



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:07 AM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.23.2  
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) : 2.23.2

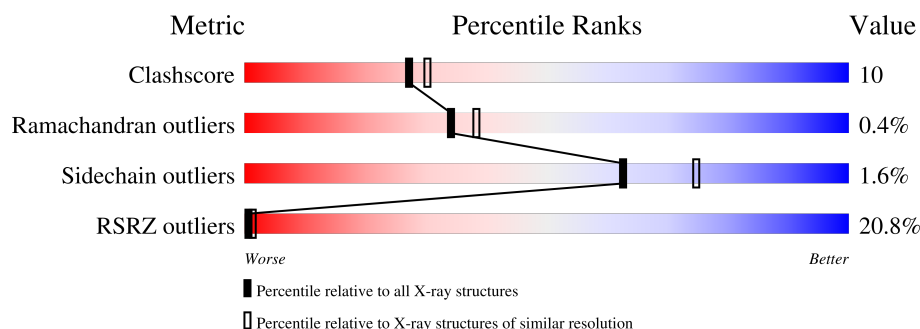
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>8%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	842	<div> <div>15%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	E	842	<div> <div>51%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>..</div> </div> </div>
2	B	207	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>
2	D	207	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>14%</div> <div>.</div> </div> </div>
2	F	207	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24682 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor 2.

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

- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1589	1002	285	302			
2	D	207	Total	C	N	O	0	0	0
			1589	1002	285	302			
2	F	207	Total	C	N	O	0	0	0
			1589	1002	285	302			

There are 12 discrepancies between the modelled and reference sequences:

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

- # NAD

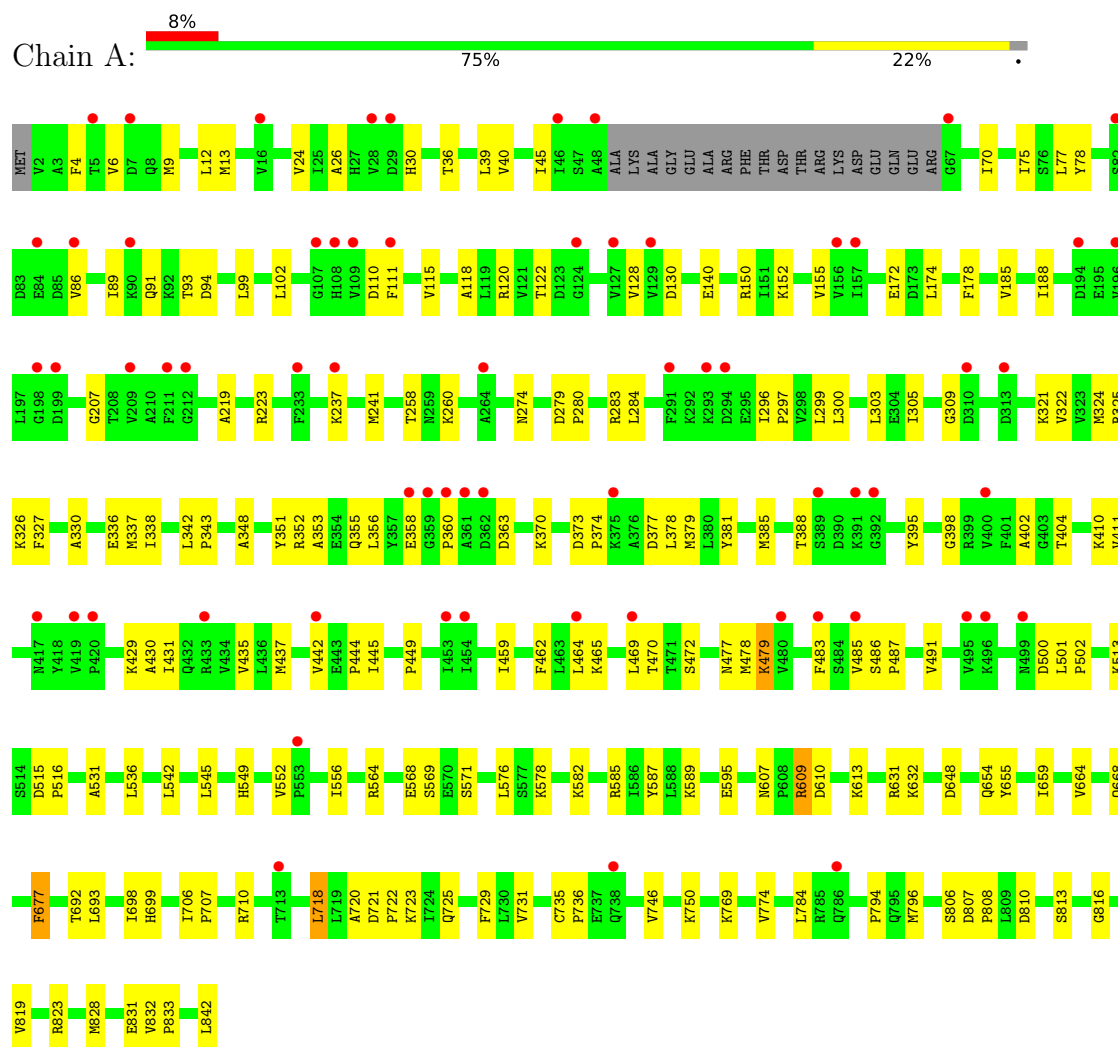
- Molecule 4 is water.

WORLDWIDE  
 **PDB**  
PROTEIN DATA BANK

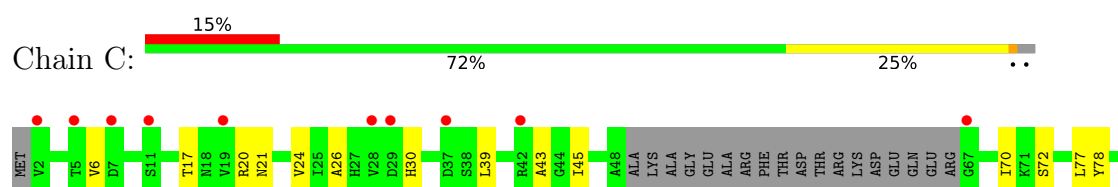
### 3 Residue-property plots

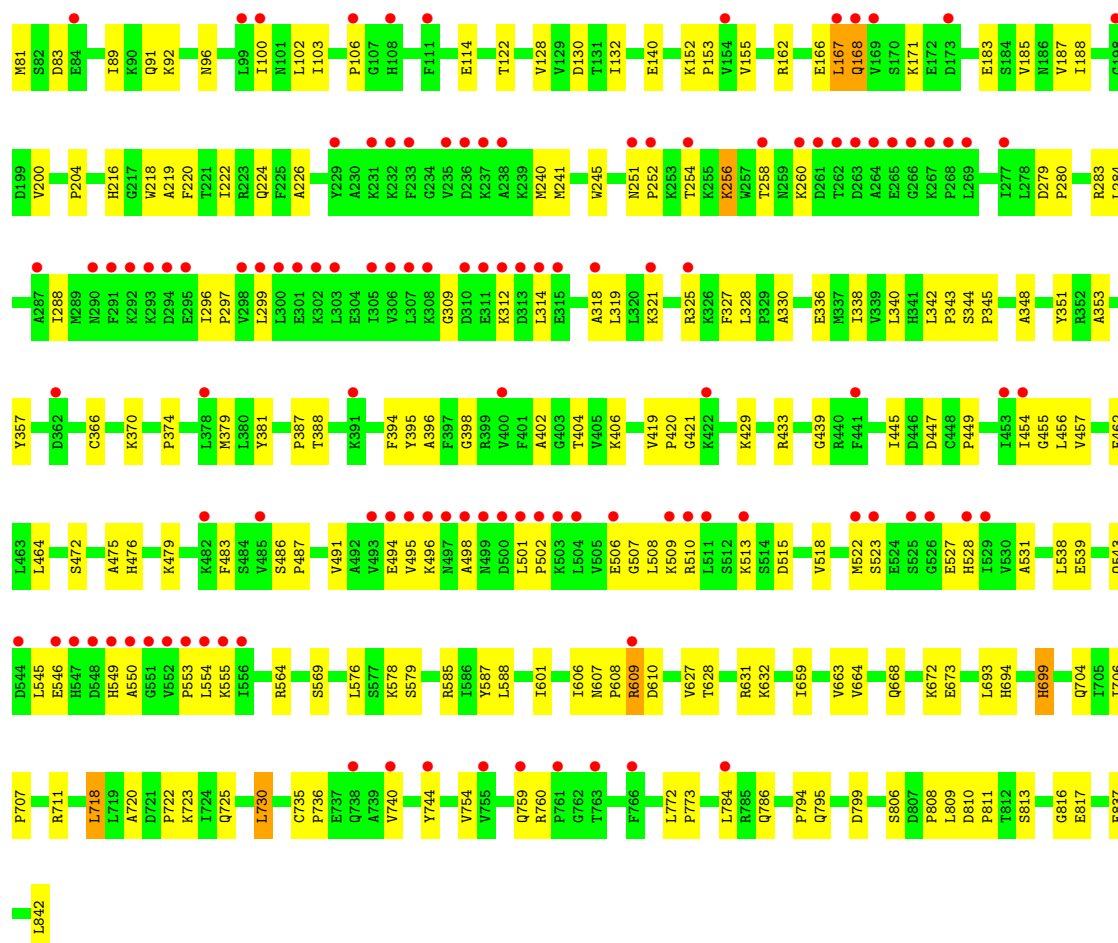
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Elongation factor 2

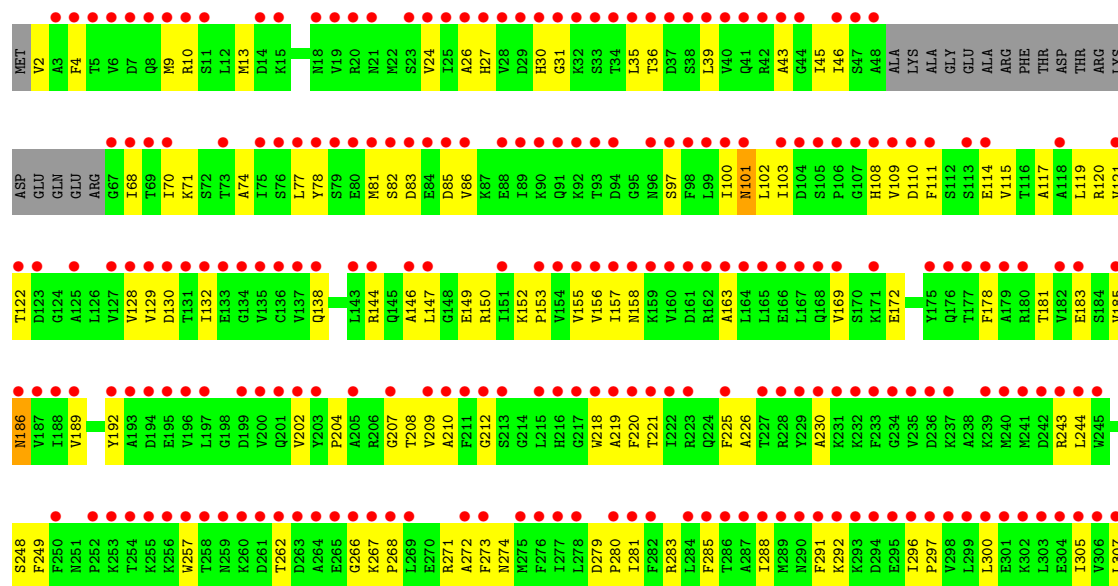


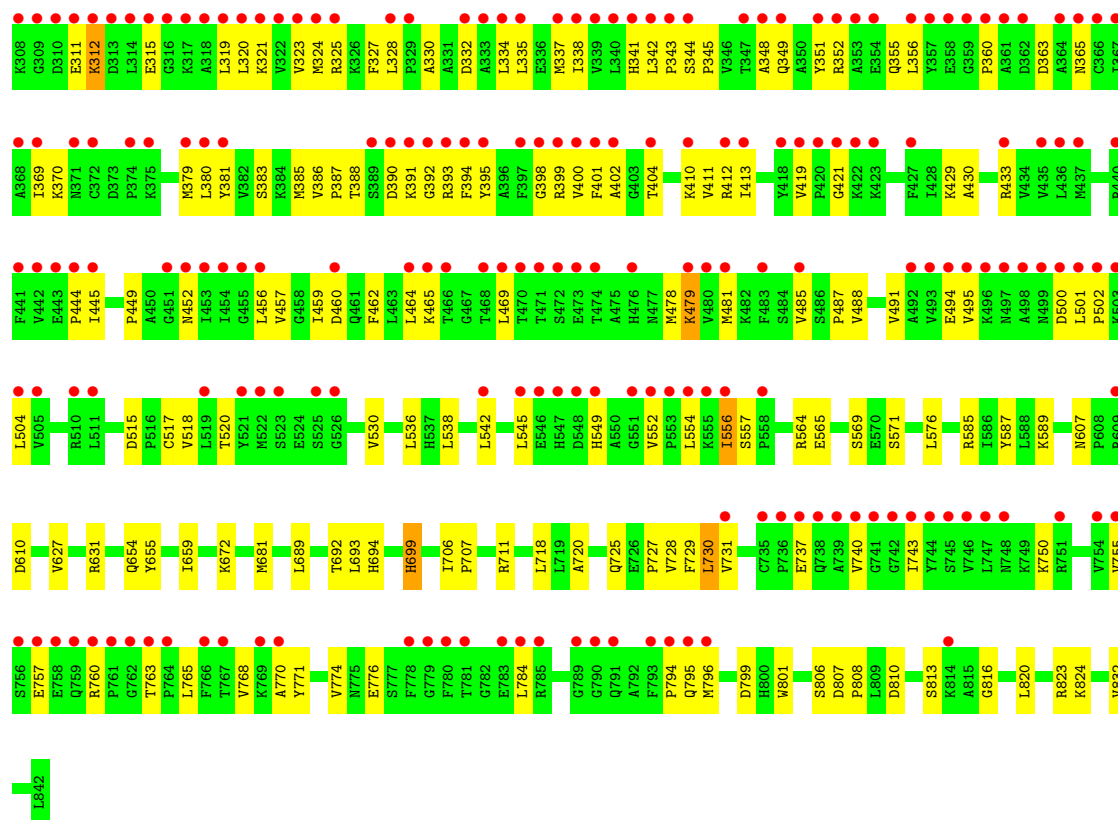
#### • Molecule 1: Elongation factor 2



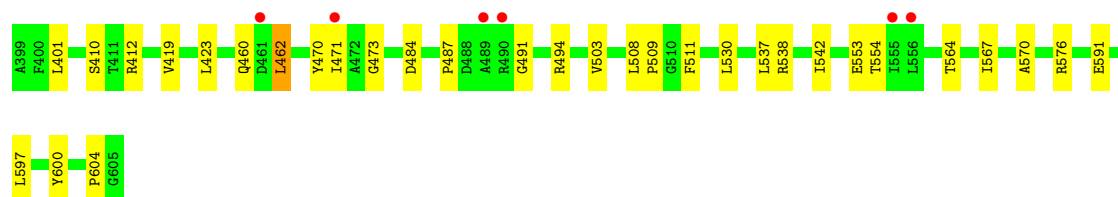
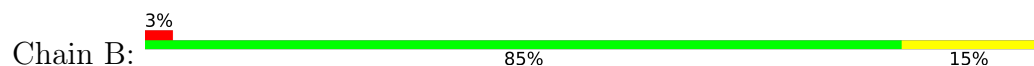


● Molecule 1: Elongation factor 2

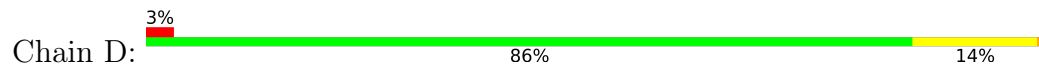




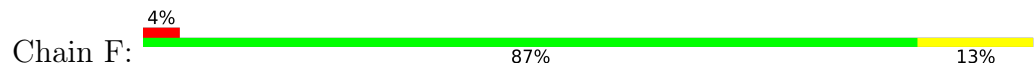
- Molecule 2: Exotoxin A



- 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, $\alpha$ , $\beta$ , $\gamma$	327.57Å 68.46Å 189.99Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35 25.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.00-2.35) 98.5 (25.00-2.35)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.36Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.257 0.209 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8973e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.20	0/6517	0.37	0/8823
1	C	0.20	0/6517	0.37	0/8823
1	E	0.20	0/6517	0.37	0/8823
2	B	0.20	0/1629	0.38	0/2219
2	D	0.20	0/1629	0.40	0/2219
2	F	0.20	0/1629	0.38	0/2219
All	All	0.20	0/24438	0.37	0/33126

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 [i](#)

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	121	0
1	C	6415	0	6488	132	0
1	E	6415	0	6488	189	0
2	B	1589	0	1543	18	0
2	D	1589	0	1543	15	0
2	F	1589	0	1543	13	0
3	B	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	26	3	0
3	F	44	0	26	1	0
4	A	83	0	0	1	0
4	B	117	0	0	1	0
4	C	85	0	0	0	0
4	D	124	0	0	1	0
4	E	45	0	0	0	0
4	F	94	0	0	1	0
All	All	24682	0	24155	488	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 (488) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:GLN:HG2	1:C:760:ARG:H	1.38	0.86
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.57	0.85
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.57	0.84
1:C:404:THR:HG22	1:C:449:PRO:HA	1.58	0.83
1:E:391:LYS:HG3	1:E:392:GLY:H	1.43	0.82
1:A:258:THR:HG22	1:A:260:LYS:H	1.45	0.81
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.62	0.81
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.61	0.81
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.64	0.79
1:E:404:THR:HG22	1:E:449:PRO:HA	1.63	0.78
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.66	0.78
1:E:571:SER:HB2	1:E:589:LYS:HG3	1.65	0.77
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.67	0.77
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.67	0.76
1:C:132:ILE:HD12	1:C:132:ILE:H	1.51	0.75
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.24	0.72
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.71	0.72
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.71	0.71
1:C:258:THR:HG22	1:C:260:LYS:H	1.56	0.71
1:C:694:HIS:CE1	1:C:699:DDE:HD2	2.26	0.70
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.26	0.70
1:E:556:ILE:HG22	1:E:557:SER:H	1.57	0.70
1:A:609:ARG:CG	1:A:609:ARG:HH11	2.04	0.69
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.74	0.69
1:A:404:THR:HG22	1:A:449:PRO:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.73	0.68
1:E:30:HIS:ND1	1:E:130:ASP:HB2	2.10	0.66
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.31	0.66
1:E:699:DDE:HAB2	1:E:699:DDE:HAT2	1.78	0.66
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.66
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.78	0.65
1:E:43:ALA:HB1	1:E:78:TYR:H	1.63	0.64
2:D:498:LEU:HD11	2:D:571:ILE:HB	1.79	0.64
1:C:496:LYS:H	1:C:554:LEU:HD22	1.63	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.78	0.64
1:C:353:ALA:HB3	1:C:370:LYS:HG3	1.79	0.63
1:A:578:LYS:HG2	1:A:585:ARG:HG2	1.80	0.63
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.38	0.63
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.80	0.63
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.80	0.63
1:C:216:HIS:ND1	1:C:321:LYS:HG2	2.14	0.62
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.81	0.62
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.81	0.62
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.80	0.62
1:C:279:ASP:O	1:C:283:ARG:HG2	1.99	0.62
1:E:810:ASP:O	1:E:816:GLY:HA3	2.00	0.62
1:A:237:LYS:O	1:A:241:MET:HB2	2.00	0.62
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.81	0.62
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.81	0.62
1:E:707:PRO:O	1:E:711:ARG:HG3	2.00	0.61
1:E:564:ARG:HB2	1:E:725:GLN:HB2	1.82	0.61
1:A:279:ASP:O	1:A:283:ARG:HG3	2.01	0.61
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.65	0.61
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.35	0.61
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.83	0.61
1:C:216:HIS:HB2	1:C:218:TRP:HD1	1.65	0.61
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.83	0.60
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.82	0.60
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.83	0.60
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.83	0.60
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.84	0.60
1:C:30:HIS:CD2	1:C:130:ASP:HB2	2.37	0.60
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.83	0.60
1:C:699:DDE:HAC2	1:C:699:DDE:NAD	2.15	0.60
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ASP:O	1:A:816:GLY:HA3	2.02	0.59
1:E:26:ALA:CB	1:E:128:VAL:HB	2.32	0.59
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.84	0.59
1:A:569:SER:O	1:A:720:ALA:HB1	2.03	0.59
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.37	0.59
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.84	0.58
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.33	0.58
1:C:707:PRO:O	1:C:711:ARG:HG3	2.03	0.58
1:C:672:LYS:HG3	1:C:673:GLU:HG3	1.86	0.58
1:A:321:LYS:O	1:A:325:ARG:HB2	2.03	0.58
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.86	0.58
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.86	0.57
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.40	0.57
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.05	0.57
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.87	0.57
1:C:722:PRO:O	1:C:723:LYS:HG3	2.05	0.57
1:E:121:VAL:HG11	1:E:383:SER:OG	2.05	0.57
1:C:374:PRO:O	1:C:404:THR:HG23	2.04	0.56
1:C:419:VAL:HG12	1:C:421:GLY:H	1.70	0.56
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.86	0.56
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.87	0.56
1:E:9:MET:O	1:E:13:MET:HG3	2.05	0.56
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.87	0.56
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.86	0.56
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.21	0.56
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.88	0.56
1:E:291:PHE:HD1	1:E:315:GLU:HB3	1.70	0.56
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.88	0.55
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.88	0.55
1:E:207:GLY:O	1:E:337:MET:HG2	2.06	0.55
1:A:30:HIS:CD2	1:A:130:ASP:HB2	2.42	0.55
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.88	0.55
1:C:772:LEU:HD12	1:C:773:PRO:HD2	1.87	0.55
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.88	0.55
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.89	0.55
1:A:324:MET:HE2	1:A:324:MET:HA	1.89	0.55
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.87	0.55
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.89	0.55
1:E:391:LYS:HG3	1:E:392:GLY:N	2.19	0.54
1:C:6:VAL:HG13	1:C:445:ILE:HG22	1.90	0.54
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.43	0.54
1:A:385:MET:HG2	1:A:465:LYS:HA	1.88	0.54
1:A:568:GLU:OE2	1:A:723:LYS:HE3	2.06	0.54
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.37	0.54
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.42	0.54
1:E:464:LEU:HG	1:E:465:LYS:HG3	1.89	0.54
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.73	0.54
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.89	0.54
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.90	0.54
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.89	0.54
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.89	0.54
1:A:500:ASP:HB3	1:A:552:VAL:HG11	1.90	0.53
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.07	0.53
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.91	0.53
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.23	0.53
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.88	0.53
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.89	0.53
1:A:823:ARG:NH2	1:A:833:PRO:HD3	2.24	0.53
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.43	0.53
2:D:537:LEU:O	2:D:538:ARG:HD3	2.09	0.53
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.91	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
1:A:819:VAL:O	1:A:823:ARG:HG2	2.08	0.53
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.44	0.53
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.90	0.53
1:A:501:LEU:N	1:A:502:PRO:HD2	2.24	0.52
1:C:627:VAL:O	1:C:631:ARG:HG3	2.08	0.52
1:E:296:ILE:O	1:E:300:LEU:HD13	2.09	0.52
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.74	0.52
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.90	0.52
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.45	0.52
1:E:257:TRP:HZ3	1:E:272:ALA:HB2	1.74	0.52
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.44	0.52
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.91	0.52
1:A:388:THR:HG21	1:A:395:TYR:CD2	2.45	0.52
1:A:609:ARG:HH11	1:A:609:ARG:HG2	1.74	0.52
1:C:296:ILE:N	1:C:297:PRO:HD2	2.25	0.52
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.52
1:A:613:LYS:HG2	1:A:631:ARG:HH11	1.75	0.51
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.92	0.51
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD13	1:A:556:ILE:HG21	1.93	0.51
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.44	0.51
1:E:74:ALA:HA	1:E:102:LEU:O	2.10	0.51
1:E:243:ARG:O	1:E:248:SER:HB2	2.08	0.51
2:F:513:ARG:HH21	2:F:513:ARG:HB2	1.75	0.51
1:A:338:ILE:O	1:A:342:LEU:HB2	2.10	0.51
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.91	0.51
1:E:755:VAL:HG23	1:E:770:ALA:HA	1.93	0.51
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.93	0.51
1:E:111:PHE:HB3	1:E:114:GLU:HG2	1.93	0.51
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.92	0.51
1:A:632:LYS:HD3	1:A:648:ASP:O	2.10	0.51
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.45	0.51
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.46	0.51
2:D:553:GLU:OE1	3:D:701:NAD:H6N	2.11	0.51
1:E:117:ALA:HA	1:E:481:MET:SD	2.49	0.51
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.92	0.51
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.92	0.51
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.93	0.51
1:A:746:VAL:O	1:A:750:LYS:HD3	2.11	0.51
1:A:381:TYR:O	1:A:398:GLY:HA3	2.11	0.51
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.75	0.51
1:E:750:LYS:HD2	1:E:776:GLU:O	2.11	0.51
2:F:537:LEU:HD11	2:F:542:ILE:HG22	1.93	0.51
1:C:321:LYS:O	1:C:325:ARG:HG3	2.11	0.50
1:E:208:THR:HG23	1:E:341:HIS:CE1	2.47	0.50
1:C:254:THR:HG22	1:C:256:LYS:HB2	1.94	0.50
1:E:291:PHE:CD1	1:E:315:GLU:HB3	2.46	0.50
1:E:654:GLN:O	1:E:655:TYR:HB2	2.12	0.50
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.93	0.50
2:D:427:ARG:HD2	2:D:431:GLU:OE2	2.12	0.50
1:E:349:GLN:O	1:E:370:LYS:HA	2.11	0.50
1:E:627:VAL:O	1:E:631:ARG:HG3	2.11	0.50
1:E:82:SER:O	1:E:86:VAL:HG23	2.11	0.50
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.93	0.50
1:E:727:PRO:HD3	1:E:801:TRP:CZ3	2.47	0.50
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.93	0.50
1:C:723:LYS:HA	1:C:808:PRO:HG3	1.93	0.50
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.93	0.50
1:A:152:LYS:HD3	1:A:343:PRO:HD3	1.94	0.50
1:A:9:MET:O	1:A:13:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.93	0.50
1:A:431:ILE:HD12	1:A:459:ILE:HD11	1.93	0.50
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.41	0.50
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.46	0.50
1:E:380:LEU:HG	1:E:400:VAL:HG22	1.94	0.49
1:A:111:PHE:O	1:A:115:VAL:HG23	2.13	0.49
1:C:17:THR:HB	1:C:92:LYS:O	2.13	0.49
1:C:338:ILE:HG23	1:C:342:LEU:HD12	1.93	0.49
1:C:487:PRO:HB3	1:C:531:ALA:HB1	1.95	0.49
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.47	0.49
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.95	0.49
1:C:759:GLN:HG2	1:C:760:ARG:N	2.17	0.49
1:C:609:ARG:H	1:C:609:ARG:HD2	1.78	0.49
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.94	0.49
1:E:185:VAL:O	1:E:189:VAL:HG23	2.13	0.49
1:E:321:LYS:O	1:E:325:ARG:HG3	2.12	0.49
1:C:314:LEU:HD22	1:C:318:ALA:HB1	1.95	0.49
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.76	0.49
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.48	0.49
1:A:731:VAL:HG22	1:A:796:MET:HB3	1.95	0.49
1:C:81:MET:O	1:C:96:ASN:HB3	2.13	0.49
1:C:806:SER:HB2	1:C:813:SER:HB2	1.95	0.49
1:C:72:SER:HA	1:C:439:GLY:O	2.13	0.48
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.95	0.48
1:E:312:LYS:HD2	1:E:312:LYS:O	2.14	0.48
1:E:538:LEU:O	1:E:542:LEU:HG	2.13	0.48
1:A:806:SER:HB2	1:A:813:SER:HB2	1.96	0.48
1:C:226:ALA:HB2	1:C:241:MET:HB3	1.94	0.48
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.96	0.48
1:A:150:ARG:HG3	1:A:355:GLN:HE22	1.79	0.48
1:E:292:LYS:O	1:E:296:ILE:HG13	2.14	0.48
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.95	0.48
1:A:118:ALA:O	1:A:122:THR:HG23	2.14	0.48
1:A:831:GLU:CD	1:A:831:GLU:H	2.16	0.48
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.14	0.48
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.96	0.48
1:C:498:ALA:HA	1:C:501:LEU:HB2	1.96	0.48
1:E:552:VAL:O	1:E:554:LEU:HG	2.14	0.48
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.49	0.48
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.96	0.48
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LYS:HG3	1:C:447:ASP:HB3	1.95	0.47
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.94	0.47
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.95	0.47
1:E:556:ILE:HG22	1:E:557:SER:N	2.27	0.47
1:E:204:PRO:HA	1:E:209:VAL:HB	1.96	0.47
1:E:365:ASN:O	1:E:369:ILE:HG12	2.13	0.47
1:A:464:LEU:HD23	1:A:483:PHE:CE1	2.50	0.47
2:D:488:ASP:HB3	4:D:795:HOH:O	2.14	0.47
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.95	0.47
1:E:391:LYS:CG	1:E:392:GLY:H	2.21	0.47
1:C:578:LYS:HB3	1:C:585:ARG:HG2	1.97	0.47
1:E:30:HIS:CE1	1:E:130:ASP:HB2	2.50	0.47
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.96	0.47
1:C:809:LEU:O	1:C:811:PRO:HD3	2.14	0.47
1:E:820:LEU:HG	1:E:824:LYS:HE2	1.96	0.47
1:A:45:ILE:HD11	1:A:78:TYR:HB2	1.96	0.47
2:B:470:TYR:CD2	3:B:700:NAD:H2D	2.50	0.47
1:C:420:PRO:HG2	1:C:476:HIS:CD2	2.50	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
2:F:513:ARG:HB2	2:F:513:ARG:NH2	2.30	0.47
1:C:515:ASP:O	1:C:518:VAL:HG12	2.15	0.47
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.50	0.47
1:A:4:PHE:HD2	1:A:45:ILE:HG23	1.79	0.46
1:A:609:ARG:HG3	1:A:609:ARG:NH1	2.30	0.46
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.97	0.46
1:E:101:ASN:N	1:E:101:ASN:HD22	2.13	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.95	0.46
1:E:419:VAL:HG12	1:E:421:GLY:H	1.80	0.46
1:C:153:PRO:HD2	1:C:200:VAL:HG12	1.96	0.46
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.46
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.97	0.46
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.50	0.46
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.98	0.46
1:E:156:VAL:HG11	1:E:334:LEU:HD21	1.98	0.46
1:A:296:ILE:O	1:A:300:LEU:HD13	2.16	0.46
1:E:352:ARG:O	1:E:356:LEU:HG	2.15	0.46
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.98	0.46
1:E:737:GLU:HA	1:E:740:VAL:HG23	1.96	0.46
1:C:43:ALA:HB1	1:C:78:TYR:O	2.16	0.46
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.51	0.46
1:C:699:DDE:HAB2	1:C:699:DDE:HAU3	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:GLU:HA	1:E:186:ASN:OD1	2.16	0.46
1:E:226:ALA:O	1:E:230:ALA:HB2	2.15	0.46
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.97	0.46
1:A:155:VAL:HG21	1:A:185:VAL:HG11	1.98	0.46
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.98	0.46
1:E:459:ILE:O	1:E:459:ILE:HG22	2.16	0.46
1:A:110:ASP:HB3	1:A:536:LEU:HD22	1.98	0.46
1:A:478:MET:O	1:A:479:LYS:C	2.54	0.46
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.46	0.46
1:E:569:SER:O	1:E:720:ALA:HB1	2.16	0.46
1:C:288:ILE:HA	1:C:296:ILE:HD11	1.97	0.45
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.97	0.45
1:A:429:LYS:HG3	1:A:462:PHE:CE2	2.51	0.45
1:C:183:GLU:O	1:C:187:VAL:HG23	2.16	0.45
2:D:538:ARG:HD2	2:D:559:PRO:HG2	1.98	0.45
1:E:381:TYR:O	1:E:398:GLY:HA3	2.15	0.45
1:A:515:ASP:HA	1:A:516:PRO:HD2	1.83	0.45
1:C:106:PRO:HG3	1:C:114:GLU:HG2	1.97	0.45
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.51	0.45
1:E:244:LEU:O	1:E:273:PHE:HB2	2.16	0.45
1:E:262:THR:HG23	1:E:266:GLY:HA2	1.98	0.45
1:E:380:LEU:HD13	1:E:456:LEU:HD11	1.99	0.45
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.99	0.45
2:F:508:LEU:N	2:F:509:PRO:CD	2.80	0.45
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.51	0.45
1:E:305:ILE:HG21	1:E:323:VAL:HG13	1.98	0.45
1:A:718:LEU:HA	1:A:722:PRO:HG3	1.98	0.45
2:B:401:LEU:HD23	2:B:567:ILE:HG22	1.98	0.45
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.98	0.45
1:E:296:ILE:N	1:E:297:PRO:HD2	2.32	0.45
1:E:459:ILE:HD12	1:E:459:ILE:N	2.32	0.45
1:E:823:ARG:HE	1:E:832:VAL:HG22	1.82	0.45
2:B:570:ALA:HB3	2:B:591:GLU:OE1	2.17	0.44
1:C:171:LYS:NZ	1:C:171:LYS:HB2	2.32	0.44
1:E:46:ILE:N	1:E:46:ILE:HD12	2.32	0.44
1:A:352:ARG:NH2	1:A:356:LEU:HD11	2.32	0.44
1:A:609:ARG:CG	1:A:609:ARG:NH1	2.68	0.44
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.98	0.44
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.52	0.44
1:E:806:SER:HB2	1:E:813:SER:HB2	1.99	0.44
1:C:664:VAL:O	1:C:668:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG21	1:A:395:TYR:CG	2.53	0.44
1:E:218:TRP:HB3	1:E:324:MET:HB3	1.99	0.44
1:E:757:GLU:HG3	1:E:768:VAL:HG22	2.00	0.44
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.99	0.44
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.99	0.44
1:E:46:ILE:HD12	1:E:46:ILE:H	1.83	0.44
1:E:279:ASP:O	1:E:283:ARG:HG2	2.17	0.44
1:E:324:MET:HE2	1:E:324:MET:HA	2.00	0.44
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.18	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.32	0.44
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.32	0.44
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.81	0.44
1:E:485:VAL:HG22	1:E:485:VAL:O	2.16	0.44
1:A:698:ILE:H	1:A:698:ILE:HG13	1.62	0.44
1:C:152:LYS:HD3	1:C:343:PRO:HD3	2.00	0.44
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.48	0.44
1:E:157:ILE:HG21	1:E:178:PHE:CD1	2.53	0.44
1:E:452:ASN:N	1:E:452:ASN:HD22	2.16	0.44
2:F:523:ALA:O	2:F:527:VAL:HG23	2.18	0.44
2:F:574:ASP:HA	2:F:575:PRO:HD2	1.84	0.44
1:A:823:ARG:HH22	1:A:833:PRO:HD3	1.82	0.44
2:B:419:VAL:O	2:B:423:LEU:HG	2.17	0.44
1:C:454:ILE:HG13	1:C:455:GLY:H	1.82	0.44
1:E:39:LEU:HD12	1:E:39:LEU:H	1.83	0.44
1:E:345:PRO:HB3	1:E:399:ARG:HH21	1.81	0.44
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.99	0.43
1:E:132:ILE:HD12	1:E:132:ILE:N	2.33	0.43
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.18	0.43
1:A:664:VAL:O	1:A:668:GLN:HG2	2.18	0.43
1:C:24:VAL:HG23	1:C:102:LEU:HD11	2.00	0.43
1:E:39:LEU:HD11	1:E:334:LEU:HD13	2.00	0.43
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.48	0.43
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.90	0.43
1:E:727:PRO:HD3	1:E:801:TRP:HZ3	1.82	0.43
1:C:579:SER:HB2	1:C:704:GLN:OE1	2.18	0.43
1:E:77:LEU:HD23	1:E:335:LEU:HD21	2.01	0.43
1:E:111:PHE:O	1:E:115:VAL:HG23	2.19	0.43
1:E:369:ILE:HD12	1:E:401:PHE:HB3	2.01	0.43
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.84	0.43
1:A:353:ALA:HB3	1:A:370:LYS:HG2	2.01	0.43
1:A:410:LYS:HA	1:A:430:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LYS:HE2	4:B:779:HOH:O	2.17	0.43
1:A:677:PHE:N	1:A:677:PHE:CD2	2.85	0.43
1:C:546:GLU:HA	1:C:550:ALA:HB3	2.00	0.43
1:C:736:PRO:O	1:C:740:VAL:HG23	2.18	0.43
1:E:485:VAL:O	1:E:487:PRO:HD3	2.18	0.43
1:E:491:VAL:HG13	1:E:538:LEU:HD21	1.99	0.43
1:E:699:DDE:HAT2	1:E:699:DDE:CAB	2.46	0.43
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.99	0.43
1:A:654:GLN:HG2	1:A:655:TYR:CE1	2.54	0.43
1:C:396:ALA:HB3	1:C:456:LEU:HB2	2.01	0.43
1:E:307:LEU:HD13	1:E:311:GLU:O	2.19	0.43
1:A:26:ALA:HB2	1:A:128:VAL:HB	2.01	0.43
1:C:608:PRO:HD2	1:C:609:ARG:NH1	2.33	0.43
2:D:499:LEU:HB3	2:D:566:VAL:CG1	2.47	0.43
1:E:150:ARG:HB3	1:E:351:TYR:HE1	1.83	0.43
1:E:181:THR:O	1:E:185:VAL:HG23	2.18	0.43
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.54	0.43
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.38	0.43
2:B:410:SER:OG	2:B:412:ARG:HG3	2.18	0.43
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.43
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.99	0.43
1:A:6:VAL:HG13	1:A:445:ILE:HG22	2.01	0.43
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.00	0.43
1:C:284:LEU:HD23	1:C:299:LEU:HD23	2.00	0.43
1:A:12:LEU:HG	1:A:99:LEU:HB2	2.01	0.42
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.53	0.42
2:B:460:GLN:HG3	2:B:462:LEU:HD11	2.00	0.42
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.18	0.42
1:E:163:ALA:O	1:E:169:VAL:HG12	2.18	0.42
1:A:731:VAL:O	1:A:769:LYS:HA	2.19	0.42
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.54	0.42
1:C:506:GLU:O	1:C:510:ARG:HG3	2.18	0.42
1:E:70:ILE:HG22	1:E:388:THR:HG22	2.01	0.42
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.83	0.42
1:C:523:SER:OG	1:C:527:GLU:HB2	2.19	0.42
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.01	0.42
1:A:120:ARG:NH1	1:A:479:LYS:HD2	2.34	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.01	0.42
1:C:167:LEU:O	1:C:168:GLN:C	2.57	0.42
1:E:149:GLU:O	1:E:352:ARG:HD2	2.19	0.42
1:A:322:VAL:O	1:A:326:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:HA	1:A:374:PRO:HD2	1.86	0.42
1:A:207:GLY:O	1:A:337:MET:HG2	2.20	0.42
1:A:464:LEU:HD23	1:A:483:PHE:HE1	1.85	0.42
1:A:698:ILE:HG13	4:A:892:HOH:O	2.19	0.42
1:E:129:VAL:HG12	1:E:130:ASP:N	2.34	0.42
1:E:565:GLU:O	1:E:681:MET:HA	2.20	0.42
1:E:731:VAL:HA	1:E:796:MET:HB3	2.02	0.42
1:E:763:THR:C	1:E:765:LEU:H	2.23	0.42
2:B:484:ASP:OD2	2:B:494:ARG:HB2	2.20	0.42
1:C:140:GLU:HG3	1:C:188:ILE:HD13	2.02	0.42
1:C:659:ILE:O	1:C:663:VAL:HG23	2.20	0.42
1:E:338:ILE:O	1:E:342:LEU:HB2	2.19	0.42
1:E:344:SER:HB2	1:E:345:PRO:HD2	2.00	0.42
1:A:40:VAL:HG12	1:A:75:ILE:HG21	2.01	0.42
1:A:223:ARG:HB3	1:A:336:GLU:OE1	2.20	0.42
1:A:832:VAL:HA	1:A:833:PRO:HD3	1.95	0.42
2:B:487:PRO:HB2	2:B:491:GLY:HA2	2.02	0.42
1:C:491:VAL:HG13	1:C:538:LEU:HD21	2.01	0.42
1:C:628:THR:O	1:C:632:LYS:HG3	2.19	0.42
1:E:296:ILE:HG21	1:E:319:LEU:HD21	2.01	0.42
1:E:355:GLN:O	1:E:479:LYS:HG3	2.20	0.42
2:B:538:ARG:HE	2:B:538:ARG:HA	1.85	0.42
1:C:501:LEU:C	1:C:501:LEU:HD23	2.40	0.42
2:D:474:ASP:HA	2:D:475:PRO:HD2	1.89	0.42
1:E:155:VAL:HG21	1:E:202:VAL:HG21	2.02	0.42
1:E:327:PHE:CD2	1:E:328:LEU:HG	2.55	0.42
1:E:410:LYS:HA	1:E:430:ALA:HA	2.02	0.42
1:C:20:ARG:NH1	1:C:344:SER:HB3	2.35	0.41
1:C:539:GLU:O	1:C:543:GLN:HG3	2.20	0.41
1:A:486:SER:HA	1:A:487:PRO:HD3	1.87	0.41
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.49	0.41
1:C:77:LEU:HB2	1:C:100:ILE:HB	2.02	0.41
1:C:132:ILE:HD11	1:C:162:ARG:HB2	2.01	0.41
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.93	0.41
1:C:588:LEU:C	1:C:588:LEU:HD12	2.41	0.41
1:C:813:SER:O	1:C:817:GLU:HB2	2.20	0.41
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.55	0.41
1:A:284:LEU:HD23	1:A:299:LEU:HD23	2.02	0.41
2:B:471:ILE:CG1	2:B:554:THR:HB	2.51	0.41
1:C:486:SER:HA	1:C:487:PRO:HD3	1.86	0.41
1:E:119:LEU:HD21	1:E:146:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.85	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.97	0.41
3:D:701:NAD:O1N	3:D:701:NAD:O2A	2.39	0.41
1:E:212:GLY:HA3	1:E:219:ALA:HA	2.02	0.41
1:E:288:ILE:HG23	1:E:319:LEU:HD23	2.01	0.41
1:A:284:LEU:HD11	1:A:303:LEU:HD12	2.01	0.41
1:A:358:GLU:HB2	1:A:477:ASN:O	2.19	0.41
1:C:153:PRO:HD2	1:C:200:VAL:CG1	2.51	0.41
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.74	0.41
1:E:491:VAL:HG21	1:E:542:LEU:HD21	2.02	0.41
1:A:305:ILE:HD11	1:A:327:PHE:CD1	2.56	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD2	2.56	0.41
1:C:699:DDE:HAA3	1:C:699:DDE:HAD2	1.85	0.41
1:C:810:ASP:O	1:C:816:GLY:HA3	2.20	0.41
1:E:152:LYS:HA	1:E:153:PRO:HD3	1.83	0.41
1:E:589:LYS:HE3	1:E:689:LEU:HD11	2.01	0.41
1:A:89:ILE:CG2	1:A:91:GLN:HG2	2.49	0.41
1:A:659:ILE:HD13	1:A:693:LEU:HD21	2.02	0.41
1:C:735:CYS:HA	1:C:736:PRO:HD3	1.96	0.41
2:D:508:LEU:N	2:D:509:PRO:CD	2.84	0.41
1:E:119:LEU:HD11	1:E:146:ALA:HA	2.02	0.41
1:A:93:THR:HG22	1:A:94:ASP:N	2.35	0.41
1:A:174:LEU:HG	1:A:178:PHE:CE2	2.56	0.41
1:A:589:LYS:HE3	1:A:589:LYS:HB2	1.95	0.41
2:B:508:LEU:N	2:B:509:PRO:CD	2.84	0.41
1:C:103:ILE:HD12	1:C:122:THR:HG22	2.01	0.41
1:C:204:PRO:HG2	1:C:245:TRP:CE2	2.55	0.41
1:C:569:SER:O	1:C:720:ALA:HB1	2.21	0.41
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.03	0.41
1:E:24:VAL:HG21	1:E:36:THR:HG22	2.02	0.41
1:E:411:VAL:HG12	1:E:412:ARG:N	2.36	0.41
1:C:718:LEU:HA	1:C:722:PRO:HG3	2.03	0.41
1:E:728:VAL:HG11	1:E:771:TYR:HB3	2.03	0.41
1:A:378:LEU:O	1:A:470:THR:HA	2.21	0.40
2:B:553:GLU:OE1	3:B:700:NAD:H6N	2.20	0.40
1:E:394:PHE:O	1:E:460:ASP:HB3	2.21	0.40
1:A:377:ASP:OD2	1:A:472:SER:HB2	2.22	0.40
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.88	0.40
1:C:70:ILE:HG22	1:C:388:THR:HG22	2.02	0.40
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.88	0.40
1:E:109:VAL:O	1:E:109:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:TYR:O	1:C:398:GLY:HA3	2.22	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.56	0.40
2:F:427:ARG:HA	4:F:755:HOH:O	2.20	0.40
1:A:120:ARG:HH12	1:A:479:LYS:HD2	1.86	0.40
1:A:609:ARG:HH11	1:A:609:ARG:HG3	1.81	0.40
2:B:511:PHE:HB3	2:B:600:TYR:CD1	2.55	0.40
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:E:103:ILE:HD13	1:E:122:THR:HG22	2.04	0.40
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.57	0.40
1:E:342:LEU:HA	1:E:343:PRO:HD2	1.85	0.40
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.85	0.40
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	818/842 (97%)	779 (95%)	36 (4%)	3 (0%)	34	38
1	C	818/842 (97%)	778 (95%)	35 (4%)	5 (1%)	25	27
1	E	818/842 (97%)	762 (93%)	53 (6%)	3 (0%)	34	38
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
2	F	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	29	32
All	All	3069/3147 (98%)	2919 (95%)	138 (4%)	12 (0%)	34	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY

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Mol	Chain	Res	Type
1	C	168	GLN
1	E	479	LYS
1	A	479	LYS
1	C	795	GLN
1	C	166	GLU
1	C	479	LYS
1	E	795	GLN
1	C	309	GLY
1	E	556	ILE
1	A	721	ASP
2	F	453	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	692 (99%)	7 (1%)	76	85
1	C	699/714 (98%)	688 (98%)	11 (2%)	62	75
1	E	699/714 (98%)	690 (99%)	9 (1%)	69	80
2	B	161/161 (100%)	160 (99%)	1 (1%)	86	93
2	D	161/161 (100%)	154 (96%)	7 (4%)	29	35
2	F	161/161 (100%)	155 (96%)	6 (4%)	34	42
All	All	2580/2625 (98%)	2539 (98%)	41 (2%)	62	75

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	MET
1	A	595	GLU
1	A	609	ARG
1	A	677	PHE
1	A	710	ARG
1	A	718	LEU
1	A	842	LEU

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Mol	Chain	Res	Type
2	B	462	LEU
1	C	83	ASP
1	C	167	LEU
1	C	240	MET
1	C	256	LYS
1	C	312	LYS
1	C	609	ARG
1	C	718	LEU
1	C	730	LEU
1	C	786	GLN
1	C	837	GLU
1	C	842	LEU
2	D	422	LEU
2	D	458	ARG
2	D	462	LEU
2	D	498	LEU
2	D	499	LEU
2	D	540	ASP
2	D	576	ARG
1	E	83	ASP
1	E	101	ASN
1	E	186	ASN
1	E	312	LYS
1	E	332	ASP
1	E	494	GLU
1	E	672	LYS
1	E	718	LEU
1	E	730	LEU
2	F	456	ARG
2	F	462	LEU
2	F	513	ARG
2	F	540	ASP
2	F	548	GLU
2	F	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	A	355	GLN
2	B	428	GLN
2	B	485	GLN

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Mol	Chain	Res	Type
1	C	528	HIS
1	C	753	GLN
1	E	476	HIS
1	E	753	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	1.02	1 (7%)	14,28,30	0.82	0
1	DDE	A	699	1	5,10,21	0.60	0	3,12,30	1.35	1 (33%)
1	DDE	E	699	1	14,20,21	0.98	2 (14%)	14,28,30	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	C	699	1	-	16/20/21/23	0/1/1/1
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1
1	DDE	E	699	1	-	5/20/21/23	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	CAT-CE1	2.31	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	CAT-CE1	2.10	1.53	1.50
1	E	699	DDE	CD2-NE2	-2.01	1.33	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	CD2-NE2-CE1	2.03	108.95	105.78

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	699	DDE	O-C-CA-CB
1	C	699	DDE	CA-CB-CG-ND1
1	C	699	DDE	CAU-CAT-CE1-NE2
1	C	699	DDE	NAD-CBI-CBW-NCB
1	C	699	DDE	OAG-CBI-CBW-NCB
1	C	699	DDE	CBI-CBW-NCB-CAB
1	C	699	DDE	CBI-CBW-NCB-CAC
1	C	699	DDE	CBI-CBW-NCB-CAA
1	C	699	DDE	CAU-CBW-NCB-CAB
1	C	699	DDE	CAU-CBW-NCB-CAC
1	C	699	DDE	CAU-CBW-NCB-CAA
1	C	699	DDE	CAT-CAU-CBW-NCB
1	E	699	DDE	CA-CB-CG-ND1
1	E	699	DDE	CAT-CAU-CBW-NCB
1	C	699	DDE	CAT-CAU-CBW-CBI
1	C	699	DDE	CA-CB-CG-CD2
1	E	699	DDE	CA-CB-CG-CD2
1	C	699	DDE	NAD-CBI-CBW-CAU
1	E	699	DDE	CAT-CAU-CBW-CBI
1	C	699	DDE	CAU-CAT-CE1-ND1
1	C	699	DDE	OAG-CBI-CBW-CAU
1	E	699	DDE	CAU-CAT-CE1-NE2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	4	0
1	E	699	DDE	3	0

## 5.5 Carbohydrates [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	0.69	0	50,73,73	1.26	3 (6%)
3	NAD	B	700	-	42,48,48	0.68	0	50,73,73	1.37	3 (6%)
3	NAD	D	701	-	42,48,48	0.68	0	50,73,73	1.36	3 (6%)

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	-	-	2/26/62/62	0/5/5/5
3	NAD	B	700	-	-	2/26/62/62	0/5/5/5
3	NAD	D	701	-	-	5/26/62/62	0/5/5/5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	C3D-C2D-C1D	4.92	108.38	100.98
3	D	701	NAD	C3D-C2D-C1D	4.63	107.95	100.98
3	D	701	NAD	N3A-C2A-N1A	-4.47	121.69	128.68
3	F	702	NAD	N3A-C2A-N1A	-4.44	121.74	128.68
3	B	700	NAD	N3A-C2A-N1A	-4.28	121.98	128.68
3	D	701	NAD	PN-O3-PA	-3.95	119.26	132.83
3	F	702	NAD	C3D-C2D-C1D	3.77	106.65	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	NAD	PN-O3-PA	-3.71	120.09	132.83
3	B	700	NAD	PN-O3-PA	-3.63	120.35	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

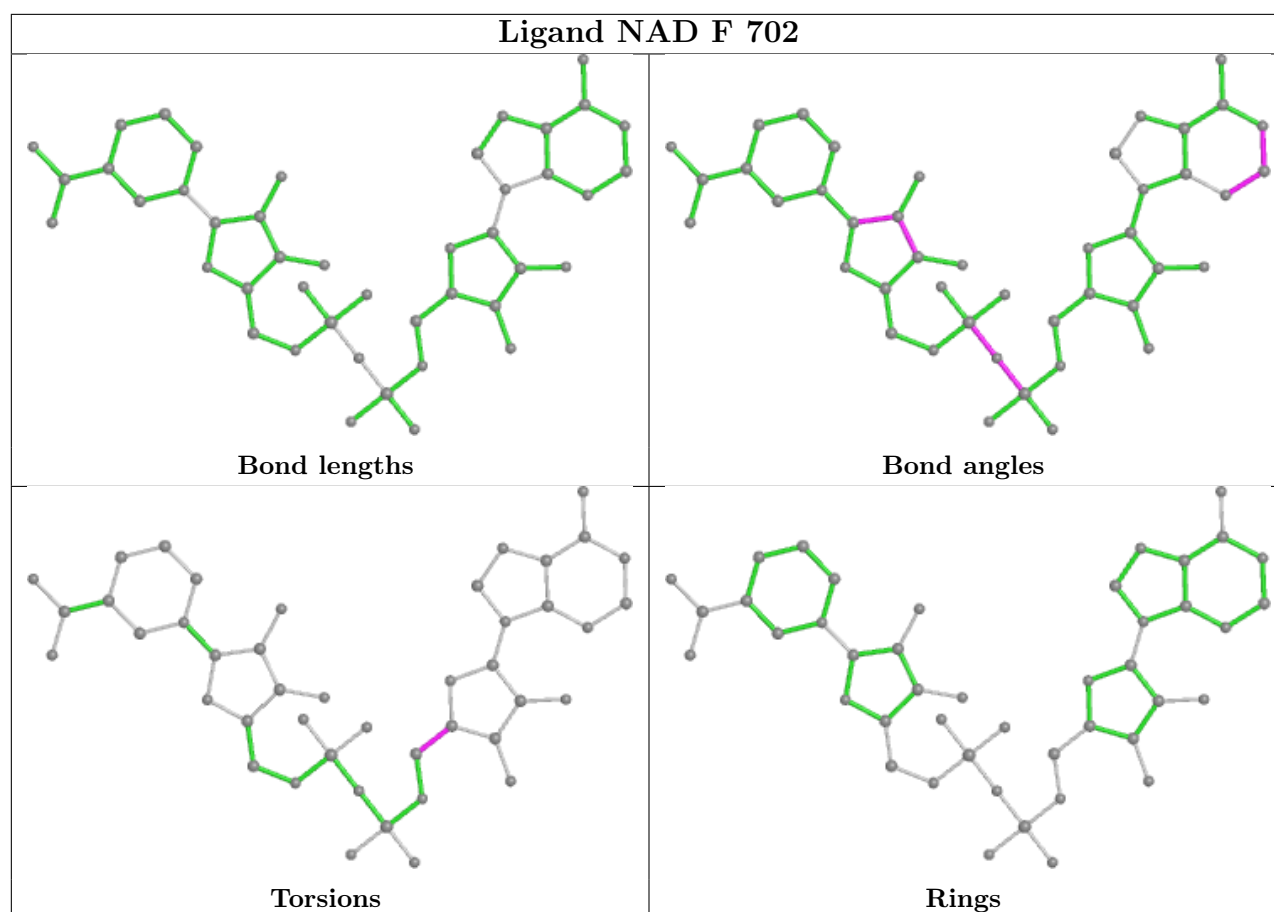
Mol	Chain	Res	Type	Atoms
3	B	700	NAD	O4B-C4B-C5B-O5B
3	B	700	NAD	C3B-C4B-C5B-O5B
3	D	701	NAD	O4B-C4B-C5B-O5B
3	F	702	NAD	O4B-C4B-C5B-O5B
3	D	701	NAD	C3B-C4B-C5B-O5B
3	F	702	NAD	C3B-C4B-C5B-O5B
3	D	701	NAD	C3D-C4D-C5D-O5D
3	D	701	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	PA-O3-PN-O1N

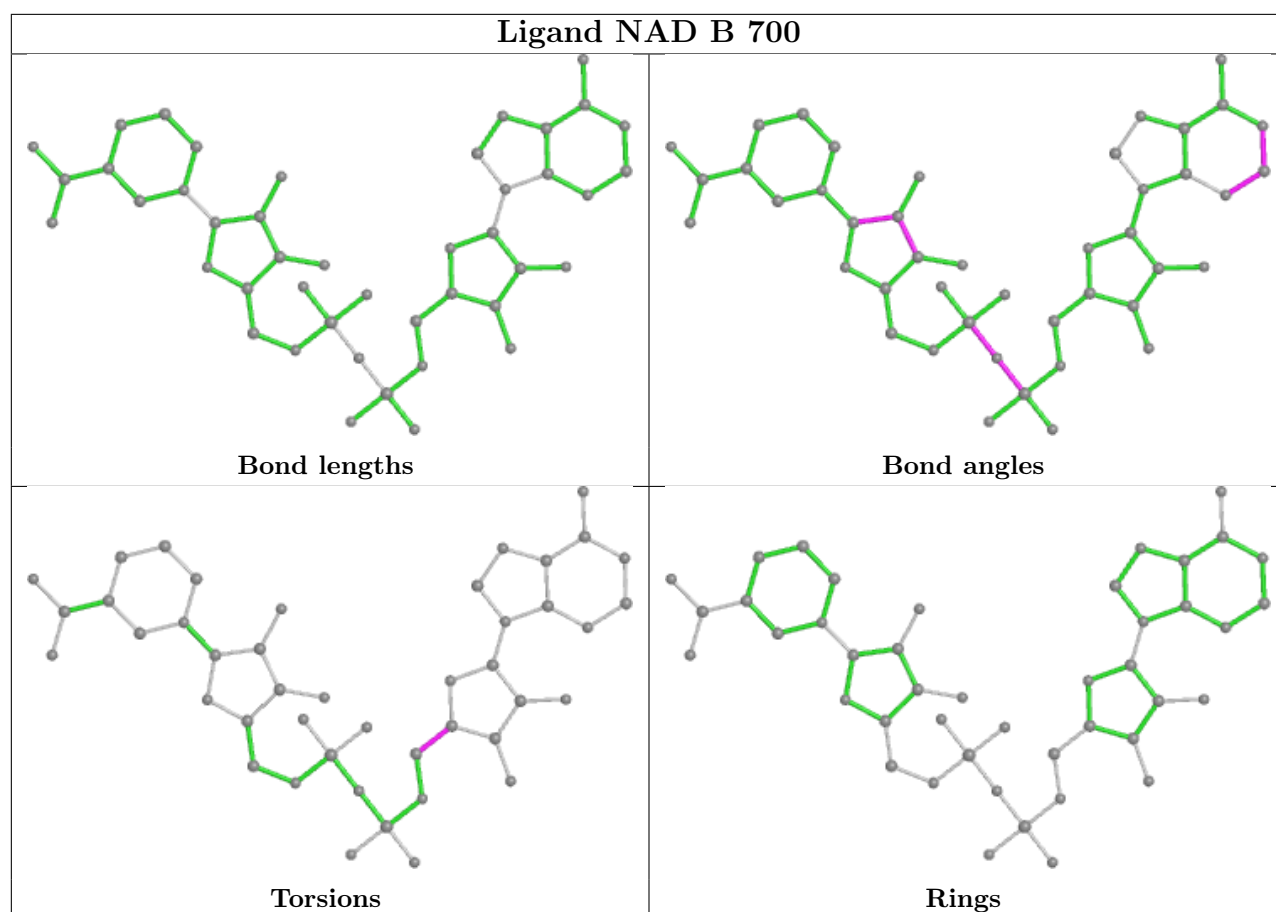
There are no ring outliers.

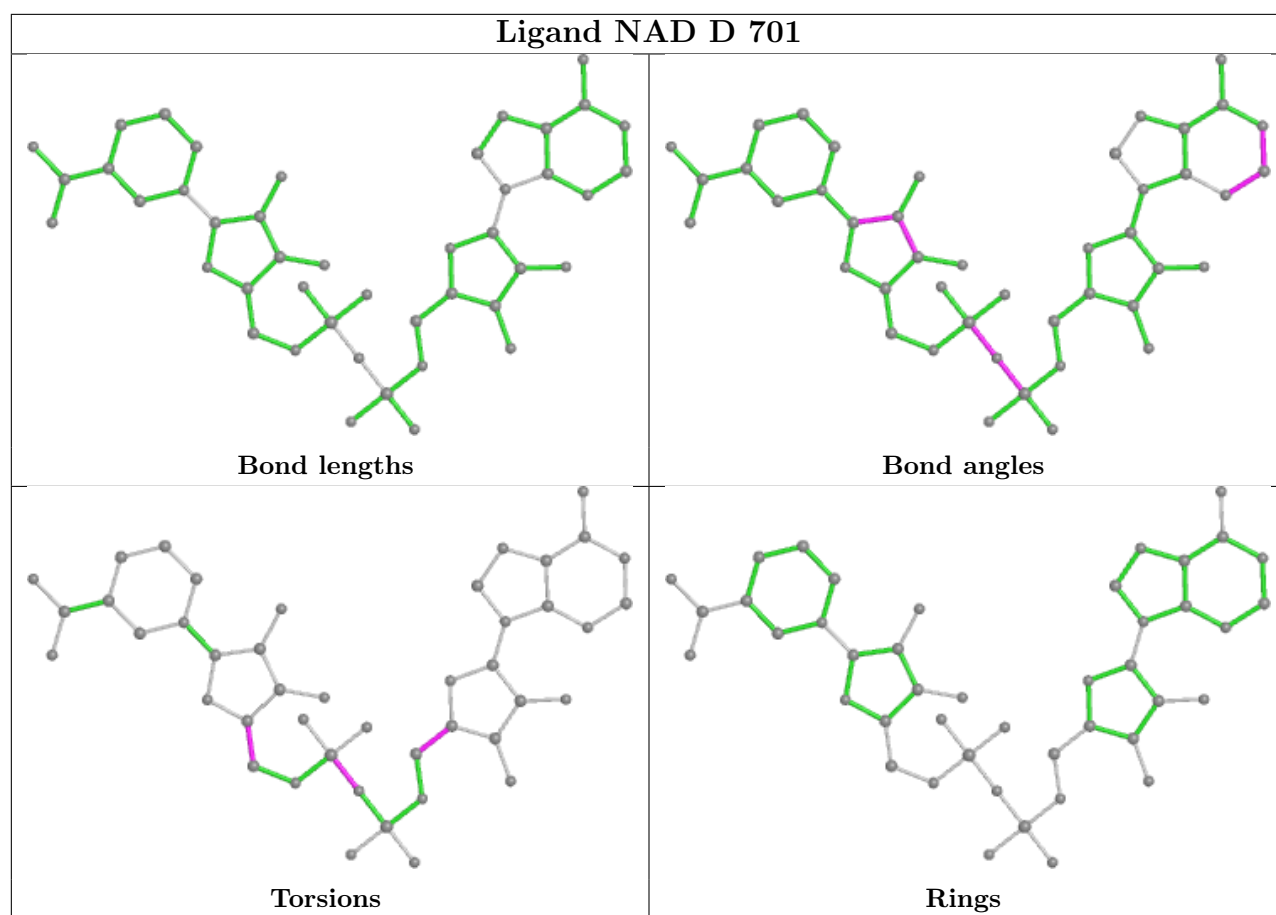
3 monomers are involved in 6 short contacts:

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

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.42	65 (7%) 12 19	14, 55, 97, 118	0
1	C	822/842 (97%)	0.82	126 (15%) 2 3	16, 61, 135, 187	0
1	E	822/842 (97%)	2.55	430 (52%) 0 0	16, 136, 189, 262	0
2	B	207/207 (100%)	0.09	6 (2%) 51 62	14, 27, 61, 94	0
2	D	207/207 (100%)	0.08	7 (3%) 45 57	12, 25, 57, 89	0
2	F	207/207 (100%)	0.08	8 (3%) 39 52	17, 29, 62, 108	0
All	All	3087/3147 (98%)	1.03	642 (20%) 1 1	12, 57, 169, 262	0

All (642) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	108	HIS	13.4
1	E	314	LEU	12.9
1	E	195	GLU	12.7
1	E	67	GLY	12.6
1	E	157	ILE	11.3
1	E	789	GLY	10.9
1	E	167	LEU	10.9
1	E	356	LEU	9.9
1	E	760	ARG	9.8
1	E	553	PRO	9.7
1	E	289	MET	9.6
1	E	166	GLU	9.5
1	E	311	GLU	9.5
1	E	766	PHE	9.4
1	E	196	VAL	9.3
1	E	310	ASP	9.2
1	E	367	ILE	9.0
1	E	315	GLU	8.6
1	E	761	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
1	E	759	GLN	8.6
1	E	361	ALA	8.5
1	E	78	TYR	8.3
1	E	498	ALA	8.2
1	C	498	ALA	8.0
1	E	268	PRO	8.0
1	C	522	MET	8.0
1	C	495	VAL	8.0
1	E	232	LYS	7.9
1	E	26	ALA	7.9
1	E	169	VAL	7.9
1	E	231	LYS	7.9
1	E	192	TYR	7.9
1	E	81	MET	7.8
1	E	48	ALA	7.8
1	C	502	PRO	7.8
1	E	156	VAL	7.8
1	E	294	ASP	7.7
1	C	499	ASN	7.7
1	E	41	GLN	7.7
1	E	128	VAL	7.7
1	E	175	TYR	7.7
1	E	281	ILE	7.7
1	E	262	THR	7.6
1	E	741	GLY	7.5
1	E	254	THR	7.5
1	E	129	VAL	7.4
1	E	240	MET	7.4
1	E	107	GLY	7.3
1	E	258	THR	7.3
1	E	163	ALA	7.3
1	E	464	LEU	7.2
1	E	194	ASP	7.2
1	E	308	LYS	7.2
1	E	179	ALA	7.1
1	E	499	ASN	7.1
1	C	550	ALA	7.1
1	E	160	VAL	7.1
1	E	106	PRO	7.1
1	E	91	GLN	7.0
1	E	211	PHE	7.0
1	E	267	LYS	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	321	LYS	7.0
1	E	755	VAL	6.9
1	C	291	PHE	6.9
1	E	203	TYR	6.9
1	E	86	VAL	6.9
1	E	790	GLY	6.7
1	E	233	PHE	6.6
1	E	332	ASP	6.5
1	E	34	THR	6.5
1	E	212	GLY	6.5
1	E	740	VAL	6.4
1	E	307	LEU	6.4
1	E	38	SER	6.4
1	E	763	THR	6.4
1	E	168	GLN	6.3
1	E	298	VAL	6.3
1	E	762	GLY	6.3
1	E	188	ILE	6.3
1	E	218	TRP	6.2
1	E	342	LEU	6.1
1	E	111	PHE	6.1
1	E	420	PRO	6.1
1	E	770	ALA	6.0
1	E	187	VAL	6.0
1	E	745	SER	6.0
1	E	32	LYS	5.9
1	C	67	GLY	5.9
1	E	127	VAL	5.8
1	E	131	THR	5.8
1	E	137	VAL	5.8
1	E	98	PHE	5.8
1	A	483	PHE	5.7
1	E	554	LEU	5.7
1	E	76	SER	5.7
1	E	230	ALA	5.7
1	E	239	LYS	5.7
1	E	256	LYS	5.7
1	E	269	LEU	5.7
1	E	317	LYS	5.7
1	C	264	ALA	5.7
1	E	162	ARG	5.7
1	E	266	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	358	GLU	5.6
1	E	282	PHE	5.6
1	E	306	VAL	5.6
1	C	167	LEU	5.6
1	E	88	GLU	5.6
1	E	316	GLY	5.5
1	E	185	VAL	5.5
1	E	216	HIS	5.5
1	E	312	LYS	5.5
1	E	737	GLU	5.5
1	E	335	LEU	5.5
1	E	299	LEU	5.5
2	D	489	ALA	5.5
1	C	306	VAL	5.5
1	E	422	LYS	5.5
1	E	442	VAL	5.5
1	E	80	GLU	5.4
1	E	90	LYS	5.4
1	E	497	ASN	5.4
1	E	143	LEU	5.4
1	E	77	LEU	5.4
1	E	496	LYS	5.4
1	E	197	LEU	5.3
1	E	89	ILE	5.3
1	E	193	ALA	5.3
1	E	366	CYS	5.3
1	E	360	PRO	5.3
1	E	764	PRO	5.3
1	E	178	PHE	5.3
1	E	546	GLU	5.3
1	E	495	VAL	5.3
1	C	504	LEU	5.3
1	E	110	ASP	5.2
1	E	180	ARG	5.2
1	C	553	PRO	5.2
1	E	421	GLY	5.2
1	E	261	ASP	5.2
1	E	263	ASP	5.2
1	C	513	LYS	5.2
1	E	237	LYS	5.2
1	E	96	ASN	5.2
1	C	496	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	501	LEU	5.1
2	B	489	ALA	5.1
1	E	375	LYS	5.1
1	E	739	ALA	5.1
1	C	252	PRO	5.0
1	E	747	LEU	5.0
1	E	255	LYS	5.0
1	E	436	LEU	5.0
1	C	311	GLU	5.0
1	E	182	VAL	5.0
1	E	278	LEU	5.0
1	E	419	VAL	4.9
1	E	210	ALA	4.9
1	C	544	ASP	4.9
1	E	215	LEU	4.9
1	E	297	PRO	4.9
1	E	453	ILE	4.9
1	E	69	THR	4.9
1	E	245	TRP	4.9
1	E	392	GLY	4.9
1	C	497	ASN	4.9
1	E	309	GLY	4.8
1	E	7	ASP	4.8
1	E	37	ASP	4.8
1	E	756	SER	4.8
1	E	794	PRO	4.8
1	E	758	GLU	4.8
1	C	233	PHE	4.8
1	E	109	VAL	4.8
1	C	290	ASN	4.8
1	E	222	ILE	4.8
1	A	196	VAL	4.7
1	E	343	PRO	4.7
1	E	503	LYS	4.7
1	E	277	ILE	4.7
1	E	260	LYS	4.7
1	A	361	ALA	4.7
1	E	47	SER	4.7
1	E	40	VAL	4.7
1	E	500	ASP	4.7
1	A	464	LEU	4.7
1	C	268	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	441	PHE	4.7
1	C	267	LYS	4.6
1	E	135	VAL	4.6
1	E	29	ASP	4.6
1	E	329	PRO	4.6
1	E	220	PHE	4.6
1	E	522	MET	4.6
1	E	42	ARG	4.6
1	E	757	GLU	4.6
1	E	736	PRO	4.6
1	E	444	PRO	4.5
1	E	265	GLU	4.5
1	E	200	VAL	4.5
1	E	738	GLN	4.5
1	E	304	GLU	4.5
1	E	290	ASN	4.5
1	E	389	SER	4.5
1	C	494	GLU	4.4
1	E	469	LEU	4.4
1	E	25	ILE	4.4
1	C	500	ASP	4.4
1	C	262	THR	4.4
1	E	395	TYR	4.4
1	E	471	THR	4.4
1	E	20	ARG	4.4
1	E	348	ALA	4.4
1	E	242	ASP	4.4
1	E	158	ASN	4.4
1	E	779	GLY	4.4
1	E	743	ILE	4.4
1	E	291	PHE	4.4
1	E	742	GLY	4.3
1	E	324	MET	4.3
1	E	795	GLN	4.3
1	E	68	ILE	4.3
1	E	46	ILE	4.3
1	C	547	HIS	4.3
1	E	555	LYS	4.2
1	C	391	LYS	4.2
1	E	257	TRP	4.2
1	E	525	SER	4.2
1	E	155	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	173	ASP	4.2
1	E	504	LEU	4.2
1	E	339	VAL	4.2
1	C	523	SER	4.2
1	E	83	ASP	4.2
1	E	36	THR	4.1
1	E	164	LEU	4.1
1	E	793	PHE	4.1
1	A	28	VAL	4.1
1	E	401	PHE	4.1
1	E	784	LEU	4.1
1	E	320	LEU	4.1
1	E	273	PHE	4.1
1	E	548	ASP	4.1
1	E	154	VAL	4.1
1	A	480	VAL	4.1
1	C	298	VAL	4.1
1	E	217	GLY	4.1
1	E	744	TYR	4.1
1	C	265	GLU	4.1
1	C	310	ASP	4.0
2	F	489	ALA	4.0
1	A	198	GLY	4.0
1	E	791	GLN	4.0
1	E	3	ALA	4.0
1	E	100	ILE	4.0
1	E	465	LYS	4.0
1	E	183	GLU	4.0
1	E	479	LYS	4.0
1	E	456	LEU	4.0
1	E	502	PRO	4.0
1	E	201	GLN	4.0
1	E	301	GLU	4.0
1	E	207	GLY	3.9
1	E	440	ARG	3.9
1	E	492	ALA	3.9
1	C	168	GLN	3.9
1	E	147	LEU	3.9
1	E	778	PHE	3.9
1	E	362	ASP	3.9
1	C	313	ASP	3.9
1	A	360	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	301	GLU	3.9
1	E	292	LYS	3.9
1	E	483	PHE	3.8
1	E	105	SER	3.8
1	E	276	PHE	3.8
1	E	391	LYS	3.8
1	C	28	VAL	3.8
1	E	209	VAL	3.8
1	E	235	VAL	3.8
1	E	783	GLU	3.8
1	C	236	ASP	3.8
1	C	251	ASN	3.8
1	E	418	TYR	3.8
1	E	302	LYS	3.8
1	E	328	LEU	3.8
1	E	243	ARG	3.7
1	E	253	LYS	3.7
1	C	235	VAL	3.7
1	E	27	HIS	3.7
1	C	761	PRO	3.7
1	E	455	GLY	3.7
1	E	767	THR	3.7
1	C	501	LEU	3.7
1	C	314	LEU	3.6
1	C	321	LYS	3.6
2	F	490	ARG	3.6
1	E	85	ASP	3.6
1	A	111	PHE	3.6
1	E	165	LEU	3.6
1	A	107	GLY	3.6
1	E	481	MET	3.6
1	E	227	THR	3.6
1	A	67	GLY	3.6
1	E	340	LEU	3.6
1	C	232	LYS	3.6
1	E	293	LYS	3.6
1	E	288	ILE	3.5
1	C	552	VAL	3.5
2	F	461	ASP	3.5
1	E	28	VAL	3.5
1	E	104	ASP	3.5
1	E	138	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	358	GLU	3.5
1	E	295	GLU	3.5
1	E	454	ILE	3.4
2	D	498	LEU	3.4
1	E	176	GLN	3.4
1	E	437	MET	3.4
1	E	466	THR	3.4
1	E	353	ALA	3.4
1	E	480	VAL	3.4
1	E	754	VAL	3.4
1	E	286	THR	3.4
1	E	305	ILE	3.4
1	E	189	VAL	3.4
1	E	177	THR	3.4
1	E	287	ALA	3.4
1	C	263	ASP	3.4
1	E	476	HIS	3.4
1	E	161	ASP	3.3
1	E	357	TYR	3.3
1	E	368	ALA	3.3
1	C	269	LEU	3.3
1	E	280	PRO	3.3
1	E	748	ASN	3.3
1	E	494	GLU	3.3
1	E	380	LEU	3.3
1	E	542	LEU	3.3
1	C	503	LYS	3.3
1	C	7	ASP	3.3
1	A	786	GLN	3.3
1	E	296	ILE	3.3
1	E	780	PHE	3.3
1	E	130	ASP	3.2
1	E	445	ILE	3.2
1	E	510	ARG	3.2
1	C	551	GLY	3.2
1	E	82	SER	3.2
1	C	11	SER	3.2
1	C	755	VAL	3.2
1	E	322	VAL	3.2
1	C	29	ASP	3.2
1	C	528	HIS	3.2
1	E	30	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	264	ALA	3.2
1	A	454	ILE	3.2
1	A	495	VAL	3.2
1	E	470	THR	3.2
1	C	482	LYS	3.2
1	A	48	ALA	3.2
1	E	8	GLN	3.2
1	E	94	ASP	3.2
1	E	93	THR	3.2
1	E	24	VAL	3.2
1	E	523	SER	3.2
1	C	318	ALA	3.2
1	E	252	PRO	3.2
1	C	261	ASP	3.2
1	C	302	LYS	3.2
1	E	551	GLY	3.2
1	C	546	GLU	3.1
1	C	295	GLU	3.1
1	E	341	HIS	3.1
1	C	277	ILE	3.1
1	A	129	VAL	3.1
1	C	84	GLU	3.1
1	C	303	LEU	3.1
1	E	159	LYS	3.1
1	C	99	LEU	3.1
1	E	472	SER	3.1
1	A	46	ILE	3.1
1	A	157	ILE	3.1
1	E	118	ALA	3.1
1	C	299	LEU	3.1
1	E	519	LEU	3.1
1	E	136	CYS	3.1
1	C	266	GLY	3.1
1	E	132	ILE	3.1
1	E	451	GLY	3.1
2	D	461	ASP	3.0
1	A	400	VAL	3.0
1	C	312	LYS	3.0
1	E	337	MET	3.0
1	C	549	HIS	3.0
1	E	769	LYS	3.0
1	C	740	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	319	LEU	3.0
1	E	338	ILE	3.0
1	A	499	ASN	3.0
1	C	108	HIS	3.0
1	E	796	MET	3.0
1	C	555	LYS	3.0
1	E	390	ASP	2.9
1	E	351	TYR	2.9
1	E	31	GLY	2.9
1	E	325	ARG	2.9
1	E	151	ILE	2.9
1	C	111	PHE	2.9
1	E	221	THR	2.9
1	E	285	PHE	2.9
1	C	231	LYS	2.9
1	E	275	MET	2.9
1	E	547	HIS	2.9
1	E	423	LYS	2.9
1	A	82	SER	2.9
1	E	10	ARG	2.9
1	E	427	PHE	2.8
1	E	443	GLU	2.8
1	C	362	ASP	2.8
1	E	146	ALA	2.8
1	A	392	GLY	2.8
1	E	44	GLY	2.8
1	C	294	ASP	2.8
1	E	334	LEU	2.8
1	E	371	ASN	2.8
1	E	323	VAL	2.8
1	E	205	ALA	2.8
1	C	784	LEU	2.8
1	E	35	LEU	2.8
1	E	234	GLY	2.8
1	E	359	GLY	2.8
1	A	310	ASP	2.8
2	B	461	ASP	2.8
1	A	90	LYS	2.8
1	E	284	LEU	2.8
1	C	526	GLY	2.8
1	E	133	GLU	2.8
1	A	264	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	97	SER	2.8
1	E	433	ARG	2.8
2	B	555	ILE	2.8
1	E	552	VAL	2.7
2	B	556	LEU	2.7
1	E	101	ASN	2.7
1	E	354	GLU	2.7
1	E	9	MET	2.7
1	E	241	MET	2.7
1	A	7	ASP	2.7
1	C	305	ILE	2.7
1	E	84	GLU	2.7
1	A	29	ASP	2.7
1	E	14	ASP	2.7
1	E	186	ASN	2.7
1	E	398	GLY	2.7
1	E	79	SER	2.7
2	F	501	VAL	2.7
1	C	763	THR	2.7
1	C	238	ALA	2.7
1	E	393	ARG	2.7
1	A	127	VAL	2.7
1	A	156	VAL	2.7
1	C	509	LYS	2.7
1	A	237	LYS	2.7
1	A	359	GLY	2.6
1	E	333	ALA	2.6
1	A	108	HIS	2.6
1	E	347	THR	2.6
1	E	474	THR	2.6
2	F	499	LEU	2.6
1	E	236	ASP	2.6
2	F	459	SER	2.6
1	E	259	ASN	2.6
1	E	369	ILE	2.6
1	E	229	TYR	2.6
2	B	490	ARG	2.6
2	F	471	ILE	2.6
1	E	404	THR	2.6
1	E	202	VAL	2.6
1	E	394	PHE	2.6
1	E	114	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	43	ALA	2.6
1	E	313	ASP	2.6
1	C	300	LEU	2.6
1	E	379	MET	2.6
1	E	746	VAL	2.6
1	A	194	ASP	2.6
1	A	375	LYS	2.6
1	A	485	VAL	2.5
1	C	2	VAL	2.5
1	E	365	ASN	2.5
1	E	144	ARG	2.5
1	E	23	SER	2.5
1	E	73	THR	2.5
1	E	15	LYS	2.5
1	A	553	PRO	2.5
1	A	391	LYS	2.5
1	E	751	ARG	2.5
2	B	471	ILE	2.5
1	A	84	GLU	2.5
1	C	293	LYS	2.5
1	E	435	VAL	2.5
1	E	272	ALA	2.5
1	E	6	VAL	2.4
1	E	505	VAL	2.4
1	E	785	ARG	2.4
1	E	399	ARG	2.4
1	C	308	LYS	2.4
1	C	485	VAL	2.4
1	E	452	ASN	2.4
1	C	254	THR	2.4
1	C	19	VAL	2.4
1	E	153	PRO	2.4
1	E	473	GLU	2.4
1	C	744	TYR	2.4
1	E	113	SER	2.4
1	E	364	ALA	2.4
1	E	103	ILE	2.4
1	A	291	PHE	2.4
1	C	5	THR	2.4
1	C	100	ILE	2.4
1	C	292	LYS	2.4
1	E	410	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	521	TYR	2.4
2	D	471	ILE	2.4
2	D	490	ARG	2.4
1	E	303	LEU	2.4
1	E	125	ALA	2.4
1	A	738	GLN	2.4
1	E	493	VAL	2.4
1	E	213	SER	2.4
1	E	372	CYS	2.4
1	E	92	LYS	2.3
1	E	171	LYS	2.3
1	E	223	ARG	2.3
1	A	453	ILE	2.3
1	C	554	LEU	2.3
1	A	5	THR	2.3
1	A	86	VAL	2.3
1	A	419	VAL	2.3
1	C	609	ARG	2.3
1	E	75	ILE	2.3
1	E	99	LEU	2.3
1	E	300	LEU	2.3
1	E	122	THR	2.3
1	A	362	ASP	2.3
1	C	493	VAL	2.3
1	E	397	PHE	2.3
1	E	134	GLY	2.3
1	E	781	THR	2.3
1	C	315	GLU	2.3
1	A	233	PHE	2.3
1	C	169	VAL	2.3
1	C	260	LYS	2.3
1	E	731	VAL	2.3
1	E	374	PRO	2.3
1	E	412	ARG	2.3
1	C	529	ILE	2.3
1	C	37	ASP	2.3
1	C	510	ARG	2.3
1	E	352	ARG	2.3
1	C	422	LYS	2.3
1	E	244	LEU	2.3
1	E	344	SER	2.3
1	E	381	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	42	ARG	2.3
1	E	549	HIS	2.3
1	A	199	ASP	2.3
1	E	545	LEU	2.2
1	A	417	ASN	2.2
1	E	18	ASN	2.2
1	E	19	VAL	2.2
1	A	420	PRO	2.2
1	C	506	GLU	2.2
1	C	237	LYS	2.2
1	C	548	ASP	2.2
1	A	16	VAL	2.2
1	C	738	GLN	2.2
1	C	766	PHE	2.2
1	A	293	LYS	2.2
1	E	485	VAL	2.2
1	E	225	PHE	2.2
1	C	258	THR	2.2
1	A	433	ARG	2.2
1	E	228	ARG	2.2
1	C	229	TYR	2.2
1	C	556	ILE	2.2
1	C	198	GLY	2.2
1	E	400	VAL	2.2
1	E	4	PHE	2.2
1	E	5	THR	2.2
1	E	402	ALA	2.2
1	E	468	THR	2.2
1	E	39	LEU	2.2
1	E	511	LEU	2.2
2	D	556	LEU	2.2
1	C	454	ILE	2.1
1	A	313	ASP	2.1
1	C	525	SER	2.1
1	C	154	VAL	2.1
1	E	121	VAL	2.1
1	C	287	ALA	2.1
1	E	814	LYS	2.1
1	C	453	ILE	2.1
1	E	11	SER	2.1
1	A	294	ASP	2.1
1	E	413	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	2.1
1	C	307	LEU	2.1
1	E	123	ASP	2.1
1	A	109	VAL	2.1
1	E	318	ALA	2.1
1	A	212	GLY	2.1
1	E	558	PRO	2.1
1	E	556	ILE	2.1
1	A	496	LYS	2.1
1	E	199	ASP	2.1
1	E	21	ASN	2.1
1	A	124	GLY	2.1
1	C	106	PRO	2.1
1	C	511	LEU	2.1
1	E	460	ASP	2.1
1	C	325	ARG	2.1
1	E	609	ARG	2.1
1	E	250	PHE	2.1
2	D	537	LEU	2.0
1	A	713	THR	2.0
1	E	33	SER	2.0
1	E	526	GLY	2.0
1	A	442	VAL	2.0
1	C	400	VAL	2.0
1	E	735	CYS	2.0
1	A	389	SER	2.0
1	C	759	GLN	2.0
1	E	349	GLN	2.0
1	A	209	VAL	2.0
1	A	211	PHE	2.0
1	C	441	PHE	2.0
1	C	378	LEU	2.0
1	E	70	ILE	2.0
2	F	555	ILE	2.0
1	E	219	ALA	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( $\text{\AA}^2$ )	Q<0.9
1	DDE	E	699	20/21	0.92	0.21	38,73,107,109	0
1	DDE	C	699	20/21	0.93	0.21	29,64,106,111	0
1	DDE	A	699	10/21	0.95	0.14	45,60,66,70	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

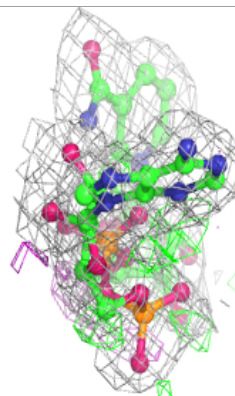
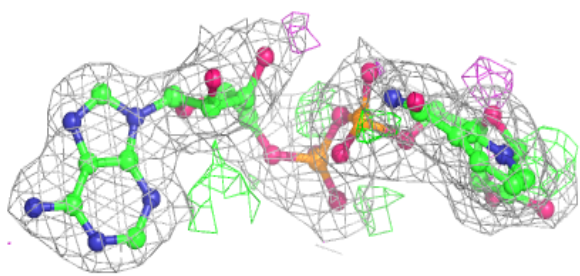
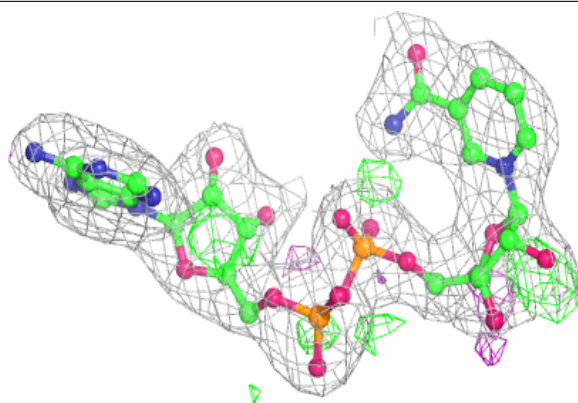
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.95	0.15	11,32,48,56	0
3	NAD	D	701	44/44	0.96	0.15	7,24,49,51	0
3	NAD	B	700	44/44	0.96	0.15	17,28,45,62	0

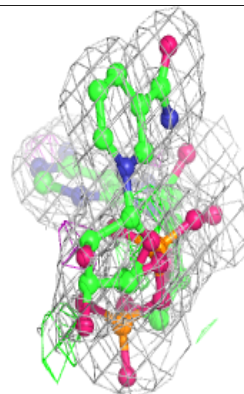
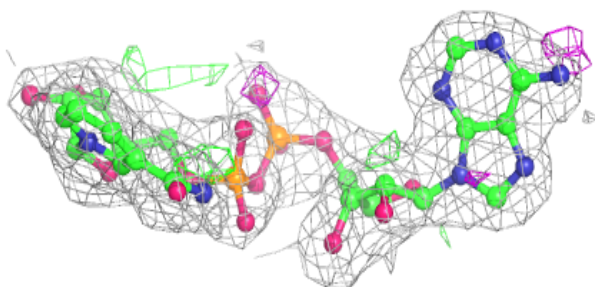
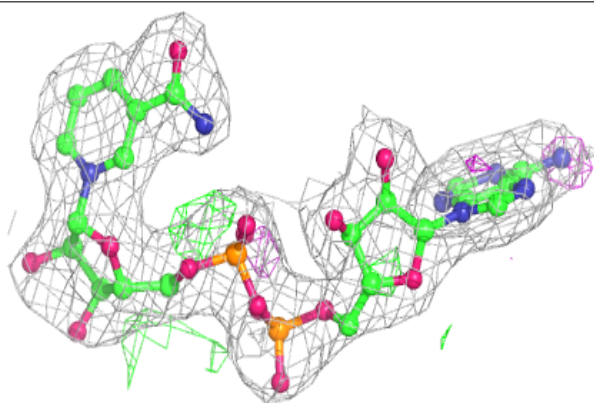
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

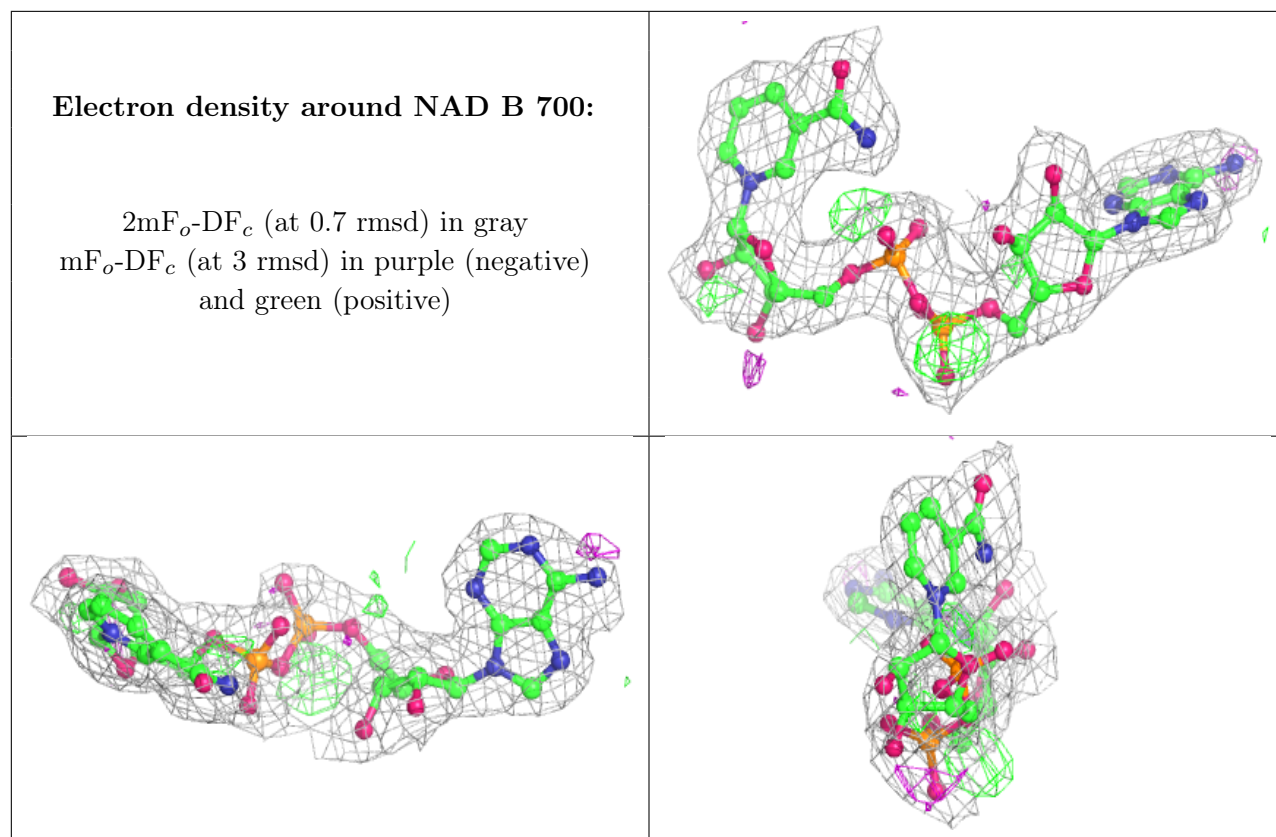
**Electron density around NAD F 702:**

$2mF_o-DF_c$  (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.