



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3B78  
Title : Structure of the eEF2-ExoA(R551H)-NAD<sup>+</sup> complex  
Authors : Jorgensen, R.; Merrill, A.R.  
Deposited on : 2007-10-30  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

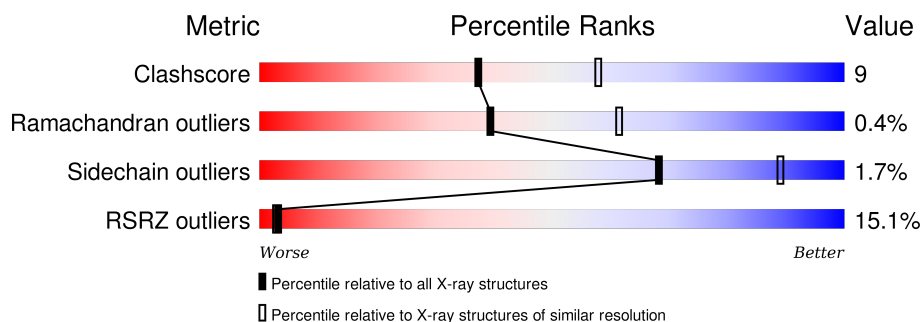
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	C	842	<div> <div>10%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	E	842	<div> <div>42%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>
2	B	207	<div> <div>84%</div> <div>16%</div> </div>
2	D	207	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
2	F	207	<div> <div>2%</div> <div>85%</div> <div>14%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Elongation factor 2.

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

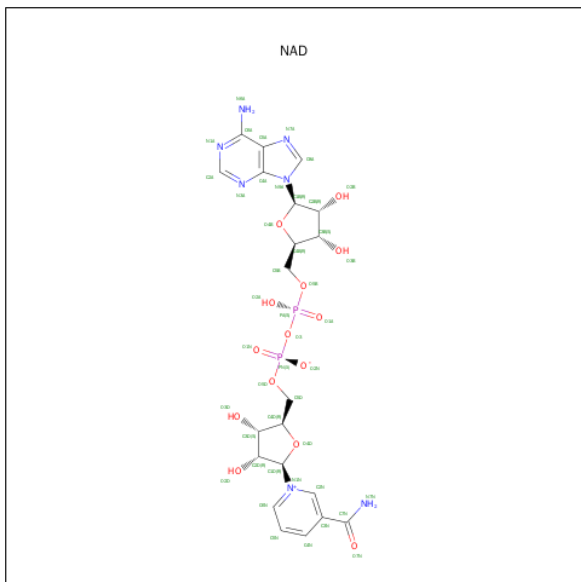
- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1587	1001	282	304			
2	D	207	Total	C	N	O	0	0	0
			1587	1001	282	304			
2	F	207	Total	C	N	O	0	0	0
			1587	1001	282	304			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	399	ALA	-	EXPRESSION TAG	UNP P11439
B	407	VAL	ILE	SEE REMARK 999	UNP P11439
B	515	SER	GLY	SEE REMARK 999	UNP P11439
B	551	HIS	ARG	ENGINEERED	UNP P11439
D	399	ALA	-	EXPRESSION TAG	UNP P11439
D	407	VAL	ILE	SEE REMARK 999	UNP P11439
D	515	SER	GLY	SEE REMARK 999	UNP P11439
D	551	HIS	ARG	ENGINEERED	UNP P11439
F	399	ALA	-	EXPRESSION TAG	UNP P11439
F	407	VAL	ILE	SEE REMARK 999	UNP P11439
F	515	SER	GLY	SEE REMARK 999	UNP P11439
F	551	HIS	ARG	ENGINEERED	UNP P11439

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

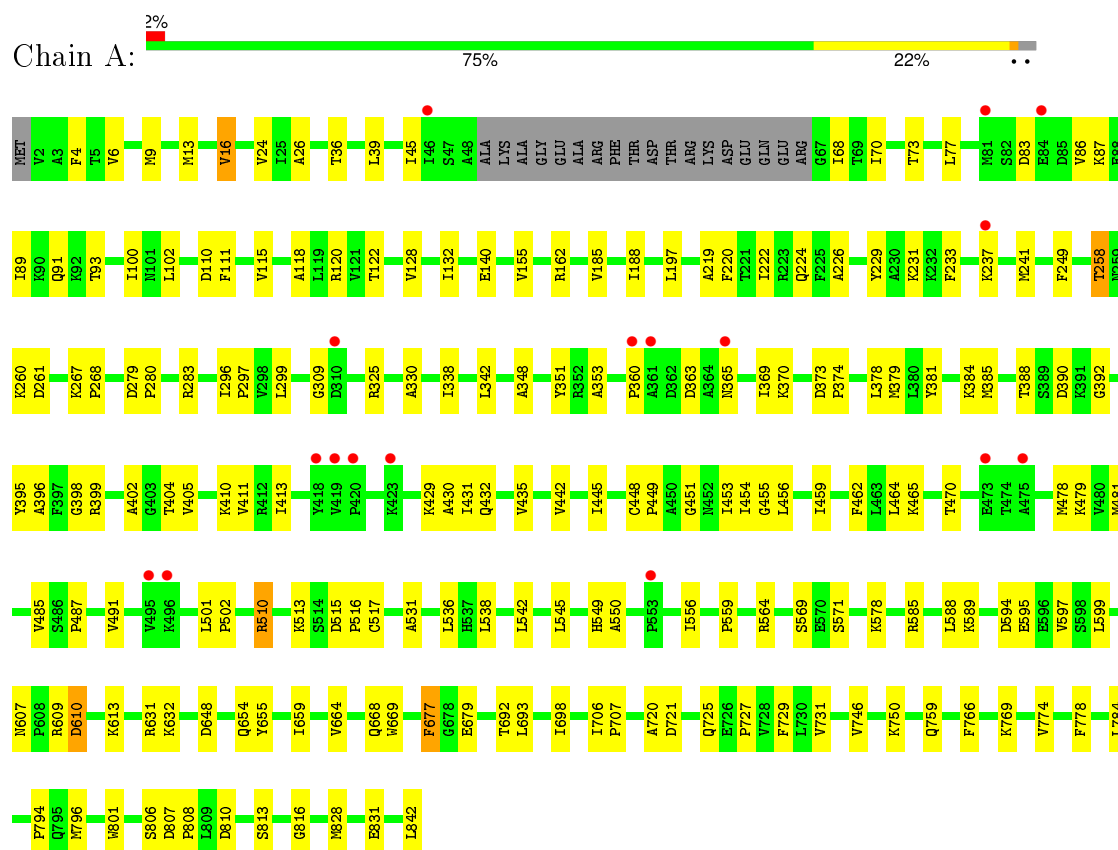
- Molecule 4 is water.

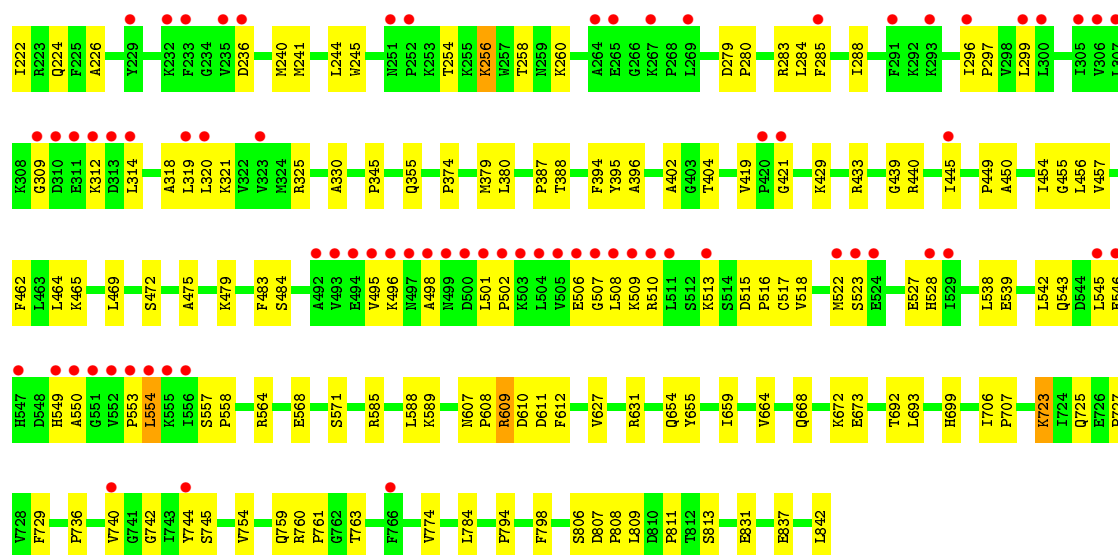
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	103	Total	O	0	0
			103	103		
4	C	84	Total	O	0	0
			84	84		
4	D	106	Total	O	0	0
			106	106		
4	E	35	Total	O	0	0
			35	35		
4	F	76	Total	O	0	0
			76	76		

### 3 Residue-property plots

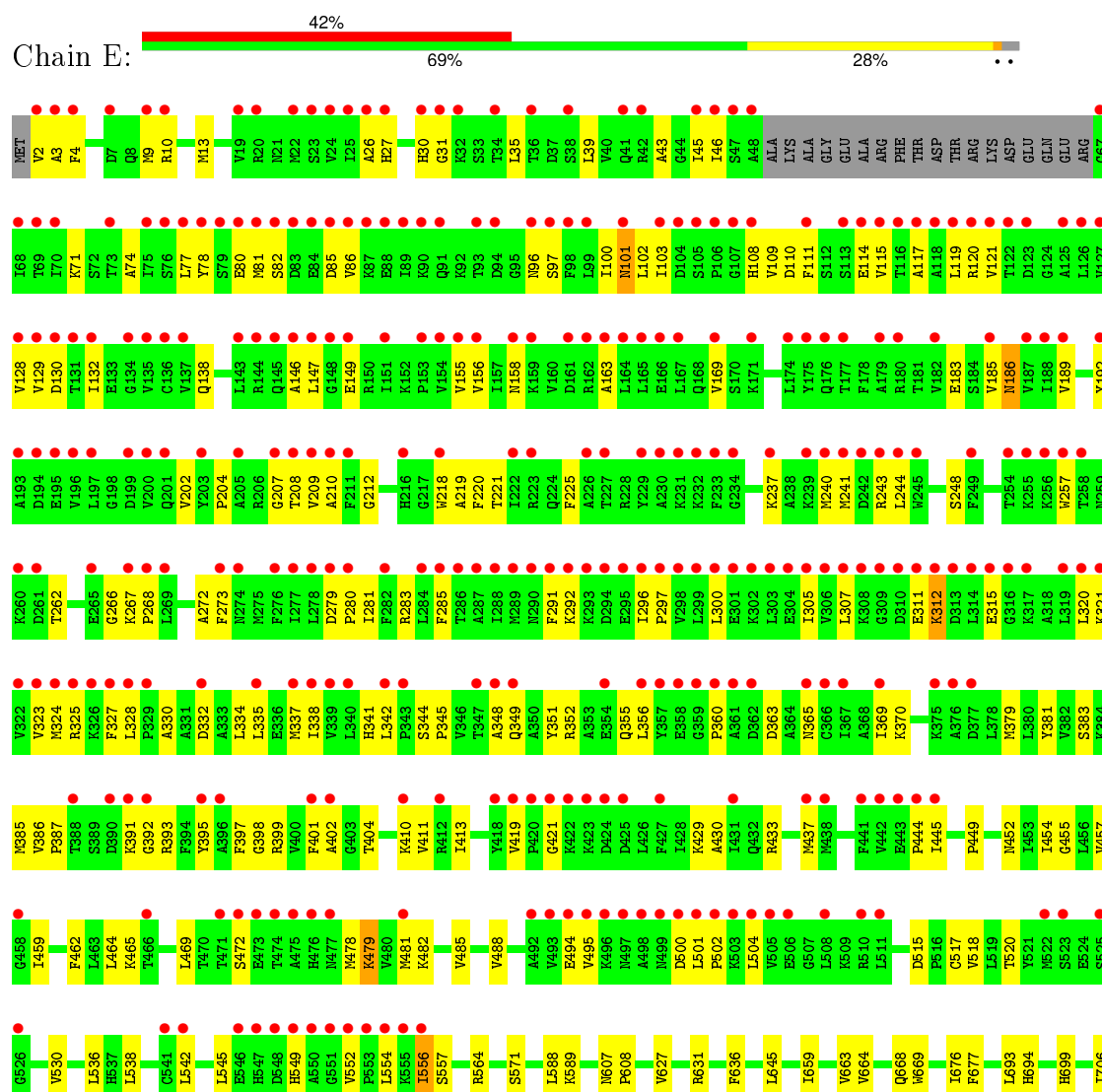
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

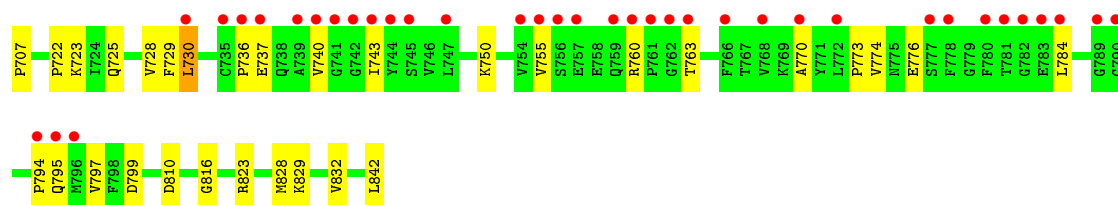
#### • Molecule 1: Elongation factor 2



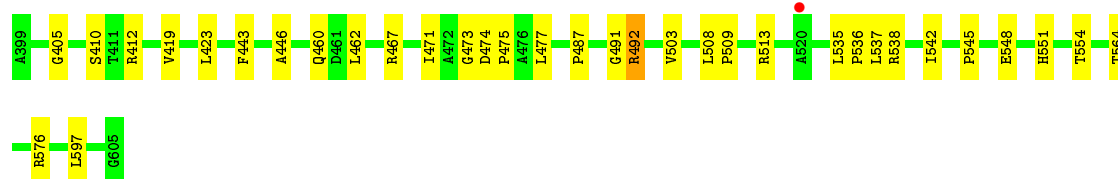
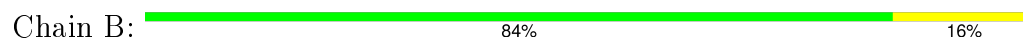


### • Molecule 1: Elongation factor 2

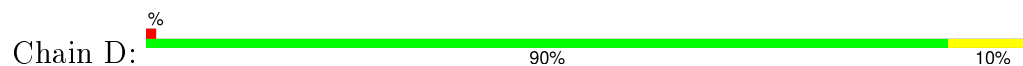




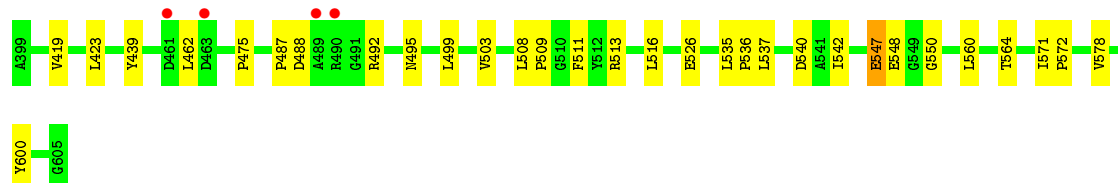
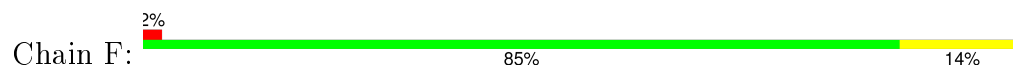
• Molecule 2: Exotoxin A



• 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, $\alpha$ , $\beta$ , $\gamma$	327.14Å 68.13Å 190.58Å 90.00° 102.99° 90.00°	Depositor
Resolution (Å)	46.55 – 2.50 46.55 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.55-2.50) 92.0 (46.55-2.48)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.206 , 0.242 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 134421 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24616	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 38.77 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5087e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.21	0/6517	0.39	0/8823
1	C	0.21	0/6517	0.38	0/8823
1	E	0.21	0/6517	0.37	0/8823
2	B	0.21	0/1627	0.40	0/2217
2	D	0.21	0/1627	0.40	0/2217
2	F	0.21	0/1627	0.38	0/2217
All	All	0.21	0/24432	0.38	0/33120

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	113	0
1	C	6415	0	6488	128	0
1	E	6405	0	6472	167	0
2	B	1587	0	1536	21	0
2	D	1587	0	1536	10	0
2	F	1587	0	1536	14	0
3	B	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	26	2	0
3	F	44	0	26	0	0
4	A	94	0	0	0	0
4	B	103	0	0	1	0
4	C	84	0	0	0	0
4	D	106	0	0	0	0
4	E	35	0	0	0	0
4	F	76	0	0	0	0
All	All	24616	0	24118	448	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 9.

All (448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:DDE:HAT2	1:C:699:DDE:HAB2	1.39	1.04
1:C:699:DDE:HAA1	3:D:701:NAD:H4D	1.52	0.89
1:E:488:VAL:HG11	1:E:774:VAL:HG21	1.55	0.88
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.55	0.88
1:C:404:THR:HG22	1:C:449:PRO:HA	1.59	0.84
1:C:568:GLU:HB2	1:C:723:LYS:HD3	1.58	0.84
1:A:571:SER:HB2	1:A:589:LYS:HG3	1.61	0.83
1:C:216:HIS:HD2	1:C:321:LYS:HG2	1.42	0.82
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.61	0.82
1:E:391:LYS:HG3	1:E:392:GLY:H	1.44	0.82
1:A:513:LYS:HA	1:A:513:LYS:HE2	1.62	0.80
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.65	0.79
1:C:132:ILE:H	1:C:132:ILE:HD12	1.46	0.79
1:C:507:GLY:HA3	1:C:549:HIS:HB3	1.64	0.79
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.65	0.77
1:E:149:GLU:HA	1:E:355:GLN:HE22	1.48	0.76
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.68	0.76
1:C:258:THR:HG22	1:C:260:LYS:H	1.51	0.75
1:A:360:PRO:HG2	1:A:363:ASP:HB2	1.69	0.74
1:A:404:THR:HG22	1:A:449:PRO:HA	1.69	0.74
1:E:404:THR:HG22	1:E:449:PRO:HA	1.67	0.74
1:C:699:DDE:CAB	1:C:699:DDE:HAT2	2.16	0.73
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.71	0.73
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.24	0.72
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.72	0.71
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.75	0.68
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.74	0.68
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.76	0.68
1:C:216:HIS:CD2	1:C:321:LYS:HG2	2.28	0.67
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.76	0.67
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.76	0.66
1:E:556:ILE:HG22	1:E:557:SER:H	1.61	0.66
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.77	0.66
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.66
1:E:43:ALA:HB1	1:E:78:TYR:H	1.61	0.65
1:E:30:HIS:ND1	1:E:130:ASP:HB2	2.12	0.64
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.79	0.64
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.33	0.64
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.79	0.63
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.80	0.63
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.82	0.62
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.80	0.62
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.81	0.62
1:A:578:LYS:HG2	1:A:585:ARG:HG2	1.81	0.62
1:C:495:VAL:HG21	1:C:501:LEU:HD12	1.80	0.62
2:F:516:LEU:HD12	2:F:526:GLU:HG2	1.81	0.62
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.80	0.61
1:C:216:HIS:HB2	1:C:218:TRP:HD1	1.66	0.61
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.81	0.61
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.82	0.61
1:E:810:ASP:O	1:E:816:GLY:HA3	2.00	0.61
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.82	0.61
1:C:759:GLN:HG2	1:C:760:ARG:H	1.67	0.60
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.84	0.60
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.84	0.60
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.82	0.60
1:C:464:LEU:HD23	1:C:483:PHE:HE1	1.67	0.59
1:A:810:ASP:O	1:A:816:GLY:HA3	2.01	0.59
1:A:510:ARG:HG3	1:A:549:HIS:HD2	1.66	0.59
1:A:399:ARG:HB2	1:A:453:ILE:HD13	1.84	0.59
1:C:699:DDE:NAD	1:C:699:DDE:HAA3	2.16	0.59
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.38	0.58
1:C:103:ILE:HD12	1:C:122:THR:HG22	1.86	0.58
1:E:121:VAL:HG11	1:E:383:SER:OG	2.02	0.58
1:A:405:VAL:HG12	1:A:448:CYS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:ASN:HB2	1:C:610:ASP:HB2	1.86	0.58
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.86	0.58
1:C:103:ILE:HD13	1:C:121:VAL:HG23	1.85	0.58
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.68	0.58
1:A:431:ILE:HD12	1:A:459:ILE:HD11	1.86	0.57
1:E:291:PHE:HD1	1:E:315:GLU:HB3	1.69	0.57
1:E:26:ALA:CB	1:E:128:VAL:HB	2.34	0.57
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.84	0.57
1:A:237:LYS:O	1:A:241:MET:HG2	2.04	0.57
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.86	0.57
1:C:496:LYS:H	1:C:554:LEU:HD22	1.70	0.57
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.39	0.57
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.40	0.57
1:A:569:SER:O	1:A:720:ALA:HB1	2.05	0.57
1:A:654:GLN:HG2	1:A:655:TYR:CD1	2.38	0.57
1:C:723:LYS:HA	1:C:808:PRO:HG3	1.87	0.57
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.86	0.57
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.19	0.57
1:E:464:LEU:HG	1:E:465:LYS:HG3	1.87	0.57
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.87	0.56
2:B:477:LEU:HD22	2:B:551:HIS:HB3	1.87	0.56
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.41	0.56
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.21	0.56
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.45	0.56
1:C:664:VAL:O	1:C:668:GLN:HG2	2.06	0.56
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.41	0.55
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.88	0.55
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.87	0.55
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.87	0.55
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.89	0.55
1:E:291:PHE:CD1	1:E:315:GLU:HB3	2.42	0.55
1:A:6:VAL:HG13	1:A:445:ILE:HG22	1.89	0.55
1:A:68:ILE:HD13	1:A:390:ASP:HB2	1.89	0.55
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.88	0.54
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.89	0.54
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.89	0.54
1:A:381:TYR:O	1:A:398:GLY:HA3	2.07	0.54
1:A:510:ARG:HG3	1:A:549:HIS:CD2	2.42	0.54
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.88	0.54
1:E:391:LYS:HG3	1:E:392:GLY:N	2.20	0.54
1:A:501:LEU:N	1:A:502:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.72	0.54
1:E:9:MET:O	1:E:13:MET:HG3	2.07	0.53
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.90	0.53
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.91	0.53
1:E:755:VAL:HG23	1:E:770:ALA:HA	1.91	0.53
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.89	0.53
1:C:609:ARG:HD2	1:C:609:ARG:H	1.73	0.53
1:C:699:DDE:CAA	3:D:701:NAD:H4D	2.33	0.53
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.89	0.53
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.91	0.53
1:A:258:THR:HG22	1:A:260:LYS:H	1.74	0.53
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.91	0.53
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.91	0.53
1:C:374:PRO:O	1:C:404:THR:HG23	2.08	0.52
1:C:727:PRO:HB2	1:C:774:VAL:HG21	1.92	0.52
1:C:699:DDE:HAA3	1:C:699:DDE:HAD2	1.75	0.52
1:C:17:THR:HB	1:C:92:LYS:O	2.09	0.52
1:E:564:ARG:HB2	1:E:725:GLN:HB2	1.90	0.52
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.91	0.52
1:C:6:VAL:HG13	1:C:445:ILE:HG22	1.91	0.52
1:A:410:LYS:HG2	1:A:430:ALA:HB2	1.92	0.52
1:E:296:ILE:O	1:E:300:LEU:HD13	2.10	0.52
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.91	0.52
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.92	0.52
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.91	0.51
1:E:207:GLY:O	1:E:337:MET:HG2	2.09	0.51
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.39	0.51
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.91	0.51
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.45	0.51
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.51
1:A:197:LEU:HD21	1:A:351:TYR:CD1	2.45	0.51
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.92	0.51
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.93	0.51
1:E:385:MET:HG2	1:E:465:LYS:HA	1.92	0.51
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.11	0.51
1:C:70:ILE:HG22	1:C:388:THR:HG22	1.91	0.51
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.93	0.50
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.92	0.50
1:A:632:LYS:HD3	1:A:648:ASP:O	2.11	0.50
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.93	0.50
1:E:74:ALA:HA	1:E:102:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ASN:O	1:A:369:ILE:HG13	2.11	0.50
1:E:243:ARG:O	1:E:248:SER:HB2	2.10	0.50
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.93	0.50
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.93	0.50
1:E:111:PHE:HB3	1:E:114:GLU:HG2	1.94	0.50
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.41	0.50
1:E:750:LYS:HD2	1:E:776:GLU:O	2.12	0.50
1:A:110:ASP:HB3	1:A:536:LEU:HD22	1.93	0.50
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.47	0.49
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.95	0.49
1:E:482:LYS:HB3	1:E:797:VAL:HG11	1.94	0.49
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.94	0.49
1:C:200:VAL:O	1:C:200:VAL:HG12	2.13	0.49
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.77	0.49
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.48	0.49
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.94	0.49
1:E:419:VAL:HG12	1:E:421:GLY:H	1.77	0.49
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.94	0.49
1:E:312:LYS:O	1:E:312:LYS:HD2	2.13	0.49
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.93	0.49
1:C:515:ASP:O	1:C:518:VAL:HG12	2.13	0.49
1:C:699:DDE:CAB	1:C:699:DDE:CAT	2.86	0.49
1:A:249:PHE:CZ	1:A:261:ASP:HB3	2.48	0.49
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.95	0.48
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.48	0.48
1:A:378:LEU:O	1:A:470:THR:HA	2.12	0.48
1:E:365:ASN:HD21	1:E:472:SER:HB3	1.77	0.48
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.95	0.48
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.48	0.48
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.95	0.48
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.78	0.48
1:C:627:VAL:O	1:C:631:ARG:HB2	2.14	0.48
1:C:538:LEU:O	1:C:542:LEU:HB2	2.14	0.48
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.95	0.48
1:A:9:MET:O	1:A:13:MET:HG3	2.14	0.48
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.96	0.48
1:E:101:ASN:N	1:E:101:ASN:HD22	2.12	0.48
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.95	0.48
1:E:292:LYS:O	1:E:296:ILE:HG13	2.14	0.48
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.49	0.47
1:C:254:THR:HG22	1:C:256:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:GLU:HA	1:C:550:ALA:HB3	1.95	0.47
1:E:823:ARG:HE	1:E:832:VAL:HG22	1.79	0.47
2:B:467:ARG:NH1	2:B:536:PRO:HG3	2.28	0.47
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.95	0.47
1:A:828:MET:HG2	2:B:576:ARG:NE	2.29	0.47
1:A:487:PRO:HB3	1:A:531:ALA:HB1	1.97	0.47
1:E:257:TRP:HZ3	1:E:272:ALA:HB2	1.79	0.47
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.97	0.47
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.95	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
1:A:746:VAL:O	1:A:750:LYS:HD3	2.15	0.47
1:C:321:LYS:O	1:C:325:ARG:HG3	2.15	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
2:D:538:ARG:HD2	2:D:538:ARG:HA	1.69	0.47
1:C:296:ILE:N	1:C:297:PRO:HD2	2.29	0.47
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.97	0.47
1:C:465:LYS:HE3	1:C:517:CYS:SG	2.55	0.47
1:E:321:LYS:O	1:E:325:ARG:HG3	2.14	0.47
1:E:627:VAL:O	1:E:631:ARG:HB2	2.14	0.47
1:A:338:ILE:O	1:A:342:LEU:HB2	2.15	0.47
1:E:39:LEU:H	1:E:39:LEU:HD12	1.79	0.47
1:A:731:VAL:HG22	1:A:796:MET:HB3	1.97	0.47
1:A:111:PHE:O	1:A:115:VAL:HG23	2.15	0.47
1:C:37:ASP:O	1:C:41:GLN:HB2	2.15	0.47
1:C:736:PRO:O	1:C:740:VAL:HG23	2.15	0.47
1:C:727:PRO:HB2	1:C:774:VAL:CG2	2.45	0.47
2:B:419:VAL:O	2:B:423:LEU:HG	2.14	0.47
2:F:547:GLU:HG3	2:F:550:GLY:HA3	1.97	0.47
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.96	0.47
1:E:391:LYS:CG	1:E:392:GLY:H	2.22	0.46
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.96	0.46
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.30	0.46
2:B:545:PRO:HA	2:B:551:HIS:O	2.15	0.46
1:A:454:ILE:HG13	1:A:455:GLY:H	1.80	0.46
1:E:30:HIS:CE1	1:E:130:ASP:HB2	2.50	0.46
1:E:459:ILE:HG22	1:E:459:ILE:O	2.16	0.46
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.98	0.46
1:A:6:VAL:CG1	1:A:445:ILE:HG22	2.45	0.46
1:A:478:MET:O	1:A:479:LYS:C	2.54	0.46
1:E:676:ILE:HG22	1:E:677:PHE:HD2	1.80	0.46
1:C:226:ALA:HB2	1:C:241:MET:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.97	0.46
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.97	0.46
1:A:731:VAL:O	1:A:769:LYS:HA	2.15	0.46
1:E:111:PHE:O	1:E:115:VAL:HG23	2.16	0.46
1:E:296:ILE:N	1:E:297:PRO:HD2	2.31	0.46
1:C:169:VAL:HG22	1:C:173:ASP:HB2	1.98	0.46
1:E:349:GLN:O	1:E:370:LYS:HA	2.15	0.46
1:E:823:ARG:HG2	1:E:828:MET:HE3	1.98	0.46
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.45	0.46
1:C:672:LYS:C	1:C:673:GLU:HG2	2.36	0.46
1:A:385:MET:HG2	1:A:465:LYS:HA	1.97	0.46
1:E:324:MET:HE2	1:E:324:MET:HA	1.98	0.45
1:E:552:VAL:O	1:E:554:LEU:HG	2.16	0.45
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.99	0.45
1:A:118:ALA:O	1:A:122:THR:HG23	2.17	0.45
1:C:126:LEU:HD12	1:C:154:VAL:HG12	1.97	0.45
1:E:185:VAL:O	1:E:189:VAL:HG23	2.16	0.45
1:A:197:LEU:HD21	1:A:351:TYR:CE1	2.52	0.45
1:C:149:GLU:HA	1:C:355:GLN:HE22	1.82	0.45
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.82	0.45
1:C:585:ARG:HB2	1:C:692:THR:OG1	2.17	0.45
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.98	0.45
1:E:183:GLU:HA	1:E:186:ASN:OD1	2.17	0.45
1:E:156:VAL:HG11	1:E:334:LEU:HD21	1.98	0.45
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.99	0.45
1:E:204:PRO:HA	1:E:209:VAL:HB	1.98	0.45
1:A:411:VAL:HG21	1:A:431:ILE:HD11	1.99	0.45
1:E:46:ILE:N	1:E:46:ILE:HD12	2.32	0.45
1:E:538:LEU:O	1:E:542:LEU:HG	2.17	0.45
1:E:659:ILE:O	1:E:663:VAL:HG23	2.17	0.45
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.99	0.45
1:E:208:THR:HG23	1:E:341:HIS:CE1	2.52	0.45
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.17	0.45
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.51	0.45
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.46	0.45
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.46	0.45
1:C:539:GLU:O	1:C:543:GLN:HG3	2.17	0.45
1:E:129:VAL:HG12	1:E:130:ASP:N	2.32	0.45
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.52	0.45
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.97	0.45
1:E:556:ILE:HG22	1:E:557:SER:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG21	1:A:451:GLY:HA3	1.98	0.45
2:F:571:ILE:HA	2:F:572:PRO:HD3	1.85	0.45
1:A:664:VAL:O	1:A:668:GLN:HG2	2.16	0.45
1:A:465:LYS:HE3	1:A:517:CYS:SG	2.57	0.44
1:C:380:LEU:HB3	1:C:469:LEU:HB2	1.99	0.44
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.44
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.16	0.44
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.85	0.44
2:F:487:PRO:HA	2:F:492:ARG:O	2.18	0.44
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.33	0.44
1:E:344:SER:HB2	1:E:345:PRO:HD2	1.99	0.44
1:E:459:ILE:N	1:E:459:ILE:HD12	2.33	0.44
2:B:487:PRO:HB2	2:B:491:GLY:HA2	1.99	0.44
1:A:231:LYS:HB3	1:A:231:LYS:HE2	1.81	0.44
1:C:498:ALA:HA	1:C:501:LEU:HB2	2.00	0.44
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.18	0.44
1:C:729:PHE:CE2	1:C:774:VAL:HG22	2.53	0.44
1:A:727:PRO:HD3	1:A:801:TRP:HZ3	1.82	0.44
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.99	0.44
2:B:474:ASP:HA	2:B:475:PRO:HD2	1.87	0.44
1:E:103:ILE:N	1:E:103:ILE:HD12	2.32	0.44
1:C:395:TYR:CD1	1:C:457:VAL:HG22	2.53	0.44
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.53	0.44
1:A:283:ARG:HB3	1:A:299:LEU:HD21	1.99	0.44
1:E:365:ASN:O	1:E:369:ILE:HG12	2.16	0.44
1:E:369:ILE:HD12	1:E:401:PHE:HB3	2.00	0.44
2:B:471:ILE:CG1	2:B:554:THR:HB	2.47	0.44
1:E:132:ILE:N	1:E:132:ILE:HD12	2.33	0.44
1:C:557:SER:HB2	1:C:558:PRO:HD2	2.00	0.44
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.79	0.44
1:E:77:LEU:HD23	1:E:335:LEU:HD21	2.00	0.43
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.00	0.43
1:C:70:ILE:O	1:C:440:ARG:HG2	2.18	0.43
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.18	0.43
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.90	0.43
1:A:515:ASP:HA	1:A:516:PRO:HD2	1.87	0.43
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.48	0.43
2:B:410:SER:OG	2:B:412:ARG:HG3	2.18	0.43
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.54	0.43
1:E:381:TYR:O	1:E:398:GLY:HA3	2.17	0.43
1:A:392:GLY:HA3	1:A:513:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PRO:O	1:A:404:THR:HG23	2.18	0.43
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.43
1:E:237:LYS:O	1:E:241:MET:HG3	2.18	0.43
1:C:807:ASP:HA	1:C:808:PRO:HD2	1.86	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.00	0.43
1:E:218:TRP:HB3	1:E:324:MET:HB3	2.00	0.43
1:C:396:ALA:HB3	1:C:456:LEU:HB2	2.01	0.43
2:F:511:PHE:HB3	2:F:600:TYR:CD1	2.54	0.43
1:C:484:SER:HB3	1:C:798:PHE:H	1.84	0.43
2:D:571:ILE:HA	2:D:572:PRO:HD3	1.88	0.43
1:C:723:LYS:HE3	1:C:723:LYS:HB3	1.67	0.43
1:C:43:ALA:HB1	1:C:78:TYR:O	2.18	0.43
1:A:36:THR:HG23	1:A:102:LEU:HD21	2.01	0.43
1:E:737:GLU:HA	1:E:740:VAL:HG23	2.00	0.43
1:A:759:GLN:HB2	1:A:766:PHE:CE2	2.53	0.43
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.54	0.43
1:A:588:LEU:HD12	1:A:588:LEU:C	2.39	0.43
1:A:73:THR:HG21	1:A:384:LYS:HD2	2.01	0.43
1:E:327:PHE:CD2	1:E:328:LEU:HG	2.54	0.43
1:E:338:ILE:O	1:E:342:LEU:HB2	2.18	0.43
1:E:279:ASP:O	1:E:283:ARG:HG2	2.18	0.43
1:A:120:ARG:NH1	1:A:479:LYS:HD2	2.33	0.43
1:A:613:LYS:HG2	1:A:631:ARG:HH11	1.83	0.43
1:C:144:ARG:HD3	1:C:192:TYR:CZ	2.54	0.43
1:C:26:ALA:HB2	1:C:128:VAL:HB	2.00	0.43
1:A:669:TRP:CZ2	2:B:492:ARG:HB2	2.53	0.43
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.78	0.43
1:E:244:LEU:O	1:E:273:PHE:HB2	2.18	0.43
1:E:485:VAL:O	1:E:485:VAL:HG22	2.18	0.43
2:F:537:LEU:HD11	2:F:542:ILE:HG22	2.00	0.43
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.99	0.43
1:A:831:GLU:H	1:A:831:GLU:CD	2.20	0.43
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.53	0.43
1:A:413:ILE:HD13	1:A:459:ILE:HG23	2.00	0.42
1:E:823:ARG:HG2	1:E:828:MET:CE	2.49	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.83	0.42
2:B:477:LEU:HD22	2:B:551:HIS:CB	2.50	0.42
1:A:545:LEU:O	1:A:550:ALA:HB3	2.19	0.42
1:A:4:PHE:HD2	1:A:45:ILE:HG23	1.83	0.42
1:E:722:PRO:O	1:E:723:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:LEU:O	1:C:811:PRO:HD3	2.20	0.42
1:A:155:VAL:HG21	1:A:185:VAL:HG11	2.01	0.42
1:A:132:ILE:HD12	1:A:162:ARG:HD3	2.01	0.42
2:D:433:GLY:O	2:D:505:ARG:HG3	2.18	0.42
1:E:39:LEU:HD11	1:E:334:LEU:HD13	2.01	0.42
2:F:495:ASN:HB3	2:F:578:VAL:HG22	2.02	0.42
1:C:806:SER:HB2	1:C:813:SER:HB2	2.02	0.42
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.50	0.42
1:A:727:PRO:HB2	1:A:774:VAL:HG21	2.02	0.42
2:F:488:ASP:HB3	2:F:492:ARG:HB2	2.01	0.42
2:F:419:VAL:O	2:F:423:LEU:HG	2.19	0.42
1:E:664:VAL:O	1:E:668:GLN:HG2	2.19	0.42
1:C:588:LEU:C	1:C:588:LEU:HD12	2.40	0.42
1:C:153:PRO:HD2	1:C:200:VAL:CG1	2.50	0.42
1:E:397:PHE:CD1	1:E:437:MET:HG3	2.54	0.42
1:E:155:VAL:HG21	1:E:202:VAL:HG21	2.02	0.42
1:A:806:SER:HB2	1:A:813:SER:HB2	2.02	0.42
1:C:654:GLN:O	1:C:655:TYR:HB2	2.20	0.42
2:D:474:ASP:HA	2:D:475:PRO:HD2	1.87	0.42
1:A:388:THR:HG21	1:A:395:TYR:CG	2.55	0.42
1:C:506:GLU:O	1:C:510:ARG:HG3	2.19	0.42
1:C:501:LEU:HD23	1:C:501:LEU:C	2.41	0.41
2:D:537:LEU:O	2:D:538:ARG:HD3	2.19	0.41
1:E:608:PRO:HG3	1:E:636:PHE:CG	2.55	0.41
1:C:3:ALA:HB2	1:C:46:ILE:HG13	2.02	0.41
1:E:410:LYS:HA	1:E:430:ALA:HA	2.02	0.41
1:A:140:GLU:HG3	1:A:188:ILE:HD13	2.02	0.41
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.20	0.41
2:B:513:ARG:HD3	4:B:779:HOH:O	2.19	0.41
1:C:285:PHE:CE1	1:C:320:LEU:HD21	2.54	0.41
1:C:288:ILE:HA	1:C:296:ILE:HD11	2.03	0.41
1:C:241:MET:HA	1:C:244:LEU:HD12	2.02	0.41
1:C:509:LYS:O	1:C:513:LYS:HG3	2.19	0.41
1:C:742:GLY:O	1:C:745:SER:HB3	2.19	0.41
1:C:284:LEU:HD23	1:C:299:LEU:HD23	2.01	0.41
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.55	0.41
1:A:410:LYS:HA	1:A:430:ALA:HA	2.01	0.41
2:B:537:LEU:O	2:B:538:ARG:HD3	2.20	0.41
1:C:26:ALA:CB	1:C:128:VAL:HB	2.51	0.41
2:F:508:LEU:N	2:F:509:PRO:CD	2.83	0.41
2:D:508:LEU:N	2:D:509:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:SER:HA	1:C:439:GLY:O	2.19	0.41
1:E:307:LEU:HD13	1:E:311:GLU:O	2.20	0.41
1:A:677:PHE:N	1:A:677:PHE:CD2	2.88	0.41
1:E:80:GLU:HA	1:E:96:ASN:O	2.20	0.41
1:C:454:ILE:HG13	1:C:455:GLY:H	1.85	0.41
1:A:226:ALA:CB	1:A:241:MET:HB3	2.44	0.41
1:A:542:LEU:HD13	1:A:556:ILE:HG21	2.01	0.41
1:E:109:VAL:O	1:E:109:VAL:HG12	2.21	0.41
1:E:212:GLY:HA3	1:E:219:ALA:HA	2.02	0.41
1:E:3:ALA:HA	1:E:46:ILE:O	2.21	0.41
1:C:314:LEU:HD22	1:C:318:ALA:HB1	2.02	0.41
1:E:119:LEU:HD11	1:E:146:ALA:HA	2.02	0.41
1:C:419:VAL:HG12	1:C:421:GLY:H	1.86	0.41
1:E:588:LEU:C	1:E:588:LEU:HD12	2.41	0.41
1:C:760:ARG:CG	1:C:761:PRO:HD2	2.51	0.41
1:A:454:ILE:HG13	1:A:455:GLY:N	2.36	0.41
1:E:237:LYS:HA	1:E:240:MET:HB3	2.03	0.41
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.91	0.41
1:C:523:SER:OG	1:C:527:GLU:HB2	2.20	0.41
1:A:83:ASP:O	1:A:87:LYS:HG3	2.20	0.41
1:A:373:ASP:HA	1:A:374:PRO:HD2	1.85	0.41
1:E:345:PRO:HB3	1:E:399:ARG:HH21	1.85	0.41
1:C:226:ALA:CB	1:C:241:MET:HB3	2.51	0.41
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.56	0.41
1:E:728:VAL:HG22	1:E:773:PRO:HA	2.02	0.41
1:E:163:ALA:O	1:E:169:VAL:HG12	2.20	0.41
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.51	0.41
1:A:559:PRO:HB2	1:A:778:PHE:CE2	2.56	0.41
1:E:736:PRO:O	1:E:740:VAL:HG23	2.21	0.41
2:F:439:TYR:CE2	2:F:475:PRO:HD3	2.56	0.40
1:C:167:LEU:O	1:C:168:GLN:C	2.59	0.40
1:A:229:TYR:HB3	1:A:233:PHE:CD2	2.56	0.40
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.84	0.40
1:C:610:ASP:OD1	1:C:611:ASP:N	2.55	0.40
1:E:352:ARG:O	1:E:356:LEU:HG	2.21	0.40
1:E:262:THR:HG23	1:E:266:GLY:HA2	2.03	0.40
1:C:454:ILE:HG13	1:C:455:GLY:N	2.36	0.40
1:A:77:LEU:HB2	1:A:100:ILE:HB	2.03	0.40
2:B:443:PHE:CZ	2:B:446:ALA:HB2	2.57	0.40
1:C:155:VAL:HG21	1:C:185:VAL:HG11	2.03	0.40
1:A:481:MET:HE2	1:A:481:MET:HB2	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.56	0.40
1:C:16:VAL:HG21	1:C:450:ALA:O	2.22	0.40
1:A:396:ALA:HB3	1:A:456:LEU:HB2	2.03	0.40
1:A:659:ILE:HD13	1:A:693:LEU:HD21	2.04	0.40
1:E:454:ILE:HG13	1:E:455:GLY:N	2.36	0.40
1:C:612:PHE:CE1	1:C:631:ARG:HG3	2.57	0.40
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.56	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.56	0.40
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.90	0.40
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.03	0.40
1:E:452:ASN:N	1:E:452:ASN:HD22	2.19	0.40
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.04	0.40
1:A:594:ASP:HB2	1:A:597:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	818/842 (97%)	781 (96%)	34 (4%)	3 (0%)	39	61
1	C	818/842 (97%)	780 (95%)	33 (4%)	5 (1%)	30	50
1	E	818/842 (97%)	763 (93%)	52 (6%)	3 (0%)	39	61
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	198 (97%)	6 (3%)	1 (0%)	34	55
2	F	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
All	All	3069/3147 (98%)	2923 (95%)	134 (4%)	12 (0%)	39	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	E	479	LYS
1	A	432	GLN
1	C	168	GLN
1	C	479	LYS
2	D	488	ASP
1	E	556	ILE
1	E	795	GLN
1	C	554	LEU
1	C	215	LEU
1	A	721	ASP
1	C	309	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	688 (98%)	11 (2%)	70	90
1	C	699/714 (98%)	688 (98%)	11 (2%)	70	90
1	E	699/714 (98%)	691 (99%)	8 (1%)	80	94
2	B	161/161 (100%)	157 (98%)	4 (2%)	55	82
2	D	161/161 (100%)	158 (98%)	3 (2%)	65	87
2	F	161/161 (100%)	154 (96%)	7 (4%)	35	61
All	All	2580/2625 (98%)	2536 (98%)	44 (2%)	68	89

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	258	THR
1	A	325	ARG
1	A	510	ARG
1	A	595	GLU
1	A	599	LEU
1	A	609	ARG

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Mol	Chain	Res	Type
1	A	610	ASP
1	A	677	PHE
1	A	698	ILE
1	A	842	LEU
2	B	460	GLN
2	B	462	LEU
2	B	492	ARG
2	B	548	GLU
1	C	41	GLN
1	C	154	VAL
1	C	236	ASP
1	C	240	MET
1	C	256	LYS
1	C	312	LYS
1	C	609	ARG
1	C	723	LYS
1	C	831	GLU
1	C	837	GLU
1	C	842	LEU
2	D	462	LEU
2	D	499	LEU
2	D	540	ASP
1	E	101	ASN
1	E	186	ASN
1	E	312	LYS
1	E	332	ASP
1	E	494	GLU
1	E	730	LEU
1	E	829	LYS
1	E	842	LEU
2	F	462	LEU
2	F	499	LEU
2	F	513	ARG
2	F	540	ASP
2	F	547	GLU
2	F	548	GLU
2	F	560	LEU

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

Mol	Chain	Res	Type
1	A	549	HIS

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Mol	Chain	Res	Type
2	B	485	GLN
1	C	216	HIS
2	D	428	GLN
1	E	355	GLN
1	E	476	HIS
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	A	699	1	5,10,21	0.56	0	3,12,30	1.66	1 (33%)
1	DDE	C	699	1	13,20,21	0.84	0	16,28,30	1.13	1 (6%)
1	DDE	E	699	1	5,10,21	0.57	0	3,12,30	1.65	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	A	699	1	-	0/4/6/23	0/1/1/1
1	DDE	C	699	1	-	0/19/21/23	0/1/1/1
1	DDE	E	699	1	-	0/4/6/23	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	CAU-CBW-CBI	-2.82	105.41	110.92
1	A	699	DDE	CD2-NE2-CE1	2.00	108.87	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	7	0
1	E	699	DDE	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	B	700	-	38,48,48	0.65	0	47,73,73	2.09	5 (10%)
3	NAD	D	701	-	38,48,48	0.66	0	47,73,73	2.08	5 (10%)
3	NAD	F	702	-	38,48,48	0.66	0	47,73,73	2.09	5 (10%)

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	B	700	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	701	-	-	0/22/62/62	0/5/5/5
3	NAD	F	702	-	-	0/22/62/62	0/5/5/5

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	N3A-C2A-N1A	-10.28	121.03	128.89
3	F	702	NAD	N3A-C2A-N1A	-10.09	121.17	128.89
3	D	701	NAD	N3A-C2A-N1A	-10.07	121.18	128.89
3	D	701	NAD	C4B-O4B-C1B	-6.85	102.19	109.72
3	F	702	NAD	C4B-O4B-C1B	-6.61	102.45	109.72
3	B	700	NAD	C4B-O4B-C1B	-6.60	102.47	109.72
3	D	701	NAD	PN-O3-PA	-3.81	122.04	132.73
3	B	700	NAD	PN-O3-PA	-3.34	123.35	132.73
3	F	702	NAD	PN-O3-PA	-3.24	123.63	132.73
3	F	702	NAD	C4A-C5A-N7A	-2.47	107.21	109.48
3	D	701	NAD	C4A-C5A-N7A	-2.39	107.28	109.48
3	B	700	NAD	C4A-C5A-N7A	-2.32	107.35	109.48
3	B	700	NAD	O4B-C1B-N9A	2.45	113.22	108.10
3	F	702	NAD	O4B-C1B-N9A	2.85	114.06	108.10
3	D	701	NAD	O4B-C1B-N9A	2.89	114.16	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	0.17	17 (2%) 67 71	17, 53, 92, 120	0
1	C	822/842 (97%)	0.59	88 (10%) 8 8	18, 60, 134, 199	0
1	E	822/842 (97%)	2.12	355 (43%) 0 0	19, 131, 186, 266	0
2	B	207/207 (100%)	0.04	1 (0%) 91 92	16, 33, 80, 99	0
2	D	207/207 (100%)	-0.04	2 (0%) 84 86	16, 30, 66, 88	0
2	F	207/207 (100%)	0.02	4 (1%) 70 73	20, 36, 82, 118	0
All	All	3087/3147 (98%)	0.77	467 (15%) 3 3	16, 57, 165, 266	0

All (467) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	195	GLU	11.1
1	E	231	LYS	10.0
1	E	311	GLU	10.0
1	E	307	LEU	9.8
1	E	314	LEU	9.8
1	C	550	ALA	9.6
1	C	495	VAL	9.5
1	E	78	TYR	9.5
1	E	179	ALA	9.1
1	E	766	PHE	8.7
1	E	277	ILE	8.7
1	E	303	LEU	8.7
1	E	280	PRO	8.4
1	E	167	LEU	8.3
1	E	310	ASP	8.1
1	E	193	ALA	8.0
1	E	239	LYS	8.0
1	E	107	GLY	7.9
1	E	553	PRO	7.8

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Mol	Chain	Res	Type	RSRZ
1	E	88	GLU	7.8
1	C	493	VAL	7.7
1	E	332	ASP	7.6
1	E	339	VAL	7.6
1	E	299	LEU	7.6
1	E	420	PRO	7.5
1	E	308	LYS	7.4
1	E	86	VAL	7.4
1	E	210	ALA	7.4
1	E	320	LEU	7.3
1	E	175	TYR	7.3
1	E	99	LEU	7.2
1	E	276	PHE	7.2
1	E	554	LEU	7.1
1	E	315	GLU	7.1
1	E	108	HIS	6.9
1	E	240	MET	6.9
1	E	81	MET	6.9
1	E	26	ALA	6.7
1	E	316	GLY	6.6
1	E	504	LEU	6.6
1	E	289	MET	6.6
1	E	321	LYS	6.6
1	E	323	VAL	6.6
1	E	366	CYS	6.5
1	C	522	MET	6.5
1	E	492	ALA	6.5
1	E	194	ASP	6.5
1	C	523	SER	6.5
1	E	233	PHE	6.5
1	E	495	VAL	6.4
1	E	278	LEU	6.4
1	E	312	LYS	6.4
1	E	745	SER	6.4
1	E	789	GLY	6.3
1	E	132	ILE	6.3
1	E	23	SER	6.3
1	E	743	ILE	6.3
1	E	98	PHE	6.2
1	E	442	VAL	6.2
1	E	282	PHE	6.0
1	C	551	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	770	ALA	6.0
1	E	128	VAL	5.9
1	A	475	ALA	5.9
1	E	97	SER	5.9
1	E	273	PHE	5.8
1	E	498	ALA	5.8
1	E	555	LYS	5.8
1	E	500	ASP	5.8
1	E	269	LEU	5.8
1	E	232	LYS	5.7
1	E	419	VAL	5.7
1	C	549	HIS	5.7
1	E	367	ILE	5.6
1	C	494	GLU	5.6
1	C	496	LYS	5.6
1	E	360	PRO	5.5
1	E	196	VAL	5.5
1	E	288	ILE	5.5
1	E	245	TRP	5.5
1	E	19	VAL	5.5
1	C	499	ASN	5.5
1	C	502	PRO	5.5
1	E	242	ASP	5.4
1	E	164	LEU	5.4
1	E	163	ALA	5.4
1	E	298	VAL	5.4
1	E	501	LEU	5.4
1	E	761	PRO	5.4
1	E	284	LEU	5.4
1	E	739	ALA	5.3
1	E	525	SER	5.3
1	E	192	TYR	5.3
1	E	80	GLU	5.3
1	C	501	LEU	5.2
1	E	418	TYR	5.2
1	C	506	GLU	5.2
1	E	77	LEU	5.2
1	E	335	LEU	5.1
1	E	89	ILE	5.1
1	E	551	GLY	5.1
1	E	476	HIS	5.1
1	C	552	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	154	VAL	5.1
1	C	508	LEU	5.1
1	E	777	SER	5.0
1	E	45	ILE	5.0
1	E	24	VAL	5.0
1	C	546	GLU	5.0
1	E	317	LYS	5.0
1	C	498	ALA	5.0
1	E	76	SER	5.0
1	E	226	ALA	4.9
1	E	227	THR	4.9
1	E	129	VAL	4.9
1	E	496	LYS	4.9
1	E	474	THR	4.9
1	C	291	PHE	4.8
1	E	83	ASP	4.8
1	E	309	GLY	4.8
1	E	290	ASN	4.8
1	E	322	VAL	4.8
1	E	329	PRO	4.8
1	E	169	VAL	4.7
1	E	306	VAL	4.7
1	E	362	ASP	4.7
1	E	741	GLY	4.7
1	E	126	LEU	4.7
1	E	143	LEU	4.7
1	E	759	GLN	4.7
1	E	105	SER	4.6
1	E	31	GLY	4.6
1	E	48	ALA	4.6
1	E	257	TRP	4.6
1	E	497	ASN	4.6
1	E	25	ILE	4.6
1	C	500	ASP	4.5
1	C	505	VAL	4.5
1	E	343	PRO	4.5
1	E	67	GLY	4.5
1	E	222	ILE	4.5
1	E	493	VAL	4.5
1	E	305	ILE	4.5
1	E	166	GLU	4.5
1	E	760	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	553	PRO	4.5
1	E	79	SER	4.4
1	E	421	GLY	4.4
1	E	740	VAL	4.4
1	E	762	GLY	4.4
1	E	319	LEU	4.4
1	E	361	ALA	4.4
1	C	528	HIS	4.4
1	A	420	PRO	4.4
1	E	499	ASN	4.4
1	E	556	ILE	4.4
1	E	747	LEU	4.4
1	E	297	PRO	4.4
1	E	506	GLU	4.3
1	E	794	PRO	4.3
1	E	241	MET	4.3
1	E	258	THR	4.3
1	E	294	ASP	4.3
1	E	475	ALA	4.3
1	C	2	VAL	4.3
1	E	296	ILE	4.3
1	C	300	LEU	4.3
1	C	504	LEU	4.3
1	E	441	PHE	4.2
1	E	127	VAL	4.2
1	E	287	ALA	4.2
1	E	176	GLN	4.2
1	E	9	MET	4.2
1	E	131	THR	4.2
1	E	229	TYR	4.2
1	E	96	ASN	4.2
1	E	254	THR	4.2
1	A	495	VAL	4.2
1	E	187	VAL	4.2
1	C	311	GLU	4.2
1	C	4	PHE	4.2
1	E	230	ALA	4.1
1	E	180	ARG	4.1
1	E	365	ASN	4.1
1	E	182	VAL	4.1
1	E	301	GLU	4.1
1	E	338	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	205	ALA	4.1
1	E	216	HIS	4.1
1	E	188	ILE	4.1
1	C	524	GLU	4.0
1	E	550	ALA	4.0
1	E	223	ARG	4.0
1	E	165	LEU	4.0
1	E	358	GLU	4.0
1	E	422	LYS	4.0
1	E	203	TYR	4.0
1	C	497	ASN	4.0
1	E	185	VAL	3.9
1	E	796	MET	3.9
1	E	737	GLU	3.9
1	E	324	MET	3.9
1	E	292	LYS	3.9
1	E	503	LYS	3.9
1	E	268	PRO	3.9
1	E	295	GLU	3.9
1	E	781	THR	3.8
1	E	730	LEU	3.8
1	E	795	GLN	3.8
1	E	155	VAL	3.8
1	E	304	GLU	3.8
1	E	736	PRO	3.8
1	E	144	ARG	3.8
1	E	106	PRO	3.8
1	E	286	THR	3.8
1	E	260	LYS	3.8
1	E	744	TYR	3.7
1	E	218	TRP	3.7
1	E	4	PHE	3.7
1	E	293	LYS	3.7
1	C	3	ALA	3.7
1	E	46	ILE	3.7
1	E	754	VAL	3.7
1	E	494	GLU	3.7
1	E	47	SER	3.7
1	E	32	LYS	3.7
1	E	134	GLY	3.6
1	E	780	PHE	3.6
1	C	306	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	323	VAL	3.6
1	E	200	VAL	3.6
1	C	513	LYS	3.6
1	E	757	GLU	3.6
1	E	93	THR	3.6
1	E	148	GLY	3.6
1	C	307	LEU	3.6
1	E	123	ASP	3.6
1	E	243	ARG	3.6
2	F	489	ALA	3.6
1	E	149	GLU	3.6
1	E	735	CYS	3.6
1	C	555	LYS	3.6
1	E	790	GLY	3.5
1	C	285	PHE	3.5
1	E	369	ILE	3.5
1	E	552	VAL	3.5
1	C	314	LEU	3.5
1	E	522	MET	3.5
1	C	556	ILE	3.5
1	C	554	LEU	3.5
1	E	326	LYS	3.5
1	E	125	ALA	3.4
1	E	161	ASP	3.4
1	E	256	LYS	3.4
1	E	137	VAL	3.4
1	E	768	VAL	3.4
1	E	340	LEU	3.3
1	E	472	SER	3.3
1	E	510	ARG	3.3
1	C	112	SER	3.3
1	E	523	SER	3.3
1	E	443	GLU	3.3
1	C	313	ASP	3.3
1	E	171	LYS	3.3
1	E	70	ILE	3.3
1	E	402	ALA	3.3
1	E	410	LYS	3.3
1	E	547	HIS	3.3
1	E	145	GLN	3.3
1	E	197	LEU	3.2
1	E	511	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	740	VAL	3.2
1	E	548	ASP	3.2
1	E	111	PHE	3.2
1	E	342	LEU	3.2
1	E	423	LYS	3.1
1	A	361	ALA	3.1
1	E	505	VAL	3.1
1	E	36	THR	3.1
1	E	302	LYS	3.1
1	E	94	ASP	3.1
1	E	113	SER	3.1
1	E	130	ASP	3.1
1	E	508	LEU	3.1
1	C	305	ILE	3.1
1	E	424	ASP	3.1
1	A	419	VAL	3.1
1	E	156	VAL	3.1
1	C	167	LEU	3.0
1	C	5	THR	3.0
1	C	299	LEU	3.0
1	C	492	ALA	3.0
1	E	291	PHE	3.0
1	E	151	ILE	3.0
1	E	755	VAL	3.0
2	F	490	ARG	3.0
1	E	103	ILE	3.0
1	E	115	VAL	2.9
1	E	162	ARG	2.9
1	E	546	GLU	2.9
1	C	547	HIS	2.9
1	E	444	PRO	2.9
1	E	42	ARG	2.9
1	E	255	LYS	2.9
1	E	104	ASP	2.9
1	E	158	ASN	2.9
1	E	431	ILE	2.9
1	E	120	ARG	2.9
1	E	376	ALA	2.9
2	D	489	ALA	2.9
1	E	147	LEU	2.9
1	E	244	LEU	2.9
1	E	34	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	509	LYS	2.9
1	C	320	LEU	2.9
1	C	545	LEU	2.9
1	E	763	THR	2.9
1	E	502	PRO	2.9
1	A	46	ILE	2.9
1	E	234	GLY	2.9
1	A	365	ASN	2.8
1	E	300	LEU	2.8
1	E	437	MET	2.8
1	E	377	ASP	2.8
1	E	3	ALA	2.8
1	C	265	GLU	2.8
1	E	135	VAL	2.8
1	E	395	TYR	2.8
1	E	121	VAL	2.8
1	E	541	CYS	2.8
1	E	412	ARG	2.8
1	E	68	ILE	2.8
1	C	503	LYS	2.8
1	C	511	LEU	2.8
1	E	85	ASP	2.8
1	C	235	VAL	2.7
1	E	69	THR	2.7
1	C	251	ASN	2.7
1	E	401	PHE	2.7
1	E	38	SER	2.7
1	E	10	ARG	2.7
1	E	357	TYR	2.7
1	E	356	LEU	2.7
1	E	784	LEU	2.7
1	C	310	ASP	2.7
1	E	261	ASP	2.7
1	C	232	LYS	2.7
1	E	199	ASP	2.7
1	E	41	GLN	2.7
1	E	91	GLN	2.7
1	E	325	ARG	2.6
1	A	553	PRO	2.6
1	E	756	SER	2.6
1	E	279	ASP	2.6
1	E	27	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	267	LYS	2.6
1	E	73	THR	2.6
1	E	82	SER	2.6
1	E	542	LEU	2.6
1	E	782	GLY	2.6
1	E	267	LYS	2.6
1	E	75	ILE	2.6
1	E	390	ASP	2.6
1	A	84	GLU	2.6
1	E	427	PHE	2.6
1	E	549	HIS	2.6
2	D	461	ASP	2.5
1	E	445	ILE	2.5
1	E	349	GLN	2.5
1	E	473	GLU	2.5
1	C	269	LEU	2.5
1	E	337	MET	2.5
1	C	7	ASP	2.5
1	E	313	ASP	2.5
1	C	421	GLY	2.5
1	E	347	THR	2.5
1	E	477	ASN	2.5
1	E	328	LEU	2.5
1	E	136	CYS	2.5
1	E	481	MET	2.5
1	C	293	LYS	2.5
1	E	265	GLU	2.5
1	E	388	THR	2.5
1	E	159	LYS	2.5
1	E	101	ASN	2.5
1	E	354	GLU	2.5
1	C	154	VAL	2.4
1	E	209	VAL	2.4
1	A	473	GLU	2.4
1	E	177	THR	2.4
1	C	445	ILE	2.4
1	C	420	PRO	2.4
1	C	510	ARG	2.4
1	E	2	VAL	2.4
1	E	208	THR	2.4
1	C	46	ILE	2.4
2	F	461	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	30	HIS	2.4
1	E	526	GLY	2.4
1	C	236	ASP	2.4
1	E	117	ALA	2.4
1	E	189	VAL	2.4
1	C	229	TYR	2.4
1	C	173	ASP	2.4
1	E	772	LEU	2.4
1	E	438	MET	2.4
1	E	90	LYS	2.3
1	E	211	PHE	2.3
1	C	109	VAL	2.3
1	E	122	THR	2.3
1	C	252	PRO	2.3
1	E	153	PRO	2.3
1	C	85	ASP	2.3
1	E	274	ASN	2.3
1	E	207	GLY	2.3
1	A	496	LYS	2.3
1	C	118	ALA	2.3
1	E	7	ASP	2.3
1	E	146	ALA	2.3
1	C	766	PHE	2.3
1	E	119	LEU	2.3
1	E	471	THR	2.3
1	E	84	GLU	2.3
1	C	312	LYS	2.3
1	E	118	ALA	2.3
1	E	249	PHE	2.3
1	E	201	GLN	2.3
1	C	309	GLY	2.3
1	E	116	THR	2.2
1	E	466	THR	2.2
1	E	783	GLU	2.2
1	C	507	GLY	2.2
1	C	264	ALA	2.2
1	A	310	ASP	2.2
1	E	22	MET	2.2
1	E	20	ARG	2.2
1	A	423	LYS	2.2
1	C	163	ALA	2.2
1	E	237	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	458	GLY	2.2
1	E	742	GLY	2.2
2	B	520	ALA	2.1
1	C	296	ILE	2.1
1	E	778	PHE	2.1
1	C	529	ILE	2.1
1	E	114	GLU	2.1
1	E	425	ASP	2.1
1	E	327	PHE	2.1
1	C	80	GLU	2.1
1	E	87	LYS	2.1
1	E	391	LYS	2.1
1	A	81	MET	2.1
1	A	360	PRO	2.1
1	E	348	ALA	2.1
1	C	744	TYR	2.1
2	F	463	ASP	2.1
1	C	319	LEU	2.0
1	E	396	ALA	2.0
1	E	392	GLY	2.0
1	C	168	GLN	2.0
1	C	233	PHE	2.0
1	A	237	LYS	2.0
1	E	359	GLY	2.0
1	E	174	LEU	2.0
1	A	418	TYR	2.0
1	E	285	PHE	2.0
1	E	375	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	DDE	A	699	10/21	0.94	0.13	-	43,61,74,78	0
1	DDE	E	699	10/21	0.96	0.13	-	38,49,69,70	0
1	DDE	C	699	20/21	0.96	0.21	-	22,85,126,129	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	D	701	44/44	0.98	0.17	-0.24	12,29,51,56	0
3	NAD	B	700	44/44	0.97	0.16	-0.25	17,33,54,59	0
3	NAD	F	702	44/44	0.98	0.16	-0.31	7,34,59,62	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.