



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:19 PM BST

PDB ID : 2ZIT  
Title : Structure of the eEF2-ExoA-NAD<sup>+</sup> complex  
Authors : Jorgensen, R.; Merrill, A.R.  
Deposited on : 2008-02-24  
Resolution : 3.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

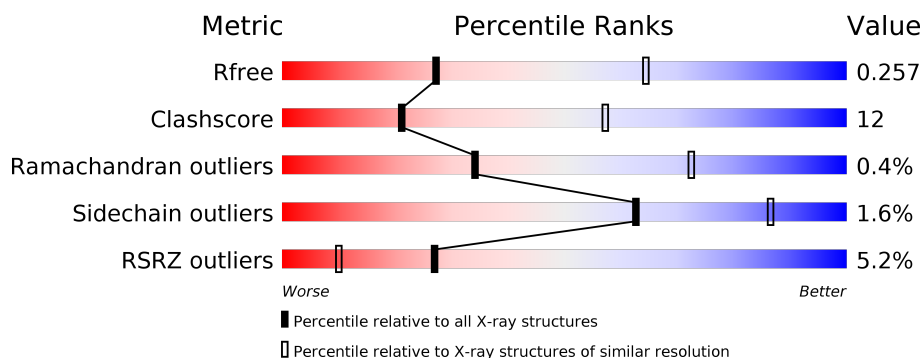
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>••</div> </div> </div>
1	C	842	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>••</div> </div> </div>
1	E	842	<div> <div>13%</div> <div> <div></div> <div>61%</div> <div>36%</div> <div>••</div> </div> </div>
2	B	207	<div> <div></div> <div> <div></div> <div>79%</div> <div>20%</div> <div>•</div> </div> </div>
2	D	207	<div> <div></div> <div> <div></div> <div>76%</div> <div>23%</div> <div></div> </div> </div>
2	F	207	<div> <div></div> <div> <div></div> <div>79%</div> <div>20%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24121 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
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			

There are 9 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
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
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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).

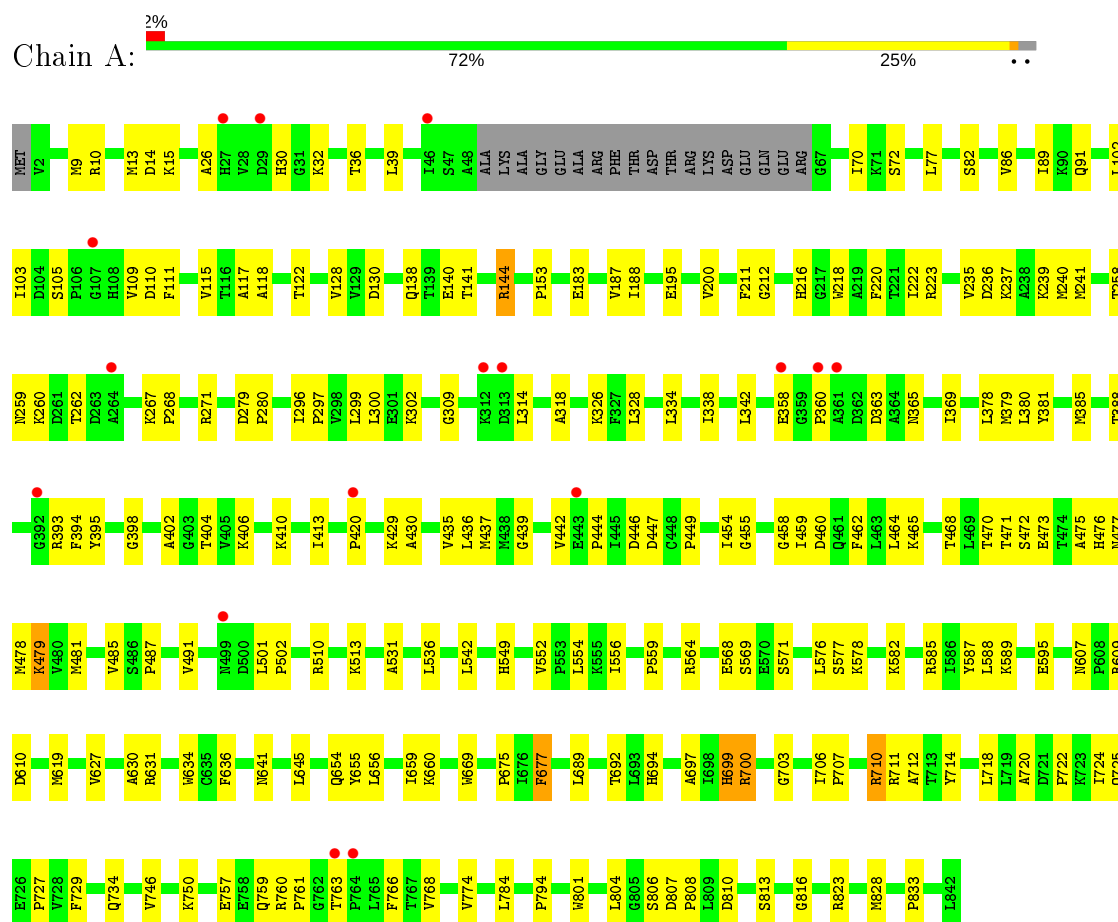


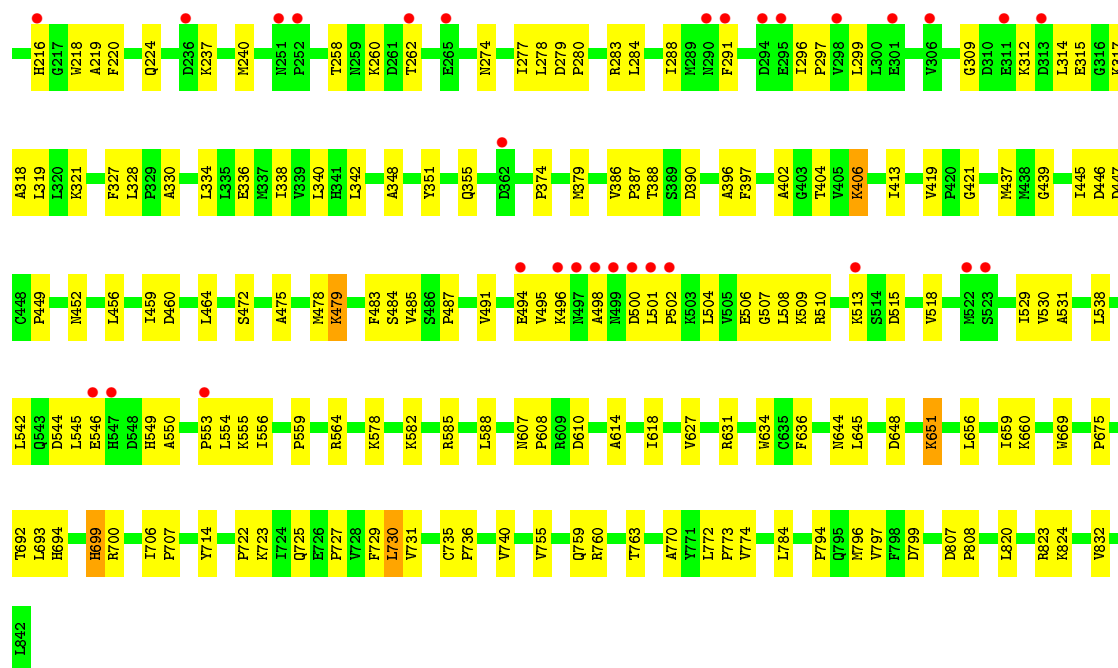
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	F	1	Total 44	C 21	N 7	O 14	P 2	0	0

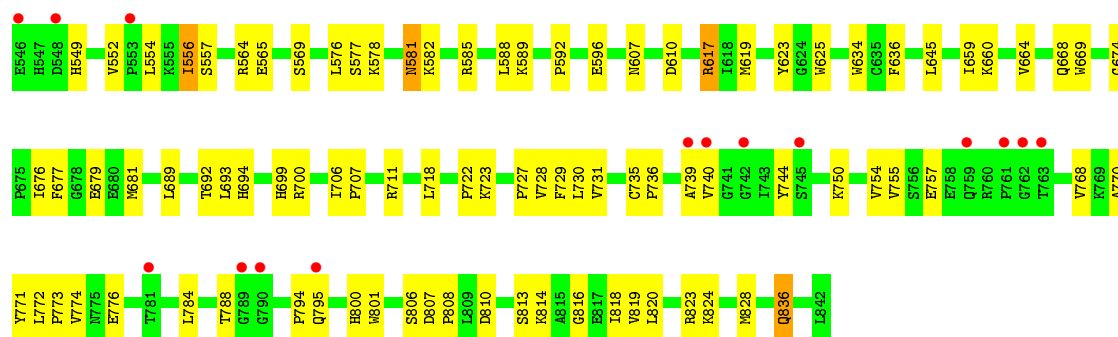
### 3 Residue-property plots

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

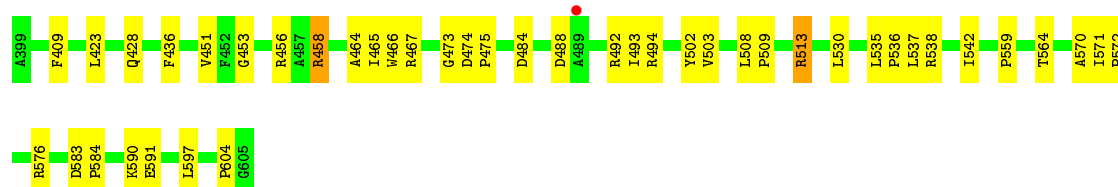
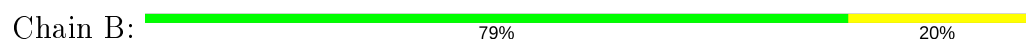
#### • Molecule 1: Elongation factor 2



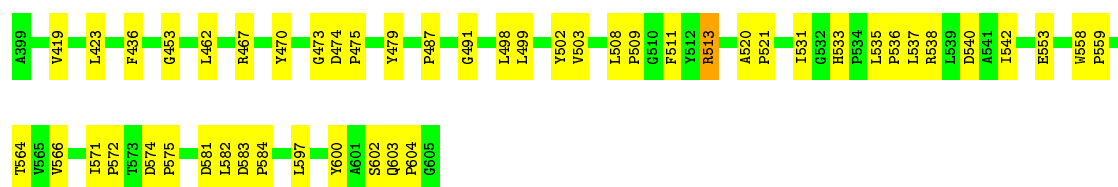
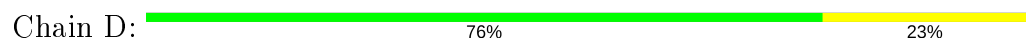




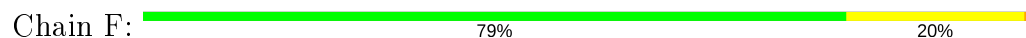
• Molecule 2: Exotoxin A



• 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, $\alpha$ , $\beta$ , $\gamma$	326.92Å 69.24Å 190.48Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	19.90 – 3.00 19.90 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.90-3.00) 97.0 (19.90-2.97)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.220 , 0.266 0.212 , 0.257	Depositor DCC
$R_{free}$ test set	1691 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	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 61.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3798e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.20	0/6517	0.38	0/8823
1	C	0.20	0/6517	0.38	0/8823
1	E	0.20	0/6517	0.37	0/8823
2	B	0.22	0/1627	0.39	0/2216
2	D	0.21	0/1627	0.40	0/2216
2	F	0.22	0/1627	0.40	0/2216
All	All	0.21	0/24432	0.38	0/33117

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	137	0
1	C	6415	0	6488	155	0
1	E	6405	0	6472	216	0
2	B	1588	0	1542	32	0
2	D	1588	0	1542	25	0
2	F	1588	0	1542	27	0
3	B	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	26	4	0
3	F	44	0	26	2	0
All	All	24121	0	24136	584	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (584) 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:HAT2	1:C:699:DDE:HAB2	1.41	0.98
1:C:699:DDE:HAA1	3:D:701:NAD:H4D	1.46	0.98
1:A:470:THR:HG22	1:A:472:SER:H	1.31	0.94
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.33	0.92
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.51	0.92
1:C:404:THR:HG22	1:C:449:PRO:HA	1.55	0.88
1:E:391:LYS:HG3	1:E:392:GLY:H	1.40	0.86
1:E:617:ARG:HG3	1:E:617:ARG:HH21	1.40	0.86
2:B:458:ARG:HG2	2:B:458:ARG:HH11	1.45	0.82
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.59	0.82
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.62	0.80
1:A:10:ARG:HH22	1:A:446:ASP:HB2	1.47	0.80
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.64	0.79
1:E:30:HIS:CD2	1:E:130:ASP:HB2	2.17	0.79
1:E:404:THR:HG22	1:E:449:PRO:HA	1.67	0.77
1:A:710:ARG:HG3	1:A:710:ARG:NH1	2.00	0.76
1:C:699:DDE:CAB	1:C:699:DDE:HAT2	2.16	0.76
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.68	0.74
1:E:836:GLN:H	1:E:836:GLN:HE21	1.33	0.74
1:A:470:THR:HG21	1:A:475:ALA:HB3	1.70	0.74
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.71	0.73
1:C:132:ILE:H	1:C:132:ILE:HD12	1.53	0.73
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.70	0.73
2:B:484:ASP:OD2	2:B:494:ARG:HG2	1.89	0.73
1:C:699:DDE:CAA	3:D:701:NAD:H4D	2.19	0.72
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.70	0.72
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.71	0.72
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.73	0.70
1:E:617:ARG:HG3	1:E:617:ARG:NH2	2.06	0.70
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.74	0.69
1:A:700:ARG:HB2	1:A:700:ARG:HH21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:VAL:HG22	1:A:631:ARG:HE	1.58	0.69
1:E:149:GLU:HA	1:E:355:GLN:HE22	1.57	0.69
1:E:556:ILE:HG22	1:E:557:SER:H	1.58	0.68
1:A:109:VAL:HG23	1:A:138:GLN:HG3	1.75	0.68
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.77	0.67
1:C:759:GLN:HG2	1:C:760:ARG:H	1.59	0.67
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.76	0.66
1:C:68:ILE:HD13	1:C:390:ASP:HB2	1.76	0.66
1:E:589:LYS:HG3	1:E:689:LEU:HD11	1.76	0.66
1:C:578:LYS:HD2	1:C:582:LYS:HD3	1.77	0.66
1:C:578:LYS:HD3	1:C:582:LYS:HA	1.78	0.65
1:C:699:DDE:NAD	1:C:699:DDE:HAA3	2.09	0.65
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.79	0.65
1:E:30:HIS:HD2	1:E:130:ASP:HB2	1.62	0.65
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.78	0.65
1:A:381:TYR:O	1:A:398:GLY:HA3	1.96	0.65
1:A:578:LYS:HD3	1:A:582:LYS:HA	1.80	0.64
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.80	0.64
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.80	0.63
1:A:542:LEU:HD13	1:A:556:ILE:HG21	1.81	0.63
1:A:810:ASP:O	1:A:816:GLY:HA3	1.99	0.63
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.80	0.62
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.79	0.62
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.81	0.62
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.80	0.62
1:E:27:HIS:HB3	1:E:30:HIS:ND1	2.14	0.62
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.82	0.62
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.82	0.62
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.80	0.62
1:C:419:VAL:HG12	1:C:421:GLY:H	1.64	0.62
2:B:453:GLY:HA3	2:B:456:ARG:NH2	2.14	0.62
2:D:513:ARG:HE	2:D:602:SER:HB3	1.65	0.61
1:A:299:LEU:HD12	1:A:302:LYS:HE2	1.81	0.61
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.65	0.61
1:C:9:MET:O	1:C:13:MET:HG3	2.01	0.61
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.82	0.61
1:C:70:ILE:HG22	1:C:388:THR:HG22	1.82	0.61
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.83	0.61
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.81	0.61
1:A:697:ALA:HA	1:A:700:ARG:HD3	1.83	0.61
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:553:GLU:OE1	3:D:701:NAD:H6N	2.01	0.61
2:F:553:GLU:OE1	3:F:702:NAD:H6N	2.01	0.61
1:A:619:MET:HE3	1:A:630:ALA:HB1	1.81	0.60
1:A:141:THR:O	1:A:144:ARG:HD2	2.01	0.60
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.82	0.60
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.84	0.60
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.83	0.60
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.83	0.60
1:E:9:MET:O	1:E:13:MET:HG3	2.02	0.60
2:B:458:ARG:CG	2:B:458:ARG:HH11	2.15	0.59
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.84	0.59
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.37	0.59
2:B:513:ARG:HB2	2:B:513:ARG:HH11	1.66	0.59
1:E:141:THR:HA	1:E:144:ARG:HH11	1.67	0.59
1:E:806:SER:HB2	1:E:813:SER:HB2	1.84	0.59
1:A:9:MET:O	1:A:13:MET:HG3	2.01	0.59
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.85	0.59
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.84	0.59
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.43	0.59
1:A:413:ILE:HD13	1:A:459:ILE:HG23	1.84	0.59
1:C:694:HIS:O	1:C:700:ARG:HD3	2.03	0.59
1:C:529:ILE:HG22	1:C:530:VAL:H	1.68	0.58
1:E:578:LYS:HD2	1:E:582:LYS:HD3	1.83	0.58
1:C:150:ARG:HG3	1:C:355:GLN:HE22	1.68	0.58
1:C:546:GLU:HA	1:C:550:ALA:HB3	1.84	0.58
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.85	0.58
1:C:627:VAL:O	1:C:631:ARG:HG3	2.03	0.58
1:A:404:THR:HG22	1:A:449:PRO:HA	1.85	0.58
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.86	0.58
1:E:385:MET:HG2	1:E:465:LYS:HA	1.86	0.58
1:A:30:HIS:NE2	1:A:130:ASP:HB2	2.19	0.57
1:C:216:HIS:ND1	1:C:321:LYS:HG2	2.19	0.57
1:C:338:ILE:HG23	1:C:342:LEU:HD12	1.85	0.57
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.86	0.57
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.84	0.57
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.34	0.57
1:C:216:HIS:HB2	1:C:218:TRP:HD1	1.67	0.57
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.87	0.57
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.85	0.57
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.85	0.57
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG21	1:A:395:TYR:CG	2.39	0.57
1:C:30:HIS:CE1	1:C:130:ASP:HB2	2.40	0.57
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.85	0.57
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.86	0.57
1:E:391:LYS:HG3	1:E:392:GLY:N	2.18	0.56
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.87	0.56
1:A:569:SER:O	1:A:720:ALA:HB1	2.05	0.56
1:E:321:LYS:O	1:E:325:ARG:HG3	2.05	0.56
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.87	0.56
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.87	0.56
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.87	0.56
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.87	0.56
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.88	0.55
1:A:406:LYS:HG2	1:A:447:ASP:HB3	1.88	0.55
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.88	0.55
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.87	0.55
1:C:237:LYS:HA	1:C:240:MET:HB3	1.87	0.55
1:A:627:VAL:O	1:A:631:ARG:HG3	2.07	0.55
1:A:314:LEU:HD22	1:A:318:ALA:HB1	1.88	0.55
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.89	0.55
1:C:169:VAL:HG22	1:C:173:ASP:HB2	1.89	0.55
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.88	0.54
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.89	0.54
1:C:71:LYS:HB3	1:C:386:VAL:HG23	1.88	0.54
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.89	0.54
1:E:349:GLN:O	1:E:370:LYS:HA	2.07	0.54
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.88	0.54
1:E:810:ASP:O	1:E:816:GLY:HA3	2.07	0.54
1:A:338:ILE:O	1:A:342:LEU:HB2	2.07	0.54
1:A:258:THR:HG22	1:A:260:LYS:H	1.71	0.54
1:C:374:PRO:O	1:C:404:THR:HG23	2.07	0.54
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.43	0.54
1:E:819:VAL:O	1:E:823:ARG:HG2	2.08	0.54
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.90	0.54
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.43	0.54
1:C:314:LEU:HD22	1:C:318:ALA:HB1	1.88	0.54
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.90	0.54
1:A:110:ASP:HB3	1:A:536:LEU:HD22	1.90	0.54
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.90	0.54
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.43	0.54
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.43	0.53
1:A:501:LEU:N	1:A:502:PRO:HD2	2.24	0.53
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.90	0.53
1:E:365:ASN:O	1:E:369:ILE:HG12	2.08	0.53
1:E:722:PRO:O	1:E:723:LYS:HD2	2.08	0.53
2:F:513:ARG:HH11	2:F:513:ARG:HB2	1.72	0.53
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.90	0.53
1:A:806:SER:HB2	1:A:813:SER:HB2	1.89	0.53
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.90	0.53
1:A:111:PHE:O	1:A:115:VAL:HG23	2.08	0.53
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.89	0.53
1:E:207:GLY:O	1:E:337:MET:HG2	2.08	0.53
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.39	0.53
1:E:410:LYS:HA	1:E:430:ALA:HA	1.91	0.53
1:E:694:HIS:O	1:E:700:ARG:HD3	2.08	0.53
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.89	0.53
1:A:237:LYS:HA	1:A:240:MET:HB3	1.91	0.52
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.44	0.52
1:C:494:GLU:HG2	1:C:495:VAL:H	1.73	0.52
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.39	0.52
1:E:117:ALA:HA	1:E:481:MET:SD	2.50	0.52
1:A:607:ASN:OD1	1:A:609:ARG:HG2	2.09	0.52
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.44	0.52
1:C:183:GLU:O	1:C:187:VAL:HG23	2.10	0.52
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.92	0.52
1:E:419:VAL:HG12	1:E:421:GLY:H	1.74	0.52
2:F:513:ARG:HB2	2:F:513:ARG:NH1	2.24	0.52
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.45	0.52
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.90	0.52
1:E:296:ILE:O	1:E:300:LEU:HD13	2.10	0.52
1:E:772:LEU:HD12	1:E:773:PRO:HD2	1.91	0.52
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.91	0.52
2:B:464:ALA:O	2:B:467:ARG:HG2	2.10	0.52
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.91	0.52
2:F:436:PHE:HB2	2:F:502:TYR:CE2	2.45	0.52
1:A:223:ARG:HA	1:A:241:MET:HE2	1.92	0.52
1:A:760:ARG:HD3	1:A:763:THR:OG1	2.08	0.52
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.92	0.52
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.52
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.92	0.51
2:F:508:LEU:N	2:F:509:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:NH2	1:A:447:ASP:H	2.08	0.51
1:C:699:DDE:HAA3	1:C:699:DDE:HAD2	1.76	0.51
1:E:121:VAL:HG11	1:E:383:SER:OG	2.09	0.51
2:F:511:PHE:HB3	2:F:600:TYR:CD1	2.45	0.51
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.92	0.51
1:A:706:ILE:HB	2:B:493:ILE:HD12	1.92	0.51
2:B:538:ARG:HD2	2:B:559:PRO:HG2	1.93	0.51
1:E:381:TYR:O	1:E:398:GLY:HA3	2.10	0.51
1:C:279:ASP:O	1:C:283:ARG:HG2	2.11	0.51
1:C:823:ARG:HE	1:C:832:VAL:HG22	1.75	0.51
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.92	0.51
1:E:26:ALA:CB	1:E:128:VAL:HB	2.41	0.51
1:C:162:ARG:O	1:C:166:GLU:HB2	2.09	0.51
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.91	0.51
1:E:617:ARG:CG	1:E:617:ARG:HH21	2.19	0.51
1:A:487:PRO:HB3	1:A:531:ALA:HB1	1.93	0.51
1:A:694:HIS:CE1	1:A:699:DDE:HD2	2.46	0.51
1:E:226:ALA:O	1:E:230:ALA:HB2	2.11	0.51
1:C:820:LEU:O	1:C:824:LYS:HG3	2.11	0.50
1:C:736:PRO:O	1:C:740:VAL:HG23	2.11	0.50
1:E:204:PRO:HA	1:E:209:VAL:HB	1.93	0.50
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.94	0.50
2:F:537:LEU:HD11	2:F:542:ILE:HG22	1.92	0.50
1:A:656:LEU:O	1:A:659:ILE:HG12	2.11	0.50
2:B:453:GLY:HA3	2:B:456:ARG:HH21	1.75	0.50
1:A:727:PRO:HD3	1:A:801:TRP:CZ3	2.46	0.50
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.94	0.50
1:E:10:ARG:NH2	1:E:449:PRO:HD3	2.27	0.50
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.93	0.50
2:F:423:LEU:HD23	2:F:594:ILE:HD13	1.92	0.50
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.92	0.50
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.27	0.50
1:E:538:LEU:O	1:E:542:LEU:HG	2.11	0.50
1:E:836:GLN:H	1:E:836:GLN:NE2	2.03	0.50
1:C:296:ILE:N	1:C:297:PRO:HD2	2.27	0.50
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.46	0.50
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.47	0.50
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.26	0.50
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.46	0.50
1:E:205:ALA:HB2	1:E:245:TRP:HB3	1.94	0.50
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.94	0.49
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.94	0.49
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.94	0.49
1:C:494:GLU:HG2	1:C:495:VAL:N	2.28	0.49
2:D:508:LEU:N	2:D:509:PRO:CD	2.75	0.49
1:A:235:VAL:HG13	1:A:239:LYS:HE3	1.93	0.49
1:A:577:SER:HB3	1:A:712:ALA:HB2	1.94	0.49
1:C:291:PHE:HD1	1:C:315:GLU:HB2	1.77	0.49
1:C:634:TRP:NE1	1:C:648:ASP:HB2	2.27	0.49
1:E:578:LYS:HD3	1:E:582:LYS:HA	1.93	0.49
1:E:74:ALA:HA	1:E:102:LEU:O	2.12	0.49
1:E:823:ARG:HB2	1:E:828:MET:HB2	1.94	0.49
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.94	0.49
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.43	0.49
1:A:491:VAL:HG12	1:A:559:PRO:HA	1.94	0.49
1:A:757:GLU:HG3	1:A:768:VAL:HG22	1.94	0.49
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.94	0.49
1:C:529:ILE:HG22	1:C:530:VAL:N	2.27	0.49
1:C:291:PHE:CD1	1:C:315:GLU:HB2	2.47	0.49
1:C:772:LEU:HD12	1:C:773:PRO:HD2	1.95	0.49
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.94	0.49
2:D:538:ARG:HD2	2:D:559:PRO:HG2	1.94	0.49
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.13	0.49
2:B:458:ARG:CG	2:B:458:ARG:NH1	2.76	0.48
1:A:183:GLU:O	1:A:187:VAL:HG23	2.13	0.48
1:A:746:VAL:O	1:A:750:LYS:HD3	2.13	0.48
2:B:465:ILE:HG13	2:B:466:TRP:CD1	2.48	0.48
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.93	0.48
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.94	0.48
1:C:578:LYS:CD	1:C:582:LYS:HD3	2.41	0.48
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.49	0.48
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.48	0.48
2:B:508:LEU:N	2:B:509:PRO:CD	2.76	0.48
2:B:513:ARG:HB2	2:B:513:ARG:NH1	2.27	0.48
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.49	0.48
1:A:669:TRP:CZ2	2:B:492:ARG:HB3	2.49	0.48
1:C:258:THR:HG22	1:C:260:LYS:HG2	1.94	0.48
2:D:467:ARG:HG3	2:D:558:TRP:CD1	2.49	0.48
1:E:69:THR:HG22	1:E:389:SER:HB3	1.95	0.48
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.34	0.48
1:E:596:GLU:HG2	1:E:623:TYR:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PHE:HB2	1:A:460:ASP:HB3	1.95	0.48
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.96	0.48
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.48
1:E:101:ASN:OD1	1:E:453:ILE:HB	2.13	0.48
1:A:153:PRO:HD2	1:A:200:VAL:HG12	1.95	0.48
1:E:578:LYS:HB3	1:E:585:ARG:HG3	1.96	0.48
1:A:707:PRO:O	1:A:711:ARG:HG3	2.14	0.47
1:C:17:THR:HB	1:C:92:LYS:O	2.13	0.47
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.13	0.47
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.49	0.47
1:A:675:PRO:HD3	1:A:714:TYR:CD1	2.50	0.47
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.49	0.47
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.97	0.47
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.80	0.47
1:C:147:LEU:HD11	1:C:189:VAL:HA	1.95	0.47
1:C:759:GLN:CG	1:C:760:ARG:H	2.21	0.47
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.79	0.47
1:E:510:ARG:HD3	1:E:549:HIS:HA	1.96	0.47
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.47
1:E:664:VAL:O	1:E:668:GLN:HG2	2.14	0.47
1:E:395:TYR:CD1	1:E:457:VAL:HG22	2.49	0.47
1:E:43:ALA:HB1	1:E:78:TYR:H	1.80	0.47
1:C:699:DDE:CAB	1:C:699:DDE:CAT	2.88	0.47
2:D:537:LEU:O	2:D:538:ARG:HD3	2.15	0.47
1:E:307:LEU:HD13	1:E:311:GLU:O	2.15	0.47
1:E:150:ARG:HB3	1:E:351:TYR:HE1	1.80	0.47
1:E:634:TRP:CE3	1:E:660:LYS:HG3	2.50	0.47
1:C:314:LEU:O	1:C:319:LEU:HD22	2.14	0.47
1:C:43:ALA:HB1	1:C:78:TYR:O	2.15	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.97	0.47
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.50	0.47
1:E:46:ILE:HG22	1:E:47:SER:N	2.30	0.47
1:E:820:LEU:HG	1:E:824:LYS:HE2	1.96	0.47
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.97	0.47
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.97	0.47
1:E:556:ILE:HG22	1:E:557:SER:N	2.28	0.47
1:A:437:MET:SD	1:A:455:GLY:HA3	2.55	0.46
1:A:552:VAL:O	1:A:554:LEU:HG	2.15	0.46
1:A:828:MET:HG2	2:B:576:ARG:NE	2.30	0.46
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.60	0.46
1:A:378:LEU:HB3	1:A:471:THR:HG23	1.98	0.46
2:B:537:LEU:O	2:B:538:ARG:HD3	2.15	0.46
1:E:132:ILE:N	1:E:132:ILE:HD12	2.30	0.46
1:E:707:PRO:O	1:E:711:ARG:HG3	2.15	0.46
1:A:118:ALA:O	1:A:122:THR:HG23	2.15	0.46
1:A:823:ARG:NH2	1:A:833:PRO:HD3	2.31	0.46
1:E:163:ALA:O	1:E:169:VAL:HG12	2.16	0.46
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.80	0.46
1:E:405:VAL:O	1:E:447:ASP:HA	2.16	0.46
1:E:540:ILE:HD12	1:E:540:ILE:H	1.79	0.46
2:D:487:PRO:HB2	2:D:491:GLY:HA2	1.97	0.46
1:C:496:LYS:H	1:C:554:LEU:HD22	1.80	0.46
1:E:129:VAL:HG12	1:E:130:ASP:N	2.31	0.46
1:E:296:ILE:N	1:E:297:PRO:HD2	2.31	0.46
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.97	0.46
1:E:20:ARG:NH1	1:E:344:SER:HB3	2.31	0.46
1:E:394:PHE:HB2	1:E:460:ASP:HB3	1.98	0.46
1:E:459:ILE:HG22	1:E:459:ILE:O	2.14	0.46
1:C:396:ALA:HB3	1:C:456:LEU:HB2	1.98	0.46
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.97	0.46
1:C:759:GLN:HG2	1:C:760:ARG:N	2.29	0.46
1:E:111:PHE:O	1:E:115:VAL:HG23	2.16	0.46
1:E:185:VAL:O	1:E:189:VAL:HG23	2.16	0.46
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.97	0.46
1:A:235:VAL:HG22	1:A:239:LYS:HE3	1.98	0.46
1:E:17:THR:HB	1:E:93:THR:HA	1.98	0.46
1:E:397:PHE:CD1	1:E:437:MET:HG3	2.51	0.46
1:E:454:ILE:HG13	1:E:455:GLY:N	2.30	0.46
1:A:385:MET:HG2	1:A:465:LYS:HA	1.98	0.46
1:E:222:ILE:HD13	1:E:245:TRP:HB2	1.98	0.46
1:E:284:LEU:HD13	1:E:324:MET:HE1	1.98	0.46
1:E:101:ASN:N	1:E:101:ASN:HD22	2.14	0.45
1:E:119:LEU:O	1:E:151:ILE:HD11	2.15	0.45
1:E:123:ASP:N	1:E:123:ASP:OD1	2.48	0.45
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.98	0.45
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.47	0.45
2:F:499:LEU:HB3	2:F:566:VAL:CG1	2.46	0.45
1:C:169:VAL:CG2	1:C:173:ASP:HB2	2.46	0.45
1:E:552:VAL:O	1:E:554:LEU:HG	2.16	0.45
1:A:334:LEU:O	1:A:338:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.16	0.45
1:C:25:ILE:HG22	1:C:139:THR:HG23	1.98	0.45
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.17	0.45
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.98	0.45
2:D:511:PHE:HB3	2:D:600:TYR:CD1	2.50	0.45
1:C:449:PRO:HG2	1:C:452:ASN:ND2	2.31	0.45
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.52	0.45
1:E:103:ILE:N	1:E:103:ILE:HD12	2.31	0.45
1:E:237:LYS:HA	1:E:240:MET:HB3	1.99	0.45
1:A:724:ILE:HD11	1:A:804:LEU:HD12	1.97	0.45
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.98	0.45
1:C:727:PRO:HB2	1:C:774:VAL:HG21	1.98	0.45
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.47	0.45
1:E:736:PRO:O	1:E:740:VAL:HG23	2.17	0.45
1:A:117:ALA:HA	1:A:481:MET:SD	2.57	0.45
1:A:30:HIS:CD2	1:A:130:ASP:HB2	2.50	0.45
1:A:727:PRO:HB2	1:A:774:VAL:HG21	1.98	0.45
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.45
1:C:478:MET:O	1:C:479:LYS:C	2.55	0.45
1:C:487:PRO:HB3	1:C:531:ALA:HB1	1.99	0.45
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.99	0.45
1:E:279:ASP:O	1:E:283:ARG:HG2	2.16	0.45
1:E:755:VAL:HG23	1:E:770:ALA:HA	1.98	0.45
1:A:410:LYS:HA	1:A:430:ALA:HA	1.99	0.45
1:A:72:SER:HA	1:A:439:GLY:O	2.17	0.45
2:D:436:PHE:HB2	2:D:502:TYR:CE2	2.52	0.45
1:E:338:ILE:O	1:E:342:LEU:HB2	2.17	0.45
1:A:14:ASP:OD1	1:A:15:LYS:HG3	2.17	0.44
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.98	0.44
1:C:699:DDE:CAA	1:C:699:DDE:NAD	2.79	0.44
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.52	0.44
1:E:46:ILE:HD12	1:E:46:ILE:N	2.32	0.44
1:A:542:LEU:HD13	1:A:556:ILE:HD13	1.98	0.44
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.82	0.44
1:E:21:ASN:HB2	1:E:123:ASP:OD1	2.17	0.44
1:E:352:ARG:O	1:E:356:LEU:HG	2.17	0.44
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.99	0.44
1:C:155:VAL:HG23	1:C:202:VAL:HG11	1.98	0.44
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.99	0.44
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.99	0.44
2:F:466:TRP:CE2	2:F:519:ALA:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:517:THR:HG23	2:F:547:GLU:HA	2.00	0.44
1:A:588:LEU:HD12	1:A:588:LEU:C	2.38	0.44
2:B:571:ILE:HA	2:B:572:PRO:HD3	1.78	0.44
1:C:274:ASN:O	1:C:279:ASP:HB2	2.17	0.44
1:E:108:HIS:O	1:E:111:PHE:HD2	2.00	0.44
1:E:744:TYR:CE1	1:E:754:VAL:HG21	2.53	0.44
1:A:510:ARG:HD2	1:A:549:HIS:HA	1.99	0.44
1:A:700:ARG:NH2	1:A:700:ARG:HB2	2.30	0.44
1:A:82:SER:O	1:A:86:VAL:HG23	2.18	0.44
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.99	0.44
1:A:326:LYS:HB2	1:A:326:LYS:HE3	1.80	0.44
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.98	0.44
1:E:244:LEU:O	1:E:273:PHE:HB2	2.18	0.44
1:E:500:ASP:HB3	1:E:552:VAL:HG21	2.00	0.44
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.83	0.44
1:C:722:PRO:O	1:C:723:LYS:HD2	2.17	0.44
1:E:243:ARG:O	1:E:248:SER:HB2	2.17	0.44
1:E:355:GLN:O	1:E:479:LYS:HG3	2.18	0.44
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.82	0.44
1:C:485:VAL:O	1:C:487:PRO:HD3	2.18	0.44
1:C:491:VAL:HG12	1:C:559:PRO:HA	1.99	0.44
1:E:422:LYS:HA	1:E:422:LYS:HE2	2.00	0.44
1:C:124:GLY:HA3	1:C:342:LEU:HD22	2.00	0.44
2:D:571:ILE:HA	2:D:572:PRO:HD3	1.83	0.44
1:E:39:LEU:H	1:E:39:LEU:HD12	1.83	0.44
1:C:498:ALA:HA	1:C:501:LEU:HB2	2.00	0.43
2:B:428:GLN:NE2	1:C:651:LYS:HE2	2.33	0.43
1:E:111:PHE:HB3	1:E:114:GLU:HG2	2.00	0.43
1:E:429:LYS:HG3	1:E:462:PHE:CE2	2.53	0.43
1:C:501:LEU:HD23	1:C:501:LEU:C	2.39	0.43
2:D:499:LEU:HB3	2:D:566:VAL:CG1	2.48	0.43
2:D:603:GLN:HG3	2:D:604:PRO:HD2	2.00	0.43
1:E:292:LYS:O	1:E:296:ILE:HG13	2.17	0.43
2:B:570:ALA:HB3	2:B:591:GLU:OE1	2.17	0.43
1:C:72:SER:HA	1:C:439:GLY:O	2.18	0.43
2:D:419:VAL:O	2:D:423:LEU:HG	2.18	0.43
1:E:659:ILE:HD13	1:E:693:LEU:HD21	2.00	0.43
1:A:420:PRO:HG2	1:A:476:HIS:CD2	2.53	0.43
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.54	0.43
1:E:12:LEU:HA	1:E:15:LYS:HE2	2.00	0.43
1:E:728:VAL:HG11	1:E:771:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:435:VAL:HG21	2:F:598:PRO:HG3	2.01	0.43
1:A:212:GLY:HA2	1:A:218:TRP:CZ3	2.53	0.43
1:C:159:LYS:HD3	1:C:162:ARG:HE	1.83	0.43
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.18	0.43
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.99	0.43
1:C:656:LEU:O	1:C:659:ILE:HG12	2.19	0.43
2:D:479:TYR:CG	2:D:582:LEU:HB2	2.54	0.43
1:E:150:ARG:HA	1:E:197:LEU:HD11	2.00	0.43
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.19	0.43
1:C:152:LYS:HA	1:C:153:PRO:HD3	1.73	0.43
1:C:314:LEU:HD13	1:C:318:ALA:O	2.18	0.43
1:E:459:ILE:N	1:E:459:ILE:HD12	2.33	0.43
1:E:588:LEU:C	1:E:588:LEU:HD12	2.39	0.43
1:E:565:GLU:OE1	1:E:674:GLY:HA3	2.18	0.43
1:E:219:ALA:HB3	1:E:330:ALA:HA	2.00	0.43
1:C:288:ILE:HG23	1:C:319:LEU:HD23	2.01	0.43
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.85	0.43
1:E:369:ILE:HD12	1:E:401:PHE:HB3	2.00	0.43
2:B:503:VAL:HG12	2:B:564:THR:HG22	2.00	0.43
1:A:634:TRP:CE3	1:A:660:LYS:HG3	2.54	0.43
1:E:111:PHE:HZ	1:E:540:ILE:HG12	1.84	0.43
1:E:30:HIS:HE1	1:E:136:CYS:SG	2.42	0.43
1:A:468:THR:HG23	1:A:478:MET:HE2	2.00	0.42
1:E:739:ALA:HB1	1:E:788:THR:HB	2.01	0.42
1:E:814:LYS:O	1:E:818:ILE:HG12	2.19	0.42
1:C:153:PRO:HD2	1:C:200:VAL:HG12	2.01	0.42
1:C:634:TRP:CE3	1:C:660:LYS:HG3	2.54	0.42
2:D:583:ASP:HA	2:D:584:PRO:HD2	1.87	0.42
1:C:515:ASP:O	1:C:518:VAL:HG12	2.19	0.42
1:E:485:VAL:HG23	1:E:517:CYS:HA	2.01	0.42
1:A:258:THR:HG22	1:A:259:ASN:N	2.34	0.42
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.34	0.42
1:C:274:ASN:HA	1:C:278:LEU:HB2	2.01	0.42
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.86	0.42
2:F:488:ASP:CG	2:F:489:ALA:H	2.23	0.42
1:A:260:LYS:HE3	1:A:262:THR:O	2.18	0.42
1:A:454:ILE:HG13	1:A:455:GLY:H	1.85	0.42
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.54	0.42
1:A:675:PRO:HD3	1:A:714:TYR:CE1	2.54	0.42
2:B:409:PHE:HZ	2:B:451:VAL:HG21	1.84	0.42
1:C:636:PHE:CE1	1:C:645:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:TRP:O	1:C:669:TRP:CD1	2.72	0.42
2:D:498:LEU:HA	2:D:498:LEU:HD23	1.83	0.42
1:E:581:ASN:C	1:E:581:ASN:HD22	2.22	0.42
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.54	0.42
1:C:338:ILE:O	1:C:342:LEU:HB2	2.19	0.42
1:C:13:MET:HB3	1:C:452:ASN:ND2	2.34	0.42
1:E:71:LYS:HB3	1:E:386:VAL:HG23	2.01	0.42
1:E:619:MET:O	1:E:625:TRP:HB2	2.18	0.42
2:F:517:THR:CG2	2:F:547:GLU:HA	2.49	0.42
1:C:109:VAL:CG2	1:C:138:GLN:HG3	2.49	0.42
1:C:39:LEU:HB3	1:C:77:LEU:HD21	2.02	0.42
1:E:411:VAL:HG13	1:E:470:THR:O	2.20	0.42
1:E:569:SER:O	1:E:592:PRO:HD3	2.20	0.42
1:E:750:LYS:HD2	1:E:776:GLU:O	2.20	0.42
1:A:473:GLU:O	1:A:473:GLU:HG2	2.19	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.87	0.42
2:D:473:GLY:HA3	2:D:597:LEU:HD11	2.02	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
1:E:718:LEU:HA	1:E:722:PRO:HG3	2.00	0.42
1:E:727:PRO:HG2	1:E:774:VAL:HB	2.02	0.42
1:A:236:ASP:OD1	1:A:239:LYS:HG2	2.20	0.42
1:A:365:ASN:O	1:A:369:ILE:HG13	2.20	0.42
1:C:317:LYS:O	1:C:321:LYS:HG3	2.19	0.42
1:E:165:LEU:HD23	1:E:317:LYS:HE2	2.01	0.42
1:E:377:ASP:OD2	1:E:472:SER:HB2	2.20	0.42
1:E:564:ARG:HD3	1:E:801:TRP:CH2	2.55	0.42
1:E:576:LEU:HD12	1:E:577:SER:H	1.84	0.42
1:A:26:ALA:CB	1:A:128:VAL:HB	2.49	0.41
1:A:296:ILE:O	1:A:300:LEU:HD13	2.20	0.41
1:A:703:GLY:HA2	2:B:493:ILE:HD13	2.01	0.41
1:E:386:VAL:HG12	1:E:395:TYR:O	2.21	0.41
1:E:46:ILE:HD12	1:E:46:ILE:H	1.85	0.41
1:E:485:VAL:O	1:E:485:VAL:HG22	2.19	0.41
1:A:393:ARG:HH21	1:A:458:GLY:HA2	1.84	0.41
1:A:478:MET:O	1:A:479:LYS:C	2.59	0.41
1:C:614:ALA:O	1:C:618:ILE:HG12	2.20	0.41
1:E:69:THR:CG2	1:E:389:SER:HB3	2.51	0.41
1:E:454:ILE:HG13	1:E:455:GLY:H	1.84	0.41
1:E:565:GLU:O	1:E:681:MET:HA	2.21	0.41
1:C:755:VAL:HG23	1:C:770:ALA:HA	2.02	0.41
1:E:358:GLU:HB2	1:E:477:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.50	0.41
2:F:467:ARG:NH2	2:F:536:PRO:HG3	2.36	0.41
1:C:807:ASP:HA	1:C:808:PRO:HD2	1.82	0.41
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.55	0.41
2:B:488:ASP:CG	2:B:492:ARG:HG2	2.40	0.41
1:C:277:ILE:O	1:C:280:PRO:HD2	2.20	0.41
1:C:538:LEU:O	1:C:542:LEU:HB2	2.21	0.41
2:D:520:ALA:HA	2:D:521:PRO:HD3	1.95	0.41
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.86	0.41
1:E:520:THR:HG22	1:E:530:VAL:HG22	2.01	0.41
1:A:380:LEU:HD23	1:A:381:TYR:N	2.36	0.41
1:A:654:GLN:HG2	1:A:655:TYR:CE1	2.56	0.41
1:C:159:LYS:HD3	1:C:162:ARG:NE	2.35	0.41
1:E:731:VAL:HG13	1:E:731:VAL:O	2.20	0.41
1:A:358:GLU:HB2	1:A:477:ASN:O	2.20	0.41
1:C:260:LYS:HG3	1:C:262:THR:O	2.21	0.41
1:C:735:CYS:HA	1:C:736:PRO:HD3	1.97	0.41
1:E:358:GLU:CG	1:E:479:LYS:HD2	2.51	0.41
2:F:445:GLU:CD	2:F:494:ARG:HH22	2.24	0.41
1:A:677:PHE:N	1:A:677:PHE:CD2	2.88	0.41
1:E:486:SER:O	1:E:488:VAL:HG23	2.20	0.41
2:F:442:THR:OG1	2:F:443:PHE:N	2.53	0.41
1:A:627:VAL:HG11	2:F:406:ASP:OD1	2.21	0.41
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.85	0.41
1:C:192:TYR:HA	1:C:763:THR:CG2	2.51	0.41
1:C:504:LEU:HD22	1:C:554:LEU:HD13	2.03	0.41
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.56	0.41
1:C:149:GLU:HA	1:C:355:GLN:OE1	2.21	0.41
2:D:474:ASP:HA	2:D:475:PRO:HD2	1.90	0.41
1:E:240:MET:O	1:E:244:LEU:HG	2.21	0.41
1:E:677:PHE:CE1	1:E:679:GLU:HG3	2.56	0.41
1:A:195:GLU:H	1:A:195:GLU:CD	2.25	0.41
2:B:474:ASP:HA	2:B:475:PRO:HD2	1.91	0.41
1:E:109:VAL:O	1:E:109:VAL:HG12	2.21	0.41
1:E:174:LEU:O	1:E:177:THR:HB	2.21	0.41
1:E:218:TRP:HZ3	1:E:220:PHE:CD2	2.38	0.41
1:E:487:PRO:HB3	1:E:531:ALA:CB	2.51	0.41
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.61	0.41
2:F:457:ALA:HA	2:F:558:TRP:CE3	2.56	0.41
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ILE:CD1	1:E:245:TRP:HB2	2.52	0.40
2:F:471:ILE:HG21	2:F:501:VAL:HG21	2.03	0.40
1:C:39:LEU:HD21	1:C:334:LEU:HB2	2.03	0.40
1:C:588:LEU:C	1:C:588:LEU:HD12	2.41	0.40
1:C:731:VAL:HA	1:C:796:MET:HA	2.03	0.40
1:E:76:SER:C	1:E:77:LEU:HD12	2.41	0.40
1:E:84:GLU:O	1:E:88:GLU:HG3	2.21	0.40
1:A:216:HIS:HB2	1:A:218:TRP:CD1	2.56	0.40
1:C:284:LEU:HD23	1:C:299:LEU:HD23	2.02	0.40
1:C:636:PHE:HA	1:C:644:ASN:O	2.21	0.40
1:E:110:ASP:HB3	1:E:536:LEU:HD22	2.03	0.40
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.89	0.40
1:E:181:THR:O	1:E:185:VAL:HG23	2.21	0.40
1:E:225:PHE:CE2	1:E:328:LEU:HD11	2.56	0.40
1:E:485:VAL:O	1:E:487:PRO:HD3	2.21	0.40
1:A:718:LEU:HA	1:A:722:PRO:HG3	2.03	0.40
1:C:506:GLU:O	1:C:510:ARG:HG3	2.21	0.40
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.21	0.40
1:E:676:ILE:HG22	1:E:677:PHE:HD2	1.87	0.40
1:E:755:VAL:HG22	1:E:771:TYR:CE2	2.57	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%)	776 (95%)	38 (5%)	4 (0%)	29 68
1	C	818/842 (97%)	767 (94%)	48 (6%)	3 (0%)	34 72
1	E	818/842 (97%)	754 (92%)	61 (8%)	3 (0%)	34 72
2	B	205/207 (99%)	199 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	205/207 (99%)	196 (96%)	8 (4%)	1 (0%)	29	68
2	F	205/207 (99%)	198 (97%)	6 (3%)	1 (0%)	29	68
All	All	3069/3147 (98%)	2890 (94%)	167 (5%)	12 (0%)	34	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	E	479	LYS
1	A	479	LYS
1	A	641	ASN
1	C	446	ASP
1	C	479	LYS
1	E	795	GLN
2	F	453	GLY
1	C	309	GLY
2	D	453	GLY
1	E	556	ILE
1	A	761	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	690 (99%)	9 (1%)	69	89
1	C	699/714 (98%)	690 (99%)	9 (1%)	69	89
1	E	699/714 (98%)	688 (98%)	11 (2%)	62	86
2	B	161/161 (100%)	159 (99%)	2 (1%)	71	90
2	D	161/161 (100%)	157 (98%)	4 (2%)	47	79
2	F	161/161 (100%)	156 (97%)	5 (3%)	40	75
All	All	2580/2625 (98%)	2540 (98%)	40 (2%)	62	86

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ARG
1	A	211	PHE
1	A	271	ARG
1	A	568	GLU
1	A	595	GLU
1	A	677	PHE
1	A	700	ARG
1	A	710	ARG
1	A	734	GLN
2	B	458	ARG
2	B	513	ARG
1	C	83	ASP
1	C	312	LYS
1	C	406	LYS
1	C	460	ASP
1	C	500	ASP
1	C	544	ASP
1	C	556	ILE
1	C	651	LYS
1	C	730	LEU
2	D	462	LEU
2	D	513	ARG
2	D	540	ASP
2	D	581	ASP
1	E	71	LYS
1	E	83	ASP
1	E	161	ASP
1	E	211	PHE
1	E	332	ASP
1	E	494	GLU
1	E	581	ASN
1	E	617	ARG
1	E	730	LEU
1	E	800	HIS
1	E	836	GLN
2	F	403	ASP
2	F	462	LEU
2	F	494	ARG
2	F	513	ARG
2	F	547	GLU

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

Mol	Chain	Res	Type
1	A	138	GLN
1	A	452	ASN
1	A	497	ASN
2	B	428	GLN
1	C	30	HIS
1	C	355	GLN
1	C	452	ASN
2	D	428	GLN
1	E	30	HIS
1	E	355	GLN
1	E	371	ASN
1	E	414	GLN
1	E	547	HIS
1	E	581	ASN
1	E	654	GLN
1	E	836	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	14,20,21	0.90	0	14,28,30	1.23	2 (14%)
1	DDE	A	699	1	5,10,21	0.58	0	3,12,30	1.36	1 (33%)
1	DDE	E	699	1	5,10,21	0.60	0	3,12,30	1.33	1 (33%)

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	-	3/20/21/23	0/1/1/1
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1
1	DDE	E	699	1	-	1/5/6/23	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	CAU-CBW-CBI	-2.39	106.45	111.20
1	C	699	DDE	CAB-NCB-CBW	2.23	116.07	110.51
1	A	699	DDE	CD2-NE2-CE1	2.09	109.03	105.78
1	E	699	DDE	CD2-NE2-CE1	2.02	108.93	105.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	8	0
1	A	699	DDE	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	-	42,48,48	0.67	0	50,73,73	1.28	3 (6%)
3	NAD	D	701	-	42,48,48	0.67	0	50,73,73	1.25	3 (6%)
3	NAD	B	700	-	42,48,48	0.67	0	50,73,73	1.28	4 (8%)

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	-	-	5/26/62/62	0/5/5/5
3	NAD	D	701	-	-	4/26/62/62	0/5/5/5
3	NAD	B	700	-	-	4/26/62/62	0/5/5/5

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	N3A-C2A-N1A	-4.61	121.47	128.68
3	D	701	NAD	N3A-C2A-N1A	-4.54	121.59	128.68
3	F	702	NAD	N3A-C2A-N1A	-4.46	121.71	128.68
3	F	702	NAD	C3D-C2D-C1D	3.66	106.49	100.98
3	D	701	NAD	C3D-C2D-C1D	3.46	106.18	100.98
3	B	700	NAD	C3D-C2D-C1D	3.40	106.09	100.98
3	F	702	NAD	PN-O3-PA	-3.19	121.89	132.83
3	D	701	NAD	PN-O3-PA	-3.14	122.04	132.83
3	B	700	NAD	PN-O3-PA	-3.05	122.38	132.83
3	B	700	NAD	C3B-C2B-C1B	2.55	104.82	100.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

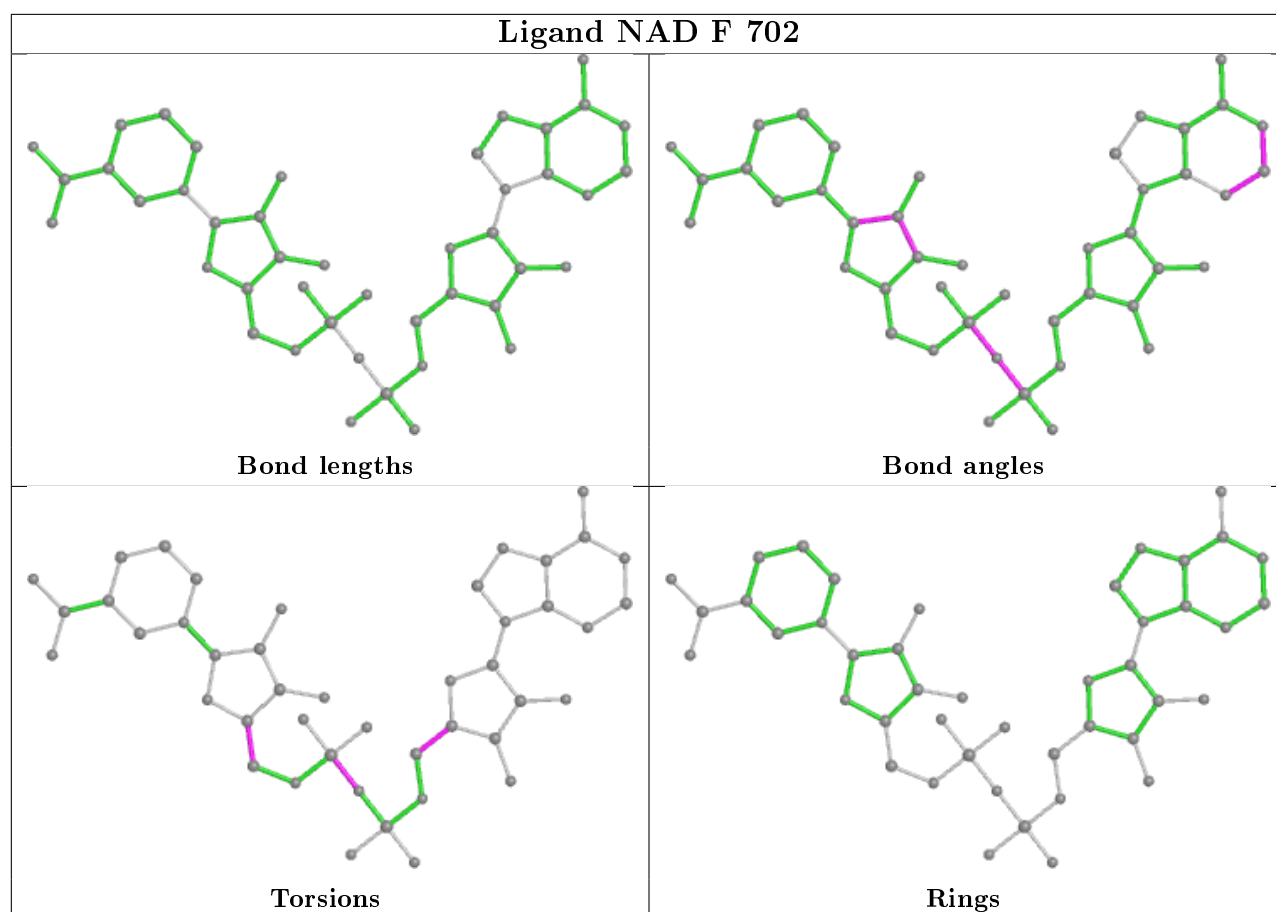
Mol	Chain	Res	Type	Atoms
3	F	702	NAD	C3D-C4D-C5D-O5D
3	B	700	NAD	C3D-C4D-C5D-O5D
3	F	702	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	C3D-C4D-C5D-O5D
3	B	700	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	O4B-C4B-C5B-O5B
3	D	701	NAD	C3B-C4B-C5B-O5B
3	B	700	NAD	O4B-C4B-C5B-O5B
3	B	700	NAD	C3B-C4B-C5B-O5B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

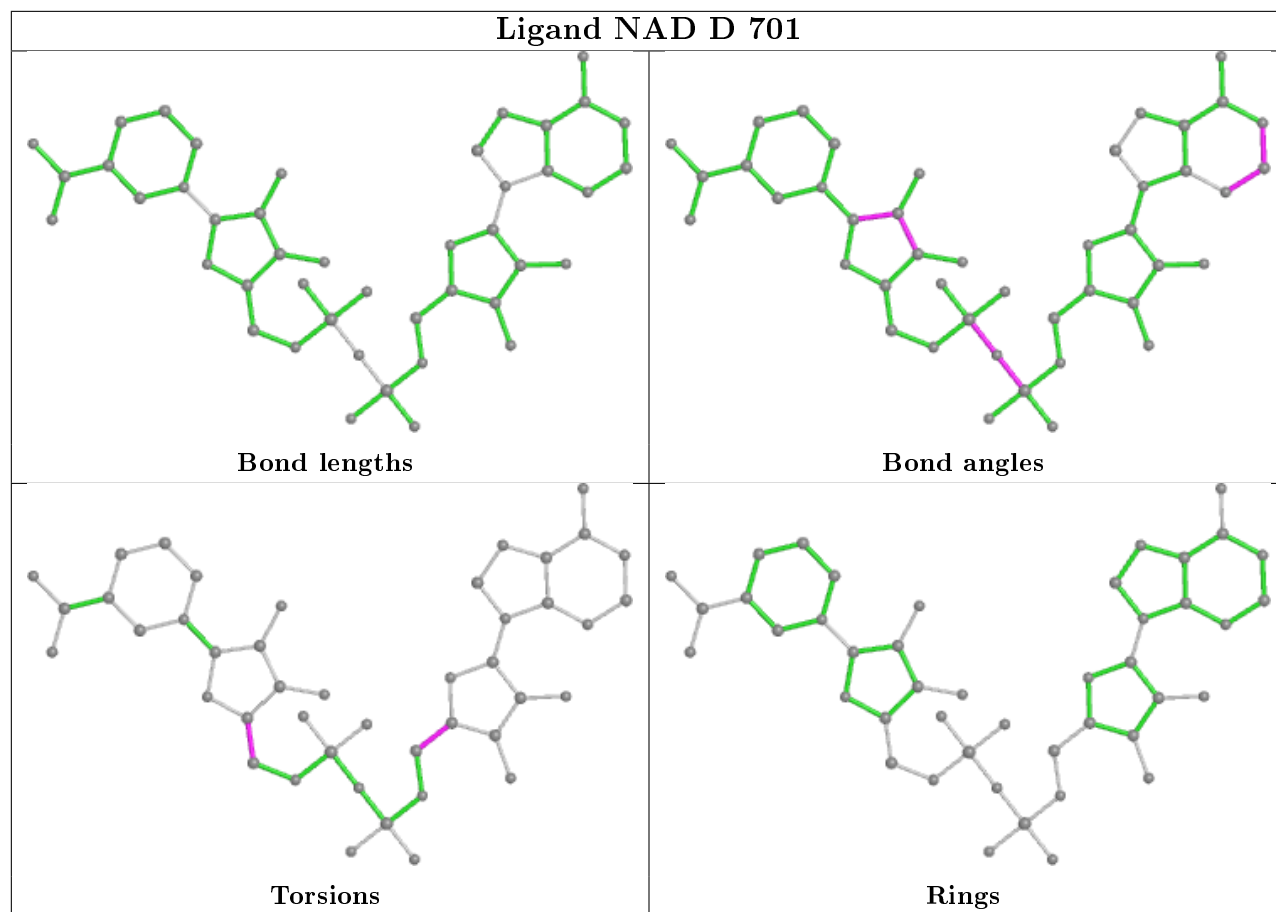
There are no ring outliers.

2 monomers are involved in 6 short contacts:

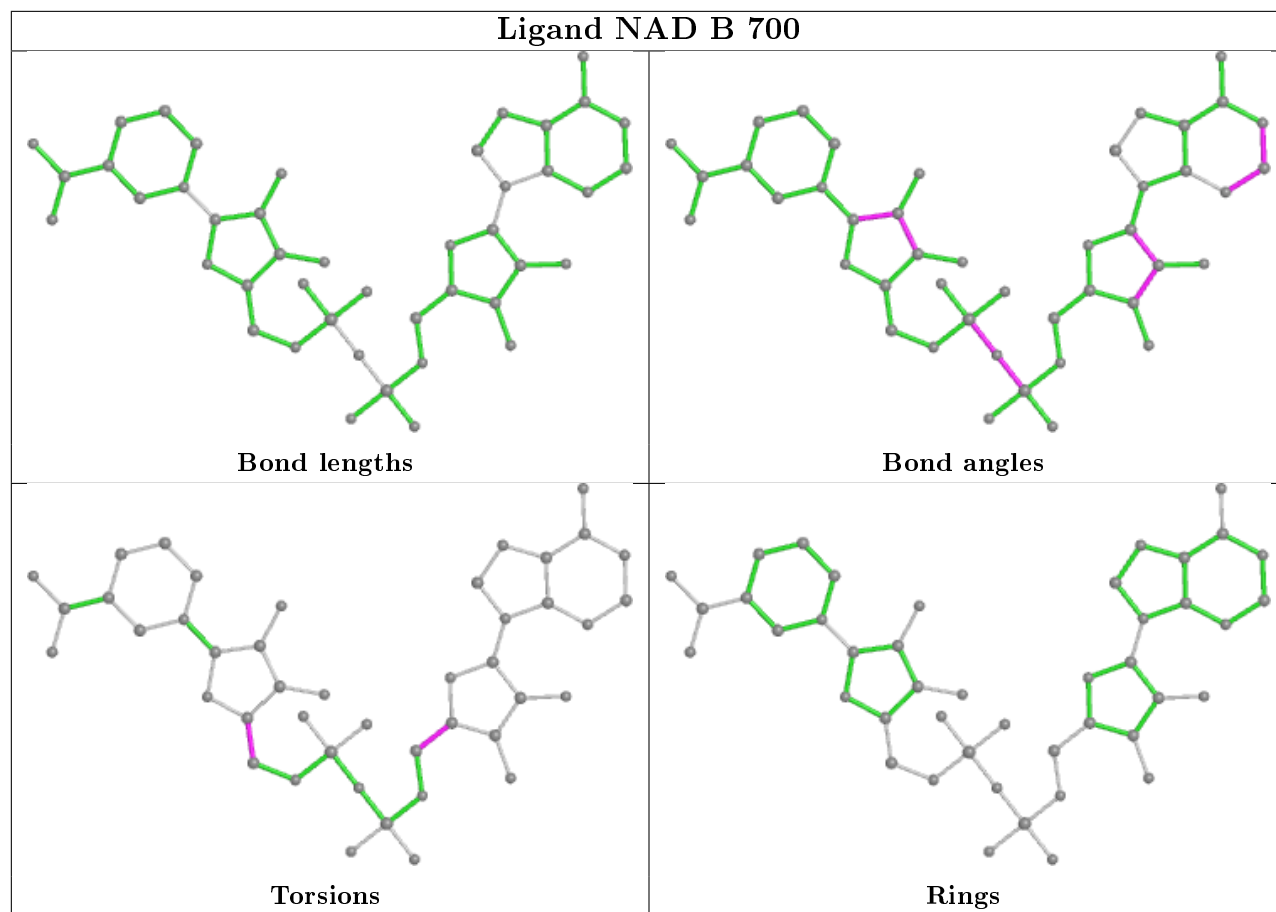
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	702	NAD	2	0
3	D	701	NAD	4	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	822/842 (97%)	-0.34	16 (1%) 66 37	18, 85, 143, 217	0
1	C	822/842 (97%)	-0.11	39 (4%) 31 11	20, 92, 182, 240	0
1	E	822/842 (97%)	0.44	106 (12%) 3 1	20, 154, 219, 298	0
2	B	207/207 (100%)	-0.73	1 (0%) 91 75	15, 37, 76, 118	0
2	D	207/207 (100%)	-0.78	0 100 100	17, 34, 75, 113	0
2	F	207/207 (100%)	-0.73	0 100 100	19, 41, 81, 123	0
All	All	3087/3147 (98%)	-0.15	162 (5%) 27 10	15, 85, 196, 298	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	ASP	7.6
1	E	739	ALA	6.4
1	C	313	ASP	6.0
1	A	29	ASP	5.2
1	E	759	GLN	5.2
1	A	358	GLU	5.1
1	E	67	GLY	4.8
1	E	137	VAL	4.8
1	E	30	HIS	4.6
1	C	311	GLU	4.4
1	E	360	PRO	4.3
1	E	107	GLY	4.3
1	E	46	ILE	4.3
1	E	268	PRO	4.2
1	E	108	HIS	4.1
1	C	291	PHE	4.0
1	A	420	PRO	4.0
1	E	80	GLU	4.0
1	E	29	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	290	ASN	3.9
1	C	494	GLU	3.8
1	E	361	ALA	3.8
1	E	166	GLU	3.8
1	A	360	PRO	3.8
1	E	392	GLY	3.8
1	E	168	GLN	3.7
1	E	195	GLU	3.7
1	C	499	ASN	3.7
1	C	502	PRO	3.6
1	E	245	TRP	3.5
1	E	91	GLN	3.5
1	E	419	VAL	3.5
1	C	33	SER	3.4
1	E	193	ALA	3.4
1	E	232	LYS	3.4
1	C	546	GLU	3.4
1	E	313	ASP	3.3
1	E	761	PRO	3.3
1	E	167	LEU	3.3
1	E	254	THR	3.2
1	E	290	ASN	3.2
1	E	314	LEU	3.2
1	E	329	PRO	3.2
1	E	27	HIS	3.2
1	E	294	ASP	3.2
1	C	498	ALA	3.1
1	E	231	LYS	3.1
1	A	361	ALA	3.1
1	E	88	GLU	3.1
1	E	32	LYS	3.1
1	E	315	GLU	3.1
1	C	108	HIS	3.1
1	E	420	PRO	3.0
1	E	293	LYS	3.0
1	A	107	GLY	3.0
1	E	740	VAL	3.0
1	C	168	GLN	3.0
1	E	781	THR	3.0
1	C	501	LEU	2.9
1	C	30	HIS	2.9
1	E	795	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	90	LYS	2.8
1	E	367	ILE	2.8
1	A	499	ASN	2.8
1	A	392	GLY	2.8
1	E	162	ARG	2.8
1	E	200	VAL	2.8
1	E	789	GLY	2.8
1	E	553	PRO	2.7
1	C	173	ASP	2.7
1	E	311	GLU	2.7
1	E	240	MET	2.7
1	C	216	HIS	2.7
1	E	548	ASP	2.7
1	E	257	TRP	2.6
1	E	762	GLY	2.6
1	E	179	ALA	2.6
1	C	262	THR	2.6
1	E	196	VAL	2.6
1	E	239	LYS	2.6
1	E	410	LYS	2.6
1	C	522	MET	2.6
1	E	376	ALA	2.5
1	C	252	PRO	2.5
1	C	513	LYS	2.5
1	E	136	CYS	2.5
1	E	308	LYS	2.5
1	E	157	ILE	2.5
1	A	763	THR	2.5
1	E	464	LEU	2.5
1	E	498	ALA	2.5
1	E	500	ASP	2.5
1	E	310	ASP	2.5
1	E	499	ASN	2.5
1	E	358	GLU	2.4
1	E	201	GLN	2.4
1	C	295	GLU	2.4
1	C	496	LYS	2.4
1	E	104	ASP	2.4
1	E	348	ALA	2.4
1	C	547	HIS	2.4
1	E	192	TYR	2.4
1	E	134	GLY	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	27	HIS	2.3
1	C	107	GLY	2.3
1	E	477	ASN	2.3
1	C	167	LEU	2.3
1	E	763	THR	2.3
1	E	353	ALA	2.3
1	E	246	GLY	2.3
1	C	500	ASP	2.3
1	C	251	ASN	2.2
1	E	366	CYS	2.2
1	E	41	GLN	2.2
1	E	210	ALA	2.2
1	E	442	VAL	2.2
1	E	89	ILE	2.2
1	C	265	GLU	2.2
1	E	295	GLU	2.2
1	E	745	SER	2.2
1	E	421	GLY	2.2
1	A	313	ASP	2.2
1	C	3	ALA	2.2
1	E	93	THR	2.2
1	E	546	GLU	2.2
1	E	212	GLY	2.2
1	E	110	ASP	2.2
1	A	46	ILE	2.2
1	C	236	ASP	2.2
1	C	362	ASP	2.2
1	E	14	ASP	2.2
1	C	298	VAL	2.1
1	E	359	GLY	2.1
1	A	264	ALA	2.1
2	B	489	ALA	2.1
1	E	132	ILE	2.1
1	E	256	LYS	2.1
1	E	160	VAL	2.1
1	A	764	PRO	2.1
1	E	742	GLY	2.1
1	E	180	ARG	2.1
1	E	130	ASP	2.1
1	C	306	VAL	2.1
1	C	294	ASP	2.1
1	E	356	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	443	GLU	2.1
1	E	354	GLU	2.1
1	E	281	ILE	2.1
1	A	312	LYS	2.1
1	C	301	GLU	2.1
1	C	553	PRO	2.1
1	E	267	LYS	2.1
1	E	790	GLY	2.1
1	E	163	ALA	2.0
1	E	44	GLY	2.0
1	E	312	LYS	2.0
1	C	497	ASN	2.0
1	E	510	ARG	2.0
1	C	523	SER	2.0
1	E	280	PRO	2.0
1	E	253	LYS	2.0
1	E	258	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	DDE	C	699	20/21	0.89	0.29	31,88,128,128	0
1	DDE	A	699	10/21	0.92	0.14	59,75,77,80	0
1	DDE	E	699	10/21	0.96	0.13	36,51,77,82	0

## 6.3 Carbohydrates ⓘ

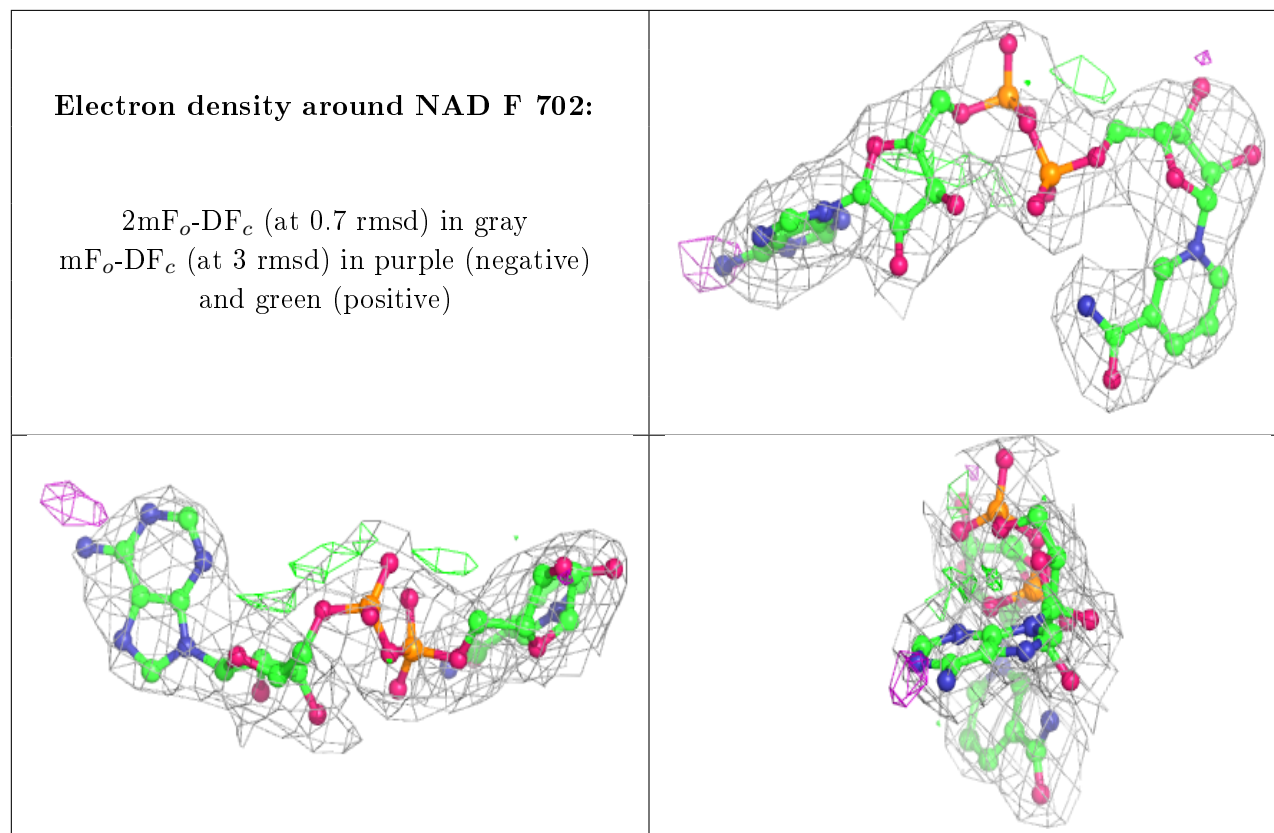
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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.

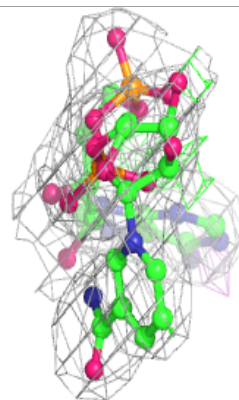
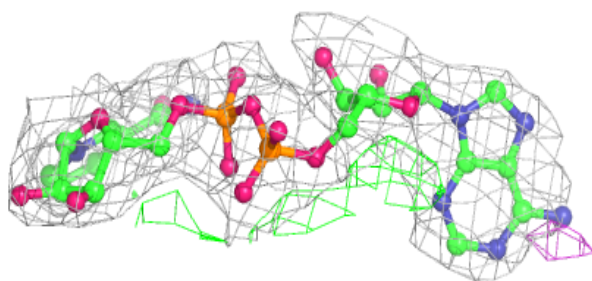
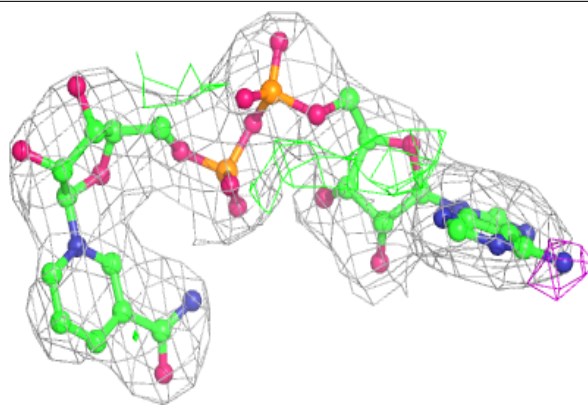
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	F	702	44/44	0.97	0.13	23,49,59,71	0
3	NAD	D	701	44/44	0.97	0.13	20,43,55,69	0
3	NAD	B	700	44/44	0.97	0.12	24,42,55,66	0

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.

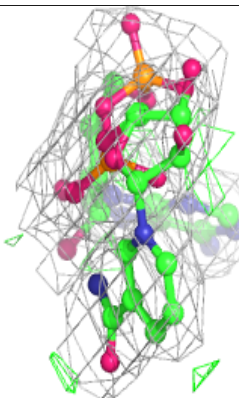
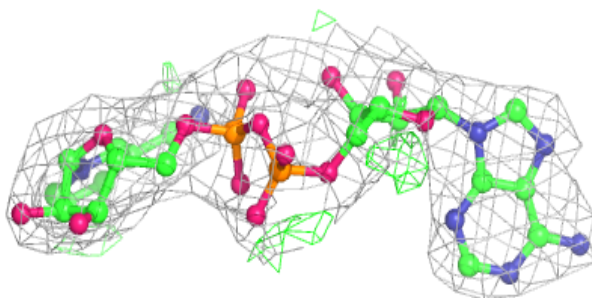
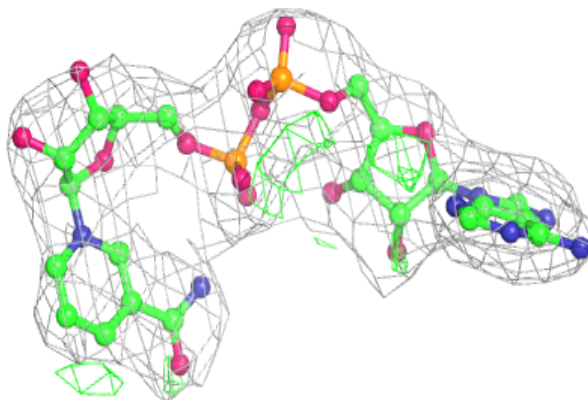


**Electron density around NAD D 701:**

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

**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

There are no such residues in this entry.