Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:39 PM GMT

PDB ID	:	1LA2
Title	:	Structural analysis of Saccharomyces cerevisiae myo-inositol phosphate synthase
Authors	:	Kniewel, R.; Buglino, J.A.; Shen, V.; Chadna, T.; Beckwith, A.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2002-03-27
Resolution	:	2.65 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 (i)) were used in the production of this report:

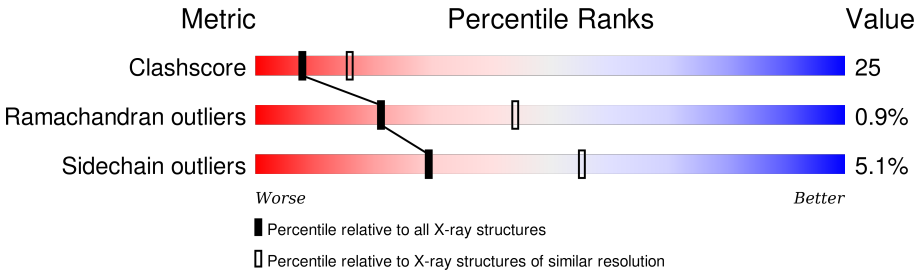
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.65 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	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	55% 39%
1	B	533	53% 41%
1	C	533	53% 40%
1	D	533	53% 40%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17040 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 Myo-inositol-1-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	B	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	C	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	D	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
A	452	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	VAL	LEU	SEE REMARK 999	UNP P11986
B	?	-	PHE	SEE REMARK 999	UNP P11986
B	60	LEU	GLU	SEE REMARK 999	UNP P11986
B	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	452	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	?	-	ARG	SEE REMARK 999	UNP P11986
C	14	VAL	LEU	SEE REMARK 999	UNP P11986
C	?	-	PHE	SEE REMARK 999	UNP P11986
C	60	LEU	GLU	SEE REMARK 999	UNP P11986
C	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	?	-	ALA	SEE REMARK 999	UNP P11986
C	98	GLU	LYS	SEE REMARK 999	UNP P11986
C	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	140	ASN	LYS	SEE REMARK 999	UNP P11986
C	141	ASP	HIS	SEE REMARK 999	UNP P11986
C	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	201	ASN	GLN	SEE REMARK 999	UNP P11986
C	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
C	444	PRO	ALA	SEE REMARK 999	UNP P11986
C	452	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	?	-	ARG	SEE REMARK 999	UNP P11986
D	14	VAL	LEU	SEE REMARK 999	UNP P11986
D	?	-	PHE	SEE REMARK 999	UNP P11986

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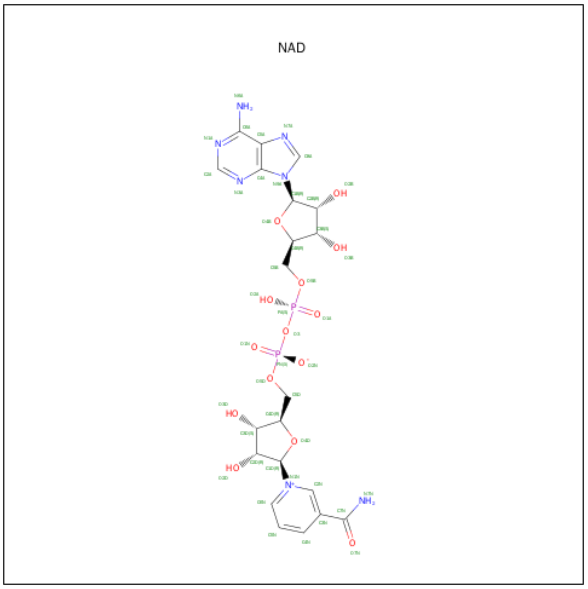
Chain	Residue	Modelled	Actual	Comment	Reference
D	60	LEU	GLU	SEE REMARK 999	UNP P11986
D	69	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	?	-	ALA	SEE REMARK 999	UNP P11986
D	98	GLU	LYS	SEE REMARK 999	UNP P11986
D	109	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	136	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	140	ASN	LYS	SEE REMARK 999	UNP P11986
D	141	ASP	HIS	SEE REMARK 999	UNP P11986
D	158	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	176	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	201	ASN	GLN	SEE REMARK 999	UNP P11986
D	261	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	405	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	415	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	423	MSE	MET	MODIFIED RESIDUE	UNP P11986
D	444	PRO	ALA	SEE REMARK 999	UNP P11986
D	452	MSE	MET	MODIFIED RESIDUE	UNP P11986

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	188	Total	O	0	0
			188	188		
3	C	194	Total	O	0	0
			194	194		
3	D	165	Total	O	0	0
			165	165		

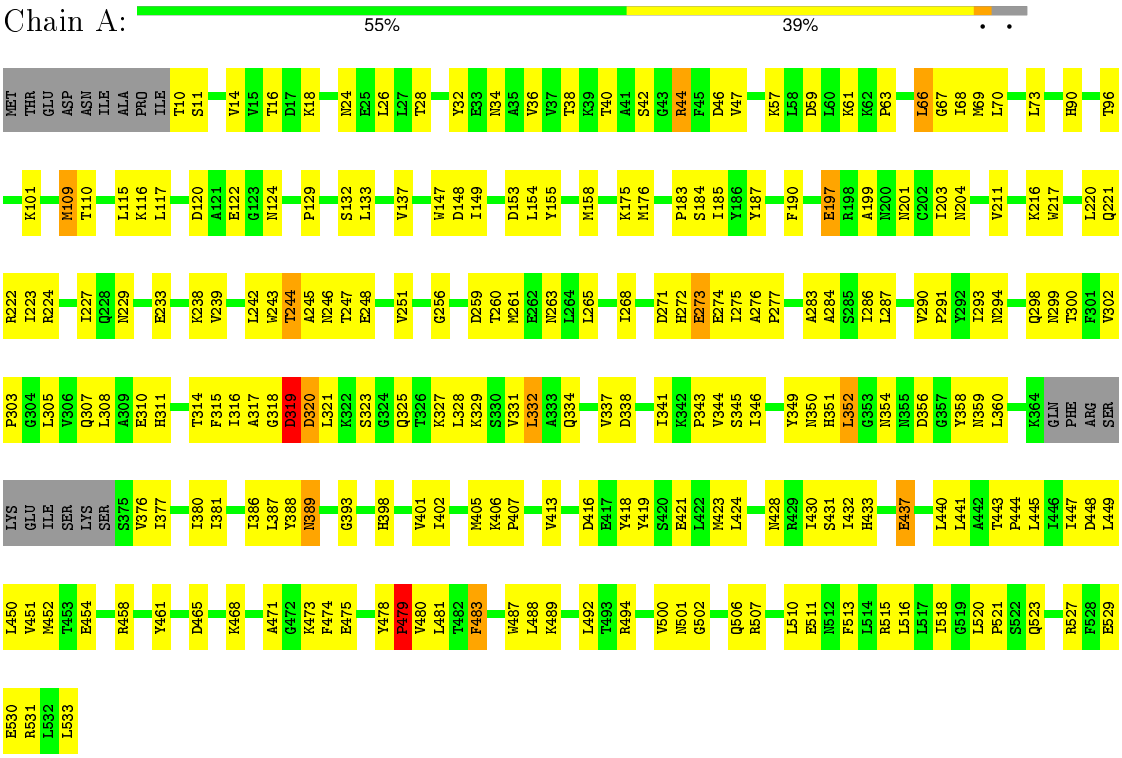
3 Residue-property plots (i)

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.

Note EDS was not executed.

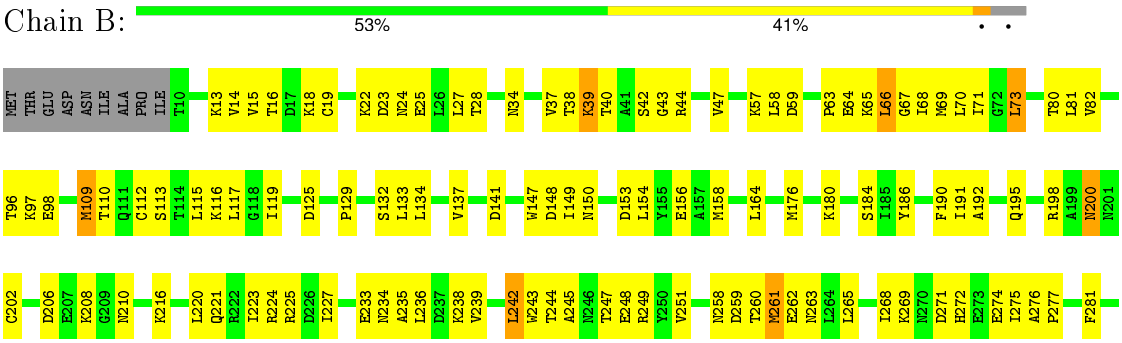
- Molecule 1: Myo-inositol-1-phosphate synthase

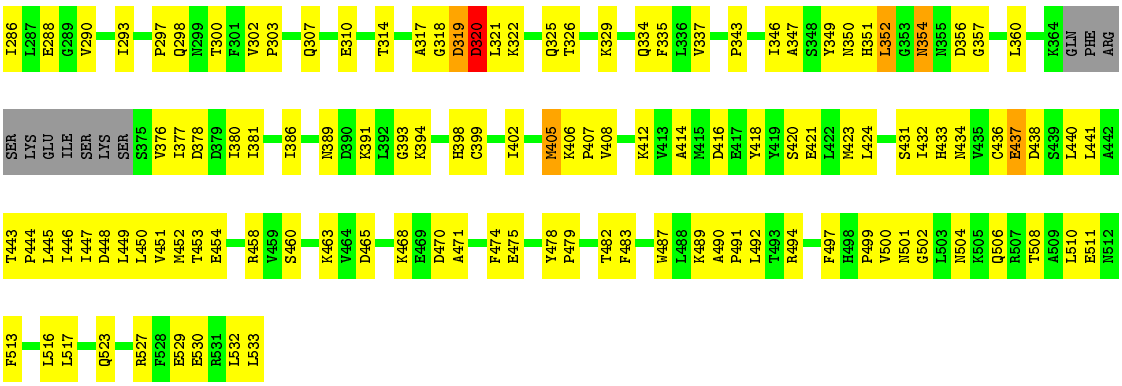
Chain A:



- Molecule 1: Myo-inositol-1-phosphate synthase

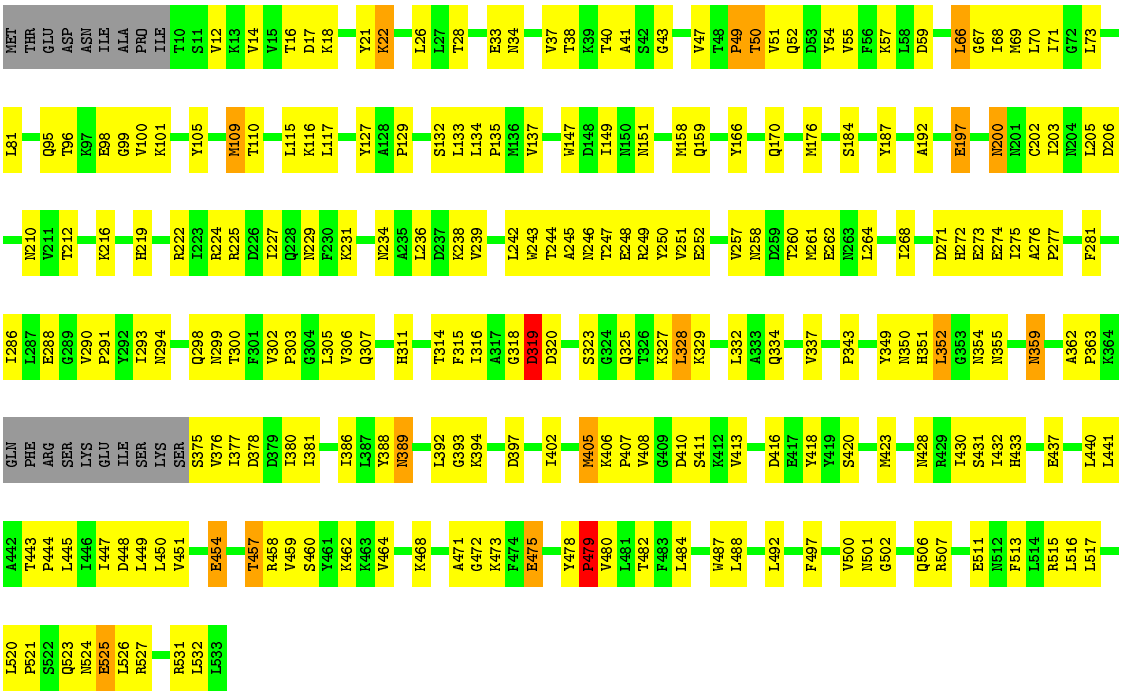
Chain B:





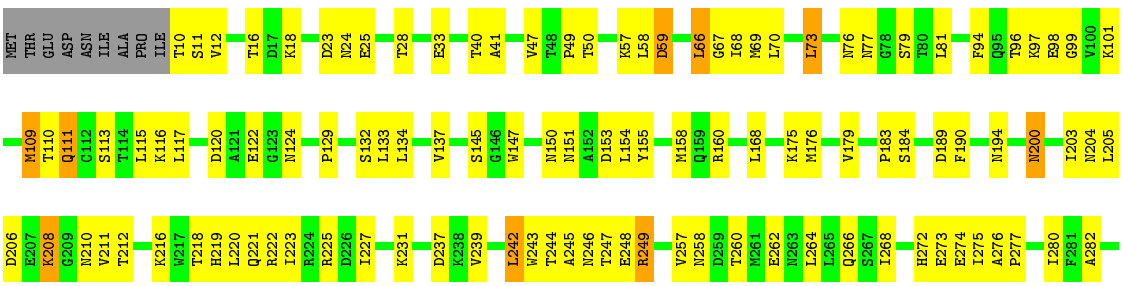
• Molecule 1: Myo-inositol-1-phosphate synthase

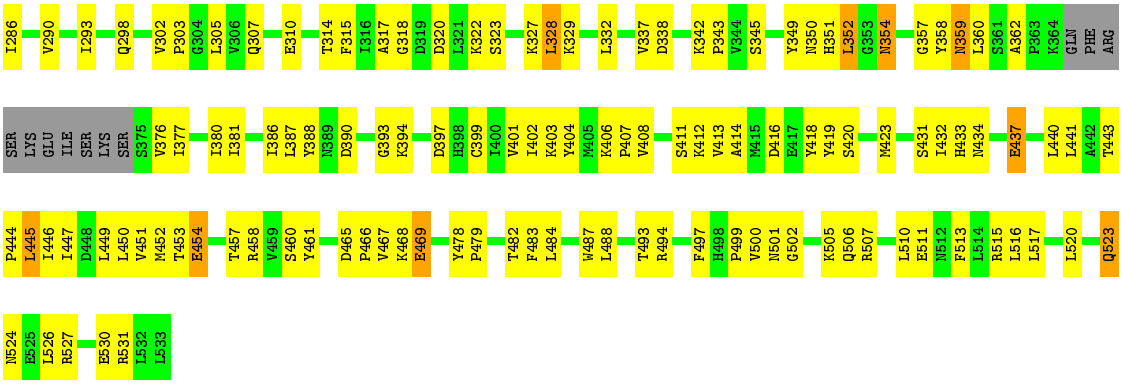
Chain C:



• Molecule 1: Myo-inositol-1-phosphate synthase

Chain D:




I286 V290 I293 Q298 V302 P303 G304 L305 V306 Q307 E310 T314 F315 I316 A317 G318 D319 D320 L321 K322 S323 K327 L328 K329 L332 V337 D338 K342 P343 V344 S345 Y349 N350 H351 L352 G353 N354 G357 Y358 N359 L360 S361 A362 P363 K364 GLN PHE ARG
SER LYS GLU ILE SER LYS SER S375 V376 I377 I380 I381 I386 L387 Y388 N389 D390 G393 K394 D397 H398 C399 I400 V401 I402 K403 Y404 M405 K406 P407 V408 S411 K412 V413 A414 M415 D416 E417 Y418 Y419 S420 M423 S431 I432 H433 N434 E437 L440 L441 A442 T443
P444 L445 I446 I447 D448 L449 L450 V451 M452 T453 E454 T457 R458 V459 S460 Y461 D465 P466 V467 K468 E469 Y478 P479 T482 F483 L484 W487 L488 T493 R494 F497 H498 P499 V500 N501 G502 K505 Q506 R507 L510 E511 N512 F513 L514 R515 L516 L517 L520 Q523
N524 E525 L526 R527 E530 R531 I532 L533

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	155.69Å 187.35Å 98.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.65	Depositor
% Data completeness (in resolution range)	99.4 (19.96-2.65)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.224 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17040	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.26	0/4112	0.47	0/5561
1	B	0.26	0/4112	0.48	0/5561
1	C	0.26	0/4112	0.48	0/5561
1	D	0.25	0/4112	0.47	0/5561
All	All	0.26	0/16448	0.47	0/22244

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4043	0	4038	216	0
1	B	4043	0	4038	212	0
1	C	4043	0	4038	216	0
1	D	4043	0	4038	226	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	145	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	188	0	0	5	0
3	C	194	0	0	11	0
3	D	165	0	0	10	0
All	All	17040	0	16256	809	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 25.

All (809) 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:423:MSE:HE3	1:D:444:PRO:HG3	1.27	1.11
1:A:437:GLU:HG3	1:A:440:LEU:HD12	1.29	1.09
1:D:437:GLU:HG3	1:D:440:LEU:HD12	1.35	1.08
1:A:129:PRO:HG2	1:A:132:SER:HB3	1.45	0.96
1:D:96:THR:HG23	1:D:98:GLU:H	1.34	0.93
1:B:73:LEU:HD22	1:B:154:LEU:HD21	1.50	0.92
1:D:69:MSE:HE2	1:D:239:VAL:HG11	1.52	0.92
1:D:242:LEU:HD22	1:D:293:ILE:HB	1.50	0.90
1:C:69:MSE:HE1	1:C:227:ILE:HG12	1.51	0.90
1:C:437:GLU:HG3	1:C:440:LEU:HD12	1.52	0.89
1:B:69:MSE:HE2	1:B:239:VAL:HG11	1.53	0.88
1:C:16:THR:HG22	1:C:18:LYS:H	1.39	0.88
1:A:492:LEU:HD23	1:A:492:LEU:H	1.39	0.87
1:A:73:LEU:HD13	1:A:154:LEU:HD21	1.56	0.87
1:B:69:MSE:HE1	1:B:227:ILE:HG12	1.57	0.87
1:B:437:GLU:HG3	1:B:440:LEU:HD12	1.57	0.86
1:B:70:LEU:HD11	1:B:81:LEU:HD13	1.56	0.86
1:D:16:THR:HG22	1:D:18:LYS:H	1.41	0.85
1:B:109:MSE:O	1:B:113:SER:HB3	1.78	0.84
1:D:69:MSE:HE1	1:D:227:ILE:HG12	1.59	0.83
1:B:129:PRO:HG2	1:B:132:SER:HB3	1.62	0.82
1:C:96:THR:HG22	1:C:99:GLY:O	1.80	0.81
1:A:423:MSE:HG2	1:A:424:LEU:HG	1.62	0.81
1:B:376:VAL:HG22	1:B:501:ASN:HB3	1.61	0.81
1:B:40:THR:HG22	1:B:42:SER:H	1.43	0.80
1:A:44:ARG:HE	1:B:13:LYS:HD2	1.46	0.80
1:A:69:MSE:HE1	1:A:227:ILE:HG12	1.60	0.80
1:D:96:THR:HG22	1:D:99:GLY:O	1.80	0.80
1:B:321:LEU:HG	1:B:445:LEU:HD22	1.61	0.80
1:C:376:VAL:HG22	1:C:501:ASN:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:ASN:HD22	1:D:526:LEU:H	1.31	0.79
1:D:110:THR:HG21	1:D:451:VAL:HG11	1.64	0.79
1:D:70:LEU:HD11	1:D:81:LEU:HD22	1.65	0.78
1:A:183:PRO:HA	1:A:201:ASN:OD1	1.84	0.78
1:C:129:PRO:HB3	1:D:386:ILE:HD11	1.67	0.76
1:A:345:SER:HB3	1:A:419:TYR:HB3	1.66	0.76
1:B:39:LYS:H	1:B:39:LYS:HD2	1.50	0.76
1:A:16:THR:HG22	1:A:18:LYS:H	1.51	0.76
1:B:242:LEU:HD22	1:B:293:ILE:HB	1.69	0.75
1:C:261:MSE:HE1	1:C:311:HIS:HB2	1.69	0.75
1:C:129:PRO:HG2	1:C:132:SER:HB3	1.68	0.75
1:D:73:LEU:HD22	1:D:154:LEU:HD11	1.69	0.74
1:D:218:THR:HA	1:D:221:GLN:HE21	1.51	0.74
1:D:129:PRO:HG2	1:D:132:SER:HB3	1.69	0.74
1:C:96:THR:HG23	1:C:98:GLU:H	1.51	0.74
1:D:293:ILE:HG23	1:D:317:ALA:HB3	1.68	0.74
1:B:59:ASP:HB3	1:B:458:ARG:HB3	1.70	0.74
1:C:318:GLY:O	1:C:319:ASP:HB2	1.87	0.74
1:D:352:LEU:HD11	1:D:360:LEU:HD12	1.70	0.74
1:C:316:ILE:HD11	1:C:480:VAL:HG22	1.70	0.74
1:B:423:MSE:HG2	1:B:424:LEU:HG	1.70	0.73
1:C:492:LEU:HD23	1:C:492:LEU:H	1.54	0.73
1:A:433:HIS:HB3	1:B:431:SER:HB2	1.69	0.73
1:B:248:GLU:OE2	1:B:277:PRO:HG2	1.89	0.73
1:B:443:THR:HB	1:B:444:PRO:HD3	1.70	0.73
1:D:115:LEU:HD22	1:D:511:GLU:HG2	1.70	0.73
1:D:343:PRO:HA	1:D:420:SER:HA	1.69	0.72
1:C:389:ASN:ND2	1:C:392:LEU:H	1.87	0.72
1:C:151:ASN:H	1:C:200:ASN:HD21	1.37	0.72
1:C:441:LEU:O	1:C:445:LEU:HD13	1.88	0.72
1:D:445:LEU:HG	1:D:487:TRP:HD1	1.55	0.71
1:C:433:HIS:HB3	1:D:431:SER:HB2	1.71	0.71
1:B:399:CYS:SG	1:C:405:MSE:HE1	2.31	0.71
1:A:117:LEU:HD21	1:A:133:LEU:HD21	1.71	0.71
1:C:511:GLU:O	1:C:515:ARG:HG3	1.91	0.71
1:D:109:MSE:O	1:D:113:SER:HB3	1.90	0.70
1:C:117:LEU:HD21	1:C:133:LEU:HD21	1.74	0.70
1:D:248:GLU:OE2	1:D:277:PRO:HG2	1.92	0.70
1:A:117:LEU:HD21	1:A:133:LEU:CD2	2.23	0.69
1:C:302:VAL:HB	1:C:303:PRO:HD2	1.75	0.68
1:C:386:ILE:HD11	1:D:129:PRO:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:GLY:O	1:D:506:GLN:HG3	1.94	0.68
1:C:68:ILE:HG12	1:C:450:LEU:HD13	1.75	0.68
1:A:69:MSE:HE2	1:A:239:VAL:HG11	1.77	0.67
1:C:147:TRP:HB3	1:C:184:SER:HB2	1.76	0.67
1:B:262:GLU:CD	1:B:262:GLU:H	1.97	0.67
1:C:22:LYS:HD2	1:C:22:LYS:O	1.95	0.67
1:A:239:VAL:O	1:A:290:VAL:HG13	1.93	0.67
1:A:533:LEU:HD23	1:B:463:LYS:NZ	2.09	0.67
1:B:153:ASP:OD2	1:B:156:GLU:HG3	1.94	0.66
1:B:116:LYS:HD3	1:B:523:GLN:HE22	1.60	0.66
1:C:329:LYS:HA	1:C:418:TYR:OH	1.96	0.66
1:A:259:ASP:HA	1:A:303:PRO:HG2	1.76	0.66
1:C:248:GLU:OE2	1:C:277:PRO:HG2	1.96	0.66
1:C:437:GLU:HG3	1:C:440:LEU:CD1	2.25	0.65
1:A:478:TYR:CE2	1:A:494:ARG:HG2	2.31	0.65
1:D:79:SER:HA	1:D:154:LEU:HD12	1.79	0.65
1:B:234:ASN:O	1:B:236:LEU:N	2.29	0.65
1:B:334:GLN:HE21	1:B:380:ILE:HG12	1.60	0.65
1:D:345:SER:HB3	1:D:419:TYR:HB3	1.79	0.65
1:B:445:LEU:HG	1:B:487:TRP:HD1	1.61	0.65
1:C:527:ARG:NH2	1:D:500:VAL:HG11	2.11	0.65
1:C:251:VAL:HG21	1:C:274:GLU:O	1.97	0.65
1:A:511:GLU:O	1:A:515:ARG:HG3	1.96	0.65
1:B:405:MSE:HE3	1:C:397:ASP:HB3	1.79	0.64
1:B:349:TYR:C	1:B:350:ASN:HD22	2.00	0.64
1:D:441:LEU:C	1:D:444:PRO:HD2	2.17	0.64
1:A:334:GLN:HE21	1:A:380:ILE:HG12	1.62	0.64
1:B:96:THR:HG22	1:B:98:GLU:H	1.62	0.64
1:A:70:LEU:CD2	1:A:242:LEU:HB3	2.28	0.64
1:D:68:ILE:HG12	1:D:450:LEU:HD13	1.78	0.64
1:C:328:LEU:HD21	1:D:332:LEU:HD21	1.79	0.64
1:D:96:THR:HG21	1:D:101:LYS:HE3	1.80	0.64
1:C:257:VAL:HG11	1:C:272:HIS:CD2	2.32	0.64
1:C:239:VAL:O	1:C:290:VAL:HG13	1.96	0.63
1:A:445:LEU:HG	1:A:487:TRP:HD1	1.64	0.63
1:D:337:VAL:HG21	1:D:380:ILE:HG22	1.79	0.63
1:D:77:ASN:HB2	1:D:244:THR:HG21	1.81	0.63
1:B:318:GLY:O	1:B:319:ASP:HB2	1.99	0.63
1:A:149:ILE:O	1:A:199:ALA:HA	1.98	0.63
1:D:208:LYS:HE3	1:D:208:LYS:H	1.64	0.63
1:D:70:LEU:HD11	1:D:81:LEU:CD2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MSE:HE3	1:A:307:GLN:HG2	1.81	0.63
1:A:61:LYS:HB3	1:A:61:LYS:NZ	2.14	0.63
1:C:59:ASP:HB3	1:C:458:ARG:HB3	1.80	0.63
1:C:95:GLN:NE2	1:C:100:VAL:HG22	2.13	0.63
1:A:129:PRO:HG2	1:A:132:SER:CB	2.26	0.62
1:A:406:LYS:N	1:A:407:PRO:HD2	2.13	0.62
1:A:203:ILE:HD13	1:A:222:ARG:HG2	1.81	0.62
1:B:437:GLU:CG	1:B:440:LEU:HD12	2.28	0.62
1:D:116:LYS:HD3	1:D:523:GLN:HE22	1.64	0.62
1:D:511:GLU:O	1:D:515:ARG:HG3	1.99	0.62
1:B:186:TYR:HE1	1:B:191:ILE:HD11	1.64	0.62
1:C:478:TYR:CD1	1:C:479:PRO:HD2	2.34	0.62
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.30	0.62
1:C:531:ARG:HG2	1:D:482:THR:OG1	1.99	0.62
1:A:70:LEU:HD23	1:A:242:LEU:HB3	1.81	0.62
1:D:246:ASN:HB3	1:D:359:ASN:ND2	2.15	0.62
1:A:349:TYR:C	1:A:350:ASN:HD22	2.04	0.62
1:D:40:THR:HG22	1:D:41:ALA:N	2.14	0.62
1:C:332:LEU:HD21	1:D:328:LEU:HD21	1.82	0.61
1:A:224:ARG:NH1	1:A:287:LEU:HB3	2.15	0.61
1:D:414:ALA:HB3	1:D:434:ASN:HB3	1.81	0.61
1:D:59:ASP:O	1:D:458:ARG:HD2	2.00	0.61
1:D:318:GLY:O	1:D:488:LEU:HD13	2.00	0.61
1:B:57:LYS:HB3	1:B:460:SER:OG	2.00	0.61
1:D:478:TYR:CE2	1:D:494:ARG:HB3	2.36	0.61
1:A:445:LEU:HD21	1:A:487:TRP:HB3	1.82	0.61
1:D:40:THR:HG22	1:D:41:ALA:H	1.64	0.61
1:A:351:HIS:CE1	1:A:413:VAL:HB	2.36	0.61
1:D:239:VAL:O	1:D:290:VAL:HG13	2.00	0.61
1:B:16:THR:HG22	1:B:18:LYS:H	1.65	0.61
1:C:242:LEU:HD22	1:C:293:ILE:HB	1.81	0.61
1:B:239:VAL:O	1:B:290:VAL:HG13	2.00	0.61
1:C:22:LYS:C	1:C:22:LYS:HD2	2.21	0.60
1:A:449:LEU:HD21	1:A:487:TRP:HB2	1.82	0.60
1:D:329:LYS:HD3	1:D:416:ASP:OD2	2.01	0.60
1:D:160:ARG:HD2	3:D:987:HOH:O	2.01	0.60
1:D:262:GLU:CD	1:D:262:GLU:H	2.04	0.60
1:A:116:LYS:HB3	1:A:523:GLN:NE2	2.16	0.60
1:A:352:LEU:HD22	1:A:354:ASN:ND2	2.17	0.60
1:A:246:ASN:HD22	1:A:359:ASN:HB2	1.66	0.60
1:D:57:LYS:HB3	1:D:460:SER:OG	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:GLU:HG3	1:D:505:LYS:HB3	1.82	0.60
1:A:203:ILE:HD11	3:A:902:HOH:O	2.01	0.60
1:C:431:SER:HB2	1:D:433:HIS:HB3	1.82	0.60
1:C:262:GLU:H	1:C:262:GLU:CD	2.03	0.60
1:C:300:THR:O	1:C:305:LEU:HD12	2.01	0.60
1:C:449:LEU:HD21	1:C:487:TRP:HB2	1.84	0.60
1:D:272:HIS:CE1	1:D:274:GLU:HG3	2.37	0.60
1:A:38:THR:OG1	1:A:46:ASP:HB2	2.01	0.60
1:D:151:ASN:H	1:D:200:ASN:HD21	1.48	0.60
1:C:225:ARG:NH1	1:C:229:ASN:HB2	2.17	0.60
1:C:129:PRO:HG2	1:C:132:SER:CB	2.32	0.60
1:A:261:MSE:HE1	1:A:311:HIS:HB2	1.84	0.60
1:A:73:LEU:CD1	1:A:154:LEU:HD21	2.30	0.59
1:A:337:VAL:HG21	1:A:380:ILE:CG2	2.31	0.59
1:D:116:LYS:HD3	1:D:523:GLN:NE2	2.16	0.59
1:C:473:LYS:HE3	1:C:475:GLU:OE1	2.02	0.59
1:C:109:MSE:HG3	1:C:110:THR:N	2.16	0.59
1:A:327:LYS:O	1:A:331:VAL:HG23	2.02	0.59
1:C:247:THR:HA	1:C:298:GLN:HE21	1.66	0.59
1:D:342:LYS:HB2	1:D:387:LEU:HD22	1.83	0.59
1:D:443:THR:HB	1:D:444:PRO:HD3	1.83	0.59
1:B:117:LEU:HD21	1:B:133:LEU:CD2	2.33	0.59
1:A:318:GLY:O	1:A:319:ASP:HB2	2.03	0.59
1:A:377:ILE:O	1:A:381:ILE:HG13	2.03	0.59
1:C:389:ASN:HD22	1:C:392:LEU:H	1.51	0.59
1:B:195:GLN:HA	1:B:195:GLN:HE21	1.66	0.59
1:A:341:ILE:O	1:A:343:PRO:HD3	2.03	0.59
1:B:247:THR:HA	1:B:298:GLN:HE21	1.67	0.58
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.37	0.58
1:B:129:PRO:HG2	1:B:132:SER:CB	2.32	0.58
1:A:437:GLU:HG3	1:A:440:LEU:CD1	2.19	0.58
1:C:224:ARG:HD2	1:C:288:GLU:OE2	2.03	0.58
1:C:323:SER:O	1:C:327:LYS:HG3	2.03	0.58
1:D:247:THR:HA	1:D:298:GLN:HE21	1.68	0.58
1:B:208:LYS:N	1:B:208:LYS:HD2	2.18	0.58
1:B:343:PRO:HA	1:B:420:SER:HA	1.86	0.58
1:A:527:ARG:HB2	1:A:531:ARG:NH1	2.17	0.58
1:A:443:THR:HB	1:A:444:PRO:HD3	1.84	0.58
1:D:515:ARG:NH1	1:D:523:GLN:HG2	2.19	0.58
1:D:150:ASN:HA	1:D:200:ASN:ND2	2.19	0.58
1:C:318:GLY:HA2	1:C:488:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ARG:NH1	1:C:458:ARG:HB2	2.19	0.57
1:A:527:ARG:NE	1:B:500:VAL:HG21	2.19	0.57
1:B:195:GLN:HE22	1:B:198:ARG:HD3	1.68	0.57
1:D:204:ASN:ND2	1:D:211:VAL:HG13	2.19	0.57
1:C:49:PRO:HG2	1:D:16:THR:OG1	2.04	0.57
1:D:449:LEU:HD21	1:D:487:TRP:HB2	1.86	0.57
1:C:272:HIS:HB3	1:C:275:ILE:HD13	1.84	0.57
1:A:10:THR:HA	1:B:43:GLY:O	2.05	0.57
1:A:221:GLN:HG2	3:A:966:HOH:O	2.03	0.57
1:B:502:GLY:O	1:B:506:GLN:HG3	2.04	0.57
1:A:26:LEU:O	1:A:57:LYS:HA	2.05	0.57
1:A:387:LEU:HD21	1:B:112:CYS:HB3	1.86	0.57
1:B:69:MSE:HE1	1:B:227:ILE:CG1	2.34	0.57
1:C:238:LYS:HE3	1:C:457:THR:HG21	1.87	0.57
1:A:109:MSE:HG3	1:A:110:THR:N	2.19	0.57
1:A:129:PRO:HB3	1:B:386:ILE:HD11	1.86	0.57
1:C:443:THR:HB	1:C:444:PRO:HD3	1.86	0.57
1:C:502:GLY:O	1:C:506:GLN:HG3	2.05	0.57
1:C:343:PRO:HA	1:C:420:SER:HA	1.87	0.57
1:A:405:MSE:HE1	1:D:399:CYS:SG	2.44	0.57
1:B:406:LYS:N	1:B:407:PRO:HD2	2.19	0.57
1:B:70:LEU:HD23	1:B:242:LEU:HB3	1.87	0.56
1:C:261:MSE:HE3	1:C:307:GLN:HG2	1.87	0.56
1:B:208:LYS:H	1:B:208:LYS:HD2	1.69	0.56
1:D:516:LEU:HD12	1:D:517:LEU:N	2.19	0.56
1:C:423:MSE:CE	1:D:444:PRO:HG3	2.19	0.56
1:C:14:VAL:HG22	1:D:47:VAL:HB	1.87	0.56
1:C:96:THR:HG21	1:C:101:LYS:HE3	1.86	0.56
1:B:260:THR:HA	1:B:307:GLN:NE2	2.20	0.56
1:D:264:LEU:O	1:D:268:ILE:HG13	2.05	0.56
1:B:337:VAL:HG21	1:B:380:ILE:HG21	1.87	0.56
1:C:242:LEU:HD12	1:C:244:THR:OG1	2.05	0.56
1:C:441:LEU:C	1:C:444:PRO:HD2	2.25	0.56
1:B:445:LEU:HD21	1:B:487:TRP:HB3	1.86	0.56
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.87	0.56
1:A:329:LYS:HA	1:A:418:TYR:OH	2.06	0.56
1:D:454:GLU:O	1:D:457:THR:HB	2.05	0.56
1:A:229:ASN:O	1:A:233:GLU:HG3	2.05	0.56
1:B:247:THR:HA	1:B:298:GLN:NE2	2.20	0.56
1:B:117:LEU:HD21	1:B:133:LEU:HD21	1.86	0.56
1:B:414:ALA:HB3	1:B:434:ASN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD22	1:A:293:ILE:HB	1.88	0.55
1:D:246:ASN:HD22	2:D:903:NAD:H8A	1.70	0.55
1:D:388:TYR:HB3	1:D:394:LYS:HA	1.89	0.55
1:B:293:ILE:HA	1:B:317:ALA:O	2.06	0.55
1:C:475:GLU:HG3	3:C:992:HOH:O	2.06	0.55
1:B:261:MSE:HG3	1:B:307:GLN:HG2	1.88	0.55
1:C:16:THR:HG22	1:C:18:LYS:N	2.17	0.55
1:B:18:LYS:O	1:B:28:THR:HA	2.06	0.55
1:D:200:ASN:HD22	1:D:200:ASN:H	1.55	0.55
1:D:247:THR:HA	1:D:298:GLN:NE2	2.21	0.55
1:A:32:TYR:HE2	1:B:529:GLU:OE2	1.89	0.55
1:B:354:ASN:H	1:B:354:ASN:ND2	2.05	0.55
1:B:468:LYS:HG2	1:B:471:ALA:HB2	1.89	0.55
1:C:458:ARG:HH11	1:C:458:ARG:HB2	1.72	0.55
1:C:329:LYS:HD3	1:C:416:ASP:OD2	2.07	0.55
1:A:428:ASN:HD21	1:A:430:ILE:HD11	1.72	0.55
1:A:203:ILE:HD13	1:A:222:ARG:CG	2.35	0.55
1:D:406:LYS:N	1:D:407:PRO:HD2	2.22	0.55
1:B:347:ALA:HB1	1:B:349:TYR:CE1	2.41	0.55
1:D:441:LEU:O	1:D:444:PRO:HD2	2.07	0.55
1:B:452:MSE:HE2	1:B:510:LEU:HD22	1.89	0.55
1:C:33:GLU:HG2	1:C:51:VAL:HG22	1.87	0.54
1:D:96:THR:HG23	1:D:98:GLU:N	2.15	0.54
1:A:468:LYS:HE3	1:A:471:ALA:CB	2.37	0.54
1:B:260:THR:HA	1:B:307:GLN:HE22	1.72	0.54
1:C:500:VAL:HG11	1:D:527:ARG:NE	2.22	0.54
1:C:216:LYS:HD2	1:C:271:ASP:HA	1.89	0.54
1:C:513:PHE:O	1:C:517:LEU:HG	2.07	0.54
1:A:251:VAL:HG12	1:A:299:ASN:ND2	2.22	0.54
1:B:356:ASP:O	1:B:360:LEU:HG	2.07	0.54
1:B:216:LYS:HD2	1:B:271:ASP:HA	1.90	0.54
1:A:445:LEU:HG	1:A:487:TRP:CD1	2.42	0.54
1:D:337:VAL:HG21	1:D:380:ILE:CG2	2.38	0.54
1:B:186:TYR:CE1	1:B:191:ILE:HD11	2.42	0.54
1:B:158:MSE:SE	1:B:176:MSE:HE2	2.58	0.54
1:A:158:MSE:HE2	1:A:176:MSE:HG3	1.88	0.54
1:D:468:LYS:HB3	1:D:468:LYS:NZ	2.22	0.54
1:D:527:ARG:HB2	1:D:531:ARG:NH1	2.22	0.54
1:A:153:ASP:OD2	1:A:155:TYR:HB3	2.07	0.54
1:B:329:LYS:HA	1:B:418:TYR:OH	2.06	0.54
1:B:96:THR:HG22	1:B:97:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:THR:HG22	1:A:448:ASP:OD1	2.07	0.54
1:A:530:GLU:HB2	1:B:497:PHE:CD2	2.43	0.54
1:A:73:LEU:HD11	1:A:154:LEU:HD11	1.90	0.54
1:A:242:LEU:CD2	1:A:293:ILE:HB	2.38	0.54
1:A:224:ARG:HH11	1:A:287:LEU:HB3	1.73	0.53
1:B:251:VAL:HG21	1:B:274:GLU:O	2.08	0.53
1:B:115:LEU:HD22	1:B:511:GLU:HG2	1.90	0.53
1:D:70:LEU:CD2	1:D:242:LEU:HB3	2.39	0.53
1:B:321:LEU:HD21	1:B:446:ILE:HG13	1.91	0.53
1:B:22:LYS:HG3	1:B:22:LYS:O	2.08	0.53
1:B:66:LEU:HB2	1:B:137:VAL:HG11	1.91	0.53
1:A:502:GLY:O	1:A:506:GLN:HG3	2.09	0.53
1:D:437:GLU:HB3	3:D:945:HOH:O	2.07	0.53
1:D:69:MSE:HE1	1:D:227:ILE:HG23	1.90	0.53
1:D:18:LYS:O	1:D:28:THR:HA	2.08	0.53
1:C:117:LEU:HD21	1:C:133:LEU:CD2	2.38	0.53
1:B:164:LEU:O	1:D:97:LYS:HG3	2.07	0.53
1:D:469:GLU:CD	1:D:469:GLU:H	2.11	0.53
1:D:310:GLU:HA	1:D:479:PRO:HG2	1.90	0.53
1:B:69:MSE:HE1	1:B:227:ILE:HG23	1.91	0.53
1:A:533:LEU:HD23	1:B:463:LYS:HZ1	1.73	0.53
1:D:150:ASN:HA	1:D:200:ASN:HD21	1.72	0.53
1:B:445:LEU:HG	1:B:487:TRP:CD1	2.41	0.53
1:C:458:ARG:CB	1:C:458:ARG:HH11	2.22	0.53
1:D:203:ILE:HD13	1:D:222:ARG:HG2	1.90	0.53
1:C:349:TYR:C	1:C:350:ASN:HD22	2.12	0.53
1:A:197:GLU:CD	1:A:197:GLU:H	2.12	0.53
1:C:468:LYS:HG2	1:C:471:ALA:HB2	1.90	0.53
1:B:350:ASN:HD22	1:B:350:ASN:N	2.06	0.53
1:D:208:LYS:HE3	1:D:208:LYS:N	2.24	0.53
1:A:432:ILE:HD12	1:B:432:ILE:HD12	1.89	0.53
1:C:516:LEU:C	1:C:516:LEU:HD12	2.29	0.53
1:D:70:LEU:HD23	1:D:242:LEU:HB3	1.90	0.53
1:B:70:LEU:CD2	1:B:242:LEU:HB3	2.39	0.53
1:C:101:LYS:HE2	3:C:923:HOH:O	2.09	0.53
1:B:354:ASN:ND2	1:B:357:GLY:H	2.07	0.53
1:A:305:LEU:HD23	1:A:308:LEU:HD23	1.91	0.53
1:C:187:TYR:OH	1:C:216:LYS:HG2	2.09	0.53
1:A:158:MSE:SE	1:A:176:MSE:HE2	2.59	0.53
1:A:220:LEU:HD21	1:A:287:LEU:HD12	1.91	0.52
1:A:248:GLU:OE2	1:A:277:PRO:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:MSE:HE1	1:D:227:ILE:CG1	2.37	0.52
1:D:282:ALA:O	1:D:286:ILE:HG13	2.09	0.52
1:D:151:ASN:H	1:D:200:ASN:ND2	2.07	0.52
1:A:14:VAL:HG22	1:B:47:VAL:HB	1.91	0.52
1:B:224:ARG:HD2	1:B:288:GLU:OE2	2.09	0.52
1:A:40:THR:HG22	1:A:42:SER:H	1.74	0.52
1:C:110:THR:HG22	1:C:448:ASP:OD1	2.09	0.52
1:C:192:ALA:HB3	1:C:359:ASN:HD22	1.74	0.52
1:B:346:ILE:O	1:B:398:HIS:HA	2.10	0.52
1:C:57:LYS:HB3	1:C:460:SER:OG	2.09	0.52
1:D:117:LEU:HD21	1:D:133:LEU:CD2	2.40	0.52
1:A:203:ILE:HG21	1:A:222:ARG:HG2	1.91	0.52
1:B:147:TRP:HB3	1:B:184:SER:HB2	1.92	0.52
1:B:394:LYS:HE3	3:B:967:HOH:O	2.09	0.52
1:D:452:MSE:HE2	1:D:510:LEU:HD22	1.91	0.52
1:A:251:VAL:HG21	1:A:274:GLU:O	2.10	0.52
1:A:247:THR:HA	1:A:298:GLN:OE1	2.10	0.52
1:A:492:LEU:CD2	1:A:492:LEU:H	2.18	0.52
1:C:246:ASN:HB3	1:C:359:ASN:OD1	2.10	0.52
1:B:421:GLU:HG2	3:B:1044:HOH:O	2.10	0.52
1:D:258:ASN:HB2	1:D:302:VAL:HG21	1.91	0.52
1:A:66:LEU:HB2	1:A:137:VAL:HG11	1.92	0.52
1:A:203:ILE:HG23	1:A:222:ARG:NH1	2.25	0.51
1:A:300:THR:HA	3:A:910:HOH:O	2.09	0.51
1:D:465:ASP:CG	1:D:466:PRO:HD2	2.31	0.51
1:A:515:ARG:NH1	1:A:523:GLN:HG2	2.25	0.51
1:A:407:PRO:HG3	1:D:397:ASP:HB2	1.92	0.51
1:B:22:LYS:HE2	1:B:27:LEU:HD11	1.92	0.51
1:D:111:GLN:HG3	3:D:918:HOH:O	2.09	0.51
1:B:150:ASN:HA	1:B:200:ASN:ND2	2.25	0.51
1:D:445:LEU:HG	1:D:487:TRP:CD1	2.42	0.51
1:C:247:THR:HA	1:C:298:GLN:NE2	2.25	0.51
1:A:261:MSE:CE	1:A:307:GLN:HG2	2.40	0.51
1:A:115:LEU:HD21	1:A:507:ARG:HH12	1.74	0.51
1:D:12:VAL:HG21	1:D:133:LEU:HD23	1.92	0.51
1:D:465:ASP:OD1	1:D:466:PRO:HD2	2.10	0.51
1:C:200:ASN:HD22	1:C:200:ASN:C	2.14	0.51
1:A:261:MSE:HE2	1:A:307:GLN:O	2.11	0.51
1:B:150:ASN:HA	1:B:200:ASN:HD21	1.75	0.51
1:D:216:LYS:HA	1:D:219:HIS:ND1	2.25	0.51
1:D:76:ASN:HD21	1:D:354:ASN:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HG22	1:B:448:ASP:OD1	2.11	0.51
1:A:242:LEU:HD13	1:A:243:TRP:N	2.26	0.51
1:C:242:LEU:CD2	1:C:293:ILE:HB	2.41	0.51
1:A:346:ILE:O	1:A:398:HIS:HA	2.11	0.51
1:A:300:THR:O	1:A:305:LEU:HD12	2.11	0.51
1:D:94:PHE:CD2	1:D:168:LEU:HD13	2.46	0.51
1:A:500:VAL:HA	3:A:1020:HOH:O	2.10	0.51
1:B:258:ASN:HD22	1:B:302:VAL:HG11	1.75	0.51
1:C:354:ASN:OD1	1:C:410:ASP:HA	2.10	0.51
1:C:351:HIS:CE1	1:C:413:VAL:HB	2.46	0.51
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.91	0.51
1:A:246:ASN:ND2	1:A:359:ASN:HB2	2.26	0.51
1:A:260:THR:HB	1:A:263:ASN:CG	2.31	0.51
1:A:69:MSE:HE1	1:A:227:ILE:CG1	2.38	0.50
1:B:261:MSE:HG3	1:B:307:GLN:CG	2.41	0.50
1:B:268:ILE:HG12	1:B:275:ILE:HG12	1.93	0.50
1:B:190:PHE:O	1:B:248:GLU:HA	2.12	0.50
1:D:225:ARG:HG3	1:D:225:ARG:HH11	1.77	0.50
1:B:192:ALA:O	1:B:195:GLN:HG2	2.10	0.50
1:B:310:GLU:HA	1:B:479:PRO:HG2	1.93	0.50
1:D:302:VAL:HB	1:D:303:PRO:HD2	1.94	0.50
1:A:63:PRO:HG2	1:A:238:LYS:HD2	1.92	0.50
1:A:533:LEU:HD23	1:B:463:LYS:HZ2	1.75	0.50
1:B:195:GLN:HA	1:B:195:GLN:NE2	2.26	0.50
1:A:389:ASN:C	1:A:389:ASN:HD22	2.15	0.50
1:D:447:ILE:O	1:D:451:VAL:HG23	2.12	0.50
1:C:482:THR:OG1	1:D:531:ARG:HG2	2.12	0.50
1:C:527:ARG:HB2	1:C:531:ARG:NH1	2.26	0.50
1:D:388:TYR:HA	1:D:393:GLY:O	2.12	0.50
1:C:246:ASN:HD22	2:C:902:NAD:H8A	1.76	0.50
1:C:261:MSE:CE	1:C:307:GLN:HG2	2.42	0.50
1:D:516:LEU:HD12	1:D:516:LEU:C	2.32	0.50
1:D:66:LEU:HB2	1:D:137:VAL:HG11	1.92	0.50
1:D:223:ILE:HD12	1:D:280:ILE:HG22	1.93	0.50
1:A:376:VAL:HG22	1:A:501:ASN:HB3	1.93	0.50
1:B:329:LYS:HD3	1:B:416:ASP:OD2	2.12	0.50
1:D:314:THR:HG22	1:D:315:PHE:N	2.27	0.50
1:A:66:LEU:HD13	1:A:68:ILE:HD11	1.94	0.50
1:B:200:ASN:H	1:B:200:ASN:HD22	1.58	0.50
1:C:260:THR:HB	1:C:262:GLU:OE2	2.11	0.49
1:C:406:LYS:N	1:C:407:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HB3	1:A:458:ARG:HB3	1.94	0.49
1:B:286:ILE:HA	1:B:314:THR:HG21	1.94	0.49
1:C:444:PRO:HG3	1:D:423:MSE:HE3	1.94	0.49
1:D:513:PHE:O	1:D:516:LEU:HG	2.12	0.49
1:A:316:ILE:O	1:A:317:ALA:HB2	2.12	0.49
1:B:272:HIS:ND1	1:B:274:GLU:HB2	2.27	0.49
1:C:166:TYR:O	1:C:170:GLN:HG2	2.13	0.49
1:C:67:GLY:C	1:C:68:ILE:HD12	2.33	0.49
1:A:388:TYR:HA	1:A:393:GLY:O	2.12	0.49
1:C:238:LYS:NZ	1:C:457:THR:HG21	2.27	0.49
1:C:394:LYS:O	1:C:394:LYS:HG2	2.11	0.49
1:A:321:LEU:HG	1:A:445:LEU:HD22	1.95	0.49
1:C:516:LEU:HD12	1:C:517:LEU:N	2.27	0.49
1:C:377:ILE:O	1:C:381:ILE:HG13	2.13	0.49
1:C:66:LEU:HB2	1:C:137:VAL:HG11	1.94	0.49
1:A:386:ILE:HD11	1:B:129:PRO:HB3	1.93	0.49
1:B:350:ASN:O	1:B:402:ILE:HA	2.13	0.49
1:A:531:ARG:HG2	1:B:482:THR:OG1	2.12	0.49
3:C:989:HOH:O	1:D:423:MSE:HG2	2.12	0.49
1:A:61:LYS:HZ2	1:A:61:LYS:HB3	1.77	0.49
1:B:261:MSE:HE2	1:B:307:GLN:HG2	1.95	0.49
1:C:192:ALA:HB3	1:C:359:ASN:ND2	2.28	0.49
1:C:447:ILE:O	1:C:451:VAL:HG23	2.13	0.49
1:A:96:THR:HG21	1:A:101:LYS:HD2	1.95	0.49
1:B:504:ASN:O	1:B:508:THR:HG23	2.12	0.49
1:D:205:LEU:HA	1:D:210:ASN:O	2.12	0.49
1:B:67:GLY:C	1:B:68:ILE:HD12	2.33	0.49
1:C:316:ILE:C	1:C:316:ILE:HD12	2.33	0.49
1:B:478:TYR:CE2	1:B:494:ARG:HB3	2.48	0.49
1:D:354:ASN:H	1:D:354:ASN:ND2	2.11	0.49
1:C:316:ILE:HD12	1:C:316:ILE:O	2.12	0.49
1:D:264:LEU:HD21	1:D:305:LEU:HG	1.95	0.49
1:B:470:ASP:HA	3:B:978:HOH:O	2.11	0.49
1:A:315:PHE:HD2	1:A:481:LEU:HD11	1.78	0.49
1:C:55:VAL:HG23	1:C:464:VAL:CG2	2.43	0.49
1:B:39:LYS:CD	1:B:39:LYS:H	2.20	0.48
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.94	0.48
1:D:357:GLY:HA3	1:D:404:TYR:CD1	2.48	0.48
1:B:15:VAL:HG23	1:B:15:VAL:O	2.13	0.48
1:C:350:ASN:O	1:C:402:ILE:HA	2.13	0.48
1:A:478:TYR:CD1	1:A:479:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:THR:HG22	2:D:903:NAD:H51N	1.96	0.48
1:B:260:THR:OG1	1:B:263:ASN:ND2	2.47	0.48
1:A:516:LEU:C	1:A:516:LEU:HD12	2.34	0.48
1:C:206:ASP:HB3	1:C:212:THR:HG21	1.96	0.48
1:D:437:GLU:HG3	1:D:440:LEU:CD1	2.25	0.48
1:B:244:THR:HG22	2:B:901:NAD:H51N	1.95	0.48
1:D:67:GLY:C	1:D:68:ILE:HD12	2.33	0.48
1:B:195:GLN:NE2	1:B:198:ARG:HD3	2.28	0.48
1:B:354:ASN:H	1:B:354:ASN:HD22	1.61	0.48
1:A:305:LEU:O	1:A:308:LEU:HB3	2.13	0.48
1:D:360:LEU:HD13	1:D:402:ILE:HG21	1.96	0.48
1:B:354:ASN:HD22	1:B:354:ASN:N	2.11	0.48
1:C:238:LYS:CE	1:C:457:THR:HG21	2.43	0.48
1:A:468:LYS:HE3	1:A:471:ALA:HB1	1.94	0.48
1:D:376:VAL:HG22	1:D:501:ASN:HB3	1.96	0.48
1:D:220:LEU:HD23	1:D:220:LEU:C	2.33	0.48
1:C:423:MSE:HE3	1:D:444:PRO:CG	2.20	0.48
1:D:446:ILE:O	1:D:450:LEU:HG	2.14	0.48
1:C:375:SER:HB2	1:C:378:ASP:OD2	2.14	0.48
1:C:203:ILE:HG21	1:C:222:ARG:HG2	1.96	0.48
1:D:58:LEU:HD22	1:D:134:LEU:HD13	1.94	0.48
1:A:423:MSE:HE3	1:B:444:PRO:HG3	1.94	0.48
1:D:129:PRO:HG2	1:D:132:SER:CB	2.40	0.48
1:B:96:THR:CG2	1:B:97:LYS:N	2.77	0.48
1:C:388:TYR:HA	1:C:393:GLY:O	2.14	0.48
1:C:302:VAL:O	1:C:306:VAL:HG23	2.13	0.47
1:A:334:GLN:NE2	1:A:380:ILE:HG12	2.28	0.47
1:A:337:VAL:HG21	1:A:380:ILE:HG21	1.96	0.47
1:A:291:PRO:HB3	1:A:315:PHE:HB2	1.95	0.47
1:D:69:MSE:HA	1:D:145:SER:O	2.14	0.47
1:A:323:SER:O	1:A:327:LYS:HG3	2.14	0.47
1:A:332:LEU:HD11	1:A:432:ILE:HD11	1.96	0.47
1:C:375:SER:HB3	3:C:929:HOH:O	2.14	0.47
1:D:322:LYS:HG2	1:D:327:LYS:HG3	1.95	0.47
1:D:147:TRP:HB3	1:D:184:SER:HB2	1.95	0.47
1:C:203:ILE:HD13	1:C:222:ARG:CG	2.44	0.47
1:C:18:LYS:HE3	3:C:1020:HOH:O	2.15	0.47
1:A:527:ARG:HD3	3:A:979:HOH:O	2.13	0.47
1:A:286:ILE:HA	1:A:314:THR:HG21	1.95	0.47
1:A:325:GLN:OE1	1:A:328:LEU:HD12	2.14	0.47
1:D:16:THR:HG23	3:D:1018:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLY:C	1:A:68:ILE:HD12	2.34	0.47
1:B:516:LEU:HD12	1:B:516:LEU:C	2.34	0.47
1:A:263:ASN:HD22	1:A:263:ASN:N	2.12	0.47
1:A:356:ASP:O	1:A:360:LEU:HG	2.15	0.47
1:B:65:LYS:HD3	1:B:141:ASP:HB3	1.95	0.47
1:D:243:TRP:CE2	1:D:245:ALA:HB3	2.50	0.47
1:B:441:LEU:C	1:B:444:PRO:HD2	2.35	0.47
1:D:116:LYS:HZ2	1:D:527:ARG:HH22	1.63	0.47
1:A:243:TRP:CE2	1:A:245:ALA:HB3	2.49	0.47
1:D:478:TYR:CD1	1:D:479:PRO:HD2	2.50	0.47
1:A:158:MSE:CE	1:A:176:MSE:HG3	2.44	0.47
1:B:447:ILE:O	1:B:451:VAL:HG23	2.14	0.47
1:D:350:ASN:HB3	1:D:412:LYS:HE2	1.97	0.47
1:D:218:THR:HA	1:D:221:GLN:NE2	2.26	0.47
1:C:454:GLU:O	1:C:457:THR:HB	2.14	0.47
1:A:350:ASN:O	1:A:402:ILE:HA	2.15	0.47
1:D:23:ASP:O	1:D:25:GLU:HG3	2.15	0.47
1:B:445:LEU:HD23	1:B:445:LEU:C	2.36	0.47
1:C:12:VAL:HG21	1:C:133:LEU:HD23	1.97	0.47
1:B:513:PHE:O	1:B:517:LEU:HG	2.15	0.47
1:A:431:SER:HB2	1:B:433:HIS:HB3	1.97	0.47
1:B:63:PRO:CG	1:B:238:LYS:HG3	2.45	0.46
1:D:153:ASP:OD2	1:D:155:TYR:HB3	2.15	0.46
1:C:158:MSE:SE	1:C:176:MSE:HE2	2.64	0.46
1:A:69:MSE:HE1	1:A:227:ILE:HG23	1.97	0.46
1:A:283:ALA:O	1:A:287:LEU:HG	2.15	0.46
1:C:352:LEU:HD22	1:C:354:ASN:HD22	1.79	0.46
1:C:205:LEU:HA	1:C:210:ASN:O	2.15	0.46
1:B:297:PRO:HD3	1:B:320:ASP:OD2	2.14	0.46
1:A:318:GLY:H	1:A:492:LEU:HD21	1.79	0.46
1:B:242:LEU:HD12	1:B:244:THR:OG1	2.14	0.46
1:B:116:LYS:HD3	1:B:523:GLN:NE2	2.28	0.46
1:A:185:ILE:CD1	1:A:223:ILE:HD11	2.45	0.46
1:C:47:VAL:HG11	1:D:520:LEU:HD21	1.98	0.46
1:A:350:ASN:N	1:A:350:ASN:HD22	2.14	0.46
1:B:184:SER:O	1:B:202:CYS:HA	2.14	0.46
1:A:473:LYS:HG2	1:A:474:PHE:H	1.80	0.46
1:C:527:ARG:H	1:C:531:ARG:HH11	1.64	0.46
1:D:257:VAL:HG11	1:D:274:GLU:OE1	2.16	0.46
1:D:260:THR:HA	1:D:307:GLN:NE2	2.31	0.46
1:D:73:LEU:CD2	1:D:154:LEU:HD11	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:PHE:O	1:C:516:LEU:HG	2.14	0.46
1:A:272:HIS:HB3	1:A:275:ILE:HD13	1.96	0.46
1:C:432:ILE:HD12	1:D:432:ILE:HD12	1.95	0.46
1:A:406:LYS:N	1:A:407:PRO:CD	2.77	0.46
1:C:359:ASN:HB2	3:C:952:HOH:O	2.15	0.46
1:B:243:TRP:CZ2	1:B:245:ALA:HB3	2.51	0.46
1:B:82:VAL:HG21	1:B:154:LEU:CD1	2.45	0.46
1:C:37:VAL:HG22	1:C:47:VAL:HG22	1.98	0.46
1:D:515:ARG:HB3	1:D:520:LEU:HB2	1.98	0.46
1:A:447:ILE:O	1:A:451:VAL:HG23	2.16	0.46
1:B:69:MSE:CE	1:B:227:ILE:HG12	2.37	0.46
1:C:389:ASN:HD22	1:C:389:ASN:C	2.18	0.45
1:C:197:GLU:CD	1:C:197:GLU:H	2.18	0.45
1:A:273:GLU:O	1:A:273:GLU:OE1	2.34	0.45
1:A:148:ASP:HA	2:A:900:NAD:N3A	2.31	0.45
1:A:18:LYS:O	1:A:28:THR:HA	2.16	0.45
1:B:248:GLU:H	1:B:298:GLN:NE2	2.14	0.45
1:B:16:THR:CG2	1:B:18:LYS:HG3	2.46	0.45
1:D:377:ILE:O	1:D:381:ILE:HG13	2.15	0.45
1:A:452:MSE:HE2	1:A:510:LEU:HD22	1.98	0.45
1:D:158:MSE:SE	1:D:176:MSE:HE2	2.66	0.45
1:D:354:ASN:HD22	1:D:354:ASN:N	2.13	0.45
1:C:497:PHE:CD2	1:D:530:GLU:HB2	2.51	0.45
1:B:223:ILE:O	1:B:227:ILE:HG13	2.17	0.45
1:C:525:GLU:O	1:C:527:ARG:HG3	2.17	0.45
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.51	0.45
1:D:243:TRP:CZ2	1:D:245:ALA:HB3	2.52	0.45
1:D:452:MSE:HG3	1:D:487:TRP:CH2	2.51	0.45
1:C:248:GLU:H	1:C:298:GLN:NE2	2.15	0.45
1:A:116:LYS:HB3	1:A:523:GLN:HE22	1.81	0.45
1:B:225:ARG:HD3	3:B:971:HOH:O	2.17	0.45
1:A:520:LEU:HA	1:A:521:PRO:HD3	1.85	0.45
1:C:105:TYR:HA	1:D:423:MSE:HE2	1.99	0.45
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.17	0.45
1:A:441:LEU:C	1:A:444:PRO:HD2	2.37	0.45
1:C:147:TRP:CD2	1:C:281:PHE:HE2	2.35	0.45
1:B:97:LYS:HB3	1:B:98:GLU:OE2	2.16	0.45
1:C:264:LEU:O	1:C:268:ILE:HG13	2.17	0.45
1:B:293:ILE:HD11	1:B:453:THR:OG1	2.17	0.45
1:C:500:VAL:HG11	1:D:527:ARG:HE	1.81	0.45
1:A:224:ARG:HD3	1:A:287:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:O	1:A:221:GLN:HG3	2.17	0.45
1:A:465:ASP:HB3	1:A:468:LYS:O	2.16	0.45
1:D:351:HIS:HB2	1:D:403:LYS:O	2.16	0.45
1:C:376:VAL:HG22	1:C:501:ASN:CB	2.40	0.45
1:C:389:ASN:ND2	1:C:392:LEU:N	2.62	0.45
1:D:276:ALA:HB1	1:D:277:PRO:HD2	1.99	0.45
1:C:33:GLU:HA	1:C:50:THR:O	2.16	0.45
1:D:376:VAL:HG13	1:D:501:ASN:HB2	1.99	0.45
1:B:326:THR:HG21	1:B:489:LYS:HG2	1.99	0.45
1:B:377:ILE:O	1:B:381:ILE:HG13	2.16	0.45
1:B:67:GLY:O	1:B:239:VAL:HA	2.17	0.45
1:B:446:ILE:O	1:B:450:LEU:HG	2.17	0.45
1:D:154:LEU:HD23	1:D:179:VAL:HG12	1.99	0.45
1:B:220:LEU:O	1:B:220:LEU:HD23	2.17	0.45
1:A:36:VAL:HA	1:B:119:ILE:O	2.17	0.45
1:D:115:LEU:HD12	1:D:133:LEU:HD11	1.98	0.44
1:D:246:ASN:HB3	1:D:359:ASN:HD21	1.82	0.44
1:A:276:ALA:HB1	1:A:277:PRO:HD2	1.99	0.44
1:A:518:ILE:HD11	1:A:520:LEU:HD12	1.99	0.44
1:C:294:ASN:ND2	1:C:319:ASP:HA	2.31	0.44
1:C:243:TRP:CE2	1:C:245:ALA:HB3	2.52	0.44
1:C:71:ILE:HG21	1:C:243:TRP:CE3	2.53	0.44
1:C:355:ASN:HB3	2:C:902:NAD:O1A	2.16	0.44
1:C:203:ILE:HD13	1:C:222:ARG:HG2	1.98	0.44
1:C:69:MSE:HE1	1:C:227:ILE:CG1	2.34	0.44
1:B:441:LEU:O	1:B:444:PRO:HD2	2.17	0.44
1:B:208:LYS:CD	1:B:208:LYS:H	2.31	0.44
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.52	0.44
1:B:200:ASN:N	1:B:200:ASN:HD22	2.13	0.44
1:A:316:ILE:O	1:A:480:VAL:HA	2.17	0.44
1:B:298:GLN:C	1:B:300:THR:H	2.21	0.44
1:A:350:ASN:HB2	1:A:402:ILE:HG12	1.98	0.44
1:D:272:HIS:HE1	1:D:274:GLU:HG3	1.82	0.44
1:D:272:HIS:HB3	1:D:275:ILE:HD13	1.99	0.44
1:C:109:MSE:HB2	1:C:109:MSE:HE3	1.87	0.44
1:A:47:VAL:HB	1:B:14:VAL:HG22	1.98	0.44
1:A:513:PHE:O	1:A:516:LEU:HG	2.16	0.44
1:A:461:TYR:CE2	1:B:532:LEU:HG	2.52	0.44
1:D:351:HIS:CE1	1:D:413:VAL:HB	2.53	0.44
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.33	0.44
1:D:242:LEU:HD13	1:D:243:TRP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:GLU:HG2	1:B:437:GLU:H	1.36	0.44
1:C:37:VAL:HG12	1:C:38:THR:N	2.32	0.44
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.99	0.44
1:C:298:GLN:C	1:C:300:THR:H	2.21	0.44
1:D:437:GLU:H	1:D:437:GLU:HG2	1.45	0.44
1:A:533:LEU:HD13	1:A:533:LEU:C	2.38	0.44
1:C:251:VAL:O	1:C:251:VAL:HG13	2.18	0.44
1:B:191:ILE:HD12	1:B:195:GLN:HG3	2.00	0.44
1:B:325:GLN:HG2	1:B:414:ALA:HB1	1.99	0.44
1:D:323:SER:O	1:D:327:LYS:HG3	2.18	0.44
1:A:120:ASP:OD2	1:A:124:ASN:N	2.51	0.44
1:C:521:PRO:HG2	1:D:33:GLU:HB3	1.99	0.44
1:C:52:GLN:HG3	1:C:54:TYR:CE1	2.53	0.44
1:A:73:LEU:HD13	1:A:73:LEU:O	2.17	0.44
1:B:109:MSE:HG3	1:B:110:THR:N	2.33	0.44
1:A:69:MSE:CE	1:A:227:ILE:HG12	2.41	0.44
1:A:327:LYS:HE2	1:B:335:PHE:CE1	2.52	0.44
1:A:344:VAL:HG11	1:A:421:GLU:HG3	2.00	0.44
1:C:337:VAL:HG21	1:C:380:ILE:CG2	2.48	0.44
1:B:68:ILE:HG12	1:B:450:LEU:HD13	1.99	0.44
1:A:327:LYS:HE2	1:B:335:PHE:HE1	1.82	0.44
1:B:259:ASP:HA	1:B:303:PRO:HG2	2.00	0.44
1:B:221:GLN:HG2	3:B:984:HOH:O	2.17	0.44
1:B:351:HIS:HD2	1:B:405:MSE:HB2	1.82	0.43
1:C:257:VAL:HG23	1:C:258:ASN:H	1.83	0.43
1:A:224:ARG:HG2	1:A:284:ALA:HB1	2.00	0.43
1:B:57:LYS:HB2	1:B:474:PHE:CE2	2.53	0.43
1:A:461:TYR:O	1:A:474:PHE:HA	2.17	0.43
1:A:529:GLU:OE1	1:A:529:GLU:N	2.49	0.43
1:C:115:LEU:O	1:C:127:TYR:HA	2.17	0.43
1:D:494:ARG:HG3	1:D:497:PHE:CD1	2.53	0.43
1:C:70:LEU:CD2	1:C:242:LEU:HB3	2.48	0.43
1:D:58:LEU:CD2	1:D:134:LEU:HD13	2.47	0.43
1:C:362:ALA:HB1	1:C:363:PRO:HD2	2.00	0.43
1:C:18:LYS:O	1:C:28:THR:HA	2.18	0.43
1:C:257:VAL:HG23	1:C:258:ASN:N	2.33	0.43
1:A:407:PRO:HD3	1:D:397:ASP:OD2	2.19	0.43
1:C:225:ARG:HH11	1:C:229:ASN:HB2	1.82	0.43
1:D:40:THR:CG2	1:D:41:ALA:N	2.82	0.43
1:C:242:LEU:HD13	1:C:243:TRP:N	2.33	0.43
1:D:203:ILE:HD11	3:D:965:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ILE:HD11	3:C:978:HOH:O	2.19	0.43
1:C:40:THR:HG22	1:C:41:ALA:N	2.33	0.43
1:D:16:THR:HB	3:D:975:HOH:O	2.19	0.43
1:C:459:VAL:HG11	1:C:513:PHE:HZ	1.83	0.43
1:C:159:GLN:HG2	3:C:956:HOH:O	2.18	0.43
1:B:265:LEU:O	1:B:269:LYS:HG3	2.19	0.43
1:B:80:THR:HG22	1:B:443:THR:HG21	2.01	0.43
1:C:527:ARG:H	1:C:531:ARG:NH1	2.16	0.43
1:A:68:ILE:HG12	1:A:450:LEU:HD13	2.00	0.43
1:D:354:ASN:H	1:D:354:ASN:HD22	1.66	0.43
1:D:350:ASN:HD22	1:D:350:ASN:N	2.15	0.43
1:A:90:HIS:CD2	1:A:175:LYS:HE2	2.53	0.43
1:C:318:GLY:HA2	1:C:488:LEU:CD2	2.46	0.43
1:B:352:LEU:CD1	1:B:357:GLY:HA3	2.48	0.43
1:B:513:PHE:O	1:B:516:LEU:HG	2.19	0.43
1:A:204:ASN:ND2	1:A:211:VAL:HG13	2.33	0.43
1:D:189:ASP:O	1:D:249:ARG:NH1	2.52	0.43
1:C:507:ARG:NH1	1:C:511:GLU:OE1	2.52	0.43
1:B:350:ASN:N	1:B:350:ASN:ND2	2.66	0.43
1:D:200:ASN:H	1:D:200:ASN:ND2	2.16	0.43
1:B:115:LEU:CD2	1:B:511:GLU:HG2	2.49	0.43
1:D:314:THR:HG22	1:D:315:PHE:H	1.84	0.43
1:A:437:GLU:HG2	1:A:437:GLU:H	1.59	0.42
1:B:449:LEU:HD21	1:B:487:TRP:HB2	2.00	0.42
1:B:277:PRO:O	1:B:281:PHE:HD1	2.01	0.42
1:D:523:GLN:HG3	3:D:923:HOH:O	2.19	0.42
1:D:381:ILE:HG23	1:D:388:TYR:CG	2.54	0.42
1:C:276:ALA:HB1	1:C:277:PRO:HD2	2.01	0.42
1:C:81:LEU:HD23	1:C:81:LEU:C	2.40	0.42
1:A:346:ILE:HD12	1:A:377:ILE:HD13	2.01	0.42
1:B:251:VAL:HG22	1:B:274:GLU:HG3	2.01	0.42
1:D:183:PRO:HG2	3:D:965:HOH:O	2.18	0.42
1:D:203:ILE:HD13	1:D:222:ARG:CG	2.49	0.42
1:A:47:VAL:O	1:B:15:VAL:HG22	2.19	0.42
1:B:190:PHE:CE2	1:B:276:ALA:HB2	2.53	0.42
1:B:347:ALA:O	1:B:416:ASP:HA	2.19	0.42
1:D:342:LYS:HG3	1:D:388:TYR:CZ	2.54	0.42
1:A:398:HIS:HB2	3:A:970:HOH:O	2.19	0.42
1:B:19:CYS:HA	1:B:27:LEU:O	2.19	0.42
1:A:59:ASP:O	1:A:458:ARG:HD2	2.20	0.42
1:B:389:ASN:HD22	1:B:391:LYS:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HA	1:C:219:HIS:ND1	2.34	0.42
1:B:405:MSE:HB3	1:B:408:VAL:CG2	2.50	0.42
1:A:445:LEU:HD23	1:A:445:LEU:C	2.40	0.42
1:B:412:LYS:HB2	1:B:438:ASP:HB2	2.01	0.42
1:D:408:VAL:HG12	1:D:411:SER:HB3	2.00	0.42
1:B:206:ASP:OD2	1:B:210:ASN:HB2	2.20	0.42
1:D:231:LYS:HG2	1:D:239:VAL:HG21	2.01	0.42
1:A:318:GLY:HA2	1:A:488:LEU:HD22	2.00	0.42
1:A:187:TYR:OH	1:A:216:LYS:HG2	2.19	0.42
1:C:337:VAL:HG21	1:C:380:ILE:HG21	2.01	0.42
1:C:532:LEU:HG	1:D:461:TYR:CE2	2.54	0.42
1:C:16:THR:HG22	1:C:17:ASP:N	2.35	0.42
1:B:16:THR:HG22	1:B:18:LYS:HG3	2.02	0.42
1:A:531:ARG:HH11	1:A:531:ARG:HG3	1.85	0.42
1:B:406:LYS:N	1:B:407:PRO:CD	2.83	0.42
1:D:443:THR:N	1:D:444:PRO:CD	2.83	0.42
1:D:360:LEU:HD13	1:D:402:ILE:CG2	2.50	0.42
1:D:329:LYS:HD2	1:D:418:TYR:OH	2.19	0.42
1:B:354:ASN:ND2	1:B:354:ASN:N	2.65	0.42
1:C:286:ILE:HA	1:C:314:THR:HG21	2.02	0.42
1:C:524:ASN:C	1:C:526:LEU:H	2.23	0.42
1:C:440:LEU:O	1:C:444:PRO:HG2	2.19	0.42
1:A:310:GLU:HA	1:A:479:PRO:HG2	2.02	0.42
1:C:192:ALA:HB2	3:C:968:HOH:O	2.20	0.42
1:B:125:ASP:CG	1:B:527:ARG:HH22	2.22	0.42
1:C:134:LEU:HB3	1:C:135:PRO:HD2	2.02	0.42
1:D:59:ASP:HB3	1:D:458:ARG:HB3	2.01	0.42
1:C:21:TYR:CZ	1:C:26:LEU:HD13	2.55	0.42
1:D:358:TYR:O	1:D:362:ALA:HB2	2.20	0.42
1:A:494:ARG:HD2	1:B:530:GLU:O	2.19	0.41
1:D:68:ILE:N	1:D:68:ILE:HD12	2.34	0.41
1:C:238:LYS:HZ1	1:C:457:THR:HG21	1.85	0.41
1:A:256:GLY:HA2	1:A:263:ASN:OD1	2.20	0.41
1:C:497:PHE:CE2	1:D:530:GLU:HB2	2.55	0.41
1:C:69:MSE:HE1	1:C:227:ILE:HG23	2.02	0.41
1:B:405:MSE:HB3	1:B:408:VAL:HG23	2.01	0.41
1:C:70:LEU:HD11	1:C:81:LEU:HD13	2.02	0.41
1:A:428:ASN:OD1	1:B:436:CYS:HB3	2.19	0.41
1:A:251:VAL:HG12	1:A:299:ASN:HD21	1.82	0.41
1:A:122:GLU:CD	1:A:122:GLU:H	2.23	0.41
1:C:116:LYS:HD3	1:C:523:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD22	1:A:354:ASN:HD22	1.84	0.41
1:D:350:ASN:HB3	1:D:412:LYS:CE	2.51	0.41
1:C:158:MSE:HE2	1:C:176:MSE:HG3	2.01	0.41
1:C:428:ASN:HD21	1:C:430:ILE:HD11	1.86	0.41
1:D:482:THR:C	1:D:484:LEU:H	2.23	0.41
1:C:532:LEU:HG	1:D:461:TYR:CD2	2.55	0.41
1:C:462:LYS:HE3	1:C:472:GLY:O	2.20	0.41
1:C:291:PRO:HA	1:C:315:PHE:O	2.20	0.41
1:C:43:GLY:O	1:D:10:THR:HA	2.19	0.41
1:B:81:LEU:C	1:B:81:LEU:HD23	2.41	0.41
1:A:423:MSE:CE	1:B:444:PRO:HG3	2.50	0.41
1:D:350:ASN:ND2	1:D:350:ASN:N	2.68	0.41
1:C:524:ASN:O	1:C:526:LEU:N	2.54	0.41
1:D:120:ASP:OD2	1:D:124:ASN:N	2.50	0.41
1:C:492:LEU:CD2	1:C:492:LEU:H	2.29	0.41
1:D:190:PHE:CE2	1:D:276:ALA:HB2	2.55	0.41
1:A:337:VAL:HG21	1:A:380:ILE:HG22	2.01	0.41
1:D:349:TYR:C	1:D:350:ASN:HD22	2.24	0.41
1:B:37:VAL:HG12	1:B:38:THR:N	2.36	0.41
1:C:318:GLY:HA2	1:C:488:LEU:HD13	2.03	0.41
1:A:332:LEU:HD13	1:A:418:TYR:CE1	2.55	0.41
1:A:500:VAL:HG21	1:B:527:ARG:NE	2.35	0.41
1:C:212:THR:HA	3:C:997:HOH:O	2.21	0.41
1:D:194:ASN:HB3	1:D:358:TYR:HD2	1.86	0.41
1:A:350:ASN:N	1:A:350:ASN:ND2	2.68	0.41
1:C:520:LEU:HA	1:C:521:PRO:HD3	1.89	0.41
1:B:58:LEU:HD22	1:B:134:LEU:HD13	2.02	0.41
1:D:175:LYS:HG3	3:D:1020:HOH:O	2.20	0.41
1:D:293:ILE:HD11	1:D:453:THR:OG1	2.21	0.41
1:C:443:THR:N	1:C:444:PRO:CD	2.83	0.41
1:A:294:ASN:O	1:A:319:ASP:N	2.52	0.41
1:C:243:TRP:CZ2	1:C:245:ALA:HB3	2.56	0.41
1:C:349:TYR:C	1:C:350:ASN:ND2	2.73	0.41
1:A:244:THR:O	2:A:900:NAD:H51N	2.21	0.41
1:C:408:VAL:HG12	1:C:408:VAL:O	2.21	0.41
1:C:231:LYS:O	1:C:234:ASN:O	2.39	0.41
1:C:234:ASN:HB2	1:C:236:LEU:HG	2.03	0.41
1:A:483:PHE:HA	1:A:483:PHE:HD2	1.76	0.41
1:B:68:ILE:HD12	1:B:68:ILE:N	2.36	0.41
1:A:318:GLY:HA2	1:A:488:LEU:CD2	2.51	0.41
1:C:478:TYR:O	1:C:480:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LEU:CD2	1:D:507:ARG:HH12	2.33	0.41
1:D:329:LYS:HA	1:D:418:TYR:OH	2.21	0.41
1:D:275:ILE:N	1:D:275:ILE:HD12	2.36	0.41
1:D:354:ASN:N	1:D:354:ASN:ND2	2.69	0.41
1:A:344:VAL:CG1	1:A:421:GLU:HG3	2.51	0.41
1:D:249:ARG:HG3	1:D:249:ARG:O	2.21	0.41
1:D:69:MSE:CE	1:D:227:ILE:HG12	2.41	0.40
1:C:482:THR:C	1:C:484:LEU:H	2.24	0.40
1:C:187:TYR:CD1	1:C:277:PRO:HD3	2.56	0.40
1:A:220:LEU:HD23	1:A:224:ARG:HG3	2.04	0.40
1:D:478:TYR:CZ	1:D:494:ARG:HB3	2.55	0.40
1:C:408:VAL:O	1:C:411:SER:HB2	2.22	0.40
1:A:320:ASP:OD1	1:A:489:LYS:HD3	2.20	0.40
1:B:491:PRO:HG2	1:B:499:PRO:HB2	2.03	0.40
1:D:109:MSE:HA	1:D:113:SER:HB2	2.03	0.40
1:D:286:ILE:HA	1:D:314:THR:HG21	2.03	0.40
1:B:71:ILE:HG21	1:B:243:TRP:CE3	2.57	0.40
1:B:243:TRP:CE2	1:B:245:ALA:HB3	2.57	0.40
1:D:122:GLU:HB2	3:D:972:HOH:O	2.20	0.40
1:B:69:MSE:CE	1:B:227:ILE:HG23	2.51	0.40
1:A:318:GLY:N	1:A:492:LEU:HD21	2.36	0.40
1:A:69:MSE:HE1	1:A:227:ILE:HA	2.03	0.40
1:B:318:GLY:O	1:B:319:ASP:CB	2.66	0.40
1:A:220:LEU:C	1:A:220:LEU:HD23	2.42	0.40
1:D:97:LYS:HG2	1:D:97:LYS:O	2.22	0.40
1:D:465:ASP:C	1:D:467:VAL:H	2.24	0.40
1:B:389:ASN:O	1:B:393:GLY:N	2.54	0.40
1:D:408:VAL:HG12	1:D:411:SER:O	2.22	0.40
1:D:206:ASP:HB3	1:D:212:THR:HG21	2.03	0.40
1:A:401:VAL:HG11	1:D:401:VAL:HG21	2.03	0.40
1:C:250:TYR:HA	1:C:299:ASN:OD1	2.21	0.40
1:C:437:GLU:CG	1:C:440:LEU:HD12	2.37	0.40
1:B:458:ARG:HB2	1:B:458:ARG:NH1	2.37	0.40
1:C:184:SER:O	1:C:202:CYS:HA	2.21	0.40
1:B:25:GLU:OE2	1:B:57:LYS:HD3	2.20	0.40
1:D:33:GLU:HA	1:D:50:THR:O	2.21	0.40
1:D:493:THR:HG21	1:D:499:PRO:HB3	2.03	0.40
1:C:334:GLN:HB2	3:C:961:HOH:O	2.22	0.40
1:B:319:ASP:HB3	1:B:490:ALA:HB3	2.04	0.40
1:C:381:ILE:HG23	1:C:388:TYR:CG	2.57	0.40
1:A:265:LEU:O	1:A:268:ILE:HB	2.21	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	510/533 (96%)	471 (92%)	36 (7%)	3 (1%)	30	54
1	B	510/533 (96%)	462 (91%)	41 (8%)	7 (1%)	14	31
1	C	510/533 (96%)	468 (92%)	37 (7%)	5 (1%)	19	41
1	D	510/533 (96%)	456 (89%)	50 (10%)	4 (1%)	24	47
All	All	2040/2132 (96%)	1857 (91%)	164 (8%)	19 (1%)	21	44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	ALA
1	B	319	ASP
1	D	320	ASP
1	D	469	GLU
1	C	319	ASP
1	B	322	LYS
1	C	525	GLU
1	B	261	MSE
1	B	320	ASP
1	D	59	ASP
1	A	319	ASP
1	A	320	ASP
1	B	148	ASP
1	C	320	ASP
1	C	479	PRO
1	D	49	PRO
1	A	479	PRO
1	B	149	ILE
1	C	49	PRO

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	452/461 (98%)	431 (95%)	21 (5%)	33	61
1	B	452/461 (98%)	427 (94%)	25 (6%)	27	51
1	C	452/461 (98%)	430 (95%)	22 (5%)	31	58
1	D	452/461 (98%)	428 (95%)	24 (5%)	28	54
All	All	1808/1844 (98%)	1716 (95%)	92 (5%)	29	55

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	24	ASN
1	A	34	ASN
1	A	44	ARG
1	A	66	LEU
1	A	109	MSE
1	A	197	GLU
1	A	244	THR
1	A	273	GLU
1	A	319	ASP
1	A	332	LEU
1	A	338	ASP
1	A	352	LEU
1	A	358	TYR
1	A	389	ASN
1	A	416	ASP
1	A	437	GLU
1	A	454	GLU
1	A	475	GLU
1	A	479	PRO
1	A	483	PHE
1	B	23	ASP
1	B	24	ASN
1	B	34	ASN

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Mol	Chain	Res	Type
1	B	39	LYS
1	B	64	GLU
1	B	66	LEU
1	B	73	LEU
1	B	109	MSE
1	B	180	LYS
1	B	200	ASN
1	B	233	GLU
1	B	242	LEU
1	B	249	ARG
1	B	320	ASP
1	B	352	LEU
1	B	354	ASN
1	B	378	ASP
1	B	405	MSE
1	B	437	GLU
1	B	454	GLU
1	B	465	ASP
1	B	475	GLU
1	B	483	PHE
1	B	492	LEU
1	B	533	LEU
1	C	22	LYS
1	C	34	ASN
1	C	50	THR
1	C	66	LEU
1	C	73	LEU
1	C	109	MSE
1	C	197	GLU
1	C	200	ASN
1	C	249	ARG
1	C	252	GLU
1	C	273	GLU
1	C	319	ASP
1	C	325	GLN
1	C	328	LEU
1	C	352	LEU
1	C	359	ASN
1	C	389	ASN
1	C	405	MSE
1	C	454	GLU
1	C	457	THR

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Mol	Chain	Res	Type
1	C	475	GLU
1	C	479	PRO
1	D	11	SER
1	D	24	ASN
1	D	66	LEU
1	D	73	LEU
1	D	109	MSE
1	D	111	GLN
1	D	200	ASN
1	D	208	LYS
1	D	237	ASP
1	D	242	LEU
1	D	249	ARG
1	D	266	GLN
1	D	273	GLU
1	D	328	LEU
1	D	338	ASP
1	D	352	LEU
1	D	354	ASN
1	D	359	ASN
1	D	390	ASP
1	D	437	GLU
1	D	445	LEU
1	D	454	GLU
1	D	483	PHE
1	D	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	ASN
1	A	159	GLN
1	A	194	ASN
1	A	221	GLN
1	A	263	ASN
1	A	266	GLN
1	A	307	GLN
1	A	334	GLN
1	A	350	ASN
1	A	351	HIS
1	A	389	ASN

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Mol	Chain	Res	Type
1	B	24	ASN
1	B	34	ASN
1	B	52	GLN
1	B	95	GLN
1	B	159	GLN
1	B	195	GLN
1	B	200	ASN
1	B	221	GLN
1	B	246	ASN
1	B	263	ASN
1	B	298	GLN
1	B	307	GLN
1	B	334	GLN
1	B	350	ASN
1	B	351	HIS
1	B	354	ASN
1	B	389	ASN
1	B	428	ASN
1	B	433	HIS
1	B	523	GLN
1	C	34	ASN
1	C	77	ASN
1	C	95	GLN
1	C	159	GLN
1	C	170	GLN
1	C	194	ASN
1	C	200	ASN
1	C	246	ASN
1	C	298	GLN
1	C	307	GLN
1	C	325	GLN
1	C	350	ASN
1	C	354	ASN
1	C	359	ASN
1	C	389	ASN
1	C	524	ASN
1	D	24	ASN
1	D	34	ASN
1	D	111	GLN
1	D	124	ASN
1	D	151	ASN
1	D	200	ASN

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Mol	Chain	Res	Type
1	D	221	GLN
1	D	228	GLN
1	D	246	ASN
1	D	263	ASN
1	D	298	GLN
1	D	307	GLN
1	D	334	GLN
1	D	350	ASN
1	D	351	HIS
1	D	354	ASN
1	D	359	ASN
1	D	433	HIS
1	D	524	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
2	NAD	A	900	-	38,48,48	2.35	8 (21%)	47,73,73	1.94	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	B	901	-	38,48,48	2.39	8 (21%)	47,73,73	1.90	12 (25%)
2	NAD	C	902	-	38,48,48	2.35	8 (21%)	47,73,73	1.99	13 (27%)
2	NAD	D	903	-	38,48,48	2.37	8 (21%)	47,73,73	1.92	12 (25%)

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
2	NAD	A	900	-	-	0/22/62/62	0/5/5/5
2	NAD	B	901	-	-	0/22/62/62	0/5/5/5
2	NAD	C	902	-	-	0/22/62/62	0/5/5/5
2	NAD	D	903	-	-	0/22/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	NAD	O4B-C1B	-3.40	1.36	1.41
2	D	903	NAD	O4B-C1B	-3.18	1.37	1.41
2	C	902	NAD	O4B-C1B	-2.88	1.37	1.41
2	A	900	NAD	O4B-C1B	-2.50	1.38	1.41
2	A	900	NAD	C7N-N7N	2.03	1.37	1.33
2	C	902	NAD	C7N-N7N	2.18	1.37	1.33
2	D	903	NAD	C7N-N7N	2.21	1.37	1.33
2	C	902	NAD	O4D-C1D	2.26	1.44	1.41
2	B	901	NAD	C7N-N7N	2.27	1.37	1.33
2	D	903	NAD	O4D-C1D	2.42	1.44	1.41
2	B	901	NAD	O4D-C1D	2.50	1.44	1.41
2	A	900	NAD	O4D-C1D	2.54	1.44	1.41
2	A	900	NAD	C2A-N1A	3.37	1.40	1.33
2	C	902	NAD	C2A-N1A	3.42	1.40	1.33
2	B	901	NAD	C2A-N1A	3.43	1.40	1.33
2	D	903	NAD	C2A-N1A	3.46	1.40	1.33
2	A	900	NAD	C6N-N1N	3.88	1.45	1.35
2	D	903	NAD	C6N-N1N	3.90	1.45	1.35
2	B	901	NAD	C6N-N1N	3.94	1.46	1.35
2	C	902	NAD	C6N-N1N	3.94	1.46	1.35
2	D	903	NAD	C2N-C3N	5.85	1.47	1.39
2	B	901	NAD	C2N-C3N	5.94	1.48	1.39
2	A	900	NAD	C2N-C3N	6.06	1.48	1.39
2	C	902	NAD	C2N-C3N	6.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	NAD	C4N-C3N	7.06	1.51	1.39
2	A	900	NAD	C4N-C3N	7.09	1.51	1.39
2	D	903	NAD	C4N-C3N	7.10	1.51	1.39
2	B	901	NAD	C4N-C3N	7.15	1.51	1.39
2	C	902	NAD	C5N-C4N	7.25	1.53	1.38
2	B	901	NAD	C5N-C4N	7.29	1.53	1.38
2	A	900	NAD	C5N-C4N	7.29	1.53	1.38
2	D	903	NAD	C5N-C4N	7.31	1.53	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	902	NAD	O7N-C7N-C3N	-5.90	113.14	119.59
2	D	903	NAD	O7N-C7N-C3N	-5.86	113.19	119.59
2	A	900	NAD	O7N-C7N-C3N	-5.83	113.23	119.59
2	B	901	NAD	O7N-C7N-C3N	-5.80	113.25	119.59
2	A	900	NAD	PN-O3-PA	-4.31	120.62	132.73
2	C	902	NAD	PN-O3-PA	-3.95	121.62	132.73
2	B	901	NAD	PN-O3-PA	-3.79	122.09	132.73
2	D	903	NAD	PN-O3-PA	-3.76	122.16	132.73
2	B	901	NAD	N3A-C2A-N1A	-3.24	126.41	128.89
2	C	902	NAD	N3A-C2A-N1A	-3.24	126.41	128.89
2	A	900	NAD	N3A-C2A-N1A	-3.16	126.47	128.89
2	D	903	NAD	N3A-C2A-N1A	-3.16	126.47	128.89
2	B	901	NAD	C5N-C4N-C3N	-2.56	117.11	120.33
2	D	903	NAD	C5N-C4N-C3N	-2.54	117.14	120.33
2	C	902	NAD	C5N-C4N-C3N	-2.52	117.16	120.33
2	A	900	NAD	C5N-C4N-C3N	-2.49	117.20	120.33
2	A	900	NAD	O5D-PN-O1N	-2.40	100.29	109.62
2	C	902	NAD	O3-PN-O5D	-2.32	96.79	102.94
2	B	901	NAD	O3-PN-O5D	-2.23	97.01	102.94
2	D	903	NAD	O3-PN-O5D	-2.22	97.04	102.94
2	C	902	NAD	O5D-PN-O1N	-2.13	101.34	109.62
2	B	901	NAD	O5D-PN-O1N	-2.10	101.47	109.62
2	D	903	NAD	O5D-PN-O1N	-2.09	101.49	109.62
2	C	902	NAD	C2D-C3D-C4D	2.09	106.91	102.61
2	D	903	NAD	C5N-C6N-N1N	2.10	124.10	120.47
2	B	901	NAD	C5N-C6N-N1N	2.11	124.13	120.47
2	A	900	NAD	C5N-C6N-N1N	2.15	124.18	120.47
2	C	902	NAD	C5N-C6N-N1N	2.21	124.30	120.47
2	A	900	NAD	O2N-PN-O3	2.31	115.57	105.09
2	C	902	NAD	O2N-PN-O3	2.40	115.98	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	NAD	O2N-PN-O3	2.41	116.03	105.09
2	A	900	NAD	C4A-C5A-N7A	2.41	111.70	109.48
2	D	903	NAD	O2N-PN-O3	2.43	116.11	105.09
2	B	901	NAD	C4A-C5A-N7A	2.43	111.72	109.48
2	C	902	NAD	C4A-C5A-N7A	2.43	111.72	109.48
2	D	903	NAD	C4A-C5A-N7A	2.44	111.72	109.48
2	A	900	NAD	O4D-C1D-N1N	2.69	111.09	108.13
2	A	900	NAD	O3-PA-O5B	2.72	110.16	102.94
2	B	901	NAD	O3-PA-O5B	2.76	110.26	102.94
2	C	902	NAD	O3-PA-O5B	2.81	110.39	102.94
2	D	903	NAD	O4D-C1D-N1N	2.81	111.22	108.13
2	D	903	NAD	O3-PA-O5B	2.82	110.41	102.94
2	B	901	NAD	O4D-C1D-N1N	2.90	111.32	108.13
2	C	902	NAD	O4D-C1D-N1N	3.77	112.28	108.13
2	B	901	NAD	C3N-C7N-N7N	6.21	124.61	117.82
2	D	903	NAD	C3N-C7N-N7N	6.24	124.65	117.82
2	C	902	NAD	C3N-C7N-N7N	6.29	124.70	117.82
2	A	900	NAD	C3N-C7N-N7N	6.44	124.86	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	NAD	2	0
2	B	901	NAD	1	0
2	C	902	NAD	2	0
2	D	903	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.