



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:02 AM UTC

PDB ID : 3B82 / pdb_00003b82
Title : Structure of the eEF2-ExoA(E546H)-NAD⁺ complex
Authors : Jorgensen, R.; Merrill, A.R.
Deposited on : 2007-10-31
Resolution : 2.35 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

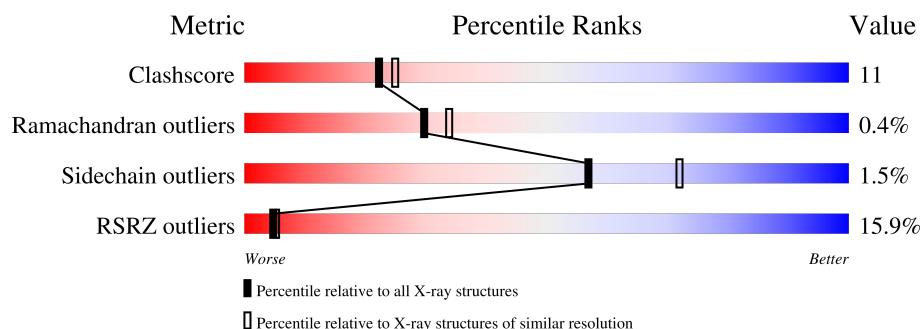
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	4% 74% 23% ..
1	C	842	9% 72% 25% ..
1	E	842	44% 64% 32% ..
2	B	207	84% 16%
2	D	207	% 86% 13% .
2	F	207	% 86% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24682 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	0	0
			1589	1002	285	302			
2	D	207	Total	C	N	O	0	0	0
			1589	1002	285	302			
2	F	207	Total	C	N	O	0	0	0
			1589	1002	285	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	HIS	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	HIS	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	HIS	GLU	engineered mutation	UNP P11439

- # NAD

- Molecule 4 is water.

WORLDWIDE
 **PDB**
PROTEIN DATA BANK

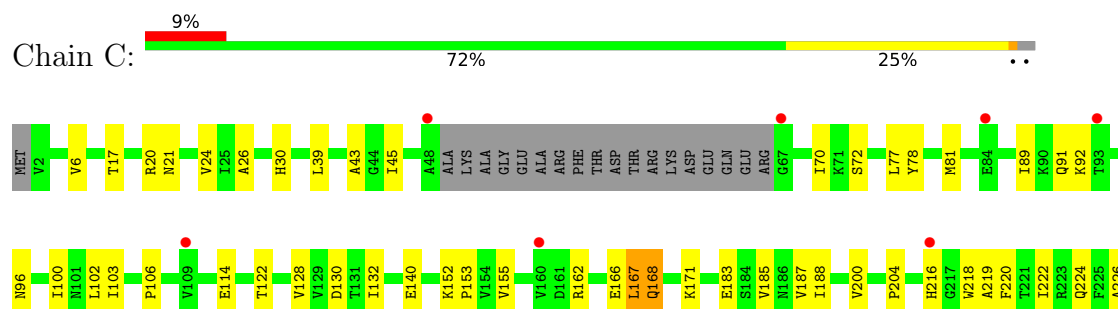
3 Residue-property plots

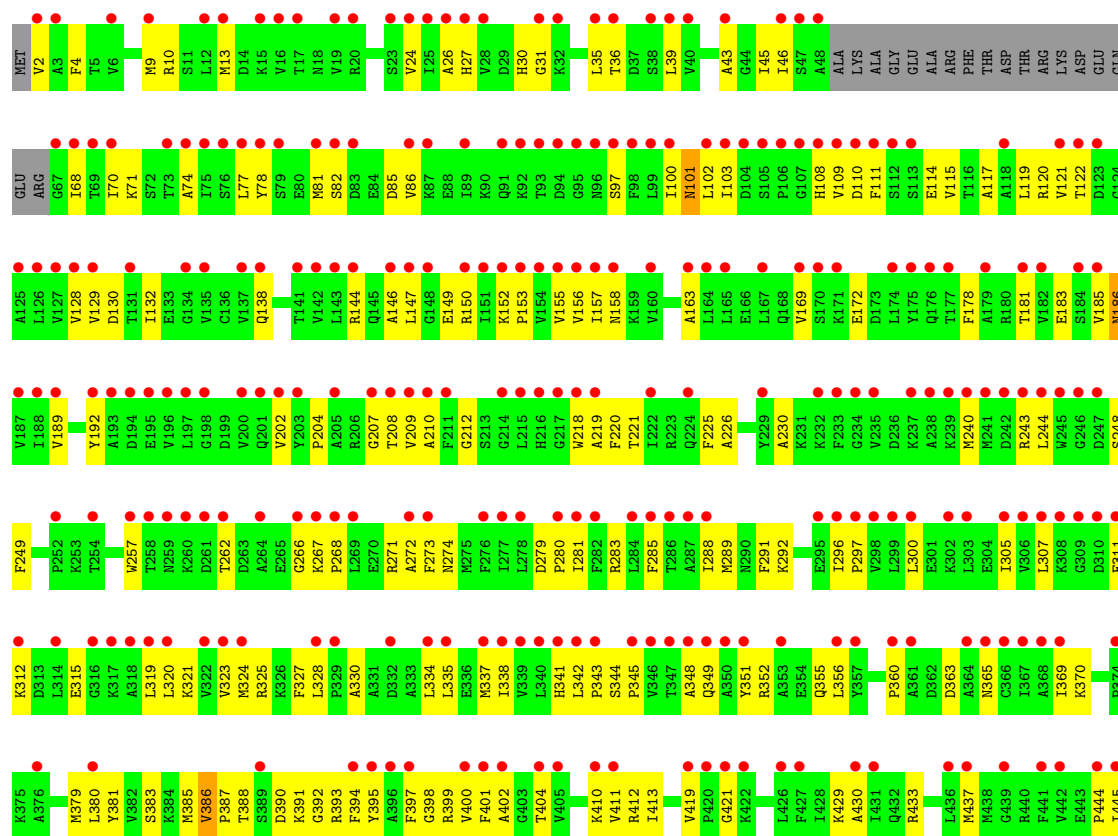
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

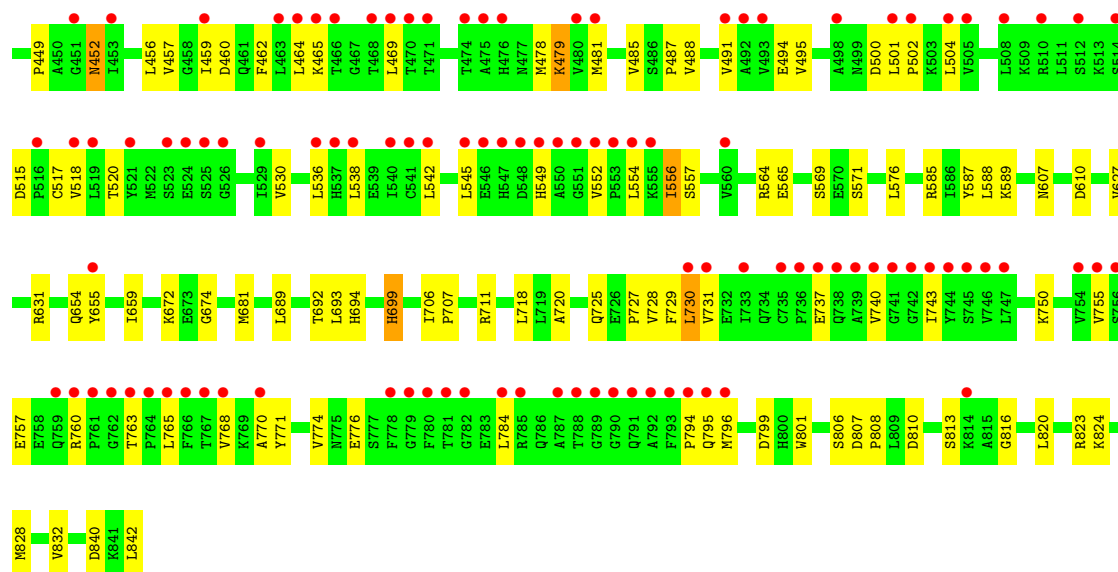
• Molecule 1: Elongation factor 2



• Molecule 1: Elongation factor 2

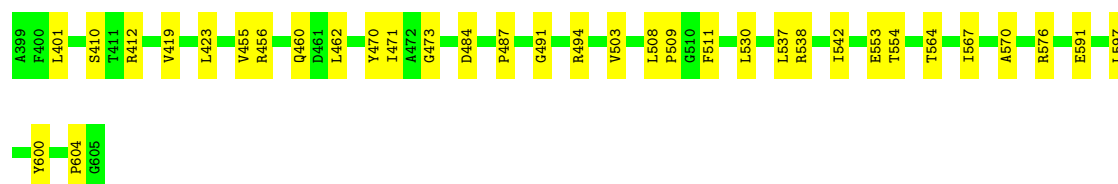






- Molecule 2: Exotoxin A

Chain B: 84% 16%



- Molecule 2: Exotoxin A

Chain D: 86% 13%



- Molecule 2: Exotoxin A

Chain F: 86% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	327.57Å 68.46Å 189.99Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35 25.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.00-2.35) 98.4 (25.00-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.36Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.257 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24682	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 40.05 % 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 2.8973e-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: NAD, DDE

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	0.25	0/6517	0.70	2/8823 (0.0%)
1	C	0.25	0/6517	0.70	2/8823 (0.0%)
1	E	0.25	0/6517	0.70	2/8823 (0.0%)
2	B	0.27	0/1629	0.71	0/2219
2	D	0.27	0/1629	0.73	3/2219 (0.1%)
2	F	0.27	0/1629	0.70	0/2219
All	All	0.26	0/24438	0.70	9/33126 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	GLY	CA-C-N	5.92	125.54	119.56
1	A	674	GLY	C-N-CA	5.92	125.54	119.56
1	E	674	GLY	CA-C-N	5.55	125.16	119.56
1	E	674	GLY	C-N-CA	5.55	125.16	119.56
1	C	674	GLY	CA-C-N	5.53	125.14	119.56
1	C	674	GLY	C-N-CA	5.53	125.14	119.56
2	D	574	ASP	CA-C-N	5.10	125.14	119.32
2	D	574	ASP	C-N-CA	5.10	125.14	119.32
2	D	438	GLY	N-CA-C	5.04	117.42	110.56

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	128	0
1	C	6415	0	6488	135	0
1	E	6415	0	6488	199	0
2	B	1589	0	1543	20	0
2	D	1589	0	1543	17	0
2	F	1589	0	1543	15	0
3	B	44	0	26	2	0
3	D	44	0	26	3	0
3	F	44	0	26	1	0
4	A	83	0	0	1	0
4	B	117	0	0	1	0
4	C	85	0	0	0	0
4	D	124	0	0	1	0
4	E	45	0	0	0	0
4	F	94	0	0	1	0
All	All	24682	0	24155	511	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 11.

All (511) 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:759:GLN:HG2	1:C:760:ARG:H	1.38	0.86
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.57	0.85
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.57	0.84
1:C:404:THR:HG22	1:C:449:PRO:HA	1.58	0.83
1:E:391:LYS:HG3	1:E:392:GLY:H	1.43	0.82
1:A:258:THR:HG22	1:A:260:LYS:H	1.45	0.81
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.62	0.81
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.61	0.81
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.64	0.79
1:E:404:THR:HG22	1:E:449:PRO:HA	1.63	0.78
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.66	0.78
1:E:571:SER:HB2	1:E:589:LYS:HG3	1.65	0.77
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.67	0.77
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.67	0.76
1:C:132:ILE:HD12	1:C:132:ILE:H	1.51	0.75
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.71	0.72
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.71	0.71
1:C:258:THR:HG22	1:C:260:LYS:H	1.56	0.71
1:A:324:MET:HE2	1:A:324:MET:HA	1.73	0.70
1:C:694:HIS:CE1	1:C:699:DDE:HD2	2.26	0.70
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.26	0.70
1:E:556:ILE:HG22	1:E:557:SER:H	1.57	0.70
1:A:609:ARG:CG	1:A:609:ARG:HH11	2.04	0.69
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.74	0.69
1:E:324:MET:HE2	1:E:324:MET:HA	1.74	0.69
1:A:404:THR:HG22	1:A:449:PRO:HA	1.76	0.68
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.73	0.68
1:C:324:MET:HE2	1:C:324:MET:HA	1.74	0.68
1:E:240:MET:HE3	1:E:240:MET:HA	1.77	0.67
1:E:30:HIS:ND1	1:E:130:ASP:HB2	2.10	0.66
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.31	0.66
1:E:699:DDE:HAB2	1:E:699:DDE:HAT2	1.78	0.66
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.66
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.78	0.65
1:E:43:ALA:HB1	1:E:78:TYR:H	1.63	0.64
2:D:498:LEU:HD11	2:D:571:ILE:HB	1.79	0.64
1:C:496:LYS:H	1:C:554:LEU:HD22	1.63	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.78	0.64
1:C:353:ALA:HB3	1:C:370:LYS:HG3	1.79	0.63
1:A:578:LYS:HG2	1:A:585:ARG:HG2	1.80	0.63
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.38	0.63
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.80	0.63
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.80	0.63
1:C:216:HIS:ND1	1:C:321:LYS:HG2	2.14	0.62
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.81	0.62
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.81	0.62
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.80	0.62
1:C:279:ASP:O	1:C:283:ARG:HG2	1.99	0.62
1:E:810:ASP:O	1:E:816:GLY:HA3	2.00	0.62
1:A:237:LYS:O	1:A:241:MET:HB2	2.00	0.62
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.81	0.62
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.81	0.62
1:E:707:PRO:O	1:E:711:ARG:HG3	2.00	0.61
1:E:564:ARG:HB2	1:E:725:GLN:HB2	1.82	0.61
1:A:279:ASP:O	1:A:283:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.65	0.61
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.35	0.61
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.83	0.61
1:C:216:HIS:HB2	1:C:218:TRP:HD1	1.65	0.61
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.83	0.60
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.82	0.60
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.83	0.60
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.83	0.60
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.84	0.60
1:C:30:HIS:CD2	1:C:130:ASP:HB2	2.37	0.60
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.83	0.60
1:C:699:DDE:HAC2	1:C:699:DDE:NAD	2.15	0.60
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.84	0.60
1:A:810:ASP:O	1:A:816:GLY:HA3	2.02	0.59
1:E:26:ALA:CB	1:E:128:VAL:HB	2.32	0.59
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.84	0.59
1:A:569:SER:O	1:A:720:ALA:HB1	2.03	0.59
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.37	0.59
1:A:828:MET:HE2	2:B:576:ARG:HE	1.67	0.58
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.84	0.58
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.33	0.58
1:C:707:PRO:O	1:C:711:ARG:HG3	2.03	0.58
1:C:672:LYS:HG3	1:C:673:GLU:HG3	1.86	0.58
1:A:321:LYS:O	1:A:325:ARG:HB2	2.03	0.58
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.86	0.58
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.86	0.57
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.40	0.57
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.05	0.57
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.87	0.57
1:C:722:PRO:O	1:C:723:LYS:HG3	2.05	0.57
1:E:121:VAL:HG11	1:E:383:SER:OG	2.05	0.57
1:C:374:PRO:O	1:C:404:THR:HG23	2.04	0.56
1:C:419:VAL:HG12	1:C:421:GLY:H	1.70	0.56
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.86	0.56
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.87	0.56
1:E:9:MET:O	1:E:13:MET:HG3	2.05	0.56
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.56
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.87	0.56
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.86	0.56
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.21	0.56
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:PHE:HD1	1:E:315:GLU:HB3	1.70	0.56
1:A:275:MET:HE2	1:A:276:PHE:CZ	2.41	0.56
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.88	0.55
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.88	0.55
1:E:207:GLY:O	1:E:337:MET:HG2	2.06	0.55
1:A:30:HIS:CD2	1:A:130:ASP:HB2	2.42	0.55
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.88	0.55
1:C:772:LEU:HD12	1:C:773:PRO:HD2	1.87	0.55
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.88	0.55
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.89	0.55
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.87	0.55
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.89	0.55
1:E:391:LYS:HG3	1:E:392:GLY:N	2.19	0.54
1:A:831:GLU:CD	1:A:831:GLU:H	2.16	0.54
1:C:6:VAL:HG13	1:C:445:ILE:HG22	1.90	0.54
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.90	0.54
1:E:156:VAL:HG22	1:E:337:MET:HE1	1.88	0.54
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.43	0.54
1:A:385:MET:HG2	1:A:465:LYS:HA	1.88	0.54
1:A:568:GLU:OE2	1:A:723:LYS:HE3	2.06	0.54
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.37	0.54
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.42	0.54
1:E:464:LEU:HG	1:E:465:LYS:HG3	1.89	0.54
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.73	0.54
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.89	0.54
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.90	0.54
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.89	0.54
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.89	0.54
1:A:250:PHE:HD2	1:A:275:MET:HE1	1.73	0.53
1:A:500:ASP:HB3	1:A:552:VAL:HG11	1.90	0.53
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.07	0.53
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.91	0.53
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.23	0.53
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.88	0.53
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.89	0.53
1:A:823:ARG:NH2	1:A:833:PRO:HD3	2.24	0.53
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.43	0.53
2:D:537:LEU:O	2:D:538:ARG:HD3	2.09	0.53
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.91	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
1:A:819:VAL:O	1:A:823:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.44	0.53
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.90	0.53
1:A:501:LEU:N	1:A:502:PRO:HD2	2.24	0.52
1:C:627:VAL:O	1:C:631:ARG:HG3	2.08	0.52
1:E:296:ILE:O	1:E:300:LEU:HD13	2.09	0.52
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.74	0.52
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.90	0.52
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.45	0.52
1:E:257:TRP:HZ3	1:E:272:ALA:HB2	1.74	0.52
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.44	0.52
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.91	0.52
1:A:388:THR:HG21	1:A:395:TYR:CD2	2.45	0.52
1:A:609:ARG:HH11	1:A:609:ARG:HG2	1.74	0.52
1:C:296:ILE:N	1:C:297:PRO:HD2	2.25	0.52
1:A:613:LYS:HG2	1:A:631:ARG:HH11	1.75	0.51
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.92	0.51
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.91	0.51
1:A:542:LEU:HD13	1:A:556:ILE:HG21	1.93	0.51
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.44	0.51
1:E:74:ALA:HA	1:E:102:LEU:O	2.10	0.51
1:E:243:ARG:O	1:E:248:SER:HB2	2.08	0.51
2:F:513:ARG:HH21	2:F:513:ARG:HB2	1.75	0.51
1:A:338:ILE:O	1:A:342:LEU:HB2	2.10	0.51
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.91	0.51
1:E:755:VAL:HG23	1:E:770:ALA:HA	1.93	0.51
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.93	0.51
1:E:111:PHE:HB3	1:E:114:GLU:HG2	1.93	0.51
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.92	0.51
1:A:632:LYS:HD3	1:A:648:ASP:O	2.10	0.51
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.45	0.51
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.46	0.51
2:D:553:GLU:OE1	3:D:701:NAD:H6N	2.11	0.51
1:E:117:ALA:HA	1:E:481:MET:SD	2.49	0.51
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.92	0.51
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.92	0.51
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.93	0.51
1:A:746:VAL:O	1:A:750:LYS:HD3	2.11	0.51
1:A:381:TYR:O	1:A:398:GLY:HA3	2.11	0.51
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.75	0.51
1:E:750:LYS:HD2	1:E:776:GLU:O	2.11	0.51
2:F:537:LEU:HD11	2:F:542:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LYS:O	1:C:325:ARG:HG3	2.11	0.50
1:E:208:THR:HG23	1:E:341:HIS:CE1	2.47	0.50
1:C:254:THR:HG22	1:C:256:LYS:HB2	1.94	0.50
1:E:291:PHE:CD1	1:E:315:GLU:HB3	2.46	0.50
1:E:654:GLN:O	1:E:655:TYR:HB2	2.12	0.50
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.93	0.50
1:A:478:MET:O	1:A:479:LYS:C	2.54	0.50
2:D:427:ARG:HD2	2:D:431:GLU:OE2	2.12	0.50
1:E:349:GLN:O	1:E:370:LYS:HA	2.11	0.50
1:E:627:VAL:O	1:E:631:ARG:HG3	2.11	0.50
1:E:82:SER:O	1:E:86:VAL:HG23	2.11	0.50
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.93	0.50
1:E:727:PRO:HD3	1:E:801:TRP:CZ3	2.47	0.50
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.93	0.50
1:C:723:LYS:HA	1:C:808:PRO:HG3	1.93	0.50
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.93	0.50
1:A:152:LYS:HD3	1:A:343:PRO:HD3	1.94	0.50
1:A:9:MET:O	1:A:13:MET:HG3	2.11	0.50
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.93	0.50
1:A:431:ILE:HD12	1:A:459:ILE:HD11	1.93	0.50
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.41	0.50
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.46	0.50
1:E:380:LEU:HG	1:E:400:VAL:HG22	1.94	0.49
1:A:111:PHE:O	1:A:115:VAL:HG23	2.13	0.49
1:C:17:THR:HB	1:C:92:LYS:O	2.13	0.49
1:C:338:ILE:HG23	1:C:342:LEU:HD12	1.93	0.49
1:C:487:PRO:HB3	1:C:531:ALA:HB1	1.95	0.49
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.47	0.49
1:C:828:MET:HE2	2:D:576:ARG:NH2	2.28	0.49
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.95	0.49
1:C:609:ARG:H	1:C:609:ARG:HD2	1.78	0.49
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.94	0.49
1:E:185:VAL:O	1:E:189:VAL:HG23	2.13	0.49
1:E:321:LYS:O	1:E:325:ARG:HG3	2.12	0.49
1:C:314:LEU:HD22	1:C:318:ALA:HB1	1.95	0.49
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.76	0.49
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.48	0.49
1:A:731:VAL:HG22	1:A:796:MET:HB3	1.95	0.49
1:C:81:MET:O	1:C:96:ASN:HB3	2.13	0.49
1:C:806:SER:HB2	1:C:813:SER:HB2	1.95	0.49
1:C:72:SER:HA	1:C:439:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.95	0.48
1:E:312:LYS:HD2	1:E:312:LYS:O	2.14	0.48
1:E:538:LEU:O	1:E:542:LEU:HG	2.13	0.48
1:A:806:SER:HB2	1:A:813:SER:HB2	1.96	0.48
1:C:226:ALA:HB2	1:C:241:MET:HB3	1.94	0.48
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.96	0.48
1:A:150:ARG:HG3	1:A:355:GLN:HE22	1.79	0.48
1:E:292:LYS:O	1:E:296:ILE:HG13	2.14	0.48
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.95	0.48
1:A:118:ALA:O	1:A:122:THR:HG23	2.14	0.48
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.14	0.48
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.96	0.48
1:C:498:ALA:HA	1:C:501:LEU:HB2	1.96	0.48
1:E:552:VAL:O	1:E:554:LEU:HG	2.14	0.48
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.49	0.48
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.96	0.48
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.38	0.48
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.95	0.47
1:C:406:LYS:HG3	1:C:447:ASP:HB3	1.95	0.47
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.94	0.47
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.95	0.47
1:E:556:ILE:HG22	1:E:557:SER:N	2.27	0.47
1:E:204:PRO:HA	1:E:209:VAL:HB	1.96	0.47
1:E:365:ASN:O	1:E:369:ILE:HG12	2.13	0.47
1:A:464:LEU:HD23	1:A:483:PHE:CE1	2.50	0.47
1:C:759:GLN:HG2	1:C:760:ARG:N	2.17	0.47
2:D:488:ASP:HB3	4:D:795:HOH:O	2.14	0.47
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.95	0.47
1:E:391:LYS:CG	1:E:392:GLY:H	2.21	0.47
1:C:578:LYS:HB3	1:C:585:ARG:HG2	1.97	0.47
1:E:30:HIS:CE1	1:E:130:ASP:HB2	2.50	0.47
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.96	0.47
1:C:809:LEU:O	1:C:811:PRO:HD3	2.14	0.47
1:E:820:LEU:HG	1:E:824:LYS:HE2	1.96	0.47
1:A:45:ILE:HD11	1:A:78:TYR:HB2	1.96	0.47
2:B:470:TYR:CD2	3:B:700:NAD:H2D	2.50	0.47
1:C:167:LEU:O	1:C:168:GLN:C	2.57	0.47
1:C:420:PRO:HG2	1:C:476:HIS:CD2	2.50	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
2:F:513:ARG:HB2	2:F:513:ARG:NH2	2.30	0.47
1:C:515:ASP:O	1:C:518:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:763:THR:C	1:E:765:LEU:H	2.23	0.47
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.50	0.47
1:A:4:PHE:HD2	1:A:45:ILE:HG23	1.79	0.46
1:A:609:ARG:HG3	1:A:609:ARG:NH1	2.30	0.46
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.97	0.46
1:C:501:LEU:C	1:C:501:LEU:HD23	2.40	0.46
1:E:101:ASN:N	1:E:101:ASN:HD22	2.13	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.95	0.46
1:E:419:VAL:HG12	1:E:421:GLY:H	1.80	0.46
1:C:153:PRO:HD2	1:C:200:VAL:HG12	1.96	0.46
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.46
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.97	0.46
1:E:289:MET:HE2	1:E:289:MET:HA	1.97	0.46
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.50	0.46
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.98	0.46
1:C:588:LEU:C	1:C:588:LEU:HD12	2.41	0.46
1:E:156:VAL:HG11	1:E:334:LEU:HD21	1.98	0.46
1:A:296:ILE:O	1:A:300:LEU:HD13	2.16	0.46
1:E:352:ARG:O	1:E:356:LEU:HG	2.15	0.46
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.98	0.46
1:E:737:GLU:HA	1:E:740:VAL:HG23	1.96	0.46
1:C:43:ALA:HB1	1:C:78:TYR:O	2.16	0.46
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.51	0.46
1:C:699:DDE:HAB2	1:C:699:DDE:HAU3	1.46	0.46
1:E:183:GLU:HA	1:E:186:ASN:OD1	2.16	0.46
1:E:226:ALA:O	1:E:230:ALA:HB2	2.15	0.46
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.97	0.46
1:A:155:VAL:HG21	1:A:185:VAL:HG11	1.98	0.46
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.98	0.46
1:E:459:ILE:O	1:E:459:ILE:HG22	2.16	0.46
1:A:110:ASP:HB3	1:A:536:LEU:HD22	1.98	0.46
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.46	0.46
1:E:397:PHE:HD1	1:E:437:MET:HE2	1.81	0.46
1:E:569:SER:O	1:E:720:ALA:HB1	2.16	0.46
1:C:288:ILE:HA	1:C:296:ILE:HD11	1.97	0.45
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.97	0.45
1:A:429:LYS:HG3	1:A:462:PHE:CE2	2.51	0.45
1:C:183:GLU:O	1:C:187:VAL:HG23	2.16	0.45
2:D:538:ARG:HD2	2:D:559:PRO:HG2	1.98	0.45
1:E:381:TYR:O	1:E:398:GLY:HA3	2.15	0.45
1:A:515:ASP:HA	1:A:516:PRO:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PRO:HG3	1:C:114:GLU:HG2	1.97	0.45
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.51	0.45
1:E:244:LEU:O	1:E:273:PHE:HB2	2.16	0.45
1:E:262:THR:HG23	1:E:266:GLY:HA2	1.98	0.45
1:E:380:LEU:HD13	1:E:456:LEU:HD11	1.99	0.45
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.99	0.45
2:F:508:LEU:N	2:F:509:PRO:CD	2.80	0.45
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.51	0.45
1:E:305:ILE:HG21	1:E:323:VAL:HG13	1.98	0.45
1:A:718:LEU:HA	1:A:722:PRO:HG3	1.98	0.45
2:B:401:LEU:HD23	2:B:567:ILE:HG22	1.98	0.45
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.98	0.45
1:E:296:ILE:N	1:E:297:PRO:HD2	2.32	0.45
1:E:459:ILE:HD12	1:E:459:ILE:N	2.32	0.45
1:E:823:ARG:HE	1:E:832:VAL:HG22	1.82	0.45
2:B:570:ALA:HB3	2:B:591:GLU:OE1	2.17	0.44
1:C:171:LYS:NZ	1:C:171:LYS:HB2	2.32	0.44
1:E:46:ILE:N	1:E:46:ILE:HD12	2.32	0.44
1:A:352:ARG:NH2	1:A:356:LEU:HD11	2.32	0.44
1:A:609:ARG:CG	1:A:609:ARG:NH1	2.68	0.44
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.98	0.44
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.52	0.44
1:E:806:SER:HB2	1:E:813:SER:HB2	1.99	0.44
1:C:664:VAL:O	1:C:668:GLN:HG2	2.17	0.44
1:A:388:THR:HG21	1:A:395:TYR:CG	2.53	0.44
1:E:218:TRP:HB3	1:E:324:MET:HB3	1.99	0.44
1:E:757:GLU:HG3	1:E:768:VAL:HG22	2.00	0.44
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.99	0.44
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.99	0.44
1:E:46:ILE:HD12	1:E:46:ILE:H	1.83	0.44
1:E:279:ASP:O	1:E:283:ARG:HG2	2.17	0.44
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.18	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.32	0.44
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.32	0.44
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.81	0.44
1:E:485:VAL:HG22	1:E:485:VAL:O	2.16	0.44
1:E:840:ASP:CG	1:E:842:LEU:HD13	2.43	0.44
1:A:698:ILE:H	1:A:698:ILE:HG13	1.62	0.44
1:C:152:LYS:HD3	1:C:343:PRO:HD3	2.00	0.44
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.48	0.44
1:E:157:ILE:HG21	1:E:178:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ASN:N	1:E:452:ASN:HD22	2.16	0.44
2:F:523:ALA:O	2:F:527:VAL:HG23	2.18	0.44
2:F:574:ASP:HA	2:F:575:PRO:HD2	1.84	0.44
1:A:823:ARG:HH22	1:A:833:PRO:HD3	1.82	0.44
2:B:419:VAL:O	2:B:423:LEU:HG	2.17	0.44
1:C:454:ILE:HG13	1:C:455:GLY:H	1.82	0.44
2:D:522:GLU:CD	2:D:522:GLU:H	2.26	0.44
1:E:39:LEU:HD12	1:E:39:LEU:H	1.83	0.44
1:E:345:PRO:HB3	1:E:399:ARG:HH21	1.81	0.44
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.99	0.43
1:E:132:ILE:HD12	1:E:132:ILE:N	2.33	0.43
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.18	0.43
1:A:664:VAL:O	1:A:668:GLN:HG2	2.18	0.43
1:C:24:VAL:HG23	1:C:102:LEU:HD11	2.00	0.43
1:E:39:LEU:HD11	1:E:334:LEU:HD13	2.00	0.43
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.48	0.43
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.90	0.43
1:E:386:VAL:HG11	1:E:437:MET:HE1	2.00	0.43
1:E:727:PRO:HD3	1:E:801:TRP:HZ3	1.82	0.43
1:A:588:LEU:HD12	1:A:588:LEU:C	2.43	0.43
1:C:579:SER:HB2	1:C:704:GLN:OE1	2.18	0.43
1:E:77:LEU:HD23	1:E:335:LEU:HD21	2.01	0.43
1:E:111:PHE:O	1:E:115:VAL:HG23	2.19	0.43
1:E:369:ILE:HD12	1:E:401:PHE:HB3	2.01	0.43
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.84	0.43
1:A:353:ALA:HB3	1:A:370:LYS:HG2	2.01	0.43
1:A:410:LYS:HA	1:A:430:ALA:HA	2.00	0.43
1:A:582:LYS:HE2	4:B:779:HOH:O	2.17	0.43
1:A:677:PHE:N	1:A:677:PHE:CD2	2.85	0.43
1:C:546:GLU:HA	1:C:550:ALA:HB3	2.00	0.43
1:C:736:PRO:O	1:C:740:VAL:HG23	2.18	0.43
1:E:485:VAL:O	1:E:487:PRO:HD3	2.18	0.43
1:E:491:VAL:HG13	1:E:538:LEU:HD21	1.99	0.43
1:E:699:DDE:HAT2	1:E:699:DDE:CAB	2.46	0.43
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.99	0.43
1:A:654:GLN:HG2	1:A:655:TYR:CE1	2.54	0.43
1:C:396:ALA:HB3	1:C:456:LEU:HB2	2.01	0.43
1:E:307:LEU:HD13	1:E:311:GLU:O	2.19	0.43
1:E:588:LEU:C	1:E:588:LEU:HD12	2.43	0.43
1:A:26:ALA:HB2	1:A:128:VAL:HB	2.01	0.43
1:C:608:PRO:HD2	1:C:609:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:499:LEU:HB3	2:D:566:VAL:CG1	2.47	0.43
1:E:150:ARG:HB3	1:E:351:TYR:HE1	1.83	0.43
1:E:181:THR:O	1:E:185:VAL:HG23	2.18	0.43
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.54	0.43
2:B:410:SER:OG	2:B:412:ARG:HG3	2.18	0.43
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.43
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.99	0.43
2:F:522:GLU:CD	2:F:522:GLU:H	2.26	0.43
1:A:6:VAL:HG13	1:A:445:ILE:HG22	2.01	0.43
1:A:81:MET:HE1	1:A:336:GLU:HA	1.99	0.43
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.00	0.43
1:C:284:LEU:HD23	1:C:299:LEU:HD23	2.00	0.43
1:A:12:LEU:HG	1:A:99:LEU:HB2	2.01	0.42
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.53	0.42
2:B:460:GLN:HG3	2:B:462:LEU:HD11	2.00	0.42
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.18	0.42
1:E:163:ALA:O	1:E:169:VAL:HG12	2.18	0.42
1:A:731:VAL:O	1:A:769:LYS:HA	2.19	0.42
2:B:455:VAL:C	2:B:456:ARG:HD2	2.44	0.42
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.54	0.42
1:C:506:GLU:O	1:C:510:ARG:HG3	2.18	0.42
1:E:70:ILE:HG22	1:E:388:THR:HG22	2.01	0.42
1:E:156:VAL:CG2	1:E:337:MET:HE1	2.50	0.42
1:E:774:VAL:C	1:E:776:GLU:H	2.27	0.42
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.83	0.42
1:C:523:SER:OG	1:C:527:GLU:HB2	2.19	0.42
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.01	0.42
1:A:120:ARG:NH1	1:A:479:LYS:HD2	2.34	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.01	0.42
1:E:149:GLU:O	1:E:352:ARG:HD2	2.19	0.42
1:A:322:VAL:O	1:A:326:LYS:HG2	2.20	0.42
1:A:373:ASP:HA	1:A:374:PRO:HD2	1.86	0.42
1:A:207:GLY:O	1:A:337:MET:HG2	2.20	0.42
1:A:464:LEU:HD23	1:A:483:PHE:HE1	1.85	0.42
1:A:698:ILE:HG13	4:A:892:HOH:O	2.19	0.42
1:E:129:VAL:HG12	1:E:130:ASP:N	2.34	0.42
1:E:565:GLU:O	1:E:681:MET:HA	2.20	0.42
1:E:731:VAL:HA	1:E:796:MET:HB3	2.02	0.42
2:B:484:ASP:OD2	2:B:494:ARG:HB2	2.20	0.42
1:C:140:GLU:HG3	1:C:188:ILE:HD13	2.02	0.42
1:C:659:ILE:O	1:C:663:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:O	1:E:342:LEU:HB2	2.19	0.42
1:E:344:SER:HB2	1:E:345:PRO:HD2	2.00	0.42
1:A:40:VAL:HG12	1:A:75:ILE:HG21	2.01	0.42
1:A:223:ARG:HB3	1:A:336:GLU:OE1	2.20	0.42
1:A:832:VAL:HA	1:A:833:PRO:HD3	1.95	0.42
2:B:487:PRO:HB2	2:B:491:GLY:HA2	2.02	0.42
1:C:491:VAL:HG13	1:C:538:LEU:HD21	2.01	0.42
1:C:628:THR:O	1:C:632:LYS:HG3	2.19	0.42
1:E:296:ILE:HG21	1:E:319:LEU:HD21	2.01	0.42
1:E:355:GLN:O	1:E:479:LYS:HG3	2.20	0.42
2:B:538:ARG:HE	2:B:538:ARG:HA	1.85	0.42
2:D:474:ASP:HA	2:D:475:PRO:HD2	1.89	0.42
1:E:155:VAL:HG21	1:E:202:VAL:HG21	2.02	0.42
1:E:327:PHE:CD2	1:E:328:LEU:HG	2.55	0.42
1:E:410:LYS:HA	1:E:430:ALA:HA	2.02	0.42
1:C:20:ARG:NH1	1:C:344:SER:HB3	2.35	0.41
1:C:539:GLU:O	1:C:543:GLN:HG3	2.20	0.41
1:A:486:SER:HA	1:A:487:PRO:HD3	1.87	0.41
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.49	0.41
1:C:77:LEU:HB2	1:C:100:ILE:HB	2.02	0.41
1:C:132:ILE:HD11	1:C:162:ARG:HB2	2.01	0.41
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.93	0.41
1:C:813:SER:O	1:C:817:GLU:HB2	2.20	0.41
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.55	0.41
1:A:284:LEU:HD23	1:A:299:LEU:HD23	2.02	0.41
1:A:721:ASP:CG	1:A:721:ASP:O	2.62	0.41
2:B:471:ILE:CG1	2:B:554:THR:HB	2.51	0.41
1:C:486:SER:HA	1:C:487:PRO:HD3	1.86	0.41
1:E:119:LEU:HD21	1:E:146:ALA:HA	2.02	0.41
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.85	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.97	0.41
3:D:701:NAD:O1N	3:D:701:NAD:O2A	2.39	0.41
1:E:212:GLY:HA3	1:E:219:ALA:HA	2.02	0.41
1:E:288:ILE:HG23	1:E:319:LEU:HD23	2.01	0.41
1:A:284:LEU:HD11	1:A:303:LEU:HD12	2.01	0.41
1:A:358:GLU:HB2	1:A:477:ASN:O	2.19	0.41
1:C:153:PRO:HD2	1:C:200:VAL:CG1	2.51	0.41
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.74	0.41
1:E:491:VAL:HG21	1:E:542:LEU:HD21	2.02	0.41
1:A:305:ILE:HD11	1:A:327:PHE:CD1	2.56	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:DDE:HAA3	1:C:699:DDE:HAD2	1.85	0.41
1:C:810:ASP:O	1:C:816:GLY:HA3	2.20	0.41
1:E:152:LYS:HA	1:E:153:PRO:HD3	1.83	0.41
1:E:589:LYS:HE3	1:E:689:LEU:HD11	2.01	0.41
1:A:89:ILE:CG2	1:A:91:GLN:HG2	2.49	0.41
1:A:659:ILE:HD13	1:A:693:LEU:HD21	2.02	0.41
1:C:735:CYS:HA	1:C:736:PRO:HD3	1.96	0.41
2:D:508:LEU:N	2:D:509:PRO:CD	2.84	0.41
1:E:119:LEU:HD11	1:E:146:ALA:HA	2.02	0.41
1:A:93:THR:HG22	1:A:94:ASP:N	2.35	0.41
1:A:174:LEU:HG	1:A:178:PHE:CE2	2.56	0.41
1:A:195:GLU:H	1:A:195:GLU:CD	2.28	0.41
1:A:589:LYS:HE3	1:A:589:LYS:HB2	1.95	0.41
2:B:508:LEU:N	2:B:509:PRO:CD	2.84	0.41
1:C:103:ILE:HD12	1:C:122:THR:HG22	2.01	0.41
1:C:204:PRO:HG2	1:C:245:TRP:CE2	2.55	0.41
1:C:250:PHE:HB3	1:C:275:MET:HE1	2.03	0.41
1:C:569:SER:O	1:C:720:ALA:HB1	2.21	0.41
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.03	0.41
1:E:24:VAL:HG21	1:E:36:THR:HG22	2.02	0.41
1:E:411:VAL:HG12	1:E:412:ARG:N	2.36	0.41
1:C:718:LEU:HA	1:C:722:PRO:HG3	2.03	0.41
1:E:728:VAL:HG11	1:E:771:TYR:HB3	2.03	0.41
1:A:378:LEU:O	1:A:470:THR:HA	2.21	0.40
2:B:553:GLU:OE1	3:B:700:NAD:H6N	2.20	0.40
1:E:394:PHE:O	1:E:460:ASP:HB3	2.21	0.40
1:A:377:ASP:OD2	1:A:472:SER:HB2	2.22	0.40
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.88	0.40
1:C:70:ILE:HG22	1:C:388:THR:HG22	2.02	0.40
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.88	0.40
1:E:109:VAL:O	1:E:109:VAL:HG12	2.21	0.40
1:C:381:TYR:O	1:C:398:GLY:HA3	2.22	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.56	0.40
2:F:427:ARG:HA	4:F:755:HOH:O	2.20	0.40
1:A:120:ARG:HH12	1:A:479:LYS:HD2	1.86	0.40
1:A:609:ARG:HH11	1:A:609:ARG:HG3	1.81	0.40
2:B:511:PHE:HB3	2:B:600:TYR:CD1	2.55	0.40
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:E:103:ILE:HD13	1:E:122:THR:HG22	2.04	0.40
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.57	0.40
1:E:342:LEU:HA	1:E:343:PRO:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.85	0.40
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.57	0.40
1:E:828:MET:HE3	2:F:576:ARG:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	779 (95%)	36 (4%)	3 (0%)	30	34
1	C	818/842 (97%)	778 (95%)	35 (4%)	5 (1%)	21	24
1	E	818/842 (97%)	762 (93%)	53 (6%)	3 (0%)	30	34
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
2	F	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	24	27
All	All	3069/3147 (98%)	2919 (95%)	138 (4%)	12 (0%)	30	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	C	168	GLN
1	E	479	LYS
1	A	479	LYS
1	C	795	GLN
1	C	166	GLU
1	C	479	LYS
1	E	795	GLN
1	C	309	GLY

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Mol	Chain	Res	Type
1	E	556	ILE
1	A	721	ASP
2	F	453	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%)	689 (99%)	10 (1%)	59	73
1	C	699/714 (98%)	689 (99%)	10 (1%)	59	73
1	E	699/714 (98%)	691 (99%)	8 (1%)	65	79
2	B	161/161 (100%)	161 (100%)	0	100	100
2	D	161/161 (100%)	156 (97%)	5 (3%)	35	47
2	F	161/161 (100%)	156 (97%)	5 (3%)	35	47
All	All	2580/2625 (98%)	2542 (98%)	38 (2%)	57	72

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	MET
1	A	479	LYS
1	A	595	GLU
1	A	599	LEU
1	A	609	ARG
1	A	677	PHE
1	A	710	ARG
1	A	718	LEU
1	A	831	GLU
1	A	842	LEU
1	C	167	LEU
1	C	240	MET
1	C	256	LYS
1	C	479	LYS
1	C	556	ILE

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Mol	Chain	Res	Type
1	C	718	LEU
1	C	730	LEU
1	C	786	GLN
1	C	837	GLU
1	C	842	LEU
2	D	422	LEU
2	D	498	LEU
2	D	499	LEU
2	D	540	ASP
2	D	576	ARG
1	E	101	ASN
1	E	186	ASN
1	E	386	VAL
1	E	452	ASN
1	E	494	GLU
1	E	672	LYS
1	E	718	LEU
1	E	730	LEU
2	F	456	ARG
2	F	513	ARG
2	F	540	ASP
2	F	548	GLU
2	F	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	274	ASN
1	A	355	GLN
2	B	428	GLN
1	C	274	ASN
1	C	341	HIS
1	C	583	HIS
1	C	753	GLN
2	D	603	GLN
1	E	21	ASN
1	E	216	HIS
1	E	476	HIS
1	E	537	HIS
1	E	573	GLN
1	E	753	GLN

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Mol	Chain	Res	Type
1	E	791	GLN
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	C	699	1	18,20,21	1.29	3 (16%)	17,28,30	0.94	0
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	1.27	3 (16%)	17,28,30	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	C	699	1	-	13/20/21/23	0/1/1/1
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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	699	DDE	CBW-NCB	-2.84	1.48	1.54
1	E	699	DDE	CBW-NCB	-2.84	1.48	1.54
1	C	699	DDE	CG-ND1	-2.52	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	CG-ND1	-2.51	1.33	1.38
1	C	699	DDE	CAT-CE1	2.37	1.53	1.49
1	E	699	DDE	CAT-CE1	2.21	1.53	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (18) 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	E	699	DDE	CAT-CAU-CBW-NCB
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	C	699	DDE	NAD-CBI-CBW-CAU
1	E	699	DDE	CAT-CAU-CBW-CBI
1	C	699	DDE	OAG-CBI-CBW-CAU

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	4	0
1	E	699	DDE	3	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	F	702	-	46,48,48	0.87	2 (4%)	64,73,73	1.61	9 (14%)
3	NAD	B	700	-	46,48,48	0.84	1 (2%)	64,73,73	1.65	10 (15%)
3	NAD	D	701	-	46,48,48	0.87	3 (6%)	64,73,73	1.65	9 (14%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	C5A-N7A	-2.29	1.34	1.39
3	F	702	NAD	C5A-N7A	-2.23	1.35	1.39
3	D	701	NAD	PN-O3	2.22	1.61	1.59
3	D	701	NAD	C5A-N7A	-2.17	1.35	1.39
3	F	702	NAD	PN-O3	2.16	1.61	1.59
3	D	701	NAD	PA-O3	2.11	1.61	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	C5A-C4A-N3A	-5.79	118.74	126.72
3	F	702	NAD	C5A-C4A-N3A	-5.65	118.94	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	NAD	C5A-C4A-N3A	-5.64	118.95	126.72
3	D	701	NAD	O4B-C1B-N9A	4.56	116.84	108.09
3	D	701	NAD	N3A-C2A-N1A	-4.55	121.69	128.58
3	F	702	NAD	N3A-C2A-N1A	-4.52	121.74	128.58
3	B	700	NAD	N3A-C2A-N1A	-4.36	121.98	128.58
3	B	700	NAD	O4B-C1B-N9A	4.34	116.43	108.09
3	F	702	NAD	O4B-C1B-N9A	4.24	116.23	108.09
3	B	700	NAD	N3A-C4A-N9A	4.09	134.12	127.17
3	D	701	NAD	N3A-C4A-N9A	3.97	133.92	127.17
3	F	702	NAD	N3A-C4A-N9A	3.86	133.73	127.17
3	F	702	NAD	C2A-N3A-C4A	3.41	120.15	111.83
3	D	701	NAD	C2A-N3A-C4A	3.37	120.06	111.83
3	B	700	NAD	C2A-N3A-C4A	3.32	119.93	111.83
3	B	700	NAD	N9A-C8A-N7A	-3.18	109.43	113.94
3	D	701	NAD	N9A-C8A-N7A	-3.12	109.50	113.94
3	F	702	NAD	N9A-C8A-N7A	-3.03	109.64	113.94
3	B	700	NAD	C5A-N7A-C8A	2.55	107.46	103.45
3	F	702	NAD	C4A-C5A-N7A	-2.44	107.80	110.58
3	D	701	NAD	C5A-N7A-C8A	2.42	107.25	103.45
3	B	700	NAD	C4A-C5A-N7A	-2.41	107.83	110.58
3	F	702	NAD	C5A-N7A-C8A	2.40	107.22	103.45
3	D	701	NAD	C4A-N9A-C8A	2.36	108.21	105.74
3	D	701	NAD	C4A-C5A-N7A	-2.34	107.90	110.58
3	B	700	NAD	C4A-N9A-C8A	2.30	108.15	105.74
3	B	700	NAD	C6A-C5A-C4A	2.23	120.23	117.18
3	F	702	NAD	C4A-N9A-C8A	2.18	108.02	105.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	O4B-C4B-C5B-O5B
3	D	701	NAD	C3B-C4B-C5B-O5B
3	F	702	NAD	C3B-C4B-C5B-O5B
3	D	701	NAD	C3D-C4D-C5D-O5D
3	D	701	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	PA-O3-PN-O1N
3	B	700	NAD	O4B-C1B-N9A-C8A
3	D	701	NAD	O4B-C1B-N9A-C8A

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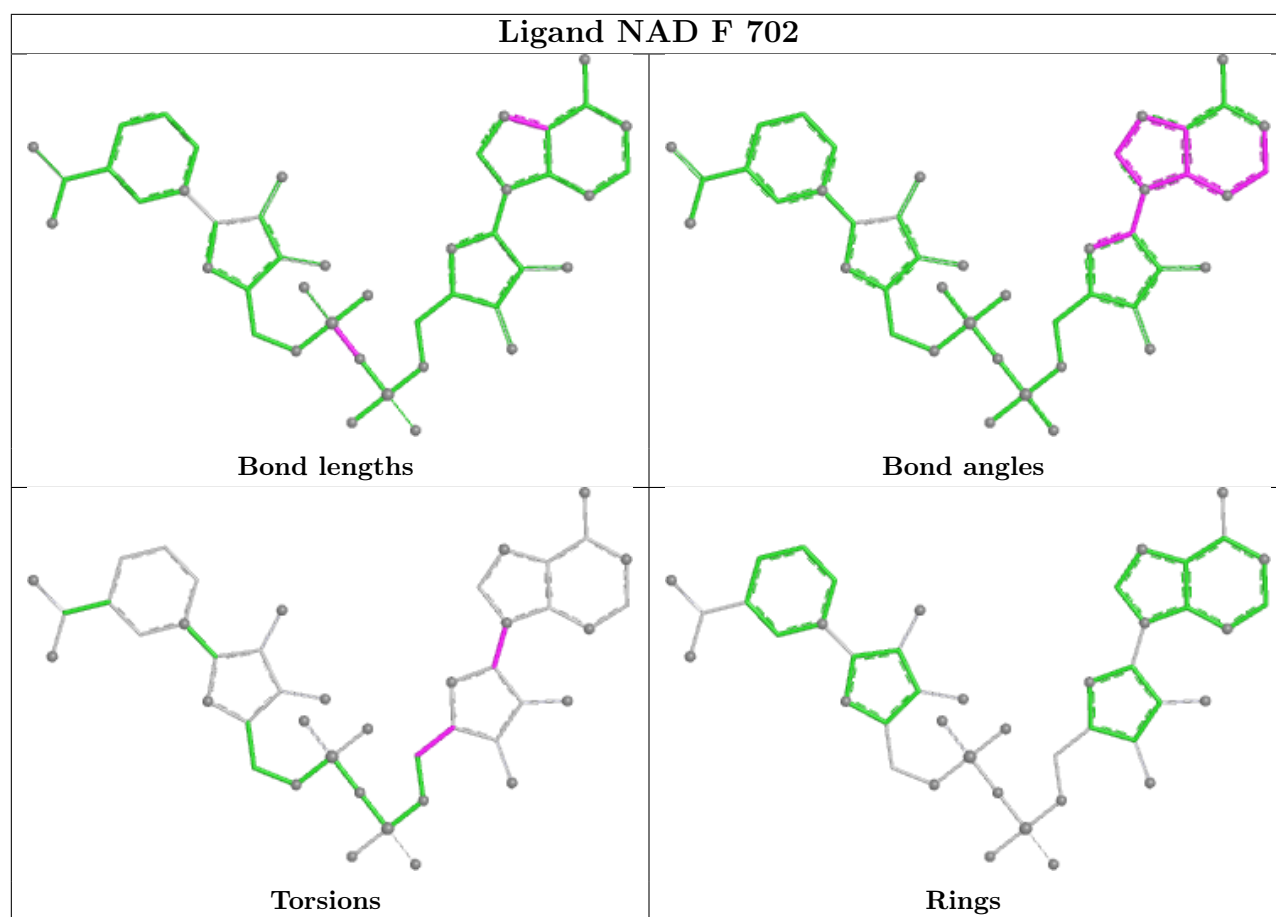
Mol	Chain	Res	Type	Atoms
3	F	702	NAD	O4B-C1B-N9A-C8A
3	D	701	NAD	PA-O3-PN-O2N

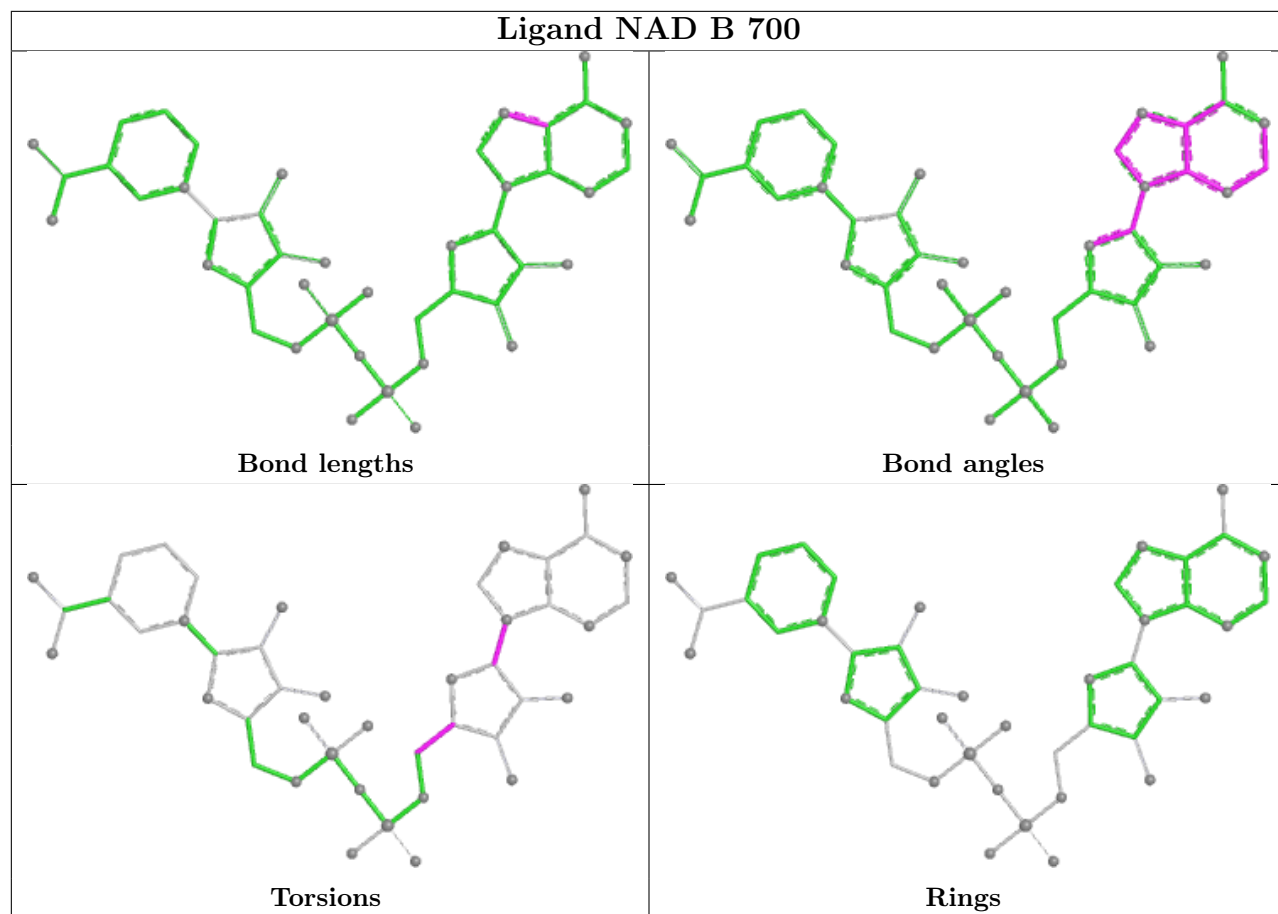
There are no ring outliers.

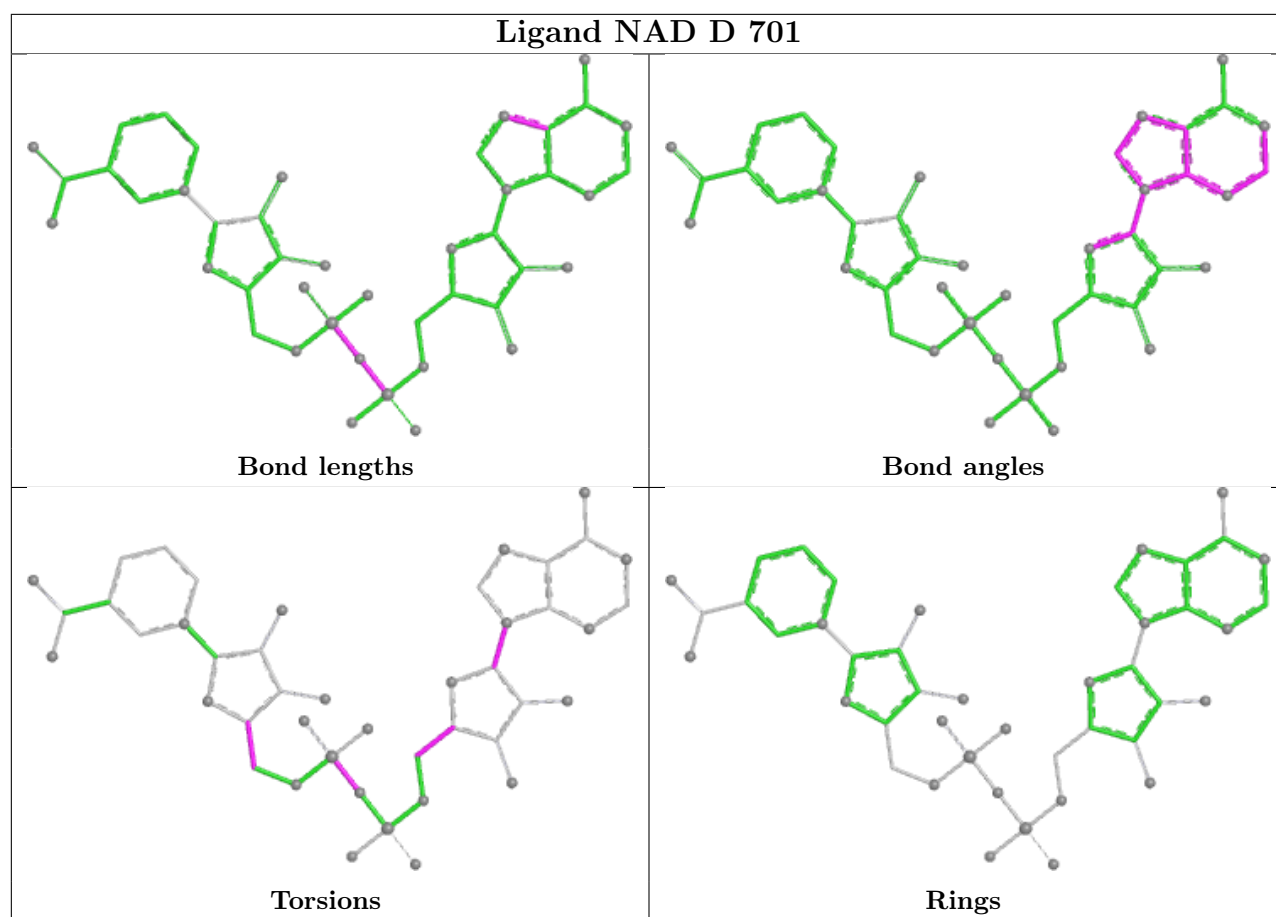
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	702	NAD	1	0
3	B	700	NAD	2	0
3	D	701	NAD	3	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%)	0.18	33 (4%) 42 48	14, 55, 97, 118	0
1	C	822/842 (97%)	0.43	79 (9%) 13 16	16, 61, 135, 187	0
1	E	822/842 (97%)	1.75	373 (45%) 0 0	16, 136, 189, 262	0
2	B	207/207 (100%)	-0.51	0 100 100	14, 27, 61, 94	0
2	D	207/207 (100%)	-0.57	2 (0%) 79 83	12, 25, 57, 89	0
2	F	207/207 (100%)	-0.46	3 (1%) 73 78	17, 29, 62, 108	0
All	All	3087/3147 (98%)	0.53	490 (15%) 5 5	12, 57, 169, 262	0

All (490) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	196	VAL	7.8
1	E	155	VAL	7.2
1	E	126	LEU	7.0
1	E	143	LEU	6.6
1	E	743	ILE	6.5
1	E	364	ALA	5.9
1	E	781	THR	5.9
1	E	306	VAL	5.9
1	E	233	PHE	5.8
1	E	129	VAL	5.4
1	E	127	VAL	5.3
1	E	26	ALA	5.3
1	E	156	VAL	5.3
1	E	245	TRP	5.2
1	E	794	PRO	5.2
1	E	282	PHE	5.2
1	C	493	VAL	5.2
1	E	109	VAL	5.2
1	E	755	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	343	PRO	5.2
1	E	86	VAL	5.1
1	E	368	ALA	5.0
1	E	342	LEU	4.9
1	E	339	VAL	4.8
1	E	335	LEU	4.8
1	C	498	ALA	4.8
1	E	492	ALA	4.8
1	E	164	LEU	4.7
1	E	278	LEU	4.7
1	E	277	ILE	4.7
1	E	273	PHE	4.6
1	E	480	VAL	4.6
1	E	338	ILE	4.6
1	E	740	VAL	4.6
1	E	360	PRO	4.5
1	E	175	TYR	4.5
1	E	493	VAL	4.5
1	E	165	LEU	4.4
1	E	307	LEU	4.4
1	E	185	VAL	4.4
1	E	442	VAL	4.4
1	E	554	LEU	4.4
1	E	78	TYR	4.4
1	E	780	PHE	4.4
1	E	188	ILE	4.4
1	E	770	ALA	4.3
1	E	128	VAL	4.3
1	E	182	VAL	4.3
1	E	553	PRO	4.3
1	E	167	LEU	4.3
1	E	81	MET	4.3
1	E	48	ALA	4.2
1	E	179	ALA	4.2
1	E	210	ALA	4.2
1	E	135	VAL	4.2
1	E	276	PHE	4.2
1	C	550	ALA	4.2
1	E	764	PRO	4.2
1	E	311	GLU	4.1
1	E	299	LEU	4.1
1	E	367	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	36	THR	4.1
1	E	25	ILE	4.1
1	C	48	ALA	4.1
1	E	784	LEU	4.0
1	E	169	VAL	4.0
1	E	99	LEU	4.0
1	E	356	LEU	4.0
1	E	782	GLY	4.0
1	E	296	ILE	4.0
1	E	19	VAL	4.0
1	E	526	GLY	4.0
1	E	504	LEU	4.0
1	E	747	LEU	3.9
1	E	163	ALA	3.9
1	E	761	PRO	3.9
1	E	314	LEU	3.9
1	E	369	ILE	3.8
1	E	192	TYR	3.8
1	E	16	VAL	3.8
1	E	147	LEU	3.8
1	E	401	PHE	3.8
1	E	151	ILE	3.8
1	C	552	VAL	3.8
1	E	536	LEU	3.7
1	C	521	TYR	3.7
1	E	257	TRP	3.7
1	E	222	ILE	3.7
1	E	197	LEU	3.7
1	E	2	VAL	3.7
1	E	209	VAL	3.7
1	E	505	VAL	3.7
1	E	207	GLY	3.6
1	E	340	LEU	3.6
1	E	187	VAL	3.6
1	E	547	HIS	3.6
1	E	793	PHE	3.6
1	E	244	LEU	3.6
1	E	519	LEU	3.6
1	E	160	VAL	3.6
1	E	525	SER	3.6
1	E	281	ILE	3.6
1	C	495	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	200	VAL	3.6
1	C	553	PRO	3.6
1	E	498	ALA	3.6
1	A	46	ILE	3.5
1	C	549	HIS	3.5
1	C	513	LYS	3.5
1	E	111	PHE	3.5
1	E	501	LEU	3.5
1	E	762	GLY	3.5
1	E	131	THR	3.5
1	E	789	GLY	3.5
1	E	790	GLY	3.5
1	E	75	ILE	3.5
1	E	203	TYR	3.5
1	E	538	LEU	3.5
1	E	471	THR	3.4
1	E	239	LYS	3.4
1	E	768	VAL	3.4
1	A	48	ALA	3.4
1	E	348	ALA	3.4
1	E	763	THR	3.4
1	E	89	ILE	3.4
1	E	280	PRO	3.4
1	E	736	PRO	3.4
1	C	109	VAL	3.4
1	E	205	ALA	3.4
1	E	264	ALA	3.4
1	E	218	TRP	3.4
1	E	444	PRO	3.4
1	E	154	VAL	3.4
1	E	146	ALA	3.4
1	E	361	ALA	3.4
1	E	202	VAL	3.3
1	E	67	GLY	3.3
1	A	411	VAL	3.3
1	E	77	LEU	3.3
1	E	320	LEU	3.3
1	E	98	PHE	3.3
1	E	766	PHE	3.3
1	E	395	TYR	3.3
1	A	109	VAL	3.3
1	C	554	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	215	LEU	3.3
1	E	82	SER	3.3
1	E	353	ALA	3.2
1	C	508	LEU	3.2
1	E	106	PRO	3.2
1	E	108	HIS	3.2
1	A	483	PHE	3.2
1	E	40	VAL	3.2
1	E	464	LEU	3.2
1	C	502	PRO	3.2
1	E	38	SER	3.2
1	E	241	MET	3.2
1	E	144	ARG	3.2
1	C	504	LEU	3.2
1	E	300	LEU	3.2
1	E	303	LEU	3.2
1	E	441	PHE	3.2
1	E	346	VAL	3.2
1	E	421	GLY	3.2
1	E	35	LEU	3.2
1	E	466	THR	3.2
1	E	93	THR	3.1
1	E	347	THR	3.1
1	E	79	SER	3.1
1	E	765	LEU	3.1
1	E	266	GLY	3.1
1	E	741	GLY	3.1
1	E	240	MET	3.1
1	E	157	ILE	3.1
1	C	551	GLY	3.1
1	E	312	LYS	3.1
1	E	258	THR	3.0
1	E	778	PHE	3.0
1	E	74	ALA	3.0
1	E	268	PRO	3.0
1	E	552	VAL	3.0
1	E	754	VAL	3.0
1	E	103	ILE	3.0
1	E	453	ILE	3.0
1	A	360	PRO	3.0
1	E	396	ALA	3.0
1	C	524	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	284	LEU	3.0
1	E	351	TYR	3.0
1	E	73	THR	3.0
1	E	404	THR	3.0
1	E	193	ALA	3.0
1	C	322	VAL	3.0
1	E	298	VAL	3.0
1	E	542	LEU	3.0
1	E	308	LYS	3.0
1	C	525	SER	3.0
1	E	419	VAL	2.9
1	C	509	LYS	2.9
1	E	445	ILE	2.9
1	E	107	GLY	2.9
1	E	238	ALA	2.9
1	E	305	ILE	2.9
1	E	744	TYR	2.9
1	A	67	GLY	2.9
1	C	309	GLY	2.9
1	E	174	LEU	2.9
1	E	219	ALA	2.9
1	E	746	VAL	2.9
1	C	523	SER	2.9
1	E	76	SER	2.9
1	E	97	SER	2.9
1	E	198	GLY	2.9
1	E	309	GLY	2.9
1	E	422	LYS	2.9
1	A	233	PHE	2.9
1	E	366	CYS	2.9
1	E	796	MET	2.9
1	E	269	LEU	2.8
1	C	306	VAL	2.8
1	C	505	VAL	2.8
1	E	24	VAL	2.8
1	C	522	MET	2.8
1	C	305	ILE	2.8
1	E	431	ILE	2.8
1	E	474	THR	2.8
1	C	500	ASP	2.8
1	E	259	ASN	2.8
1	E	785	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	761	PRO	2.8
1	E	9	MET	2.8
1	E	541	CYS	2.8
1	C	544	ASP	2.8
1	E	451	GLY	2.8
1	E	502	PRO	2.8
1	E	334	LEU	2.8
1	E	427	PHE	2.8
1	E	437	MET	2.8
1	E	286	THR	2.8
1	E	47	SER	2.8
1	E	39	LEU	2.8
1	E	357	TYR	2.8
1	E	32	LYS	2.8
2	F	489	ALA	2.8
1	A	495	VAL	2.8
1	E	6	VAL	2.8
1	E	731	VAL	2.8
1	C	529	ILE	2.7
1	E	70	ILE	2.7
1	E	254	THR	2.7
1	E	767	THR	2.7
1	E	332	ASP	2.7
1	E	95	GLY	2.7
1	E	134	GLY	2.7
1	E	374	PRO	2.7
1	E	420	PRO	2.7
1	E	655	TYR	2.7
1	E	137	VAL	2.7
1	E	322	VAL	2.7
1	E	323	VAL	2.7
1	C	497	ASN	2.7
1	E	46	ILE	2.7
1	E	123	ASP	2.7
1	E	242	ASP	2.7
2	D	489	ALA	2.7
1	A	466	THR	2.7
1	E	742	GLY	2.7
1	C	320	LEU	2.7
1	E	376	ALA	2.7
1	E	217	GLY	2.7
1	E	3	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	318	ALA	2.6
1	A	459	ILE	2.6
1	E	20	ARG	2.6
1	E	243	ARG	2.6
1	E	112	SER	2.6
1	E	436	LEU	2.6
1	E	545	LEU	2.6
1	E	232	LYS	2.6
1	E	302	LYS	2.6
1	A	2	VAL	2.6
1	E	141	THR	2.6
1	E	405	VAL	2.6
1	E	113	SER	2.6
1	E	514	SER	2.6
1	E	795	GLN	2.6
1	C	264	ALA	2.6
1	C	526	GLY	2.6
1	C	740	VAL	2.6
1	E	28	VAL	2.6
1	E	121	VAL	2.6
1	E	788	THR	2.6
1	C	528	HIS	2.6
1	E	328	LEU	2.6
1	A	361	ALA	2.6
1	E	792	ALA	2.6
1	C	548	ASP	2.6
1	E	110	ASP	2.6
1	C	316	GLY	2.6
1	E	142	VAL	2.6
1	E	411	VAL	2.6
1	C	744	TYR	2.6
1	E	68	ILE	2.6
1	E	733	ILE	2.6
1	C	547	HIS	2.6
1	E	194	ASP	2.5
1	E	397	PHE	2.5
1	E	529	ILE	2.5
1	E	91	GLN	2.5
1	E	43	ALA	2.5
1	C	254	THR	2.5
1	E	17	THR	2.5
1	E	23	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	170	SER	2.5
1	E	189	VAL	2.5
1	E	201	GLN	2.5
1	E	760	ARG	2.5
1	E	83	ASP	2.5
1	E	125	ALA	2.5
2	F	461	ASP	2.5
1	E	148	GLY	2.5
1	E	262	THR	2.5
1	A	485	VAL	2.5
1	E	389	SER	2.5
1	E	27	HIS	2.5
1	C	252	PRO	2.5
1	E	153	PRO	2.5
1	E	345	PRO	2.5
1	E	510	ARG	2.4
1	E	735	CYS	2.4
1	E	105	SER	2.4
1	E	400	VAL	2.4
1	E	491	VAL	2.4
1	E	469	LEU	2.4
1	E	216	HIS	2.4
2	D	461	ASP	2.4
1	E	791	GLN	2.4
1	A	475	ALA	2.4
1	E	779	GLY	2.4
1	E	184	SER	2.4
1	E	235	VAL	2.4
1	C	496	LYS	2.4
1	E	87	LYS	2.4
1	E	508	LEU	2.4
1	E	94	ASP	2.4
1	E	349	GLN	2.4
1	E	548	ASP	2.4
1	E	118	ALA	2.4
1	E	272	ALA	2.4
1	E	350	ALA	2.4
1	E	224	GLN	2.4
1	C	236	ASP	2.4
1	C	527	GLU	2.4
1	E	158	ASN	2.4
1	E	246	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	2.4
1	E	285	PHE	2.4
1	E	540	ILE	2.4
1	C	545	LEU	2.4
1	E	252	PRO	2.3
1	C	67	GLY	2.3
1	E	324	MET	2.3
1	A	442	VAL	2.3
1	A	552	VAL	2.3
1	C	541	CYS	2.3
1	E	537	HIS	2.3
1	E	380	LEU	2.3
1	C	260	LYS	2.3
1	E	465	LYS	2.3
1	E	516	PRO	2.3
1	E	551	GLY	2.3
1	C	93	THR	2.3
1	C	291	PHE	2.3
1	E	102	LEU	2.3
1	E	730	LEU	2.3
1	E	171	LYS	2.3
1	E	365	ASN	2.3
1	E	31	GLY	2.3
1	E	229	TYR	2.3
1	C	216	HIS	2.3
1	E	100	ILE	2.3
1	A	480	VAL	2.3
1	C	235	VAL	2.3
1	C	323	VAL	2.3
1	C	307	LEU	2.3
1	C	511	LEU	2.3
1	A	310	ASP	2.3
1	E	104	ASP	2.3
1	C	318	ALA	2.3
1	E	150	ARG	2.3
1	E	787	ALA	2.3
1	E	177	THR	2.3
1	E	176	GLN	2.3
1	E	546	GLU	2.3
1	C	292	LYS	2.3
1	E	15	LYS	2.3
1	E	92	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	314	LEU	2.2
1	E	12	LEU	2.2
1	E	316	GLY	2.2
1	E	341	HIS	2.2
1	E	550	ALA	2.2
1	E	459	ILE	2.2
1	A	235	VAL	2.2
1	C	300	LEU	2.2
1	C	303	LEU	2.2
1	C	285	PHE	2.2
1	E	261	ASP	2.2
1	A	481	MET	2.2
1	E	214	GLY	2.2
1	E	295	GLU	2.2
1	C	555	LYS	2.2
1	E	430	ALA	2.2
1	C	514	SER	2.2
1	C	501	LEU	2.2
1	E	463	LEU	2.2
1	C	298	VAL	2.2
1	E	297	PRO	2.2
1	E	555	LYS	2.2
1	E	475	ALA	2.2
1	E	756	SER	2.2
1	E	288	ILE	2.2
1	C	480	VAL	2.2
1	E	518	VAL	2.2
1	E	260	LYS	2.2
1	E	317	LYS	2.2
1	A	392	GLY	2.2
1	E	234	GLY	2.2
1	E	439	GLY	2.2
1	E	476	HIS	2.2
1	E	402	ALA	2.2
1	C	290	ASN	2.1
1	C	312	LYS	2.1
1	C	317	LYS	2.1
1	E	814	LYS	2.1
1	A	761	PRO	2.1
1	E	759	GLN	2.1
1	E	287	ALA	2.1
1	E	523	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	745	SER	2.1
1	A	433	ARG	2.1
2	F	490	ARG	2.1
1	A	464	LEU	2.1
1	C	519	LEU	2.1
1	E	247	ASP	2.1
1	A	427	PHE	2.1
1	C	233	PHE	2.1
1	C	276	PHE	2.1
1	E	394	PHE	2.1
1	E	468	THR	2.1
1	E	470	THR	2.1
1	E	737	GLU	2.1
1	C	313	ASP	2.1
1	A	434	VAL	2.1
1	E	560	VAL	2.1
1	E	211	PHE	2.1
1	A	458	GLY	2.1
1	E	69	THR	2.1
1	E	512	SER	2.1
1	E	237	LYS	2.1
1	E	410	LYS	2.1
1	E	13	MET	2.1
1	E	337	MET	2.1
1	E	481	MET	2.1
1	E	524	GLU	2.1
1	A	356	LEU	2.1
1	E	319	LEU	2.1
1	E	96	ASN	2.1
1	E	549	HIS	2.1
1	A	420	PRO	2.1
1	A	553	PRO	2.1
1	E	267	LYS	2.0
1	E	122	THR	2.0
1	E	208	THR	2.0
1	C	494	GLU	2.0
1	E	195	GLU	2.0
1	E	739	ALA	2.0
1	E	138	GLN	2.0
1	C	319	LEU	2.0
1	E	329	PRO	2.0
1	E	521	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	160	VAL	2.0
1	A	107	GLY	2.0
1	E	152	LYS	2.0
1	C	84	GLU	2.0
1	E	181	THR	2.0
1	E	738	GLN	2.0
1	E	310	ASP	2.0
1	E	426	LEU	2.0
1	C	743	ILE	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	45,60,66,70	0
1	DDE	E	699	20/21	0.91	0.14	38,73,107,109	0
1	DDE	C	699	20/21	0.93	0.12	29,64,106,111	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.

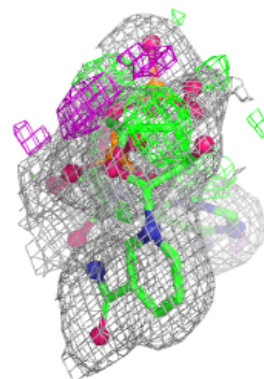
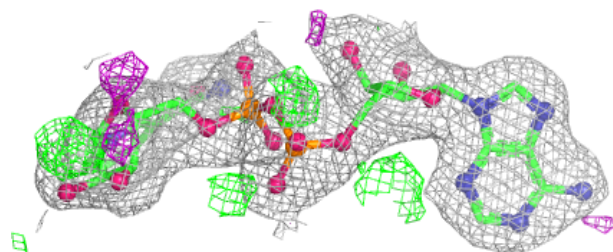
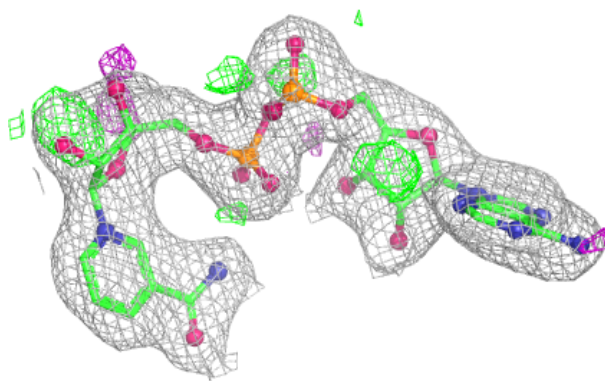
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAD	F	702	44/44	0.95	0.07	11,32,48,56	0
3	NAD	B	700	44/44	0.96	0.07	17,28,45,62	0
3	NAD	D	701	44/44	0.97	0.07	7,24,49,51	0

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.

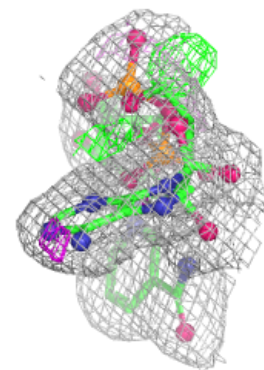
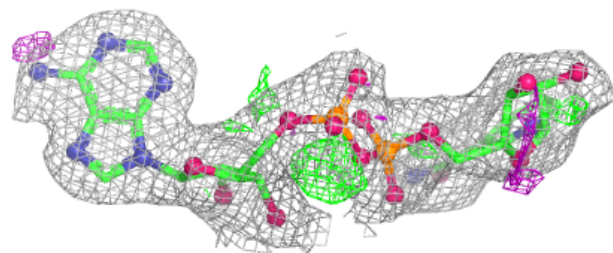
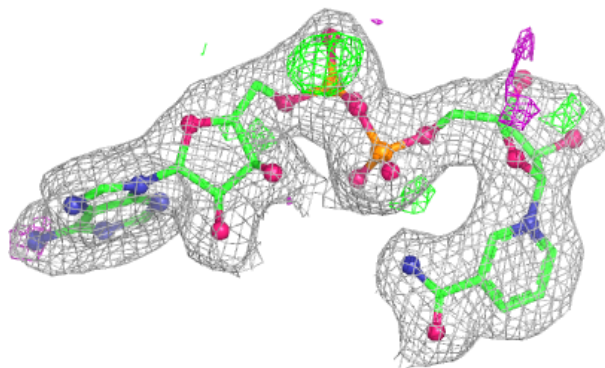
Electron density around NAD F 702:

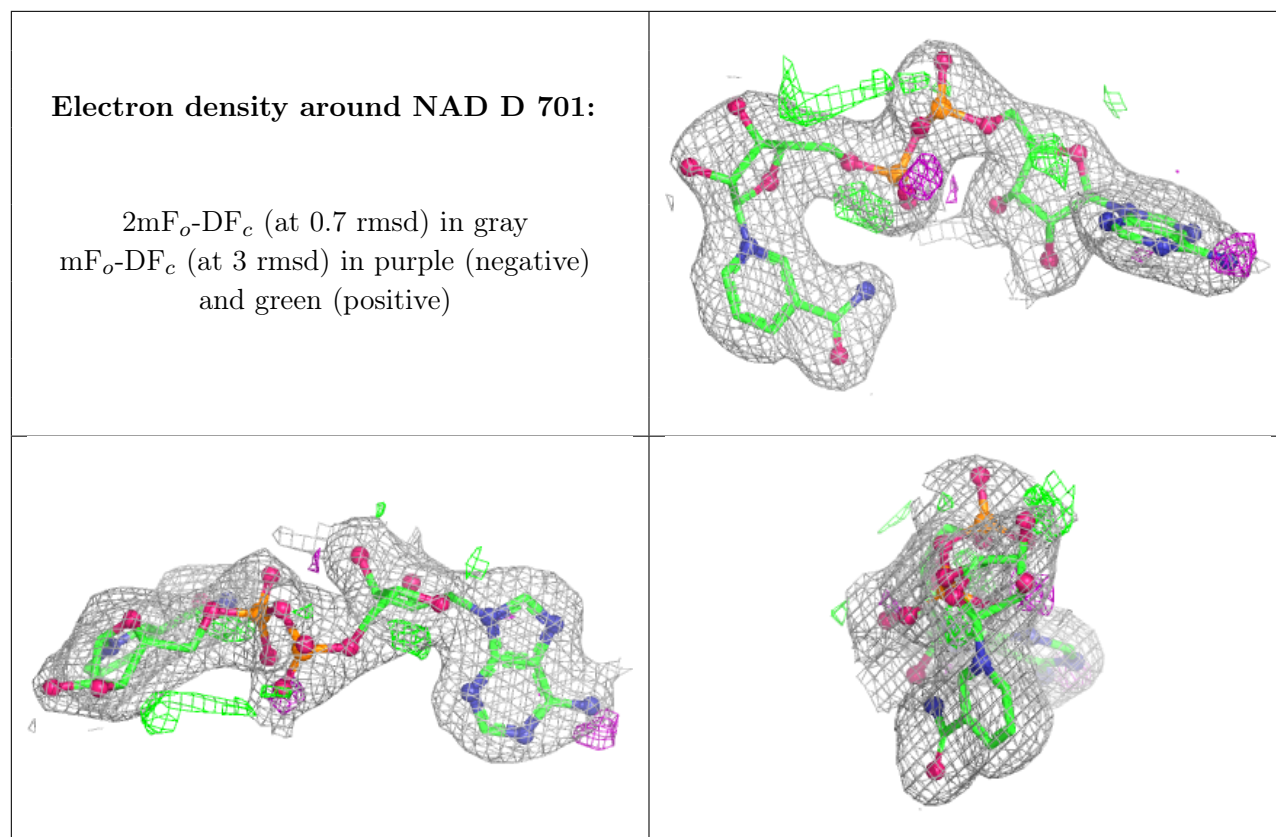
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.