Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:34 AM GMT

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

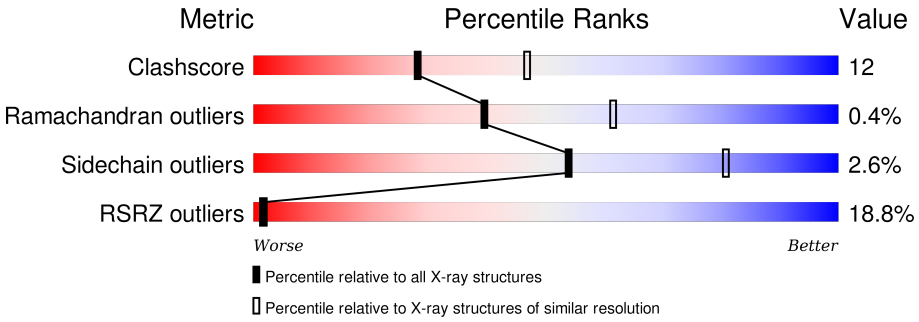
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	6% 72% 25%
1	C	842	16% 71% 26%
1	E	842	45% 61% 37%
2	B	207	2% 86% 14%
2	D	207	% 86% 14%
2	F	207	% 86% 13%

2 Entry composition

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

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

- Molecule 1 is a protein called Elongation factor 2.

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

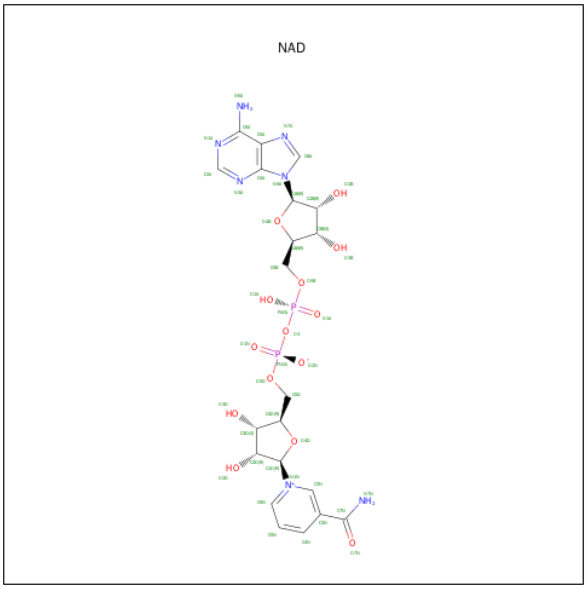
- Molecule 2 is a protein called Exotoxin A.

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

There are 12 discrepancies between the modelled and reference sequences:

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

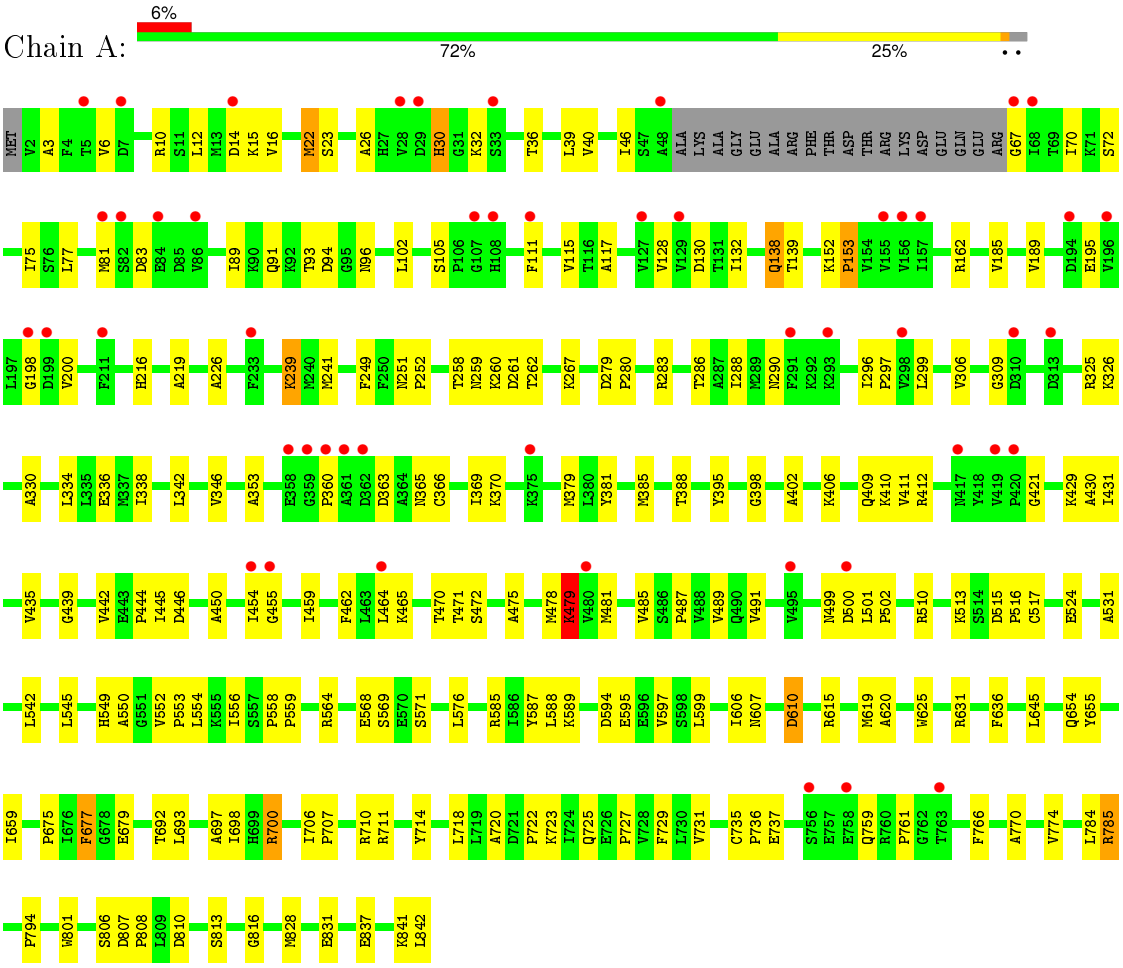
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	116	Total	O	0	0
			116	116		
4	C	77	Total	O	0	0
			77	77		
4	D	142	Total	O	0	0
			142	142		
4	E	60	Total	O	0	0
			60	60		
4	F	88	Total	O	0	0
			88	88		

3 Residue-property plots (i)

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

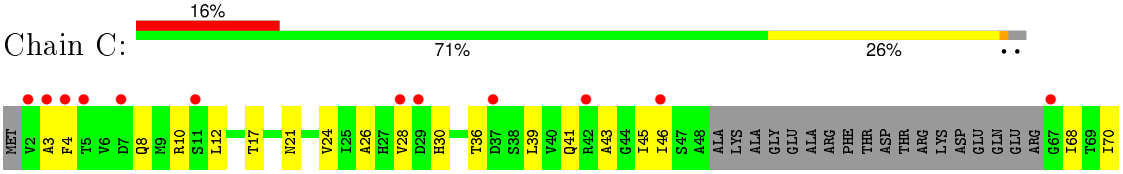
- Molecule 1: Elongation factor 2

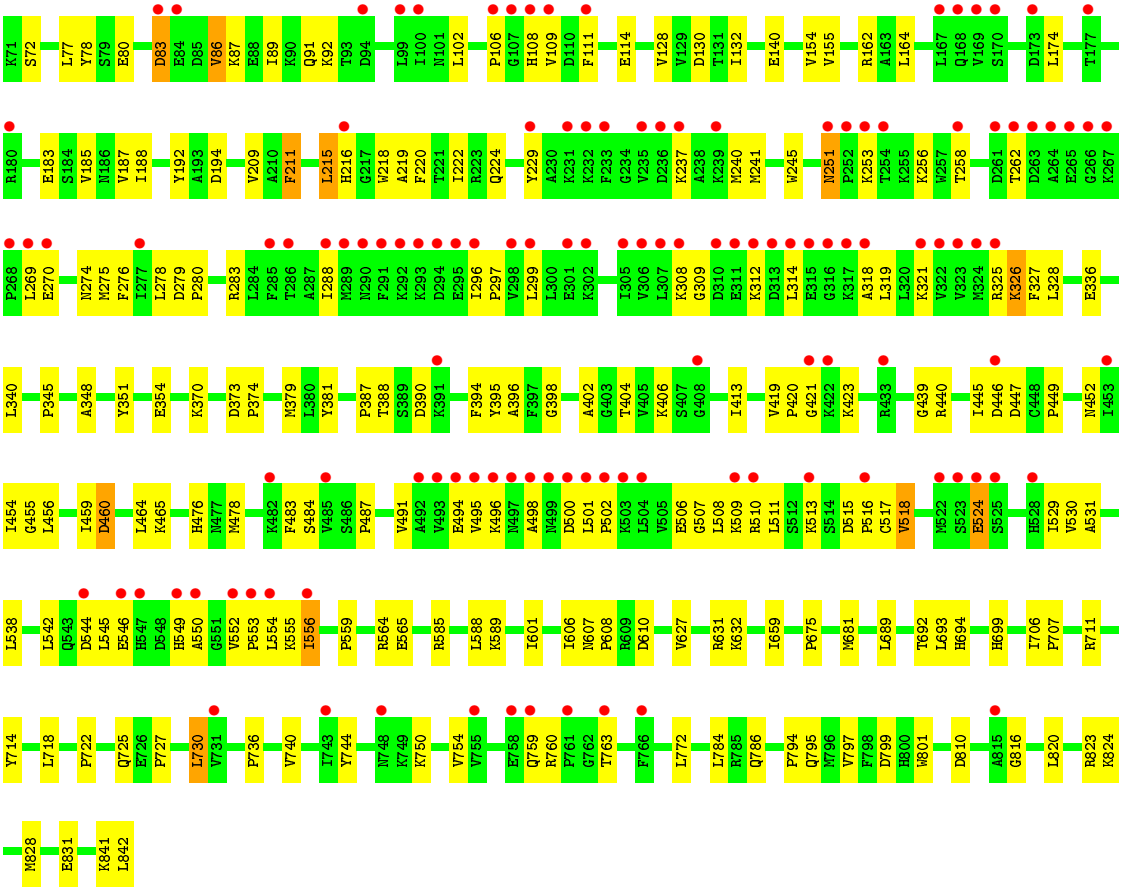
Chain A:



- Molecule 1: Elongation factor 2

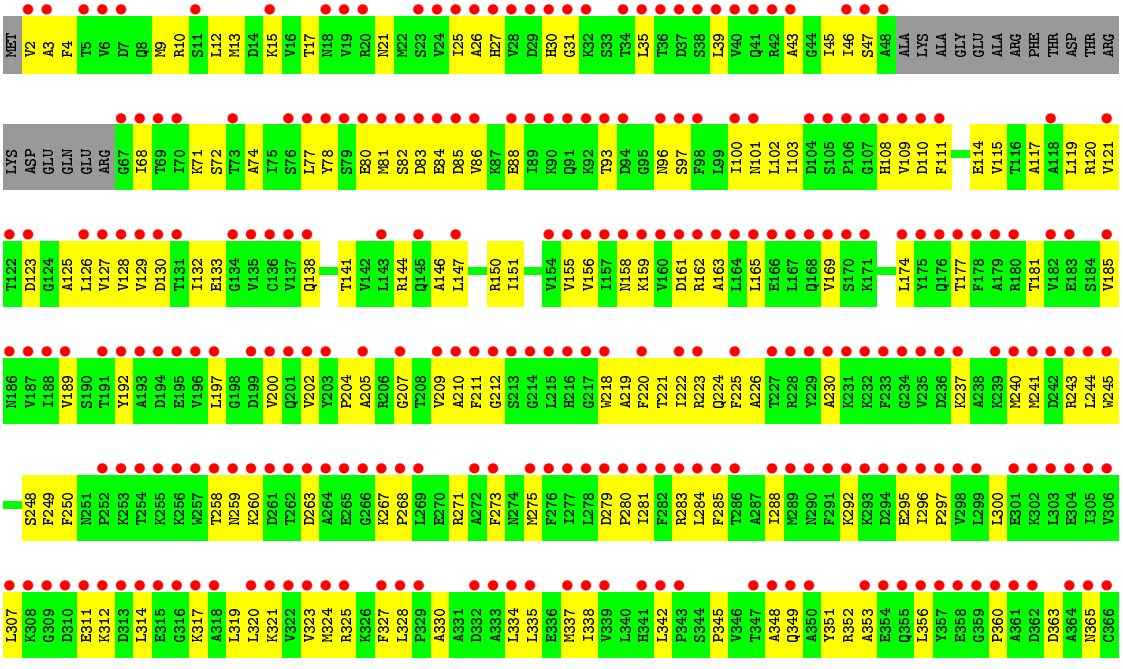
Chain C:

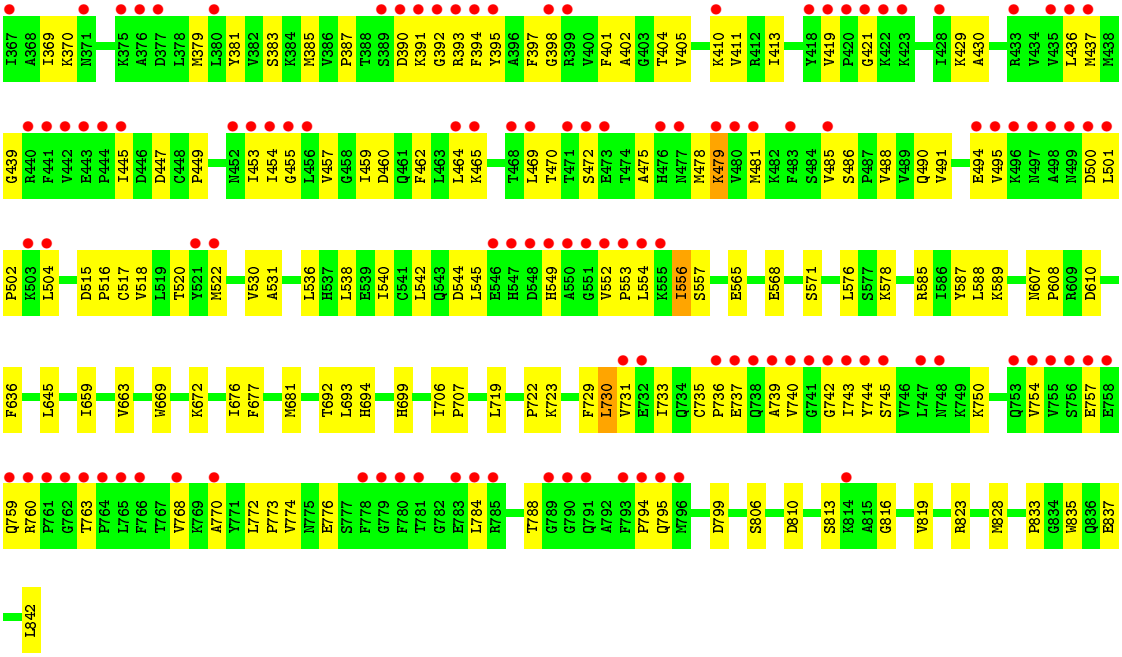




- Molecule 1: Elongation factor 2

Chain E:





- Molecule 2: Exotoxin A

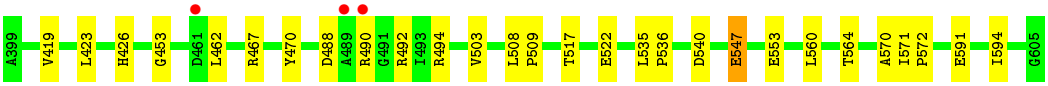
Chain B:

- Molecule 2: Exotoxin A

Chain D:

- Molecule 2: Exotoxin A

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	329.44Å 68.16Å 191.63Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	24.99 – 2.50 24.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.99-2.50) 99.0 (24.99-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	3 of 162490 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24719	wwPDB-VP
Average B, all atoms (Å^2)	66.0	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 42.86 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9175e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.21	0/6517	0.40	1/8823 (0.0%)
1	C	0.21	0/6517	0.40	0/8823
1	E	0.21	0/6517	0.38	0/8823
2	B	0.21	0/1634	0.40	0/2225
2	D	0.21	0/1623	0.41	0/2211
2	F	0.21	0/1623	0.39	0/2211
All	All	0.21	0/24431	0.39	1/33116 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6405	0	6472	145	0
1	C	6415	0	6488	148	0
1	E	6415	0	6488	226	0
2	B	1592	0	1554	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1584	0	1541	16	0
2	F	1584	0	1541	19	0
3	B	44	0	26	1	0
3	D	44	0	26	1	0
3	F	44	0	26	2	0
4	A	109	0	0	2	0
4	B	116	0	0	1	0
4	C	77	0	0	0	0
4	D	142	0	0	2	0
4	E	60	0	0	1	0
4	F	88	0	0	0	0
All	All	24719	0	24162	567	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:PRO:HD3	1:A:714:TYR:CD1	2.45	0.51
1:A:40:VAL:HG22	1:A:75:ILE:HG21	1.90	0.51
1:E:419:VAL:HG12	1:E:421:GLY:H	1.75	0.51
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.92	0.51
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.45	0.51
1:E:495:VAL:HG13	1:E:504:LEU:HD22	1.91	0.51
1:C:274:ASN:HA	1:C:278:LEU:HB2	1.93	0.51
1:E:391:LYS:CG	1:E:392:GLY:H	2.18	0.51
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.40	0.51
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.46	0.51
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.93	0.51
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.93	0.51
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.74	0.51
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.92	0.51
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.93	0.51
1:E:750:LYS:HD2	1:E:776:GLU:O	2.11	0.51
1:E:25:ILE:HG13	1:E:125:ALA:HB1	1.93	0.51
1:C:736:PRO:O	1:C:740:VAL:HG23	2.11	0.51
1:E:165:LEU:HD23	1:E:317:LYS:HE2	1.93	0.50
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.93	0.50
1:E:120:ARG:NH1	1:E:479:LYS:HB3	2.26	0.50
1:E:410:LYS:HA	1:E:430:ALA:HA	1.94	0.50
1:E:27:HIS:HB3	1:E:30:HIS:CD2	2.47	0.50
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.93	0.50
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.41	0.50
1:E:515:ASP:HB3	1:E:518:VAL:HG12	1.92	0.50
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.94	0.50
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.94	0.50
1:C:24:VAL:HG23	1:C:102:LEU:HD11	1.94	0.50
1:C:759:GLN:CG	1:C:760:ARG:H	2.12	0.49
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.47	0.49
1:C:72:SER:HA	1:C:439:GLY:O	2.12	0.49
1:C:546:GLU:HA	1:C:550:ALA:HB3	1.92	0.49
1:E:108:HIS:O	1:E:111:PHE:HD2	1.95	0.49
1:C:524:GLU:OE1	1:C:524:GLU:HA	2.11	0.49
1:C:494:GLU:HB3	1:C:555:LYS:HB3	1.93	0.49
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.94	0.49
1:E:82:SER:O	1:E:86:VAL:HG23	2.12	0.49
1:C:8:GLN:O	1:C:12:LEU:HB2	2.12	0.49
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.47	0.49
1:E:123:ASP:N	1:E:123:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.78	0.49
1:E:608:PRO:HA	1:E:636:PHE:CE2	2.47	0.49
1:E:699:DDE:HAT2	1:E:699:DDE:HAB2	1.93	0.49
1:A:22:MET:HG2	1:A:23:SER:N	2.26	0.49
1:A:30:HIS:NE2	1:A:130:ASP:HB2	2.27	0.49
1:E:369:ILE:HD13	1:E:402:ALA:HB2	1.94	0.49
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.95	0.49
1:E:397:PHE:CD1	1:E:437:MET:HG3	2.47	0.49
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.94	0.49
1:A:93:THR:HG22	1:A:94:ASP:H	1.78	0.49
1:C:589:LYS:HD2	1:C:689:LEU:HD11	1.95	0.49
1:E:556:ILE:HG22	1:E:557:SER:N	2.24	0.49
1:E:117:ALA:HA	1:E:481:MET:SD	2.53	0.49
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.48	0.49
2:D:470:TYR:CD2	3:D:701:NAD:H2D	2.47	0.49
1:E:222:ILE:HD13	1:E:245:TRP:HB2	1.94	0.49
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.95	0.49
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.43	0.48
1:C:321:LYS:O	1:C:325:ARG:HG3	2.12	0.48
1:E:459:ILE:HG22	1:E:459:ILE:O	2.12	0.48
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.95	0.48
1:C:30:HIS:CE1	1:C:130:ASP:HB2	2.48	0.48
1:A:72:SER:HA	1:A:439:GLY:O	2.13	0.48
1:E:31:GLY:HA3	1:E:158:ASN:ND2	2.28	0.48
1:E:163:ALA:O	1:E:169:VAL:HG12	2.14	0.48
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.96	0.48
1:E:210:ALA:HB2	1:E:221:THR:HG22	1.94	0.48
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.94	0.48
1:A:510:ARG:HD2	1:A:549:HIS:HA	1.96	0.48
1:E:454:ILE:HG13	1:E:455:GLY:N	2.28	0.48
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.49	0.48
1:E:181:THR:O	1:E:185:VAL:HG23	2.14	0.48
1:C:3:ALA:HA	1:C:46:ILE:O	2.14	0.48
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.96	0.48
2:F:488:ASP:HB3	2:F:492:ARG:HB2	1.96	0.47
1:A:478:MET:O	1:A:479:LYS:C	2.52	0.47
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.29	0.47
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.96	0.47
2:F:508:LEU:N	2:F:509:PRO:CD	2.77	0.47
1:C:237:LYS:O	1:C:241:MET:HG2	2.14	0.47
1:A:785:ARG:NH1	1:A:785:ARG:CG	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:659:ILE:O	1:E:663:VAL:HG23	2.14	0.47
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.14	0.47
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.29	0.47
1:C:494:GLU:O	1:C:554:LEU:HB3	2.15	0.47
1:E:132:ILE:N	1:E:132:ILE:HD12	2.29	0.47
1:A:216:HIS:O	1:A:325:ARG:HG3	2.14	0.47
1:A:93:THR:HG22	1:A:94:ASP:N	2.29	0.47
1:A:722:PRO:O	1:A:723:LYS:HG2	2.15	0.47
1:A:479:LYS:HA	1:A:479:LYS:HE3	1.96	0.47
1:C:509:LYS:O	1:C:513:LYS:HG3	2.15	0.47
1:C:627:VAL:O	1:C:631:ARG:HG3	2.14	0.47
1:E:369:ILE:HD12	1:E:401:PHE:HB3	1.96	0.47
1:E:223:ARG:HG3	1:E:241:MET:SD	2.54	0.47
1:E:39:LEU:HD23	1:E:335:LEU:HD23	1.96	0.47
1:E:10:ARG:NH2	1:E:449:PRO:HD3	2.29	0.47
1:A:568:GLU:HG3	1:A:723:LYS:CG	2.44	0.47
1:E:218:TRP:HB3	1:E:324:MET:HB3	1.96	0.47
1:E:279:ASP:O	1:E:283:ARG:HG2	2.14	0.47
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.95	0.47
1:A:406:LYS:HB2	1:A:409:GLN:HB2	1.96	0.47
1:A:501:LEU:N	1:A:502:PRO:HD2	2.29	0.47
1:A:607:ASN:O	1:A:615:ARG:HD3	2.15	0.47
1:E:731:VAL:HG12	1:E:770:ALA:O	2.15	0.47
2:B:516:LEU:O	2:B:545:PRO:HD2	2.14	0.47
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.97	0.47
1:A:286:THR:O	1:A:290:ASN:HB2	2.15	0.47
1:E:80:GLU:HA	1:E:96:ASN:O	2.14	0.47
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.50	0.47
1:C:296:ILE:N	1:C:297:PRO:HD2	2.29	0.47
1:C:498:ALA:HA	1:C:501:LEU:HB2	1.97	0.47
1:E:772:LEU:HD12	1:E:773:PRO:HD2	1.96	0.47
1:E:225:PHE:CE2	1:E:328:LEU:HD11	2.50	0.46
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.97	0.46
1:E:520:THR:HG22	1:E:530:VAL:HG22	1.97	0.46
1:C:108:HIS:ND1	1:C:109:VAL:N	2.64	0.46
1:E:669:TRP:CZ2	2:F:492:ARG:HG3	2.50	0.46
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.97	0.46
1:E:185:VAL:O	1:E:189:VAL:HG23	2.16	0.46
2:D:537:LEU:HD11	2:D:542:ILE:HG22	1.97	0.46
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.51	0.46
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:LEU:O	1:E:273:PHE:HB2	2.15	0.46
1:C:491:VAL:HG13	1:C:538:LEU:HD21	1.98	0.46
1:C:501:LEU:HD23	1:C:501:LEU:C	2.36	0.46
1:E:338:ILE:O	1:E:342:LEU:HB2	2.15	0.46
1:E:736:PRO:O	1:E:740:VAL:HG23	2.16	0.46
1:E:204:PRO:HA	1:E:209:VAL:HB	1.96	0.46
1:A:3:ALA:HA	1:A:46:ILE:O	2.15	0.46
1:C:251:ASN:ND2	1:C:253:LYS:H	2.13	0.46
2:F:419:VAL:O	2:F:423:LEU:HG	2.16	0.46
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.50	0.46
1:C:760:ARG:HD3	1:C:763:THR:OG1	2.15	0.46
1:E:109:VAL:O	1:E:109:VAL:HG12	2.15	0.46
1:E:111:PHE:O	1:E:115:VAL:HG23	2.16	0.46
1:A:677:PHE:N	1:A:677:PHE:CD2	2.83	0.46
1:A:262:THR:HA	1:A:267:LYS:O	2.16	0.46
1:E:110:ASP:HB3	1:E:536:LEU:HD22	1.96	0.46
1:C:699:DDE:HAU3	1:C:699:DDE:HAB2	1.46	0.46
1:A:258:THR:HG21	4:A:912:HOH:O	2.15	0.46
2:D:420:GLU:HG2	4:D:734:HOH:O	2.17	0.45
1:E:3:ALA:HA	1:E:46:ILE:O	2.17	0.45
1:C:750:LYS:HB3	1:C:772:LEU:HD11	1.97	0.45
1:E:119:LEU:O	1:E:151:ILE:HD11	2.16	0.45
1:E:669:TRP:CE2	2:F:492:ARG:HG3	2.51	0.45
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.97	0.45
1:E:429:LYS:HG3	1:E:462:PHE:CE2	2.51	0.45
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.98	0.45
1:A:81:MET:HE1	1:A:336:GLU:HA	1.98	0.45
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.36	0.45
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.98	0.45
1:A:500:ASP:HB3	1:A:552:VAL:HG21	1.99	0.45
2:B:490:ARG:NH2	2:B:492[B]:ARG:HE	2.15	0.45
1:E:394:PHE:HB2	1:E:460:ASP:HB3	1.99	0.45
1:A:807:ASP:HA	1:A:808:PRO:HD2	1.87	0.45
1:E:111:PHE:CE1	1:E:540:ILE:HD13	2.52	0.45
1:E:731:VAL:HG13	1:E:731:VAL:O	2.17	0.45
1:A:152:LYS:HA	1:A:153:PRO:HD3	1.71	0.45
1:E:676:ILE:HG22	1:E:677:PHE:HD2	1.82	0.45
1:A:542:LEU:HD22	1:A:556:ILE:HD13	1.99	0.45
1:E:352:ARG:O	1:E:356:LEU:HG	2.17	0.45
1:E:43:ALA:HB1	1:E:78:TYR:H	1.82	0.45
1:E:411:VAL:HG13	1:E:470:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.85	0.45
1:E:405:VAL:O	1:E:447:ASP:HA	2.17	0.45
1:C:727:PRO:HD3	1:C:801:TRP:CZ3	2.52	0.45
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.48	0.45
1:E:129:VAL:HG12	1:E:130:ASP:H	1.82	0.44
1:C:222:ILE:CD1	1:C:245:TRP:HB2	2.47	0.44
1:E:296:ILE:N	1:E:297:PRO:HD2	2.33	0.44
1:A:675:PRO:HD3	1:A:714:TYR:CE1	2.52	0.44
1:A:454:ILE:HG13	1:A:455:GLY:N	2.30	0.44
1:E:486:SER:O	1:E:488:VAL:HG23	2.17	0.44
1:E:307:LEU:HD13	1:E:311:GLU:O	2.17	0.44
1:C:506:GLU:O	1:C:510:ARG:HG3	2.17	0.44
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.88	0.44
1:E:485:VAL:O	1:E:485:VAL:HG22	2.17	0.44
1:E:237:LYS:HA	1:E:240:MET:HB3	2.00	0.44
1:C:460:ASP:OD1	1:C:460:ASP:N	2.51	0.44
1:C:707:PRO:O	1:C:711:ARG:HG3	2.17	0.44
1:E:121:VAL:HG11	1:E:383:SER:OG	2.18	0.44
1:E:739:ALA:HB1	1:E:788:THR:HB	2.00	0.44
1:A:727:PRO:HD3	1:A:801:TRP:CZ3	2.52	0.44
1:E:263:ASP:HB3	1:E:267:LYS:HB2	1.98	0.44
1:C:464:LEU:HD23	1:C:483:PHE:CE1	2.50	0.44
1:E:314:LEU:O	1:E:319:LEU:HB2	2.18	0.44
1:A:454:ILE:HG13	1:A:455:GLY:H	1.83	0.44
1:A:251:ASN:HA	1:A:252:PRO:HD3	1.86	0.44
1:A:470:THR:HG22	1:A:471:THR:N	2.33	0.44
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.53	0.44
1:E:454:ILE:HG13	1:E:455:GLY:H	1.82	0.44
1:C:491:VAL:HG12	1:C:559:PRO:HA	2.00	0.44
1:C:21:ASN:ND2	1:C:345:PRO:HG3	2.33	0.44
1:E:578:LYS:HE3	1:E:578:LYS:HB2	1.87	0.44
2:F:470:TYR:CD2	3:F:702:NAD:H2D	2.53	0.44
1:E:46:ILE:HD12	1:E:46:ILE:N	2.33	0.44
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.91	0.44
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.00	0.44
1:E:103:ILE:N	1:E:103:ILE:HD12	2.32	0.44
1:C:552:VAL:HG13	1:C:553:PRO:HD2	2.00	0.44
1:E:46:ILE:HG22	1:E:47:SER:N	2.33	0.44
2:D:535:LEU:HB3	2:D:536:PRO:HA	2.00	0.44
1:E:744:TYR:CE1	1:E:754:VAL:HG21	2.53	0.43
1:E:760:ARG:HD3	1:E:763:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:GLU:O	1:E:88:GLU:HG3	2.18	0.43
1:E:464:LEU:HG	1:E:465:LYS:HG3	2.00	0.43
1:A:552:VAL:HG13	1:A:553:PRO:HD2	2.01	0.43
1:A:14:ASP:OD1	1:A:15:LYS:HG3	2.18	0.43
1:A:837:GLU:HG3	4:A:871:HOH:O	2.18	0.43
1:E:30:HIS:HE1	1:E:133:GLU:OE1	2.01	0.43
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.00	0.43
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.19	0.43
1:A:6:VAL:CG1	1:A:445:ILE:HG22	2.48	0.43
2:B:440:HIS:HB2	2:B:471:ILE:HG22	2.00	0.43
1:E:588:LEU:C	1:E:588:LEU:HD12	2.38	0.43
1:C:327:PHE:CD2	1:C:328:LEU:HG	2.54	0.43
1:A:698:ILE:HG13	1:A:698:ILE:H	1.56	0.43
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.53	0.43
1:E:39:LEU:HB3	1:E:77:LEU:HD23	2.01	0.43
1:E:459:ILE:N	1:E:459:ILE:HD12	2.33	0.43
1:E:72:SER:HA	1:E:439:GLY:O	2.19	0.43
1:E:819:VAL:O	1:E:823:ARG:HG3	2.18	0.43
1:E:488:VAL:CG1	1:E:774:VAL:HG11	2.48	0.43
1:E:353:ALA:HB3	1:E:370:LYS:HG3	1.99	0.43
1:E:117:ALA:O	1:E:121:VAL:HG13	2.18	0.43
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.52	0.43
2:B:508:LEU:N	2:B:509:PRO:CD	2.81	0.43
1:C:314:LEU:HD13	1:C:318:ALA:O	2.19	0.43
1:A:26:ALA:CB	1:A:128:VAL:HB	2.48	0.43
1:E:292:LYS:O	1:E:296:ILE:HG13	2.18	0.43
1:C:155:VAL:O	1:C:209:VAL:HA	2.19	0.43
1:E:258:THR:HG22	1:E:259:ASN:N	2.34	0.43
1:C:24:VAL:HG21	1:C:36:THR:HG22	2.00	0.43
2:B:574:ASP:HA	2:B:575:PRO:HD2	1.84	0.43
1:A:185:VAL:O	1:A:189:VAL:HG23	2.19	0.43
1:C:542:LEU:HA	1:C:542:LEU:HD12	1.84	0.43
1:A:588:LEU:C	1:A:588:LEU:HD12	2.39	0.43
1:A:552:VAL:O	1:A:554:LEU:HG	2.18	0.43
1:A:727:PRO:HD3	1:A:801:TRP:HZ3	1.84	0.43
1:E:706:ILE:HB	1:E:707:PRO:HD3	2.01	0.43
1:A:731:VAL:HG12	1:A:770:ALA:O	2.19	0.43
2:D:517:THR:HG23	2:D:547:GLU:HA	2.00	0.43
1:C:820:LEU:O	1:C:824:LYS:HG3	2.19	0.43
1:E:285:PHE:CE1	1:E:320:LEU:HD21	2.54	0.42
1:E:150:ARG:HA	1:E:197:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:O	1:E:127:VAL:HA	2.19	0.42
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.54	0.42
1:E:585:ARG:HB2	1:E:692:THR:OG1	2.19	0.42
1:C:381:TYR:O	1:C:398:GLY:HA3	2.18	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
2:B:471:ILE:HG13	2:B:554:THR:HB	2.01	0.42
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.35	0.42
1:E:81:MET:HB3	1:E:85:ASP:HB2	2.01	0.42
1:A:239:LYS:HE3	1:A:239:LYS:HB2	1.65	0.42
1:C:487:PRO:HB2	1:C:531:ALA:HB1	2.00	0.42
1:E:833:PRO:HB3	1:E:837:GLU:OE1	2.19	0.42
1:A:841:LYS:HE3	4:B:806:HOH:O	2.18	0.42
1:C:449:PRO:HG2	1:C:452:ASN:ND2	2.34	0.42
1:C:554:LEU:HB3	1:C:555:LYS:H	1.69	0.42
2:D:428:GLN:O	2:D:432:ARG:HD3	2.19	0.42
1:A:429:LYS:HG3	1:A:462:PHE:CE2	2.54	0.42
1:A:594:ASP:HB2	1:A:597:VAL:HG23	2.00	0.42
1:C:588:LEU:C	1:C:588:LEU:HD12	2.40	0.42
1:C:256:LYS:HE3	1:C:256:LYS:HB3	1.92	0.42
1:E:250:PHE:HD2	1:E:275:MET:HE1	1.85	0.42
1:E:552:VAL:HG13	1:E:553:PRO:HD2	2.00	0.42
1:E:552:VAL:O	1:E:554:LEU:HG	2.20	0.42
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.87	0.42
2:F:467:ARG:CZ	2:F:536:PRO:HG3	2.49	0.42
1:E:119:LEU:HD21	1:E:146:ALA:HA	2.02	0.42
1:E:126:LEU:HD11	1:E:156:VAL:HG21	2.01	0.42
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.54	0.42
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.17	0.42
1:A:366:CYS:O	1:A:370:LYS:HG3	2.20	0.42
1:C:373:ASP:HA	1:C:374:PRO:HD2	1.88	0.42
1:E:522:MET:HB2	2:F:490:ARG:HH22	1.84	0.42
1:A:288:ILE:HA	1:A:296:ILE:HD11	2.02	0.42
1:E:515:ASP:HA	1:E:516:PRO:HD2	1.86	0.42
1:E:205:ALA:HB2	1:E:245:TRP:HB3	2.01	0.42
1:C:336:GLU:HG2	1:C:340:LEU:HD12	2.02	0.42
1:C:841:LYS:O	1:C:842:LEU:HD23	2.20	0.42
1:E:39:LEU:HD11	1:E:334:LEU:CB	2.50	0.42
1:A:385:MET:HG2	1:A:465:LYS:HA	2.02	0.42
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.54	0.42
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.89	0.42
1:E:249:PHE:CD1	1:E:271:ARG:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.02	0.42
1:E:39:LEU:HD11	1:E:334:LEU:HB3	2.02	0.42
1:C:192:TYR:HA	1:C:763:THR:CG2	2.50	0.42
1:E:111:PHE:HB3	1:E:114:GLU:HG2	2.02	0.42
1:E:222:ILE:CD1	1:E:245:TRP:HB2	2.50	0.42
1:E:733:ILE:HG21	1:E:743:ILE:HD11	2.01	0.42
1:E:719:LEU:HD21	1:E:835:TRP:CD2	2.54	0.42
1:E:101:ASN:OD1	1:E:453:ILE:HB	2.20	0.42
1:E:565:GLU:O	1:E:681:MET:HA	2.20	0.42
1:E:141:THR:HA	1:E:144:ARG:NH1	2.31	0.42
1:C:251:ASN:C	1:C:251:ASN:ND2	2.73	0.42
1:A:334:LEU:O	1:A:338:ILE:HG13	2.20	0.42
1:C:45:ILE:HD11	1:C:78:TYR:HB2	2.01	0.42
1:E:240:MET:O	1:E:244:LEU:HG	2.19	0.42
2:D:574:ASP:HA	2:D:575:PRO:HD2	1.79	0.42
1:A:258:THR:HG22	1:A:259:ASN:N	2.34	0.41
1:A:707:PRO:O	1:A:711:ARG:HG3	2.20	0.41
1:E:737:GLU:HA	1:E:740:VAL:HG23	2.02	0.41
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.60	0.41
1:E:759:GLN:HG2	1:E:760:ARG:N	2.34	0.41
1:C:215:LEU:HD23	1:C:216:HIS:N	2.35	0.41
1:A:249:PHE:CZ	1:A:261:ASP:HB3	2.55	0.41
2:B:511:PHE:HB3	2:B:600:TYR:CD1	2.55	0.41
1:E:150:ARG:HB3	1:E:351:TYR:CE1	2.53	0.41
1:E:395:TYR:CD1	1:E:457:VAL:HG22	2.55	0.41
1:A:410:LYS:HG2	1:A:430:ALA:HB2	2.01	0.41
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.35	0.41
1:C:759:GLN:CG	1:C:760:ARG:N	2.81	0.41
1:E:307:LEU:HB2	1:E:312:LYS:HE2	2.02	0.41
1:A:429:LYS:HE3	1:A:462:PHE:CE1	2.56	0.41
1:A:677:PHE:N	1:A:677:PHE:HD2	2.19	0.41
1:A:6:VAL:HG13	1:A:445:ILE:HG22	2.01	0.41
1:C:718:LEU:HA	1:C:722:PRO:HG3	2.02	0.41
1:A:831:GLU:CD	1:A:831:GLU:H	2.21	0.41
1:C:192:TYR:HA	1:C:763:THR:HG22	2.01	0.41
1:C:823:ARG:HA	1:C:828:MET:CE	2.47	0.41
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.84	0.41
1:C:494:GLU:HG2	1:C:495:VAL:N	2.34	0.41
1:A:132:ILE:HD12	1:A:162:ARG:HD3	2.02	0.41
1:A:411:VAL:HG12	1:A:412:ARG:N	2.35	0.41
1:A:410:LYS:HA	1:A:430:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:PHE:O	1:C:219:ALA:HA	2.20	0.41
1:A:524:GLU:CD	1:A:710:ARG:HH22	2.23	0.41
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.56	0.41
1:E:742:GLY:O	1:E:745:SER:HB3	2.21	0.41
1:E:200:VAL:O	1:E:200:VAL:HG22	2.20	0.41
2:F:426:HIS:CG	2:F:594:ILE:HD12	2.56	0.41
2:D:479:TYR:CG	2:D:582:LEU:HB2	2.56	0.41
1:C:354:GLU:HG3	1:C:370:LYS:HE3	2.02	0.41
1:A:279:ASP:HB3	1:A:280:PRO:HD3	2.01	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.97	0.41
2:B:498:LEU:HD23	2:B:498:LEU:HA	1.92	0.41
1:E:174:LEU:O	1:E:177:THR:HB	2.20	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.56	0.41
1:A:381:TYR:HB2	1:A:478:MET:CE	2.51	0.41
1:C:111:PHE:HB3	1:C:114:GLU:HB2	2.02	0.41
1:E:114:GLU:O	1:E:117:ALA:HB3	2.21	0.41
1:C:12:LEU:HD12	1:C:12:LEU:HA	1.93	0.41
1:A:545:LEU:O	1:A:550:ALA:HB3	2.21	0.41
1:C:237:LYS:HA	1:C:240:MET:HB3	2.03	0.41
2:F:571:ILE:HA	2:F:572:PRO:HD3	1.84	0.41
1:C:270:GLU:OE1	1:C:275:MET:HG3	2.20	0.41
1:A:620:ALA:HA	1:A:625:TRP:O	2.21	0.41
1:A:326:LYS:HB2	1:A:326:LYS:HE3	1.80	0.41
1:C:132:ILE:HD11	1:C:162:ARG:HB2	2.03	0.41
1:E:292:LYS:HD3	1:E:295:GLU:OE2	2.21	0.41
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.51	0.41
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.55	0.41
1:C:459:ILE:HG22	1:C:459:ILE:O	2.21	0.40
1:E:258:THR:HG22	1:E:260:LYS:H	1.85	0.40
1:C:420:PRO:HG2	1:C:476:HIS:CE1	2.56	0.40
1:C:556:ILE:HG12	1:C:556:ILE:O	2.21	0.40
1:C:831:GLU:N	1:C:831:GLU:OE1	2.51	0.40
1:A:470:THR:HG22	1:A:472:SER:N	2.25	0.40
1:C:501:LEU:N	1:C:502:PRO:CD	2.84	0.40
1:A:697:ALA:HA	1:A:700:ARG:CD	2.51	0.40
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.56	0.40
2:F:522:GLU:H	2:F:522:GLU:CD	2.24	0.40
1:C:699:DDE:HAC2	1:C:699:DDE:HAD2	1.82	0.40
1:E:225:PHE:HZ	1:E:327:PHE:CZ	2.39	0.40
1:E:491:VAL:HG21	1:E:542:LEU:HD21	2.03	0.40
2:F:553:GLU:OE1	3:F:702:NAD:H6N	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.56	0.40
1:C:565:GLU:O	1:C:681:MET:HA	2.22	0.40
1:A:558:PRO:HA	1:A:559:PRO:HD3	1.98	0.40
1:C:454:ILE:HG13	1:C:455:GLY:H	1.86	0.40
1:E:17:THR:HB	1:E:93:THR:HA	2.04	0.40
1:E:218:TRP:HZ3	1:E:220:PHE:CD2	2.39	0.40
1:C:711:ARG:HD2	2:D:578:VAL:O	2.22	0.40
1:A:431:ILE:CD1	1:A:459:ILE:HD11	2.51	0.40
2:D:484:ASP:OD2	2:D:494:ARG:HB2	2.21	0.40
1:E:284:LEU:HD22	1:E:323:VAL:HG11	2.03	0.40
1:E:12:LEU:HA	1:E:15:LYS:HE2	2.04	0.40
1:E:243:ARG:O	1:E:248:SER:HB2	2.22	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%)	780 (95%)	34 (4%)	4 (0%)	34	55
1	C	818/842 (97%)	776 (95%)	39 (5%)	3 (0%)	39	61
1	E	818/842 (97%)	750 (92%)	65 (8%)	3 (0%)	39	61
2	B	206/207 (100%)	200 (97%)	6 (3%)	0	100	100
2	D	205/207 (99%)	199 (97%)	5 (2%)	1 (0%)	34	55
2	F	205/207 (99%)	201 (98%)	3 (2%)	1 (0%)	34	55
All	All	3070/3147 (98%)	2906 (95%)	152 (5%)	12 (0%)	39	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	699/714 (98%)	678 (97%)	21 (3%)	48 76
1	C	699/714 (98%)	674 (96%)	25 (4%)	42 69
1	E	699/714 (98%)	689 (99%)	10 (1%)	74 91
2	B	161/160 (101%)	158 (98%)	3 (2%)	65 87
2	D	160/160 (100%)	156 (98%)	4 (2%)	55 82
2	F	160/160 (100%)	155 (97%)	5 (3%)	47 75
All	All	2578/2622 (98%)	2510 (97%)	68 (3%)	54 81

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

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

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

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

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

Mol	Chain	Res	Type
2	B	428	GLN
1	C	30	HIS
1	C	452	ASN
2	D	428	GLN
1	E	30	HIS
1	E	414	GLN
2	F	428	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.86	0	16,28,30	0.67	0
1	DDE	E	699	1	13,20,21	0.86	0	16,28,30	0.69	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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	699	DDE	CD2-NE2-CE1	2.06	108.96	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	4	0
1	E	699	DDE	2	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	0.63	0	47,73,73	1.97	4 (8%)
3	NAD	D	701	-	38,48,48	0.63	0	47,73,73	1.92	4 (8%)
3	NAD	F	702	-	38,48,48	0.66	0	47,73,73	2.04	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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	700	NAD	N3A-C2A-N1A	-9.97	121.26	128.89
3	F	702	NAD	N3A-C2A-N1A	-9.83	121.36	128.89
3	D	701	NAD	N3A-C2A-N1A	-9.71	121.46	128.89
3	F	702	NAD	C4B-O4B-C1B	-6.05	103.08	109.72
3	B	700	NAD	C4B-O4B-C1B	-5.25	103.95	109.72
3	D	701	NAD	C4B-O4B-C1B	-4.75	104.50	109.72
3	F	702	NAD	PN-O3-PA	-3.80	122.05	132.73
3	D	701	NAD	PN-O3-PA	-3.48	122.95	132.73
3	B	700	NAD	PN-O3-PA	-3.45	123.04	132.73
3	D	701	NAD	O4B-C1B-N9A	3.40	115.22	108.10
3	B	700	NAD	O4B-C1B-N9A	3.75	115.95	108.10
3	F	702	NAD	O4B-C1B-N9A	4.34	117.19	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	822/842 (97%)	0.30	50 (6%) 25 27	12, 51, 91, 113	0
1	C	822/842 (97%)	0.83	137 (16%) 2 2	13, 60, 136, 178	0
1	E	822/842 (97%)	2.24	382 (46%) 0 0	10, 124, 182, 229	0
2	B	207/207 (100%)	-0.10	4 (1%) 70 73	10, 22, 54, 89	0
2	D	207/207 (100%)	-0.10	3 (1%) 78 80	9, 21, 52, 95	0
2	F	207/207 (100%)	-0.12	3 (1%) 78 80	12, 27, 62, 91	0
All	All	3087/3147 (98%)	0.88	579 (18%) 2 1	9, 53, 159, 229	0

All (579) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	314	LEU	15.5
1	E	67	GLY	11.5
1	E	163	ALA	10.8
1	E	315	GLU	10.8
1	E	108	HIS	10.5
1	E	761	PRO	10.3
1	E	167	LEU	10.1
1	E	193	ALA	10.1
1	E	789	GLY	9.9
1	E	166	GLU	9.8
1	E	310	ASP	9.7
1	E	311	GLU	9.4
1	E	196	VAL	8.9
1	C	504	LEU	8.9
1	E	157	ILE	8.6
1	E	245	TRP	8.6
1	E	759	GLN	8.3
1	E	298	VAL	8.3
1	E	231	LYS	8.2

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Mol	Chain	Res	Type	RSRZ
1	E	175	TYR	8.1
1	E	32	LYS	8.1
1	E	107	GLY	7.9
1	E	321	LYS	7.8
1	E	200	VAL	7.8
1	C	498	ALA	7.8
1	E	290	ASN	7.6
1	E	740	VAL	7.6
1	E	361	ALA	7.5
1	E	179	ALA	7.5
1	E	790	GLY	7.3
1	E	187	VAL	7.3
1	E	766	PHE	7.3
1	E	420	PRO	7.2
1	C	499	ASN	7.1
1	E	316	GLY	7.1
1	C	167	LEU	7.0
1	E	281	ILE	7.0
1	E	47	SER	7.0
1	E	160	VAL	6.9
1	E	367	ILE	6.9
1	E	499	ASN	6.9
1	E	795	GLN	6.9
1	E	197	LEU	6.9
1	E	211	PHE	6.9
1	E	356	LEU	6.8
1	E	419	VAL	6.8
1	E	262	THR	6.8
1	E	195	GLU	6.8
1	E	81	MET	6.8
1	E	317	LYS	6.8
1	E	289	MET	6.7
1	E	212	GLY	6.7
1	E	307	LEU	6.7
1	E	335	LEU	6.7
1	C	298	VAL	6.6
1	E	68	ILE	6.6
1	E	498	ALA	6.6
1	E	129	VAL	6.6
1	E	257	TRP	6.6
1	C	502	PRO	6.6
1	E	254	THR	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	744	TYR	6.5
2	D	489	ALA	6.5
1	E	192	TYR	6.5
1	C	306	VAL	6.5
1	E	760	ARG	6.5
1	E	169	VAL	6.4
1	E	233	PHE	6.4
1	E	97	SER	6.4
1	E	232	LYS	6.3
1	E	360	PRO	6.3
1	C	522	MET	6.3
1	C	494	GLU	6.3
1	C	501	LEU	6.3
1	C	252	PRO	6.2
1	E	216	HIS	6.2
1	E	770	ALA	6.2
1	E	26	ALA	6.2
1	E	91	GLN	6.2
1	C	251	ASN	6.1
1	C	67	GLY	6.1
1	C	311	GLU	6.1
1	A	361	ALA	6.1
1	E	36	THR	6.1
1	E	269	LEU	6.1
1	E	218	TRP	6.0
1	E	739	ALA	6.0
1	E	268	PRO	6.0
1	C	168	GLN	6.0
1	E	48	ALA	6.0
1	E	343	PRO	6.0
1	E	737	GLU	6.0
1	E	741	GLY	6.0
1	E	194	ASP	5.9
1	E	78	TYR	5.9
1	E	168	GLN	5.9
1	E	27	HIS	5.9
1	E	553	PRO	5.9
1	E	306	VAL	5.9
1	A	67	GLY	5.9
1	E	86	VAL	5.9
1	E	763	THR	5.9
1	E	89	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	267	LYS	5.8
1	E	342	LEU	5.8
1	C	495	VAL	5.8
1	E	90	LYS	5.8
1	E	88	GLU	5.7
1	E	178	PHE	5.7
1	E	237	LYS	5.7
1	E	358	GLU	5.7
1	E	131	THR	5.6
1	E	239	LYS	5.6
1	E	240	MET	5.6
1	E	359	GLY	5.5
1	C	235	VAL	5.5
1	E	215	LEU	5.5
1	C	299	LEU	5.5
1	E	745	SER	5.5
1	C	523	SER	5.4
1	E	278	LEU	5.4
1	C	291	PHE	5.4
1	E	256	LYS	5.3
1	C	269	LEU	5.3
1	E	137	VAL	5.2
2	B	489	ALA	5.2
1	E	28	VAL	5.2
1	E	277	ILE	5.2
1	E	764	PRO	5.1
1	E	98	PHE	5.1
1	E	354	GLU	5.1
1	E	264	ALA	5.1
1	E	128	VAL	5.1
1	C	549	HIS	5.1
1	E	203	TYR	5.1
1	C	173	ASP	5.1
1	C	493	VAL	5.1
1	E	76	SER	5.1
1	E	299	LEU	5.0
1	E	180	ARG	5.0
1	E	258	THR	5.0
1	C	267	LYS	5.0
1	C	290	ASN	5.0
1	E	40	VAL	5.0
1	A	198	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	41	GLN	5.0
1	C	108	HIS	5.0
1	E	497	ASN	5.0
1	E	755	VAL	5.0
1	C	496	LYS	5.0
1	E	96	ASN	5.0
1	E	308	LYS	4.9
1	E	189	VAL	4.9
1	E	266	GLY	4.9
1	E	756	SER	4.9
1	E	30	HIS	4.9
1	E	442	VAL	4.9
1	E	46	ILE	4.9
1	C	264	ALA	4.9
1	E	111	PHE	4.9
1	E	263	ASP	4.9
1	E	294	ASP	4.9
1	A	107	GLY	4.8
1	E	260	LYS	4.8
1	E	297	PRO	4.8
1	C	268	PRO	4.8
1	E	453	ILE	4.8
1	E	302	LYS	4.8
1	E	296	ILE	4.8
1	E	20	ARG	4.8
1	E	332	ASP	4.7
1	C	321	LYS	4.7
1	E	156	VAL	4.7
1	E	436	LEU	4.7
1	E	282	PHE	4.7
1	C	513	LYS	4.7
1	E	324	MET	4.7
1	E	441	PHE	4.6
1	E	444	PRO	4.6
1	C	265	GLU	4.6
1	E	158	ASN	4.6
1	E	366	CYS	4.5
1	E	164	LEU	4.5
1	E	747	LEU	4.5
1	E	376	ALA	4.5
1	E	188	ILE	4.5
1	E	253	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	4.5
1	E	293	LYS	4.5
1	E	391	LYS	4.4
1	C	216	HIS	4.4
1	C	233	PHE	4.4
1	E	291	PHE	4.4
1	A	196	VAL	4.4
1	E	210	ALA	4.4
1	E	227	THR	4.4
1	E	162	ARG	4.3
1	E	500	ASP	4.3
1	E	554	LEU	4.3
1	A	111	PHE	4.3
1	E	312	LYS	4.3
1	E	83	ASP	4.3
1	C	310	ASP	4.3
1	C	556	ILE	4.3
1	E	201	GLN	4.3
1	E	135	VAL	4.2
1	E	265	GLU	4.2
1	C	547	HIS	4.2
1	E	503	LYS	4.2
1	E	329	PRO	4.2
1	E	110	ASP	4.2
1	E	781	THR	4.2
1	C	107	GLY	4.2
1	E	762	GLY	4.2
1	C	497	ASN	4.2
1	E	422	LYS	4.1
1	C	262	THR	4.1
1	C	550	ALA	4.1
1	E	134	GLY	4.1
1	E	421	GLY	4.1
1	E	235	VAL	4.1
1	C	317	LYS	4.1
1	A	48	ALA	4.0
1	E	230	ALA	4.0
1	C	553	PRO	4.0
1	C	314	LEU	4.0
1	E	476	HIS	4.0
1	C	301	GLU	4.0
1	E	29	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	390	ASP	4.0
1	E	743	ILE	4.0
1	E	24	VAL	4.0
1	E	220	PHE	4.0
1	A	7	ASP	3.9
1	E	109	VAL	3.9
1	C	236	ASP	3.9
1	E	80	GLU	3.9
1	E	255	LYS	3.9
1	E	758	GLU	3.9
1	C	111	PHE	3.9
1	E	273	PHE	3.9
1	C	313	ASP	3.9
1	C	500	ASP	3.9
1	E	742	GLY	3.9
1	E	155	VAL	3.9
1	E	38	SER	3.9
1	E	338	ILE	3.8
1	C	29	ASP	3.8
1	E	34	THR	3.8
1	E	288	ILE	3.8
1	C	761	PRO	3.8
1	C	546	GLU	3.8
1	E	304	GLU	3.8
1	E	7	ASP	3.8
1	E	205	ALA	3.8
1	C	232	LYS	3.7
1	E	494	GLU	3.7
1	E	318	ALA	3.7
1	E	455	GLY	3.7
1	E	261	ASP	3.7
1	E	768	VAL	3.7
1	A	28	VAL	3.7
1	E	170	SER	3.7
1	E	242	ASP	3.7
1	C	266	GLY	3.7
1	E	42	ARG	3.7
1	E	323	VAL	3.6
1	E	437	MET	3.6
1	C	258	THR	3.6
1	E	757	GLU	3.6
1	E	389	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	138	GLN	3.6
1	E	548	ASP	3.6
2	B	461	ASP	3.6
1	C	305	ILE	3.6
1	E	736	PRO	3.6
1	C	318	ALA	3.6
1	A	358	GLU	3.5
1	E	479	LYS	3.5
1	E	276	PHE	3.5
1	E	496	LYS	3.5
1	C	46	ILE	3.5
1	E	82	SER	3.5
1	E	100	ILE	3.5
1	E	222	ILE	3.5
1	C	231	LYS	3.5
1	E	348	ALA	3.5
1	A	360	PRO	3.5
1	E	738	GLN	3.5
1	E	469	LEU	3.5
1	E	94	ASP	3.5
1	E	106	PRO	3.5
1	E	454	ILE	3.5
1	C	552	VAL	3.5
1	E	395	TYR	3.4
1	E	127	VAL	3.4
1	E	754	VAL	3.4
1	E	154	VAL	3.4
1	E	37	ASP	3.4
1	E	456	LEU	3.4
1	E	213	SER	3.4
1	E	309	GLY	3.4
1	E	325	ARG	3.4
1	C	763	THR	3.4
1	E	333	ALA	3.4
1	E	472	SER	3.4
1	E	794	PRO	3.4
1	A	480	VAL	3.3
1	E	362	ASP	3.4
1	E	177	THR	3.3
1	E	748	ASN	3.3
1	E	23	SER	3.3
1	E	783	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	325	ARG	3.3
1	E	375	LYS	3.3
1	E	286	THR	3.3
1	C	293	LYS	3.3
1	C	391	LYS	3.3
1	E	418	TYR	3.3
1	E	423	LYS	3.3
1	E	176	GLN	3.3
1	A	419	VAL	3.3
1	E	199	ASP	3.3
1	E	313	ASP	3.3
1	E	301	GLU	3.2
1	E	25	ILE	3.2
1	E	320	LEU	3.2
1	E	435	VAL	3.2
1	C	544	ASP	3.2
1	A	454	ILE	3.2
1	E	15	LYS	3.2
1	E	555	LYS	3.2
1	E	105	SER	3.2
1	E	779	GLY	3.2
1	E	796	MET	3.2
1	E	70	ILE	3.2
1	C	294	ASP	3.2
1	A	108	HIS	3.2
1	E	284	LEU	3.1
1	C	263	ASP	3.1
1	E	322	VAL	3.1
1	E	130	ASP	3.1
1	E	31	GLY	3.1
1	E	392	GLY	3.1
1	E	3	ALA	3.1
1	E	104	ASP	3.1
1	C	289	MET	3.1
1	C	237	LYS	3.1
1	C	421	GLY	3.1
1	A	417	ASN	3.0
1	C	510	ARG	3.0
1	E	182	VAL	3.0
1	E	126	LEU	3.0
1	C	485	VAL	3.0
1	A	5	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	93	THR	3.0
1	E	214	GLY	3.0
1	E	202	VAL	3.0
1	A	81	MET	3.0
1	A	157	ILE	3.0
1	E	504	LEU	3.0
2	B	549	GLY	3.0
1	E	229	TYR	3.0
1	E	481	MET	2.9
1	A	464	LEU	2.9
1	E	92	LYS	2.9
1	C	554	LEU	2.9
1	E	79	SER	2.9
1	E	784	LEU	2.9
1	E	371	ASN	2.9
1	C	42	ARG	2.9
1	E	243	ARG	2.9
1	E	185	VAL	2.9
1	E	443	GLU	2.9
1	C	177	THR	2.9
1	C	446	ASP	2.9
1	E	473	GLU	2.8
1	C	323	VAL	2.8
1	C	759	GLN	2.8
1	E	353	ALA	2.8
1	E	279	ASP	2.8
1	C	528	HIS	2.8
1	E	303	LEU	2.8
2	F	461	ASP	2.8
1	E	785	ARG	2.8
1	E	272	ALA	2.8
1	C	11	SER	2.8
1	E	85	ASP	2.8
1	E	159	LYS	2.8
1	E	123	ASP	2.8
1	E	69	THR	2.8
1	E	477	ASN	2.8
1	A	420	PRO	2.7
1	E	793	PHE	2.7
1	E	236	ASP	2.7
1	E	145	GLN	2.7
1	E	77	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	399	ARG	2.7
1	C	109	VAL	2.7
1	A	375	LYS	2.7
1	C	509	LYS	2.7
1	E	464	LEU	2.7
1	C	261	ASP	2.7
1	C	292	LYS	2.7
1	E	161	ASP	2.7
1	E	522	MET	2.7
1	C	7	ASP	2.7
1	A	86	VAL	2.7
1	E	18	ASN	2.7
1	E	445	ILE	2.7
1	C	106	PRO	2.7
1	E	292	LYS	2.7
1	A	362	ASP	2.6
1	C	180	ARG	2.6
1	E	501	LEU	2.6
1	E	2	VAL	2.6
1	C	83	ASP	2.6
1	A	194	ASP	2.6
1	A	199	ASP	2.6
1	C	3	ALA	2.6
2	D	490	ARG	2.6
1	E	252	PRO	2.6
1	C	315	GLU	2.6
1	E	209	VAL	2.6
1	E	791	GLN	2.6
1	E	234	GLY	2.6
1	E	393	ARG	2.6
1	E	186	ASN	2.6
1	C	748	ASN	2.5
1	E	546	GLU	2.5
1	E	285	PHE	2.5
1	E	480	VAL	2.5
1	C	503	LYS	2.5
1	E	814	LYS	2.5
1	E	549	HIS	2.5
1	C	4	PHE	2.5
1	A	82	SER	2.5
1	A	495	VAL	2.5
1	E	495	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	136	CYS	2.5
1	C	286	THR	2.5
1	E	365	ASN	2.5
1	E	334	LEU	2.5
1	E	547	HIS	2.5
1	E	280	PRO	2.5
1	E	35	LEU	2.5
1	E	174	LEU	2.5
1	E	341	HIS	2.5
1	E	275	MET	2.5
1	C	295	GLU	2.5
1	A	291	PHE	2.4
1	E	39	LEU	2.4
1	C	239	LYS	2.4
1	C	253	LYS	2.4
1	C	302	LYS	2.4
1	E	357	TYR	2.4
1	E	377	ASP	2.4
1	C	169	VAL	2.4
1	C	492	ALA	2.4
1	A	310	ASP	2.4
1	E	183	GLU	2.4
1	E	483	PHE	2.4
1	E	19	VAL	2.4
1	E	780	PHE	2.4
1	A	313	ASP	2.4
1	E	394	PHE	2.4
1	C	100	ILE	2.4
1	A	156	VAL	2.4
1	E	731	VAL	2.4
2	F	490	ARG	2.4
1	E	5	THR	2.4
1	C	84	GLU	2.4
1	E	364	ALA	2.4
1	E	295	GLU	2.3
1	E	305	ILE	2.3
1	E	428	ILE	2.3
1	E	355	GLN	2.3
1	C	322	VAL	2.3
1	E	73	THR	2.3
1	C	482	LYS	2.3
1	E	433	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	815	ALA	2.3
1	E	84	GLU	2.3
1	E	171	LYS	2.3
1	E	551	GLY	2.3
1	C	288	ILE	2.3
2	D	461	ASP	2.3
1	A	293	LYS	2.3
1	C	229	TYR	2.3
1	E	11	SER	2.3
1	E	328	LEU	2.3
1	E	380	LEU	2.3
1	E	440	ARG	2.3
1	C	28	VAL	2.3
1	E	241	MET	2.3
1	C	170	SER	2.3
1	E	244	LEU	2.3
1	E	122	THR	2.3
1	E	347	THR	2.3
1	E	118	ALA	2.3
1	E	283	ARG	2.3
1	A	758	GLU	2.3
1	A	500	ASP	2.3
2	F	489	ALA	2.2
1	A	29	ASP	2.2
1	E	732	GLU	2.2
1	E	410	LYS	2.2
1	C	525	SER	2.2
1	E	452	ASN	2.2
1	A	14	ASP	2.2
1	E	778	PHE	2.2
1	E	147	LEU	2.2
1	A	155	VAL	2.2
1	C	296	ILE	2.2
1	A	756	SER	2.2
1	E	225	PHE	2.2
1	E	471	THR	2.2
1	E	43	ALA	2.2
1	C	94	ASP	2.2
1	E	349	GLN	2.2
1	A	127	VAL	2.2
1	E	552	VAL	2.2
1	C	308	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	33	SER	2.2
1	E	398	GLY	2.2
1	A	233	PHE	2.2
1	E	339	VAL	2.2
1	E	350	ALA	2.2
1	C	5	THR	2.2
1	C	516	PRO	2.2
1	E	259	ASN	2.2
1	E	121	VAL	2.1
1	A	455	GLY	2.1
1	E	521	TYR	2.1
1	A	211	PHE	2.1
1	E	753	GLN	2.1
1	E	101	ASN	2.1
1	E	765	LEU	2.1
1	C	254	THR	2.1
1	A	129	VAL	2.1
1	C	2	VAL	2.1
1	C	731	VAL	2.1
1	E	337	MET	2.1
1	A	84	GLU	2.1
1	C	270	GLU	2.1
1	C	307	LEU	2.1
1	E	165	LEU	2.1
1	E	465	LYS	2.1
1	E	217	GLY	2.1
1	C	433	ARG	2.1
1	C	755	VAL	2.1
1	C	324	MET	2.1
1	E	228	ARG	2.1
1	E	468	THR	2.1
1	A	298	VAL	2.1
1	E	550	ALA	2.1
1	C	99	LEU	2.1
1	C	766	PHE	2.1
1	E	327	PHE	2.1
1	C	524	GLU	2.1
1	C	758	GLU	2.1
1	C	422	LYS	2.1
1	E	6	VAL	2.1
1	E	485	VAL	2.1
1	E	223	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	68	ILE	2.1
1	A	359	GLY	2.1
1	C	37	ASP	2.1
1	C	453	ILE	2.0
1	C	743	ILE	2.0
1	E	207	GLY	2.0
1	A	763	THR	2.0
2	B	490	ARG	2.0
1	C	312	LYS	2.0
1	C	316	GLY	2.0
1	C	408	GLY	2.0
1	C	277	ILE	2.0
1	C	285	PHE	2.0
1	E	191	THR	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^{th} 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^2)	Q<0.9
1	DDE	C	699	20/21	0.92	0.20	-	14,61,107,114	0
1	DDE	A	699	10/21	0.95	0.19	-	40,49,57,57	0
1	DDE	E	699	20/21	0.91	0.24	-	30,62,75,79	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^{th} 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^2)	Q<0.9
3	NAD	B	700	44/44	0.96	0.15	-0.50	4,20,39,42	0
3	NAD	F	702	44/44	0.96	0.14	-0.64	11,24,38,48	0
3	NAD	D	701	44/44	0.96	0.15	-0.67	7,22,38,45	0

6.5 Other polymers (i)

There are no such residues in this entry.