



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

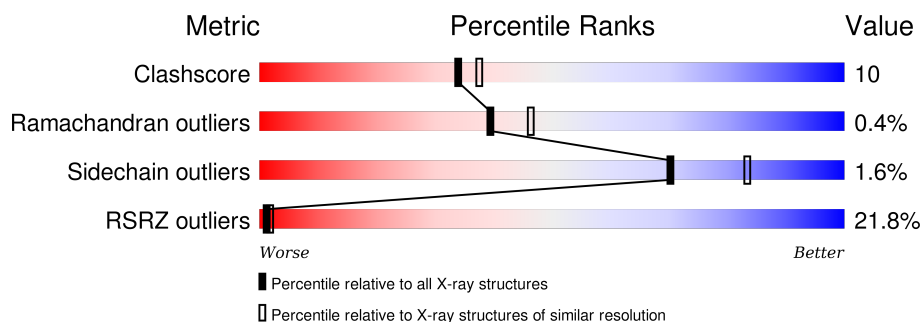
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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>9%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	C	842	<div> <div>16%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	E	842	<div> <div>52%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
2	B	207	<div> <div>4%</div> <div>85%</div> <div>15%</div> </div>
2	D	207	<div> <div>4%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
2	F	207	<div> <div>4%</div> <div>87%</div> <div>13%</div> </div>

## 2 Entry composition

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

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

- Molecule 1 is a protein called Elongation factor 2.

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

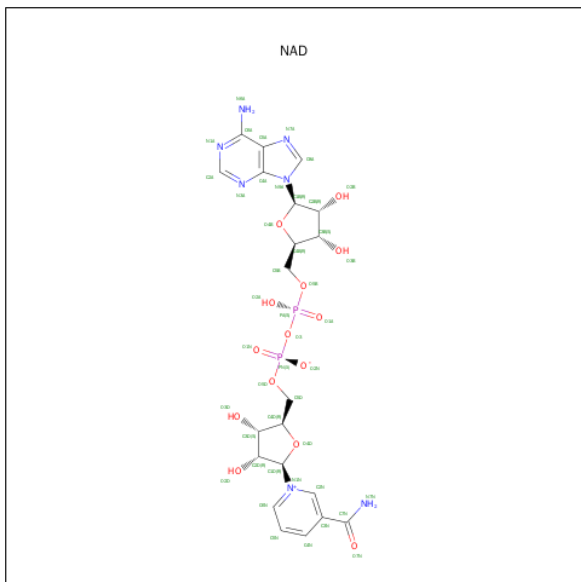
- Molecule 2 is a protein called Exotoxin A.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	399	ALA	-	EXPRESSION TAG	UNP P11439
B	407	VAL	ILE	SEE REMARK 999	UNP P11439
B	515	SER	GLY	SEE REMARK 999	UNP P11439
B	546	HIS	GLU	ENGINEERED	UNP P11439
D	399	ALA	-	EXPRESSION TAG	UNP P11439
D	407	VAL	ILE	SEE REMARK 999	UNP P11439
D	515	SER	GLY	SEE REMARK 999	UNP P11439
D	546	HIS	GLU	ENGINEERED	UNP P11439
F	399	ALA	-	EXPRESSION TAG	UNP P11439
F	407	VAL	ILE	SEE REMARK 999	UNP P11439
F	515	SER	GLY	SEE REMARK 999	UNP P11439
F	546	HIS	GLU	ENGINEERED	UNP P11439

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

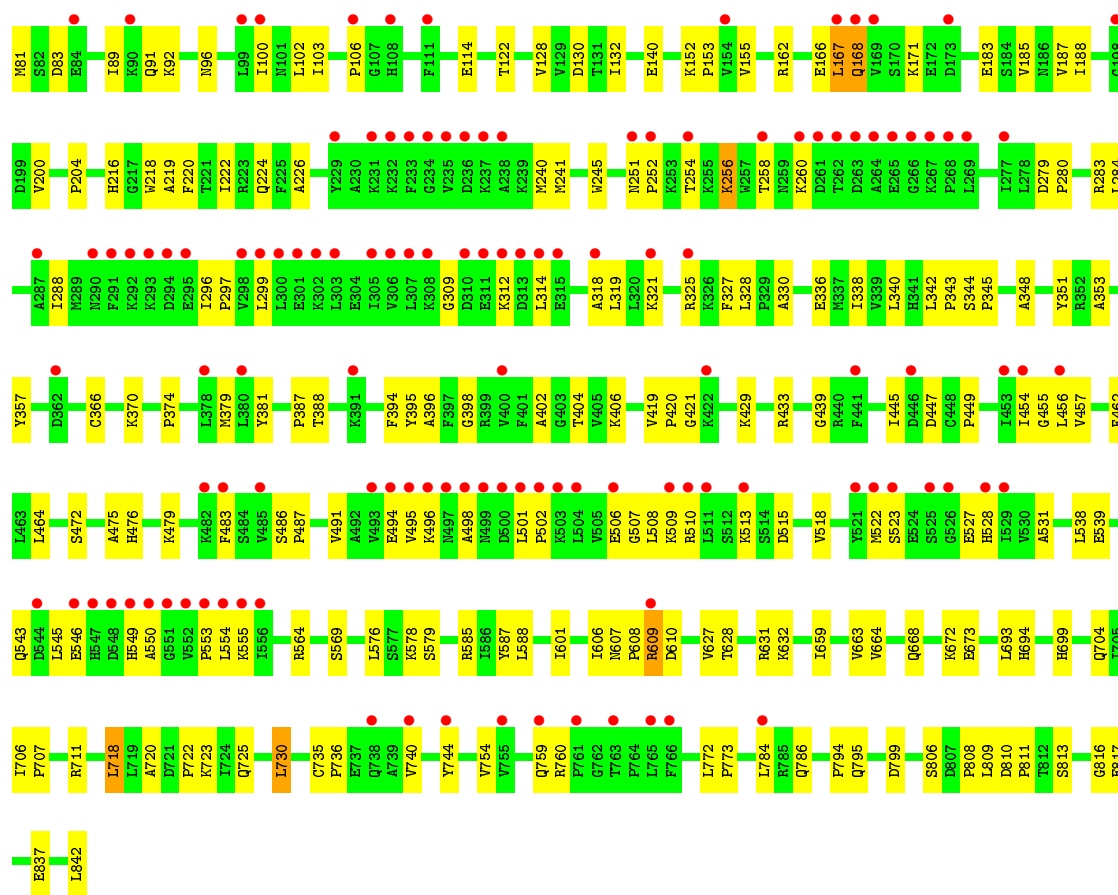


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

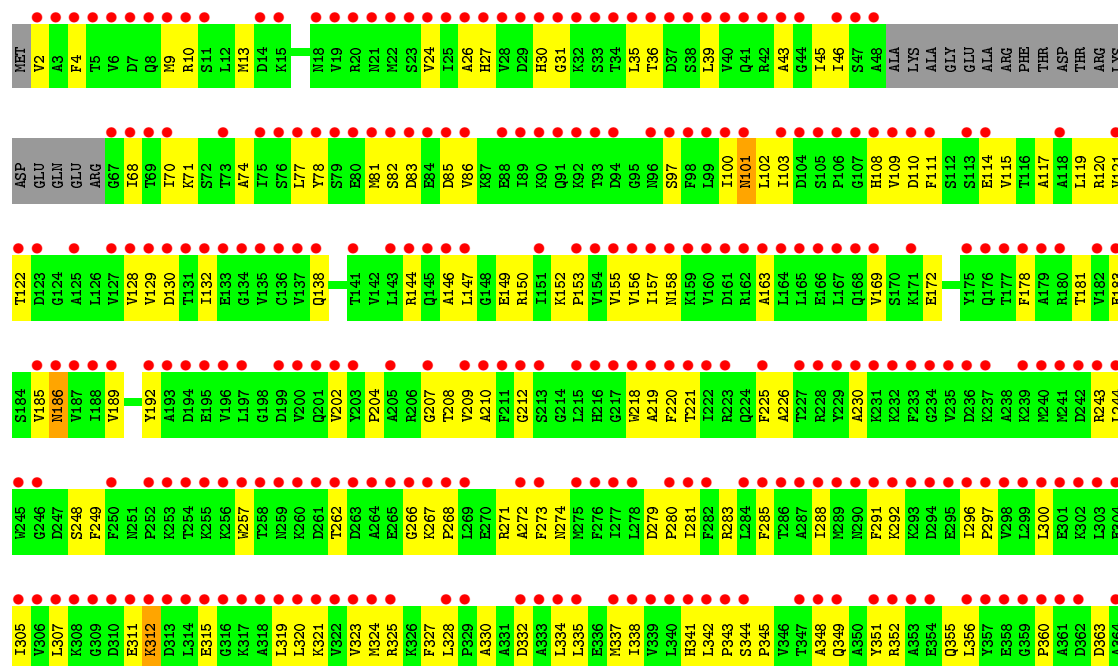
- Molecule 4 is water.

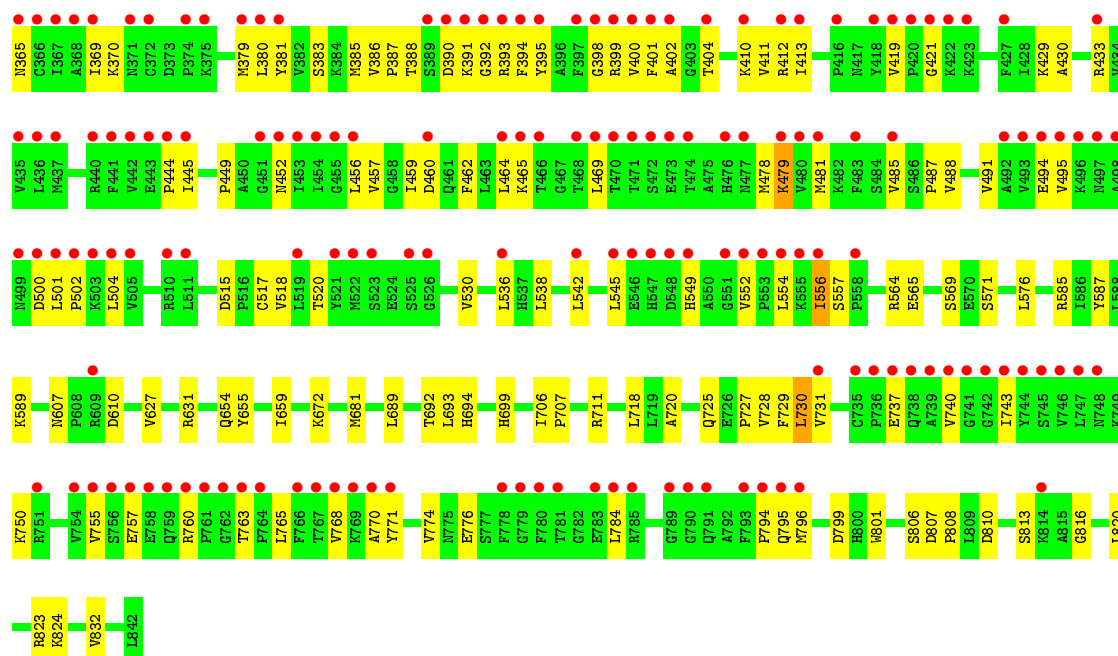
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	117	Total	O	0	0
			117	117		
4	C	85	Total	O	0	0
			85	85		
4	D	124	Total	O	0	0
			124	124		
4	E	45	Total	O	0	0
			45	45		
4	F	94	Total	O	0	0
			94	94		



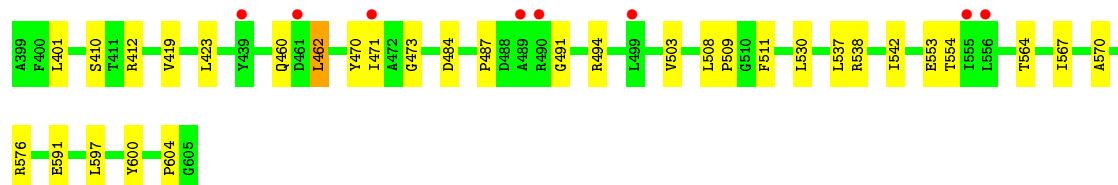
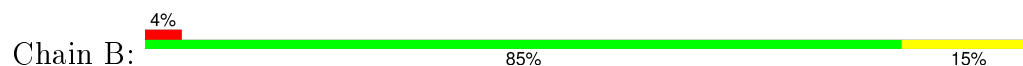


• Molecule 1: Elongation factor 2

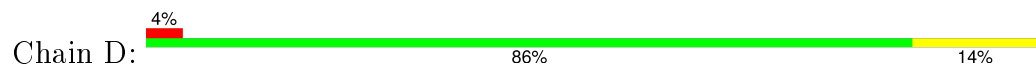




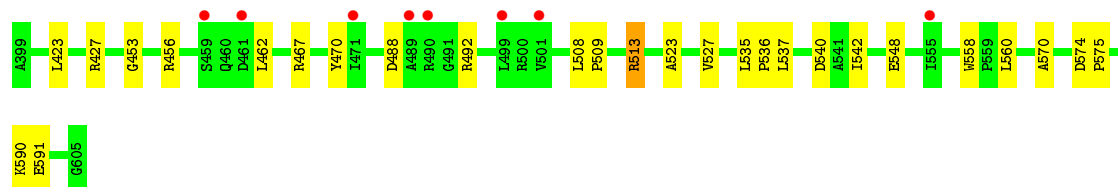
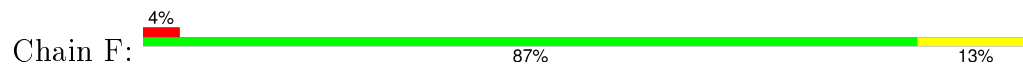
• Molecule 2: Exotoxin A



• Molecule 2: Exotoxin A



• Molecule 2: Exotoxin A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	327.57Å 68.46Å 189.99Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	25.00 – 2.35 25.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.00-2.35) 98.5 (25.00-2.35)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.36Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.257 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 169195 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

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

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.20	0/6517	0.37	0/8823
1	C	0.20	0/6517	0.37	0/8823
1	E	0.20	0/6517	0.37	0/8823
2	B	0.20	0/1629	0.38	0/2219
2	D	0.20	0/1629	0.40	0/2219
2	F	0.20	0/1629	0.38	0/2219
All	All	0.20	0/24438	0.37	0/33126

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	6472	121	0
1	C	6415	0	6488	132	0
1	E	6415	0	6488	189	0
2	B	1589	0	1543	18	0
2	D	1589	0	1543	15	0
2	F	1589	0	1543	13	0
3	B	44	0	26	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	26	3	0
3	F	44	0	26	1	0
4	A	83	0	0	1	0
4	B	117	0	0	1	0
4	C	85	0	0	0	0
4	D	124	0	0	1	0
4	E	45	0	0	0	0
4	F	94	0	0	1	0
All	All	24682	0	24155	488	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (488) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ASP:O	1:A:816:GLY:HA3	2.02	0.59
1:E:26:ALA:CB	1:E:128:VAL:HB	2.32	0.59
1:A:569:SER:O	1:A:720:ALA:HB1	2.03	0.59
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.84	0.59
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.37	0.59
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.84	0.58
1:A:828:MET:HG2	2:B:576:ARG:CZ	2.33	0.58
1:C:707:PRO:O	1:C:711:ARG:HG3	2.03	0.58
1:C:672:LYS:HG3	1:C:673:GLU:HG3	1.86	0.58
1:A:321:LYS:O	1:A:325:ARG:HB2	2.03	0.58
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.86	0.58
1:A:435:VAL:HB	1:A:442:VAL:HG13	1.86	0.57
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.05	0.57
1:E:285:PHE:CD1	1:E:320:LEU:HD21	2.40	0.57
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.87	0.57
1:E:121:VAL:HG11	1:E:383:SER:OG	2.05	0.57
1:C:722:PRO:O	1:C:723:LYS:HG3	2.05	0.57
1:C:374:PRO:O	1:C:404:THR:HG23	2.04	0.56
1:C:419:VAL:HG12	1:C:421:GLY:H	1.70	0.56
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.86	0.56
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.87	0.56
1:E:9:MET:O	1:E:13:MET:HG3	2.05	0.56
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.87	0.56
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.86	0.56
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.21	0.56
1:E:291:PHE:HD1	1:E:315:GLU:HB3	1.70	0.56
1:A:70:ILE:HG22	1:A:388:THR:HG22	1.88	0.56
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.88	0.55
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.88	0.55
1:E:207:GLY:O	1:E:337:MET:HG2	2.06	0.55
1:C:772:LEU:HD12	1:C:773:PRO:HD2	1.87	0.55
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.88	0.55
1:A:30:HIS:CD2	1:A:130:ASP:HB2	2.42	0.55
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.89	0.55
2:B:537:LEU:HD11	2:B:542:ILE:HG22	1.88	0.55
1:A:324:MET:HA	1:A:324:MET:HE2	1.89	0.55
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.87	0.55
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.89	0.55
1:E:391:LYS:HG3	1:E:392:GLY:N	2.19	0.54
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.43	0.54
1:C:6:VAL:HG13	1:C:445:ILE:HG22	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.90	0.54
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.37	0.54
1:A:568:GLU:OE2	1:A:723:LYS:HE3	2.06	0.54
1:A:385:MET:HG2	1:A:465:LYS:HA	1.88	0.54
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.42	0.54
1:E:464:LEU:HG	1:E:465:LYS:HG3	1.89	0.54
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.89	0.54
1:E:433:ARG:HE	1:E:444:PRO:HB3	1.73	0.54
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.90	0.54
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.89	0.54
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.89	0.54
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.07	0.53
1:A:500:ASP:HB3	1:A:552:VAL:HG11	1.90	0.53
2:D:503:VAL:HG12	2:D:564:THR:HG22	1.91	0.53
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.23	0.53
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.88	0.53
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.89	0.53
1:A:823:ARG:NH2	1:A:833:PRO:HD3	2.24	0.53
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.43	0.53
2:D:537:LEU:O	2:D:538:ARG:HD3	2.09	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.91	0.53
1:A:819:VAL:O	1:A:823:ARG:HG2	2.08	0.53
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.44	0.53
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.90	0.53
1:A:501:LEU:N	1:A:502:PRO:HD2	2.24	0.52
1:E:296:ILE:O	1:E:300:LEU:HD13	2.09	0.52
1:C:627:VAL:O	1:C:631:ARG:HG3	2.08	0.52
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.90	0.52
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.74	0.52
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.45	0.52
1:E:257:TRP:HZ3	1:E:272:ALA:HB2	1.74	0.52
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.44	0.52
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.91	0.52
1:A:609:ARG:HH11	1:A:609:ARG:HG2	1.74	0.52
1:A:388:THR:HG21	1:A:395:TYR:CD2	2.45	0.52
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.52
1:C:296:ILE:N	1:C:297:PRO:HD2	2.25	0.52
1:E:35:LEU:HD22	1:E:334:LEU:HD11	1.92	0.51
1:A:613:LYS:HG2	1:A:631:ARG:HH11	1.75	0.51
1:E:74:ALA:HA	1:E:102:LEU:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD13	1:A:556:ILE:HG21	1.93	0.51
1:A:24:VAL:HG23	1:A:102:LEU:HD11	1.91	0.51
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.44	0.51
1:E:243:ARG:O	1:E:248:SER:HB2	2.08	0.51
2:F:513:ARG:HH21	2:F:513:ARG:HB2	1.75	0.51
1:A:338:ILE:O	1:A:342:LEU:HB2	2.10	0.51
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.91	0.51
1:E:755:VAL:HG23	1:E:770:ALA:HA	1.93	0.51
1:E:111:PHE:HB3	1:E:114:GLU:HG2	1.93	0.51
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.93	0.51
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.92	0.51
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.46	0.51
2:D:553:GLU:OE1	3:D:701:NAD:H6N	2.11	0.51
1:E:117:ALA:HA	1:E:481:MET:SD	2.49	0.51
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.45	0.51
1:A:632:LYS:HD3	1:A:648:ASP:O	2.10	0.51
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.92	0.51
1:A:491:VAL:HG21	1:A:542:LEU:HD11	1.92	0.51
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.93	0.51
1:A:746:VAL:O	1:A:750:LYS:HD3	2.11	0.51
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.75	0.51
1:A:381:TYR:O	1:A:398:GLY:HA3	2.11	0.51
2:F:537:LEU:HD11	2:F:542:ILE:HG22	1.93	0.51
1:E:750:LYS:HD2	1:E:776:GLU:O	2.11	0.51
1:C:321:LYS:O	1:C:325:ARG:HG3	2.11	0.50
1:E:208:THR:HG23	1:E:341:HIS:CE1	2.47	0.50
1:E:291:PHE:CD1	1:E:315:GLU:HB3	2.46	0.50
1:E:654:GLN:O	1:E:655:TYR:HB2	2.12	0.50
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.93	0.50
1:C:254:THR:HG22	1:C:256:LYS:HB2	1.94	0.50
1:E:349:GLN:O	1:E:370:LYS:HA	2.11	0.50
2:D:427:ARG:HD2	2:D:431:GLU:OE2	2.12	0.50
1:E:627:VAL:O	1:E:631:ARG:HG3	2.11	0.50
1:E:82:SER:O	1:E:86:VAL:HG23	2.11	0.50
1:E:413:ILE:HD13	1:E:459:ILE:HG23	1.93	0.50
1:E:727:PRO:HD3	1:E:801:TRP:CZ3	2.47	0.50
1:C:723:LYS:HA	1:C:808:PRO:HG3	1.93	0.50
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.93	0.50
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.93	0.50
1:A:152:LYS:HD3	1:A:343:PRO:HD3	1.94	0.50
1:A:9:MET:O	1:A:13:MET:HG3	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.93	0.50
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.41	0.50
1:A:431:ILE:HD12	1:A:459:ILE:HD11	1.93	0.50
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.46	0.50
1:E:380:LEU:HG	1:E:400:VAL:HG22	1.94	0.49
1:C:17:THR:HB	1:C:92:LYS:O	2.13	0.49
1:A:111:PHE:O	1:A:115:VAL:HG23	2.13	0.49
1:C:338:ILE:HG23	1:C:342:LEU:HD12	1.93	0.49
1:C:522:MET:HG2	1:C:528:HIS:CE1	2.47	0.49
1:C:487:PRO:HB3	1:C:531:ALA:HB1	1.95	0.49
1:C:759:GLN:HG2	1:C:760:ARG:N	2.17	0.49
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.95	0.49
1:C:609:ARG:HD2	1:C:609:ARG:H	1.78	0.49
1:E:321:LYS:O	1:E:325:ARG:HG3	2.12	0.49
1:E:10:ARG:HD3	1:E:445:ILE:HD11	1.94	0.49
1:E:185:VAL:O	1:E:189:VAL:HG23	2.13	0.49
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.76	0.49
1:C:314:LEU:HD22	1:C:318:ALA:HB1	1.95	0.49
1:C:81:MET:O	1:C:96:ASN:HB3	2.13	0.49
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.48	0.49
1:A:731:VAL:HG22	1:A:796:MET:HB3	1.95	0.49
1:C:806:SER:HB2	1:C:813:SER:HB2	1.95	0.49
1:C:72:SER:HA	1:C:439:GLY:O	2.13	0.48
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.95	0.48
1:E:312:LYS:O	1:E:312:LYS:HD2	2.14	0.48
1:E:538:LEU:O	1:E:542:LEU:HG	2.13	0.48
1:C:226:ALA:HB2	1:C:241:MET:HB3	1.94	0.48
1:A:806:SER:HB2	1:A:813:SER:HB2	1.96	0.48
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.96	0.48
1:E:292:LYS:O	1:E:296:ILE:HG13	2.14	0.48
1:A:150:ARG:HG3	1:A:355:GLN:HE22	1.79	0.48
1:E:488:VAL:HG12	1:E:774:VAL:HG11	1.95	0.48
1:A:118:ALA:O	1:A:122:THR:HG23	2.14	0.48
1:A:831:GLU:CD	1:A:831:GLU:H	2.16	0.48
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.14	0.48
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.96	0.48
1:C:498:ALA:HA	1:C:501:LEU:HB2	1.96	0.48
1:E:552:VAL:O	1:E:554:LEU:HG	2.14	0.48
1:E:576:LEU:HD13	1:E:587:TYR:CE1	2.49	0.48
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.96	0.48
1:E:556:ILE:HG22	1:E:557:SER:N	2.27	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.95	0.47
1:C:406:LYS:HG3	1:C:447:ASP:HB3	1.95	0.47
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.94	0.47
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.95	0.47
1:E:365:ASN:O	1:E:369:ILE:HG12	2.13	0.47
1:E:204:PRO:HA	1:E:209:VAL:HB	1.96	0.47
1:E:391:LYS:CG	1:E:392:GLY:H	2.21	0.47
1:A:464:LEU:HD23	1:A:483:PHE:CE1	2.50	0.47
2:D:488:ASP:HB3	4:D:795:HOH:O	2.14	0.47
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.95	0.47
1:E:30:HIS:CE1	1:E:130:ASP:HB2	2.50	0.47
1:C:578:LYS:HB3	1:C:585:ARG:HG2	1.97	0.47
1:C:809:LEU:O	1:C:811:PRO:HD3	2.14	0.47
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.96	0.47
1:E:820:LEU:HG	1:E:824:LYS:HE2	1.96	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
2:F:513:ARG:NH2	2:F:513:ARG:HB2	2.30	0.47
2:B:470:TYR:CD2	3:B:700:NAD:H2D	2.50	0.47
1:C:420:PRO:HG2	1:C:476:HIS:CD2	2.50	0.47
1:A:45:ILE:HD11	1:A:78:TYR:HB2	1.96	0.47
1:C:515:ASP:O	1:C:518:VAL:HG12	2.15	0.47
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.50	0.47
1:A:609:ARG:NH1	1:A:609:ARG:HG3	2.30	0.46
1:A:4:PHE:HD2	1:A:45:ILE:HG23	1.79	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.95	0.46
1:E:419:VAL:HG12	1:E:421:GLY:H	1.80	0.46
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.97	0.46
1:E:101:ASN:N	1:E:101:ASN:HD22	2.13	0.46
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.46
1:C:153:PRO:HD2	1:C:200:VAL:HG12	1.96	0.46
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.97	0.46
1:E:2:VAL:HG12	1:E:4:PHE:CE1	2.50	0.46
1:E:156:VAL:HG11	1:E:334:LEU:HD21	1.98	0.46
1:A:435:VAL:HG12	1:A:444:PRO:HA	1.98	0.46
1:E:352:ARG:O	1:E:356:LEU:HG	2.15	0.46
1:A:296:ILE:O	1:A:300:LEU:HD13	2.16	0.46
1:E:737:GLU:HA	1:E:740:VAL:HG23	1.96	0.46
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.98	0.46
1:C:699:DDE:HAU3	1:C:699:DDE:HAB2	1.46	0.46
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.97	0.46
1:C:43:ALA:HB1	1:C:78:TYR:O	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.51	0.46
1:E:226:ALA:O	1:E:230:ALA:HB2	2.15	0.46
1:E:183:GLU:HA	1:E:186:ASN:OD1	2.16	0.46
1:A:155:VAL:HG21	1:A:185:VAL:HG11	1.98	0.46
1:E:459:ILE:O	1:E:459:ILE:HG22	2.16	0.46
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.98	0.46
1:E:569:SER:O	1:E:720:ALA:HB1	2.16	0.46
1:A:478:MET:O	1:A:479:LYS:C	2.54	0.46
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.46	0.46
1:A:110:ASP:HB3	1:A:536:LEU:HD22	1.98	0.46
1:C:288:ILE:HA	1:C:296:ILE:HD11	1.97	0.45
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.97	0.45
2:D:538:ARG:HD2	2:D:559:PRO:HG2	1.98	0.45
1:A:429:LYS:HG3	1:A:462:PHE:CE2	2.51	0.45
1:E:381:TYR:O	1:E:398:GLY:HA3	2.15	0.45
1:C:183:GLU:O	1:C:187:VAL:HG23	2.16	0.45
1:A:515:ASP:HA	1:A:516:PRO:HD2	1.83	0.45
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.51	0.45
1:E:380:LEU:HD13	1:E:456:LEU:HD11	1.99	0.45
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.99	0.45
2:F:508:LEU:N	2:F:509:PRO:CD	2.80	0.45
1:E:244:LEU:O	1:E:273:PHE:HB2	2.16	0.45
1:E:262:THR:HG23	1:E:266:GLY:HA2	1.98	0.45
1:C:106:PRO:HG3	1:C:114:GLU:HG2	1.97	0.45
1:E:305:ILE:HG21	1:E:323:VAL:HG13	1.98	0.45
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.51	0.45
1:A:718:LEU:HA	1:A:722:PRO:HG3	1.98	0.45
2:B:401:LEU:HD23	2:B:567:ILE:HG22	1.98	0.45
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.98	0.45
1:E:296:ILE:N	1:E:297:PRO:HD2	2.32	0.45
1:E:459:ILE:N	1:E:459:ILE:HD12	2.32	0.45
1:E:823:ARG:HE	1:E:832:VAL:HG22	1.82	0.45
2:B:570:ALA:HB3	2:B:591:GLU:OE1	2.17	0.44
1:E:46:ILE:N	1:E:46:ILE:HD12	2.32	0.44
1:C:171:LYS:NZ	1:C:171:LYS:HB2	2.32	0.44
1:A:609:ARG:NH1	1:A:609:ARG:CG	2.68	0.44
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.52	0.44
1:A:352:ARG:NH2	1:A:356:LEU:HD11	2.32	0.44
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.98	0.44
1:E:806:SER:HB2	1:E:813:SER:HB2	1.99	0.44
1:C:664:VAL:O	1:C:668:GLN:HG2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG21	1:A:395:TYR:CG	2.53	0.44
1:E:757:GLU:HG3	1:E:768:VAL:HG22	2.00	0.44
1:E:218:TRP:HB3	1:E:324:MET:HB3	1.99	0.44
1:E:279:ASP:O	1:E:283:ARG:HG2	2.17	0.44
1:E:46:ILE:HD12	1:E:46:ILE:H	1.83	0.44
1:E:324:MET:HA	1:E:324:MET:HE2	2.00	0.44
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.18	0.44
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.99	0.44
1:C:564:ARG:HB2	1:C:725:GLN:HB2	1.99	0.44
1:E:103:ILE:N	1:E:103:ILE:HD12	2.32	0.44
1:E:485:VAL:O	1:E:485:VAL:HG22	2.16	0.44
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.81	0.44
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.32	0.44
1:E:157:ILE:HG21	1:E:178:PHE:CD1	2.53	0.44
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.48	0.44
2:F:574:ASP:HA	2:F:575:PRO:HD2	1.84	0.44
1:C:152:LYS:HD3	1:C:343:PRO:HD3	2.00	0.44
1:E:452:ASN:N	1:E:452:ASN:HD22	2.16	0.44
1:A:698:ILE:H	1:A:698:ILE:HG13	1.62	0.44
2:F:523:ALA:O	2:F:527:VAL:HG23	2.18	0.44
1:E:39:LEU:H	1:E:39:LEU:HD12	1.83	0.44
1:E:345:PRO:HB3	1:E:399:ARG:HH21	1.81	0.44
1:A:823:ARG:HH22	1:A:833:PRO:HD3	1.82	0.44
2:B:419:VAL:O	2:B:423:LEU:HG	2.17	0.44
1:C:454:ILE:HG13	1:C:455:GLY:H	1.82	0.44
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.99	0.43
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.18	0.43
1:E:132:ILE:N	1:E:132:ILE:HD12	2.33	0.43
1:E:39:LEU:HD11	1:E:334:LEU:HD13	2.00	0.43
1:E:727:PRO:HD3	1:E:801:TRP:HZ3	1.82	0.43
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.48	0.43
1:A:664:VAL:O	1:A:668:GLN:HG2	2.18	0.43
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.90	0.43
1:C:24:VAL:HG23	1:C:102:LEU:HD11	2.00	0.43
1:E:77:LEU:HD23	1:E:335:LEU:HD21	2.01	0.43
1:E:369:ILE:HD12	1:E:401:PHE:HB3	2.01	0.43
1:E:111:PHE:O	1:E:115:VAL:HG23	2.19	0.43
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.84	0.43
1:C:579:SER:HB2	1:C:704:GLN:OE1	2.18	0.43
1:E:699:DDE:HAT2	1:E:699:DDE:CAB	2.46	0.43
1:E:485:VAL:O	1:E:487:PRO:HD3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LYS:HA	1:A:430:ALA:HA	2.00	0.43
1:E:491:VAL:HG13	1:E:538:LEU:HD21	1.99	0.43
1:A:353:ALA:HB3	1:A:370:LYS:HG2	2.01	0.43
1:C:546:GLU:HA	1:C:550:ALA:HB3	2.00	0.43
1:A:582:LYS:HE2	4:B:779:HOH:O	2.17	0.43
1:A:677:PHE:N	1:A:677:PHE:CD2	2.85	0.43
1:C:736:PRO:O	1:C:740:VAL:HG23	2.18	0.43
1:A:654:GLN:HG2	1:A:655:TYR:CE1	2.54	0.43
1:A:564:ARG:HB2	1:A:725:GLN:HB2	1.99	0.43
1:E:307:LEU:HD13	1:E:311:GLU:O	2.19	0.43
1:C:396:ALA:HB3	1:C:456:LEU:HB2	2.01	0.43
1:C:608:PRO:HD2	1:C:609:ARG:NH1	2.33	0.43
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.54	0.43
1:E:150:ARG:HB3	1:E:351:TYR:HE1	1.83	0.43
1:E:181:THR:O	1:E:185:VAL:HG23	2.18	0.43
2:D:499:LEU:HB3	2:D:566:VAL:CG1	2.47	0.43
1:A:26:ALA:HB2	1:A:128:VAL:HB	2.01	0.43
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.38	0.43
1:E:144:ARG:HA	1:E:147:LEU:HD12	1.99	0.43
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.43
2:B:410:SER:OG	2:B:412:ARG:HG3	2.18	0.43
1:C:284:LEU:HD23	1:C:299:LEU:HD23	2.00	0.43
1:A:6:VAL:HG13	1:A:445:ILE:HG22	2.01	0.43
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.00	0.43
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.53	0.42
1:A:12:LEU:HG	1:A:99:LEU:HB2	2.01	0.42
1:C:546:GLU:OE1	1:C:553:PRO:HD3	2.18	0.42
1:E:163:ALA:O	1:E:169:VAL:HG12	2.18	0.42
2:B:460:GLN:HG3	2:B:462:LEU:HD11	2.00	0.42
1:A:731:VAL:O	1:A:769:LYS:HA	2.19	0.42
1:E:70:ILE:HG22	1:E:388:THR:HG22	2.01	0.42
1:C:506:GLU:O	1:C:510:ARG:HG3	2.18	0.42
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.54	0.42
1:C:523:SER:OG	1:C:527:GLU:HB2	2.19	0.42
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.01	0.42
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.83	0.42
1:E:149:GLU:O	1:E:352:ARG:HD2	2.19	0.42
1:A:120:ARG:NH1	1:A:479:LYS:HD2	2.34	0.42
1:C:167:LEU:O	1:C:168:GLN:C	2.57	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.01	0.42
1:A:373:ASP:HA	1:A:374:PRO:HD2	1.86	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:O	1:A:326:LYS:HG2	2.20	0.42
1:A:464:LEU:HD23	1:A:483:PHE:HE1	1.85	0.42
1:E:129:VAL:HG12	1:E:130:ASP:N	2.34	0.42
1:E:763:THR:C	1:E:765:LEU:H	2.23	0.42
1:A:698:ILE:HG13	4:A:892:HOH:O	2.19	0.42
1:E:565:GLU:O	1:E:681:MET:HA	2.20	0.42
1:E:731:VAL:HA	1:E:796:MET:HB3	2.02	0.42
1:A:207:GLY:O	1:A:337:MET:HG2	2.20	0.42
1:E:344:SER:HB2	1:E:345:PRO:HD2	2.00	0.42
1:E:338:ILE:O	1:E:342:LEU:HB2	2.19	0.42
1:C:659:ILE:O	1:C:663:VAL:HG23	2.20	0.42
1:C:140:GLU:HG3	1:C:188:ILE:HD13	2.02	0.42
2:B:484:ASP:OD2	2:B:494:ARG:HB2	2.20	0.42
1:E:355:GLN:O	1:E:479:LYS:HG3	2.20	0.42
1:A:832:VAL:HA	1:A:833:PRO:HD3	1.95	0.42
1:E:296:ILE:HG21	1:E:319:LEU:HD21	2.01	0.42
2:B:487:PRO:HB2	2:B:491:GLY:HA2	2.02	0.42
1:A:40:VAL:HG12	1:A:75:ILE:HG21	2.01	0.42
1:C:628:THR:O	1:C:632:LYS:HG3	2.19	0.42
1:C:491:VAL:HG13	1:C:538:LEU:HD21	2.01	0.42
1:A:223:ARG:HB3	1:A:336:GLU:OE1	2.20	0.42
1:C:501:LEU:HD23	1:C:501:LEU:C	2.40	0.42
1:E:327:PHE:CD2	1:E:328:LEU:HG	2.55	0.42
1:E:155:VAL:HG21	1:E:202:VAL:HG21	2.02	0.42
1:E:410:LYS:HA	1:E:430:ALA:HA	2.02	0.42
2:B:538:ARG:HA	2:B:538:ARG:HE	1.85	0.42
2:D:474:ASP:HA	2:D:475:PRO:HD2	1.89	0.42
1:C:539:GLU:O	1:C:543:GLN:HG3	2.20	0.41
1:C:20:ARG:NH1	1:C:344:SER:HB3	2.35	0.41
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.49	0.41
1:A:486:SER:HA	1:A:487:PRO:HD3	1.87	0.41
1:C:132:ILE:HD11	1:C:162:ARG:HB2	2.01	0.41
1:C:77:LEU:HB2	1:C:100:ILE:HB	2.02	0.41
1:C:813:SER:O	1:C:817:GLU:HB2	2.20	0.41
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.93	0.41
1:C:588:LEU:C	1:C:588:LEU:HD12	2.41	0.41
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.55	0.41
1:C:486:SER:HA	1:C:487:PRO:HD3	1.86	0.41
1:A:284:LEU:HD23	1:A:299:LEU:HD23	2.02	0.41
1:E:119:LEU:HD21	1:E:146:ALA:HA	2.02	0.41
2:B:471:ILE:CG1	2:B:554:THR:HB	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.56	0.40
1:C:381:TYR:O	1:C:398:GLY:HA3	2.22	0.40
2:F:427:ARG:HA	4:F:755:HOH:O	2.20	0.40
1:A:609:ARG:HH11	1:A:609:ARG:HG3	1.81	0.40
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:E:342:LEU:HA	1:E:343:PRO:HD2	1.85	0.40
1:A:120:ARG:HH12	1:A:479:LYS:HD2	1.86	0.40
1:E:103:ILE:HD13	1:E:122:THR:HG22	2.04	0.40
2:B:511:PHE:HB3	2:B:600:TYR:CD1	2.55	0.40
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.57	0.40
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.57	0.40
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.85	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%)	779 (95%)	36 (4%)	3 (0%)	39	46
1	C	818/842 (97%)	778 (95%)	35 (4%)	5 (1%)	30	34
1	E	818/842 (97%)	762 (93%)	53 (6%)	3 (0%)	39	46
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
2	F	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	34	39
All	All	3069/3147 (98%)	2919 (95%)	138 (4%)	12 (0%)	39	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY

Continued on next page...

*Continued from previous page...*

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/714 (98%)	692 (99%)	7 (1%)	82	91
1	C	699/714 (98%)	688 (98%)	11 (2%)	70	83
1	E	699/714 (98%)	690 (99%)	9 (1%)	76	87
2	B	161/161 (100%)	160 (99%)	1 (1%)	90	96
2	D	161/161 (100%)	154 (96%)	7 (4%)	35	45
2	F	161/161 (100%)	155 (96%)	6 (4%)	41	53
All	All	2580/2625 (98%)	2539 (98%)	41 (2%)	70	83

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	528	HIS
1	C	753	GLN
1	E	476	HIS
1	E	753	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	DDE	A	699	1	5,10,21	0.55	0	3,12,30	1.69	1 (33%)
1	DDE	C	699	1	13,20,21	0.84	0	16,28,30	0.65	0
1	DDE	E	699	1	13,20,21	0.85	1 (7%)	16,28,30	0.71	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	-	0/19/21/23	0/1/1/1

All (1) bond length outliers are listed below:

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

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	CD2-NE2-CE1	2.05	108.95	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no 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	1 (2%)	47,73,73	1.84	4 (8%)
3	NAD	D	701	-	38,48,48	0.65	1 (2%)	47,73,73	1.92	4 (8%)
3	NAD	F	702	-	38,48,48	0.66	0	47,73,73	1.89	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	700	-	-	0/22/62/62	0/5/5/5
3	NAD	D	701	-	-	0/22/62/62	0/5/5/5
3	NAD	F	702	-	-	0/22/62/62	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	NAD	O4B-C1B	2.01	1.43	1.41
3	D	701	NAD	O4B-C1B	2.04	1.43	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	NAD	N3A-C2A-N1A	-9.40	121.69	128.89
3	F	702	NAD	N3A-C2A-N1A	-9.35	121.74	128.89
3	B	700	NAD	N3A-C2A-N1A	-9.02	121.98	128.89
3	D	701	NAD	PN-O3-PA	-4.80	119.26	132.73
3	F	702	NAD	PN-O3-PA	-4.50	120.09	132.73
3	B	700	NAD	PN-O3-PA	-4.41	120.35	132.73
3	F	702	NAD	C4B-O4B-C1B	-4.14	105.17	109.72
3	D	701	NAD	C4B-O4B-C1B	-3.36	106.03	109.72
3	B	700	NAD	C4B-O4B-C1B	-2.66	106.79	109.72
3	F	702	NAD	O4B-C1B-N9A	3.89	116.23	108.10
3	B	700	NAD	O4B-C1B-N9A	3.98	116.43	108.10
3	D	701	NAD	O4B-C1B-N9A	4.18	116.84	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	NAD	2	0
3	D	701	NAD	3	0
3	F	702	NAD	1	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%)	0.48	75 (9%) 11 18	14, 55, 97, 118	0
1	C	822/842 (97%)	0.89	134 (16%) 2 4	16, 61, 135, 187	0
1	E	822/842 (97%)	2.66	440 (53%) 0 0	16, 136, 189, 262	0
2	B	207/207 (100%)	0.15	8 (3%) 43 57	14, 27, 61, 94	0
2	D	207/207 (100%)	0.14	8 (3%) 43 57	12, 25, 57, 89	0
2	F	207/207 (100%)	0.14	8 (3%) 43 57	17, 29, 62, 108	0
All	All	3087/3147 (98%)	1.10	673 (21%) 1 2	12, 57, 169, 262	0

All (673) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	108	HIS	13.8
1	E	314	LEU	13.2
1	E	195	GLU	13.1
1	E	67	GLY	13.0
1	E	157	ILE	11.7
1	E	789	GLY	11.2
1	E	167	LEU	11.2
1	E	356	LEU	10.2
1	E	553	PRO	10.0
1	E	760	ARG	10.0
1	E	289	MET	9.8
1	E	166	GLU	9.7
1	E	766	PHE	9.6
1	E	311	GLU	9.6
1	E	196	VAL	9.6
1	E	367	ILE	9.4
1	E	310	ASP	9.3
1	E	315	GLU	9.0
1	E	361	ALA	8.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	761	PRO	8.8
1	E	759	GLN	8.7
1	E	78	TYR	8.5
1	E	498	ALA	8.4
1	C	495	VAL	8.3
1	E	268	PRO	8.2
1	E	169	VAL	8.2
1	C	498	ALA	8.1
1	E	26	ALA	8.1
1	E	48	ALA	8.1
1	C	522	MET	8.1
1	C	502	PRO	8.1
1	E	156	VAL	8.1
1	E	128	VAL	8.0
1	E	294	ASP	8.0
1	E	231	LYS	8.0
1	E	192	TYR	8.0
1	E	232	LYS	8.0
1	E	741	GLY	8.0
1	E	41	GLN	8.0
1	E	81	MET	8.0
1	C	499	ASN	7.9
1	E	262	THR	7.9
1	E	281	ILE	7.9
1	E	175	TYR	7.8
1	E	254	THR	7.8
1	E	258	THR	7.7
1	E	240	MET	7.6
1	E	129	VAL	7.6
1	E	163	ALA	7.6
1	E	107	GLY	7.6
1	E	499	ASN	7.4
1	E	194	ASP	7.4
1	E	464	LEU	7.4
1	C	550	ALA	7.3
1	E	211	PHE	7.3
1	E	160	VAL	7.3
1	E	179	ALA	7.3
1	E	106	PRO	7.2
1	E	308	LYS	7.2
1	E	755	VAL	7.2
1	E	321	LYS	7.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	91	GLN	7.2
1	E	267	LYS	7.1
1	E	86	VAL	7.1
1	C	291	PHE	7.1
1	E	203	TYR	7.0
1	E	790	GLY	6.9
1	E	233	PHE	6.9
1	E	34	THR	6.8
1	E	332	ASP	6.8
1	E	212	GLY	6.7
1	E	38	SER	6.6
1	E	740	VAL	6.6
1	E	298	VAL	6.6
1	E	188	ILE	6.6
1	E	307	LEU	6.5
1	E	763	THR	6.5
1	E	762	GLY	6.4
1	E	342	LEU	6.4
1	E	168	GLN	6.4
1	E	420	PRO	6.4
1	E	111	PHE	6.3
1	E	218	TRP	6.3
1	E	187	VAL	6.3
1	E	745	SER	6.2
1	E	127	VAL	6.1
1	E	137	VAL	6.1
1	E	32	LYS	6.1
1	C	67	GLY	6.1
1	E	770	ALA	6.0
1	E	131	THR	6.0
1	E	269	LEU	6.0
1	A	483	PHE	5.9
1	C	264	ALA	5.9
1	E	76	SER	5.9
1	E	98	PHE	5.9
1	E	554	LEU	5.9
1	E	230	ALA	5.9
1	E	266	GLY	5.8
1	E	317	LYS	5.8
1	E	239	LYS	5.8
1	E	185	VAL	5.8
1	E	216	HIS	5.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	737	GLU	5.8
1	C	167	LEU	5.8
1	E	256	LYS	5.8
1	E	282	PHE	5.8
1	E	335	LEU	5.8
1	E	316	GLY	5.7
1	E	162	ARG	5.7
1	E	299	LEU	5.7
1	E	306	VAL	5.7
1	E	358	GLU	5.7
1	E	442	VAL	5.7
2	D	489	ALA	5.7
1	E	77	LEU	5.6
1	C	306	VAL	5.6
1	E	366	CYS	5.6
1	E	422	LYS	5.6
1	E	193	ALA	5.6
1	E	88	GLU	5.6
1	E	89	ILE	5.6
1	E	497	ASN	5.6
1	E	360	PRO	5.6
1	E	143	LEU	5.6
1	E	197	LEU	5.6
1	E	312	LYS	5.5
1	E	178	PHE	5.5
1	E	764	PRO	5.5
1	E	496	LYS	5.5
1	E	80	GLU	5.5
1	C	504	LEU	5.4
1	C	553	PRO	5.4
1	E	90	LYS	5.4
1	E	546	GLU	5.4
1	E	495	VAL	5.4
1	E	421	GLY	5.4
2	B	489	ALA	5.4
1	E	110	ASP	5.4
1	E	237	LYS	5.4
1	E	261	ASP	5.4
1	E	263	ASP	5.3
1	C	496	LYS	5.3
1	E	375	LYS	5.3
1	E	501	LEU	5.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	513	LYS	5.3
1	E	180	ARG	5.2
1	E	436	LEU	5.2
1	E	96	ASN	5.2
1	C	252	PRO	5.2
1	C	311	GLU	5.2
1	E	182	VAL	5.2
1	E	739	ALA	5.2
1	E	309	GLY	5.1
1	E	747	LEU	5.1
1	E	245	TRP	5.1
1	C	544	ASP	5.1
1	E	419	VAL	5.1
1	E	278	LEU	5.1
1	E	210	ALA	5.1
1	E	255	LYS	5.1
1	E	215	LEU	5.1
1	E	297	PRO	5.1
1	E	453	ILE	5.1
1	A	196	VAL	5.0
1	E	69	THR	5.0
1	E	7	ASP	5.0
1	E	794	PRO	5.0
1	E	37	ASP	5.0
1	E	756	SER	5.0
1	C	290	ASN	5.0
1	E	343	PRO	4.9
1	C	497	ASN	4.9
1	A	361	ALA	4.9
1	E	222	ILE	4.9
1	E	40	VAL	4.9
1	E	135	VAL	4.9
1	E	392	GLY	4.9
1	C	233	PHE	4.9
1	E	277	ILE	4.9
1	E	441	PHE	4.9
1	E	500	ASP	4.8
1	E	758	GLU	4.8
1	A	464	LEU	4.8
1	E	47	SER	4.8
1	E	29	ASP	4.8
1	E	260	LYS	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	503	LYS	4.8
1	E	736	PRO	4.8
1	E	522	MET	4.8
1	E	220	PHE	4.8
1	E	109	VAL	4.7
1	C	268	PRO	4.7
1	E	200	VAL	4.7
1	C	267	LYS	4.7
1	E	304	GLU	4.7
1	E	444	PRO	4.7
1	E	738	GLN	4.7
1	E	757	GLU	4.7
1	E	290	ASN	4.7
1	E	42	ARG	4.7
1	E	265	GLU	4.7
1	E	329	PRO	4.6
1	E	158	ASN	4.6
1	C	494	GLU	4.6
1	E	389	SER	4.6
1	E	471	THR	4.6
1	E	742	GLY	4.6
1	C	500	ASP	4.6
1	E	46	ILE	4.6
1	E	324	MET	4.6
1	E	469	LEU	4.6
1	E	242	ASP	4.6
1	E	743	ILE	4.5
1	E	395	TYR	4.5
1	C	262	THR	4.5
1	E	25	ILE	4.5
1	E	20	ARG	4.5
1	E	291	PHE	4.5
1	E	348	ALA	4.5
1	E	779	GLY	4.5
1	E	257	TRP	4.5
1	E	68	ILE	4.4
1	E	525	SER	4.4
1	E	154	VAL	4.4
1	E	339	VAL	4.4
1	E	504	LEU	4.4
1	E	795	GLN	4.4
1	E	36	THR	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	28	VAL	4.4
1	E	555	LYS	4.4
1	E	548	ASP	4.4
1	E	155	VAL	4.4
1	C	547	HIS	4.4
1	E	784	LEU	4.4
1	C	173	ASP	4.4
1	E	83	ASP	4.4
1	E	320	LEU	4.3
1	E	3	ALA	4.3
1	E	273	PHE	4.3
1	E	401	PHE	4.3
1	C	523	SER	4.3
1	C	298	VAL	4.3
1	E	217	GLY	4.3
1	E	793	PHE	4.3
1	E	492	ALA	4.3
2	F	489	ALA	4.3
1	C	391	LYS	4.2
1	A	480	VAL	4.2
1	E	744	TYR	4.2
1	C	310	ASP	4.2
1	E	164	LEU	4.2
1	C	265	GLU	4.2
1	E	502	PRO	4.2
1	E	456	LEU	4.2
1	A	198	GLY	4.2
1	E	362	ASP	4.2
1	E	100	ILE	4.1
1	E	183	GLU	4.1
1	E	791	GLN	4.1
1	E	207	GLY	4.1
1	E	465	LYS	4.1
1	E	479	LYS	4.1
1	E	483	PHE	4.1
1	C	168	GLN	4.0
1	E	235	VAL	4.0
1	C	301	GLU	4.0
1	E	301	GLU	4.0
1	E	778	PHE	4.0
1	A	360	PRO	4.0
1	E	201	GLN	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	28	VAL	4.0
1	E	147	LEU	4.0
1	E	440	ARG	4.0
1	C	313	ASP	4.0
1	E	276	PHE	3.9
1	E	209	VAL	3.9
1	E	292	LYS	3.9
1	E	783	GLU	3.9
1	C	236	ASP	3.9
1	C	251	ASN	3.9
1	E	27	HIS	3.9
1	E	105	SER	3.9
1	E	302	LYS	3.9
1	E	328	LEU	3.9
1	E	391	LYS	3.9
1	C	235	VAL	3.9
1	C	761	PRO	3.8
1	C	501	LEU	3.8
1	E	253	LYS	3.8
1	E	418	TYR	3.8
1	E	455	GLY	3.8
1	A	107	GLY	3.8
1	E	243	ARG	3.8
1	C	321	LYS	3.8
2	F	490	ARG	3.8
1	E	767	THR	3.7
1	C	552	VAL	3.7
1	E	227	THR	3.7
1	C	314	LEU	3.7
1	A	67	GLY	3.7
1	E	288	ILE	3.7
1	E	28	VAL	3.7
1	E	481	MET	3.7
1	E	85	ASP	3.7
1	E	340	LEU	3.7
1	C	232	LYS	3.7
1	E	480	VAL	3.7
1	A	111	PHE	3.7
1	E	165	LEU	3.6
2	F	461	ASP	3.6
1	E	353	ALA	3.6
1	E	454	ILE	3.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	466	THR	3.6
1	E	293	LYS	3.6
1	E	437	MET	3.6
2	D	498	LEU	3.6
1	E	286	THR	3.6
1	E	189	VAL	3.6
1	E	754	VAL	3.6
1	E	305	ILE	3.5
1	A	358	GLU	3.5
1	C	503	LYS	3.5
1	E	104	ASP	3.5
1	E	380	LEU	3.5
1	C	263	ASP	3.5
1	E	287	ALA	3.5
1	E	542	LEU	3.5
1	E	494	GLU	3.5
1	E	138	GLN	3.5
1	E	295	GLU	3.5
1	E	177	THR	3.5
1	E	476	HIS	3.5
1	E	748	ASN	3.5
1	E	357	TYR	3.5
1	C	551	GLY	3.4
1	C	528	HIS	3.4
1	C	7	ASP	3.4
1	E	161	ASP	3.4
1	C	11	SER	3.4
1	E	176	GLN	3.4
1	C	269	LEU	3.4
1	E	280	PRO	3.4
1	C	318	ALA	3.4
1	A	786	GLN	3.4
1	E	368	ALA	3.4
1	E	296	ILE	3.4
1	E	445	ILE	3.4
1	C	755	VAL	3.4
1	E	322	VAL	3.4
1	E	93	THR	3.4
1	E	130	ASP	3.4
1	E	780	PHE	3.3
1	A	46	ILE	3.3
1	A	129	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	454	ILE	3.3
1	A	495	VAL	3.3
1	E	8	GLN	3.3
1	E	82	SER	3.3
1	C	546	GLU	3.3
1	E	510	ARG	3.3
1	C	29	ASP	3.3
1	E	94	ASP	3.3
1	E	470	THR	3.3
1	C	99	LEU	3.3
1	E	523	SER	3.3
1	A	157	ILE	3.3
1	E	551	GLY	3.3
1	E	30	HIS	3.3
1	C	84	GLU	3.3
1	C	277	ILE	3.2
1	C	303	LEU	3.2
1	A	400	VAL	3.2
1	E	264	ALA	3.2
1	E	252	PRO	3.2
1	E	132	ILE	3.2
1	E	159	LYS	3.2
1	E	24	VAL	3.2
1	E	31	GLY	3.2
1	C	302	LYS	3.2
1	C	482	LYS	3.2
1	C	295	GLU	3.2
1	C	299	LEU	3.2
1	E	341	HIS	3.2
1	C	266	GLY	3.2
2	D	461	ASP	3.2
1	C	549	HIS	3.2
1	E	338	ILE	3.2
1	C	740	VAL	3.2
1	E	472	SER	3.2
1	E	451	GLY	3.1
1	E	118	ALA	3.1
1	A	499	ASN	3.1
1	C	261	ASP	3.1
1	C	312	LYS	3.1
1	A	48	ALA	3.1
1	E	319	LEU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	337	MET	3.1
1	E	519	LEU	3.1
1	C	108	HIS	3.1
1	E	796	MET	3.1
1	E	151	ILE	3.1
1	E	136	CYS	3.1
1	E	351	TYR	3.1
1	E	769	LYS	3.1
1	E	285	PHE	3.1
1	C	555	LYS	3.0
1	E	221	THR	3.0
1	C	111	PHE	3.0
1	E	44	GLY	3.0
1	E	275	MET	3.0
1	C	231	LYS	3.0
1	E	547	HIS	3.0
1	E	146	ALA	3.0
1	E	390	ASP	3.0
1	E	334	LEU	3.0
1	A	392	GLY	3.0
1	E	427	PHE	3.0
1	E	97	SER	3.0
1	E	323	VAL	3.0
1	A	82	SER	3.0
1	C	784	LEU	3.0
1	E	443	GLU	2.9
1	E	325	ARG	2.9
1	E	423	LYS	2.9
2	B	461	ASP	2.9
1	E	133	GLU	2.9
1	E	10	ARG	2.9
1	E	101	ASN	2.9
1	E	234	GLY	2.9
1	C	362	ASP	2.9
2	B	555	ILE	2.9
1	E	35	LEU	2.9
1	E	284	LEU	2.9
1	E	371	ASN	2.9
1	A	310	ASP	2.9
1	C	294	ASP	2.9
1	E	552	VAL	2.9
1	C	305	ILE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	556	LEU	2.9
1	E	241	MET	2.9
1	E	186	ASN	2.9
1	A	7	ASP	2.9
1	C	238	ALA	2.8
1	E	205	ALA	2.8
1	E	433	ARG	2.8
2	F	501	VAL	2.8
1	C	763	THR	2.8
1	E	14	ASP	2.8
1	A	264	ALA	2.8
1	A	90	LYS	2.8
1	E	359	GLY	2.8
1	E	9	MET	2.8
1	E	333	ALA	2.8
1	E	398	GLY	2.8
1	A	156	VAL	2.8
1	E	84	GLU	2.8
1	A	29	ASP	2.8
1	E	347	THR	2.8
1	A	127	VAL	2.8
1	E	79	SER	2.8
1	A	108	HIS	2.8
1	E	354	GLU	2.8
1	A	194	ASP	2.8
1	C	300	LEU	2.8
1	C	526	GLY	2.8
1	E	394	PHE	2.8
1	E	393	ARG	2.8
1	E	229	TYR	2.8
2	F	459	SER	2.7
1	E	236	ASP	2.7
2	F	471	ILE	2.7
2	F	499	LEU	2.7
1	A	237	LYS	2.7
1	E	259	ASN	2.7
1	C	509	LYS	2.7
1	E	369	ILE	2.7
1	E	43	ALA	2.7
1	E	114	GLU	2.7
1	E	505	VAL	2.7
1	E	746	VAL	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	404	THR	2.7
1	E	474	THR	2.7
1	A	485	VAL	2.7
1	A	375	LYS	2.7
1	A	359	GLY	2.7
1	E	73	THR	2.7
1	C	2	VAL	2.7
1	E	6	VAL	2.7
1	E	202	VAL	2.7
1	E	23	SER	2.6
1	E	144	ARG	2.6
2	B	490	ARG	2.6
1	E	379	MET	2.6
1	E	272	ALA	2.6
1	E	15	LYS	2.6
1	E	313	ASP	2.6
1	A	391	LYS	2.6
1	E	435	VAL	2.6
1	E	751	ARG	2.6
1	A	553	PRO	2.6
1	C	485	VAL	2.6
2	B	471	ILE	2.6
1	E	153	PRO	2.6
1	A	84	GLU	2.6
1	E	134	GLY	2.6
1	C	19	VAL	2.6
1	E	300	LEU	2.6
1	C	254	THR	2.6
1	E	365	ASN	2.6
1	E	125	ALA	2.5
1	C	493	VAL	2.5
1	E	103	ILE	2.5
1	A	291	PHE	2.5
1	C	293	LYS	2.5
1	E	785	ARG	2.5
1	A	86	VAL	2.5
1	C	308	LYS	2.5
1	C	100	ILE	2.5
1	E	113	SER	2.5
1	A	5	THR	2.5
1	E	303	LEU	2.5
1	C	169	VAL	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	19	VAL	2.5
1	E	75	ILE	2.5
2	D	471	ILE	2.5
1	E	372	CYS	2.5
1	C	744	TYR	2.5
1	E	213	SER	2.5
1	A	419	VAL	2.5
1	E	493	VAL	2.5
1	E	731	VAL	2.5
1	E	452	ASN	2.5
1	E	399	ARG	2.5
1	E	473	GLU	2.5
1	C	5	THR	2.5
1	A	453	ILE	2.5
2	D	490	ARG	2.5
1	E	397	PHE	2.5
1	E	92	LYS	2.4
1	E	364	ALA	2.4
1	E	781	THR	2.4
1	A	362	ASP	2.4
1	A	738	GLN	2.4
1	E	381	TYR	2.4
1	E	122	THR	2.4
1	E	244	LEU	2.4
1	E	18	ASN	2.4
1	E	410	LYS	2.4
1	E	521	TYR	2.4
1	C	315	GLU	2.4
1	C	37	ASP	2.4
1	C	292	LYS	2.4
1	E	549	HIS	2.4
1	A	420	PRO	2.4
1	E	374	PRO	2.4
1	E	99	LEU	2.4
1	E	545	LEU	2.4
1	E	412	ARG	2.4
1	A	16	VAL	2.4
1	C	260	LYS	2.4
1	C	529	ILE	2.4
1	A	233	PHE	2.4
1	E	5	THR	2.4
1	C	42	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	554	LEU	2.4
1	C	738	GLN	2.4
1	E	171	LYS	2.4
1	A	199	ASP	2.4
1	E	344	SER	2.4
1	C	287	ALA	2.4
1	C	422	LYS	2.4
1	C	609	ARG	2.4
1	E	352	ARG	2.4
1	C	506	GLU	2.3
1	E	485	VAL	2.3
1	E	223	ARG	2.3
1	C	548	ASP	2.3
1	E	556	ILE	2.3
1	E	225	PHE	2.3
1	E	318	ALA	2.3
1	C	198	GLY	2.3
1	E	228	ARG	2.3
1	C	258	THR	2.3
1	C	766	PHE	2.3
1	C	510	ARG	2.3
1	A	417	ASN	2.3
1	C	556	ILE	2.3
1	E	400	VAL	2.3
1	E	4	PHE	2.3
1	A	293	LYS	2.3
1	E	558	PRO	2.3
1	A	109	VAL	2.3
1	C	154	VAL	2.3
1	E	402	ALA	2.3
1	E	468	THR	2.3
2	D	556	LEU	2.3
1	C	453	ILE	2.2
1	C	454	ILE	2.2
1	E	121	VAL	2.2
1	A	313	ASP	2.2
1	E	123	ASP	2.2
1	E	413	ILE	2.2
1	C	229	TYR	2.2
1	A	433	ARG	2.2
1	C	237	LYS	2.2
1	A	469	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	511	LEU	2.2
1	A	212	GLY	2.2
1	A	294	ASP	2.2
1	C	525	SER	2.2
1	E	21	ASN	2.2
1	C	106	PRO	2.2
1	C	307	LEU	2.2
1	E	39	LEU	2.2
1	E	511	LEU	2.2
1	A	713	THR	2.2
1	A	124	GLY	2.2
1	E	735	CYS	2.2
2	D	537	LEU	2.2
1	E	814	LYS	2.2
1	E	11	SER	2.2
1	E	70	ILE	2.2
1	C	400	VAL	2.2
1	E	199	ASP	2.2
1	A	209	VAL	2.1
1	E	2	VAL	2.1
1	C	378	LEU	2.1
1	E	33	SER	2.1
1	A	496	LYS	2.1
2	F	555	ILE	2.1
1	E	349	GLN	2.1
1	A	442	VAL	2.1
1	A	389	SER	2.1
1	C	325	ARG	2.1
1	C	441	PHE	2.1
1	E	460	ASP	2.1
1	E	609	ARG	2.1
1	C	521	TYR	2.1
1	C	456	LEU	2.1
1	E	141	THR	2.1
2	B	499	LEU	2.1
1	E	526	GLY	2.1
1	E	250	PHE	2.1
1	A	466	THR	2.1
1	A	434	VAL	2.1
1	E	768	VAL	2.1
1	A	211	PHE	2.1
1	A	81	MET	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	455	GLY	2.1
1	A	37	ASP	2.1
1	C	446	ASP	2.1
1	C	759	GLN	2.1
1	E	145	GLN	2.1
1	C	234	GLY	2.0
1	E	219	ALA	2.0
1	E	771	TYR	2.0
1	C	90	LYS	2.0
1	A	552	VAL	2.0
1	A	87	LYS	2.0
1	C	380	LEU	2.0
1	C	483	PHE	2.0
1	C	765	LEU	2.0
1	E	22	MET	2.0
2	B	439	TYR	2.0
1	A	33	SER	2.0
1	E	246	GLY	2.0
1	E	477	ASN	2.0
1	A	473	GLU	2.0
1	A	437	MET	2.0
1	E	536	LEU	2.0
2	D	499	LEU	2.0
1	E	416	PRO	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. 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	0.95	0.14	-	45,60,66,70	0
1	DDE	C	699	20/21	0.93	0.21	-	29,64,106,111	0
1	DDE	E	699	20/21	0.92	0.21	-	38,73,107,109	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	B	700	44/44	0.96	0.15	-0.34	17,28,45,62	0
3	NAD	F	702	44/44	0.95	0.15	-0.42	11,32,48,56	0
3	NAD	D	701	44/44	0.96	0.15	-0.55	7,24,49,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.