2.15	0.46
1:E:338:ILE:O	1:E:342:LEU:HB2	2.15	0.46
1:A:3:ALA:HA	1:A:46:ILE:O	2.15	0.46
1:C:379:MET:HB3	1:C:478:MET:CE	2.46	0.46
1:E:204:PRO:HA	1:E:209:VAL:HB	1.96	0.46
1:E:736:PRO:O	1:E:740:VAL:HG23	2.16	0.46
1:C:251:ASN:ND2	1:C:253:LYS:H	2.13	0.46
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.50	0.46
2:F:419:VAL:O	2:F:423:LEU:HG	2.16	0.46
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.15	0.46
1:E:109:VAL:HG12	1:E:109:VAL:O	2.15	0.46
1:A:524:GLU:CD	1:A:710:ARG:HH22	2.23	0.46
1:A:262:THR:HA	1:A:267:LYS:O	2.16	0.46
1:A:677:PHE:N	1:A:677:PHE:CD2	2.83	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.96	0.46
1:E:111:PHE:O	1:E:115:VAL:HG23	2.16	0.46
1:A:258:THR:HG21	4:A:912:HOH:O	2.15	0.46
1:C:699:DDE:HAB2	1:C:699:DDE:HAU3	1.46	0.46
2:D:420:GLU:HG2	4:D:734:HOH:O	2.17	0.45
2:F:522:GLU:CD	2:F:522:GLU:H	2.24	0.45
1:C:750:LYS:HB3	1:C:772:LEU:HD11	1.97	0.45
1:E:3:ALA:HA	1:E:46:ILE:O	2.17	0.45
1:E:119:LEU:O	1:E:151:ILE:HD11	2.16	0.45
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.97	0.45
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.98	0.45
1:E:429:LYS:HG3	1:E:462:PHE:CE2	2.51	0.45
1:E:669:TRP:CE2	2:F:492:ARG:HG3	2.51	0.45
1:A:13:MET:HE1	1:A:436:LEU:HD22	1.98	0.45
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.98	0.45
1:A:500:ASP:HB3	1:A:552:VAL:HG21	1.99	0.45
1:C:436:LEU:CD1	1:C:438:MET:HE2	2.45	0.45
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.87	0.45
2:B:490:ARG:NH2	2:B:492[B]:ARG:HE	2.15	0.45
1:E:394:PHE:HB2	1:E:460:ASP:HB3	1.99	0.45
1:A:152:LYS:HA	1:A:153:PRO:HD3	1.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:PHE:CE1	1:E:540:ILE:HD13	2.52	0.45
1:E:676:ILE:HG22	1:E:677:PHE:HD2	1.82	0.45
1:E:731:VAL:O	1:E:731:VAL:HG13	2.17	0.45
1:A:542:LEU:HD22	1:A:556:ILE:HD13	1.99	0.45
1:E:352:ARG:O	1:E:356:LEU:HG	2.17	0.45
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.48	0.45
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.85	0.45
1:C:727:PRO:HD3	1:C:801:TRP:CZ3	2.52	0.45
1:E:43:ALA:HB1	1:E:78:TYR:H	1.82	0.45
1:E:314:LEU:C	1:E:319:LEU:HB2	2.41	0.45
1:E:405:VAL:O	1:E:447:ASP:HA	2.17	0.45
1:E:411:VAL:HG13	1:E:470:THR:O	2.17	0.45
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.47	0.44
1:E:129:VAL:HG12	1:E:130:ASP:H	1.82	0.44
1:A:454:ILE:HG13	1:A:455:GLY:N	2.30	0.44
1:A:675:PRO:HD3	1:A:714:TYR:CE1	2.52	0.44
1:E:296:ILE:N	1:E:297:PRO:HD2	2.33	0.44
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.88	0.44
1:C:506:GLU:O	1:C:510:ARG:HG3	2.17	0.44
1:E:307:LEU:HD13	1:E:311:GLU:O	2.17	0.44
1:E:486:SER:O	1:E:488:VAL:HG23	2.17	0.44
1:C:460:ASP:OD1	1:C:460:ASP:N	2.51	0.44
1:E:237:LYS:HA	1:E:240:MET:HB3	2.00	0.44
1:E:485:VAL:HG22	1:E:485:VAL:O	2.17	0.44
1:A:727:PRO:HD3	1:A:801:TRP:CZ3	2.52	0.44
1:C:707:PRO:O	1:C:711:ARG:HG3	2.17	0.44
1:E:121:VAL:HG11	1:E:383:SER:OG	2.18	0.44
1:E:263:ASP:HB3	1:E:267:LYS:HB2	1.98	0.44
1:E:739:ALA:HB1	1:E:788:THR:HB	2.00	0.44
1:A:251:ASN:HA	1:A:252:PRO:HD3	1.86	0.44
1:A:454:ILE:HG13	1:A:455:GLY:H	1.83	0.44
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.44
1:E:314:LEU:O	1:E:319:LEU:HB2	2.18	0.44
1:A:470:THR:HG22	1:A:471:THR:N	2.33	0.44
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.33	0.44
1:C:491:VAL:HG12	1:C:559:PRO:HA	2.00	0.44
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.53	0.44
1:E:454:ILE:HG13	1:E:455:GLY:H	1.82	0.44
1:E:578:LYS:HB2	1:E:578:LYS:HE3	1.87	0.44
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.53	0.44
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ILE:N	1:E:46:ILE:HD12	2.33	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.32	0.44
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.91	0.44
1:C:552:VAL:HG13	1:C:553:PRO:HD2	2.00	0.44
2:D:535:LEU:HB3	2:D:536:PRO:HA	2.00	0.44
1:E:46:ILE:HG22	1:E:47:SER:N	2.33	0.44
1:E:84:GLU:O	1:E:88:GLU:HG3	2.18	0.43
1:E:501:LEU:HD23	1:E:501:LEU:C	2.43	0.43
1:E:744:TYR:CE1	1:E:754:VAL:HG21	2.53	0.43
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.18	0.43
1:A:14:ASP:OD1	1:A:15:LYS:HG3	2.18	0.43
1:A:552:VAL:HG13	1:A:553:PRO:HD2	2.01	0.43
1:A:837:GLU:HG3	4:A:871:HOH:O	2.18	0.43
1:E:464:LEU:HG	1:E:465:LYS:HG3	2.00	0.43
1:A:6:VAL:CG1	1:A:445:ILE:HG22	2.48	0.43
2:B:440:HIS:HB2	2:B:471:ILE:HG22	2.00	0.43
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.00	0.43
1:E:30:HIS:HE1	1:E:133:GLU:OE1	2.01	0.43
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.19	0.43
1:A:698:ILE:H	1:A:698:ILE:HG13	1.56	0.43
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.54	0.43
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.53	0.43
1:C:436:LEU:HD12	1:C:438:MET:HE2	2.00	0.43
1:E:39:LEU:HB3	1:E:77:LEU:HD23	2.01	0.43
1:E:72:SER:HA	1:E:439:GLY:O	2.19	0.43
1:E:288:ILE:HG22	1:E:289:MET:HE2	2.01	0.43
1:E:459:ILE:HD12	1:E:459:ILE:N	2.33	0.43
1:E:819:VAL:O	1:E:823:ARG:HG3	2.18	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.52	0.43
1:E:117:ALA:O	1:E:121:VAL:HG13	2.18	0.43
1:E:353:ALA:HB3	1:E:370:LYS:HG3	1.99	0.43
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.48	0.43
1:A:26:ALA:CB	1:A:128:VAL:HB	2.48	0.43
1:C:155:VAL:O	1:C:209:VAL:HA	2.19	0.43
1:C:314:LEU:HD13	1:C:318:ALA:O	2.19	0.43
1:E:258:THR:HG22	1:E:259:ASN:N	2.34	0.43
1:E:292:LYS:O	1:E:296:ILE:HG13	2.18	0.43
1:A:185:VAL:O	1:A:189:VAL:HG23	2.19	0.43
1:A:501:LEU:C	1:A:501:LEU:HD23	2.43	0.43
2:B:574:ASP:HA	2:B:575:PRO:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:HG21	1:C:36:THR:HG22	2.00	0.43
1:C:542:LEU:HD12	1:C:542:LEU:HA	1.84	0.43
1:E:80:GLU:C	1:E:81:MET:HE2	2.44	0.43
1:A:552:VAL:O	1:A:554:LEU:HG	2.18	0.43
1:A:727:PRO:HD3	1:A:801:TRP:HZ3	1.84	0.43
1:A:731:VAL:HG12	1:A:770:ALA:O	2.19	0.43
1:C:820:LEU:O	1:C:824:LYS:HG3	2.19	0.43
2:D:517:THR:HG23	2:D:547:GLU:HA	2.00	0.43
1:E:706:ILE:HB	1:E:707:PRO:HD3	2.01	0.43
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.54	0.42
1:C:381:TYR:O	1:C:398:GLY:HA3	2.18	0.42
1:E:25:ILE:O	1:E:127:VAL:HA	2.19	0.42
1:E:76:SER:C	1:E:77:LEU:HD12	2.44	0.42
1:E:150:ARG:HA	1:E:197:LEU:HD11	2.01	0.42
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.54	0.42
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.19	0.42
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.35	0.42
1:A:239:LYS:HB2	1:A:239:LYS:HE3	1.65	0.42
2:B:471:ILE:HG13	2:B:554:THR:HB	2.01	0.42
1:C:487:PRO:HB2	1:C:531:ALA:HB1	2.00	0.42
1:E:81:MET:HB3	1:E:85:ASP:HB2	2.01	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
1:A:841:LYS:HE3	4:B:806:HOH:O	2.18	0.42
1:E:833:PRO:HB3	1:E:837:GLU:OE1	2.19	0.42
1:A:429:LYS:HG3	1:A:462:PHE:CE2	2.54	0.42
1:A:594:ASP:HB2	1:A:597:VAL:HG23	2.00	0.42
1:C:256:LYS:HE3	1:C:256:LYS:HB3	1.92	0.42
1:C:449:PRO:HG2	1:C:452:ASN:ND2	2.34	0.42
1:C:554:LEU:HB3	1:C:555:LYS:H	1.69	0.42
2:D:428:GLN:O	2:D:432:ARG:HD3	2.19	0.42
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.54	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.87	0.42
1:E:119:LEU:HD21	1:E:146:ALA:HA	2.02	0.42
1:E:126:LEU:HD11	1:E:156:VAL:HG21	2.01	0.42
1:E:552:VAL:HG13	1:E:553:PRO:HD2	2.00	0.42
1:E:552:VAL:O	1:E:554:LEU:HG	2.20	0.42
2:F:467:ARG:CZ	2:F:536:PRO:HG3	2.49	0.42
1:A:366:CYS:O	1:A:370:LYS:HG3	2.20	0.42
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.17	0.42
1:A:288:ILE:HA	1:A:296:ILE:HD11	2.02	0.42
1:C:336:GLU:HG2	1:C:340:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ASP:HA	1:C:374:PRO:HD2	1.88	0.42
1:C:841:LYS:O	1:C:842:LEU:HD23	2.20	0.42
1:E:4:PHE:HD2	1:E:8:GLN:CD	2.27	0.42
1:E:205:ALA:HB2	1:E:245:TRP:HB3	2.01	0.42
1:E:515:ASP:HA	1:E:516:PRO:HD2	1.86	0.42
1:E:522:MET:HB2	2:F:490:ARG:HH22	1.84	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.02	0.42
1:A:385:MET:HG2	1:A:465:LYS:HA	2.02	0.42
1:E:39:LEU:HD11	1:E:334:LEU:CB	2.50	0.42
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.54	0.42
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.55	0.42
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.89	0.42
1:C:192:TYR:HA	1:C:763:THR:CG2	2.50	0.42
1:E:39:LEU:HD11	1:E:334:LEU:HB3	2.02	0.42
1:E:101:ASN:OD1	1:E:453:ILE:HB	2.20	0.42
1:E:111:PHE:HB3	1:E:114:GLU:HG2	2.02	0.42
1:E:222:ILE:CD1	1:E:245:TRP:HB2	2.50	0.42
1:E:565:GLU:O	1:E:681:MET:HA	2.20	0.42
1:E:719:LEU:HD21	1:E:835:TRP:CD2	2.54	0.42
1:E:733:ILE:HG21	1:E:743:ILE:HD11	2.01	0.42
1:A:334:LEU:O	1:A:338:ILE:HG13	2.20	0.42
1:C:45:ILE:HD11	1:C:78:TYR:HB2	2.01	0.42
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.79	0.42
1:E:141:THR:HA	1:E:144:ARG:NH1	2.31	0.42
1:E:240:MET:O	1:E:244:LEU:HG	2.19	0.42
1:A:249:PHE:CZ	1:A:261:ASP:HB3	2.55	0.41
1:A:258:THR:HG22	1:A:259:ASN:N	2.34	0.41
1:A:707:PRO:O	1:A:711:ARG:HG3	2.20	0.41
2:B:511:PHE:HB3	2:B:600:TYR:CD1	2.55	0.41
1:C:215:LEU:HD23	1:C:216:HIS:N	2.35	0.41
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.60	0.41
1:E:737:GLU:HA	1:E:740:VAL:HG23	2.02	0.41
1:E:759:GLN:HG2	1:E:760:ARG:N	2.34	0.41
1:A:410:LYS:HG2	1:A:430:ALA:HB2	2.01	0.41
1:E:150:ARG:HB3	1:E:351:TYR:CE1	2.53	0.41
1:E:156:VAL:CG2	1:E:337:MET:HE1	2.50	0.41
1:E:395:TYR:CD1	1:E:457:VAL:HG22	2.55	0.41
1:A:6:VAL:HG13	1:A:445:ILE:HG22	2.01	0.41
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.56	0.41
1:A:677:PHE:N	1:A:677:PHE:HD2	2.19	0.41
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:LEU:HA	1:C:722:PRO:HG3	2.02	0.41
1:C:759:GLN:CG	1:C:760:ARG:N	2.81	0.41
1:E:307:LEU:HB2	1:E:312:LYS:HE2	2.02	0.41
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.84	0.41
1:C:192:TYR:HA	1:C:763:THR:HG22	2.01	0.41
1:A:132:ILE:HD12	1:A:162:ARG:HD3	2.02	0.41
1:A:411:VAL:HG12	1:A:412:ARG:N	2.35	0.41
1:C:494:GLU:HG2	1:C:495:VAL:N	2.34	0.41
1:E:111:PHE:O	1:E:112:SER:C	2.63	0.41
1:E:204:PRO:C	1:E:222:ILE:HD12	2.45	0.41
1:A:410:LYS:HA	1:A:430:ALA:HA	2.02	0.41
1:C:211:PHE:O	1:C:219:ALA:HA	2.20	0.41
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.56	0.41
1:A:565:GLU:CD	1:A:676:ILE:HB	2.45	0.41
2:D:479:TYR:CG	2:D:582:LEU:HB2	2.56	0.41
1:E:200:VAL:O	1:E:200:VAL:HG22	2.20	0.41
1:E:742:GLY:O	1:E:745:SER:HB3	2.21	0.41
2:F:426:HIS:CG	2:F:594:ILE:HD12	2.56	0.41
1:A:279:ASP:HB3	1:A:280:PRO:HD3	2.01	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.97	0.41
2:B:498:LEU:HD23	2:B:498:LEU:HA	1.92	0.41
1:C:354:GLU:HG3	1:C:370:LYS:HE3	2.02	0.41
1:E:47:SER:HB3	1:E:438:MET:HE2	2.03	0.41
1:E:174:LEU:O	1:E:177:THR:HB	2.20	0.41
1:A:326:LYS:HB2	1:A:326:LYS:HE3	1.80	0.41
1:A:381:TYR:HB2	1:A:478:MET:CE	2.51	0.41
1:A:545:LEU:O	1:A:550:ALA:HB3	2.21	0.41
1:A:620:ALA:HA	1:A:625:TRP:O	2.21	0.41
1:C:12:LEU:HD12	1:C:12:LEU:HA	1.93	0.41
1:C:111:PHE:HB3	1:C:114:GLU:HB2	2.02	0.41
1:C:237:LYS:HA	1:C:240:MET:HB3	2.03	0.41
1:C:270:GLU:OE1	1:C:275:MET:HG3	2.20	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.56	0.41
1:E:114:GLU:O	1:E:117:ALA:HB3	2.21	0.41
2:F:571:ILE:HA	2:F:572:PRO:HD3	1.84	0.41
1:C:132:ILE:HD11	1:C:162:ARG:HB2	2.03	0.41
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.55	0.41
1:E:292:LYS:HD3	1:E:295:GLU:OE2	2.21	0.41
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.51	0.41
1:C:420:PRO:HG2	1:C:476:HIS:CE1	2.56	0.40
1:C:556:ILE:O	1:C:556:ILE:HG12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:831:GLU:OE1	1:C:831:GLU:N	2.51	0.40
1:E:258:THR:HG22	1:E:260:LYS:H	1.85	0.40
1:A:308:LYS:O	1:A:309:GLY:C	2.63	0.40
1:A:470:THR:HG22	1:A:472:SER:N	2.25	0.40
1:A:697:ALA:HA	1:A:700:ARG:CD	2.51	0.40
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:C:545:LEU:C	1:C:547:HIS:H	2.28	0.40
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.56	0.40
1:A:231:LYS:C	1:A:233:PHE:H	2.29	0.40
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.56	0.40
1:C:699:DDE:HAC2	1:C:699:DDE:HAD2	1.82	0.40
1:E:225:PHE:HZ	1:E:327:PHE:CZ	2.39	0.40
1:E:491:VAL:HG21	1:E:542:LEU:HD21	2.03	0.40
2:F:553:GLU:OE1	3:F:702:NAD:H6N	2.21	0.40
1:A:558:PRO:HA	1:A:559:PRO:HD3	1.98	0.40
1:C:454:ILE:HG13	1:C:455:GLY:H	1.86	0.40
1:C:565:GLU:O	1:C:681:MET:HA	2.22	0.40
1:E:17:THR:HB	1:E:93:THR:HA	2.04	0.40
1:A:431:ILE:CD1	1:A:459:ILE:HD11	2.51	0.40
1:C:711:ARG:HD2	2:D:578:VAL:O	2.22	0.40
2:D:484:ASP:OD2	2:D:494:ARG:HB2	2.21	0.40
1:E:12:LEU:HA	1:E:15:LYS:HE2	2.04	0.40
1:E:218:TRP:HZ3	1:E:220:PHE:CD2	2.39	0.40
1:E:218:TRP:C	1:E:330:ALA:HB2	2.47	0.40
1:E:243:ARG:O	1:E:248:SER:HB2	2.22	0.40
1:E:284:LEU:HD22	1:E:323:VAL:HG11	2.03	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	818/842 (97%)	780 (95%)	34 (4%)	4 (0%)	24	43
1	C	818/842 (97%)	776 (95%)	39 (5%)	3 (0%)	30	49
1	E	818/842 (97%)	750 (92%)	65 (8%)	3 (0%)	30	49
2	B	206/207 (100%)	200 (97%)	6 (3%)	0	100	100
2	D	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	24	43
2	F	205/207 (99%)	201 (98%)	3 (2%)	1 (0%)	24	43
All	All	3070/3147 (98%)	2906 (95%)	152 (5%)	12 (0%)	30	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	C	309	GLY
1	E	479	LYS
1	A	479	LYS
1	A	761	PRO
2	D	453	GLY
1	E	795	GLN
2	F	453	GLY
1	C	446	ASP
1	C	795	GLN
1	E	556	ILE
1	A	421	GLY

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	699/714 (98%)	676 (97%)	23 (3%)	33	61
1	C	699/714 (98%)	680 (97%)	19 (3%)	39	67
1	E	699/714 (98%)	694 (99%)	5 (1%)	76	89
2	B	161/160 (101%)	157 (98%)	4 (2%)	42	69
2	D	160/160 (100%)	156 (98%)	4 (2%)	42	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	160/160 (100%)	154 (96%)	6 (4%)	29 56
All	All	2578/2622 (98%)	2517 (98%)	61 (2%)	43 70

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	22	MET
1	A	138	GLN
1	A	195	GLU
1	A	235	VAL
1	A	239	LYS
1	A	306	VAL
1	A	479	LYS
1	A	480	VAL
1	A	489	VAL
1	A	499	ASN
1	A	595	GLU
1	A	599	LEU
1	A	610	ASP
1	A	631	ARG
1	A	677	PHE
1	A	698	ILE
1	A	700	ARG
1	A	718	LEU
1	A	734	GLN
1	A	785	ARG
1	A	831	GLU
1	A	842	LEU
2	B	460	GLN
2	B	462	LEU
2	B	513	ARG
2	B	540	ASP
1	C	28	VAL
1	C	41	GLN
1	C	68	ILE
1	C	80	GLU
1	C	83	ASP
1	C	86	VAL
1	C	87	LYS
1	C	154	VAL
1	C	166	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	215	LEU
1	C	251	ASN
1	C	258	THR
1	C	262	THR
1	C	460	ASP
1	C	518	VAL
1	C	524	GLU
1	C	556	ILE
1	C	730	LEU
1	C	786	GLN
2	D	462	LEU
2	D	488	ASP
2	D	538	ARG
2	D	540	ASP
1	E	211	PHE
1	E	494	GLU
1	E	672	LYS
1	E	730	LEU
1	E	842	LEU
2	F	462	LEU
2	F	494	ARG
2	F	499	LEU
2	F	540	ASP
2	F	547	GLU
2	F	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	355	GLN
1	A	414	GLN
1	A	528	HIS
1	A	791	GLN
1	A	795	GLN
2	B	428	GLN
1	C	30	HIS
1	C	96	ASN
1	C	145	GLN
1	C	452	ASN
1	C	791	GLN
2	D	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	30	HIS
1	E	259	ASN
1	E	414	GLN
1	E	583	HIS
2	F	428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	DDE	A	699	1	9,10,21	0.44	0	8,12,30	0.99	0
1	DDE	E	699	1	18,20,21	1.29	3 (16%)	17,28,30	0.93	1 (5%)
1	DDE	C	699	1	18,20,21	1.26	3 (16%)	17,28,30	0.98	1 (5%)

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
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1
1	DDE	E	699	1	-	4/20/21/23	0/1/1/1
1	DDE	C	699	1	-	12/20/21/23	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	CAT-CE1	2.73	1.54	1.49
1	E	699	DDE	CBW-NCB	-2.65	1.48	1.54
1	C	699	DDE	CG-ND1	-2.51	1.33	1.38
1	C	699	DDE	CAT-CE1	2.49	1.53	1.49
1	C	699	DDE	CBW-NCB	-2.48	1.49	1.54
1	E	699	DDE	CG-ND1	-2.36	1.34	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	699	DDE	CB-CG-CD2	-2.19	124.85	129.33
1	C	699	DDE	CB-CG-CD2	-2.06	125.12	129.33

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	699	DDE	O-C-CA-CB
1	C	699	DDE	NAD-CBI-CBW-NCB
1	C	699	DDE	CBI-CBW-NCB-CAB
1	C	699	DDE	CBI-CBW-NCB-CAC
1	C	699	DDE	CBI-CBW-NCB-CAA
1	C	699	DDE	CAU-CBW-NCB-CAB
1	C	699	DDE	CAU-CBW-NCB-CAC
1	C	699	DDE	CAU-CBW-NCB-CAA
1	C	699	DDE	CAT-CAU-CBW-CBI
1	C	699	DDE	CA-CB-CG-ND1
1	E	699	DDE	CA-CB-CG-ND1
1	C	699	DDE	CA-CB-CG-CD2
1	E	699	DDE	CA-CB-CG-CD2
1	C	699	DDE	CAT-CAU-CBW-NCB
1	E	699	DDE	CAT-CAU-CBW-NCB
1	E	699	DDE	CAT-CAU-CBW-CBI
1	C	699	DDE	NAD-CBI-CBW-CAU

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	699	DDE	2	0
1	C	699	DDE	4	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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	NAD	B	700	-	46,48,48	0.90	3 (6%)	64,73,73	1.59	10 (15%)
3	NAD	D	701	-	46,48,48	0.89	3 (6%)	64,73,73	1.58	10 (15%)
3	NAD	F	702	-	46,48,48	0.92	4 (8%)	64,73,73	1.67	11 (17%)

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	NAD	B	700	-	-	3/30/62/62	0/5/5/5
3	NAD	D	701	-	-	7/30/62/62	0/5/5/5
3	NAD	F	702	-	-	5/30/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	702	NAD	PN-O3	2.42	1.62	1.59
3	B	700	NAD	PN-O3	2.33	1.62	1.59
3	D	701	NAD	PN-O3	2.21	1.61	1.59
3	D	701	NAD	C5A-N7A	-2.11	1.35	1.39
3	B	700	NAD	C5A-N7A	-2.10	1.35	1.39
3	B	700	NAD	PA-O3	2.09	1.61	1.59
3	F	702	NAD	PA-O3	2.04	1.61	1.59
3	F	702	NAD	C5A-N7A	-2.03	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	701	NAD	C8A-N7A	2.01	1.35	1.31
3	F	702	NAD	C8A-N9A	-2.01	1.34	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	NAD	C5A-C4A-N3A	-5.47	119.19	126.72
3	D	701	NAD	C5A-C4A-N3A	-5.05	119.77	126.72
3	B	700	NAD	C5A-C4A-N3A	-4.94	119.92	126.72
3	B	700	NAD	N3A-C2A-N1A	-4.84	121.26	128.58
3	F	702	NAD	N3A-C2A-N1A	-4.77	121.36	128.58
3	F	702	NAD	O4B-C1B-N9A	4.74	117.19	108.09
3	D	701	NAD	N3A-C2A-N1A	-4.71	121.46	128.58
3	B	700	NAD	O4B-C1B-N9A	4.09	115.95	108.09
3	F	702	NAD	N3A-C4A-N9A	3.72	133.50	127.17
3	D	701	NAD	O4B-C1B-N9A	3.71	115.22	108.09
3	F	702	NAD	C2A-N3A-C4A	3.44	120.23	111.83
3	B	700	NAD	N9A-C8A-N7A	-3.37	109.16	113.94
3	B	700	NAD	C2A-N3A-C4A	3.35	120.01	111.83
3	D	701	NAD	C2A-N3A-C4A	3.34	119.98	111.83
3	D	701	NAD	N9A-C8A-N7A	-3.28	109.29	113.94
3	B	700	NAD	N3A-C4A-N9A	3.22	132.65	127.17
3	D	701	NAD	N3A-C4A-N9A	3.20	132.61	127.17
3	F	702	NAD	N9A-C8A-N7A	-3.07	109.58	113.94
3	F	702	NAD	C4B-O4B-C1B	-2.89	103.08	109.47
3	D	701	NAD	C4A-C5A-N7A	-2.55	107.67	110.58
3	B	700	NAD	C4A-N9A-C8A	2.54	108.40	105.74
3	F	702	NAD	C4A-N9A-C8A	2.51	108.38	105.74
3	B	700	NAD	C4B-O4B-C1B	-2.50	103.95	109.47
3	B	700	NAD	C4A-C5A-N7A	-2.48	107.74	110.58
3	F	702	NAD	C4A-C5A-N7A	-2.47	107.76	110.58
3	B	700	NAD	C5A-N7A-C8A	2.44	107.28	103.45
3	D	701	NAD	C5A-N7A-C8A	2.42	107.25	103.45
3	D	701	NAD	C4A-N9A-C8A	2.32	108.17	105.74
3	D	701	NAD	C4B-O4B-C1B	-2.25	104.50	109.47
3	F	702	NAD	C5A-N7A-C8A	2.24	106.98	103.45
3	F	702	NAD	C5N-C4N-C3N	-2.01	118.39	120.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

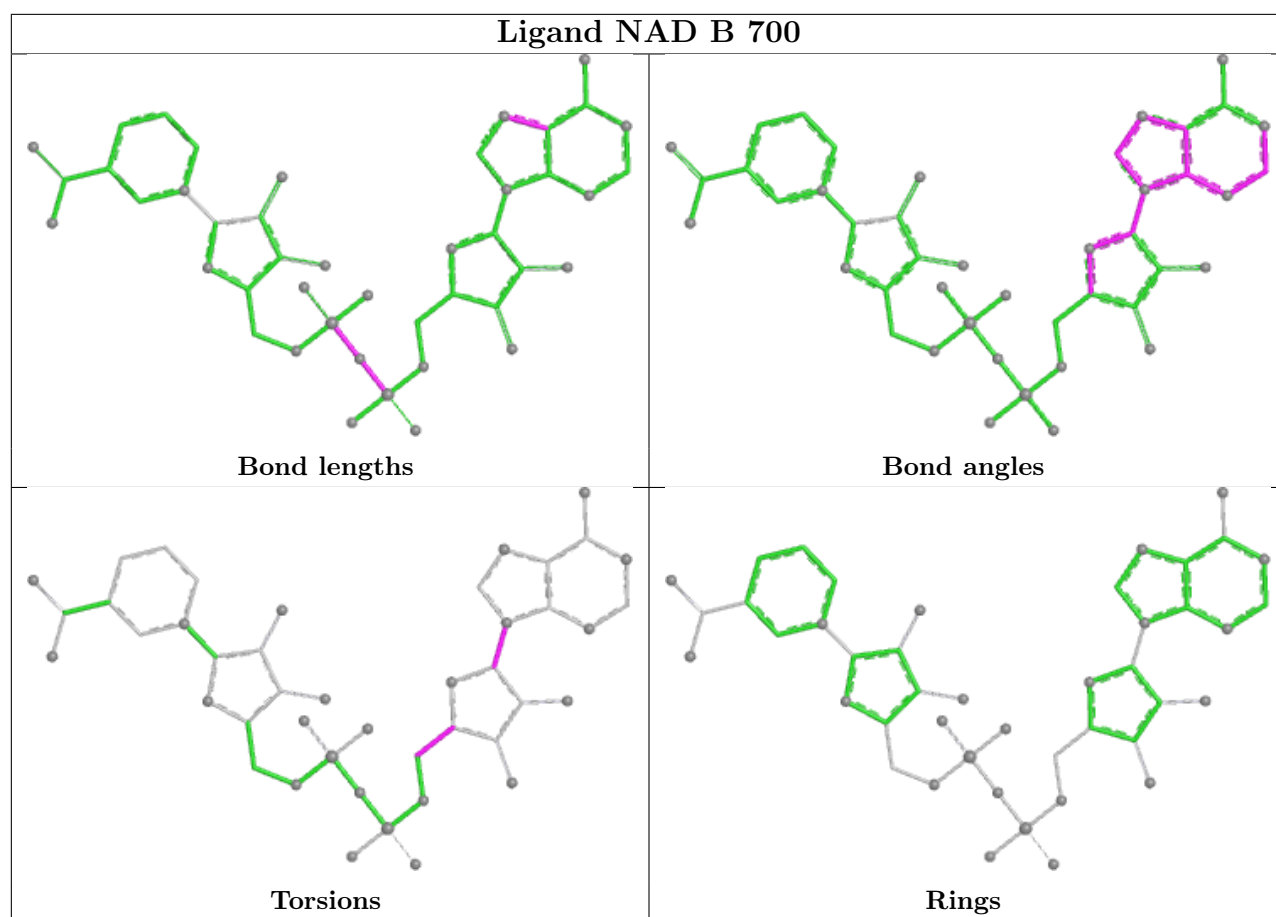
Mol	Chain	Res	Type	Atoms
3	D	701	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	C3D-C4D-C5D-O5D
3	B	700	NAD	O4B-C4B-C5B-O5B
3	B	700	NAD	C3B-C4B-C5B-O5B
3	D	701	NAD	O4B-C4B-C5B-O5B
3	F	702	NAD	O4D-C1D-N1N-C2N
3	F	702	NAD	O4D-C1D-N1N-C6N
3	D	701	NAD	PN-O3-PA-O1A
3	D	701	NAD	O4B-C1B-N9A-C8A
3	D	701	NAD	PN-O3-PA-O2A
3	B	700	NAD	O4B-C1B-N9A-C8A
3	F	702	NAD	O4B-C1B-N9A-C8A
3	F	702	NAD	O4B-C4B-C5B-O5B
3	D	701	NAD	PA-O3-PN-O2N
3	F	702	NAD	PN-O3-PA-O2A

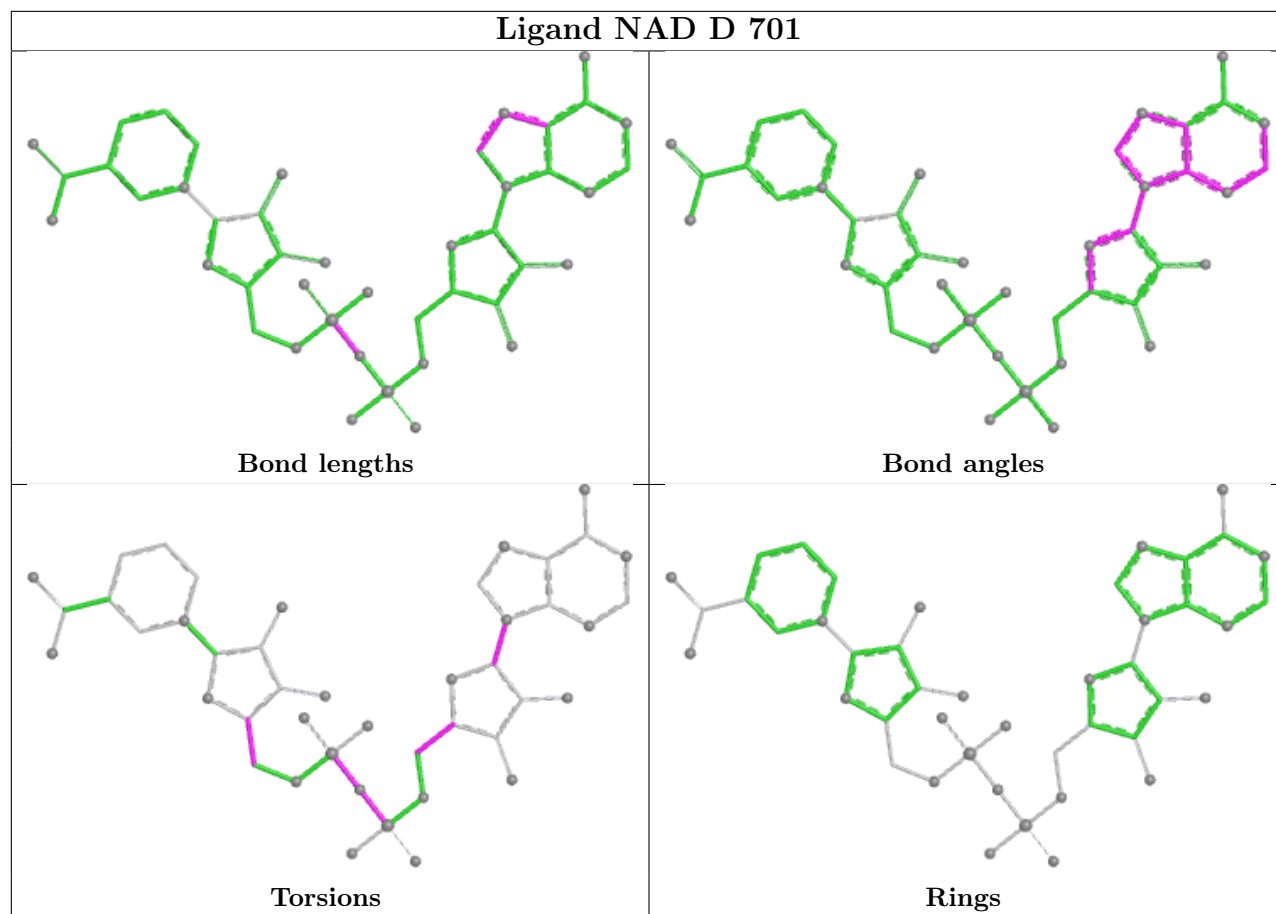
There are no ring outliers.

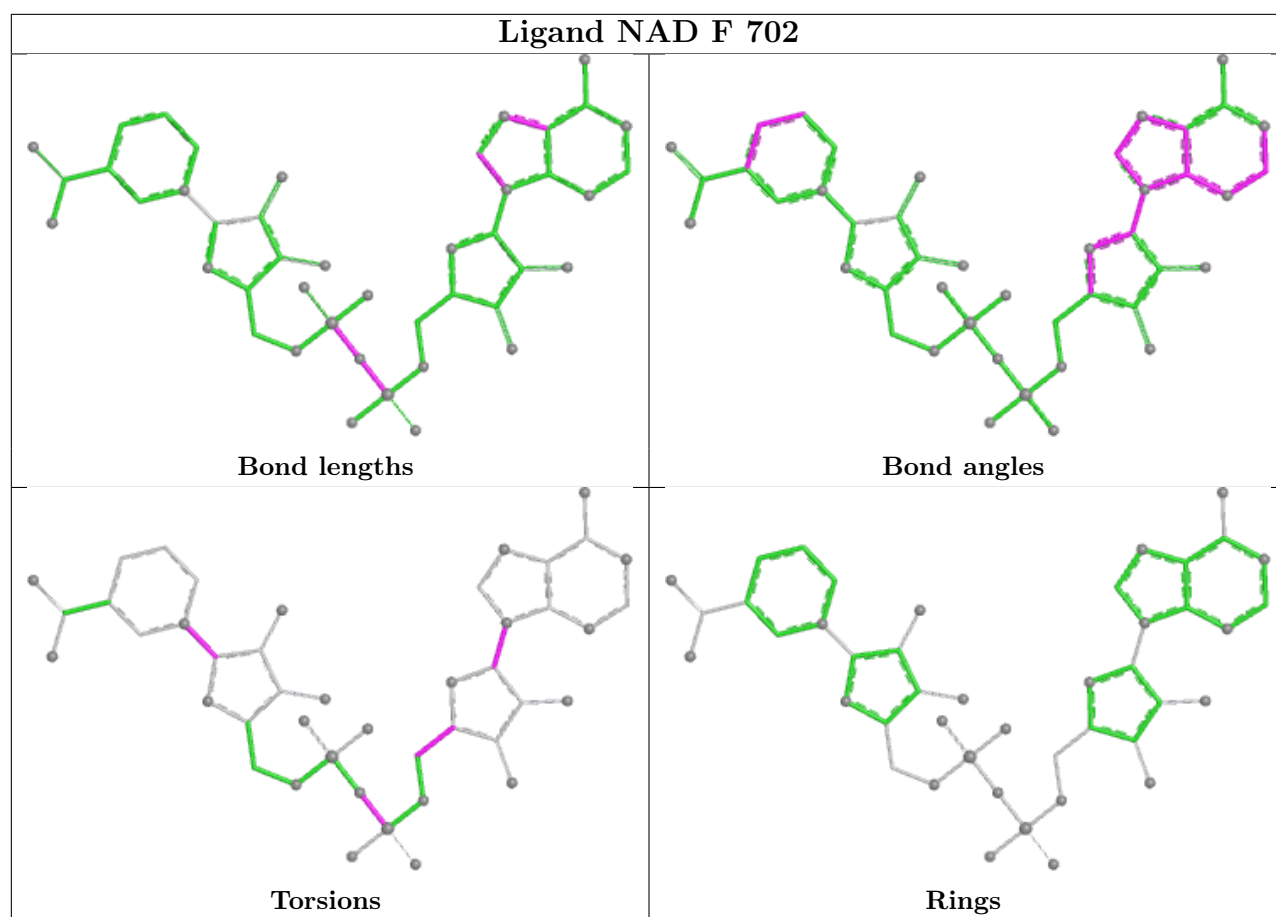
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	NAD	1	0
3	D	701	NAD	1	0
3	F	702	NAD	2	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 than 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.







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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	822/842 (97%)	0.06	19 (2%) 61 57	12, 51, 91, 113	0
1	C	822/842 (97%)	0.49	90 (10%) 10 9	13, 60, 136, 178	0
1	E	822/842 (97%)	1.71	363 (44%) 0 0	10, 124, 182, 229	0
2	B	207/207 (100%)	-0.60	2 (0%) 79 76	10, 22, 54, 89	1 (0%)
2	D	207/207 (100%)	-0.65	1 (0%) 87 85	9, 21, 52, 95	0
2	F	207/207 (100%)	-0.52	2 (0%) 79 76	12, 27, 62, 91	0
All	All	3087/3147 (98%)	0.49	477 (15%) 5 4	9, 53, 159, 229	1 (0%)

All (477) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	743	ILE	8.0
1	E	781	THR	7.0
1	E	277	ILE	6.7
1	E	196	VAL	6.5
1	C	493	VAL	6.2
1	E	175	TYR	5.9
1	E	364	ALA	5.8
1	E	755	VAL	5.8
1	E	109	VAL	5.7
1	E	306	VAL	5.7
1	E	740	VAL	5.6
1	E	245	TRP	5.5
1	E	335	LEU	5.5
1	E	768	VAL	5.5
1	E	143	LEU	5.5
1	E	78	TYR	5.4
1	E	126	LEU	5.4
1	E	155	VAL	5.3
1	C	504	LEU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	86	VAL	5.3
1	E	179	ALA	5.3
1	E	338	ILE	5.1
1	E	744	TYR	5.1
1	E	794	PRO	4.9
1	E	156	VAL	4.9
1	E	343	PRO	4.9
1	E	278	LEU	4.9
1	E	26	ALA	4.8
1	E	163	ALA	4.8
1	E	342	LEU	4.8
1	C	553	PRO	4.8
1	E	273	PHE	4.7
1	E	200	VAL	4.7
1	E	307	LEU	4.7
1	E	741	GLY	4.7
1	E	368	ALA	4.7
1	E	164	LEU	4.7
1	E	233	PHE	4.7
1	E	127	VAL	4.6
1	E	762	GLY	4.6
1	C	505	VAL	4.6
1	E	299	LEU	4.6
1	C	549	HIS	4.6
1	E	36	THR	4.6
1	E	780	PHE	4.5
1	E	339	VAL	4.5
1	E	107	GLY	4.5
1	C	216	HIS	4.4
1	E	193	ALA	4.4
1	E	19	VAL	4.3
1	E	764	PRO	4.3
1	E	553	PRO	4.3
1	E	367	ILE	4.2
1	E	276	PHE	4.2
1	E	282	PHE	4.2
1	E	68	ILE	4.2
1	C	109	VAL	4.2
1	E	770	ALA	4.2
1	E	209	VAL	4.2
1	C	521	TYR	4.1
1	E	754	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	361	ALA	4.1
1	E	97	SER	4.1
1	E	281	ILE	4.1
1	E	296	ILE	4.1
1	C	556	ILE	4.1
1	E	128	VAL	4.1
1	E	135	VAL	4.1
1	E	210	ALA	4.1
1	C	523	SER	4.1
1	E	81	MET	4.0
1	E	360	PRO	4.0
1	E	308	LYS	4.0
1	E	779	GLY	4.0
1	E	736	PRO	4.0
1	E	99	LEU	4.0
1	C	322	VAL	4.0
1	E	167	LEU	4.0
1	C	306	VAL	4.0
1	C	550	ALA	3.9
1	C	508	LEU	3.9
1	E	284	LEU	3.9
1	E	129	VAL	3.9
1	E	197	LEU	3.9
1	E	763	THR	3.9
1	E	89	ILE	3.9
1	E	98	PHE	3.9
1	A	67	GLY	3.9
1	E	747	LEU	3.9
1	C	495	VAL	3.9
1	E	67	GLY	3.8
1	C	309	GLY	3.8
1	E	158	ASN	3.8
1	E	541	CYS	3.8
1	C	498	ALA	3.8
1	E	790	GLY	3.8
1	E	311	GLU	3.8
1	C	554	LEU	3.7
1	E	493	VAL	3.7
1	E	205	ALA	3.7
1	E	70	ILE	3.7
1	E	215	LEU	3.7
1	E	32	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	288	ILE	3.7
1	E	795	GLN	3.7
1	E	192	TYR	3.7
1	E	474	THR	3.6
1	E	239	LYS	3.6
1	E	93	THR	3.6
1	E	442	VAL	3.6
1	C	524	GLU	3.6
1	E	793	PHE	3.6
1	E	323	VAL	3.6
1	E	82	SER	3.6
1	A	48	ALA	3.6
1	E	314	LEU	3.6
1	E	108	HIS	3.5
1	E	471	THR	3.5
1	E	25	ILE	3.5
1	E	476	HIS	3.5
1	C	298	VAL	3.5
1	E	536	LEU	3.5
1	E	498	ALA	3.5
1	E	240	MET	3.4
1	E	346	VAL	3.4
1	E	165	LEU	3.4
1	E	9	MET	3.4
1	E	31	GLY	3.4
1	E	366	CYS	3.4
1	E	160	VAL	3.4
1	E	194	ASP	3.4
1	E	746	VAL	3.4
1	E	761	PRO	3.4
1	E	134	GLY	3.4
1	E	492	ALA	3.4
1	E	280	PRO	3.3
1	E	316	GLY	3.3
1	E	789	GLY	3.3
1	E	188	ILE	3.3
1	E	796	MET	3.3
1	E	174	LEU	3.3
1	E	244	LEU	3.3
1	E	187	VAL	3.3
1	E	202	VAL	3.3
1	E	73	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	547	HIS	3.3
1	C	67	GLY	3.3
1	E	151	ILE	3.3
1	E	475	ALA	3.3
1	E	111	PHE	3.3
1	E	340	LEU	3.3
1	E	756	SER	3.2
1	E	734	GLN	3.2
1	E	123	ASP	3.2
1	E	16	VAL	3.2
1	E	137	VAL	3.2
1	E	154	VAL	3.2
1	E	317	LYS	3.2
1	E	79	SER	3.2
1	C	48	ALA	3.2
1	E	348	ALA	3.2
1	E	329	PRO	3.2
1	E	784	LEU	3.2
1	E	2	VAL	3.2
1	E	131	THR	3.2
1	E	742	GLY	3.2
1	E	218	TRP	3.2
1	E	184	SER	3.2
1	E	766	PHE	3.2
1	C	494	GLU	3.2
1	E	235	VAL	3.2
1	E	309	GLY	3.2
2	D	489	ALA	3.1
1	E	480	VAL	3.1
1	E	420	PRO	3.1
1	E	320	LEU	3.1
1	C	235	VAL	3.1
1	E	445	ILE	3.1
1	C	312	LYS	3.1
1	E	260	LYS	3.1
1	E	321	LYS	3.1
1	E	285	PHE	3.1
1	C	299	LEU	3.1
1	E	356	LEU	3.1
1	E	264	ALA	3.1
1	E	178	PHE	3.1
1	C	497	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	24	VAL	3.1
1	C	509	LYS	3.0
1	E	146	ALA	3.0
1	E	421	GLY	3.0
1	E	189	VAL	3.0
1	C	546	GLU	3.0
1	E	464	LEU	3.0
1	E	501	LEU	3.0
1	E	23	SER	3.0
1	E	76	SER	3.0
1	E	312	LYS	3.0
1	E	169	VAL	3.0
1	E	322	VAL	3.0
1	E	17	THR	3.0
1	E	334	LEU	3.0
1	A	233	PHE	3.0
1	E	349	GLN	3.0
1	E	733	ILE	2.9
1	E	257	TRP	2.9
1	E	444	PRO	2.9
1	E	357	TYR	2.9
1	E	427	PHE	2.9
1	C	552	VAL	2.9
1	E	185	VAL	2.9
1	E	27	HIS	2.9
1	E	347	THR	2.9
1	E	353	ALA	2.9
1	E	85	ASP	2.9
1	C	107	GLY	2.9
1	E	136	CYS	2.9
1	E	222	ILE	2.9
1	A	480	VAL	2.9
1	E	402	ALA	2.9
1	C	511	LEU	2.9
1	E	147	LEU	2.9
1	E	765	LEU	2.9
1	E	401	PHE	2.9
1	E	512	SER	2.9
1	C	496	LYS	2.9
1	C	502	PRO	2.9
2	B	489	ALA	2.9
1	E	211	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	44	GLY	2.9
1	C	323	VAL	2.8
1	E	6	VAL	2.8
1	E	142	VAL	2.8
1	E	505	VAL	2.8
1	E	268	PRO	2.8
1	E	303	LEU	2.8
1	E	554	LEU	2.8
1	E	224	GLN	2.8
1	E	171	LYS	2.8
1	E	298	VAL	2.8
1	E	254	THR	2.8
1	E	538	LEU	2.8
1	E	242	ASP	2.8
1	E	20	ARG	2.8
1	E	479	LYS	2.8
1	E	745	SER	2.8
1	E	121	VAL	2.8
1	E	405	VAL	2.8
1	C	492	ALA	2.8
1	E	91	GLN	2.8
1	E	77	LEU	2.8
1	E	258	THR	2.8
1	A	107	GLY	2.7
1	E	451	GLY	2.7
1	E	453	ILE	2.7
1	C	307	LEU	2.7
1	E	404	THR	2.7
1	E	550	ALA	2.7
1	C	285	PHE	2.7
1	C	551	GLY	2.7
1	E	40	VAL	2.7
1	E	229	TYR	2.7
1	E	208	THR	2.7
1	E	350	ALA	2.7
1	E	341	HIS	2.7
1	E	94	ASP	2.7
1	E	392	GLY	2.7
1	C	4	PHE	2.7
1	C	317	LYS	2.7
1	E	422	LYS	2.7
1	A	109	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	269	LEU	2.7
1	A	361	ALA	2.7
1	E	785	ARG	2.6
1	C	319	LEU	2.6
1	C	545	LEU	2.6
1	E	182	VAL	2.6
1	E	300	LEU	2.6
1	E	552	VAL	2.6
1	E	525	SER	2.6
1	E	30	HIS	2.6
1	C	288	ILE	2.6
1	E	369	ILE	2.6
1	E	731	VAL	2.6
1	E	355	GLN	2.6
1	E	216	HIS	2.6
1	C	513	LYS	2.6
1	E	266	GLY	2.6
1	E	46	ILE	2.6
1	E	75	ILE	2.6
1	E	385	MET	2.6
1	E	477	ASN	2.6
1	C	11	SER	2.6
1	E	112	SER	2.6
1	E	777	SER	2.6
1	C	252	PRO	2.6
1	E	100	ILE	2.6
1	E	225	PHE	2.6
1	E	778	PHE	2.6
1	C	251	ASN	2.6
1	C	763	THR	2.6
1	C	767	THR	2.6
1	E	48	ALA	2.6
1	E	760	ARG	2.5
1	C	500	ASP	2.5
1	E	110	ASP	2.5
1	C	529	ILE	2.5
1	C	233	PHE	2.5
1	A	12	LEU	2.5
1	C	269	LEU	2.5
1	C	320	LEU	2.5
1	E	759	GLN	2.5
1	C	525	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	333	ALA	2.5
1	E	177	THR	2.5
1	E	87	LYS	2.5
1	E	237	LYS	2.5
1	E	259	ASN	2.5
1	E	419	VAL	2.5
1	E	396	ALA	2.5
1	E	286	THR	2.5
1	E	223	ARG	2.5
1	A	360	PRO	2.5
1	E	395	TYR	2.5
1	E	397	PHE	2.5
1	E	92	LYS	2.5
1	E	252	PRO	2.5
1	E	359	GLY	2.5
1	C	321	LYS	2.5
1	C	501	LEU	2.5
1	E	255	LYS	2.5
1	E	302	LYS	2.5
1	E	176	GLN	2.5
1	E	441	PHE	2.5
1	E	105	SER	2.5
1	E	466	THR	2.5
1	E	214	GLY	2.4
1	E	439	GLY	2.4
1	E	351	TYR	2.4
1	E	497	ASN	2.4
1	A	470	THR	2.4
1	E	246	GLY	2.4
1	E	782	GLY	2.4
1	E	83	ASP	2.4
1	C	167	LEU	2.4
1	E	35	LEU	2.4
1	E	201	GLN	2.4
1	C	108	HIS	2.4
1	C	547	HIS	2.4
1	E	180	ARG	2.4
1	E	241	MET	2.4
1	E	274	ASN	2.4
1	E	386	VAL	2.4
1	E	792	ALA	2.4
1	E	227	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	256	LYS	2.4
1	E	504	LEU	2.4
1	E	418	TYR	2.4
1	E	96	ASN	2.4
1	C	507	GLY	2.4
1	E	198	GLY	2.4
1	E	138	GLN	2.4
1	E	325	ARG	2.4
1	E	436	LEU	2.4
1	E	4	PHE	2.4
1	E	203	TYR	2.4
1	C	264	ALA	2.4
1	A	358	GLU	2.4
1	A	46	ILE	2.3
1	C	528	HIS	2.3
2	F	488	ASP	2.3
1	E	337	MET	2.3
1	E	735	CYS	2.3
1	E	739	ALA	2.3
1	E	757	GLU	2.3
1	E	95	GLY	2.3
1	E	103	ILE	2.3
1	E	448	CYS	2.3
1	A	419	VAL	2.3
1	E	28	VAL	2.3
1	E	737	GLU	2.3
1	E	43	ALA	2.3
1	E	767	THR	2.3
1	E	207	GLY	2.3
1	E	305	ILE	2.3
1	E	545	LEU	2.3
1	E	769	LYS	2.3
1	C	757	GLU	2.3
1	E	354	GLU	2.3
1	E	21	ASN	2.3
1	E	365	ASN	2.3
1	E	34	THR	2.3
1	C	266	GLY	2.3
1	C	421	GLY	2.3
1	C	503	LYS	2.3
1	E	195	GLU	2.3
1	E	394	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	434	VAL	2.3
1	E	145	GLN	2.2
1	C	512	SER	2.2
1	C	544	ASP	2.2
1	C	527	GLU	2.2
1	A	111	PHE	2.2
1	E	144	ARG	2.2
1	E	74	ALA	2.2
1	C	762	GLY	2.2
1	C	46	ILE	2.2
1	E	387	PRO	2.2
1	E	376	ALA	2.2
1	E	499	ASN	2.2
1	E	391	LYS	2.2
1	A	763	THR	2.2
1	E	753	GLN	2.2
1	C	522	MET	2.2
1	E	519	LEU	2.2
1	E	542	LEU	2.2
1	E	130	ASP	2.2
1	E	80	GLU	2.2
1	E	411	VAL	2.2
1	E	549	HIS	2.2
1	E	324	MET	2.2
1	C	536	LEU	2.2
1	E	132	ILE	2.2
1	E	435	VAL	2.1
1	E	3	ALA	2.1
1	C	519	LEU	2.1
1	C	526	GLY	2.1
1	E	443	GLU	2.1
1	C	555	LYS	2.1
1	E	153	PRO	2.1
1	E	374	PRO	2.1
1	E	13	MET	2.1
1	E	39	LEU	2.1
1	A	357	TYR	2.1
1	C	506	GLU	2.1
2	F	461	ASP	2.1
1	C	232	LYS	2.1
1	E	106	PRO	2.1
1	E	345	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	476	HIS	2.1
1	C	169	VAL	2.1
1	E	331	ALA	2.1
1	E	228	ARG	2.1
1	E	295	GLU	2.1
1	E	358	GLU	2.1
1	E	293	LYS	2.1
1	E	190	SER	2.1
1	E	472	SER	2.1
1	E	204	PRO	2.1
1	E	272	ALA	2.1
1	C	303	LEU	2.1
1	E	378	LEU	2.1
1	E	463	LEU	2.1
1	C	234	GLY	2.1
1	C	316	GLY	2.1
1	A	471	THR	2.1
1	C	445	ILE	2.1
1	E	310	ASP	2.1
1	E	47	SER	2.1
1	A	420	PRO	2.1
1	E	738	GLN	2.0
1	E	148	GLY	2.0
1	C	308	LYS	2.0
1	E	15	LYS	2.0
1	E	71	LYS	2.0
1	E	423	LYS	2.0
1	E	548	ASP	2.0
1	E	72	SER	2.0
1	C	111	PHE	2.0
1	C	291	PHE	2.0
1	C	739	ALA	2.0
1	E	328	LEU	2.0
1	E	730	LEU	2.0
1	E	161	ASP	2.0
2	B	461	ASP	2.0
1	C	229	TYR	2.0
1	E	38	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	DDE	A	699	10/21	0.88	0.10	40,49,57,57	0
1	DDE	C	699	20/21	0.91	0.15	14,61,107,114	0
1	DDE	E	699	20/21	0.91	0.15	30,62,75,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

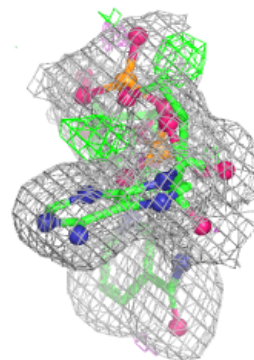
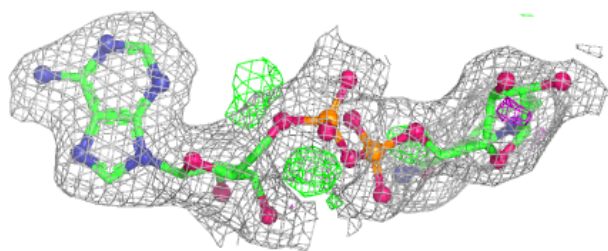
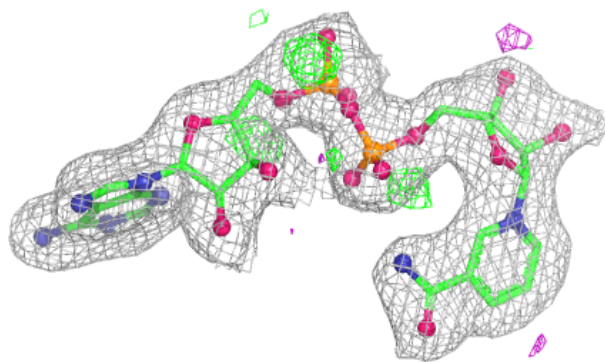
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAD	B	700	44/44	0.97	0.07	4,20,39,42	0
3	NAD	D	701	44/44	0.97	0.07	7,22,38,45	0
3	NAD	F	702	44/44	0.97	0.06	11,24,38,48	0

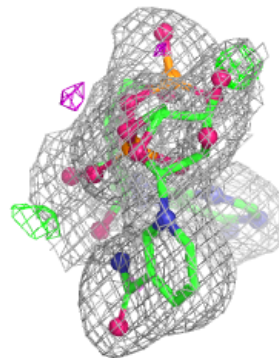
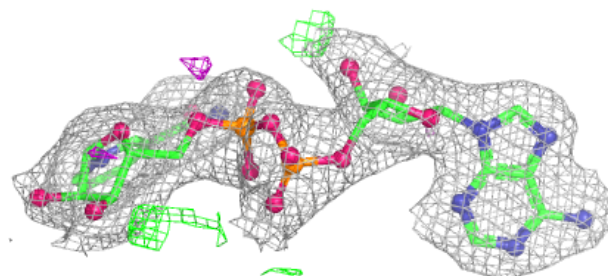
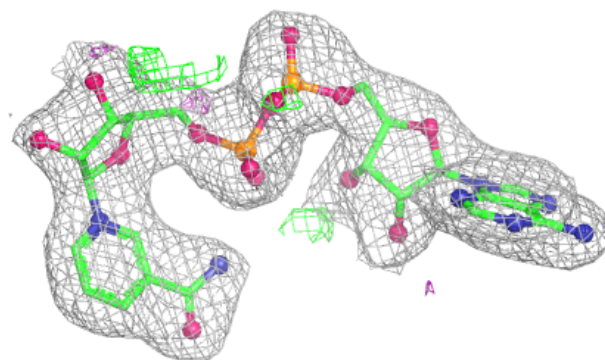
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

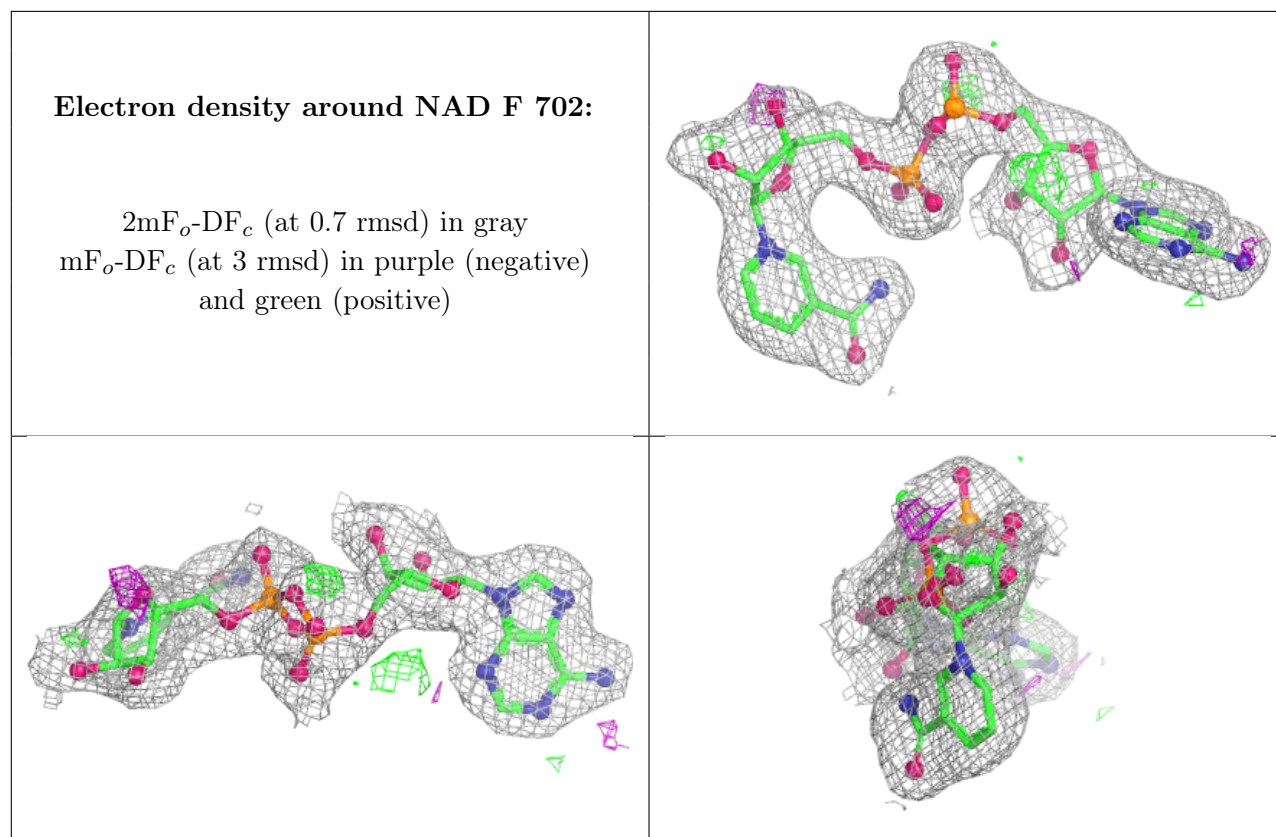
Electron density around NAD B 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD D 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.