



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:02 AM EDT

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

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

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

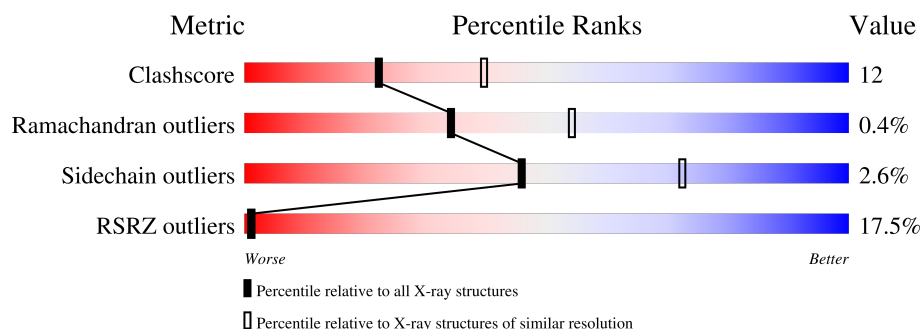
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>5%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	C	842	<div> <div>14%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	E	842	<div> <div>44%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>
2	B	207	<div> <div>%</div> <div>86%</div> <div>14%</div> <div></div> </div>
2	D	207	<div> <div>%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
2	F	207	<div> <div>%</div> <div>86%</div> <div>13%</div> <div></div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor 2.

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

- Molecule 2 is a protein called Exotoxin A.

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

There are 12 discrepancies between the modelled and reference sequences:

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

- # NAD

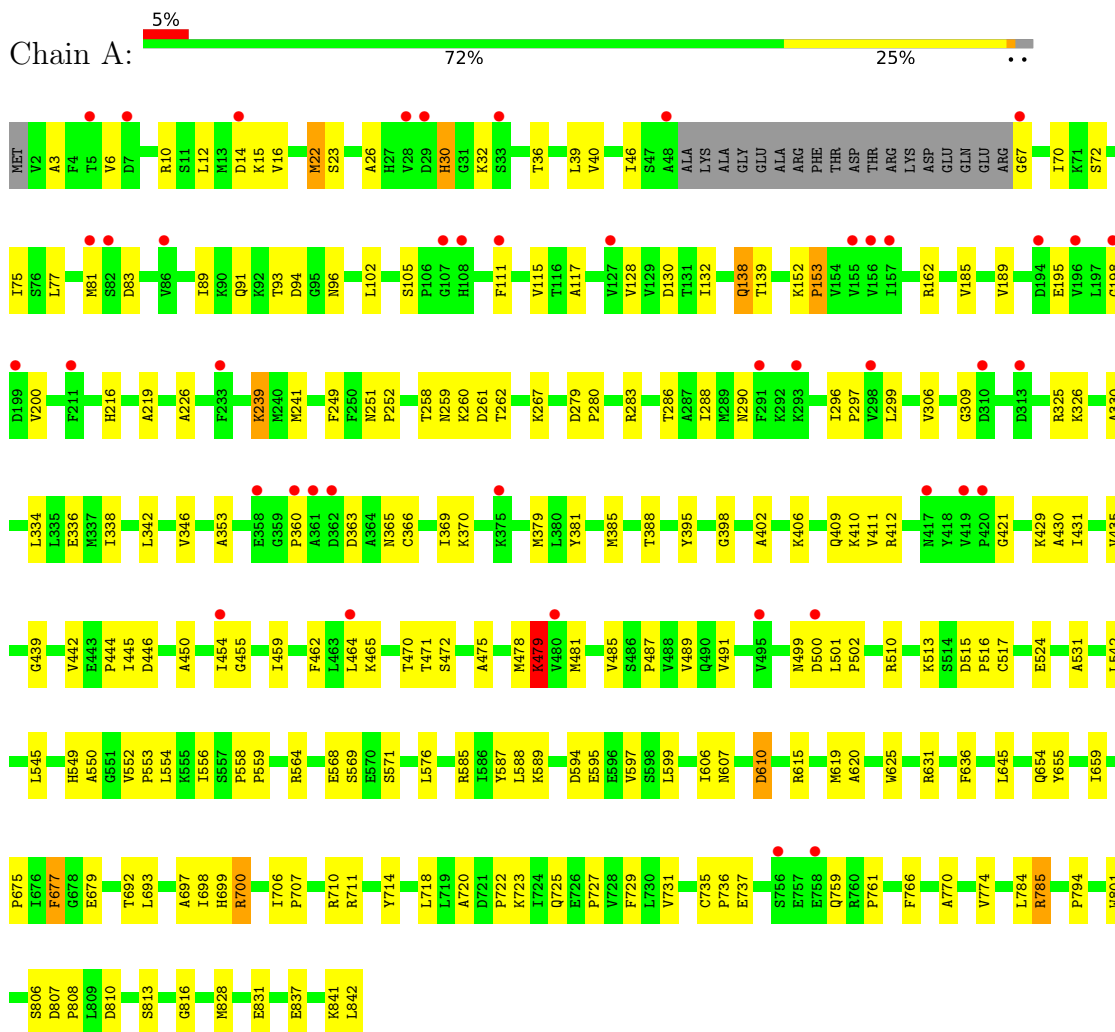
- Molecule 4 is water.

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

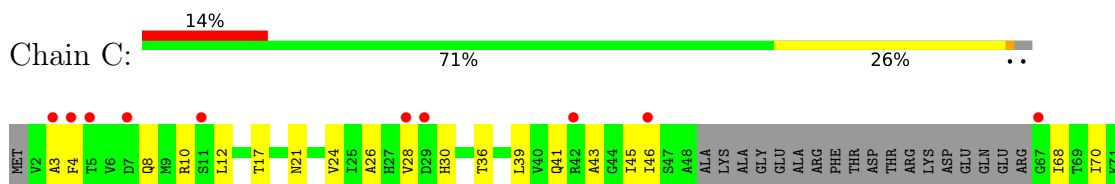
### 3 Residue-property plots

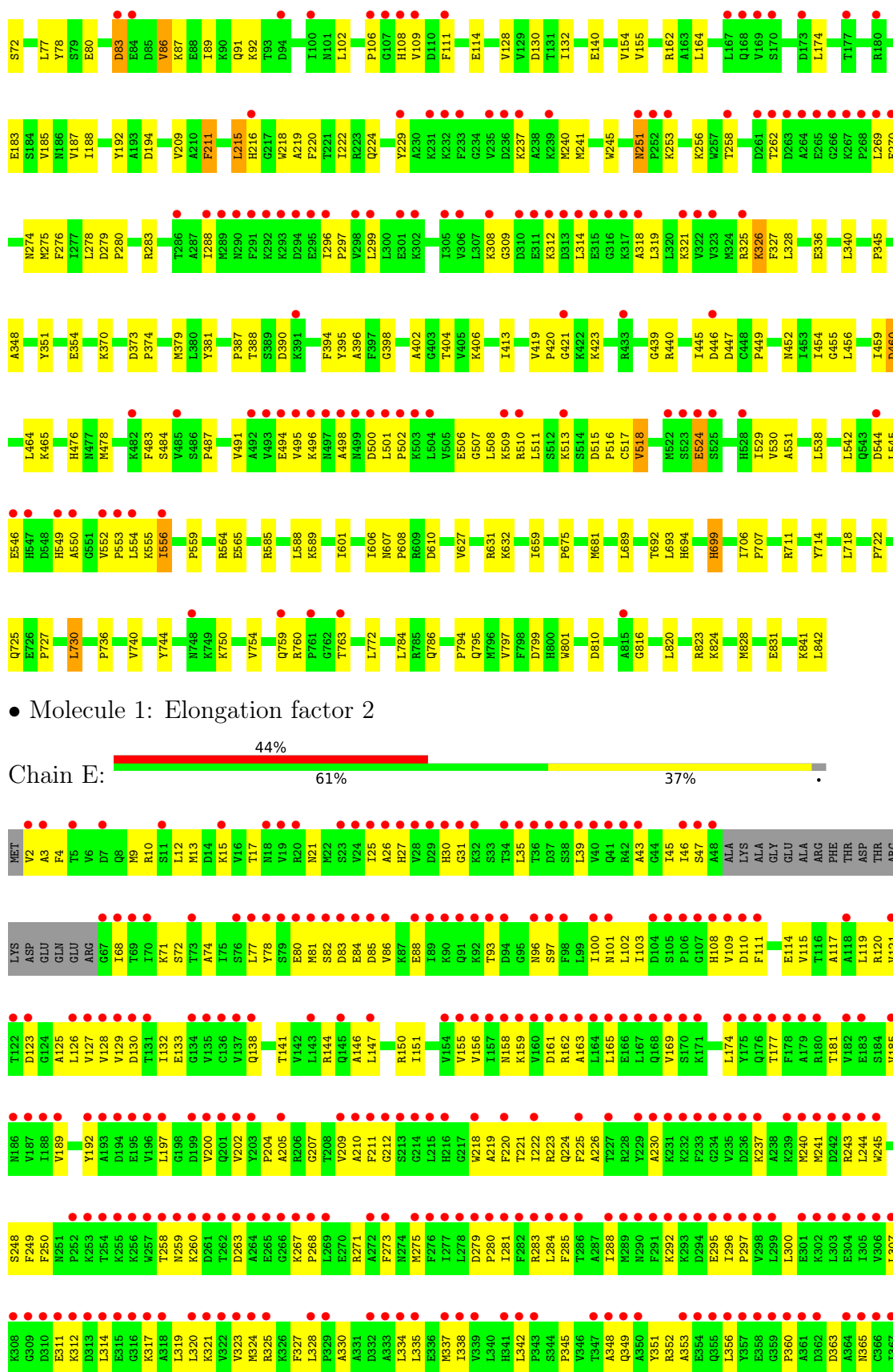
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

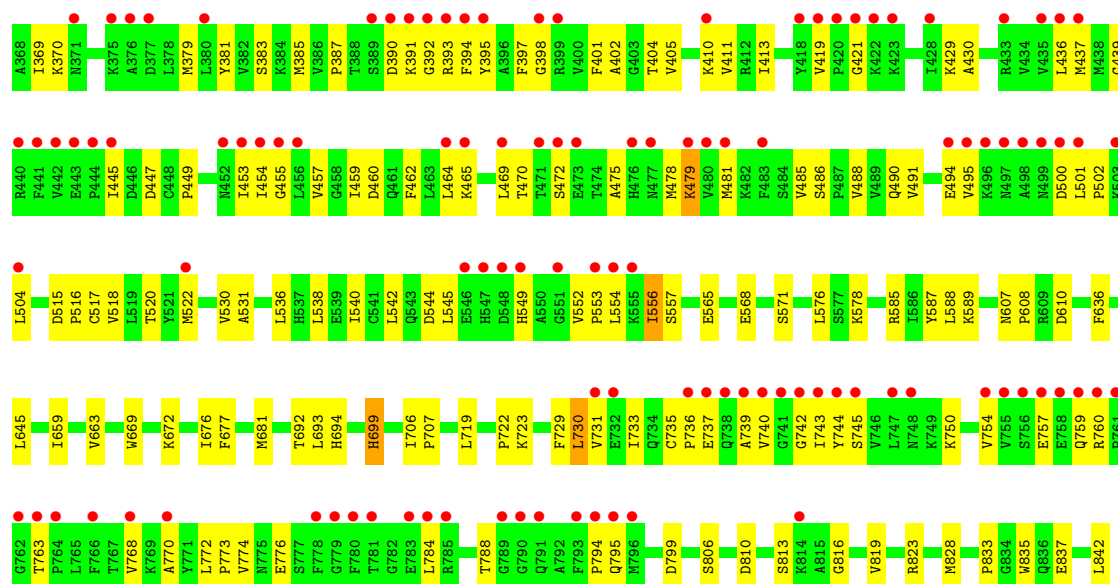
#### • Molecule 1: Elongation factor 2



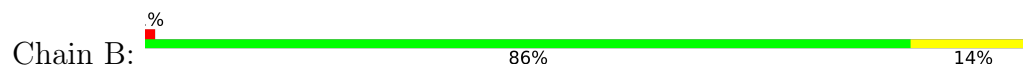
#### • Molecule 1: Elongation factor 2



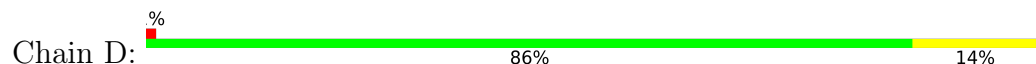




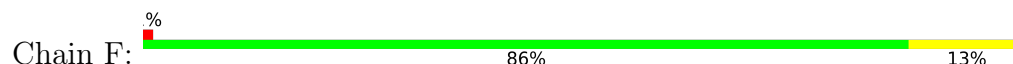
• Molecule 2: Exotoxin A



• 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, $\alpha$ , $\beta$ , $\gamma$	329.44Å 68.16Å 191.63Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	24.99 – 2.50 24.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.99-2.50) 99.0 (24.99-2.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.214 , 0.256 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

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

<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: 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	0.21	0/6517	0.40	1/8823 (0.0%)
1	C	0.21	0/6517	0.40	0/8823
1	E	0.21	0/6517	0.38	0/8823
2	B	0.21	0/1634	0.40	0/2225
2	D	0.21	0/1623	0.41	0/2211
2	F	0.21	0/1623	0.39	0/2211
All	All	0.21	0/24431	0.39	1/33116 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	GLY	N-CA-C	-5.72	98.79	113.10

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	145	0
1	C	6415	0	6488	148	0
1	E	6415	0	6488	226	0
2	B	1592	0	1554	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1584	0	1541	16	0
2	F	1584	0	1541	19	0
3	B	44	0	26	1	0
3	D	44	0	26	1	0
3	F	44	0	26	2	0
4	A	109	0	0	2	0
4	B	116	0	0	1	0
4	C	77	0	0	0	0
4	D	142	0	0	2	0
4	E	60	0	0	1	0
4	F	88	0	0	0	0
All	All	24719	0	24162	567	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 (567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:ARG:HG2	1:A:785:ARG:HH11	1.18	1.02
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.44	0.98
1:C:404:THR:HG22	1:C:449:PRO:HA	1.48	0.95
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.54	0.89
1:C:694:HIS:CE1	1:C:699:DDE:HD2	2.09	0.88
1:E:391:LYS:HG3	1:E:392:GLY:H	1.38	0.88
1:C:759:GLN:HG2	1:C:760:ARG:H	1.43	0.84
2:B:490:ARG:HH22	2:B:492[B]:ARG:HH21	1.19	0.84
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.60	0.84
1:A:258:THR:HG22	1:A:260:LYS:H	1.43	0.83
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.58	0.82
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.61	0.82
1:C:132:ILE:HD12	1:C:132:ILE:H	1.46	0.81
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.64	0.79
1:E:404:THR:HG22	1:E:449:PRO:HA	1.64	0.79
1:A:470:THR:HG22	1:A:472:SER:H	1.47	0.78
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.66	0.78
1:E:556:ILE:HG22	1:E:557:SER:H	1.50	0.76
1:A:785:ARG:HH11	1:A:785:ARG:CG	1.99	0.75
1:C:823:ARG:HA	1:C:828:MET:HE3	1.69	0.74
1:A:568:GLU:HG3	1:A:723:LYS:HD2	1.69	0.73
2:B:490:ARG:HH22	2:B:492[B]:ARG:NH2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:HG21	1:A:475:ALA:HB3	1.69	0.72
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.72	0.71
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.26	0.70
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.73	0.70
1:C:379:MET:HB3	1:C:478:MET:HE2	1.73	0.70
1:E:141:THR:HA	1:E:144:ARG:HH11	1.57	0.69
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.75	0.69
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.74	0.68
1:C:699:DDE:HAC2	1:C:699:DDE:NAD	2.08	0.68
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.28	0.68
1:C:529:ILE:HG22	1:C:530:VAL:H	1.58	0.68
1:C:465:LYS:HE3	1:C:517:CYS:SG	2.34	0.68
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.74	0.67
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.75	0.67
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.76	0.67
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.76	0.67
1:C:68:ILE:HG12	1:C:390:ASP:HB2	1.77	0.66
1:C:70:ILE:HG22	1:C:388:THR:HG22	1.77	0.66
1:A:810:ASP:O	1:A:816:GLY:HA3	1.96	0.66
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.78	0.65
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.79	0.65
1:C:70:ILE:O	1:C:440:ARG:HG2	1.97	0.64
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.78	0.64
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.79	0.64
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.64
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.80	0.64
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.79	0.64
2:F:490:ARG:HD3	2:F:492:ARG:HD3	1.79	0.63
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.81	0.63
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.80	0.63
2:F:517:THR:HG23	2:F:547:GLU:HA	1.79	0.63
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.78	0.63
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.34	0.63
1:C:396:ALA:HB3	1:C:456:LEU:HB2	1.81	0.62
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.64	0.62
1:A:283:ARG:HB3	1:A:299:LEU:HD21	1.82	0.62
1:A:381:TYR:O	1:A:398:GLY:HA3	1.98	0.62
1:C:419:VAL:HG12	1:C:421:GLY:H	1.65	0.62
1:A:697:ALA:HA	1:A:700:ARG:HD2	1.81	0.62
1:E:26:ALA:CB	1:E:128:VAL:HB	2.30	0.62
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASN:HB2	1:C:269:LEU:HD22	1.82	0.61
1:E:207:GLY:O	1:E:337:MET:HG2	1.99	0.61
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.81	0.61
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.82	0.61
1:C:374:PRO:O	1:C:404:THR:HG23	1.98	0.61
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.83	0.61
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.82	0.61
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.31	0.61
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.82	0.61
1:A:10:ARG:HH22	1:A:446:ASP:HB2	1.66	0.60
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.82	0.60
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.83	0.60
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.82	0.60
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.82	0.60
2:B:460:GLN:HG3	2:B:462:LEU:HD11	1.84	0.60
1:A:568:GLU:HG3	1:A:723:LYS:HG3	1.83	0.59
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.84	0.59
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.85	0.59
1:A:606:ILE:HD12	1:A:619:MET:HG2	1.82	0.59
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.42	0.59
1:C:106:PRO:HG3	1:C:114:GLU:HB3	1.84	0.59
2:D:488:ASP:HB2	2:D:490:ARG:H	1.67	0.59
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.84	0.59
2:B:490:ARG:NH2	2:B:492[B]:ARG:HH21	1.97	0.58
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.85	0.58
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.85	0.58
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.38	0.58
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.85	0.58
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.84	0.58
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.44	0.58
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.69	0.58
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.85	0.58
1:E:321:LYS:O	1:E:325:ARG:HG3	2.02	0.58
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.84	0.58
2:D:598:PRO:HG2	2:D:600:TYR:CE1	2.38	0.58
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.84	0.58
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.69	0.58
1:E:391:LYS:HG3	1:E:392:GLY:N	2.16	0.58
1:E:9:MET:O	1:E:13:MET:HG3	2.03	0.58
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.86	0.57
1:A:785:ARG:HG2	1:A:785:ARG:NH1	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:GLN:HG2	1:C:760:ARG:N	2.16	0.57
1:C:308:LYS:HE2	1:C:326:LYS:NZ	2.20	0.57
1:C:585:ARG:HB2	1:C:692:THR:OG1	2.05	0.57
1:E:150:ARG:HB3	1:E:351:TYR:HE1	1.69	0.57
1:A:138:GLN:HG3	1:A:139:THR:N	2.20	0.56
1:A:568:GLU:HG3	1:A:723:LYS:CD	2.35	0.56
1:E:349:GLN:O	1:E:370:LYS:HA	2.05	0.56
2:D:432:ARG:HD2	4:D:802:HOH:O	2.05	0.56
2:D:460:GLN:HG3	2:D:462:LEU:HD11	1.88	0.56
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.88	0.56
1:C:496:LYS:H	1:C:554:LEU:HD22	1.71	0.56
1:E:385:MET:HG2	1:E:465:LYS:HA	1.87	0.56
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.86	0.56
1:A:111:PHE:O	1:A:115:VAL:HG23	2.06	0.56
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.88	0.56
1:A:81:MET:O	1:A:96:ASN:HB3	2.05	0.56
1:A:198:GLY:O	1:A:200:VAL:HG23	2.06	0.56
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.87	0.56
1:C:314:LEU:HD22	1:C:318:ALA:HB1	1.87	0.56
1:C:529:ILE:HG22	1:C:530:VAL:N	2.21	0.56
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.88	0.56
1:A:10:ARG:NH2	1:A:446:ASP:H	2.04	0.55
1:A:569:SER:O	1:A:720:ALA:HB1	2.06	0.55
1:C:17:THR:HB	1:C:92:LYS:O	2.06	0.55
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.88	0.55
1:E:365:ASN:O	1:E:369:ILE:HG12	2.06	0.55
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.88	0.55
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.89	0.55
1:A:388:THR:HG21	1:A:395:TYR:CG	2.41	0.55
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.87	0.55
1:C:83:ASP:O	1:C:86:VAL:HG12	2.06	0.55
1:C:511:LEU:HG	1:C:518:VAL:HG11	1.88	0.55
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.89	0.55
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.89	0.55
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.41	0.55
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.88	0.55
1:E:784:LEU:HD12	4:E:850:HOH:O	2.07	0.55
1:A:16:VAL:HG21	1:A:450:ALA:O	2.07	0.54
1:E:226:ALA:O	1:E:230:ALA:HB2	2.07	0.54
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.07	0.54
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:TYR:O	1:E:398:GLY:HA3	2.07	0.54
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.89	0.54
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.90	0.54
1:A:200:VAL:HG12	1:A:200:VAL:O	2.07	0.54
1:C:279:ASP:O	1:C:283:ARG:HG2	2.07	0.54
1:E:296:ILE:O	1:E:300:LEU:HD13	2.08	0.54
1:A:654:GLN:HG2	1:A:655:TYR:CE1	2.43	0.54
1:A:258:THR:HG22	1:A:260:LYS:N	2.19	0.53
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.08	0.53
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.89	0.53
1:E:522:MET:HB2	2:F:490:ARG:NH2	2.23	0.53
1:A:365:ASN:O	1:A:369:ILE:HG13	2.09	0.53
1:E:810:ASP:O	1:E:816:GLY:HA3	2.08	0.53
1:A:117:ALA:HA	1:A:481:MET:SD	2.49	0.53
1:E:806:SER:HB2	1:E:813:SER:HB2	1.91	0.53
1:A:737:GLU:HB2	1:A:766:PHE:HE2	1.74	0.53
1:E:722:PRO:O	1:E:723:LYS:HD2	2.09	0.53
1:E:74:ALA:HA	1:E:102:LEU:O	2.09	0.53
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.90	0.53
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.89	0.53
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.90	0.53
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.44	0.53
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.39	0.53
1:C:183:GLU:O	1:C:187:VAL:HG23	2.09	0.53
1:E:21:ASN:HB2	1:E:123:ASP:OD1	2.09	0.53
2:B:470:TYR:CD2	3:B:700:NAD:H2D	2.44	0.52
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.90	0.52
1:A:806:SER:HB2	1:A:813:SER:HB2	1.91	0.52
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.90	0.52
1:E:538:LEU:O	1:E:542:LEU:HG	2.09	0.52
1:A:338:ILE:O	1:A:342:LEU:HB2	2.08	0.52
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.92	0.52
1:C:43:ALA:HB1	1:C:78:TYR:O	2.09	0.52
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.90	0.52
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.44	0.52
2:F:517:THR:CG2	2:F:547:GLU:HA	2.40	0.52
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.75	0.52
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.92	0.52
1:E:129:VAL:HG12	1:E:130:ASP:N	2.25	0.52
1:E:478:MET:O	1:E:479:LYS:C	2.48	0.52
1:C:810:ASP:O	1:C:816:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG22	1:A:75:ILE:HG21	1.90	0.51
1:A:675:PRO:HD3	1:A:714:TYR:CD1	2.45	0.51
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.92	0.51
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.45	0.51
1:E:419:VAL:HG12	1:E:421:GLY:H	1.75	0.51
1:C:274:ASN:HA	1:C:278:LEU:HB2	1.93	0.51
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.91	0.51
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.93	0.51
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.93	0.51
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.40	0.51
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.46	0.51
1:E:391:LYS:CG	1:E:392:GLY:H	2.18	0.51
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.92	0.51
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.74	0.51
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.93	0.51
1:C:736:PRO:O	1:C:740:VAL:HG23	2.11	0.51
1:E:25:ILE:HG13	1:E:125:ALA:HB1	1.93	0.51
1:E:750:LYS:HD2	1:E:776:GLU:O	2.11	0.51
1:E:165:LEU:HD23	1:E:317:LYS:HE2	1.93	0.50
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.93	0.50
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.26	0.50
1:E:410:LYS:HA	1:E:430:ALA:HA	1.94	0.50
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.47	0.50
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.93	0.50
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.41	0.50
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.92	0.50
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.94	0.50
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.94	0.50
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.94	0.50
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.47	0.49
1:C:72:SER:HA	1:C:439:GLY:O	2.12	0.49
1:C:759:GLN:CG	1:C:760:ARG:H	2.12	0.49
1:C:524:GLU:HA	1:C:524:GLU:OE1	2.11	0.49
1:C:546:GLU:HA	1:C:550:ALA:HB3	1.92	0.49
1:E:108:HIS:O	1:E:111:PHE:HD2	1.95	0.49
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.94	0.49
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.93	0.49
1:C:8:GLN:O	1:C:12:LEU:HB2	2.12	0.49
1:E:82:SER:O	1:E:86:VAL:HG23	2.12	0.49
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.47	0.49
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ASP:OD1	1:E:123:ASP:N	2.44	0.49
1:E:608:PRO:HA	1:E:636:PHE:CE2	2.47	0.49
1:A:22:MET:HG2	1:A:23:SER:N	2.26	0.49
1:A:30:HIS:NE2	1:A:130:ASP:HB2	2.27	0.49
1:E:699:DDE:HAB2	1:E:699:DDE:HAT2	1.93	0.49
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.94	0.49
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.95	0.49
1:A:93:THR:HG22	1:A:94:ASP:H	1.78	0.49
1:C:589:LYS:HD2	1:C:689:LEU:HD11	1.95	0.49
1:E:397:PHE:CD1	1:E:437:MET:HG3	2.47	0.49
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.94	0.49
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.48	0.49
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.47	0.49
1:E:117:ALA:HA	1:E:481:MET:SD	2.53	0.49
1:E:222:ILE:HD13	1:E:245:TRP:HB2	1.94	0.49
1:E:556:ILE:HG22	1:E:557:SER:N	2.24	0.49
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.95	0.49
1:C:321:LYS:O	1:C:325:ARG:HG3	2.12	0.48
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.43	0.48
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.95	0.48
1:E:459:ILE:O	1:E:459:ILE:HG22	2.12	0.48
1:C:30:HIS:CE1	1:C:130:ASP:HB2	2.48	0.48
1:A:72:SER:HA	1:A:439:GLY:O	2.13	0.48
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.28	0.48
1:E:163:ALA:O	1:E:169:VAL:HG12	2.14	0.48
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.96	0.48
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.94	0.48
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.94	0.48
1:A:510:ARG:HD2	1:A:549:HIS:HA	1.96	0.48
1:E:454:ILE:HG13	1:E:455:GLY:N	2.28	0.48
1:E:181:THR:O	1:E:185:VAL:HG23	2.14	0.48
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.49	0.48
1:C:3:ALA:HA	1:C:46:ILE:O	2.14	0.48
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.96	0.48
1:A:478:MET:O	1:A:479:LYS:C	2.52	0.47
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.96	0.47
1:C:237:LYS:O	1:C:241:MET:HG2	2.14	0.47
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.29	0.47
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.96	0.47
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.47
1:A:785:ARG:CG	1:A:785:ARG:NH1	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.14	0.47
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.29	0.47
1:E:659:ILE:O	1:E:663:VAL:HG23	2.14	0.47
1:A:216:HIS:O	1:A:325:ARG:HG3	2.14	0.47
1:C:494:GLU:O	1:C:554:LEU:HB3	2.15	0.47
1:E:132:ILE:HD12	1:E:132:ILE:N	2.29	0.47
1:A:93:THR:HG22	1:A:94:ASP:N	2.29	0.47
1:A:479:LYS:HE3	1:A:479:LYS:HA	1.96	0.47
1:A:722:PRO:O	1:A:723:LYS:HG2	2.15	0.47
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.47
1:C:627:VAL:O	1:C:631:ARG:HG3	2.14	0.47
1:E:223:ARG:HG3	1:E:241:MET:SD	2.54	0.47
1:E:369:ILE:HD12	1:E:401:PHE:HB3	1.96	0.47
1:A:406:LYS:HB2	1:A:409:GLN:HB2	1.96	0.47
1:A:501:LEU:N	1:A:502:PRO:HD2	2.29	0.47
1:A:568:GLU:HG3	1:A:723:LYS:CG	2.44	0.47
1:E:10:ARG:NH2	1:E:449:PRO:HD3	2.29	0.47
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.96	0.47
1:E:218:TRP:HB3	1:E:324:MET:HB3	1.96	0.47
1:E:279:ASP:O	1:E:283:ARG:HG2	2.14	0.47
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.95	0.47
1:A:607:ASN:O	1:A:615:ARG:HD3	2.15	0.47
2:B:516:LEU:O	2:B:545:PRO:HD2	2.14	0.47
1:E:731:VAL:HG12	1:E:770:ALA:O	2.15	0.47
1:A:286:THR:O	1:A:290:ASN:HB2	2.15	0.47
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.50	0.47
1:C:296:ILE:N	1:C:297:PRO:HD2	2.29	0.47
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.97	0.47
1:E:80:GLU:HA	1:E:96:ASN:O	2.14	0.47
1:C:498:ALA:HA	1:C:501:LEU:HB2	1.97	0.47
1:E:772:LEU:HD12	1:E:773:PRO:HD2	1.96	0.47
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.97	0.46
1:C:108:HIS:ND1	1:C:109:VAL:N	2.64	0.46
1:E:225:PHE:CE2	1:E:328:LEU:HD11	2.50	0.46
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.97	0.46
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.97	0.46
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.97	0.46
1:E:185:VAL:O	1:E:189:VAL:HG23	2.16	0.46
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.50	0.46
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.96	0.46
1:C:491:VAL:HG13	1:C:538:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.51	0.46
1:E:244:LEU:O	1:E:273:PHE:HB2	2.15	0.46
1:C:501:LEU:C	1:C:501:LEU:HD23	2.36	0.46
1:E:338:ILE:O	1:E:342:LEU:HB2	2.15	0.46
1:A:3:ALA:HA	1:A:46:ILE:O	2.15	0.46
1:E:204:PRO:HA	1:E:209:VAL:HB	1.96	0.46
1:E:736:PRO:O	1:E:740:VAL:HG23	2.16	0.46
1:C:251:ASN:ND2	1:C:253:LYS:H	2.13	0.46
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.50	0.46
2:F:419:VAL:O	2:F:423:LEU:HG	2.16	0.46
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.15	0.46
1:E:109:VAL:HG12	1:E:109:VAL:O	2.15	0.46
1:A:262:THR:HA	1:A:267:LYS:O	2.16	0.46
1:A:677:PHE:N	1:A:677:PHE:CD2	2.83	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.96	0.46
1:E:111:PHE:O	1:E:115:VAL:HG23	2.16	0.46
1:A:258:THR:HG21	4:A:912:HOH:O	2.15	0.46
1:C:699:DDE:HAB2	1:C:699:DDE:HAU3	1.46	0.46
2:D:420:GLU:HG2	4:D:734:HOH:O	2.17	0.45
1:C:750:LYS:HB3	1:C:772:LEU:HD11	1.97	0.45
1:E:3:ALA:HA	1:E:46:ILE:O	2.17	0.45
1:E:119:LEU:O	1:E:151:ILE:HD11	2.16	0.45
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.97	0.45
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.98	0.45
1:E:429:LYS:HG3	1:E:462:PHE:CE2	2.51	0.45
1:E:669:TRP:CE2	2:F:492:ARG:HG3	2.51	0.45
1:A:81:MET:HE1	1:A:336:GLU:HA	1.98	0.45
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.36	0.45
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.98	0.45
1:A:500:ASP:HB3	1:A:552:VAL:HG21	1.99	0.45
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.87	0.45
2:B:490:ARG:NH2	2:B:492[B]:ARG:HE	2.15	0.45
1:E:394:PHE:HB2	1:E:460:ASP:HB3	1.99	0.45
1:A:152:LYS:HA	1:A:153:PRO:HD3	1.71	0.45
1:E:111:PHE:CE1	1:E:540:ILE:HD13	2.52	0.45
1:E:676:ILE:HG22	1:E:677:PHE:HD2	1.82	0.45
1:E:731:VAL:O	1:E:731:VAL:HG13	2.17	0.45
1:A:542:LEU:HD22	1:A:556:ILE:HD13	1.99	0.45
1:E:352:ARG:O	1:E:356:LEU:HG	2.17	0.45
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.48	0.45
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:727:PRO:HD3	1:C:801:TRP:CZ3	2.52	0.45
1:E:43:ALA:HB1	1:E:78:TYR:H	1.82	0.45
1:E:405:VAL:O	1:E:447:ASP:HA	2.17	0.45
1:E:411:VAL:HG13	1:E:470:THR:O	2.17	0.45
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.47	0.44
1:E:129:VAL:HG12	1:E:130:ASP:H	1.82	0.44
1:A:454:ILE:HG13	1:A:455:GLY:N	2.30	0.44
1:A:675:PRO:HD3	1:A:714:TYR:CE1	2.52	0.44
1:E:296:ILE:N	1:E:297:PRO:HD2	2.33	0.44
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.88	0.44
1:C:506:GLU:O	1:C:510:ARG:HG3	2.17	0.44
1:E:307:LEU:HD13	1:E:311:GLU:O	2.17	0.44
1:E:486:SER:O	1:E:488:VAL:HG23	2.17	0.44
1:C:460:ASP:N	1:C:460:ASP:OD1	2.51	0.44
1:E:237:LYS:HA	1:E:240:MET:HB3	2.00	0.44
1:E:485:VAL:HG22	1:E:485:VAL:O	2.17	0.44
1:A:727:PRO:HD3	1:A:801:TRP:CZ3	2.52	0.44
1:C:707:PRO:O	1:C:711:ARG:HG3	2.17	0.44
1:E:121:VAL:HG11	1:E:383:SER:OG	2.18	0.44
1:E:263:ASP:HB3	1:E:267:LYS:HB2	1.98	0.44
1:E:739:ALA:HB1	1:E:788:THR:HB	2.00	0.44
1:A:251:ASN:HA	1:A:252:PRO:HD3	1.86	0.44
1:A:454:ILE:HG13	1:A:455:GLY:H	1.83	0.44
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.44
1:E:314:LEU:O	1:E:319:LEU:HB2	2.18	0.44
1:A:470:THR:HG22	1:A:471:THR:N	2.33	0.44
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.33	0.44
1:C:491:VAL:HG12	1:C:559:PRO:HA	2.00	0.44
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.53	0.44
1:E:454:ILE:HG13	1:E:455:GLY:H	1.82	0.44
1:E:578:LYS:HB2	1:E:578:LYS:HE3	1.87	0.44
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.53	0.44
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.00	0.44
1:E:46:ILE:N	1:E:46:ILE:HD12	2.33	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.32	0.44
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.91	0.44
1:C:552:VAL:HG13	1:C:553:PRO:HD2	2.00	0.44
2:D:535:LEU:HB3	2:D:536:PRO:HA	2.00	0.44
1:E:46:ILE:HG22	1:E:47:SER:N	2.33	0.44
1:E:84:GLU:O	1:E:88:GLU:HG3	2.18	0.43
1:E:744:TYR:CE1	1:E:754:VAL:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.18	0.43
1:A:14:ASP:OD1	1:A:15:LYS:HG3	2.18	0.43
1:A:552:VAL:HG13	1:A:553:PRO:HD2	2.01	0.43
1:A:837:GLU:HG3	4:A:871:HOH:O	2.18	0.43
1:E:464:LEU:HG	1:E:465:LYS:HG3	2.00	0.43
1:A:6:VAL:CG1	1:A:445:ILE:HG22	2.48	0.43
2:B:440:HIS:HB2	2:B:471:ILE:HG22	2.00	0.43
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.00	0.43
1:E:30:HIS:HE1	1:E:133:GLU:OE1	2.01	0.43
1:E:588:LEU:C	1:E:588:LEU:HD12	2.38	0.43
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.19	0.43
1:A:698:ILE:H	1:A:698:ILE:HG13	1.56	0.43
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.54	0.43
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.53	0.43
1:E:39:LEU:HB3	1:E:77:LEU:HD23	2.01	0.43
1:E:72:SER:HA	1:E:439:GLY:O	2.19	0.43
1:E:459:ILE:HD12	1:E:459:ILE:N	2.33	0.43
1:E:819:VAL:O	1:E:823:ARG:HG3	2.18	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.52	0.43
1:E:117:ALA:O	1:E:121:VAL:HG13	2.18	0.43
1:E:353:ALA:HB3	1:E:370:LYS:HG3	1.99	0.43
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.48	0.43
1:A:26:ALA:CB	1:A:128:VAL:HB	2.48	0.43
1:C:155:VAL:O	1:C:209:VAL:HA	2.19	0.43
1:C:314:LEU:HD13	1:C:318:ALA:O	2.19	0.43
1:E:258:THR:HG22	1:E:259:ASN:N	2.34	0.43
1:E:292:LYS:O	1:E:296:ILE:HG13	2.18	0.43
1:A:185:VAL:O	1:A:189:VAL:HG23	2.19	0.43
1:A:588:LEU:HD12	1:A:588:LEU:C	2.39	0.43
2:B:574:ASP:HA	2:B:575:PRO:HD2	1.84	0.43
1:C:24:VAL:HG21	1:C:36:THR:HG22	2.00	0.43
1:C:542:LEU:HD12	1:C:542:LEU:HA	1.84	0.43
1:A:552:VAL:O	1:A:554:LEU:HG	2.18	0.43
1:A:727:PRO:HD3	1:A:801:TRP:HZ3	1.84	0.43
1:A:731:VAL:HG12	1:A:770:ALA:O	2.19	0.43
1:C:820:LEU:O	1:C:824:LYS:HG3	2.19	0.43
2:D:517:THR:HG23	2:D:547:GLU:HA	2.00	0.43
1:E:706:ILE:HB	1:E:707:PRO:HD3	2.01	0.43
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.54	0.42
1:C:381:TYR:O	1:C:398:GLY:HA3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:O	1:E:127:VAL:HA	2.19	0.42
1:E:150:ARG:HA	1:E:197:LEU:HD11	2.01	0.42
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.54	0.42
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.19	0.42
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.35	0.42
1:A:239:LYS:HB2	1:A:239:LYS:HE3	1.65	0.42
2:B:471:ILE:HG13	2:B:554:THR:HB	2.01	0.42
1:C:487:PRO:HB2	1:C:531:ALA:HB1	2.00	0.42
1:E:81:MET:HB3	1:E:85:ASP:HB2	2.01	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
1:A:841:LYS:HE3	4:B:806:HOH:O	2.18	0.42
1:E:833:PRO:HB3	1:E:837:GLU:OE1	2.19	0.42
1:A:429:LYS:HG3	1:A:462:PHE:CE2	2.54	0.42
1:A:594:ASP:HB2	1:A:597:VAL:HG23	2.00	0.42
1:C:256:LYS:HE3	1:C:256:LYS:HB3	1.92	0.42
1:C:449:PRO:HG2	1:C:452:ASN:ND2	2.34	0.42
1:C:554:LEU:HB3	1:C:555:LYS:H	1.69	0.42
1:C:588:LEU:C	1:C:588:LEU:HD12	2.40	0.42
2:D:428:GLN:O	2:D:432:ARG:HD3	2.19	0.42
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.85	0.42
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.54	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.87	0.42
1:E:119:LEU:HD21	1:E:146:ALA:HA	2.02	0.42
1:E:126:LEU:HD11	1:E:156:VAL:HG21	2.01	0.42
1:E:552:VAL:HG13	1:E:553:PRO:HD2	2.00	0.42
1:E:552:VAL:O	1:E:554:LEU:HG	2.20	0.42
2:F:467:ARG:CZ	2:F:536:PRO:HG3	2.49	0.42
1:A:366:CYS:O	1:A:370:LYS:HG3	2.20	0.42
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.17	0.42
1:A:288:ILE:HA	1:A:296:ILE:HD11	2.02	0.42
1:C:336:GLU:HG2	1:C:340:LEU:HD12	2.02	0.42
1:C:373:ASP:HA	1:C:374:PRO:HD2	1.88	0.42
1:C:841:LYS:O	1:C:842:LEU:HD23	2.20	0.42
1:E:205:ALA:HB2	1:E:245:TRP:HB3	2.01	0.42
1:E:515:ASP:HA	1:E:516:PRO:HD2	1.86	0.42
1:E:522:MET:HB2	2:F:490:ARG:HH22	1.84	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.02	0.42
1:A:385:MET:HG2	1:A:465:LYS:HA	2.02	0.42
1:E:39:LEU:HD11	1:E:334:LEU:CB	2.50	0.42
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.54	0.42
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.89	0.42
1:C:192:TYR:HA	1:C:763:THR:CG2	2.50	0.42
1:E:39:LEU:HD11	1:E:334:LEU:HB3	2.02	0.42
1:E:101:ASN:OD1	1:E:453:ILE:HB	2.20	0.42
1:E:111:PHE:HB3	1:E:114:GLU:HG2	2.02	0.42
1:E:222:ILE:CD1	1:E:245:TRP:HB2	2.50	0.42
1:E:565:GLU:O	1:E:681:MET:HA	2.20	0.42
1:E:719:LEU:HD21	1:E:835:TRP:CD2	2.54	0.42
1:E:733:ILE:HG21	1:E:743:ILE:HD11	2.01	0.42
1:A:334:LEU:O	1:A:338:ILE:HG13	2.20	0.42
1:C:45:ILE:HD11	1:C:78:TYR:HB2	2.01	0.42
1:C:251:ASN:ND2	1:C:251:ASN:C	2.73	0.42
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.79	0.42
1:E:141:THR:HA	1:E:144:ARG:NH1	2.31	0.42
1:E:240:MET:O	1:E:244:LEU:HG	2.19	0.42
1:A:249:PHE:CZ	1:A:261:ASP:HB3	2.55	0.41
1:A:258:THR:HG22	1:A:259:ASN:N	2.34	0.41
1:A:707:PRO:O	1:A:711:ARG:HG3	2.20	0.41
2:B:511:PHE:HB3	2:B:600:TYR:CD1	2.55	0.41
1:C:215:LEU:HD23	1:C:216:HIS:N	2.35	0.41
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.60	0.41
1:E:737:GLU:HA	1:E:740:VAL:HG23	2.02	0.41
1:E:759:GLN:HG2	1:E:760:ARG:N	2.34	0.41
1:A:410:LYS:HG2	1:A:430:ALA:HB2	2.01	0.41
1:E:150:ARG:HB3	1:E:351:TYR:CE1	2.53	0.41
1:E:395:TYR:CD1	1:E:457:VAL:HG22	2.55	0.41
1:A:6:VAL:HG13	1:A:445:ILE:HG22	2.01	0.41
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.56	0.41
1:A:677:PHE:N	1:A:677:PHE:HD2	2.19	0.41
1:A:831:GLU:CD	1:A:831:GLU:H	2.21	0.41
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.35	0.41
1:C:718:LEU:HA	1:C:722:PRO:HG3	2.02	0.41
1:C:759:GLN:CG	1:C:760:ARG:N	2.81	0.41
1:E:307:LEU:HB2	1:E:312:LYS:HE2	2.02	0.41
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.84	0.41
1:C:192:TYR:HA	1:C:763:THR:HG22	2.01	0.41
1:C:823:ARG:HA	1:C:828:MET:CE	2.47	0.41
1:A:132:ILE:HD12	1:A:162:ARG:HD3	2.02	0.41
1:A:411:VAL:HG12	1:A:412:ARG:N	2.35	0.41
1:C:494:GLU:HG2	1:C:495:VAL:N	2.34	0.41
1:A:410:LYS:HA	1:A:430:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:CD	1:A:710:ARG:HH22	2.23	0.41
1:C:211:PHE:O	1:C:219:ALA:HA	2.20	0.41
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.56	0.41
2:D:479:TYR:CG	2:D:582:LEU:HB2	2.56	0.41
1:E:200:VAL:O	1:E:200:VAL:HG22	2.20	0.41
1:E:742:GLY:O	1:E:745:SER:HB3	2.21	0.41
2:F:426:HIS:CG	2:F:594:ILE:HD12	2.56	0.41
1:A:279:ASP:HB3	1:A:280:PRO:HD3	2.01	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.97	0.41
2:B:498:LEU:HD23	2:B:498:LEU:HA	1.92	0.41
1:C:354:GLU:HG3	1:C:370:LYS:HE3	2.02	0.41
1:E:174:LEU:O	1:E:177:THR:HB	2.20	0.41
1:A:326:LYS:HB2	1:A:326:LYS:HE3	1.80	0.41
1:A:381:TYR:HB2	1:A:478:MET:CE	2.51	0.41
1:A:545:LEU:O	1:A:550:ALA:HB3	2.21	0.41
1:A:620:ALA:HA	1:A:625:TRP:O	2.21	0.41
1:C:12:LEU:HD12	1:C:12:LEU:HA	1.93	0.41
1:C:111:PHE:HB3	1:C:114:GLU:HB2	2.02	0.41
1:C:237:LYS:HA	1:C:240:MET:HB3	2.03	0.41
1:C:270:GLU:OE1	1:C:275:MET:HG3	2.20	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.56	0.41
1:E:114:GLU:O	1:E:117:ALA:HB3	2.21	0.41
2:F:571:ILE:HA	2:F:572:PRO:HD3	1.84	0.41
1:C:132:ILE:HD11	1:C:162:ARG:HB2	2.03	0.41
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.55	0.41
1:E:292:LYS:HD3	1:E:295:GLU:OE2	2.21	0.41
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.51	0.41
1:C:420:PRO:HG2	1:C:476:HIS:CE1	2.56	0.40
1:C:459:ILE:HG22	1:C:459:ILE:O	2.21	0.40
1:C:556:ILE:O	1:C:556:ILE:HG12	2.21	0.40
1:C:831:GLU:OE1	1:C:831:GLU:N	2.51	0.40
1:E:258:THR:HG22	1:E:260:LYS:H	1.85	0.40
1:A:470:THR:HG22	1:A:472:SER:N	2.25	0.40
1:A:697:ALA:HA	1:A:700:ARG:CD	2.51	0.40
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.56	0.40
2:F:522:GLU:CD	2:F:522:GLU:H	2.24	0.40
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.56	0.40
1:C:699:DDE:HAC2	1:C:699:DDE:HAD2	1.82	0.40
1:E:225:PHE:HZ	1:E:327:PHE:CZ	2.39	0.40
1:E:491:VAL:HG21	1:E:542:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:553:GLU:OE1	3:F:702:NAD:H6N	2.21	0.40
1:A:558:PRO:HA	1:A:559:PRO:HD3	1.98	0.40
1:C:454:ILE:HG13	1:C:455:GLY:H	1.86	0.40
1:C:565:GLU:O	1:C:681:MET:HA	2.22	0.40
1:E:17:THR:HB	1:E:93:THR:HA	2.04	0.40
1:A:431:ILE:CD1	1:A:459:ILE:HD11	2.51	0.40
1:C:711:ARG:HD2	2:D:578:VAL:O	2.22	0.40
2:D:484:ASP:OD2	2:D:494:ARG:HB2	2.21	0.40
1:E:12:LEU:HA	1:E:15:LYS:HE2	2.04	0.40
1:E:218:TRP:HZ3	1:E:220:PHE:CD2	2.39	0.40
1:E:243:ARG:O	1:E:248:SER:HB2	2.22	0.40
1:E:284:LEU:HD22	1:E:323:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	818/842 (97%)	780 (95%)	34 (4%)	4 (0%)	29	48
1	C	818/842 (97%)	776 (95%)	39 (5%)	3 (0%)	34	54
1	E	818/842 (97%)	750 (92%)	65 (8%)	3 (0%)	34	54
2	B	206/207 (100%)	200 (97%)	6 (3%)	0	100	100
2	D	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	29	48
2	F	205/207 (99%)	201 (98%)	3 (2%)	1 (0%)	29	48
All	All	3070/3147 (98%)	2906 (95%)	152 (5%)	12 (0%)	34	54

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	678 (97%)	21 (3%)	41	68
1	C	699/714 (98%)	674 (96%)	25 (4%)	35	61
1	E	699/714 (98%)	689 (99%)	10 (1%)	67	86
2	B	161/160 (101%)	158 (98%)	3 (2%)	57	80
2	D	160/160 (100%)	156 (98%)	4 (2%)	47	73
2	F	160/160 (100%)	155 (97%)	5 (3%)	40	67
All	All	2578/2622 (98%)	2510 (97%)	68 (3%)	46	72

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	22	MET
1	A	30	HIS
1	A	83	ASP
1	A	138	GLN
1	A	153	PRO
1	A	195	GLU

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Mol	Chain	Res	Type
1	A	239	LYS
1	A	306	VAL
1	A	479	LYS
1	A	489	VAL
1	A	499	ASN
1	A	595	GLU
1	A	599	LEU
1	A	610	ASP
1	A	631	ARG
1	A	677	PHE
1	A	700	ARG
1	A	718	LEU
1	A	785	ARG
1	A	842	LEU
2	B	462	LEU
2	B	513	ARG
2	B	540	ASP
1	C	28	VAL
1	C	41	GLN
1	C	80	GLU
1	C	83	ASP
1	C	86	VAL
1	C	87	LYS
1	C	154	VAL
1	C	194	ASP
1	C	211	PHE
1	C	215	LEU
1	C	251	ASN
1	C	258	THR
1	C	262	THR
1	C	312	LYS
1	C	326	LYS
1	C	423	LYS
1	C	460	ASP
1	C	500	ASP
1	C	518	VAL
1	C	524	GLU
1	C	544	ASP
1	C	556	ILE
1	C	632	LYS
1	C	730	LEU
1	C	786	GLN

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Mol	Chain	Res	Type
2	D	462	LEU
2	D	488	ASP
2	D	538	ARG
2	D	540	ASP
1	E	83	ASP
1	E	161	ASP
1	E	211	PHE
1	E	494	GLU
1	E	544	ASP
1	E	568	GLU
1	E	672	LYS
1	E	730	LEU
1	E	828	MET
1	E	842	LEU
2	F	462	LEU
2	F	494	ARG
2	F	540	ASP
2	F	547	GLU
2	F	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	428	GLN
1	C	30	HIS
1	C	452	ASN
2	D	428	GLN
1	E	30	HIS
1	E	414	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	E	699	1	14,20,21	1.12	1 (7%)	14,28,30	0.94	0
1	DDE	A	699	1	5,10,21	0.60	0	3,12,30	1.32	1 (33%)
1	DDE	C	699	1	14,20,21	1.05	1 (7%)	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	E	699	1	-	4/20/21/23	0/1/1/1
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1
1	DDE	C	699	1	-	14/20/21/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	CAT-CE1	2.80	1.54	1.50
1	C	699	DDE	CAT-CE1	2.48	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	CD2-NE2-CE1	2.04	108.96	105.78

There are no chirality outliers.

All (19) 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	CBI-CBW-NCB-CAB

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Mol	Chain	Res	Type	Atoms
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	OAG-CBI-CBW-NCB
1	E	699	DDE	CAT-CAU-CBW-CBI
1	E	699	DDE	CA-CB-CG-CD2
1	C	699	DDE	CA-CB-CG-CD2
1	C	699	DDE	NAD-CBI-CBW-CAU

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates [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	D	701	-	42,48,48	0.67	0	50,73,73	1.26	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAD	B	700	-	42,48,48	0.67	0	50,73,73	1.25	3 (6%)
3	NAD	F	702	-	42,48,48	0.69	0	50,73,73	1.25	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	D	701	-	-	5/26/62/62	0/5/5/5
3	NAD	B	700	-	-	2/26/62/62	0/5/5/5
3	NAD	F	702	-	-	1/26/62/62	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	N3A-C2A-N1A	-4.74	121.26	128.68
3	F	702	NAD	N3A-C2A-N1A	-4.68	121.36	128.68
3	D	701	NAD	N3A-C2A-N1A	-4.62	121.46	128.68
3	D	701	NAD	C3D-C2D-C1D	3.72	106.58	100.98
3	B	700	NAD	C3D-C2D-C1D	3.67	106.50	100.98
3	F	702	NAD	C3D-C2D-C1D	3.59	106.38	100.98
3	F	702	NAD	PN-O3-PA	-3.14	122.05	132.83
3	D	701	NAD	PN-O3-PA	-2.88	122.95	132.83
3	B	700	NAD	PN-O3-PA	-2.85	123.04	132.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

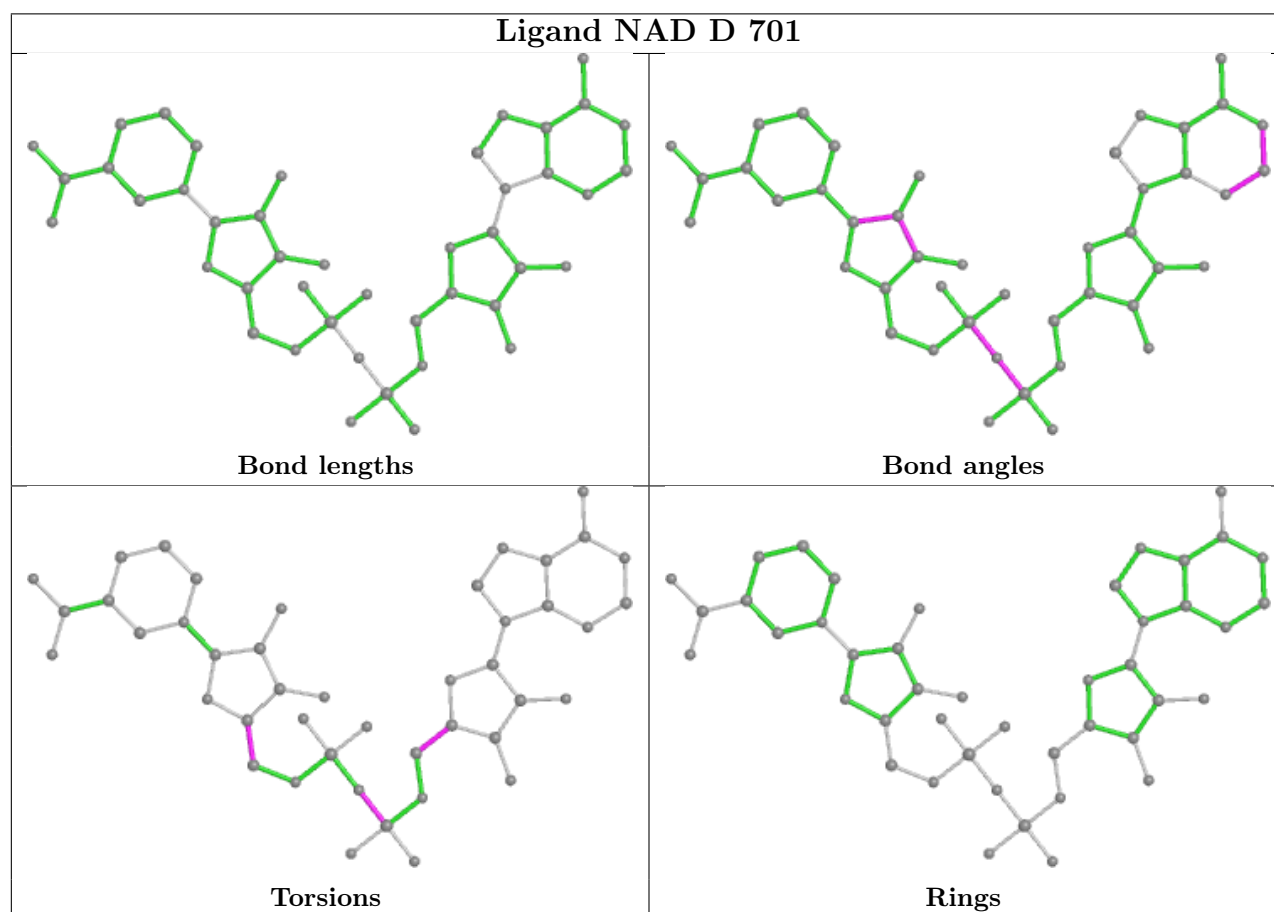
Mol	Chain	Res	Type	Atoms
3	D	701	NAD	O4D-C4D-C5D-O5D
3	D	701	NAD	C3D-C4D-C5D-O5D
3	B	700	NAD	O4B-C4B-C5B-O5B
3	B	700	NAD	C3B-C4B-C5B-O5B
3	D	701	NAD	O4B-C4B-C5B-O5B
3	D	701	NAD	PN-O3-PA-O1A
3	F	702	NAD	O4B-C4B-C5B-O5B
3	D	701	NAD	PN-O3-PA-O2A

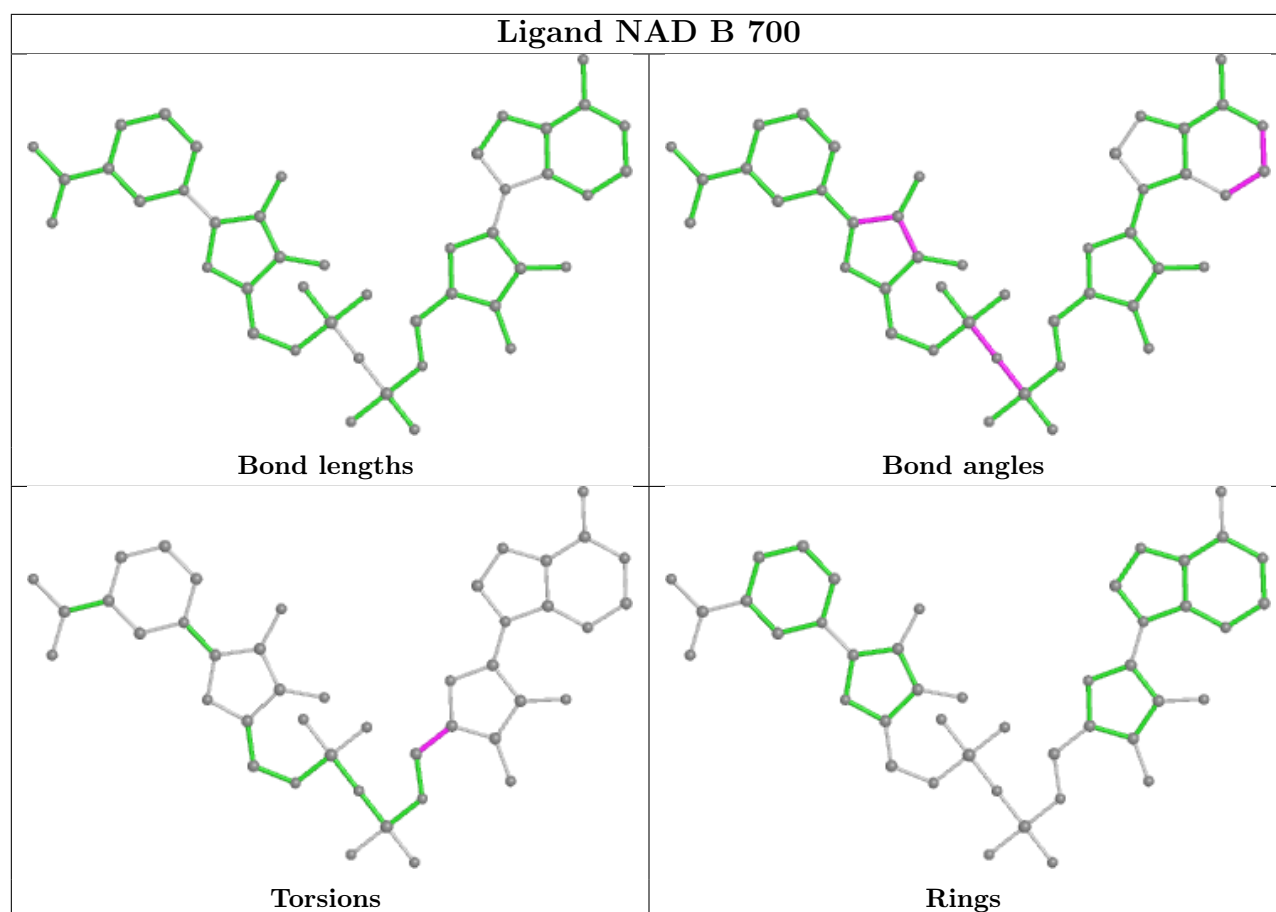
There are no ring outliers.

3 monomers are involved in 4 short contacts:

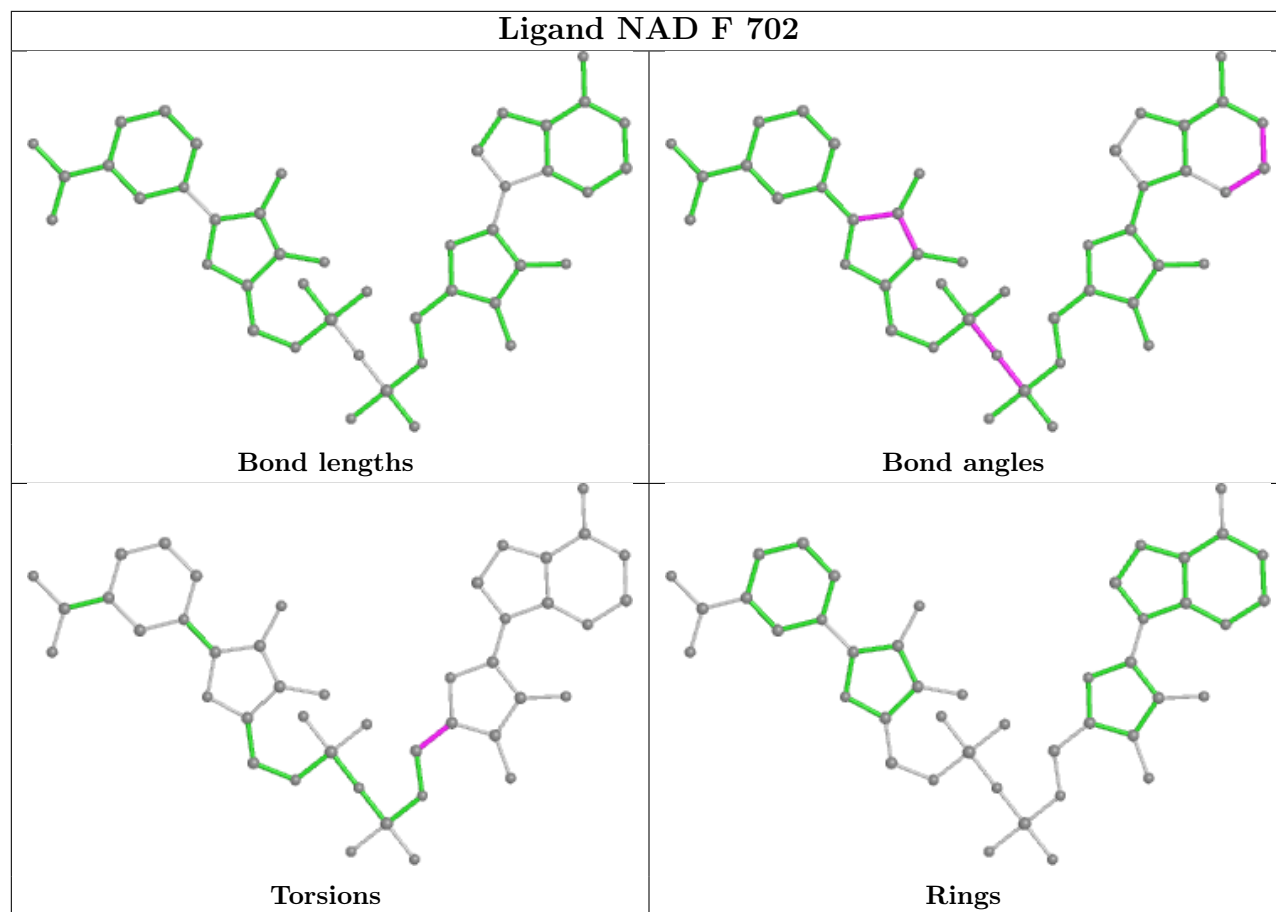
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	NAD	1	0
3	B	700	NAD	1	0
3	F	702	NAD	2	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.24	44 (5%) 25 27	12, 51, 91, 113	0
1	C	822/842 (97%)	0.75	120 (14%) 2 2	13, 60, 136, 178	0
1	E	822/842 (97%)	2.12	368 (44%) 0 0	10, 124, 182, 229	0
2	B	207/207 (100%)	-0.15	3 (1%) 75 77	10, 22, 54, 89	0
2	D	207/207 (100%)	-0.15	3 (1%) 75 77	9, 21, 52, 95	0
2	F	207/207 (100%)	-0.17	3 (1%) 75 77	12, 27, 62, 91	0
All	All	3087/3147 (98%)	0.80	541 (17%) 1 1	9, 53, 159, 229	0

All (541) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	314	LEU	15.0
1	E	67	GLY	11.3
1	E	315	GLU	10.4
1	E	163	ALA	10.4
1	E	108	HIS	10.4
1	E	193	ALA	9.9
1	E	167	LEU	9.7
1	E	761	PRO	9.7
1	E	166	GLU	9.6
1	E	789	GLY	9.3
1	E	310	ASP	9.3
1	E	311	GLU	9.1
1	E	245	TRP	8.6
1	E	196	VAL	8.5
1	C	504	LEU	8.4
1	E	157	ILE	8.2
1	E	231	LYS	8.1
1	E	298	VAL	8.0
1	E	32	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
1	E	759	GLN	7.9
1	E	175	TYR	7.8
1	E	107	GLY	7.7
1	E	200	VAL	7.5
1	E	321	LYS	7.5
1	C	498	ALA	7.4
1	E	361	ALA	7.4
1	E	290	ASN	7.4
1	E	740	VAL	7.3
1	E	179	ALA	7.1
1	E	766	PHE	7.1
1	E	187	VAL	6.9
1	E	420	PRO	6.9
1	E	499	ASN	6.8
1	E	367	ILE	6.8
1	C	499	ASN	6.8
1	E	790	GLY	6.7
1	E	795	GLN	6.7
1	E	316	GLY	6.7
1	E	281	ILE	6.7
1	E	211	PHE	6.7
1	C	167	LEU	6.7
1	E	195	GLU	6.6
1	E	160	VAL	6.6
1	E	197	LEU	6.6
1	E	356	LEU	6.6
1	E	262	THR	6.6
1	E	289	MET	6.5
1	E	335	LEU	6.5
1	E	47	SER	6.5
1	E	419	VAL	6.5
1	E	317	LYS	6.5
1	E	744	TYR	6.5
1	E	192	TYR	6.4
1	E	307	LEU	6.4
1	E	81	MET	6.4
1	E	212	GLY	6.4
1	C	502	PRO	6.4
1	E	68	ILE	6.4
1	C	306	VAL	6.4
1	C	298	VAL	6.3
1	E	257	TRP	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	129	VAL	6.3
1	E	498	ALA	6.3
1	E	233	PHE	6.2
2	D	489	ALA	6.2
1	E	360	PRO	6.2
1	E	97	SER	6.2
1	E	760	ARG	6.2
1	E	254	THR	6.2
1	C	501	LEU	6.1
1	E	169	VAL	6.1
1	E	232	LYS	6.1
1	C	522	MET	6.0
1	E	216	HIS	6.0
1	E	91	GLN	6.0
1	E	26	ALA	5.9
1	C	494	GLU	5.9
1	C	252	PRO	5.9
1	E	268	PRO	5.9
1	E	343	PRO	5.9
1	C	251	ASN	5.9
1	C	168	GLN	5.9
1	E	770	ALA	5.9
1	E	36	THR	5.8
1	C	67	GLY	5.8
1	E	269	LEU	5.8
1	C	311	GLU	5.8
1	E	218	TRP	5.8
1	E	27	HIS	5.8
1	E	737	GLU	5.8
1	A	361	ALA	5.8
1	E	739	ALA	5.7
1	E	48	ALA	5.7
1	E	741	GLY	5.7
1	E	89	ILE	5.7
1	E	78	TYR	5.7
1	E	88	GLU	5.7
1	E	267	LYS	5.7
1	E	194	ASP	5.7
1	E	90	LYS	5.6
1	E	168	GLN	5.6
1	E	763	THR	5.6
1	A	67	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	342	LEU	5.6
1	E	131	THR	5.5
1	E	553	PRO	5.5
1	E	86	VAL	5.5
1	E	358	GLU	5.5
1	E	306	VAL	5.5
1	E	178	PHE	5.5
1	E	239	LYS	5.4
1	E	237	LYS	5.4
1	E	240	MET	5.4
1	E	215	LEU	5.4
1	C	235	VAL	5.4
1	E	359	GLY	5.4
1	C	523	SER	5.4
1	C	495	VAL	5.3
1	C	291	PHE	5.3
1	E	745	SER	5.3
1	E	278	LEU	5.3
1	C	299	LEU	5.3
1	E	256	LYS	5.1
1	C	496	LYS	5.0
1	C	269	LEU	5.0
1	E	28	VAL	5.0
1	E	203	TYR	5.0
1	E	137	VAL	4.9
1	C	290	ASN	4.9
1	C	267	LYS	4.9
2	B	489	ALA	4.9
1	E	96	ASN	4.9
1	E	98	PHE	4.9
1	C	549	HIS	4.9
1	E	277	ILE	4.9
1	E	258	THR	4.9
1	E	299	LEU	4.9
1	E	76	SER	4.8
1	E	180	ARG	4.8
1	E	46	ILE	4.8
1	E	41	GLN	4.8
1	E	40	VAL	4.8
1	E	354	GLU	4.8
1	E	264	ALA	4.8
1	E	497	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	128	VAL	4.8
1	C	173	ASP	4.8
1	E	189	VAL	4.8
1	E	308	LYS	4.8
1	E	266	GLY	4.8
1	E	764	PRO	4.8
1	A	198	GLY	4.7
1	E	442	VAL	4.7
1	E	755	VAL	4.7
1	C	493	VAL	4.7
1	C	108	HIS	4.7
1	E	260	LYS	4.7
1	E	30	HIS	4.7
1	C	264	ALA	4.7
1	E	302	LYS	4.6
1	E	294	ASP	4.6
1	E	297	PRO	4.6
1	E	263	ASP	4.6
1	E	111	PHE	4.6
1	C	268	PRO	4.6
1	C	321	LYS	4.6
1	E	282	PHE	4.6
1	A	107	GLY	4.5
1	E	296	ILE	4.5
1	E	20	ARG	4.5
1	E	156	VAL	4.5
1	E	453	ILE	4.5
1	E	756	SER	4.5
1	E	436	LEU	4.5
1	E	441	PHE	4.5
1	E	332	ASP	4.5
1	C	513	LYS	4.5
1	E	158	ASN	4.4
1	C	265	GLU	4.4
1	E	164	LEU	4.4
1	E	366	CYS	4.4
1	E	747	LEU	4.4
1	E	324	MET	4.4
1	E	253	LYS	4.3
1	E	291	PHE	4.3
1	E	391	LYS	4.3
1	E	293	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	444	PRO	4.3
1	C	216	HIS	4.3
1	C	233	PHE	4.3
1	E	376	ALA	4.3
1	E	188	ILE	4.2
1	E	227	THR	4.2
1	E	143	LEU	4.2
1	E	210	ALA	4.2
1	C	550	ALA	4.2
1	E	312	LYS	4.2
1	A	196	VAL	4.2
1	A	111	PHE	4.2
1	C	556	ILE	4.1
1	E	500	ASP	4.1
1	C	310	ASP	4.1
1	E	503	LYS	4.1
1	E	162	ARG	4.1
1	E	554	LEU	4.1
1	E	329	PRO	4.0
1	E	201	GLN	4.0
1	E	135	VAL	4.0
1	E	83	ASP	4.0
1	E	265	GLU	4.0
1	C	107	GLY	4.0
1	E	781	THR	4.0
1	E	422	LYS	4.0
1	E	110	ASP	4.0
1	C	547	HIS	4.0
1	E	235	VAL	4.0
1	C	262	THR	4.0
1	E	421	GLY	4.0
1	C	497	ASN	3.9
1	E	134	GLY	3.9
1	E	29	ASP	3.9
1	E	220	PHE	3.8
1	E	762	GLY	3.8
1	C	317	LYS	3.8
1	A	48	ALA	3.8
1	E	743	ILE	3.8
1	A	7	ASP	3.8
1	C	301	GLU	3.8
1	C	553	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	230	ALA	3.8
1	E	476	HIS	3.8
1	E	34	THR	3.8
1	C	314	LEU	3.8
1	E	80	GLU	3.8
1	E	390	ASP	3.8
1	E	109	VAL	3.7
1	E	255	LYS	3.7
1	E	338	ILE	3.7
1	C	29	ASP	3.7
1	C	500	ASP	3.7
1	C	111	PHE	3.7
1	E	24	VAL	3.7
1	E	318	ALA	3.7
1	E	273	PHE	3.7
1	C	546	GLU	3.7
1	E	288	ILE	3.7
1	E	38	SER	3.7
1	E	304	GLU	3.7
1	C	236	ASP	3.7
1	E	758	GLU	3.6
1	E	7	ASP	3.6
1	C	232	LYS	3.6
1	E	155	VAL	3.6
1	E	742	GLY	3.6
1	C	313	ASP	3.6
1	E	138	GLN	3.6
1	C	761	PRO	3.6
1	E	242	ASP	3.6
1	E	323	VAL	3.6
1	E	768	VAL	3.6
1	E	455	GLY	3.5
1	A	28	VAL	3.5
1	E	42	ARG	3.5
1	E	494	GLU	3.5
1	E	261	ASP	3.5
1	E	496	LYS	3.5
1	E	170	SER	3.5
1	E	548	ASP	3.5
1	E	736	PRO	3.5
1	E	437	MET	3.5
1	C	231	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	479	LYS	3.5
1	C	258	THR	3.4
1	E	205	ALA	3.4
1	E	389	SER	3.4
1	C	266	GLY	3.4
2	B	461	ASP	3.4
1	A	358	GLU	3.4
1	C	305	ILE	3.4
1	E	757	GLU	3.4
1	E	738	GLN	3.4
1	E	94	ASP	3.4
1	E	222	ILE	3.4
1	E	276	PHE	3.4
1	A	360	PRO	3.4
1	E	82	SER	3.3
1	E	100	ILE	3.3
1	E	325	ARG	3.3
1	C	552	VAL	3.3
1	E	286	THR	3.3
1	C	46	ILE	3.3
1	E	106	PRO	3.3
1	E	469	LEU	3.3
1	C	318	ALA	3.3
1	E	309	GLY	3.3
1	C	325	ARG	3.3
1	E	395	TYR	3.3
1	E	348	ALA	3.2
1	C	293	LYS	3.2
1	E	375	LYS	3.2
1	E	23	SER	3.2
1	E	456	LEU	3.2
1	E	748	ASN	3.2
1	E	423	LYS	3.2
1	E	794	PRO	3.2
1	C	763	THR	3.2
1	E	154	VAL	3.2
1	E	754	VAL	3.2
1	E	454	ILE	3.2
1	E	213	SER	3.2
1	E	472	SER	3.2
1	E	37	ASP	3.2
1	E	127	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	391	LYS	3.2
1	A	480	VAL	3.2
1	E	320	LEU	3.2
1	E	418	TYR	3.1
1	E	333	ALA	3.1
1	E	362	ASP	3.1
1	A	108	HIS	3.1
1	E	15	LYS	3.1
1	E	177	THR	3.1
1	E	435	VAL	3.1
1	A	454	ILE	3.1
1	E	301	GLU	3.1
1	E	783	GLU	3.1
1	E	176	GLN	3.1
1	E	199	ASP	3.1
1	A	419	VAL	3.1
1	E	105	SER	3.1
1	E	3	ALA	3.1
1	E	313	ASP	3.1
1	C	263	ASP	3.0
1	E	25	ILE	3.0
1	E	70	ILE	3.0
1	E	555	LYS	3.0
1	E	779	GLY	3.0
1	E	182	VAL	3.0
1	E	796	MET	3.0
1	C	294	ASP	3.0
1	C	544	ASP	3.0
1	E	284	LEU	3.0
1	E	104	ASP	2.9
1	E	130	ASP	2.9
1	E	93	THR	2.9
1	E	392	GLY	2.9
1	E	31	GLY	2.9
1	E	126	LEU	2.9
1	C	237	LYS	2.9
1	C	289	MET	2.9
1	C	510	ARG	2.9
1	A	5	THR	2.9
1	E	322	VAL	2.9
1	C	421	GLY	2.9
1	C	485	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	202	VAL	2.8
2	B	549	GLY	2.8
1	E	504	LEU	2.8
1	E	229	TYR	2.8
1	A	157	ILE	2.8
1	A	417	ASN	2.8
1	E	371	ASN	2.8
1	A	464	LEU	2.8
1	E	92	LYS	2.8
1	E	79	SER	2.8
1	E	481	MET	2.8
1	E	243	ARG	2.8
1	C	528	HIS	2.8
1	C	42	ARG	2.8
1	E	214	GLY	2.7
1	C	177	THR	2.7
1	E	784	LEU	2.7
1	E	473	GLU	2.7
1	E	185	VAL	2.7
1	C	323	VAL	2.7
1	C	11	SER	2.7
1	C	554	LEU	2.7
1	E	292	LYS	2.7
1	A	81	MET	2.7
1	E	785	ARG	2.7
1	E	443	GLU	2.7
1	C	759	GLN	2.7
1	E	159	LYS	2.7
1	E	279	ASP	2.7
1	E	69	THR	2.7
1	A	375	LYS	2.7
1	E	236	ASP	2.7
1	E	353	ALA	2.6
1	E	303	LEU	2.6
2	F	461	ASP	2.6
1	E	477	ASN	2.6
1	E	464	LEU	2.6
1	E	793	PHE	2.6
1	E	399	ARG	2.6
1	E	145	GLN	2.6
1	E	272	ALA	2.6
1	C	292	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	446	ASP	2.6
1	A	420	PRO	2.6
1	C	7	ASP	2.6
1	E	85	ASP	2.6
1	E	285	PHE	2.6
1	E	445	ILE	2.6
1	C	509	LYS	2.6
2	D	490	ARG	2.6
1	C	109	VAL	2.5
1	E	77	LEU	2.5
1	C	261	ASP	2.5
1	E	123	ASP	2.5
1	E	522	MET	2.5
1	E	252	PRO	2.5
1	E	501	LEU	2.5
1	E	161	ASP	2.5
1	A	199	ASP	2.5
1	C	83	ASP	2.5
1	E	18	ASN	2.5
1	E	546	GLU	2.5
1	E	234	GLY	2.5
1	A	194	ASP	2.5
1	C	3	ALA	2.5
1	C	106	PRO	2.5
1	A	86	VAL	2.5
1	A	362	ASP	2.5
1	E	186	ASN	2.5
1	C	180	ARG	2.4
1	C	315	GLU	2.4
1	E	547	HIS	2.4
1	E	2	VAL	2.4
1	E	209	VAL	2.4
1	E	814	LYS	2.4
1	E	393	ARG	2.4
1	E	35	LEU	2.4
1	E	791	GLN	2.4
1	C	4	PHE	2.4
1	E	136	CYS	2.4
1	E	549	HIS	2.4
1	C	169	VAL	2.4
1	C	295	GLU	2.4
1	E	183	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	503	LYS	2.4
1	A	82	SER	2.4
1	E	11	SER	2.4
1	A	495	VAL	2.4
1	E	365	ASN	2.4
1	E	495	VAL	2.4
1	A	291	PHE	2.4
1	C	302	LYS	2.3
1	E	480	VAL	2.3
1	C	748	ASN	2.3
1	E	334	LEU	2.3
1	E	780	PHE	2.3
1	C	253	LYS	2.3
1	C	286	THR	2.3
1	E	19	VAL	2.3
1	E	394	PHE	2.3
1	E	483	PHE	2.3
1	E	357	TYR	2.3
1	E	39	LEU	2.3
1	E	341	HIS	2.3
1	C	84	GLU	2.3
1	E	275	MET	2.3
1	E	295	GLU	2.3
1	C	239	LYS	2.3
1	C	815	ALA	2.3
1	E	355	GLN	2.3
1	E	280	PRO	2.3
1	A	310	ASP	2.3
1	E	5	THR	2.3
2	F	490	ARG	2.2
1	A	313	ASP	2.2
1	C	288	ILE	2.2
1	E	174	LEU	2.2
1	C	482	LYS	2.2
1	E	364	ALA	2.2
1	E	73	THR	2.2
1	C	229	TYR	2.2
1	A	156	VAL	2.2
1	E	241	MET	2.2
1	E	731	VAL	2.2
1	C	100	ILE	2.2
1	E	305	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	244	LEU	2.2
1	E	84	GLU	2.2
1	E	377	ASP	2.2
1	A	293	LYS	2.2
1	E	410	LYS	2.2
1	E	428	ILE	2.2
1	E	171	LYS	2.2
1	A	29	ASP	2.2
1	E	440	ARG	2.2
1	C	170	SER	2.2
1	C	492	ALA	2.2
1	C	296	ILE	2.2
1	E	122	THR	2.2
1	E	347	THR	2.2
1	E	551	GLY	2.2
1	E	147	LEU	2.2
2	F	489	ALA	2.1
1	A	758	GLU	2.1
1	E	732	GLU	2.1
1	A	756	SER	2.1
1	C	525	SER	2.1
2	D	461	ASP	2.1
1	A	155	VAL	2.1
1	C	322	VAL	2.1
1	E	433	ARG	2.1
1	E	380	LEU	2.1
1	A	500	ASP	2.1
1	E	225	PHE	2.1
1	E	778	PHE	2.1
1	E	259	ASN	2.1
1	E	452	ASN	2.1
1	C	28	VAL	2.1
1	A	14	ASP	2.1
1	C	308	LYS	2.1
1	E	118	ALA	2.1
1	E	339	VAL	2.1
1	E	283	ARG	2.1
1	E	350	ALA	2.1
1	A	33	SER	2.1
1	A	211	PHE	2.1
1	E	328	LEU	2.1
1	C	270	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	127	VAL	2.0
1	E	471	THR	2.0
1	E	101	ASN	2.0
1	C	5	THR	2.0
1	E	349	GLN	2.0
1	E	398	GLY	2.0
1	A	233	PHE	2.0
1	C	94	ASP	2.0
1	C	524	GLU	2.0
1	E	43	ALA	2.0
1	E	465	LYS	2.0
1	A	298	VAL	2.0
1	E	121	VAL	2.0
1	C	316	GLY	2.0
1	C	433	ARG	2.0
1	E	165	LEU	2.0
1	C	312	LYS	2.0
1	E	337	MET	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	E	699	20/21	0.91	0.24	30,62,75,79	0
1	DDE	C	699	20/21	0.93	0.20	14,61,107,114	0
1	DDE	A	699	10/21	0.95	0.19	40,49,57,57	0

## 6.3 Carbohydrates [i](#)

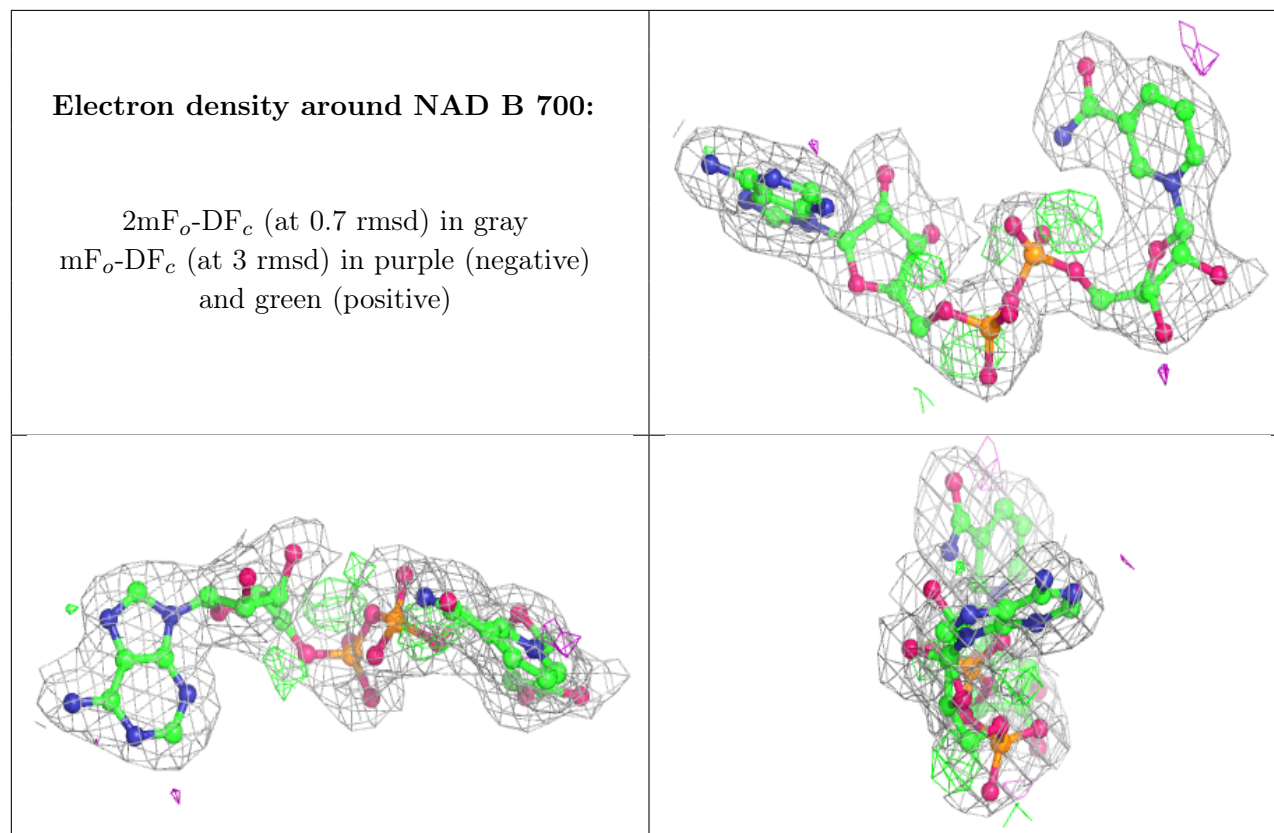
There are no monosaccharides in this entry.

## 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	B	700	44/44	0.96	0.15	4,20,39,42	0
3	NAD	D	701	44/44	0.96	0.15	7,22,38,45	0
3	NAD	F	702	44/44	0.96	0.15	11,24,38,48	0

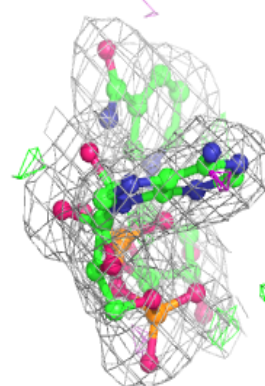
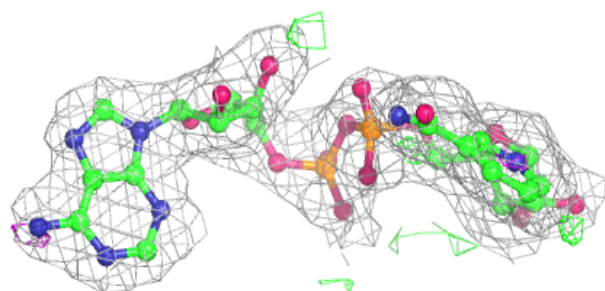
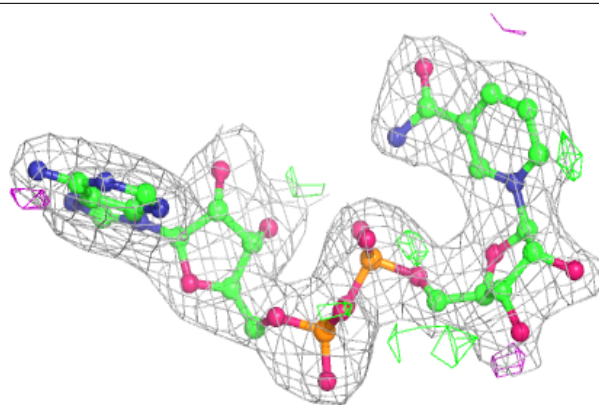
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



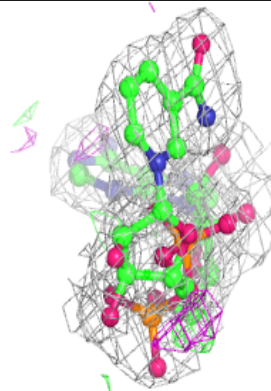
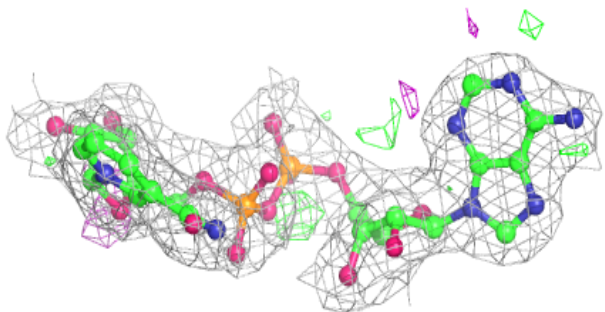
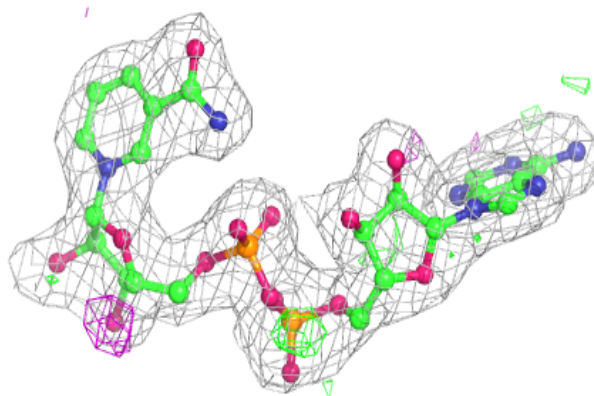


**Electron density around NAD D 701:**

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

**Electron density around NAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.