



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 09:21 AM EDT

PDB ID : 3B78  
Title : Structure of the eEF2-ExoA(R551H)-NAD<sup>+</sup> complex  
Authors : Jorgensen, R.; Merrill, A.R.  
Deposited on : unknown  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

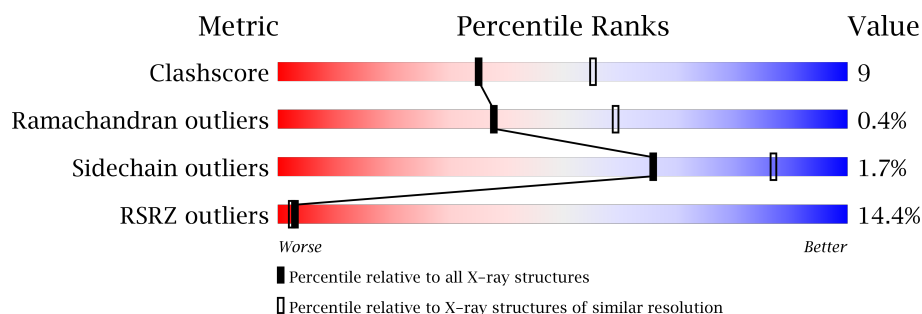
# 1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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	 2% 75% 22% ..
1	C	842	 10% 74% 22% ..
1	E	842	 41% 69% 28% ..
2	B	207	 84% 16%
2	D	207	 90% 10%
2	F	207	 85% 14%

## 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:

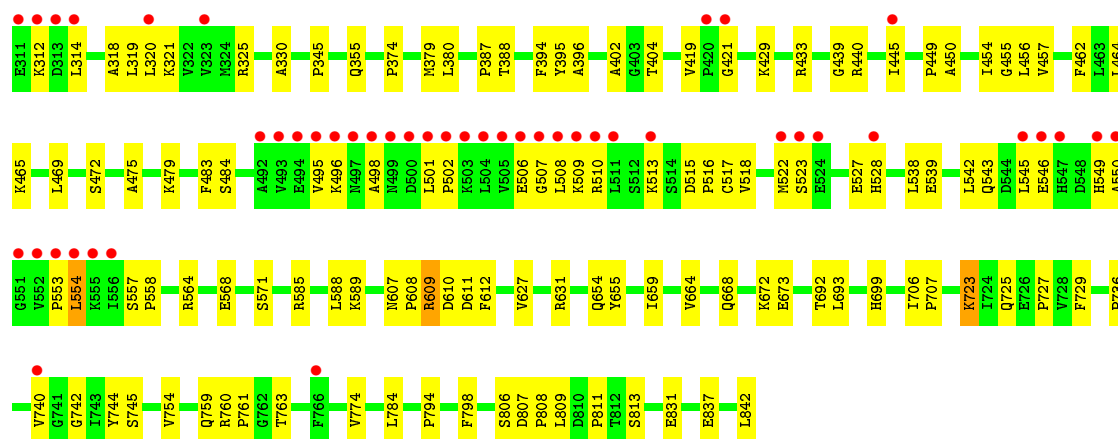
Chain	Residue	Modelled	Actual	Comment	Reference
B	399	ALA	-	EXPRESSION TAG	UNP P11439
B	407	VAL	ILE	SEE REMARK 999	UNP P11439
B	515	SER	GLY	SEE REMARK 999	UNP P11439
B	551	HIS	ARG	ENGINEERED	UNP P11439
D	399	ALA	-	EXPRESSION TAG	UNP P11439
D	407	VAL	ILE	SEE REMARK 999	UNP P11439
D	515	SER	GLY	SEE REMARK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

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- The chemical structure of NADH (Nicotinamide Adenine Dinucleotide) is shown. It consists of a nicotinamide ring (top) connected to a ribose sugar (middle), which is linked via a pyrophosphate bridge to another ribose sugar (bottom) attached to an adenine ring (bottom). The structure is color-coded: blue for the nitrogenous bases, red for the ribose sugars, and purple for the phosphate groups. The nicotinamide ring is in its oxidized state (NAD<sup>+</sup>), and the adenine ring is in its reduced state (adenine).

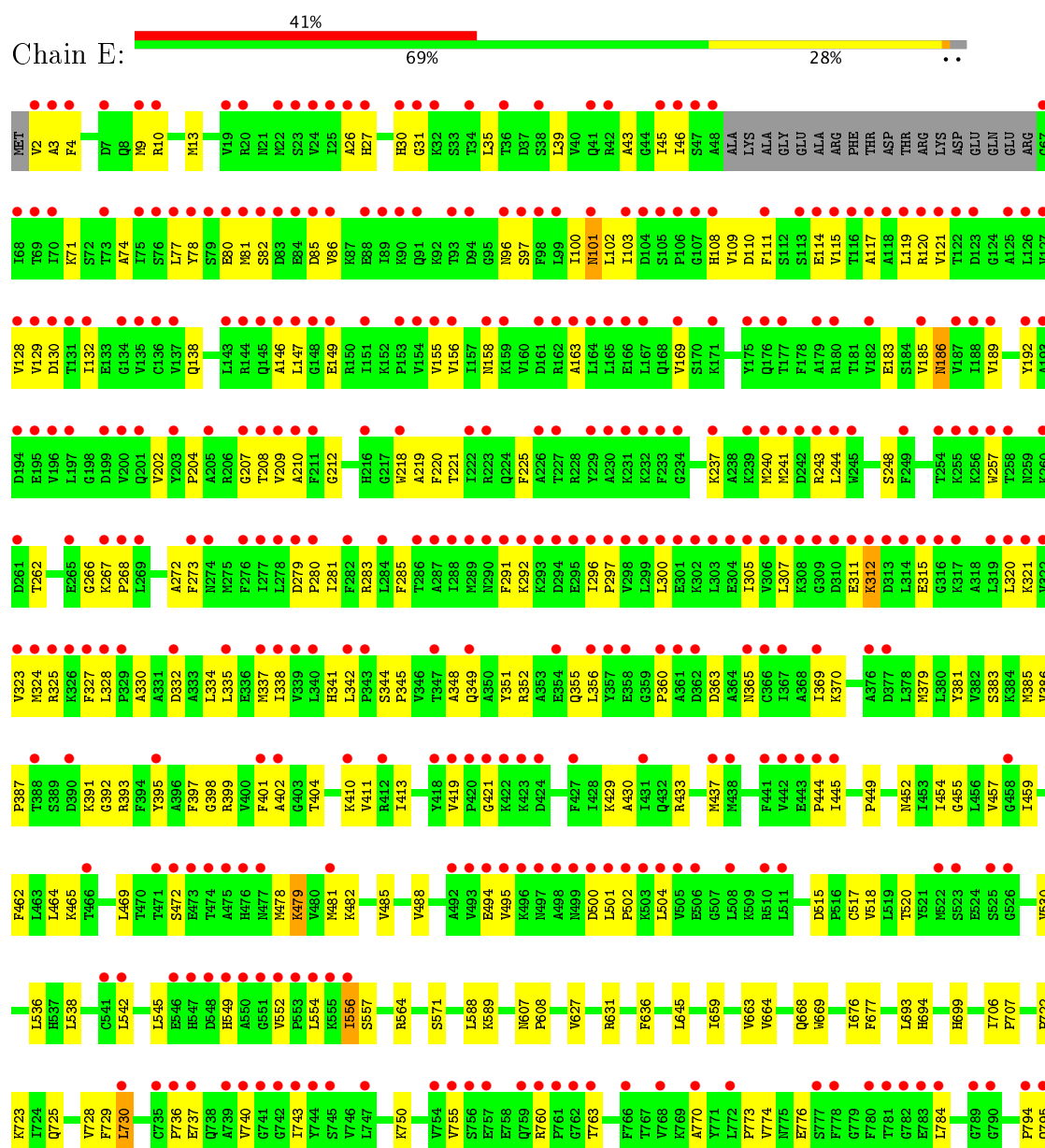
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	F	1	Total 44	C 21	N 7	O 14	P 2	0	0

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





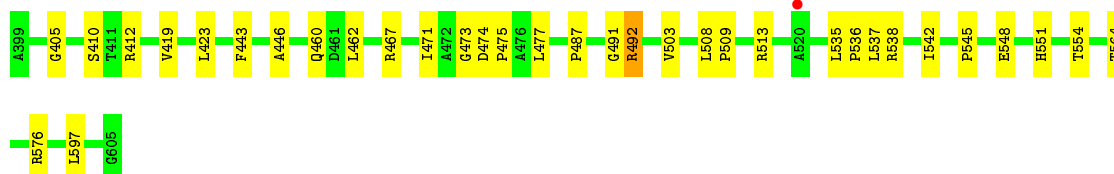
• Molecule 1: Elongation factor 2





## ● Molecule 2: Exotoxin A

Chain B: 84% 16%



## ● Molecule 2: Exotoxin A

Chain D: 90% 10%



## ● Molecule 2: Exotoxin A

Chain F: 85% 14%



## 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 0.185 , (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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.21	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:70:ILE:HG22	1:A:388:THR:HG22	1.74	0.68
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.75	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:26:ALA:HB2	1:E:128:VAL:HB	1.77	0.66
1:E:520:THR:HG22	1:E:530:VAL:HG22	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:A:578:LYS:HG2	1:A:585:ARG:HG2	1.81	0.62
1:C:433:ARG:HB3	1:C:457:VAL:HB	1.81	0.62
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: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:379:MET:HB2	1:E:402:ALA:HB3	1.82	0.61
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.81	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:510:ARG:HG3	1:A:549:HIS:HD2	1.66	0.59
1:A:810:ASP:O	1:A:816:GLY:HA3	2.01	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
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.84	0.57
1:E:26:ALA:CB	1:E:128:VAL:HB	2.34	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:654:GLN:HG2	1:A:655:TYR:CD1	2.38	0.57
1:A:569:SER:O	1:A:720:ALA:HB1	2.05	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: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:291:PHE:CD1	1:E:315:GLU:HB3	2.42	0.55
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.89	0.54
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.88	0.54
1:A:381:TYR:O	1:A:398:GLY:HA3	2.07	0.54
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.89	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:755:VAL:HG23	1:E:770:ALA:HA	1.91	0.53
1:E:488:VAL:HG12	1:E:774:VAL:HG11	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: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:C:699:DDE:CAA	3:D:701:NAD:H4D	2.33	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:A:379:MET:HB2	1:A:402:ALA:HB3	1.92	0.50
1:E:120:ARG:HG3	1:E:356:LEU:HD22	1.93	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:A:365:ASN:O	1:A:369:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ALA:HA	1:E:102:LEU:O	2.12	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:482:LYS:HB3	1:E:797:VAL:HG11	1.94	0.49
1:E:81:MET:HB3	1:E:85:ASP:HB2	1.95	0.49
1:C:200:VAL:O	1:C:200:VAL:HG12	2.13	0.49
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.94	0.49
1:C:495:VAL:HG11	1:C:501:LEU:HG	1.94	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: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:A:249:PHE:CZ	1:A:261:ASP:HB3	2.48	0.49
1:C:699:DDE:CAB	1:C:699:DDE:CAT	2.86	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: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:365:ASN:HD21	1:E:472:SER:HB3	1.77	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:A:89:ILE:HG22	1:A:91:GLN:HG2	1.95	0.48
1:C:538:LEU:O	1:C:542:LEU:HB2	2.14	0.48
1:C:627:VAL:O	1:C:631:ARG:HB2	2.14	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:487:PRO:HB3	1:A:531:ALA:HB1	1.97	0.47
1:A:828:MET:HG2	2:B:576:ARG:NE	2.29	0.47
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.95	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:A:746:VAL:O	1:A:750:LYS:HD3	2.15	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
1:A:607:ASN:HB3	1:A:610:ASP:HB2	1.97	0.47
1:C:321:LYS:O	1:C:325:ARG:HG3	2.15	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:C:465:LYS:HE3	1:C:517:CYS:SG	2.55	0.47
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.97	0.47
1:A:338:ILE:O	1:A:342:LEU:HB2	2.15	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:111:PHE:O	1:A:115:VAL:HG23	2.15	0.47
1:A:731:VAL:HG22	1:A:796:MET:HB3	1.97	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:E:39:LEU:H	1:E:39:LEU:HD12	1.79	0.47
2:B:419:VAL:O	2:B:423:LEU:HG	2.14	0.47
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.96	0.47
1:C:727:PRO:HB2	1:C:774:VAL:CG2	2.45	0.47
2:F:547:GLU:HG3	2:F:550:GLY:HA3	1.97	0.47
1:E:391:LYS:CG	1:E:392:GLY:H	2.22	0.46
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.30	0.46
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.96	0.46
1:A:454:ILE:HG13	1:A:455:GLY:H	1.80	0.46
2:B:545:PRO:HA	2:B:551:HIS:O	2.15	0.46
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.98	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:A:478:MET:O	1:A:479:LYS:C	2.54	0.46
1:A:6:VAL:CG1	1:A:445:ILE:HG22	2.45	0.46
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.97	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:E:676:ILE:HG22	1:E:677:PHE:HD2	1.80	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:C:169:VAL:HG22	1:C:173:ASP:HB2	1.98	0.46
1:E:296:ILE:N	1:E:297:PRO:HD2	2.31	0.46
1:E:349:GLN:O	1:E:370:LYS:HA	2.15	0.46
1:A:385:MET:HG2	1:A:465:LYS:HA	1.97	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:E:823:ARG:HG2	1:E:828:MET:HE3	1.98	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: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:E:39:LEU:HD23	1:E:335:LEU:HD23	1.99	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:204:PRO:HA	1:E:209:VAL:HB	1.98	0.45
1:E:500:ASP:HB3	1:E:552:VAL:HG21	1.99	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
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:659:ILE:O	1:E:663:VAL:HG23	2.17	0.45
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.17	0.45
1:C:539:GLU:O	1:C:543:GLN:HG3	2.17	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:E:729:PHE:CE2	1:E:774:VAL:HG22	2.51	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:A:16:VAL:HG21	1:A:451:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:VAL:O	1:A:668:GLN:HG2	2.16	0.45
1:E:556:ILE:HG22	1:E:557:SER:N	2.29	0.45
2:F:571:ILE:HA	2:F:572:PRO:HD3	1.85	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:A:807:ASP:HA	1:A:808:PRO:HD2	1.85	0.44
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.16	0.44
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	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:A:231:LYS:HB3	1:A:231:LYS:HE2	1.81	0.44
2:B:487:PRO:HB2	2:B:491:GLY:HA2	1.99	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
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.99	0.44
1:A:727:PRO:HD3	1:A:801:TRP:HZ3	1.82	0.44
2:B:474:ASP:HA	2:B:475:PRO:HD2	1.87	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:E:103:ILE:N	1:E:103:ILE:HD12	2.32	0.44
1:A:283:ARG:HB3	1:A:299:LEU:HD21	1.99	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
2:B:471:ILE:CG1	2:B:554:THR:HB	2.47	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:132:ILE:N	1:E:132:ILE:HD12	2.33	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
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.18	0.43
1:A:515:ASP:HA	1:A:516:PRO:HD2	1.87	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:E:267:LYS:HA	1:E:268:PRO:HD3	1.90	0.43
1:E:77:LEU:HD23	1:E:335:LEU:HD21	2.00	0.43
2:B:410:SER:OG	2:B:412:ARG:HG3	2.18	0.43
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.48	0.43
1:E:381:TYR:O	1:E:398:GLY:HA3	2.17	0.43
1:E:399:ARG:HD3	1:E:401:PHE:CZ	2.54	0.43
1:A:374:PRO:O	1:A:404:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLY:HA3	1:A:513:LYS:HD3	1.99	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:A:219:ALA:HB3	1:A:330:ALA:HA	2.00	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:C:807:ASP:HA	1:C:808:PRO:HD2	1.86	0.43
1:C:396:ALA:HB3	1:C:456:LEU:HB2	2.01	0.43
1:E:218:TRP:HB3	1:E:324:MET:HB3	2.00	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
2:F:511:PHE:HB3	2:F:600:TYR:CD1	2.54	0.43
1:A:36:THR:HG23	1:A:102:LEU:HD21	2.01	0.43
1:A:588:LEU:HD12	1:A:588:LEU:C	2.39	0.43
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.54	0.43
1:A:73:THR:HG21	1:A:384:LYS:HD2	2.01	0.43
1:A:759:GLN:HB2	1:A:766:PHE:CE2	2.53	0.43
1:C:723:LYS:HB3	1:C:723:LYS:HE3	1.67	0.43
1:C:43:ALA:HB1	1:C:78:TYR:O	2.18	0.43
1:E:737:GLU:HA	1:E:740:VAL:HG23	2.00	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:A:669:TRP:CZ2	2:B:492:ARG:HB2	2.53	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:E:244:LEU:O	1:E:273:PHE:HB2	2.18	0.43
1:E:279:ASP:O	1:E:283:ARG:HG2	2.18	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:607:ASN:HA	1:E:608:PRO:HD3	1.78	0.43
1:A:831:GLU:H	1:A:831:GLU:CD	2.20	0.43
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.99	0.43
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.53	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: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:A:545:LEU:O	1:A:550:ALA:HB3	2.19	0.42
2:B:477:LEU:HD22	2:B:551:HIS:CB	2.50	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.83	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:A:155:VAL:HG21	1:A:185:VAL:HG11	2.01	0.42
1:C:809:LEU:O	1:C:811:PRO:HD3	2.20	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: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: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:A:727:PRO:HB2	1:A:774:VAL:HG21	2.02	0.42
1:C:588:LEU:C	1:C:588:LEU:HD12	2.40	0.42
1:E:664:VAL:O	1:E:668:GLN:HG2	2.19	0.42
2:F:419:VAL:O	2:F:423:LEU:HG	2.19	0.42
2:F:488:ASP:HB3	2:F:492:ARG:HB2	2.01	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: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:E:155:VAL:HG21	1:E:202:VAL:HG21	2.02	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:A:140:GLU:HG3	1:A:188:ILE:HD13	2.02	0.41
1:C:3:ALA:HB2	1:C:46:ILE:HG13	2.02	0.41
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:410:LYS:HA	1:E:430:ALA:HA	2.02	0.41
1:E:608:PRO:HG3	1:E:636:PHE:CG	2.55	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:546:GLU:OE1	1:C:553:PRO:HD3	2.20	0.41
1:C:241:MET:HA	1:C:244:LEU:HD12	2.02	0.41
1:C:288:ILE:HA	1:C:296:ILE:HD11	2.03	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
1:C:72:SER:HA	1:C:439:GLY:O	2.19	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:E:307:LEU:HD13	1:E:311:GLU:O	2.20	0.41
2:F:508:LEU:N	2:F:509:PRO:CD	2.83	0.41
1:A:677:PHE:N	1:A:677:PHE:CD2	2.88	0.41
1:C:454:ILE:HG13	1:C:455:GLY:H	1.85	0.41
1:E:80:GLU:HA	1:E:96:ASN:O	2.20	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:C:314:LEU:HD22	1:C:318:ALA:HB1	2.02	0.41
1:C:419:VAL:HG12	1:C:421:GLY:H	1.86	0.41
1:E:109:VAL:O	1:E:109:VAL:HG12	2.21	0.41
1:E:119:LEU:HD11	1:E:146:ALA:HA	2.02	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:E:588:LEU:C	1:E:588:LEU:HD12	2.41	0.41
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.91	0.41
1:A:454:ILE:HG13	1:A:455:GLY:N	2.36	0.41
1:A:83:ASP:O	1:A:87:LYS:HG3	2.20	0.41
1:C:523:SER:OG	1:C:527:GLU:HB2	2.20	0.41
1:C:760:ARG:CG	1:C:761:PRO:HD2	2.51	0.41
1:E:237:LYS:HA	1:E:240:MET:HB3	2.03	0.41
1:E:163:ALA:O	1:E:169:VAL:HG12	2.20	0.41
1:E:345:PRO:HB3	1:E:399:ARG:HH21	1.85	0.41
1:E:728:VAL:HG22	1:E:773:PRO:HA	2.02	0.41
1:A:373:ASP:HA	1:A:374:PRO:HD2	1.85	0.41
1:A:559:PRO:HB2	1:A:778:PHE:CE2	2.56	0.41
1:C:226:ALA:CB	1:C:241:MET:HB3	2.51	0.41
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.51	0.41
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.56	0.41
1:E:736:PRO:O	1:E:740:VAL:HG23	2.21	0.41
1:A:229:TYR:HB3	1:A:233:PHE:CD2	2.56	0.40
1:C:167:LEU:O	1:C:168:GLN:C	2.59	0.40
2:F:439:TYR:CE2	2:F:475:PRO:HD3	2.56	0.40
1:A:481:MET:HE2	1:A:481:MET:HB2	1.81	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:C:454:ILE:HG13	1:C:455:GLY:N	2.36	0.40
1:C:610:ASP:OD1	1:C:611:ASP:N	2.55	0.40
1:E:262:THR:HG23	1:E:266:GLY:HA2	2.03	0.40
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.84	0.40
1:E:352:ARG:O	1:E:356:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:16:VAL:HG21	1:C:450:ALA:O	2.22	0.40
1:E:454:ILE:HG13	1:E:455:GLY:N	2.36	0.40
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.56	0.40
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.03	0.40
1:A:429:LYS:HG3	1:A:462:PHE:CZ	2.56	0.40
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.90	0.40
1:C:612:PHE:CE1	1:C:631:ARG:HG3	2.57	0.40
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.56	0.40
1:E:452:ASN:N	1:E:452:ASN:HD22	2.19	0.40
1:A:594:ASP:HB2	1:A:597:VAL:HG23	2.02	0.40
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.04	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%)	38	59
1	C	818/842 (97%)	780 (95%)	33 (4%)	5 (1%)	28	48
1	E	818/842 (97%)	763 (93%)	52 (6%)	3 (0%)	38	59
2	B	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
2	D	205/207 (99%)	198 (97%)	6 (3%)	1 (0%)	32	53
2	F	205/207 (99%)	200 (98%)	5 (2%)	0	100	100
All	All	3069/3147 (98%)	2923 (95%)	134 (4%)	12 (0%)	38	59

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%)	68	88
1	C	699/714 (98%)	688 (98%)	11 (2%)	68	88
1	E	699/714 (98%)	691 (99%)	8 (1%)	78	92
2	B	161/161 (100%)	157 (98%)	4 (2%)	53	79
2	D	161/161 (100%)	158 (98%)	3 (2%)	62	85
2	F	161/161 (100%)	154 (96%)	7 (4%)	33	58
All	All	2580/2625 (98%)	2536 (98%)	44 (2%)	66	87

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	6,10,21	0.98	1 (16%)	5,12,30	1.27	0
1	DDE	C	699	1	15,20,21	1.28	2 (13%)	15,28,30	1.25	1 (6%)
1	DDE	E	699	1	6,10,21	1.05	1 (16%)	5,12,30	1.29	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

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	DDE	CA-C	2.01	1.52	1.50
1	E	699	DDE	CA-C	2.20	1.53	1.50
1	C	699	DDE	CA-C	2.57	1.53	1.50
1	C	699	DDE	CAT-CE1	2.95	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	CAU-CBW-CBI	-2.90	105.41	111.12

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	-	41,48,48	0.62	0	43,73,73	1.96	3 (6%)
3	NAD	D	701	-	41,48,48	0.64	0	43,73,73	1.94	3 (6%)
3	NAD	F	702	-	41,48,48	0.63	0	43,73,73	1.95	4 (9%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	NAD	N3A-C2A-N1A	-8.99	121.03	128.86
3	F	702	NAD	N3A-C2A-N1A	-8.83	121.17	128.86
3	D	701	NAD	N3A-C2A-N1A	-8.81	121.18	128.86
3	D	701	NAD	C4B-O4B-C1B	-7.12	102.19	109.77
3	F	702	NAD	C4B-O4B-C1B	-6.87	102.45	109.77
3	B	700	NAD	C4B-O4B-C1B	-6.86	102.47	109.77
3	F	702	NAD	C4A-C5A-N7A	-2.28	107.21	109.41
3	D	701	NAD	C4A-C5A-N7A	-2.21	107.28	109.41
3	B	700	NAD	C4A-C5A-N7A	-2.13	107.35	109.41
3	F	702	NAD	C5D-C4D-C3D	-2.02	107.58	115.29

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%)	0.11	13 (1%) 72 73	17, 53, 92, 120	0
1	C	822/842 (97%)	0.52	82 (9%) 8 7	18, 60, 134, 199	0
1	E	822/842 (97%)	2.00	345 (41%) 0 0	19, 131, 186, 266	0
2	B	207/207 (100%)	-0.01	1 (0%) 90 91	16, 33, 80, 99	0
2	D	207/207 (100%)	-0.09	2 (0%) 82 83	16, 30, 66, 88	0
2	F	207/207 (100%)	-0.03	3 (1%) 75 76	20, 36, 82, 118	0
All	All	3087/3147 (98%)	0.69	446 (14%) 3 2	16, 57, 165, 266	0

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	195	GLU	10.7
1	E	231	LYS	9.7
1	E	311	GLU	9.7
1	E	307	LEU	9.5
1	E	314	LEU	9.5
1	E	78	TYR	9.3
1	C	550	ALA	9.2
1	C	495	VAL	9.1
1	E	179	ALA	8.7
1	E	766	PHE	8.5
1	E	303	LEU	8.4
1	E	277	ILE	8.4
1	E	280	PRO	8.0
1	E	167	LEU	8.0
1	E	310	ASP	7.8
1	E	239	LYS	7.8
1	E	193	ALA	7.7
1	E	107	GLY	7.6
1	E	88	GLU	7.6

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Mol	Chain	Res	Type	RSRZ
1	E	553	PRO	7.5
1	C	493	VAL	7.3
1	E	299	LEU	7.3
1	E	332	ASP	7.3
1	E	339	VAL	7.2
1	E	308	LYS	7.2
1	E	420	PRO	7.1
1	E	175	TYR	7.1
1	E	320	LEU	7.1
1	E	86	VAL	7.1
1	E	210	ALA	7.0
1	E	276	PHE	6.9
1	E	99	LEU	6.9
1	E	554	LEU	6.9
1	E	315	GLU	6.8
1	E	108	HIS	6.7
1	E	240	MET	6.5
1	E	81	MET	6.5
1	E	26	ALA	6.4
1	E	504	LEU	6.4
1	E	321	LYS	6.4
1	E	316	GLY	6.3
1	C	523	SER	6.3
1	E	233	PHE	6.3
1	E	289	MET	6.3
1	E	323	VAL	6.3
1	E	366	CYS	6.3
1	E	492	ALA	6.2
1	E	194	ASP	6.2
1	C	522	MET	6.2
1	E	312	LYS	6.2
1	E	278	LEU	6.2
1	E	495	VAL	6.1
1	E	745	SER	6.1
1	E	23	SER	6.1
1	E	98	PHE	6.0
1	E	789	GLY	6.0
1	E	132	ILE	6.0
1	E	743	ILE	6.0
1	E	442	VAL	5.9
1	E	282	PHE	5.8
1	C	551	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	770	ALA	5.7
1	E	97	SER	5.7
1	E	128	VAL	5.6
1	A	475	ALA	5.6
1	E	273	PHE	5.6
1	E	555	LYS	5.6
1	E	232	LYS	5.6
1	E	269	LEU	5.5
1	E	498	ALA	5.5
1	E	500	ASP	5.5
1	C	549	HIS	5.5
1	E	419	VAL	5.4
1	C	496	LYS	5.4
1	C	494	GLU	5.4
1	E	367	ILE	5.4
1	E	245	TRP	5.3
1	E	288	ILE	5.3
1	C	499	ASN	5.3
1	E	360	PRO	5.3
1	E	196	VAL	5.3
1	E	19	VAL	5.2
1	E	164	LEU	5.2
1	E	501	LEU	5.2
1	C	502	PRO	5.2
1	E	242	ASP	5.2
1	E	163	ALA	5.2
1	E	298	VAL	5.2
1	E	284	LEU	5.2
1	E	525	SER	5.1
1	E	761	PRO	5.1
1	E	192	TYR	5.1
1	E	739	ALA	5.1
1	E	80	GLU	5.1
1	E	418	TYR	5.0
1	C	501	LEU	5.0
1	C	506	GLU	5.0
1	E	77	LEU	5.0
1	E	476	HIS	4.9
1	E	335	LEU	4.9
1	E	89	ILE	4.9
1	E	551	GLY	4.9
1	E	777	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	508	LEU	4.9
1	C	552	VAL	4.9
1	E	317	LYS	4.9
1	C	546	GLU	4.8
1	E	45	ILE	4.8
1	E	154	VAL	4.8
1	E	24	VAL	4.8
1	E	76	SER	4.8
1	C	498	ALA	4.8
1	E	496	LYS	4.7
1	E	227	THR	4.7
1	E	226	ALA	4.7
1	C	291	PHE	4.7
1	E	129	VAL	4.7
1	E	474	THR	4.7
1	E	290	ASN	4.6
1	E	83	ASP	4.6
1	E	309	GLY	4.6
1	E	322	VAL	4.5
1	E	329	PRO	4.5
1	E	169	VAL	4.5
1	E	306	VAL	4.5
1	E	362	ASP	4.5
1	E	126	LEU	4.5
1	E	105	SER	4.5
1	E	759	GLN	4.5
1	E	143	LEU	4.5
1	E	257	TRP	4.5
1	E	741	GLY	4.5
1	E	497	ASN	4.4
1	E	48	ALA	4.4
1	E	31	GLY	4.4
1	E	25	ILE	4.4
1	C	500	ASP	4.3
1	E	222	ILE	4.3
1	E	166	GLU	4.3
1	C	505	VAL	4.3
1	E	760	ARG	4.3
1	E	305	ILE	4.3
1	E	343	PRO	4.3
1	E	67	GLY	4.3
1	E	79	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	493	VAL	4.3
1	C	528	HIS	4.2
1	C	553	PRO	4.2
1	E	499	ASN	4.2
1	E	319	LEU	4.2
1	E	556	ILE	4.2
1	E	747	LEU	4.2
1	E	740	VAL	4.2
1	E	361	ALA	4.2
1	E	421	GLY	4.2
1	E	762	GLY	4.2
1	E	506	GLU	4.2
1	A	420	PRO	4.2
1	E	297	PRO	4.1
1	E	258	THR	4.1
1	E	794	PRO	4.1
1	E	294	ASP	4.1
1	E	441	PHE	4.1
1	E	296	ILE	4.1
1	E	241	MET	4.1
1	E	475	ALA	4.1
1	C	300	LEU	4.1
1	C	504	LEU	4.1
1	C	2	VAL	4.1
1	E	176	GLN	4.1
1	E	229	TYR	4.1
1	E	96	ASN	4.0
1	E	131	THR	4.0
1	E	287	ALA	4.0
1	E	127	VAL	4.0
1	C	4	PHE	4.0
1	E	254	THR	4.0
1	C	311	GLU	4.0
1	E	9	MET	4.0
1	E	180	ARG	4.0
1	A	495	VAL	4.0
1	E	365	ASN	4.0
1	E	187	VAL	4.0
1	E	230	ALA	3.9
1	E	301	GLU	3.9
1	E	216	HIS	3.9
1	E	338	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	182	VAL	3.9
1	E	188	ILE	3.9
1	E	223	ARG	3.9
1	C	524	GLU	3.9
1	E	205	ALA	3.9
1	E	422	LYS	3.8
1	E	165	LEU	3.8
1	E	203	TYR	3.8
1	E	358	GLU	3.8
1	E	550	ALA	3.8
1	C	497	ASN	3.8
1	E	292	LYS	3.8
1	E	503	LYS	3.8
1	E	737	GLU	3.8
1	E	185	VAL	3.7
1	E	796	MET	3.7
1	E	295	GLU	3.7
1	E	324	MET	3.7
1	E	268	PRO	3.7
1	E	781	THR	3.7
1	E	795	GLN	3.6
1	E	730	LEU	3.6
1	E	304	GLU	3.6
1	E	144	ARG	3.6
1	E	260	LYS	3.6
1	E	218	TRP	3.6
1	E	744	TYR	3.6
1	E	293	LYS	3.6
1	E	4	PHE	3.6
1	E	286	THR	3.6
1	E	155	VAL	3.6
1	E	736	PRO	3.6
1	E	106	PRO	3.6
1	E	46	ILE	3.5
1	E	47	SER	3.5
1	E	494	GLU	3.5
1	E	32	LYS	3.5
1	C	3	ALA	3.5
1	E	754	VAL	3.5
1	E	780	PHE	3.5
1	C	513	LYS	3.5
1	E	757	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	93	THR	3.5
1	E	243	ARG	3.5
1	C	306	VAL	3.5
1	C	323	VAL	3.5
1	E	134	GLY	3.5
1	E	200	VAL	3.5
1	C	307	LEU	3.4
1	E	149	GLU	3.4
1	C	555	LYS	3.4
1	E	148	GLY	3.4
1	E	123	ASP	3.4
2	F	489	ALA	3.4
1	E	735	CYS	3.4
1	E	790	GLY	3.3
1	C	285	PHE	3.3
1	E	326	LYS	3.3
1	C	314	LEU	3.3
1	E	369	ILE	3.3
1	E	256	LYS	3.3
1	C	554	LEU	3.3
1	C	556	ILE	3.3
1	E	552	VAL	3.3
1	E	125	ALA	3.3
1	E	161	ASP	3.3
1	E	522	MET	3.3
1	E	472	SER	3.2
1	E	510	ARG	3.2
1	E	137	VAL	3.2
1	E	340	LEU	3.2
1	E	768	VAL	3.2
1	E	171	LYS	3.2
1	C	112	SER	3.2
1	E	523	SER	3.2
1	E	443	GLU	3.2
1	E	410	LYS	3.2
1	C	313	ASP	3.1
1	E	70	ILE	3.1
1	E	547	HIS	3.1
1	E	145	GLN	3.1
1	E	402	ALA	3.1
1	E	111	PHE	3.0
1	E	197	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	511	LEU	3.0
1	E	342	LEU	3.0
1	E	423	LYS	3.0
1	E	548	ASP	3.0
1	C	740	VAL	3.0
1	E	302	LYS	3.0
1	E	113	SER	3.0
1	A	361	ALA	3.0
1	E	36	THR	3.0
1	E	505	VAL	2.9
1	E	508	LEU	2.9
1	E	94	ASP	2.9
1	E	130	ASP	2.9
1	C	305	ILE	2.9
1	E	424	ASP	2.9
1	C	167	LEU	2.9
1	A	419	VAL	2.9
1	E	156	VAL	2.9
1	E	291	PHE	2.9
1	C	5	THR	2.9
1	C	299	LEU	2.9
2	F	490	ARG	2.8
1	E	151	ILE	2.8
1	C	492	ALA	2.8
1	E	162	ARG	2.8
1	E	255	LYS	2.8
1	C	547	HIS	2.8
1	E	103	ILE	2.8
1	E	546	GLU	2.8
1	E	42	ARG	2.8
1	E	755	VAL	2.8
1	E	115	VAL	2.8
1	E	158	ASN	2.8
1	E	120	ARG	2.8
1	E	104	ASP	2.8
1	E	444	PRO	2.8
1	E	431	ILE	2.8
1	C	509	LYS	2.8
1	E	147	LEU	2.7
1	E	244	LEU	2.7
1	E	34	THR	2.7
1	E	376	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	489	ALA	2.7
1	C	320	LEU	2.7
1	C	545	LEU	2.7
1	A	365	ASN	2.7
1	C	265	GLU	2.7
1	A	46	ILE	2.7
1	E	763	THR	2.7
1	E	300	LEU	2.7
1	E	395	TYR	2.7
1	E	234	GLY	2.7
1	E	502	PRO	2.7
1	E	377	ASP	2.7
1	E	3	ALA	2.7
1	E	412	ARG	2.7
1	C	503	LYS	2.7
1	E	437	MET	2.7
1	E	135	VAL	2.7
1	E	121	VAL	2.6
1	C	511	LEU	2.6
1	E	68	ILE	2.6
1	E	541	CYS	2.6
1	E	401	PHE	2.6
1	E	38	SER	2.6
1	C	251	ASN	2.6
1	E	85	ASP	2.6
1	E	10	ARG	2.6
1	E	69	THR	2.6
1	E	357	TYR	2.6
1	C	235	VAL	2.6
1	E	356	LEU	2.6
1	E	784	LEU	2.6
1	C	232	LYS	2.6
1	E	41	GLN	2.5
1	E	91	GLN	2.5
1	E	325	ARG	2.5
1	C	310	ASP	2.5
1	E	261	ASP	2.5
1	E	756	SER	2.5
1	C	267	LYS	2.5
1	E	199	ASP	2.5
1	E	27	HIS	2.5
1	E	82	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	553	PRO	2.5
1	E	73	THR	2.5
1	E	267	LYS	2.5
1	E	279	ASP	2.5
1	E	542	LEU	2.5
1	E	75	ILE	2.4
1	E	427	PHE	2.4
1	A	84	GLU	2.4
1	E	782	GLY	2.4
1	E	549	HIS	2.4
1	E	390	ASP	2.4
1	E	349	GLN	2.4
1	E	473	GLU	2.4
1	E	445	ILE	2.4
1	C	269	LEU	2.4
2	D	461	ASP	2.4
1	C	293	LYS	2.4
1	E	477	ASN	2.4
1	C	7	ASP	2.4
1	E	313	ASP	2.4
1	E	347	THR	2.4
1	E	328	LEU	2.4
1	C	421	GLY	2.4
1	E	265	GLU	2.4
1	E	159	LYS	2.4
1	E	337	MET	2.4
1	E	354	GLU	2.3
1	E	388	THR	2.3
1	E	101	ASN	2.3
1	E	136	CYS	2.3
1	A	473	GLU	2.3
1	E	481	MET	2.3
1	C	510	ARG	2.3
1	C	154	VAL	2.3
1	E	209	VAL	2.3
1	C	445	ILE	2.3
1	E	177	THR	2.3
1	E	30	HIS	2.3
1	C	46	ILE	2.3
1	E	208	THR	2.3
1	C	420	PRO	2.3
1	E	2	VAL	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	461	ASP	2.3
1	C	229	TYR	2.3
1	E	90	LYS	2.2
1	E	526	GLY	2.2
1	C	236	ASP	2.2
1	E	117	ALA	2.2
1	E	211	PHE	2.2
1	E	772	LEU	2.2
1	E	189	VAL	2.2
1	C	173	ASP	2.2
1	A	496	LYS	2.2
1	E	122	THR	2.2
1	E	274	ASN	2.2
1	C	109	VAL	2.2
1	E	438	MET	2.2
1	C	766	PHE	2.2
1	C	85	ASP	2.2
1	C	252	PRO	2.2
1	E	153	PRO	2.2
1	E	84	GLU	2.2
1	C	312	LYS	2.2
1	E	119	LEU	2.2
1	E	207	GLY	2.2
1	C	118	ALA	2.2
1	E	146	ALA	2.2
1	E	7	ASP	2.2
1	E	471	THR	2.2
1	E	249	PHE	2.2
1	E	201	GLN	2.1
1	E	118	ALA	2.1
1	E	783	GLU	2.1
1	C	309	GLY	2.1
1	E	116	THR	2.1
1	E	466	THR	2.1
1	E	20	ARG	2.1
1	A	423	LYS	2.1
1	C	507	GLY	2.1
1	C	264	ALA	2.1
1	A	310	ASP	2.1
1	E	237	LYS	2.1
1	E	22	MET	2.0
1	C	163	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	296	ILE	2.0
1	E	458	GLY	2.0
1	E	742	GLY	2.0
1	E	778	PHE	2.0
2	B	520	ALA	2.0
1	E	327	PHE	2.0
1	E	114	GLU	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	0.94	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(Å <sup>2</sup> )	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

There are no such residues in this entry.