



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 PM UTC

PDB ID : 3B78 / pdb_00003b78
Title : Structure of the eEF2-ExoA(R551H)-NAD⁺ complex
Authors : Jorgensen, R.; Merrill, A.R.
Deposited on : 2007-10-30
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

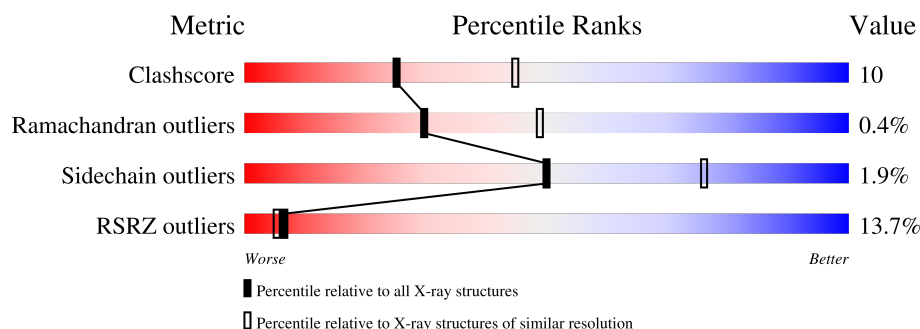
1 Overall quality at a glance ⓘ

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% 74% 23% ..
1	C	842	7% 73% 24% ..
1	E	842	40% 69% 28% ..
2	B	207	% 84% 15%
2	D	207	% 88% 12%
2	F	207	2% 86% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24616 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
			6405	4075	1093	1207	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
			1587	1001	282	304			
2	D	207	Total	C	N	O	0	0	0
			1587	1001	282	304			
2	F	207	Total	C	N	O	0	0	0
			1587	1001	282	304			

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	551	HIS	ARG	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	551	HIS	ARG	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	551	HIS	ARG	engineered mutation	UNP P11439

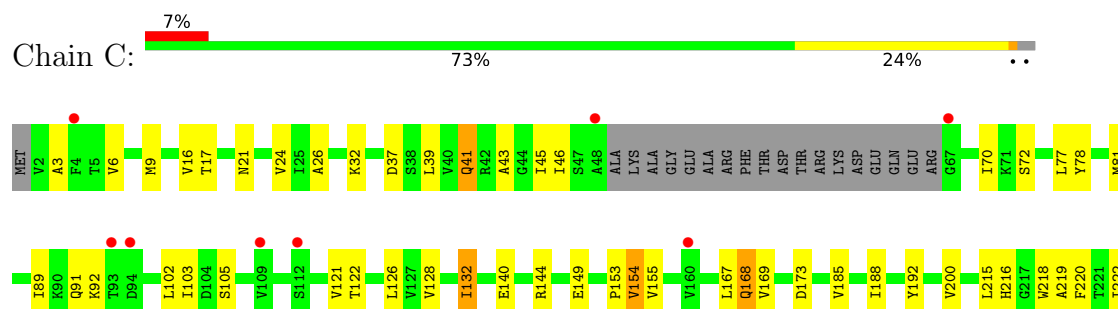
3 Residue-property plots

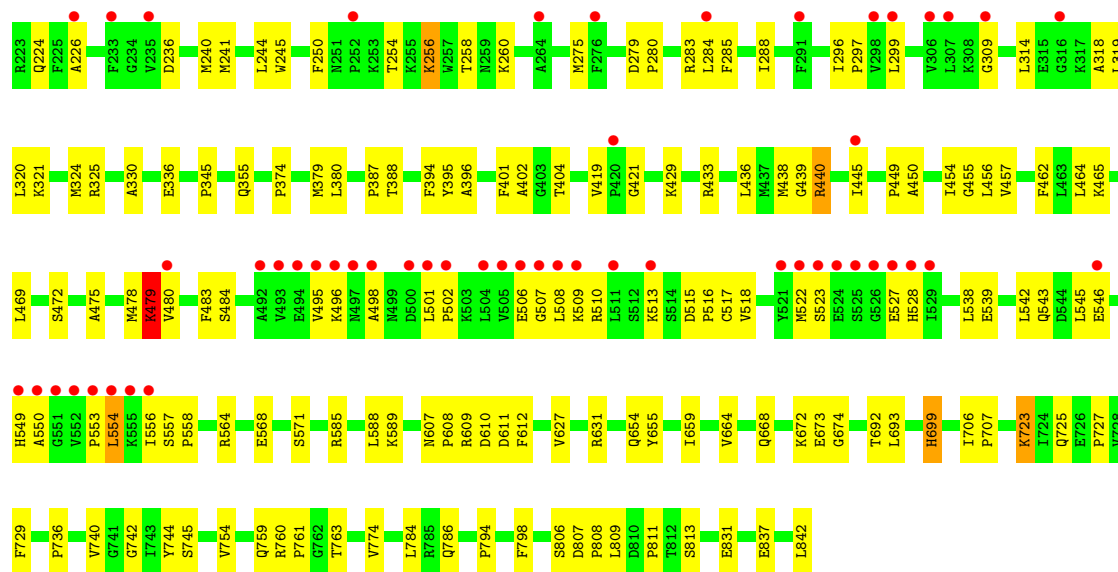
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



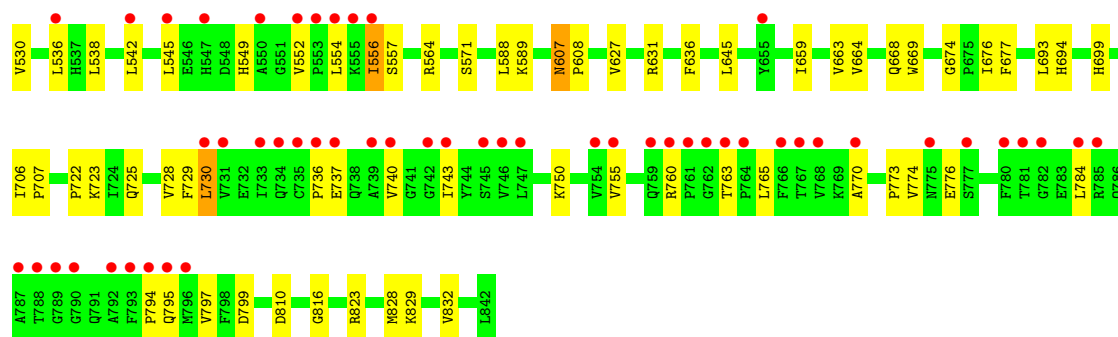
• Molecule 1: Elongation factor 2



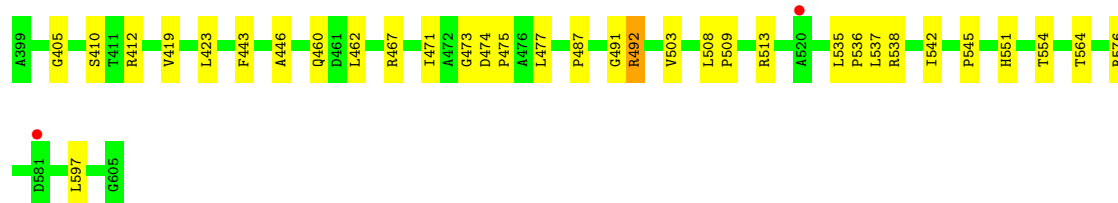
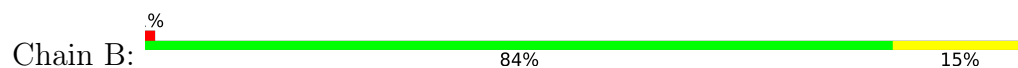


• Molecule 1: Elongation factor 2

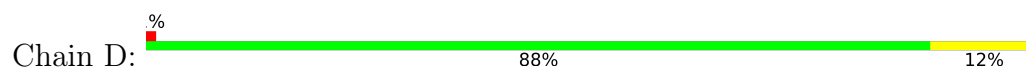




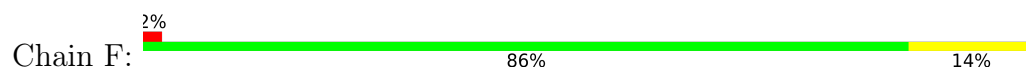
● Molecule 2: Exotoxin A



● 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	327.14Å 68.13Å 190.58Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	46.55 – 2.50 46.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.55-2.50) 93.3 (46.55-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.242 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24616	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 38.77 % 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 3.5087e-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	4/8823 (0.0%)
1	C	0.27	0/6517	0.72	2/8823 (0.0%)
1	E	0.26	0/6517	0.71	4/8823 (0.0%)
2	B	0.28	0/1627	0.74	0/2217
2	D	0.28	0/1627	0.72	2/2217 (0.1%)
2	F	0.28	0/1627	0.70	0/2217
All	All	0.27	0/24432	0.72	12/33120 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	607	ASN	CA-C-N	8.45	128.18	119.56
1	E	607	ASN	C-N-CA	8.45	128.18	119.56
1	A	674	GLY	CA-C-N	5.99	125.61	119.56
1	A	674	GLY	C-N-CA	5.99	125.61	119.56
1	E	674	GLY	CA-C-N	5.56	125.18	119.56
1	E	674	GLY	C-N-CA	5.56	125.18	119.56
1	C	674	GLY	CA-C-N	5.41	125.49	119.87
1	C	674	GLY	C-N-CA	5.41	125.49	119.87
2	D	489	ALA	N-CA-C	-5.19	106.46	112.89
1	A	793	PHE	CA-C-N	5.06	125.03	120.03
1	A	793	PHE	C-N-CA	5.06	125.03	120.03
2	D	438	GLY	N-CA-C	5.01	117.50	110.38

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	120	0
1	C	6415	0	6488	135	0
1	E	6405	0	6472	174	0
2	B	1587	0	1536	21	0
2	D	1587	0	1536	11	0
2	F	1587	0	1536	14	0
3	B	44	0	26	0	0
3	D	44	0	26	2	0
3	F	44	0	26	0	0
4	A	94	0	0	0	0
4	B	103	0	0	1	0
4	C	84	0	0	0	0
4	D	106	0	0	0	0
4	E	35	0	0	0	0
4	F	76	0	0	0	0
All	All	24616	0	24118	470	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 10.

All (470) 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:699:DDE:HAB2	1:C:699:DDE:HAT2	1.39	1.04
1:C:699:DDE:HAA1	3:D:701:NAD:H4D	1.52	0.89
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.55	0.88
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.55	0.88
1:C:404:THR:HG22	1:C:449:PRO:HA	1.59	0.84
1:C:568:GLU:HB2	1:C:723:LYS:HD3	1.58	0.84
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.61	0.83
1:C:216:HIS:HD2	1:C:321:LYS:HG2	1.42	0.82
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.61	0.82
1:E:391:LYS:HG3	1:E:392:GLY:H	1.44	0.82
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.62	0.80
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HD12	1:C:132:ILE:H	1.46	0.79
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.64	0.79
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.65	0.77
1:A:437:MET:HE3	1:A:455:GLY:HA3	1.66	0.77
1:E:149:GLU:HA	1:E:355:GLN:HE22	1.48	0.76
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.68	0.76
1:C:258:THR:HG22	1:C:260:LYS:H	1.51	0.75
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.69	0.74
1:A:404:THR:HG22	1:A:449:PRO:HA	1.69	0.74
1:E:404:THR:HG22	1:E:449:PRO:HA	1.67	0.74
1:C:699:DDE:HAT2	1:C:699:DDE:CAB	2.16	0.73
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.71	0.73
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.24	0.72
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.71	0.72
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.72	0.71
1:C:324:MET:HE2	1:C:324:MET:HA	1.72	0.70
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.74	0.68
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.75	0.68
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.76	0.68
1:E:324:MET:HE2	1:E:324:MET:HA	1.76	0.68
1:C:216:HIS:CD2	1:C:321:LYS:HG2	2.28	0.67
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.76	0.67
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.76	0.66
1:E:556:ILE:HG22	1:E:557:SER:H	1.61	0.66
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.66
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.77	0.66
1:E:240:MET:HE3	1:E:240:MET:HA	1.77	0.65
1:E:43:ALA:HB1	1:E:78:TYR:H	1.61	0.65
1:E:30:HIS:ND1	1:E:130:ASP:HB2	2.12	0.64
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.79	0.64
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.33	0.64
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.79	0.63
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.80	0.63
1:A:578:LYS:HG2	1:A:585:ARG:HG2	1.81	0.62
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.81	0.62
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.82	0.62
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.80	0.62
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.80	0.62
2:F:516:LEU:HD12	2:F:526:GLU:HG2	1.81	0.62
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.80	0.61
1:C:216:HIS:HB2	1:C:218:TRP:HD1	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.82	0.61
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.81	0.61
1:E:810:ASP:O	1:E:816:GLY:HA3	2.00	0.61
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.82	0.61
1:C:759:GLN:HG2	1:C:760:ARG:H	1.67	0.60
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.84	0.60
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.84	0.60
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.82	0.60
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.67	0.59
1:A:510:ARG:HG3	1:A:549:HIS:HD2	1.66	0.59
1:A:810:ASP:O	1:A:816:GLY:HA3	2.01	0.59
1:A:399:ARG:HB2	1:A:453:ILE:HD13	1.84	0.59
1:C:699:DDE:HAA3	1:C:699:DDE:NAD	2.16	0.59
1:A:250:PHE:HD2	1:A:275:MET:HE1	1.67	0.59
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.38	0.58
1:C:103:ILE:HD12	1:C:122:THR:HG22	1.86	0.58
1:E:121:VAL:HG11	1:E:383:SER:OG	2.02	0.58
1:A:405:VAL:HG12	1:A:448:CYS:HB3	1.86	0.58
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.86	0.58
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.86	0.58
1:C:103:ILE:HD13	1:C:121:VAL:HG23	1.85	0.58
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.68	0.58
1:A:431:ILE:HD12	1:A:459:ILE:HD11	1.86	0.57
1:E:291:PHE:HD1	1:E:315:GLU:HB3	1.69	0.57
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.84	0.57
1:E:26:ALA:CB	1:E:128:VAL:HB	2.34	0.57
1:A:237:LYS:O	1:A:241:MET:HG2	2.04	0.57
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.86	0.57
1:C:496:LYS:H	1:C:554:LEU:HD22	1.70	0.57
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.39	0.57
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.40	0.57
1:A:569:SER:O	1:A:720:ALA:HB1	2.05	0.57
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.38	0.57
1:C:436:LEU:HD13	1:C:438:MET:HE3	1.87	0.57
1:C:723:LYS:HA	1:C:808:PRO:HG3	1.87	0.57
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.86	0.57
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.19	0.57
1:E:464:LEU:HG	1:E:465:LYS:HG3	1.87	0.57
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.87	0.56
2:B:477:LEU:HD22	2:B:551:HIS:HB3	1.87	0.56
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.21	0.56
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.45	0.56
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.56
1:C:664:VAL:O	1:C:668:GLN:HG2	2.06	0.56
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.41	0.55
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.88	0.55
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.87	0.55
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.87	0.55
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.89	0.55
1:A:6:VAL:HG13	1:A:445:ILE:HG22	1.89	0.55
1:A:68:ILE:HD13	1:A:390:ASP:HB2	1.89	0.55
1:E:291:PHE:CD1	1:E:315:GLU:HB3	2.42	0.55
1:A:275:MET:HE2	1:A:276:PHE:CZ	2.42	0.54
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.89	0.54
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.88	0.54
1:A:381:TYR:O	1:A:398:GLY:HA3	2.07	0.54
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.89	0.54
1:A:510:ARG:HG3	1:A:549:HIS:CD2	2.42	0.54
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.88	0.54
1:E:391:LYS:HG3	1:E:392:GLY:N	2.20	0.54
1:A:501:LEU:N	1:A:502:PRO:HD2	2.23	0.54
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.72	0.54
1:E:9:MET:O	1:E:13:MET:HG3	2.07	0.53
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.90	0.53
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.91	0.53
1:E:755:VAL:HG23	1:E:770:ALA:HA	1.91	0.53
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.89	0.53
1:C:609:ARG:H	1:C:609:ARG:HD2	1.73	0.53
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.89	0.53
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.91	0.53
1:C:699:DDE:CAA	3:D:701:NAD:H4D	2.33	0.53
1:A:258:THR:HG22	1:A:260:LYS:H	1.74	0.53
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.91	0.53
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.91	0.53
1:C:374:PRO:O	1:C:404:THR:HG23	2.08	0.52
1:C:727:PRO:HB2	1:C:774:VAL:HG21	1.92	0.52
1:C:699:DDE:HAA3	1:C:699:DDE:HAD2	1.75	0.52
1:C:17:THR:HB	1:C:92:LYS:O	2.09	0.52
1:E:564:ARG:HB2	1:E:725:GLN:HB2	1.90	0.52
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.91	0.52
1:C:6:VAL:HG13	1:C:445:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.92	0.52
1:E:296:ILE:O	1:E:300:LEU:HD13	2.10	0.52
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.91	0.52
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.92	0.52
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.91	0.51
1:E:207:GLY:O	1:E:337:MET:HG2	2.09	0.51
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.39	0.51
1:E:156:VAL:HG22	1:E:337:MET:HE1	1.92	0.51
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.91	0.51
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.45	0.51
1:A:197:LEU:HD21	1:A:351:TYR:CD1	2.45	0.51
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.92	0.51
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.93	0.51
1:E:385:MET:HG2	1:E:465:LYS:HA	1.92	0.51
1:A:478:MET:O	1:A:479:LYS:C	2.54	0.51
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.11	0.51
1:C:70:ILE:HG22	1:C:388:THR:HG22	1.91	0.51
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.92	0.50
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.93	0.50
1:A:632:LYS:HD3	1:A:648:ASP:O	2.11	0.50
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.93	0.50
1:A:365:ASN:O	1:A:369:ILE:HG13	2.11	0.50
1:E:74:ALA:HA	1:E:102:LEU:O	2.12	0.50
1:E:243:ARG:O	1:E:248:SER:HB2	2.10	0.50
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.93	0.50
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.93	0.50
1:C:672:LYS:C	1:C:673:GLU:HG2	2.36	0.50
1:E:111:PHE:HB3	1:E:114:GLU:HG2	1.94	0.50
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.41	0.50
1:E:750:LYS:HD2	1:E:776:GLU:O	2.12	0.50
1:A:110:ASP:HB3	1:A:536:LEU:HD22	1.93	0.50
1:E:289:MET:HE2	1:E:289:MET:HA	1.94	0.50
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.47	0.49
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.95	0.49
1:E:482:LYS:HB3	1:E:797:VAL:HG11	1.94	0.49
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.94	0.49
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.94	0.49
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.48	0.49
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.77	0.49
1:E:419:VAL:HG12	1:E:421:GLY:H	1.77	0.49
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:VAL:HG12	1:C:200:VAL:O	2.13	0.49
1:E:312:LYS:HD2	1:E:312:LYS:O	2.13	0.49
1:A:831:GLU:CD	1:A:831:GLU:H	2.20	0.49
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.93	0.49
1:C:515:ASP:O	1:C:518:VAL:HG12	2.13	0.49
1:A:249:PHE:CZ	1:A:261:ASP:HB3	2.48	0.49
1:C:699:DDE:CAB	1:C:699:DDE:CAT	2.86	0.49
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.95	0.48
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.48	0.48
1:A:378:LEU:O	1:A:470:THR:HA	2.12	0.48
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.95	0.48
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.48	0.48
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.95	0.48
1:E:365:ASN:HD21	1:E:472:SER:HB3	1.77	0.48
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.78	0.48
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.95	0.48
1:C:538:LEU:O	1:C:542:LEU:HB2	2.14	0.48
1:C:627:VAL:O	1:C:631:ARG:HB2	2.14	0.48
1:A:9:MET:O	1:A:13:MET:HG3	2.14	0.48
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.96	0.48
1:E:101:ASN:N	1:E:101:ASN:HD22	2.12	0.48
1:C:250:PHE:HB3	1:C:275:MET:HE1	1.96	0.48
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.95	0.48
1:E:292:LYS:O	1:E:296:ILE:HG13	2.14	0.48
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.49	0.47
1:A:588:LEU:HD12	1:A:588:LEU:C	2.39	0.47
1:C:254:THR:HG22	1:C:256:LYS:HB2	1.95	0.47
1:C:546:GLU:HA	1:C:550:ALA:HB3	1.95	0.47
1:E:823:ARG:HE	1:E:832:VAL:HG22	1.79	0.47
2:B:467:ARG:NH1	2:B:536:PRO:HG3	2.28	0.47
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.95	0.47
1:A:487:PRO:HB3	1:A:531:ALA:HB1	1.97	0.47
1:A:828:MET:HG2	2:B:576:ARG:NE	2.29	0.47
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.95	0.47
1:E:257:TRP:HZ3	1:E:272:ALA:HB2	1.79	0.47
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.97	0.47
1:A:746:VAL:O	1:A:750:LYS:HD3	2.15	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.97	0.47
1:C:296:ILE:N	1:C:297:PRO:HD2	2.29	0.47
1:C:321:LYS:O	1:C:325:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:LYS:HE3	1:C:517:CYS:SG	2.55	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
2:D:538:ARG:HD2	2:D:538:ARG:HA	1.69	0.47
1:A:338:ILE:O	1:A:342:LEU:HB2	2.15	0.47
1:E:321:LYS:O	1:E:325:ARG:HG3	2.14	0.47
1:E:627:VAL:O	1:E:631:ARG:HB2	2.14	0.47
1:A:111:PHE:O	1:A:115:VAL:HG23	2.15	0.47
1:A:731:VAL:HG22	1:A:796:MET:HB3	1.97	0.47
1:C:37:ASP:O	1:C:41:GLN:HB2	2.15	0.47
1:C:588:LEU:C	1:C:588:LEU:HD12	2.40	0.47
1:C:736:PRO:O	1:C:740:VAL:HG23	2.15	0.47
1:E:39:LEU:HD12	1:E:39:LEU:H	1.79	0.47
2:B:419:VAL:O	2:B:423:LEU:HG	2.14	0.47
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.96	0.47
1:C:727:PRO:HB2	1:C:774:VAL:CG2	2.45	0.47
2:F:547:GLU:HG3	2:F:550:GLY:HA3	1.97	0.47
1:E:391:LYS:CG	1:E:392:GLY:H	2.22	0.46
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.30	0.46
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.96	0.46
1:A:454:ILE:HG13	1:A:455:GLY:H	1.80	0.46
2:B:545:PRO:HA	2:B:551:HIS:O	2.15	0.46
1:C:501:LEU:C	1:C:501:LEU:HD23	2.41	0.46
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.98	0.46
1:E:30:HIS:CE1	1:E:130:ASP:HB2	2.50	0.46
1:E:459:ILE:O	1:E:459:ILE:HG22	2.16	0.46
1:A:6:VAL:CG1	1:A:445:ILE:HG22	2.45	0.46
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.97	0.46
1:C:226:ALA:HB2	1:C:241:MET:HB3	1.97	0.46
1:E:676:ILE:HG22	1:E:677:PHE:HD2	1.80	0.46
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.97	0.46
1:A:731:VAL:O	1:A:769:LYS:HA	2.15	0.46
1:E:111:PHE:O	1:E:115:VAL:HG23	2.16	0.46
1:C:169:VAL:HG22	1:C:173:ASP:HB2	1.98	0.46
1:E:296:ILE:N	1:E:297:PRO:HD2	2.31	0.46
1:E:349:GLN:O	1:E:370:LYS:HA	2.15	0.46
1:A:385:MET:HG2	1:A:465:LYS:HA	1.97	0.46
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.45	0.46
1:E:552:VAL:O	1:E:554:LEU:HG	2.16	0.45
1:A:118:ALA:O	1:A:122:THR:HG23	2.17	0.45
1:C:126:LEU:HD12	1:C:154:VAL:HG12	1.97	0.45
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:VAL:O	1:E:189:VAL:HG23	2.16	0.45
1:A:197:LEU:HD21	1:A:351:TYR:CE1	2.52	0.45
1:C:149:GLU:HA	1:C:355:GLN:HE22	1.82	0.45
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.82	0.45
1:C:585:ARG:HB2	1:C:692:THR:OG1	2.17	0.45
1:E:588:LEU:C	1:E:588:LEU:HD12	2.41	0.45
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.98	0.45
1:C:167:LEU:O	1:C:168:GLN:C	2.59	0.45
1:E:183:GLU:HA	1:E:186:ASN:OD1	2.17	0.45
1:C:9:MET:HG3	1:C:438:MET:HE1	1.98	0.45
1:E:156:VAL:HG11	1:E:334:LEU:HD21	1.98	0.45
1:E:204:PRO:HA	1:E:209:VAL:HB	1.98	0.45
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.99	0.45
1:A:411:VAL:HG21	1:A:431:ILE:HD11	1.99	0.45
1:E:46:ILE:N	1:E:46:ILE:HD12	2.32	0.45
1:E:538:LEU:O	1:E:542:LEU:HG	2.17	0.45
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.99	0.45
1:E:208:THR:HG23	1:E:341:HIS:CE1	2.52	0.45
1:E:659:ILE:O	1:E:663:VAL:HG23	2.17	0.45
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.17	0.45
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.46	0.45
1:C:539:GLU:O	1:C:543:GLN:HG3	2.17	0.45
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.46	0.45
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.51	0.45
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.52	0.45
1:E:129:VAL:HG12	1:E:130:ASP:N	2.32	0.45
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.97	0.45
1:A:16:VAL:HG21	1:A:451:GLY:HA3	1.98	0.45
1:A:664:VAL:O	1:A:668:GLN:HG2	2.16	0.45
1:E:556:ILE:HG22	1:E:557:SER:N	2.29	0.45
2:F:571:ILE:HA	2:F:572:PRO:HD3	1.85	0.45
1:A:465:LYS:HE3	1:A:517:CYS:SG	2.57	0.44
1:C:380:LEU:HB3	1:C:469:LEU:HB2	1.99	0.44
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.85	0.44
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.16	0.44
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.44
1:E:823:ARG:HG2	1:E:828:MET:HE3	1.99	0.44
2:F:487:PRO:HA	2:F:492:ARG:O	2.18	0.44
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.33	0.44
1:C:478:MET:O	1:C:479:LYS:C	2.60	0.44
1:A:231:LYS:HB3	1:A:231:LYS:HE2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:ASP:CG	1:A:721:ASP:O	2.60	0.44
2:B:487:PRO:HB2	2:B:491:GLY:HA2	1.99	0.44
1:E:344:SER:HB2	1:E:345:PRO:HD2	1.99	0.44
1:E:459:ILE:HD12	1:E:459:ILE:N	2.33	0.44
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.99	0.44
1:A:727:PRO:HD3	1:A:801:TRP:HZ3	1.82	0.44
2:B:474:ASP:HA	2:B:475:PRO:HD2	1.87	0.44
1:C:498:ALA:HA	1:C:501:LEU:HB2	2.00	0.44
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.53	0.44
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.18	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.32	0.44
1:A:45:ILE:HG22	1:A:438:MET:HE1	1.99	0.44
1:E:763:THR:C	1:E:765:LEU:H	2.26	0.44
1:A:283:ARG:HB3	1:A:299:LEU:HD21	1.99	0.44
1:C:395:TYR:CD1	1:C:457:VAL:HG22	2.53	0.44
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.53	0.44
2:B:471:ILE:CG1	2:B:554:THR:HB	2.47	0.44
1:C:557:SER:HB2	1:C:558:PRO:HD2	2.00	0.44
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.79	0.44
1:E:132:ILE:HD12	1:E:132:ILE:N	2.33	0.44
1:E:365:ASN:O	1:E:369:ILE:HG12	2.16	0.44
1:E:369:ILE:HD12	1:E:401:PHE:HB3	2.00	0.44
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.18	0.43
1:A:250:PHE:CD2	1:A:275:MET:HE1	2.52	0.43
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.00	0.43
1:A:515:ASP:HA	1:A:516:PRO:HD2	1.87	0.43
1:C:70:ILE:O	1:C:440:ARG:HG2	2.18	0.43
1:E:77:LEU:HD23	1:E:335:LEU:HD21	2.00	0.43
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.90	0.43
2:B:410:SER:OG	2:B:412:ARG:HG3	2.18	0.43
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.48	0.43
1:E:381:TYR:O	1:E:398:GLY:HA3	2.17	0.43
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.54	0.43
1:A:374:PRO:O	1:A:404:THR:HG23	2.18	0.43
1:A:392:GLY:HA3	1:A:513:LYS:HD3	1.99	0.43
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.43
1:E:237:LYS:O	1:E:241:MET:HG3	2.18	0.43
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.00	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:C:807:ASP:HA	1:C:808:PRO:HD2	1.86	0.43
1:C:396:ALA:HB3	1:C:456:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:TRP:HB3	1:E:324:MET:HB3	2.00	0.43
1:C:484:SER:HB3	1:C:798:PHE:H	1.84	0.43
2:D:571:ILE:HA	2:D:572:PRO:HD3	1.88	0.43
2:F:511:PHE:HB3	2:F:600:TYR:CD1	2.54	0.43
1:A:36:THR:HG23	1:A:102:LEU:HD21	2.01	0.43
1:A:73:THR:HG21	1:A:384:LYS:HD2	2.01	0.43
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.54	0.43
1:A:759:GLN:HB2	1:A:766:PHE:CE2	2.53	0.43
1:C:43:ALA:HB1	1:C:78:TYR:O	2.18	0.43
1:C:723:LYS:HB3	1:C:723:LYS:HE3	1.67	0.43
1:E:737:GLU:HA	1:E:740:VAL:HG23	2.00	0.43
1:A:120:ARG:NH1	1:A:479:LYS:HD2	2.33	0.43
1:A:613:LYS:HG2	1:A:631:ARG:HH11	1.83	0.43
1:A:669:TRP:CZ2	2:B:492:ARG:HB2	2.53	0.43
1:C:26:ALA:HB2	1:C:128:VAL:HB	2.00	0.43
1:C:144:ARG:HD3	1:C:192:TYR:CZ	2.54	0.43
1:E:244:LEU:O	1:E:273:PHE:HB2	2.18	0.43
1:E:279:ASP:O	1:E:283:ARG:HG2	2.18	0.43
1:E:327:PHE:CD2	1:E:328:LEU:HG	2.54	0.43
1:E:338:ILE:O	1:E:342:LEU:HB2	2.18	0.43
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.78	0.43
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.99	0.43
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.53	0.43
1:E:485:VAL:HG22	1:E:485:VAL:O	2.18	0.43
2:F:537:LEU:HD11	2:F:542:ILE:HG22	2.00	0.43
1:A:413:ILE:HD13	1:A:459:ILE:HG23	2.00	0.42
1:E:823:ARG:HG2	1:E:828:MET:CE	2.49	0.42
1:A:545:LEU:O	1:A:550:ALA:HB3	2.19	0.42
2:B:477:LEU:HD22	2:B:551:HIS:CB	2.50	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.83	0.42
1:A:4:PHE:HD2	1:A:45:ILE:HG23	1.83	0.42
1:E:722:PRO:O	1:E:723:LYS:HD2	2.19	0.42
1:A:155:VAL:HG21	1:A:185:VAL:HG11	2.01	0.42
1:C:809:LEU:O	1:C:811:PRO:HD3	2.20	0.42
1:A:132:ILE:HD12	1:A:162:ARG:HD3	2.01	0.42
2:D:433:GLY:O	2:D:505:ARG:HG3	2.18	0.42
1:E:774:VAL:C	1:E:776:GLU:H	2.28	0.42
1:C:806:SER:HB2	1:C:813:SER:HB2	2.02	0.42
1:E:39:LEU:HD11	1:E:334:LEU:HD13	2.01	0.42
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.50	0.42
2:F:495:ASN:HB3	2:F:578:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:PRO:HB2	1:A:774:VAL:HG21	2.02	0.42
1:E:664:VAL:O	1:E:668:GLN:HG2	2.19	0.42
2:F:419:VAL:O	2:F:423:LEU:HG	2.19	0.42
2:F:488:ASP:HB3	2:F:492:ARG:HB2	2.01	0.42
1:C:153:PRO:HD2	1:C:200:VAL:CG1	2.50	0.42
1:C:401:PHE:CD2	1:C:478:MET:HE1	2.55	0.42
1:E:397:PHE:CD1	1:E:437:MET:HG3	2.54	0.42
1:A:806:SER:HB2	1:A:813:SER:HB2	2.02	0.42
1:C:654:GLN:O	1:C:655:TYR:HB2	2.20	0.42
2:D:474:ASP:HA	2:D:475:PRO:HD2	1.87	0.42
1:E:155:VAL:HG21	1:E:202:VAL:HG21	2.02	0.42
1:A:388:THR:HG21	1:A:395:TYR:CG	2.55	0.42
1:C:506:GLU:O	1:C:510:ARG:HG3	2.19	0.42
1:A:140:GLU:HG3	1:A:188:ILE:HD13	2.02	0.41
1:C:3:ALA:HB2	1:C:46:ILE:HG13	2.02	0.41
2:D:537:LEU:O	2:D:538:ARG:HD3	2.19	0.41
1:E:410:LYS:HA	1:E:430:ALA:HA	2.02	0.41
1:E:608:PRO:HG3	1:E:636:PHE:CG	2.55	0.41
2:B:513:ARG:HD3	4:B:779:HOH:O	2.19	0.41
1:C:285:PHE:CE1	1:C:320:LEU:HD21	2.54	0.41
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.20	0.41
1:C:241:MET:HA	1:C:244:LEU:HD12	2.02	0.41
1:C:288:ILE:HA	1:C:296:ILE:HD11	2.03	0.41
1:C:509:LYS:O	1:C:513:LYS:HG3	2.19	0.41
1:C:742:GLY:O	1:C:745:SER:HB3	2.19	0.41
1:C:284:LEU:HD23	1:C:299:LEU:HD23	2.01	0.41
2:D:522:GLU:CD	2:D:522:GLU:H	2.28	0.41
1:E:250:PHE:O	1:E:275:MET:HE1	2.20	0.41
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.55	0.41
1:A:410:LYS:HA	1:A:430:ALA:HA	2.01	0.41
2:B:537:LEU:O	2:B:538:ARG:HD3	2.20	0.41
1:C:26:ALA:CB	1:C:128:VAL:HB	2.51	0.41
1:C:72:SER:HA	1:C:439:GLY:O	2.19	0.41
2:D:508:LEU:N	2:D:509:PRO:CD	2.84	0.41
1:E:307:LEU:HD13	1:E:311:GLU:O	2.20	0.41
2:F:508:LEU:N	2:F:509:PRO:CD	2.83	0.41
1:A:677:PHE:N	1:A:677:PHE:CD2	2.88	0.41
1:C:454:ILE:HG13	1:C:455:GLY:H	1.85	0.41
1:E:80:GLU:HA	1:E:96:ASN:O	2.20	0.41
1:A:226:ALA:CB	1:A:241:MET:HB3	2.44	0.41
1:A:542:LEU:HD13	1:A:556:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HD22	1:C:318:ALA:HB1	2.02	0.41
1:C:419:VAL:HG12	1:C:421:GLY:H	1.86	0.41
1:E:3:ALA:HA	1:E:46:ILE:O	2.21	0.41
1:E:109:VAL:O	1:E:109:VAL:HG12	2.21	0.41
1:E:119:LEU:HD11	1:E:146:ALA:HA	2.02	0.41
1:E:212:GLY:HA3	1:E:219:ALA:HA	2.02	0.41
1:A:83:ASP:O	1:A:87:LYS:HG3	2.20	0.41
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.91	0.41
1:A:454:ILE:HG13	1:A:455:GLY:N	2.36	0.41
1:C:523:SER:OG	1:C:527:GLU:HB2	2.20	0.41
1:C:760:ARG:CG	1:C:761:PRO:HD2	2.51	0.41
1:E:76:SER:C	1:E:77:LEU:HD12	2.46	0.41
1:E:237:LYS:HA	1:E:240:MET:HB3	2.03	0.41
1:A:373:ASP:HA	1:A:374:PRO:HD2	1.85	0.41
1:A:559:PRO:HB2	1:A:778:PHE:CE2	2.56	0.41
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.51	0.41
1:C:226:ALA:CB	1:C:241:MET:HB3	2.51	0.41
1:E:163:ALA:O	1:E:169:VAL:HG12	2.20	0.41
1:E:345:PRO:HB3	1:E:399:ARG:HH21	1.85	0.41
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.56	0.41
1:E:728:VAL:HG22	1:E:773:PRO:HA	2.02	0.41
1:E:736:PRO:O	1:E:740:VAL:HG23	2.21	0.41
1:A:229:TYR:HB3	1:A:233:PHE:CD2	2.56	0.40
2:F:439:TYR:CE2	2:F:475:PRO:HD3	2.56	0.40
1:A:77:LEU:HB2	1:A:100:ILE:HB	2.03	0.40
1:A:565:GLU:CD	1:A:676:ILE:HB	2.45	0.40
2:B:443:PHE:CZ	2:B:446:ALA:HB2	2.57	0.40
1:C:155:VAL:HG21	1:C:185:VAL:HG11	2.03	0.40
1:C:454:ILE:HG13	1:C:455:GLY:N	2.36	0.40
1:C:610:ASP:OD1	1:C:611:ASP:N	2.55	0.40
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.84	0.40
1:E:262:THR:HG23	1:E:266:GLY:HA2	2.03	0.40
1:E:352:ARG:O	1:E:356:LEU:HG	2.21	0.40
1:A:47:SER:HB3	1:A:438:MET:HE2	2.02	0.40
1:A:396:ALA:HB3	1:A:456:LEU:HB2	2.03	0.40
1:A:659:ILE:HD13	1:A:693:LEU:HD21	2.04	0.40
1:C:16:VAL:HG21	1:C:450:ALA:O	2.22	0.40
1:C:81:MET:HE1	1:C:336:GLU:HA	2.03	0.40
1:E:454:ILE:HG13	1:E:455:GLY:N	2.36	0.40
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.56	0.40
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.56	0.40
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.90	0.40
1:C:612:PHE:CE1	1:C:631:ARG:HG3	2.57	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.56	0.40
1:E:452:ASN:HD22	1:E:452:ASN:N	2.19	0.40
1:A:594:ASP:HB2	1:A:597:VAL:HG23	2.02	0.40
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.04	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%)	781 (96%)	34 (4%)	3 (0%)	30 49
1	C	818/842 (97%)	780 (95%)	33 (4%)	5 (1%)	21 38
1	E	818/842 (97%)	763 (93%)	52 (6%)	3 (0%)	30 49
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100 100
2	D	205/207 (99%)	198 (97%)	6 (3%)	1 (0%)	24 43
2	F	205/207 (99%)	200 (98%)	5 (2%)	0	100 100
All	All	3069/3147 (98%)	2923 (95%)	134 (4%)	12 (0%)	30 49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	E	479	LYS
1	A	432	GLN
1	C	168	GLN
1	C	479	LYS

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Mol	Chain	Res	Type
2	D	488	ASP
1	E	556	ILE
1	E	795	GLN
1	C	554	LEU
1	C	215	LEU
1	A	721	ASP
1	C	309	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%)	683 (98%)	16 (2%)	44	72
1	C	699/714 (98%)	684 (98%)	15 (2%)	47	74
1	E	699/714 (98%)	693 (99%)	6 (1%)	70	87
2	B	161/161 (100%)	158 (98%)	3 (2%)	50	76
2	D	161/161 (100%)	158 (98%)	3 (2%)	50	76
2	F	161/161 (100%)	155 (96%)	6 (4%)	30	57
All	All	2580/2625 (98%)	2531 (98%)	49 (2%)	50	76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	258	THR
1	A	300	LEU
1	A	325	ARG
1	A	479	LYS
1	A	510	ARG
1	A	578	LYS
1	A	595	GLU
1	A	599	LEU
1	A	609	ARG
1	A	610	ASP

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Mol	Chain	Res	Type
1	A	677	PHE
1	A	698	ILE
1	A	795	GLN
1	A	831	GLU
1	A	842	LEU
2	B	460	GLN
2	B	462	LEU
2	B	492	ARG
1	C	41	GLN
1	C	132	ILE
1	C	154	VAL
1	C	236	ASP
1	C	240	MET
1	C	256	LYS
1	C	440	ARG
1	C	479	LYS
1	C	480	VAL
1	C	556	ILE
1	C	723	LYS
1	C	786	GLN
1	C	831	GLU
1	C	837	GLU
1	C	842	LEU
2	D	462	LEU
2	D	499	LEU
2	D	540	ASP
1	E	101	ASN
1	E	186	ASN
1	E	452	ASN
1	E	494	GLU
1	E	730	LEU
1	E	829	LYS
2	F	462	LEU
2	F	499	LEU
2	F	513	ARG
2	F	547	GLU
2	F	548	GLU
2	F	560	LEU

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	145	GLN
1	A	528	HIS
1	A	549	HIS
1	A	657	HIS
1	A	795	GLN
2	B	551	HIS
1	C	138	GLN
1	C	216	HIS
1	C	341	HIS
1	C	414	GLN
1	C	607	ASN
1	C	759	GLN
2	D	428	GLN
2	D	603	GLN
1	E	21	ASN
1	E	365	ASN
1	E	452	ASN
1	E	476	HIS
1	E	738	GLN
1	E	791	GLN
2	F	428	GLN
2	F	551	HIS

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	E	699	1	9,10,21	0.48	0	8,12,30	0.94	0

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	1.10	1 (5%)
1	DDE	A	699	1	9,10,21	0.46	0	8,12,30	0.95	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	E	699	1	-	1/5/6/23	0/1/1/1
1	DDE	C	699	1	-	2/20/21/23	0/1/1/1
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	699	DDE	CG-ND1	-2.87	1.33	1.38
1	C	699	DDE	CBW-NCB	-2.46	1.49	1.54
1	C	699	DDE	CAT-CE1	2.43	1.53	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	CAU-CBW-CBI	-2.97	105.41	111.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	699	DDE	O-C-CA-CB
1	C	699	DDE	O-C-CA-CB
1	E	699	DDE	O-C-CA-CB
1	C	699	DDE	NAD-CBI-CBW-NCB

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	699	DDE	1	0
1	C	699	DDE	7	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	D	701	-	46,48,48	0.92	3 (6%)	64,73,73	1.59	10 (15%)
3	NAD	B	700	-	46,48,48	0.91	4 (8%)	64,73,73	1.60	10 (15%)
3	NAD	F	702	-	46,48,48	0.94	6 (13%)	64,73,73	1.62	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	D	701	-	-	8/30/62/62	0/5/5/5
3	NAD	B	700	-	-	7/30/62/62	0/5/5/5
3	NAD	F	702	-	-	7/30/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	702	NAD	PN-O3	2.37	1.62	1.59
3	D	701	NAD	C8A-N9A	-2.32	1.33	1.37
3	F	702	NAD	PA-O3	2.23	1.61	1.59
3	B	700	NAD	C8A-N9A	-2.21	1.33	1.37
3	D	701	NAD	PN-O3	2.12	1.61	1.59
3	F	702	NAD	O4D-C1D	2.12	1.43	1.40
3	F	702	NAD	C8A-N9A	-2.12	1.33	1.37
3	D	701	NAD	O4D-C1D	2.10	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	C4A-N9A	-2.06	1.33	1.37
3	F	702	NAD	C5A-N7A	-2.02	1.35	1.39
3	B	700	NAD	C5A-N7A	-2.01	1.35	1.39
3	B	700	NAD	C8A-N7A	2.01	1.35	1.31
3	F	702	NAD	C4A-N9A	-2.00	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	N3A-C2A-N1A	-4.99	121.03	128.58
3	D	701	NAD	C5A-C4A-N3A	-4.99	119.85	126.72
3	F	702	NAD	C5A-C4A-N3A	-4.95	119.91	126.72
3	F	702	NAD	N3A-C2A-N1A	-4.90	121.17	128.58
3	D	701	NAD	N3A-C2A-N1A	-4.89	121.18	128.58
3	B	700	NAD	C5A-C4A-N3A	-4.73	120.21	126.72
3	D	701	NAD	C2A-N3A-C4A	3.39	120.10	111.83
3	F	702	NAD	C2A-N3A-C4A	3.37	120.06	111.83
3	B	700	NAD	C2A-N3A-C4A	3.33	119.95	111.83
3	D	701	NAD	C4B-O4B-C1B	-3.30	102.19	109.47
3	F	702	NAD	C4B-O4B-C1B	-3.18	102.45	109.47
3	B	700	NAD	C4B-O4B-C1B	-3.17	102.47	109.47
3	D	701	NAD	O4B-C1B-N9A	3.16	114.16	108.09
3	B	700	NAD	N9A-C8A-N7A	-3.12	109.52	113.94
3	F	702	NAD	O4B-C1B-N9A	3.11	114.06	108.09
3	D	701	NAD	N3A-C4A-N9A	3.10	132.43	127.17
3	F	702	NAD	N9A-C8A-N7A	-2.96	109.74	113.94
3	F	702	NAD	C4A-C5A-N7A	-2.95	107.21	110.58
3	F	702	NAD	N3A-C4A-N9A	2.95	132.18	127.17
3	B	700	NAD	N3A-C4A-N9A	2.89	132.09	127.17
3	D	701	NAD	C4A-C5A-N7A	-2.89	107.28	110.58
3	D	701	NAD	N9A-C8A-N7A	-2.87	109.86	113.94
3	B	700	NAD	C4A-C5A-N7A	-2.83	107.35	110.58
3	B	700	NAD	O4B-C1B-N9A	2.67	113.22	108.09
3	B	700	NAD	C4A-N9A-C8A	2.51	108.38	105.74
3	F	702	NAD	C5A-N7A-C8A	2.32	107.09	103.45
3	B	700	NAD	C5A-N7A-C8A	2.30	107.06	103.45
3	D	701	NAD	C4A-N9A-C8A	2.29	108.14	105.74
3	D	701	NAD	C5A-N7A-C8A	2.26	107.01	103.45
3	F	702	NAD	C4A-N9A-C8A	2.19	108.04	105.74
3	F	702	NAD	C5D-C4D-C3D	-2.12	107.58	115.21

There are no chirality outliers.

All (22) torsion outliers are listed below:

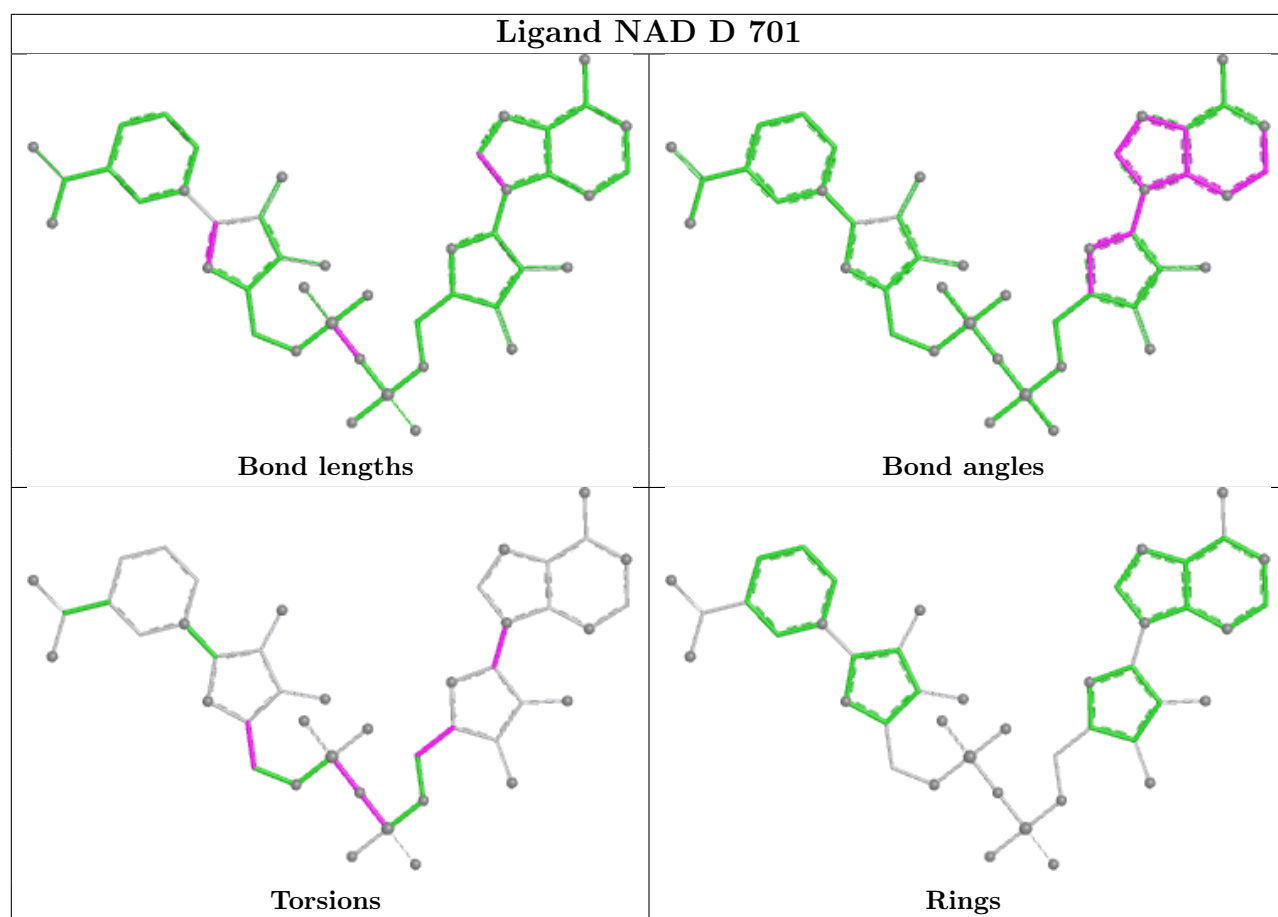
Mol	Chain	Res	Type	Atoms
3	B	700	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	O4D-C4D-C5D-O5D
3	B	700	NAD	C3D-C4D-C5D-O5D
3	D	701	NAD	C3D-C4D-C5D-O5D
3	F	702	NAD	O4D-C4D-C5D-O5D
3	F	702	NAD	C3D-C4D-C5D-O5D
3	B	700	NAD	O4B-C4B-C5B-O5B
3	F	702	NAD	O4B-C4B-C5B-O5B
3	B	700	NAD	C3B-C4B-C5B-O5B
3	F	702	NAD	C3B-C4B-C5B-O5B
3	D	701	NAD	PA-O3-PN-O1N
3	D	701	NAD	O4B-C4B-C5B-O5B
3	B	700	NAD	PN-O3-PA-O1A
3	D	701	NAD	PN-O3-PA-O1A
3	F	702	NAD	PN-O3-PA-O1A
3	B	700	NAD	PN-O3-PA-O2A
3	D	701	NAD	PN-O3-PA-O2A
3	D	701	NAD	PA-O3-PN-O2N
3	F	702	NAD	PN-O3-PA-O2A
3	B	700	NAD	O4B-C1B-N9A-C8A
3	D	701	NAD	O4B-C1B-N9A-C8A
3	F	702	NAD	O4B-C1B-N9A-C8A

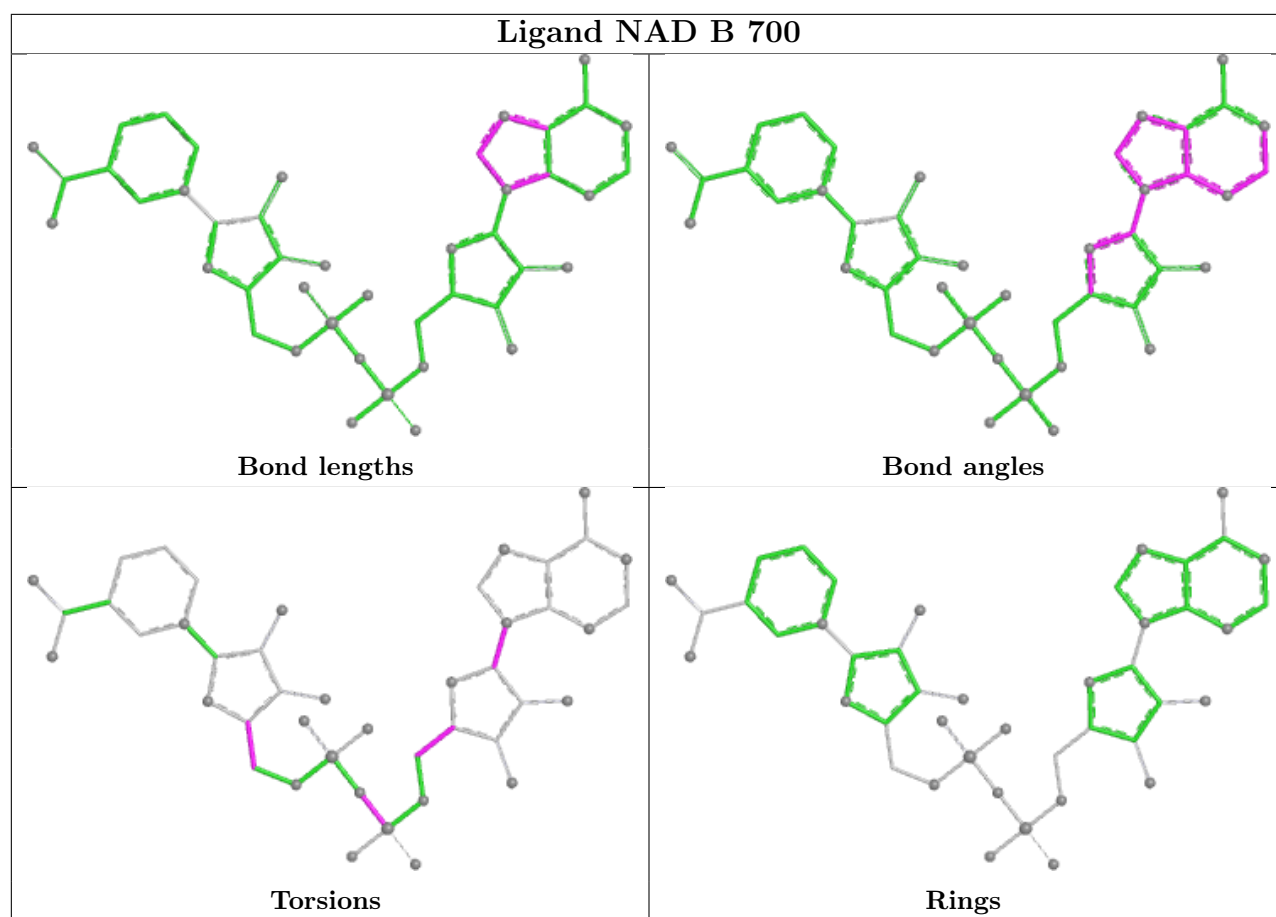
There are no ring outliers.

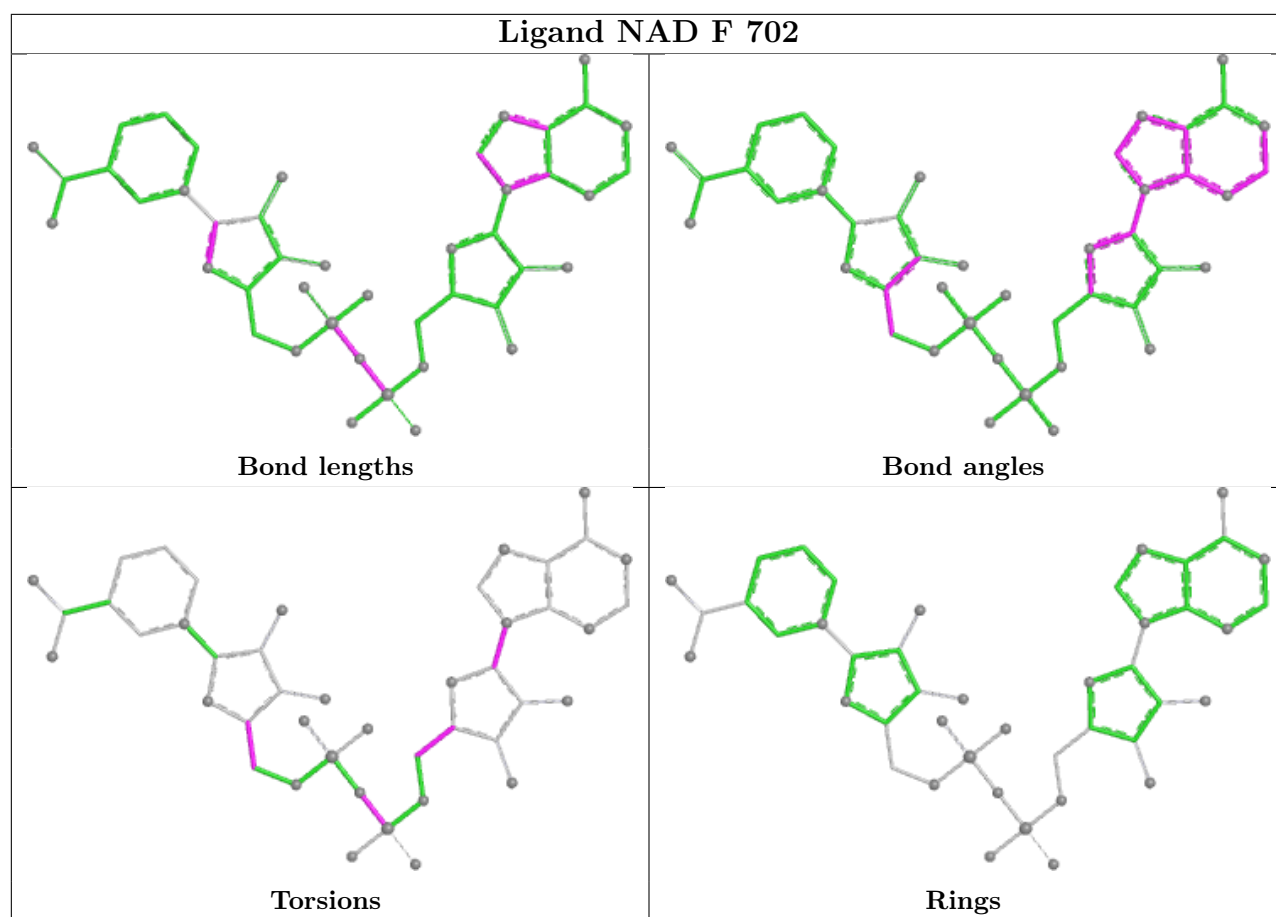
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	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%)	0.13	18 (2%) 62 58	17, 53, 92, 120	0
1	C	822/842 (97%)	0.42	61 (7%) 20 18	18, 60, 134, 199	0
1	E	822/842 (97%)	1.68	333 (40%) 0 0	19, 131, 186, 266	0
2	B	207/207 (100%)	-0.28	2 (0%) 79 76	16, 33, 80, 99	0
2	D	207/207 (100%)	-0.36	3 (1%) 73 70	16, 30, 66, 88	0
2	F	207/207 (100%)	-0.16	5 (2%) 59 55	20, 36, 82, 118	0
All	All	3087/3147 (98%)	0.54	422 (13%) 6 5	16, 57, 165, 266	0

All (422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	26	ALA	8.2
1	E	143	LEU	7.5
1	E	126	LEU	7.1
1	E	277	ILE	6.8
1	E	127	VAL	6.6
1	E	129	VAL	6.2
1	E	128	VAL	6.2
1	C	493	VAL	6.0
1	E	196	VAL	6.0
1	E	179	ALA	6.0
1	E	123	ASP	5.8
1	E	794	PRO	5.7
1	E	743	ILE	5.7
1	E	781	THR	5.7
1	E	155	VAL	5.6
1	E	278	LEU	5.4
1	E	188	ILE	5.3
1	E	276	PHE	5.2
1	E	343	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	147	LEU	5.2
1	E	156	VAL	5.1
1	C	109	VAL	5.0
1	E	185	VAL	5.0
1	E	175	TYR	5.0
1	E	273	PHE	4.9
1	E	154	VAL	4.9
1	E	25	ILE	4.9
1	E	280	PRO	4.9
1	E	338	ILE	4.8
1	E	504	LEU	4.8
1	E	99	LEU	4.7
1	E	241	MET	4.7
1	E	763	THR	4.7
1	E	36	THR	4.6
1	E	86	VAL	4.6
1	E	730	LEU	4.5
1	E	796	MET	4.5
1	E	24	VAL	4.4
1	E	525	SER	4.4
1	E	442	VAL	4.4
1	C	550	ALA	4.4
1	E	770	ALA	4.4
1	E	205	ALA	4.4
1	E	233	PHE	4.3
1	E	193	ALA	4.3
1	C	549	HIS	4.3
1	E	146	ALA	4.2
1	E	364	ALA	4.2
1	E	19	VAL	4.2
1	E	782	GLY	4.2
1	E	335	LEU	4.2
1	E	493	VAL	4.2
1	E	78	TYR	4.1
1	E	125	ALA	4.1
1	E	182	VAL	4.1
1	C	553	PRO	4.1
1	E	492	ALA	4.1
1	E	192	TYR	4.1
1	E	187	VAL	4.1
1	E	501	LEU	4.1
1	E	342	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	755	VAL	4.0
1	E	303	LEU	4.0
1	E	474	THR	4.0
1	E	348	ALA	4.0
1	E	245	TRP	4.0
1	E	103	ILE	3.9
1	E	222	ILE	3.9
1	E	210	ALA	3.8
1	E	766	PHE	3.8
1	E	203	TYR	3.8
1	E	169	VAL	3.8
1	E	761	PRO	3.8
1	E	789	GLY	3.7
1	E	167	LEU	3.7
1	E	200	VAL	3.7
1	E	339	VAL	3.7
1	C	504	LEU	3.7
1	E	23	SER	3.7
1	C	508	LEU	3.7
1	E	73	THR	3.7
1	C	523	SER	3.7
1	E	77	LEU	3.7
1	E	189	VAL	3.6
1	E	788	THR	3.6
1	E	536	LEU	3.6
1	E	89	ILE	3.6
1	E	526	GLY	3.6
1	E	107	GLY	3.6
1	E	284	LEU	3.6
1	E	340	LEU	3.6
1	E	735	CYS	3.6
1	E	282	PHE	3.6
1	E	306	VAL	3.5
1	A	48	ALA	3.5
1	E	197	LEU	3.5
1	E	366	CYS	3.5
1	E	131	THR	3.5
1	E	347	THR	3.5
1	A	475	ALA	3.5
1	E	46	ILE	3.5
1	E	332	ASP	3.4
1	E	202	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	323	VAL	3.4
2	B	520	ALA	3.4
1	E	164	LEU	3.4
1	E	300	LEU	3.4
1	E	480	VAL	3.4
1	E	163	ALA	3.4
1	E	79	SER	3.4
1	E	777	SER	3.4
1	E	346	VAL	3.3
1	E	740	VAL	3.3
1	E	144	ARG	3.3
1	E	176	GLN	3.3
1	E	35	LEU	3.3
1	C	298	VAL	3.3
1	E	27	HIS	3.3
1	E	135	VAL	3.3
1	E	246	GLY	3.3
1	C	4	PHE	3.3
1	E	98	PHE	3.3
1	E	242	ASP	3.3
1	E	174	LEU	3.3
1	E	215	LEU	3.3
1	E	109	VAL	3.3
1	E	207	GLY	3.3
1	E	75	ILE	3.3
1	E	780	PHE	3.2
1	E	547	HIS	3.2
1	E	209	VAL	3.2
1	E	254	THR	3.2
1	E	76	SER	3.2
1	E	194	ASP	3.2
1	E	21	ASN	3.2
1	C	501	LEU	3.2
1	C	554	LEU	3.2
1	C	527	GLU	3.2
1	E	762	GLY	3.2
1	E	745	SER	3.2
1	C	528	HIS	3.2
1	E	81	MET	3.2
1	E	177	THR	3.2
1	A	46	ILE	3.2
1	E	438	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	184	SER	3.1
1	E	553	PRO	3.1
1	C	445	ILE	3.1
2	F	489	ALA	3.1
1	E	795	GLN	3.1
1	E	121	VAL	3.1
1	E	32	LYS	3.1
1	E	299	LEU	3.1
1	E	784	LEU	3.1
1	E	16	VAL	3.1
1	E	171	LYS	3.1
1	E	240	MET	3.1
1	E	437	MET	3.1
1	E	476	HIS	3.1
1	E	211	PHE	3.1
1	E	401	PHE	3.1
1	E	420	PRO	3.0
1	E	260	LYS	3.0
1	E	6	VAL	3.0
1	E	731	VAL	3.0
1	E	368	ALA	3.0
1	C	546	GLU	3.0
1	E	736	PRO	3.0
1	E	104	ASP	3.0
1	A	365	ASN	3.0
1	E	768	VAL	3.0
1	C	498	ALA	3.0
1	E	739	ALA	3.0
1	E	243	ARG	3.0
1	A	237	LYS	3.0
1	E	157	ILE	3.0
1	C	494	GLU	3.0
1	E	329	PRO	3.0
1	C	555	LYS	3.0
1	C	505	VAL	2.9
1	E	151	ILE	2.9
1	E	281	ILE	2.9
1	C	524	GLU	2.9
1	E	195	GLU	2.9
1	E	74	ALA	2.9
1	E	349	GLN	2.9
1	C	492	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	350	ALA	2.9
1	E	361	ALA	2.9
1	E	764	PRO	2.9
1	E	320	LEU	2.9
1	C	112	SER	2.9
1	A	81	MET	2.9
1	C	235	VAL	2.9
1	E	505	VAL	2.9
1	E	475	ALA	2.9
1	E	747	LEU	2.9
2	D	461	ASP	2.9
1	C	495	VAL	2.9
1	E	239	LYS	2.9
1	E	17	THR	2.9
1	C	507	GLY	2.9
1	E	170	SER	2.8
1	E	40	VAL	2.8
1	E	466	THR	2.8
1	C	500	ASP	2.8
1	E	247	ASP	2.8
1	C	513	LYS	2.8
1	E	44	GLY	2.8
1	C	497	ASN	2.8
1	E	259	ASN	2.8
1	E	445	ILE	2.8
1	C	93	THR	2.8
1	E	742	GLY	2.8
1	C	521	TYR	2.8
1	E	733	ILE	2.8
1	E	112	SER	2.8
1	E	506	GLU	2.7
2	F	490	ARG	2.7
1	E	2	VAL	2.7
1	E	47	SER	2.7
2	D	489	ALA	2.7
1	E	444	PRO	2.7
1	E	248	SER	2.7
1	E	312	LYS	2.7
1	E	351	TYR	2.7
1	E	519	LEU	2.7
1	E	20	ARG	2.7
1	E	498	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	148	GLY	2.7
1	E	153	PRO	2.7
1	A	196	VAL	2.7
1	E	443	GLU	2.7
1	C	526	GLY	2.6
1	E	67	GLY	2.6
1	E	68	ILE	2.6
1	E	178	PHE	2.6
1	E	264	ALA	2.6
1	E	331	ALA	2.6
1	E	341	HIS	2.6
1	E	554	LEU	2.6
1	E	754	VAL	2.6
1	E	82	SER	2.6
1	E	229	TYR	2.6
1	A	433	ARG	2.6
1	E	70	ILE	2.6
1	E	785	ARG	2.6
1	E	356	LEU	2.6
1	E	238	ALA	2.6
1	E	134	GLY	2.6
1	E	217	GLY	2.6
1	E	334	LEU	2.6
1	E	160	VAL	2.6
1	E	759	GLN	2.6
1	E	787	ALA	2.6
1	E	256	LYS	2.6
1	E	418	TYR	2.6
1	C	502	PRO	2.5
1	E	83	ASP	2.5
2	F	461	ASP	2.5
1	C	529	ILE	2.5
1	C	233	PHE	2.5
1	E	111	PHE	2.5
1	C	48	ALA	2.5
1	E	38	SER	2.5
1	E	337	MET	2.5
1	C	316	GLY	2.5
1	C	556	ILE	2.5
1	E	441	PHE	2.5
1	E	545	LEU	2.5
1	E	93	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	268	PRO	2.5
1	E	367	ILE	2.5
2	D	459	SER	2.5
1	E	9	MET	2.5
1	E	556	ILE	2.5
1	C	291	PHE	2.5
1	E	225	PHE	2.5
1	E	734	GLN	2.5
1	E	417	ASN	2.5
1	C	522	MET	2.5
1	E	316	GLY	2.4
1	E	737	GLU	2.4
1	E	244	LEU	2.4
1	E	314	LEU	2.4
1	E	542	LEU	2.4
1	E	201	GLN	2.4
1	E	355	GLN	2.4
1	E	218	TRP	2.4
1	E	101	ASN	2.4
1	E	48	ALA	2.4
1	E	289	MET	2.4
1	E	792	ALA	2.4
1	E	471	THR	2.4
1	C	420	PRO	2.4
1	C	309	GLY	2.4
1	C	551	GLY	2.4
1	E	305	ILE	2.4
1	E	369	ILE	2.4
2	F	488	ASP	2.4
1	C	299	LEU	2.4
1	E	395	TYR	2.4
1	A	495	VAL	2.4
1	C	306	VAL	2.4
1	E	142	VAL	2.4
1	E	71	LYS	2.4
1	E	145	GLN	2.4
1	E	108	HIS	2.4
1	E	352	ARG	2.4
1	E	655	TYR	2.4
1	E	322	VAL	2.4
1	E	552	VAL	2.4
1	E	746	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	186	ASN	2.4
1	E	365	ASN	2.4
1	A	84	GLU	2.4
1	C	252	PRO	2.4
1	E	190	SER	2.4
1	E	94	ASP	2.4
1	E	372	CYS	2.4
1	E	357	TYR	2.4
1	E	775	ASN	2.4
1	A	761	PRO	2.3
1	E	258	THR	2.3
1	C	525	SER	2.3
1	E	132	ILE	2.3
1	E	307	LEU	2.3
1	E	328	LEU	2.3
1	A	109	VAL	2.3
1	E	158	ASN	2.3
1	E	226	ALA	2.3
1	E	523	SER	2.3
1	A	548	ASP	2.3
1	E	478	MET	2.3
1	E	555	LYS	2.3
1	E	180	ARG	2.3
1	E	198	GLY	2.3
1	E	790	GLY	2.3
1	C	284	LEU	2.3
1	E	793	PHE	2.3
1	C	552	VAL	2.3
1	E	333	ALA	2.3
1	E	387	PRO	2.3
1	E	550	ALA	2.3
1	E	296	ILE	2.3
1	E	130	ASP	2.3
1	E	425	ASP	2.3
1	C	276	PHE	2.3
1	A	480	VAL	2.3
1	E	106	PRO	2.3
1	E	477	ASN	2.2
1	E	767	THR	2.2
1	E	31	GLY	2.2
1	E	105	SER	2.2
1	E	344	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	354	GLU	2.2
1	E	510	ARG	2.2
1	E	274	ASN	2.2
1	E	122	THR	2.2
1	E	421	GLY	2.2
1	A	524	GLU	2.2
1	E	149	GLU	2.2
1	E	311	GLU	2.2
1	E	431	ILE	2.2
1	C	506	GLU	2.2
1	E	257	TRP	2.2
1	E	760	ARG	2.2
1	E	502	PRO	2.2
1	C	480	VAL	2.2
1	E	28	VAL	2.2
1	E	191	THR	2.2
1	C	307	LEU	2.2
1	C	511	LEU	2.2
2	F	492	ARG	2.2
1	C	160	VAL	2.1
1	E	39	LEU	2.1
1	E	139	THR	2.1
1	E	208	THR	2.1
1	E	80	GLU	2.1
1	C	509	LYS	2.1
1	E	422	LYS	2.1
1	E	483	PHE	2.1
1	E	224	GLN	2.1
1	E	3	ALA	2.1
1	E	118	ALA	2.1
1	E	141	THR	2.1
2	B	581	ASP	2.1
1	E	216	HIS	2.1
1	E	419	VAL	2.1
1	C	67	GLY	2.1
1	E	88	GLU	2.1
1	E	288	ILE	2.1
1	A	194	ASP	2.1
1	A	310	ASP	2.1
1	E	302	LYS	2.1
1	E	360	PRO	2.1
1	E	386	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	405	VAL	2.1
1	E	427	PHE	2.1
1	C	226	ALA	2.1
1	C	264	ALA	2.1
1	E	165	LEU	2.1
1	E	214	GLY	2.1
1	E	309	GLY	2.1
1	E	439	GLY	2.1
1	A	16	VAL	2.0
1	E	206	ARG	2.0
1	E	219	ALA	2.0
1	E	102	LEU	2.0
1	C	94	ASP	2.0
1	E	199	ASP	2.0
1	E	374	PRO	2.0
1	E	521	TYR	2.0
1	E	269	LEU	2.0
1	E	376	ALA	2.0
1	E	436	LEU	2.0
1	C	496	LYS	2.0
1	E	524	GLU	2.0
1	E	95	GLY	2.0
1	E	467	GLY	2.0
1	E	468	THR	2.0
1	E	113	SER	2.0

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

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	0.92	0.10	43,61,74,78	0
1	DDE	E	699	10/21	0.93	0.10	38,49,69,70	0
1	DDE	C	699	20/21	0.94	0.16	22,85,126,129	0

6.3 Carbohydrates ⓘ

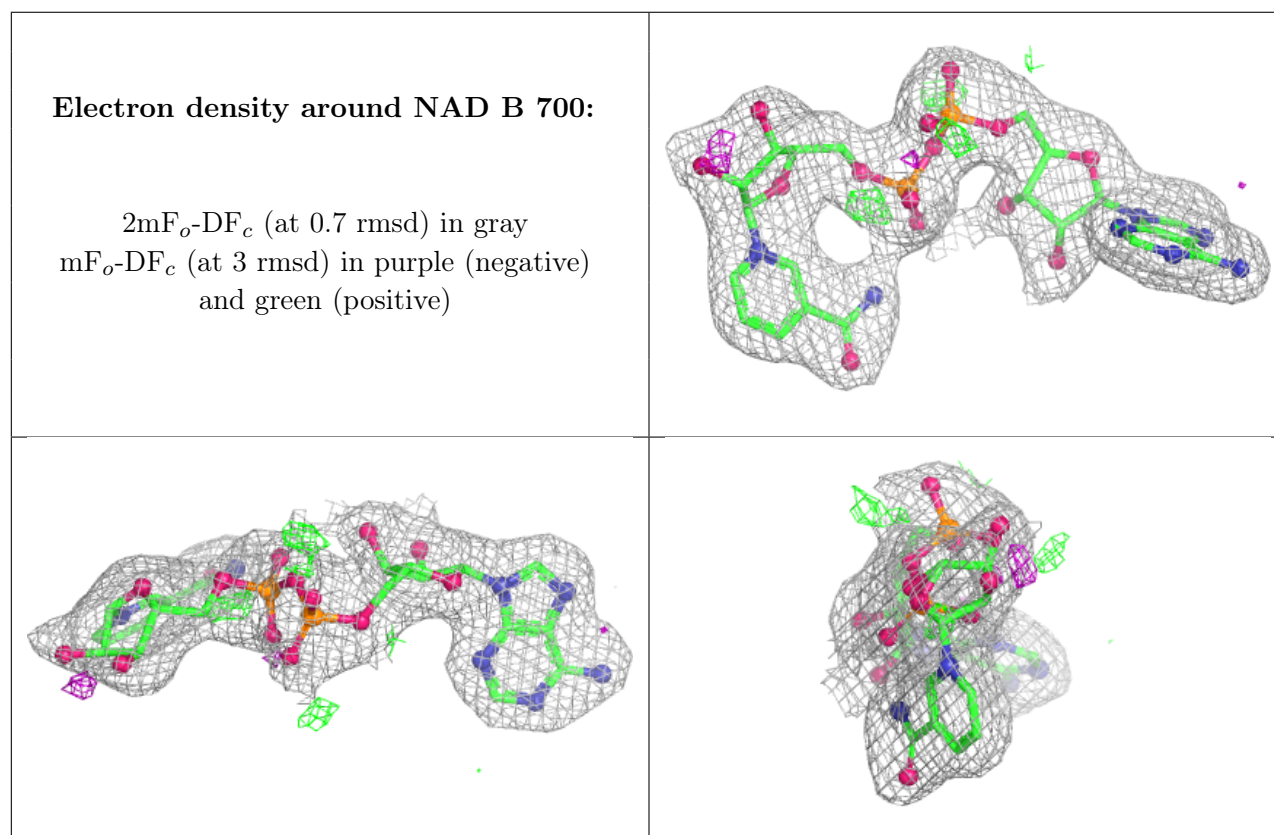
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

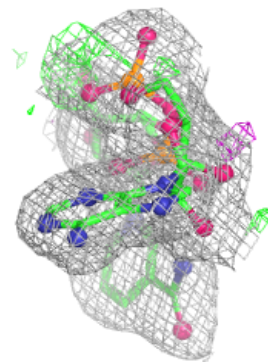
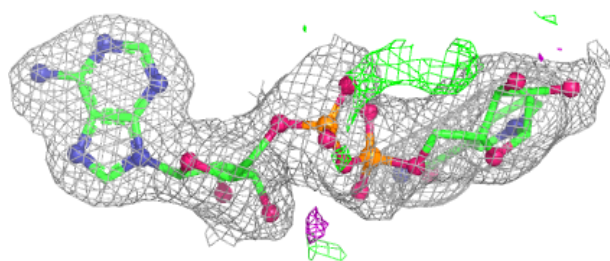
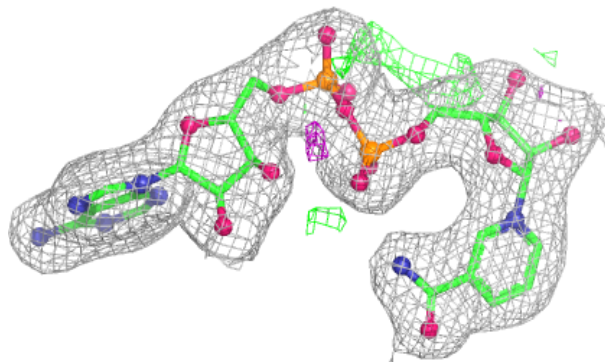
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAD	B	700	44/44	0.96	0.07	17,33,54,59	0
3	NAD	F	702	44/44	0.96	0.08	7,34,59,62	0
3	NAD	D	701	44/44	0.97	0.08	12,29,51,56	0

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.

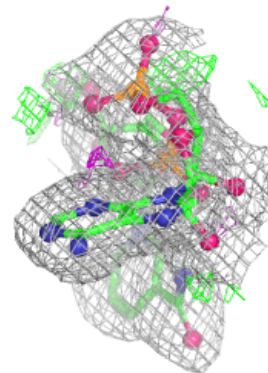
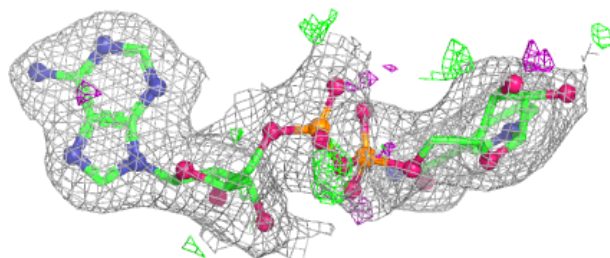
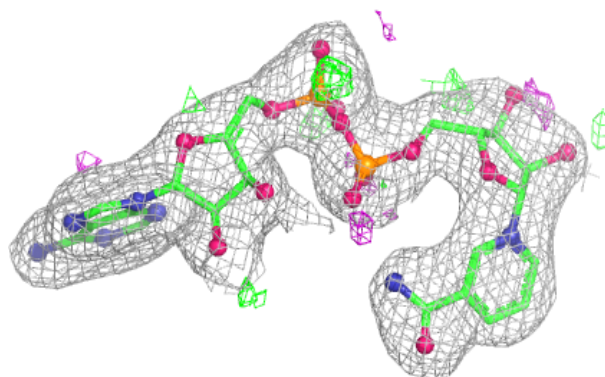


Electron density around NAD F 702:

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

**Electron density around NAD 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 [i](#)

There are no such residues in this entry.