



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:27 PM GMT

PDB ID : 1P1H
Title : Crystal structure of the 1L-myo-inositol/NAD⁺ complex
Authors : Jin, X.; Geiger, J.H.
Deposited on : 2003-04-12
Resolution : 1.95 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

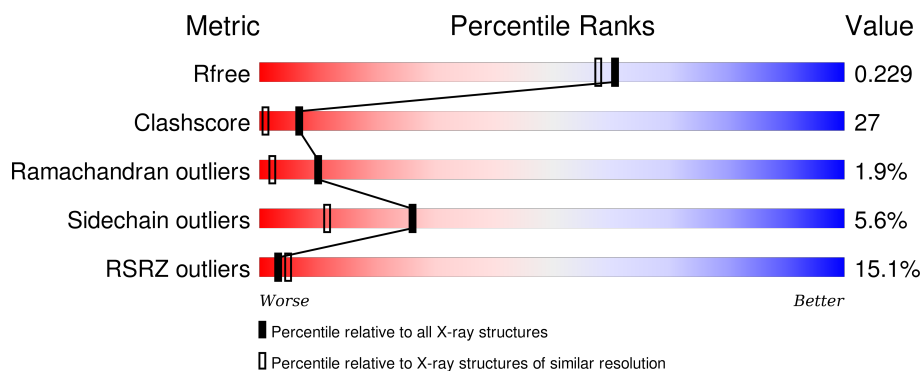
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	533	<div> <div>14%</div> <div>56%</div> <div>35%</div> <div>5%</div> <div>5%</div> </div>
1	B	533	<div> <div>15%</div> <div>54%</div> <div>34%</div> <div>•</div> <div>8%</div> </div>
1	C	533	<div> <div>14%</div> <div>58%</div> <div>34%</div> <div>5%</div> <div>•</div> </div>
1	D	533	<div> <div>13%</div> <div>52%</div> <div>34%</div> <div>5%</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17489 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 Inositol-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3988	2538	669	765	16			
1	B	491	Total	C	N	O	S	0	0	0
			3876	2467	652	741	16			
1	C	517	Total	C	N	O	S	0	0	0
			4081	2596	686	783	16			
1	D	487	Total	C	N	O	S	0	0	0
			3839	2439	643	743	14			

There are 40 discrepancies between the modelled and reference sequences:

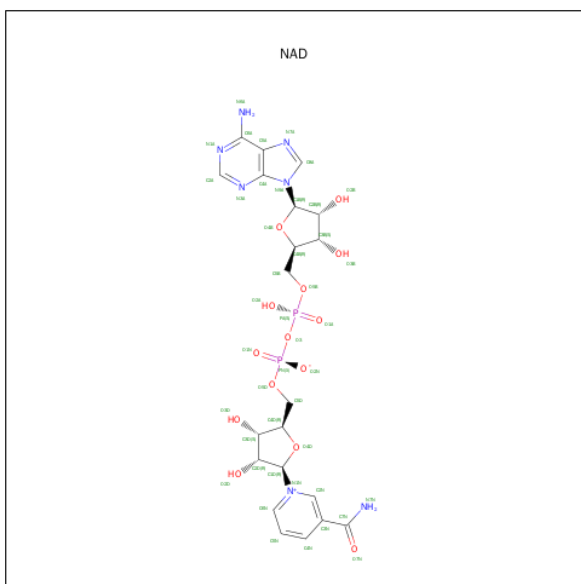
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986
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	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986
C	?	-	ARG	SEE REMARK 999	UNP P11986

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Chain	Residue	Modelled	Actual	Comment	Reference
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	?	-	ALA	SEE REMARK 999	UNP P11986
C	98	GLU	LYS	SEE REMARK 999	UNP P11986
C	140	ASN	LYS	SEE REMARK 999	UNP P11986
C	141	ASP	HIS	SEE REMARK 999	UNP P11986
C	201	ASN	GLN	SEE REMARK 999	UNP P11986
C	444	PRO	ALA	SEE REMARK 999	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
D	60	LEU	GLU	SEE REMARK 999	UNP P11986
D	?	-	ALA	SEE REMARK 999	UNP P11986
D	98	GLU	LYS	SEE REMARK 999	UNP P11986
D	140	ASN	LYS	SEE REMARK 999	UNP P11986
D	141	ASP	HIS	SEE REMARK 999	UNP P11986
D	201	ASN	GLN	SEE REMARK 999	UNP P11986
D	444	PRO	ALA	SEE REMARK 999	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
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	425	Total	O	0	0
			425	425		
3	B	354	Total	O	0	0
			354	354		
3	C	383	Total	O	0	0
			383	383		
3	D	367	Total	O	0	0
			367	367		

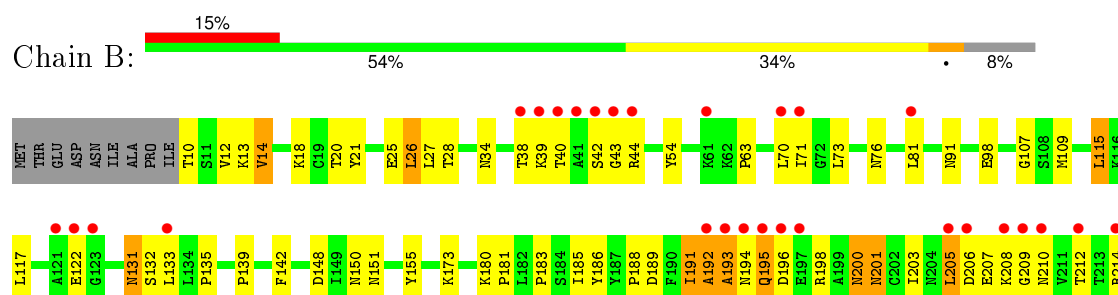
3 Residue-property plots

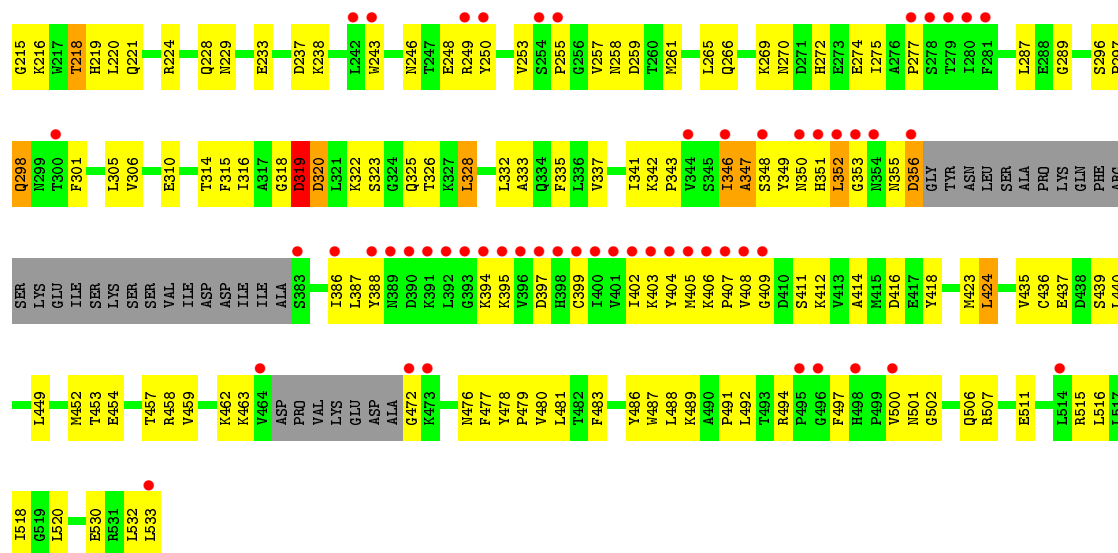
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Inositol-3-phosphate synthase

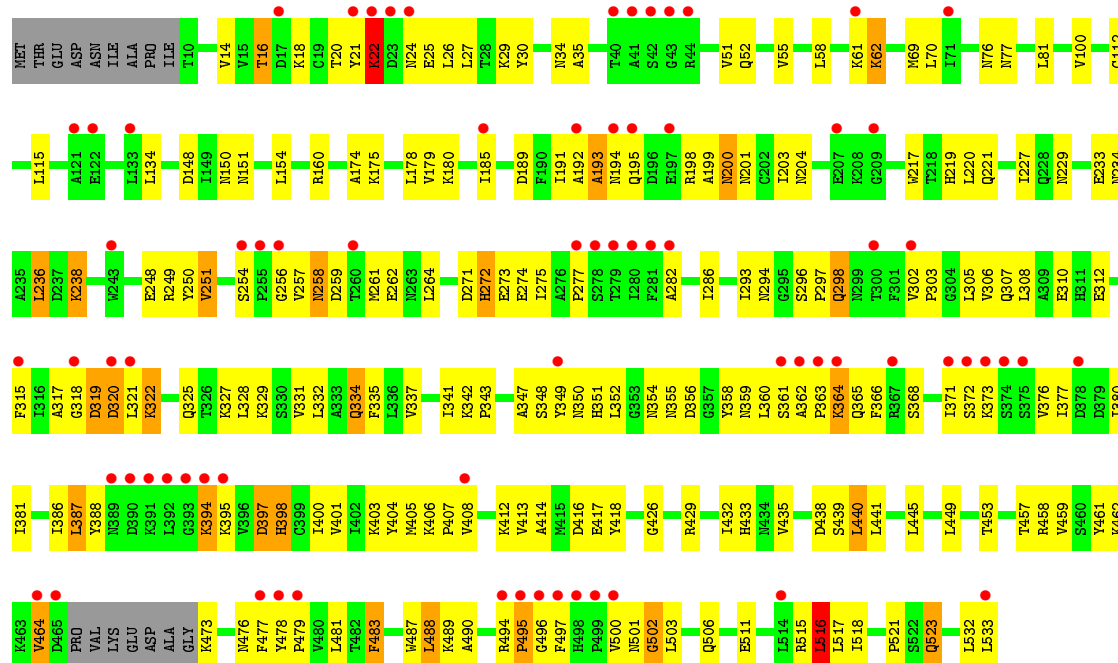


• Molecule 1: Inositol-3-phosphate synthase

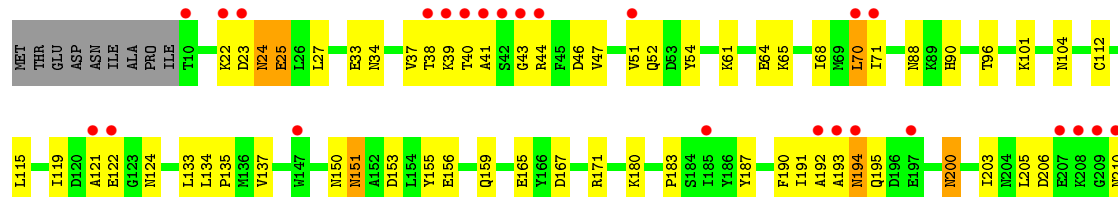


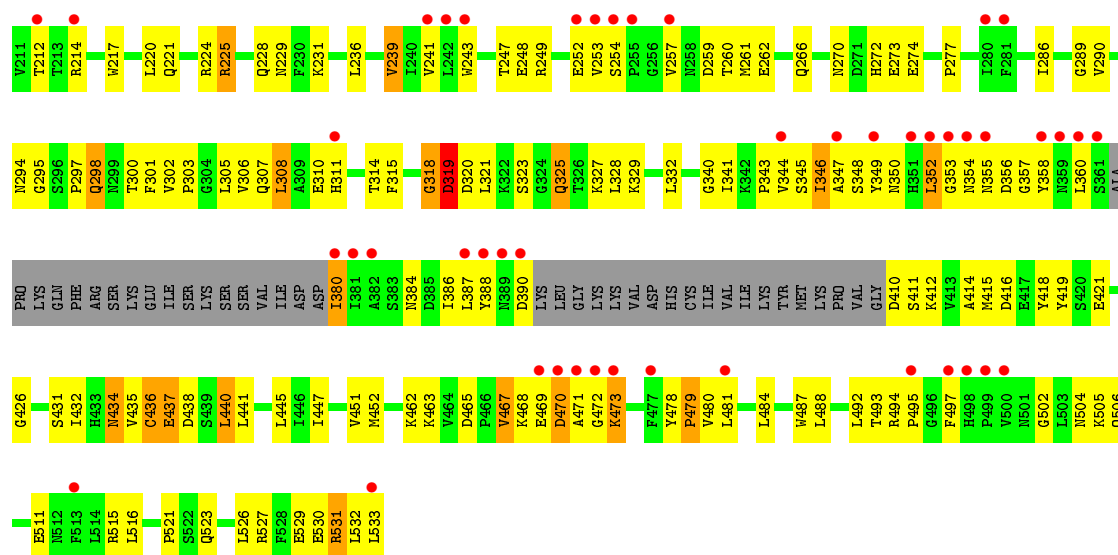


• Molecule 1: Inositol-3-phosphate synthase



• Molecule 1: Inositol-3-phosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 185.58Å 94.08Å 90.00° 114.77° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 26.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.95) 96.3 (26.35-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.249 0.232 , 0.229	Depositor DCC
R_{free} test set	10055 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 89.9	EDS
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 214414 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17489	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/4066	0.61	0/5513
1	B	0.35	0/3951	0.60	0/5354
1	C	0.36	0/4160	0.60	1/5637 (0.0%)
1	D	0.37	0/3913	0.62	1/5308 (0.0%)
All	All	0.36	0/16090	0.61	2/21812 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	318	GLY	N-CA-C	5.40	126.59	113.10
1	C	516	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3988	0	3989	213	0
1	B	3876	0	3879	220	0
1	C	4081	0	4088	258	0
1	D	3839	0	3816	229	0
2	A	44	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	3	0
2	C	44	0	26	5	0
2	D	44	0	26	1	0
3	A	425	0	0	27	0
3	B	354	0	0	20	0
3	C	383	0	0	25	0
3	D	367	0	0	18	0
All	All	17489	0	15876	856	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 27.

All (856) 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:494:ARG:HB3	1:C:495:PRO:HD2	1.34	1.08
1:C:494:ARG:HH22	1:D:533:LEU:HB3	0.94	1.06
1:A:352:LEU:HD21	1:A:357:GLY:HA3	1.37	1.06
1:C:69:MET:HE1	1:C:227:ILE:HG12	1.42	1.01
1:D:191:ILE:HG22	1:D:192:ALA:H	1.25	1.01
1:A:69:MET:HE1	1:A:227:ILE:HA	1.42	1.00
1:B:191:ILE:HG13	1:B:192:ALA:H	1.20	1.00
1:C:320:ASP:HB3	1:C:489:LYS:HB3	1.39	1.00
1:C:494:ARG:NH2	1:D:533:LEU:HB3	1.78	0.97
1:B:322:LYS:HA	1:B:489:LYS:HG3	1.46	0.96
1:A:318:GLY:HA2	1:A:488:LEU:HG	1.48	0.96
1:B:437:GLU:HG3	1:B:440:LEU:HD12	1.47	0.94
1:A:115:LEU:HD22	1:A:511:GLU:HG3	1.50	0.93
1:D:437:GLU:HG3	1:D:440:LEU:HD22	1.49	0.93
1:A:502:GLY:HA3	1:A:505:LYS:HE2	1.50	0.93
1:C:533:LEU:HB3	1:D:494:ARG:HH22	1.36	0.90
1:C:494:ARG:HH22	1:D:533:LEU:CB	1.83	0.89
1:B:323:SER:H	1:B:489:LYS:HE3	1.36	0.89
1:B:347:ALA:HA	1:B:399:CYS:HB3	1.53	0.89
1:C:302:VAL:HG22	1:C:303:PRO:HD2	1.57	0.87
1:B:151:ASN:H	1:B:200:ASN:HD21	1.21	0.87
1:D:22:LYS:HE3	1:D:27:LEU:HD11	1.57	0.86
1:C:22:LYS:HZ2	1:C:25:GLU:HB2	1.41	0.85
1:C:533:LEU:HD13	1:D:494:ARG:HH12	1.41	0.84
1:B:289:GLY:HA2	1:B:314:THR:HG21	1.59	0.84
1:B:408:VAL:HG21	3:B:1000:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:HG13	1:B:192:ALA:N	1.92	0.84
1:C:24:ASN:HD22	1:C:61:LYS:HB2	1.42	0.84
1:A:381:ILE:HD11	1:A:396:VAL:HG23	1.58	0.84
1:C:337:VAL:HG21	1:C:380:ILE:HG23	1.57	0.83
1:D:225:ARG:HH21	1:D:229:ASN:HB2	1.42	0.83
1:D:415:MET:HE3	1:D:431:SER:HB2	1.62	0.82
1:B:198:ARG:HD2	3:B:973:HOH:O	1.79	0.82
1:D:40:THR:HG21	1:D:44:ARG:NH1	1.95	0.82
1:C:254:SER:HB2	1:C:257:VAL:HG11	1.62	0.81
1:B:195:GLN:HG3	1:B:198:ARG:HH21	1.43	0.81
1:D:115:LEU:HD22	1:D:511:GLU:HG3	1.60	0.80
1:C:515:ARG:NH1	1:C:521:PRO:O	2.15	0.80
1:D:325:GLN:HA	1:D:325:GLN:HE21	1.45	0.80
1:D:352:LEU:HA	1:D:412:LYS:HA	1.64	0.79
1:C:261:MET:HG2	1:C:307:GLN:NE2	1.97	0.79
1:D:191:ILE:HG22	1:D:192:ALA:N	1.98	0.78
1:C:310:GLU:HG2	1:C:479:PRO:HG2	1.65	0.78
1:C:494:ARG:HB3	1:C:495:PRO:CD	2.13	0.78
1:C:347:ALA:HB2	3:C:920:HOH:O	1.82	0.78
1:B:342:LYS:HB2	1:B:387:LEU:HD22	1.66	0.78
1:C:494:ARG:HH12	1:D:533:LEU:HG	1.49	0.78
1:C:302:VAL:CG2	1:C:303:PRO:HD2	2.14	0.78
1:D:306:VAL:O	1:D:310:GLU:HG3	1.83	0.78
1:A:532:LEU:HB3	1:A:533:LEU:HD12	1.66	0.78
1:C:191:ILE:HG22	1:C:192:ALA:H	1.48	0.77
1:A:389:ASN:HD21	1:A:392:LEU:HD21	1.48	0.77
1:C:191:ILE:HG22	1:C:192:ALA:N	1.99	0.77
1:C:69:MET:CE	1:C:227:ILE:HG12	2.13	0.76
1:D:352:LEU:HD11	1:D:357:GLY:HA3	1.66	0.76
1:B:20:THR:HB	1:B:27:LEU:HB2	1.65	0.76
1:C:151:ASN:H	1:C:200:ASN:HD21	1.30	0.76
1:B:212:THR:HG22	1:B:214:ARG:H	1.49	0.76
1:B:478:TYR:HD2	1:B:480:VAL:HG22	1.51	0.76
1:D:156:GLU:HA	1:D:159:GLN:HE21	1.51	0.76
1:D:318:GLY:HA2	1:D:488:LEU:HD13	1.68	0.76
1:C:478:TYR:HB2	1:C:494:ARG:HH21	1.52	0.74
1:A:251:VAL:H	1:A:299:ASN:HD21	1.35	0.74
1:D:515:ARG:NH1	1:D:521:PRO:O	2.21	0.74
1:A:352:LEU:HD23	1:A:354:ASN:ND2	2.02	0.74
1:C:322:LYS:CD	1:C:327:LYS:HG2	2.18	0.73
1:D:33:GLU:HG2	1:D:51:VAL:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LYS:HB3	1:C:458:ARG:CZ	2.19	0.73
1:B:248:GLU:H	1:B:298:GLN:HG2	1.50	0.73
1:C:500:VAL:HG21	1:D:527:ARG:NE	2.04	0.73
1:C:264:LEU:HD21	1:C:305:LEU:HD13	1.69	0.73
1:C:377:ILE:O	1:C:381:ILE:HG13	1.88	0.72
1:B:310:GLU:HG2	1:B:479:PRO:HG3	1.70	0.72
1:A:407:PRO:HG3	1:C:395:LYS:HE2	1.72	0.72
1:B:205:LEU:HA	1:B:210:ASN:O	1.90	0.72
1:A:352:LEU:CD2	1:A:357:GLY:HA3	2.18	0.72
1:B:478:TYR:CD2	1:B:480:VAL:HG22	2.25	0.71
1:C:533:LEU:HD13	1:D:494:ARG:NH1	2.05	0.71
1:B:437:GLU:HG3	1:B:440:LEU:CD1	2.21	0.71
1:D:352:LEU:HB3	1:D:412:LYS:HB2	1.72	0.71
1:C:320:ASP:CB	1:C:489:LYS:HB3	2.19	0.71
1:B:318:GLY:O	1:B:319:ASP:HB2	1.91	0.70
1:A:221:GLN:HG2	3:A:881:HOH:O	1.90	0.70
1:B:14:VAL:HG11	1:B:518:ILE:O	1.90	0.70
1:C:272:HIS:CD2	1:C:274:GLU:H	2.09	0.70
1:D:310:GLU:HG2	1:D:479:PRO:HG3	1.73	0.70
1:A:352:LEU:HD21	1:A:357:GLY:CA	2.19	0.70
1:C:337:VAL:HG21	1:C:380:ILE:CG2	2.21	0.70
1:A:256:GLY:HA2	1:A:263:ASN:HD22	1.56	0.69
1:D:532:LEU:O	1:D:533:LEU:HB2	1.90	0.69
1:C:334:GLN:HG2	1:C:335:PHE:N	2.05	0.69
1:C:373:LYS:HE3	1:C:489:LYS:HD3	1.72	0.69
1:D:415:MET:CE	1:D:431:SER:HB2	2.23	0.69
1:C:150:ASN:ND2	1:C:160:ARG:HH12	1.90	0.69
1:C:331:VAL:HA	1:C:334:GLN:NE2	2.06	0.69
1:A:257:VAL:HG13	1:A:258:ASN:H	1.58	0.69
1:C:115:LEU:CD2	1:C:511:GLU:HG2	2.23	0.69
1:A:39:LYS:O	1:A:40:THR:HG23	1.93	0.68
1:A:486:TYR:HA	1:A:506:GLN:NE2	2.09	0.68
1:A:328:LEU:HD13	3:A:935:HOH:O	1.92	0.68
1:B:318:GLY:HA2	1:B:488:LEU:HD13	1.76	0.68
1:C:22:LYS:HB3	1:C:22:LYS:HZ2	1.59	0.67
1:A:64:GLU:O	1:A:65:LYS:HD2	1.93	0.67
1:A:254:SER:O	1:A:257:VAL:HG12	1.94	0.67
1:C:154:LEU:HD22	1:C:179:VAL:HG11	1.77	0.67
1:C:350:ASN:HD22	1:C:412:LYS:HE3	1.59	0.67
1:A:318:GLY:O	1:A:319:ASP:HB2	1.93	0.67
1:C:515:ARG:HD2	3:C:911:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ALA:HB3	1:C:365:GLN:HG2	1.77	0.67
1:A:10:THR:HG22	1:B:43:GLY:HA3	1.76	0.67
1:C:494:ARG:CB	1:C:495:PRO:HD2	2.20	0.67
1:C:154:LEU:HD22	1:C:179:VAL:CG1	2.25	0.67
1:B:404:TYR:OH	1:B:406:LYS:HE3	1.94	0.66
1:C:70:LEU:HD11	1:C:81:LEU:HD23	1.76	0.66
1:C:478:TYR:CD1	1:C:479:PRO:HD2	2.31	0.66
1:C:533:LEU:HB3	1:D:494:ARG:NH2	2.08	0.66
1:A:217:TRP:O	1:A:221:GLN:HG3	1.95	0.66
1:C:296:SER:HB2	1:C:298:GLN:OE1	1.96	0.66
1:B:352:LEU:H	1:B:352:LEU:HD13	1.61	0.66
1:B:98:GLU:HB2	3:B:806:HOH:O	1.95	0.66
1:D:437:GLU:HG3	1:D:440:LEU:CD2	2.24	0.66
1:B:388:TYR:HB3	1:B:394:LYS:HA	1.77	0.66
1:D:38:THR:HG23	1:D:46:ASP:HB2	1.76	0.66
1:D:191:ILE:CG2	1:D:192:ALA:H	2.06	0.65
1:A:256:GLY:HA2	1:A:263:ASN:ND2	2.10	0.65
1:D:341:ILE:O	1:D:343:PRO:HD3	1.95	0.65
1:D:318:GLY:CA	1:D:488:LEU:HD13	2.26	0.65
1:C:115:LEU:HD21	1:C:511:GLU:HG2	1.78	0.65
1:A:151:ASN:HB2	1:A:180:LYS:HE2	1.77	0.65
1:B:405:MET:SD	1:D:347:ALA:HB2	2.36	0.65
1:C:321:LEU:O	1:C:321:LEU:HD23	1.96	0.65
1:A:47:VAL:HG22	1:B:14:VAL:HA	1.79	0.65
1:D:273:GLU:HG2	3:D:822:HOH:O	1.96	0.65
1:D:434:ASN:HD22	1:D:435:VAL:N	1.95	0.65
1:C:178:LEU:HD12	3:C:936:HOH:O	1.95	0.65
1:C:322:LYS:HA	1:C:489:LYS:HE3	1.79	0.64
1:D:318:GLY:O	1:D:319:ASP:HB2	1.96	0.64
1:A:322:LYS:NZ	1:A:506:GLN:HE22	1.95	0.64
1:D:345:SER:HB3	1:D:419:TYR:HB3	1.78	0.64
1:D:473:LYS:HA	3:D:895:HOH:O	1.97	0.64
1:B:322:LYS:NZ	1:B:506:GLN:HE22	1.96	0.64
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.13	0.64
1:C:361:SER:HB2	3:C:1031:HOH:O	1.97	0.63
1:C:191:ILE:HG21	1:C:195:GLN:HG3	1.80	0.63
1:C:322:LYS:HD3	1:C:327:LYS:HG2	1.79	0.63
1:A:505:LYS:HG3	3:A:777:HOH:O	1.97	0.63
1:B:195:GLN:HG3	1:B:198:ARG:NH2	2.14	0.63
1:C:14:VAL:HG22	1:D:47:VAL:HB	1.79	0.63
1:B:409:GLY:HA3	3:B:844:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LYS:HA	1:C:489:LYS:HB2	1.80	0.63
1:C:426:GLY:HA3	1:D:440:LEU:HD23	1.81	0.63
1:B:405:MET:O	1:B:408:VAL:HG22	1.99	0.62
1:B:353:GLY:HA3	1:B:406:LYS:HA	1.80	0.62
1:C:302:VAL:HG22	1:C:303:PRO:CD	2.29	0.62
1:B:395:LYS:HE2	1:B:397:ASP:OD2	1.99	0.62
1:A:405:MET:HE2	3:C:920:HOH:O	1.99	0.62
1:C:248:GLU:OE1	1:C:277:PRO:HD2	2.00	0.62
1:D:321:LEU:HB3	3:D:712:HOH:O	2.00	0.62
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.34	0.62
1:A:321:LEU:HD22	1:A:445:LEU:CD2	2.30	0.62
1:C:248:GLU:H	1:C:298:GLN:HG2	1.65	0.62
1:C:151:ASN:N	1:C:200:ASN:HD21	1.97	0.62
1:B:395:LYS:HD2	3:B:825:HOH:O	1.99	0.62
1:C:445:LEU:HD21	1:C:487:TRP:HB3	1.82	0.62
1:B:12:VAL:HG21	1:B:133:LEU:HD23	1.83	0.61
1:D:329:LYS:HD2	1:D:416:ASP:OD2	2.00	0.61
1:C:58:LEU:HD22	1:C:134:LEU:HD13	1.80	0.61
1:D:357:GLY:O	1:D:360:LEU:HB3	2.00	0.61
1:C:328:LEU:O	1:C:332:LEU:HG	2.01	0.61
1:B:341:ILE:O	1:B:343:PRO:HD3	2.00	0.61
1:B:186:TYR:OH	1:B:196:ASP:HA	2.01	0.61
1:B:191:ILE:CG1	1:B:192:ALA:H	2.02	0.61
1:A:392:LEU:HB3	3:B:854:HOH:O	2.00	0.61
1:D:192:ALA:HA	3:D:970:HOH:O	2.00	0.61
1:B:195:GLN:H	1:B:195:GLN:NE2	1.98	0.61
1:B:109:MET:HE2	1:B:507:ARG:HE	1.65	0.60
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.36	0.60
1:D:289:GLY:HA2	1:D:314:THR:CG2	2.31	0.60
1:A:501:ASN:HA	1:A:506:GLN:OE1	2.01	0.60
1:C:387:LEU:HD11	1:D:112:CYS:HB3	1.82	0.60
1:C:432:ILE:HG13	3:C:1034:HOH:O	2.01	0.60
1:A:332:LEU:HD21	1:B:328:LEU:HD12	1.82	0.60
1:D:225:ARG:NH2	1:D:229:ASN:HB2	2.14	0.60
1:B:480:VAL:O	1:B:480:VAL:HG23	2.01	0.60
1:D:289:GLY:HA2	1:D:314:THR:HG21	1.83	0.60
1:C:478:TYR:CB	1:C:494:ARG:HH21	2.14	0.60
1:C:394:LYS:NZ	1:C:394:LYS:HB3	2.17	0.60
1:A:257:VAL:HG13	1:A:258:ASN:N	2.15	0.60
1:A:449:LEU:HD21	1:A:487:TRP:HB2	1.82	0.60
1:B:325:GLN:HA	1:B:325:GLN:HE21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:THR:HG22	1:D:165:GLU:HG2	1.84	0.60
1:C:100:VAL:HG12	3:C:797:HOH:O	2.00	0.60
1:A:341:ILE:O	1:A:343:PRO:HD3	2.01	0.60
1:B:70:LEU:HD11	1:B:81:LEU:HD23	1.84	0.60
1:C:22:LYS:NZ	1:C:25:GLU:HB2	2.16	0.60
1:D:511:GLU:O	1:D:515:ARG:HG3	2.02	0.60
1:A:75:GLY:O	1:A:79:SER:HB2	2.01	0.60
1:C:150:ASN:HA	1:C:200:ASN:ND2	2.17	0.59
1:B:437:GLU:CG	1:B:440:LEU:HD12	2.28	0.59
1:C:453:THR:O	1:C:457:THR:HG23	2.02	0.59
1:A:352:LEU:N	1:A:352:LEU:HD13	2.17	0.59
1:D:412:LYS:HE3	1:D:438:ASP:OD1	2.02	0.59
1:B:200:ASN:C	1:B:200:ASN:HD22	2.05	0.59
1:B:266:GLN:HE21	1:B:270:ASN:HD21	1.48	0.59
1:A:286:ILE:HG22	1:A:312:GLU:HG3	1.84	0.59
1:C:440:LEU:HD23	1:D:426:GLY:HA3	1.84	0.59
1:D:344:VAL:HG11	1:D:421:GLU:OE2	2.03	0.59
1:C:325:GLN:NE2	1:C:412:LYS:HD3	2.17	0.59
1:C:329:LYS:HG3	1:C:418:TYR:OH	2.03	0.59
1:B:42:SER:C	1:B:44:ARG:H	2.06	0.59
1:C:273:GLU:H	1:C:273:GLU:CD	2.05	0.59
1:B:215:GLY:O	1:B:218:THR:HB	2.02	0.59
1:A:310:GLU:HG2	1:A:479:PRO:HG3	1.84	0.59
1:A:116:LYS:HB3	1:A:523:GLN:NE2	2.18	0.59
1:C:18:LYS:HE2	3:C:820:HOH:O	2.03	0.59
1:C:258:ASN:HD22	1:C:258:ASN:C	2.07	0.59
1:C:325:GLN:HB3	3:C:1035:HOH:O	2.02	0.59
1:B:185:ILE:HG12	1:B:203:ILE:HD11	1.85	0.59
1:A:332:LEU:HG	1:A:432:ILE:HD11	1.84	0.58
1:A:21:TYR:HD2	1:A:60:LEU:HD11	1.67	0.58
1:C:516:LEU:HD23	1:C:516:LEU:C	2.22	0.58
1:A:438:ASP:HB3	2:A:650:NAD:O7N	2.03	0.58
1:C:191:ILE:CG2	1:C:195:GLN:HG3	2.33	0.58
1:C:523:GLN:HA	1:C:523:GLN:HE21	1.67	0.58
1:A:220:LEU:HD23	1:A:280:ILE:HG23	1.85	0.58
1:B:193:ALA:N	1:B:196:ASP:HB2	2.17	0.58
1:C:254:SER:HB2	1:C:257:VAL:CG1	2.32	0.58
1:A:405:MET:HE3	1:C:397:ASP:HB3	1.84	0.58
1:B:318:GLY:CA	1:B:488:LEU:HD13	2.33	0.58
1:C:319:ASP:HB3	1:C:490:ALA:HB3	1.85	0.58
1:C:272:HIS:HB3	1:C:275:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:SER:H	1:B:489:LYS:CE	2.12	0.58
1:A:351:HIS:HD2	1:C:349:TYR:OH	1.87	0.58
1:C:351:HIS:HA	1:C:403:LYS:O	2.03	0.58
1:C:302:VAL:O	1:C:306:VAL:HG23	2.04	0.58
1:C:494:ARG:HH12	1:D:533:LEU:CG	2.16	0.58
1:B:63:PRO:HG3	1:B:238:LYS:HG3	1.85	0.58
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.86	0.58
1:D:346:ILE:HG12	1:D:418:TYR:CD2	2.38	0.58
1:A:47:VAL:HG22	1:B:14:VAL:HB	1.85	0.57
1:D:411:SER:HB3	3:D:867:HOH:O	2.04	0.57
1:C:191:ILE:CG2	1:C:192:ALA:H	2.16	0.57
1:B:478:TYR:CE2	1:B:494:ARG:HG2	2.38	0.57
1:B:306:VAL:O	1:B:310:GLU:HG3	2.04	0.57
1:D:286:ILE:HG21	1:D:308:LEU:HD13	1.84	0.57
1:C:25:GLU:HB3	3:C:922:HOH:O	2.03	0.57
1:D:325:GLN:HA	1:D:325:GLN:NE2	2.16	0.57
1:C:192:ALA:O	1:C:193:ALA:HB2	2.04	0.57
1:D:122:GLU:HB2	1:D:124:ASN:OD1	2.04	0.57
1:C:302:VAL:HG12	1:C:305:LEU:HB2	1.86	0.57
1:A:15:VAL:HG11	3:A:788:HOH:O	2.04	0.57
1:C:297:PRO:HB3	1:C:320:ASP:OD1	2.04	0.57
1:A:497:PHE:CD2	1:B:530:GLU:HG2	2.40	0.56
1:A:407:PRO:CG	1:C:395:LYS:HE2	2.36	0.56
1:C:405:MET:O	1:C:408:VAL:HG22	2.06	0.56
1:A:462:LYS:HA	3:A:1072:HOH:O	2.05	0.56
1:C:432:ILE:HD12	1:D:432:ILE:HD12	1.88	0.56
1:C:533:LEU:CD1	1:D:494:ARG:HH12	2.14	0.56
1:C:221:GLN:HG2	3:C:799:HOH:O	2.06	0.56
1:D:380:ILE:N	1:D:380:ILE:HD13	2.21	0.56
1:C:350:ASN:ND2	1:C:412:LYS:HE3	2.20	0.56
1:A:231:LYS:HE3	3:A:790:HOH:O	2.05	0.56
1:D:38:THR:CG2	1:D:46:ASP:HB2	2.36	0.56
1:D:183:PRO:HB2	1:D:203:ILE:HG23	1.88	0.56
1:D:259:ASP:HA	1:D:303:PRO:HG2	1.88	0.56
1:C:191:ILE:CG2	1:C:192:ALA:N	2.69	0.56
1:B:348:SER:HB3	1:B:399:CYS:O	2.06	0.55
1:A:39:LYS:HB2	1:A:45:PHE:CD1	2.41	0.55
1:C:77:ASN:ND2	2:C:670:NAD:N7N	2.54	0.55
1:B:10:THR:HG22	1:B:132:SER:HB2	1.87	0.55
1:D:350:ASN:OD1	1:D:412:LYS:HD3	2.06	0.55
1:A:248:GLU:H	1:A:298:GLN:NE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:THR:O	1:D:305:LEU:HD12	2.07	0.55
1:D:220:LEU:HD23	1:D:220:LEU:C	2.27	0.55
1:A:124:ASN:HB3	3:B:991:HOH:O	2.05	0.55
1:B:506:GLN:HG3	3:B:916:HOH:O	2.07	0.55
1:C:417:GLU:OE1	1:C:429:ARG:HD3	2.05	0.55
1:D:318:GLY:HA2	1:D:488:LEU:CD1	2.36	0.55
1:A:256:GLY:CA	1:A:263:ASN:HD22	2.18	0.55
1:B:348:SER:HB2	1:B:416:ASP:OD2	2.07	0.55
1:D:470:ASP:O	1:D:471:ALA:HB3	2.06	0.55
1:B:353:GLY:CA	1:B:406:LYS:HA	2.37	0.55
1:D:321:LEU:HG	1:D:445:LEU:HD22	1.88	0.55
1:D:478:TYR:CD2	1:D:479:PRO:HD2	2.42	0.55
1:A:325:GLN:NE2	3:A:935:HOH:O	2.40	0.55
1:A:185:ILE:CD1	1:A:223:ILE:HD11	2.37	0.55
1:D:191:ILE:HG21	1:D:195:GLN:HG3	1.88	0.55
1:C:403:LYS:NZ	1:C:403:LYS:HB3	2.21	0.55
1:D:40:THR:CG2	1:D:44:ARG:HB3	2.37	0.54
1:A:351:HIS:HA	1:A:403:LYS:O	2.07	0.54
1:B:155:TYR:CE2	1:B:173:LYS:HE3	2.42	0.54
1:C:318:GLY:O	1:C:319:ASP:HB2	2.07	0.54
1:B:76:ASN:HB3	1:B:439:SER:OG	2.07	0.54
1:A:325:GLN:HE22	1:A:434:ASN:HB2	1.72	0.54
1:C:24:ASN:ND2	1:C:61:LYS:HB2	2.19	0.54
1:B:459:VAL:HB	1:B:477:PHE:HE1	1.73	0.54
1:B:131:ASN:HD22	1:B:131:ASN:C	2.10	0.54
1:C:296:SER:HB3	1:C:297:PRO:HD2	1.89	0.54
1:A:301:PHE:HB2	3:A:942:HOH:O	2.08	0.54
1:A:381:ILE:HD11	1:A:396:VAL:CG2	2.35	0.54
1:A:299:ASN:ND2	1:A:299:ASN:H	2.06	0.54
1:D:302:VAL:HB	1:D:303:PRO:HD2	1.88	0.54
1:A:116:LYS:HB3	1:A:523:GLN:HE22	1.72	0.54
1:A:158:MET:CE	1:A:176:MET:HG3	2.37	0.54
1:C:238:LYS:HG2	3:C:1015:HOH:O	2.08	0.54
1:C:354:ASN:HB2	3:C:688:HOH:O	2.08	0.54
1:C:341:ILE:O	1:C:343:PRO:HD3	2.08	0.53
1:A:47:VAL:CG2	1:B:14:VAL:HB	2.38	0.53
1:A:246:ASN:HD22	1:A:359:ASN:ND2	2.06	0.53
1:B:352:LEU:HD13	1:B:352:LEU:N	2.23	0.53
1:B:20:THR:HG22	1:B:21:TYR:N	2.23	0.53
1:B:117:LEU:HD21	1:B:133:LEU:HD21	1.90	0.53
1:D:480:VAL:HG11	1:D:492:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:O	1:A:211:VAL:O	2.26	0.53
1:B:454:GLU:OE2	1:B:458:ARG:HD3	2.08	0.53
1:D:151:ASN:H	1:D:200:ASN:HD21	1.55	0.53
1:C:21:TYR:CE2	1:C:26:LEU:HD13	2.43	0.53
1:C:18:LYS:HA	1:C:29:LYS:HE2	1.90	0.53
1:C:234:ASN:HB2	1:C:236:LEU:HD22	1.90	0.53
1:D:502:GLY:O	1:D:506:GLN:HG3	2.08	0.53
1:D:225:ARG:NH2	3:D:819:HOH:O	2.40	0.53
1:C:381:ILE:HG23	1:C:388:TYR:CG	2.44	0.53
1:B:325:GLN:HG2	1:B:414:ALA:HB1	1.90	0.53
1:C:352:LEU:H	1:C:352:LEU:HD23	1.74	0.53
1:B:351:HIS:HB3	1:B:403:LYS:HB2	1.91	0.53
1:D:165:GLU:HG3	3:D:734:HOH:O	2.09	0.53
1:B:224:ARG:O	1:B:228:GLN:HG3	2.09	0.53
1:C:250:TYR:HD1	1:C:368:SER:HG	1.55	0.53
1:C:58:LEU:HD13	1:C:459:VAL:HG22	1.91	0.53
1:C:325:GLN:HE21	1:C:412:LYS:HD3	1.74	0.53
1:D:206:ASP:HB3	1:D:212:THR:HB	1.90	0.53
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.44	0.53
1:C:533:LEU:HD22	1:D:494:ARG:HH12	1.72	0.53
1:D:224:ARG:O	1:D:228:GLN:HG3	2.09	0.53
1:B:180:LYS:HE3	3:B:982:HOH:O	2.08	0.53
1:A:500:VAL:HG22	3:A:943:HOH:O	2.07	0.53
1:B:491:PRO:HD2	1:B:501:ASN:HD21	1.74	0.52
1:A:183:PRO:HB2	1:A:203:ILE:HG23	1.91	0.52
1:C:134:LEU:HD21	1:C:518:ILE:HG22	1.91	0.52
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.09	0.52
1:A:470:ASP:O	1:A:471:ALA:HB3	2.09	0.52
1:B:188:PRO:O	1:B:192:ALA:HB2	2.09	0.52
1:C:328:LEU:CD2	1:C:432:ILE:HG21	2.38	0.52
1:C:532:LEU:HD23	1:D:54:TYR:CE2	2.44	0.52
1:C:192:ALA:HB2	1:C:359:ASN:OD1	2.09	0.52
1:D:183:PRO:HB2	1:D:203:ILE:CG2	2.40	0.52
1:D:467:VAL:O	1:D:467:VAL:HG13	2.08	0.52
1:B:350:ASN:ND2	1:B:402:ILE:HG12	2.24	0.52
1:C:112:CYS:HB3	1:D:387:LEU:CD1	2.39	0.52
1:D:360:LEU:O	1:D:360:LEU:HD22	2.10	0.52
1:D:434:ASN:HD22	1:D:434:ASN:C	2.12	0.52
1:A:360:LEU:HD23	3:A:1059:HOH:O	2.09	0.52
1:D:516:LEU:HD12	1:D:516:LEU:C	2.29	0.52
1:B:208:LYS:HE3	3:B:974:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLY:HA3	1:A:236:LEU:HD13	1.91	0.52
1:C:294:ASN:HB3	1:C:318:GLY:HA3	1.92	0.52
1:B:326:THR:OG1	1:B:489:LYS:HE2	2.09	0.52
1:A:328:LEU:HD21	1:B:332:LEU:CD2	2.39	0.52
1:A:272:HIS:ND1	1:A:273:GLU:N	2.57	0.52
1:C:400:ILE:HG23	1:C:400:ILE:O	2.10	0.52
1:C:55:VAL:HG23	1:C:464:VAL:HG11	1.90	0.52
1:B:12:VAL:HG21	1:B:133:LEU:CD2	2.40	0.52
1:C:373:LYS:CE	1:C:489:LYS:HD3	2.37	0.52
1:A:238:LYS:HG3	3:A:1034:HOH:O	2.09	0.52
1:D:484:LEU:HA	1:D:487:TRP:CZ3	2.45	0.52
1:A:307:GLN:HA	1:A:310:GLU:OE1	2.09	0.52
1:D:88:ASN:HD21	1:D:104:ASN:CA	2.23	0.52
1:A:206:ASP:HB3	1:A:212:THR:OG1	2.09	0.51
1:A:515:ARG:NH1	1:A:521:PRO:O	2.43	0.51
1:A:417:GLU:OE2	1:A:429:ARG:HD3	2.10	0.51
1:C:306:VAL:O	1:C:310:GLU:HG3	2.10	0.51
1:A:502:GLY:HA3	1:A:505:LYS:CE	2.30	0.51
1:A:341:ILE:HD13	1:B:107:GLY:HA2	1.92	0.51
1:C:440:LEU:CD2	1:D:426:GLY:HA3	2.40	0.51
1:C:348:SER:HA	1:C:416:ASP:OD1	2.11	0.51
1:D:360:LEU:C	1:D:360:LEU:HD13	2.30	0.51
1:C:329:LYS:HE2	1:C:348:SER:OG	2.10	0.51
1:A:358:TYR:O	1:A:361:SER:HB3	2.10	0.51
1:C:478:TYR:HB2	1:C:494:ARG:NH2	2.23	0.51
1:B:301:PHE:CD1	1:B:492:LEU:HD22	2.45	0.51
1:B:301:PHE:HD1	1:B:492:LEU:HD22	1.75	0.51
1:D:438:ASP:N	1:D:438:ASP:OD2	2.44	0.51
1:A:405:MET:HG3	3:C:920:HOH:O	2.10	0.51
1:D:295:GLY:HA3	1:D:321:LEU:HD13	1.93	0.51
1:B:325:GLN:HA	1:B:325:GLN:NE2	2.26	0.51
1:C:438:ASP:HB3	2:C:670:NAD:O7N	2.10	0.51
1:C:347:ALA:HB1	1:C:349:TYR:CE2	2.45	0.51
1:B:248:GLU:OE1	1:B:277:PRO:HD2	2.11	0.51
1:A:39:LYS:HD2	1:A:45:PHE:CZ	2.46	0.50
1:C:445:LEU:HG	1:C:487:TRP:HD1	1.76	0.50
1:A:437:GLU:HG3	3:A:658:HOH:O	2.11	0.50
1:A:350:ASN:HD21	1:A:402:ILE:HG23	1.76	0.50
1:B:356:ASP:HB2	2:B:660:NAD:H3D	1.93	0.50
1:A:306:VAL:O	1:A:310:GLU:HG3	2.11	0.50
1:C:185:ILE:HG12	1:C:203:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ALA:HB3	1:C:305:LEU:HD21	1.93	0.50
2:C:670:NAD:O5D	2:C:670:NAD:H2N	2.11	0.50
1:A:344:VAL:HG22	1:A:419:TYR:O	2.12	0.50
1:A:296:SER:HA	2:A:650:NAD:O2D	2.11	0.50
1:D:340:GLY:O	1:D:387:LEU:HD21	2.10	0.50
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.92	0.50
1:B:150:ASN:HD22	1:B:198:ARG:HG3	1.77	0.50
1:B:310:GLU:HG2	1:B:479:PRO:CG	2.41	0.50
1:B:122:GLU:N	1:B:122:GLU:OE2	2.42	0.50
1:A:253:VAL:HG13	1:A:253:VAL:O	2.10	0.50
1:C:433:HIS:HB3	1:D:431:SER:OG	2.12	0.50
1:C:150:ASN:HA	1:C:200:ASN:HD21	1.77	0.50
1:C:354:ASN:OD1	1:C:356:ASP:HB3	2.12	0.50
1:A:18:LYS:HE3	3:A:988:HOH:O	2.11	0.50
1:B:476:ASN:HB3	3:B:827:HOH:O	2.10	0.50
1:C:500:VAL:HG11	3:D:864:HOH:O	2.11	0.50
1:C:372:SER:CB	1:C:490:ALA:HB2	2.42	0.50
1:C:319:ASP:O	1:C:320:ASP:HB2	2.11	0.49
1:B:200:ASN:ND2	1:B:200:ASN:C	2.65	0.49
1:A:286:ILE:HG23	1:A:314:THR:HG21	1.94	0.49
1:C:516:LEU:HD23	1:C:517:LEU:N	2.27	0.49
1:C:51:VAL:HG22	1:C:52:GLN:N	2.27	0.49
1:B:221:GLN:HG2	3:B:983:HOH:O	2.12	0.49
1:D:40:THR:HG22	1:D:44:ARG:HB3	1.93	0.49
1:A:47:VAL:HG22	1:B:14:VAL:CB	2.42	0.49
1:D:115:LEU:HD22	1:D:511:GLU:CG	2.39	0.49
1:A:191:ILE:HD12	1:A:195:GLN:HG2	1.94	0.49
3:C:996:HOH:O	1:D:463:LYS:HD2	2.13	0.49
1:D:231:LYS:HE2	1:D:239:VAL:HG13	1.94	0.49
1:C:55:VAL:HG23	1:C:464:VAL:CG1	2.42	0.49
1:A:349:TYR:O	1:A:350:ASN:HB3	2.13	0.49
1:B:253:VAL:O	1:B:253:VAL:HG13	2.12	0.49
1:B:272:HIS:HE1	1:B:274:GLU:HG2	1.77	0.49
1:C:180:LYS:HB3	3:C:881:HOH:O	2.11	0.49
1:B:216:LYS:HA	1:B:219:HIS:ND1	2.28	0.49
1:C:297:PRO:HB3	1:C:320:ASP:CG	2.33	0.49
1:B:491:PRO:CD	1:B:501:ASN:HD21	2.25	0.49
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.25	0.49
1:A:204:ASN:O	1:A:211:VAL:O	2.30	0.49
1:A:408:VAL:HG12	1:A:411:SER:O	2.12	0.49
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:HIS:CE1	1:B:274:GLU:HG2	2.48	0.49
1:C:502:GLY:O	1:C:506:GLN:HG3	2.13	0.49
1:A:151:ASN:CB	1:A:180:LYS:HE2	2.42	0.49
1:B:63:PRO:CG	1:B:238:LYS:HG3	2.43	0.49
1:C:310:GLU:CG	1:C:479:PRO:HG2	2.41	0.48
1:A:211:VAL:O	1:A:212:THR:HB	2.13	0.48
1:B:296:SER:O	1:B:320:ASP:N	2.46	0.48
1:D:68:ILE:HG22	1:D:70:LEU:HD13	1.95	0.48
1:A:391:LYS:HD3	3:A:761:HOH:O	2.12	0.48
1:D:328:LEU:HD23	1:D:432:ILE:HG21	1.94	0.48
1:B:405:MET:HE3	3:D:874:HOH:O	2.12	0.48
1:C:500:VAL:HG21	1:D:527:ARG:CZ	2.43	0.48
1:B:318:GLY:HA2	1:B:488:LEU:CD1	2.42	0.48
1:D:286:ILE:CG2	1:D:308:LEU:HD13	2.43	0.48
1:A:88:ASN:HD21	1:A:104:ASN:HA	1.77	0.48
1:D:504:ASN:HB2	1:D:505:LYS:NZ	2.28	0.48
1:D:88:ASN:HD21	1:D:104:ASN:HA	1.79	0.48
1:B:297:PRO:HB3	1:B:320:ASP:OD2	2.13	0.48
1:C:272:HIS:HD2	1:C:274:GLU:HB2	1.77	0.48
1:A:47:VAL:HG22	1:B:14:VAL:CA	2.43	0.48
1:A:45:PHE:HE2	1:B:10:THR:HG21	1.78	0.48
1:D:343:PRO:HD2	1:D:388:TYR:OH	2.13	0.48
1:A:183:PRO:HB2	1:A:203:ILE:CG2	2.43	0.48
1:A:95:GLN:NE2	1:A:100:VAL:HG22	2.28	0.48
1:C:328:LEU:HD22	1:C:432:ILE:HG21	1.95	0.48
1:C:334:GLN:HB2	3:C:980:HOH:O	2.14	0.48
1:A:39:LYS:HD2	1:A:45:PHE:CE1	2.48	0.48
1:A:452:MET:HG3	1:A:487:TRP:CH2	2.49	0.48
1:D:261:MET:H	1:D:307:GLN:NE2	2.11	0.48
1:D:193:ALA:C	1:D:195:GLN:H	2.17	0.48
1:C:533:LEU:HD22	1:D:494:ARG:NH1	2.28	0.48
1:C:257:VAL:HG13	1:C:258:ASN:N	2.29	0.48
1:A:151:ASN:ND2	1:A:200:ASN:HD21	2.12	0.48
1:A:308:LEU:O	1:A:312:GLU:HG2	2.13	0.48
1:A:494:ARG:CG	1:A:495:PRO:HD2	2.43	0.48
1:C:343:PRO:HD2	1:C:388:TYR:OH	2.14	0.48
1:D:441:LEU:HD12	3:D:946:HOH:O	2.14	0.48
1:B:435:VAL:O	1:B:436:CYS:HB3	2.14	0.48
1:C:376:VAL:HG22	1:C:501:ASN:HB3	1.96	0.48
1:B:407:PRO:HB3	1:D:344:VAL:HG23	1.95	0.48
1:D:24:ASN:OD1	1:D:61:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:HD2	3:B:851:HOH:O	2.14	0.48
1:A:225:ARG:HG3	3:A:882:HOH:O	2.13	0.48
1:D:325:GLN:CA	1:D:325:GLN:HE21	2.17	0.48
1:A:299:ASN:N	1:A:299:ASN:HD22	2.11	0.48
1:D:64:GLU:O	1:D:65:LYS:HE3	2.14	0.48
1:D:180:LYS:HD2	3:D:928:HOH:O	2.13	0.48
1:A:131:ASN:HD22	1:A:131:ASN:N	2.10	0.48
1:B:257:VAL:HG13	1:B:272:HIS:CD2	2.49	0.47
1:D:247:THR:CG2	1:D:297:PRO:HG2	2.43	0.47
1:A:112:CYS:HA	1:B:386:ILE:HG21	1.96	0.47
1:A:122:GLU:OE1	1:A:122:GLU:N	2.48	0.47
1:D:360:LEU:O	1:D:360:LEU:HD13	2.14	0.47
1:B:20:THR:CG2	1:B:21:TYR:N	2.77	0.47
1:D:261:MET:HE1	1:D:311:HIS:HB2	1.95	0.47
1:C:386:ILE:HG21	1:D:112:CYS:HA	1.95	0.47
1:C:394:LYS:HB3	1:C:394:LYS:HZ3	1.78	0.47
1:D:71:ILE:HD13	1:D:243:TRP:HE3	1.79	0.47
1:D:137:VAL:HG13	3:D:696:HOH:O	2.14	0.47
1:B:229:ASN:O	1:B:233:GLU:HG3	2.15	0.47
1:C:412:LYS:HE2	1:C:414:ALA:HB2	1.96	0.47
1:D:220:LEU:O	1:D:224:ARG:HG3	2.14	0.47
1:D:266:GLN:NE2	1:D:270:ASN:HD21	2.12	0.47
1:D:254:SER:HB2	1:D:257:VAL:HB	1.97	0.47
1:B:500:VAL:O	1:B:500:VAL:HG13	2.13	0.47
1:D:248:GLU:H	1:D:298:GLN:NE2	2.12	0.47
1:C:372:SER:HB3	1:C:490:ALA:HB2	1.96	0.47
1:C:251:VAL:HG21	1:C:274:GLU:O	2.14	0.47
1:D:200:ASN:HD22	1:D:200:ASN:C	2.16	0.47
1:B:224:ARG:HD2	1:B:287:LEU:HD23	1.96	0.47
1:D:504:ASN:ND2	3:D:827:HOH:O	2.47	0.47
1:D:253:VAL:O	1:D:253:VAL:HG13	2.15	0.47
1:B:352:LEU:HD22	1:B:352:LEU:C	2.34	0.47
1:D:325:GLN:HG2	1:D:414:ALA:HB1	1.96	0.47
1:A:39:LYS:HB2	1:A:45:PHE:CE1	2.49	0.47
1:B:332:LEU:O	1:B:335:PHE:HB3	2.15	0.47
1:C:342:LYS:HB2	1:C:387:LEU:HG	1.97	0.47
1:C:229:ASN:HB3	1:C:233:GLU:OE1	2.14	0.47
1:C:481:LEU:HA	3:C:852:HOH:O	2.15	0.47
1:C:445:LEU:HG	1:C:487:TRP:CD1	2.50	0.47
1:D:71:ILE:HG21	1:D:243:TRP:CE3	2.49	0.47
1:C:296:SER:C	1:C:320:ASP:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:HIS:CD2	1:C:274:GLU:HB2	2.49	0.47
1:C:200:ASN:HD22	1:C:200:ASN:C	2.17	0.47
2:D:680:NAD:O2N	2:D:680:NAD:N7N	2.48	0.47
1:D:231:LYS:HE2	1:D:239:VAL:CG1	2.45	0.47
1:B:193:ALA:H	1:B:196:ASP:HB2	1.79	0.46
1:B:489:LYS:O	1:B:491:PRO:HD3	2.15	0.46
1:A:151:ASN:HB2	1:A:180:LYS:CE	2.45	0.46
1:A:345:SER:HA	1:A:397:ASP:O	2.15	0.46
1:D:22:LYS:HB2	1:D:25:GLU:HB3	1.97	0.46
1:C:257:VAL:HG13	1:C:258:ASN:H	1.79	0.46
1:A:476:ASN:HB3	3:A:875:HOH:O	2.15	0.46
1:B:198:ARG:NH2	1:B:355:ASN:HD21	2.12	0.46
1:B:38:THR:HG22	1:B:39:LYS:N	2.30	0.46
1:B:131:ASN:ND2	1:B:131:ASN:C	2.69	0.46
1:A:84:SER:HB3	1:B:423:MET:HE3	1.96	0.46
1:A:54:TYR:CE2	1:B:532:LEU:HD23	2.50	0.46
1:D:167:ASP:O	1:D:171:ARG:HG3	2.15	0.46
1:D:262:GLU:HA	1:D:262:GLU:OE2	2.16	0.46
1:B:216:LYS:O	1:B:219:HIS:HB2	2.15	0.46
1:C:217:TRP:O	1:C:220:LEU:HB3	2.14	0.46
1:D:151:ASN:C	1:D:151:ASN:HD22	2.17	0.46
1:A:131:ASN:HD22	1:A:131:ASN:H	1.63	0.46
1:B:73:LEU:HD23	1:B:181:PRO:HB3	1.98	0.46
1:D:37:VAL:HG22	1:D:47:VAL:HG22	1.97	0.46
1:A:206:ASP:OD1	1:A:208:LYS:N	2.48	0.46
1:D:206:ASP:N	1:D:210:ASN:O	2.38	0.46
1:A:45:PHE:HB2	1:B:12:VAL:HG22	1.98	0.46
1:A:453:THR:O	1:A:457:THR:HG23	2.15	0.46
1:A:516:LEU:C	1:A:516:LEU:HD12	2.35	0.46
1:B:10:THR:N	3:B:917:HOH:O	2.48	0.46
1:B:248:GLU:HB2	1:B:298:GLN:HG2	1.97	0.46
1:B:39:LYS:HE2	1:B:43:GLY:HA2	1.98	0.46
1:A:192:ALA:O	1:A:193:ALA:C	2.53	0.46
1:C:262:GLU:HB2	3:C:830:HOH:O	2.16	0.46
1:D:40:THR:CG2	1:D:44:ARG:H	2.28	0.46
1:D:153:ASP:OD2	1:D:155:TYR:HB3	2.16	0.46
1:A:299:ASN:HD22	1:A:299:ASN:H	1.64	0.46
1:D:38:THR:HG23	1:D:38:THR:O	2.16	0.46
1:D:121:ALA:HB3	1:D:122:GLU:OE2	2.16	0.46
1:A:494:ARG:HG3	1:A:495:PRO:HD2	1.98	0.46
1:B:489:LYS:C	1:B:491:PRO:HD3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TYR:CE1	1:B:26:LEU:HD23	2.51	0.45
1:D:329:LYS:NZ	1:D:348:SER:HB2	2.31	0.45
1:D:452:MET:HG3	1:D:487:TRP:CH2	2.50	0.45
1:C:473:LYS:O	1:C:473:LYS:HG2	2.16	0.45
1:C:363:PRO:HA	1:C:366:PHE:HB3	1.98	0.45
1:D:150:ASN:HA	1:D:200:ASN:ND2	2.31	0.45
1:B:250:TYR:HD1	3:B:858:HOH:O	1.98	0.45
1:C:413:VAL:HG22	1:C:435:VAL:HG22	1.97	0.45
1:B:453:THR:O	1:B:457:THR:HG23	2.16	0.45
1:B:246:ASN:HB3	3:B:987:HOH:O	2.15	0.45
1:A:389:ASN:OD1	1:A:392:LEU:HD23	2.16	0.45
1:A:131:ASN:ND2	1:A:131:ASN:H	2.14	0.45
1:A:187:TYR:HA	1:A:188:PRO:HD2	1.79	0.45
1:B:18:LYS:O	1:B:28:THR:HA	2.16	0.45
1:B:220:LEU:O	1:B:220:LEU:HD23	2.16	0.45
1:A:404:TYR:OH	1:A:406:LYS:HG2	2.17	0.45
1:B:323:SER:N	1:B:489:LYS:HE3	2.17	0.45
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.96	0.45
1:D:71:ILE:HG21	1:D:243:TRP:CZ3	2.52	0.45
1:A:76:ASN:HB3	1:A:439:SER:OG	2.17	0.45
1:B:480:VAL:CG2	1:B:480:VAL:O	2.63	0.45
1:C:175:LYS:NZ	3:C:962:HOH:O	2.49	0.45
1:A:405:MET:O	1:A:408:VAL:HG23	2.16	0.45
1:C:198:ARG:NH2	1:C:355:ASN:ND2	2.65	0.45
1:A:328:LEU:HD21	1:B:332:LEU:HD23	1.98	0.45
1:B:115:LEU:HG	1:B:511:GLU:HG3	1.97	0.45
1:C:293:ILE:HA	1:C:317:ALA:O	2.17	0.45
1:B:198:ARG:HH22	1:B:355:ASN:ND2	2.15	0.45
1:D:445:LEU:HD23	1:D:445:LEU:C	2.37	0.45
1:A:248:GLU:OE2	1:A:277:PRO:HD2	2.17	0.45
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.52	0.45
1:B:192:ALA:O	1:B:193:ALA:HB3	2.17	0.45
1:C:364:LYS:HB2	1:C:365:GLN:NE2	2.31	0.45
1:A:208:LYS:HB2	1:A:210:ASN:OD1	2.17	0.45
1:B:206:ASP:OD1	1:B:209:GLY:N	2.49	0.45
1:C:371:ILE:HG22	1:C:372:SER:N	2.31	0.45
1:B:348:SER:C	1:B:349:TYR:CD1	2.90	0.45
1:B:195:GLN:N	1:B:195:GLN:NE2	2.65	0.45
1:D:412:LYS:HE3	1:D:438:ASP:CG	2.38	0.45
1:C:500:VAL:HG21	1:D:527:ARG:HE	1.79	0.45
1:D:121:ALA:N	3:D:740:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:TRP:O	1:D:221:GLN:HG3	2.17	0.45
1:B:452:MET:HG3	1:B:487:TRP:CH2	2.52	0.45
1:D:526:LEU:O	1:D:531:ARG:NE	2.43	0.45
1:B:322:LYS:HA	1:B:489:LYS:CG	2.32	0.45
1:D:352:LEU:HA	1:D:412:LYS:CA	2.42	0.45
1:A:225:ARG:HH11	1:A:228:GLN:NE2	2.14	0.45
1:B:315:PHE:CD1	1:B:481:LEU:HD11	2.51	0.45
1:A:489:LYS:HD3	3:A:986:HOH:O	2.16	0.45
1:D:261:MET:HE2	1:D:308:LEU:HA	1.99	0.44
1:B:218:THR:HG23	3:B:984:HOH:O	2.18	0.44
1:C:352:LEU:N	1:C:352:LEU:HD23	2.32	0.44
1:C:55:VAL:CG2	1:C:464:VAL:HG11	2.47	0.44
1:C:34:ASN:CG	1:C:35:ALA:H	2.20	0.44
1:C:319:ASP:HB2	1:C:490:ALA:O	2.18	0.44
1:C:22:LYS:HB3	1:C:22:LYS:NZ	2.32	0.44
1:A:299:ASN:N	1:A:299:ASN:ND2	2.65	0.44
1:A:65:LYS:NZ	3:A:996:HOH:O	2.50	0.44
1:B:272:HIS:HB3	1:B:275:ILE:HG12	1.99	0.44
1:C:315:PHE:CD1	1:C:481:LEU:HD11	2.53	0.44
1:D:190:PHE:O	1:D:249:ARG:HG3	2.17	0.44
1:A:351:HIS:CD2	1:C:349:TYR:OH	2.69	0.44
1:C:148:ASP:HA	2:C:670:NAD:N3A	2.32	0.44
1:C:204:ASN:HB3	1:C:219:HIS:CE1	2.52	0.44
1:C:335:PHE:HE2	1:D:327:LYS:HB3	1.82	0.44
1:B:148:ASP:HA	2:B:660:NAD:N3A	2.32	0.44
1:A:452:MET:HG3	1:A:487:TRP:HH2	1.83	0.44
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.99	0.44
1:A:352:LEU:HD22	1:A:352:LEU:O	2.18	0.44
1:B:198:ARG:NH2	1:B:355:ASN:ND2	2.66	0.44
1:B:180:LYS:HB3	3:B:732:HOH:O	2.17	0.44
1:D:505:LYS:HG2	3:D:950:HOH:O	2.15	0.44
1:C:497:PHE:CD2	1:D:530:GLU:HG2	2.53	0.44
1:C:335:PHE:CE2	1:D:327:LYS:HB3	2.53	0.44
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.17	0.44
1:A:322:LYS:NZ	3:A:847:HOH:O	2.50	0.44
1:A:224:ARG:NH1	1:A:287:LEU:HD13	2.33	0.44
1:D:247:THR:HG21	1:D:297:PRO:HG2	1.99	0.44
1:D:523:GLN:HE21	1:D:523:GLN:HA	1.83	0.44
1:C:296:SER:O	1:C:319:ASP:HA	2.17	0.44
1:C:372:SER:O	1:C:489:LYS:HG2	2.17	0.44
1:B:349:TYR:N	1:B:349:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LEU:HD22	1:D:308:LEU:O	2.18	0.44
1:D:134:LEU:HB3	1:D:135:PRO:HD2	1.99	0.44
1:D:315:PHE:CZ	1:D:481:LEU:HD21	2.52	0.44
1:A:234:ASN:HB2	1:A:236:LEU:HG	2.00	0.44
1:C:503:LEU:HA	1:C:506:GLN:OE1	2.18	0.44
1:D:347:ALA:HB1	1:D:349:TYR:CE2	2.52	0.43
1:C:445:LEU:C	1:C:445:LEU:HD23	2.38	0.43
1:D:96:THR:HG21	1:D:101:LYS:HD2	1.99	0.43
1:A:158:MET:HE2	1:A:176:MET:HG3	1.98	0.43
1:A:246:ASN:HD22	1:A:359:ASN:HD22	1.66	0.43
1:B:348:SER:CB	1:B:416:ASP:OD2	2.66	0.43
1:D:119:ILE:HA	1:D:124:ASN:O	2.18	0.43
1:D:315:PHE:CD1	1:D:481:LEU:HD11	2.53	0.43
1:B:71:ILE:HG21	1:B:243:TRP:CZ3	2.53	0.43
1:D:22:LYS:HE3	1:D:27:LEU:CD1	2.40	0.43
1:B:352:LEU:HD21	1:B:356:ASP:O	2.18	0.43
1:D:352:LEU:HB3	1:D:412:LYS:CB	2.46	0.43
1:A:172:LEU:O	1:A:176:MET:HG2	2.18	0.43
1:C:112:CYS:HB3	1:D:387:LEU:HD11	1.99	0.43
1:C:259:ASP:N	1:C:259:ASP:OD2	2.51	0.43
1:D:272:HIS:CD2	1:D:274:GLU:H	2.36	0.43
1:A:117:LEU:HB3	3:A:798:HOH:O	2.18	0.43
1:A:134:LEU:HD11	1:A:517:LEU:HB2	2.00	0.43
1:B:91:ASN:HB3	3:B:752:HOH:O	2.17	0.43
1:B:310:GLU:HA	1:B:479:PRO:HG3	2.00	0.43
1:C:358:TYR:HB2	1:C:404:TYR:CE1	2.54	0.43
1:B:462:LYS:HD2	1:B:472:GLY:O	2.17	0.43
1:D:465:ASP:HB3	1:D:468:LYS:HB3	2.00	0.43
1:A:381:ILE:HG23	1:A:388:TYR:CB	2.49	0.43
1:B:355:ASN:HB3	2:B:660:NAD:O1A	2.18	0.43
1:B:117:LEU:HD21	1:B:133:LEU:CD2	2.48	0.43
1:D:295:GLY:CA	1:D:321:LEU:HD13	2.48	0.43
1:B:183:PRO:HB2	1:B:203:ILE:CG2	2.48	0.43
1:D:447:ILE:O	1:D:451:VAL:HG23	2.18	0.43
1:C:478:TYR:CE2	1:C:494:ARG:HG2	2.53	0.43
1:C:22:LYS:HB3	1:C:25:GLU:HB2	2.00	0.43
1:C:350:ASN:HB3	1:C:414:ALA:HA	2.00	0.43
1:B:333:ALA:O	1:B:337:VAL:HG22	2.18	0.43
1:B:352:LEU:CD1	1:B:352:LEU:N	2.82	0.43
1:D:40:THR:HG21	1:D:44:ARG:HH12	1.75	0.43
1:C:257:VAL:HG21	1:C:272:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:LEU:HD21	1:C:487:TRP:HB2	2.01	0.43
1:A:148:ASP:HA	2:A:650:NAD:N3A	2.33	0.43
1:D:266:GLN:HE21	1:D:270:ASN:ND2	2.16	0.43
1:C:256:GLY:H	1:C:259:ASP:CG	2.22	0.43
1:C:174:ALA:HB2	3:C:933:HOH:O	2.18	0.43
1:C:282:ALA:O	1:C:286:ILE:HG13	2.19	0.43
1:B:109:MET:HE3	1:B:486:TYR:CZ	2.54	0.43
1:D:352:LEU:HD22	1:D:354:ASN:OD1	2.18	0.43
1:B:266:GLN:HE21	1:B:270:ASN:ND2	2.14	0.43
1:A:286:ILE:HG23	1:A:314:THR:CG2	2.48	0.43
1:D:200:ASN:ND2	1:D:200:ASN:C	2.71	0.43
1:A:224:ARG:O	1:A:228:GLN:HG3	2.19	0.43
1:C:272:HIS:HD2	1:C:274:GLU:H	1.62	0.43
1:C:115:LEU:HD22	1:C:511:GLU:HG2	1.99	0.43
1:A:501:ASN:ND2	3:A:795:HOH:O	2.51	0.43
1:D:286:ILE:HG23	1:D:314:THR:OG1	2.19	0.43
1:D:452:MET:HG3	1:D:487:TRP:HH2	1.84	0.43
1:A:134:LEU:HD11	1:A:517:LEU:CB	2.49	0.43
1:D:497:PHE:N	1:D:497:PHE:CD1	2.87	0.43
1:C:483:PHE:HA	1:D:531:ARG:NH2	2.34	0.43
1:B:195:GLN:HG2	1:B:246:ASN:ND2	2.34	0.43
1:C:14:VAL:O	1:C:16:THR:HG22	2.18	0.43
1:A:286:ILE:HG21	1:A:308:LEU:HD22	2.01	0.43
1:B:351:HIS:CD2	1:D:349:TYR:OH	2.72	0.42
1:D:90:HIS:HE1	3:D:790:HOH:O	2.01	0.42
1:C:476:ASN:HA	3:C:991:HOH:O	2.18	0.42
1:C:335:PHE:CE1	1:D:328:LEU:CD1	3.03	0.42
1:D:435:VAL:O	1:D:436:CYS:HB3	2.19	0.42
1:B:40:THR:OG1	1:B:44:ARG:HB3	2.19	0.42
1:D:301:PHE:CD1	1:D:492:LEU:HD12	2.54	0.42
1:C:112:CYS:HB3	1:D:387:LEU:HD13	2.01	0.42
1:B:449:LEU:HD21	1:B:487:TRP:HB2	2.01	0.42
1:B:412:LYS:HE3	1:B:412:LYS:HB2	1.78	0.42
1:A:352:LEU:CD2	1:A:354:ASN:ND2	2.78	0.42
2:C:670:NAD:O2N	2:C:670:NAD:N7N	2.52	0.42
1:A:22:LYS:O	1:A:25:GLU:HB3	2.20	0.42
1:B:261:MET:O	1:B:265:LEU:HG	2.19	0.42
1:C:362:ALA:HB3	1:C:365:GLN:CG	2.46	0.42
1:A:448:ASP:HB3	1:A:487:TRP:CE2	2.54	0.42
1:B:42:SER:C	1:B:44:ARG:N	2.72	0.42
1:A:250:TYR:CE2	1:A:298:GLN:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HE2	3:A:699:HOH:O	2.19	0.42
1:D:194:ASN:HB2	1:D:358:TYR:CE2	2.55	0.42
1:C:495:PRO:HG2	1:C:496:GLY:H	1.82	0.42
1:C:461:TYR:OH	1:D:533:LEU:N	2.52	0.42
1:D:155:TYR:O	1:D:159:GLN:HG3	2.20	0.42
1:C:18:LYS:HA	1:C:29:LYS:CE	2.50	0.42
1:A:220:LEU:CD2	1:A:280:ILE:HG23	2.47	0.42
1:C:112:CYS:HA	1:D:386:ILE:HG21	2.00	0.42
1:A:418:TYR:O	1:A:429:ARG:HA	2.20	0.42
1:B:189:ASP:O	1:B:249:ARG:HD2	2.19	0.42
1:A:96:THR:HG21	1:A:101:LYS:HD2	2.02	0.42
1:D:187:TYR:CD1	1:D:277:PRO:HG3	2.55	0.42
1:B:201:ASN:HA	1:B:201:ASN:HD22	1.65	0.42
1:C:322:LYS:HD2	1:C:327:LYS:HE2	2.00	0.42
1:A:407:PRO:HG3	1:C:395:LYS:CE	2.47	0.42
1:A:322:LYS:HZ1	1:A:506:GLN:HE22	1.66	0.42
1:B:459:VAL:HB	1:B:477:PHE:CE1	2.54	0.42
1:B:139:PRO:HA	1:B:142:PHE:CD2	2.54	0.42
1:C:76:ASN:HB3	1:C:439:SER:OG	2.19	0.42
1:A:110:THR:HA	1:A:130:PHE:CD2	2.54	0.42
1:A:137:VAL:HG12	3:A:651:HOH:O	2.19	0.42
1:A:354:ASN:HD22	1:A:354:ASN:C	2.22	0.42
1:B:405:MET:C	1:B:407:PRO:HD2	2.40	0.42
1:B:310:GLU:CG	1:B:479:PRO:HG3	2.45	0.42
1:B:42:SER:O	1:B:44:ARG:N	2.50	0.42
1:D:205:LEU:HA	1:D:210:ASN:O	2.20	0.42
1:A:259:ASP:HA	1:A:303:PRO:HG2	2.02	0.42
1:D:239:VAL:O	1:D:290:VAL:HG13	2.20	0.42
1:A:187:TYR:CD1	1:A:213:THR:HG22	2.55	0.42
1:A:405:MET:CE	1:C:397:ASP:HB3	2.50	0.42
1:C:200:ASN:C	1:C:200:ASN:ND2	2.73	0.42
1:B:350:ASN:HD21	1:B:402:ILE:HG12	1.85	0.42
1:C:69:MET:HE2	1:C:227:ILE:HG23	2.01	0.42
1:D:325:GLN:HG2	3:D:785:HOH:O	2.19	0.42
1:B:26:LEU:HD22	1:B:27:LEU:N	2.34	0.42
1:B:454:GLU:OE1	1:B:458:ARG:NH2	2.53	0.42
1:A:79:SER:HB3	3:A:740:HOH:O	2.19	0.42
1:B:183:PRO:HB2	1:B:203:ILE:HG23	2.02	0.42
1:A:184:SER:OG	1:A:185:ILE:N	2.52	0.42
1:A:90:HIS:HE1	3:A:784:HOH:O	2.02	0.42
1:A:389:ASN:ND2	1:A:392:LEU:HD21	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG23	1:D:290:VAL:HG11	2.02	0.41
1:C:406:LYS:HB3	1:C:407:PRO:HD3	2.01	0.41
1:D:294:ASN:ND2	3:D:726:HOH:O	2.53	0.41
1:D:492:LEU:HD23	1:D:493:THR:N	2.35	0.41
1:A:350:ASN:ND2	1:A:412:LYS:HE3	2.35	0.41
1:C:22:LYS:HE3	3:C:773:HOH:O	2.20	0.41
1:D:384:ASN:O	1:D:388:TYR:HB2	2.21	0.41
1:A:185:ILE:HD11	1:A:223:ILE:CD1	2.51	0.41
1:B:350:ASN:O	1:B:402:ILE:HA	2.20	0.41
1:D:266:GLN:HE21	1:D:270:ASN:HD21	1.69	0.41
1:C:462:LYS:HD2	1:C:473:LYS:HD3	2.02	0.41
1:A:247:THR:CG2	1:A:297:PRO:HG2	2.51	0.41
1:C:398:HIS:CD2	1:C:398:HIS:N	2.89	0.41
1:D:530:GLU:O	1:D:531:ARG:C	2.58	0.41
1:D:352:LEU:HD11	1:D:357:GLY:CA	2.44	0.41
1:B:27:LEU:HD22	1:B:27:LEU:N	2.35	0.41
1:D:527:ARG:C	1:D:529:GLU:H	2.23	0.41
1:D:39:LYS:HE2	1:D:43:GLY:HA2	2.03	0.41
1:B:253:VAL:O	1:B:253:VAL:HG22	2.21	0.41
1:D:353:GLY:O	1:D:410:ASP:N	2.53	0.41
1:C:532:LEU:O	1:C:533:LEU:OXT	2.39	0.41
1:B:408:VAL:HB	1:B:411:SER:O	2.21	0.41
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.21	0.41
1:C:254:SER:N	1:C:258:ASN:HD21	2.18	0.41
1:C:30:TYR:CD1	1:C:516:LEU:HG	2.56	0.41
1:B:253:VAL:HA	1:B:258:ASN:OD1	2.21	0.41
1:C:312:GLU:OE1	3:C:873:HOH:O	2.22	0.41
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.56	0.41
1:A:285:SER:HB3	1:A:290:VAL:CG2	2.51	0.41
1:D:530:GLU:O	1:D:532:LEU:N	2.53	0.41
1:C:327:LYS:O	1:C:331:VAL:HG23	2.21	0.41
1:C:193:ALA:C	1:C:195:GLN:H	2.23	0.41
1:C:356:ASP:O	1:C:360:LEU:HD23	2.20	0.41
1:C:477:PHE:HD1	3:C:991:HOH:O	2.04	0.41
1:C:298:GLN:H	1:C:298:GLN:HG3	1.45	0.41
1:D:323:SER:O	1:D:327:LYS:HG3	2.21	0.41
1:D:494:ARG:HB3	1:D:495:PRO:HD2	2.03	0.41
1:B:351:HIS:HD2	1:D:349:TYR:OH	2.03	0.41
1:A:532:LEU:HD23	1:B:54:TYR:CE2	2.56	0.41
1:A:528:PHE:C	1:A:530:GLU:H	2.24	0.41
1:C:349:TYR:CD1	1:C:401:VAL:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ASN:HB2	1:C:198:ARG:HG2	2.03	0.41
1:B:212:THR:HG22	1:B:214:ARG:N	2.27	0.41
1:B:248:GLU:N	1:B:298:GLN:HG2	2.27	0.41
1:A:256:GLY:C	1:A:263:ASN:HD22	2.24	0.41
1:A:65:LYS:HE2	1:A:141:ASP:HA	2.03	0.41
1:C:362:ALA:HA	1:C:363:PRO:HD2	1.90	0.41
1:C:134:LEU:HD21	1:C:518:ILE:CG2	2.51	0.41
1:D:289:GLY:HA2	1:D:314:THR:HG22	2.01	0.41
1:D:261:MET:HE3	1:D:307:GLN:HG2	2.03	0.41
1:A:347:ALA:HB1	1:A:349:TYR:CE2	2.55	0.41
1:A:285:SER:HB3	1:A:290:VAL:HG23	2.01	0.41
1:A:175:LYS:NZ	3:A:806:HOH:O	2.48	0.41
1:A:44:ARG:HH11	1:B:13:LYS:CB	2.34	0.41
1:B:516:LEU:C	1:B:516:LEU:HD12	2.41	0.41
1:C:249:ARG:HG3	1:C:249:ARG:HH21	1.86	0.41
1:A:69:MET:HE1	1:A:227:ILE:CA	2.30	0.41
1:D:437:GLU:H	1:D:437:GLU:HG2	1.44	0.41
1:C:112:CYS:SG	1:D:387:LEU:HD11	2.61	0.41
1:B:423:MET:CE	1:B:424:LEU:HD22	2.50	0.41
1:D:41:ALA:C	1:D:43:GLY:H	2.24	0.41
1:C:69:MET:CE	1:C:227:ILE:HA	2.51	0.40
1:D:52:GLN:HG3	1:D:54:TYR:CE1	2.56	0.40
1:A:533:LEU:HD21	1:B:463:LYS:HE2	2.03	0.40
1:B:494:ARG:HB2	1:B:497:PHE:CD1	2.56	0.40
1:D:527:ARG:C	1:D:529:GLU:N	2.74	0.40
1:B:404:TYR:OH	1:B:406:LYS:HB2	2.21	0.40
1:D:297:PRO:HD3	1:D:320:ASP:OD1	2.21	0.40
1:D:523:GLN:HA	1:D:523:GLN:NE2	2.36	0.40
1:A:394:LYS:O	1:A:394:LYS:CG	2.69	0.40
1:C:318:GLY:HA2	1:C:488:LEU:HD21	2.03	0.40
1:D:354:ASN:C	1:D:356:ASP:H	2.25	0.40
1:A:403:LYS:HE3	1:C:401:VAL:HG22	2.04	0.40
1:B:325:GLN:CA	1:B:325:GLN:HE21	2.29	0.40
1:A:266:GLN:HA	1:A:269:LYS:HD2	2.04	0.40
1:C:20:THR:HB	1:C:27:LEU:HB2	2.04	0.40
1:D:133:LEU:HD12	1:D:133:LEU:N	2.37	0.40
1:B:316:ILE:HD11	1:B:480:VAL:HG12	2.03	0.40
1:A:158:MET:HE1	1:A:176:MET:HG3	2.02	0.40
1:A:445:LEU:HG	1:A:487:TRP:CD1	2.56	0.40
1:B:183:PRO:HD2	3:B:811:HOH:O	2.21	0.40
1:A:191:ILE:HG22	1:A:359:ASN:HD21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PRO:HG2	1:B:458:ARG:NH1	2.36	0.40
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.96	0.40
1:D:462:LYS:HE2	1:D:472:GLY:O	2.22	0.40
1:C:248:GLU:HB2	1:C:298:GLN:HE21	1.85	0.40
1:C:271:ASP:O	1:C:272:HIS:C	2.59	0.40
1:A:478:TYR:HA	1:B:533:LEU:HD21	2.04	0.40
1:D:260:THR:HB	1:D:307:GLN:HE22	1.86	0.40
1:B:70:LEU:HD11	1:B:81:LEU:CD2	2.50	0.40
1:B:265:LEU:O	1:B:269:LYS:HG3	2.20	0.40
1:A:102:GLN:NE2	3:A:811:HOH:O	2.46	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	502/533 (94%)	465 (93%)	28 (6%)	9 (2%)	11	2
1	B	485/533 (91%)	445 (92%)	32 (7%)	8 (2%)	12	3
1	C	513/533 (96%)	474 (92%)	27 (5%)	12 (2%)	8	1
1	D	481/533 (90%)	445 (92%)	28 (6%)	8 (2%)	11	3
All	All	1981/2132 (93%)	1829 (92%)	115 (6%)	37 (2%)	10	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	A	211	VAL
1	A	319	ASP
1	A	495	PRO
1	B	192	ALA

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Mol	Chain	Res	Type
1	B	319	ASP
1	C	193	ALA
1	D	319	ASP
1	B	191	ILE
1	C	199	ALA
1	C	319	ASP
1	D	531	ARG
1	A	195	GLN
1	B	193	ALA
1	B	347	ALA
1	C	22	LYS
1	C	189	ASP
1	C	194	ASN
1	C	272	HIS
1	C	322	LYS
1	D	23	ASP
1	D	470	ASP
1	B	320	ASP
1	A	212	THR
1	C	320	ASP
1	C	502	GLY
1	D	355	ASN
1	A	42	SER
1	A	479	PRO
1	A	502	GLY
1	D	194	ASN
1	B	502	GLY
1	B	346	ILE
1	C	495	PRO
1	D	346	ILE
1	D	479	PRO
1	C	464	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/471 (95%)	418 (94%)	28 (6%)	22	8
1	B	434/471 (92%)	412 (95%)	22 (5%)	29	13
1	C	458/471 (97%)	435 (95%)	23 (5%)	30	14
1	D	429/471 (91%)	403 (94%)	26 (6%)	23	9
All	All	1767/1884 (94%)	1668 (94%)	99 (6%)	26	11

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	47	VAL
1	A	65	LYS
1	A	79	SER
1	A	122	GLU
1	A	131	ASN
1	A	151	ASN
1	A	154	LEU
1	A	191	ILE
1	A	194	ASN
1	A	207	GLU
1	A	237	ASP
1	A	251	VAL
1	A	262	GLU
1	A	298	GLN
1	A	299	ASN
1	A	308	LEU
1	A	319	ASP
1	A	328	LEU
1	A	332	LEU
1	A	352	LEU
1	A	354	ASN
1	A	392	LEU
1	A	398	HIS
1	A	438	ASP
1	A	483	PHE
1	A	495	PRO
1	A	497	PHE
1	B	14	VAL
1	B	25	GLU
1	B	26	LEU
1	B	34	ASN
1	B	115	LEU

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Mol	Chain	Res	Type
1	B	131	ASN
1	B	194	ASN
1	B	195	GLN
1	B	200	ASN
1	B	201	ASN
1	B	205	LEU
1	B	207	GLU
1	B	218	THR
1	B	237	ASP
1	B	298	GLN
1	B	319	ASP
1	B	328	LEU
1	B	352	LEU
1	B	356	ASP
1	B	424	LEU
1	B	483	PHE
1	B	520	LEU
1	C	16	THR
1	C	22	LYS
1	C	62	LYS
1	C	200	ASN
1	C	201	ASN
1	C	236	LEU
1	C	238	LYS
1	C	251	VAL
1	C	258	ASN
1	C	298	GLN
1	C	308	LEU
1	C	334	GLN
1	C	364	LYS
1	C	387	LEU
1	C	394	LYS
1	C	397	ASP
1	C	398	HIS
1	C	440	LEU
1	C	441	LEU
1	C	483	PHE
1	C	488	LEU
1	C	516	LEU
1	C	523	GLN
1	D	24	ASN
1	D	25	GLU

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Mol	Chain	Res	Type
1	D	34	ASN
1	D	70	LEU
1	D	151	ASN
1	D	200	ASN
1	D	214	ARG
1	D	225	ARG
1	D	236	LEU
1	D	239	VAL
1	D	252	GLU
1	D	298	GLN
1	D	308	LEU
1	D	319	ASP
1	D	325	GLN
1	D	332	LEU
1	D	352	LEU
1	D	380	ILE
1	D	390	ASP
1	D	434	ASN
1	D	436	CYS
1	D	437	GLU
1	D	440	LEU
1	D	467	VAL
1	D	469	GLU
1	D	473	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	ASN
1	A	88	ASN
1	A	90	HIS
1	A	102	GLN
1	A	131	ASN
1	A	151	ASN
1	A	159	GLN
1	A	169	GLN
1	A	170	GLN
1	A	228	GLN
1	A	266	GLN
1	A	298	GLN
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	325	GLN
1	A	351	HIS
1	A	354	ASN
1	A	359	ASN
1	A	398	HIS
1	A	428	ASN
1	A	433	HIS
1	A	506	GLN
1	A	512	ASN
1	B	34	ASN
1	B	95	GLN
1	B	102	GLN
1	B	131	ASN
1	B	159	GLN
1	B	169	GLN
1	B	170	GLN
1	B	195	GLN
1	B	200	ASN
1	B	201	ASN
1	B	228	GLN
1	B	229	ASN
1	B	263	ASN
1	B	270	ASN
1	B	298	GLN
1	B	325	GLN
1	B	351	HIS
1	B	501	ASN
1	B	506	GLN
1	B	512	ASN
1	B	523	GLN
1	C	24	ASN
1	C	77	ASN
1	C	90	HIS
1	C	150	ASN
1	C	151	ASN
1	C	169	GLN
1	C	170	GLN
1	C	195	GLN
1	C	200	ASN
1	C	201	ASN
1	C	221	GLN
1	C	228	GLN

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	263	ASN
1	C	272	HIS
1	C	298	GLN
1	C	307	GLN
1	C	325	GLN
1	C	334	GLN
1	C	355	ASN
1	C	365	GLN
1	C	512	ASN
1	C	523	GLN
1	D	24	ASN
1	D	34	ASN
1	D	52	GLN
1	D	76	ASN
1	D	88	ASN
1	D	90	HIS
1	D	151	ASN
1	D	159	GLN
1	D	169	GLN
1	D	195	GLN
1	D	200	ASN
1	D	228	GLN
1	D	246	ASN
1	D	263	ASN
1	D	266	GLN
1	D	270	ASN
1	D	272	HIS
1	D	294	ASN
1	D	298	GLN
1	D	307	GLN
1	D	325	GLN
1	D	334	GLN
1	D	434	ASN
1	D	476	ASN
1	D	504	ASN
1	D	512	ASN
1	D	523	GLN

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	650	-	38,48,48	1.81	6 (15%)	47,73,73	1.49	6 (12%)
2	NAD	B	660	-	38,48,48	1.93	8 (21%)	47,73,73	1.39	6 (12%)
2	NAD	C	670	-	38,48,48	1.68	6 (15%)	47,73,73	1.60	7 (14%)
2	NAD	D	680	-	38,48,48	1.82	7 (18%)	47,73,73	1.58	8 (17%)

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	650	-	-	0/22/62/62	0/5/5/5
2	NAD	B	660	-	-	0/22/62/62	0/5/5/5
2	NAD	C	670	-	-	0/22/62/62	0/5/5/5
2	NAD	D	680	-	-	0/22/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	680	NAD	O4B-C1B	-2.85	1.37	1.41
2	B	660	NAD	O4B-C1B	-2.32	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	670	NAD	C4A-N3A	2.06	1.38	1.35
2	A	650	NAD	C4A-N3A	2.40	1.39	1.35
2	D	680	NAD	C4A-N3A	2.41	1.39	1.35
2	B	660	NAD	C2N-C3N	2.48	1.42	1.39
2	B	660	NAD	C4A-N3A	2.49	1.39	1.35
2	A	650	NAD	C3N-C7N	2.56	1.54	1.50
2	D	680	NAD	C3N-C7N	2.83	1.55	1.50
2	C	670	NAD	C2A-N1A	2.86	1.39	1.33
2	C	670	NAD	C3N-C7N	3.18	1.55	1.50
2	C	670	NAD	C5N-C4N	3.19	1.45	1.38
2	D	680	NAD	C5N-C4N	3.25	1.45	1.38
2	A	650	NAD	C5N-C4N	3.29	1.45	1.38
2	D	680	NAD	C2A-N1A	3.54	1.40	1.33
2	A	650	NAD	C2A-N1A	3.60	1.40	1.33
2	B	660	NAD	C3N-C7N	3.68	1.56	1.50
2	B	660	NAD	C6N-N1N	3.74	1.45	1.35
2	B	660	NAD	C5N-C4N	3.74	1.46	1.38
2	B	660	NAD	C2A-N1A	3.85	1.41	1.33
2	C	670	NAD	C6N-N1N	4.08	1.46	1.35
2	A	650	NAD	C6N-N1N	4.13	1.46	1.35
2	D	680	NAD	C6N-N1N	4.21	1.46	1.35
2	C	670	NAD	C4N-C3N	5.50	1.48	1.39
2	D	680	NAD	C4N-C3N	6.08	1.49	1.39
2	A	650	NAD	C4N-C3N	6.14	1.49	1.39
2	B	660	NAD	C4N-C3N	6.23	1.50	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	670	NAD	O7N-C7N-N7N	-3.52	117.64	122.59
2	D	680	NAD	O7N-C7N-N7N	-3.18	118.12	122.59
2	D	680	NAD	C1B-N9A-C4A	-3.09	122.28	126.94
2	B	660	NAD	O7N-C7N-N7N	-2.88	118.54	122.59
2	C	670	NAD	C1B-N9A-C4A	-2.76	122.77	126.94
2	A	650	NAD	O7N-C7N-N7N	-2.68	118.82	122.59
2	C	670	NAD	N3A-C2A-N1A	-2.63	126.88	128.89
2	A	650	NAD	N3A-C2A-N1A	-2.55	126.94	128.89
2	B	660	NAD	C1B-N9A-C4A	-2.45	123.25	126.94
2	D	680	NAD	N3A-C2A-N1A	-2.10	127.29	128.89
2	B	660	NAD	N3A-C2A-N1A	-2.05	127.33	128.89
2	B	660	NAD	C4A-C5A-N7A	2.07	111.38	109.48
2	D	680	NAD	O4D-C4D-C3D	2.09	109.35	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	670	NAD	O2A-PA-O3	2.16	114.90	105.09
2	D	680	NAD	C4A-C5A-N7A	2.18	111.49	109.48
2	D	680	NAD	O2A-PA-O3	2.42	116.07	105.09
2	A	650	NAD	O2A-PA-O3	2.46	116.25	105.09
2	A	650	NAD	C4A-C5A-N7A	2.68	111.94	109.48
2	C	670	NAD	C3N-C7N-N7N	2.88	120.97	117.82
2	C	670	NAD	C4A-C5A-N7A	2.89	112.13	109.48
2	D	680	NAD	C3N-C7N-N7N	3.39	121.53	117.82
2	A	650	NAD	C3N-C7N-N7N	3.81	121.99	117.82
2	B	660	NAD	C3N-C7N-N7N	4.13	122.34	117.82
2	B	660	NAD	O4D-C1D-N1N	5.12	113.76	108.13
2	A	650	NAD	O4D-C1D-N1N	6.10	114.84	108.13
2	D	680	NAD	O4D-C1D-N1N	7.09	115.92	108.13
2	C	670	NAD	O4D-C1D-N1N	7.22	116.06	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	650	NAD	3	0
2	B	660	NAD	3	0
2	C	670	NAD	5	0
2	D	680	NAD	1	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, 95th 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	506/533 (94%)	0.71	76 (15%) 3 5	24, 45, 85, 90	0
1	B	491/533 (92%)	0.77	82 (16%) 2 3	23, 45, 88, 90	0
1	C	517/533 (96%)	0.71	73 (14%) 4 6	22, 45, 86, 90	0
1	D	487/533 (91%)	0.67	71 (14%) 3 5	21, 41, 88, 90	0
All	All	2001/2132 (93%)	0.71	302 (15%) 3 5	21, 44, 87, 90	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	ALA	9.2
1	B	193	ALA	8.9
1	C	41	ALA	8.3
1	B	41	ALA	8.2
1	D	353	GLY	8.2
1	D	472	GLY	7.9
1	A	496	GLY	7.7
1	A	471	ALA	7.6
1	D	40	THR	7.5
1	B	404	TYR	7.0
1	B	396	VAL	6.9
1	C	496	GLY	6.5
1	B	40	THR	6.5
1	A	41	ALA	6.5
1	A	392	LEU	6.4
1	A	212	THR	6.4
1	B	394	LYS	6.2
1	A	40	THR	6.2
1	B	42	SER	6.2
1	D	381	ILE	6.1
1	A	42	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	471	ALA	6.0
1	B	194	ASN	6.0
1	D	43	GLY	5.9
1	B	399	CYS	5.9
1	D	354	ASN	5.9
1	A	360	LEU	5.7
1	B	464	VAL	5.7
1	C	465	ASP	5.7
1	D	41	ALA	5.7
1	C	42	SER	5.7
1	D	352	LEU	5.5
1	D	194	ASN	5.5
1	C	497	PHE	5.4
1	A	497	PHE	5.3
1	D	358	TYR	5.3
1	B	472	GLY	5.2
1	A	358	TYR	5.1
1	C	533	LEU	5.0
1	B	393	GLY	5.0
1	C	495	PRO	5.0
1	C	390	ASP	5.0
1	D	473	LYS	5.0
1	C	363	PRO	5.0
1	D	499	PRO	4.9
1	A	194	ASN	4.8
1	C	255	PRO	4.8
1	B	43	GLY	4.7
1	B	390	ASP	4.7
1	A	44	ARG	4.7
1	D	390	ASP	4.7
1	C	374	SER	4.6
1	D	361	SER	4.5
1	C	254	SER	4.4
1	D	193	ALA	4.4
1	C	372	SER	4.3
1	D	197	GLU	4.3
1	D	387	LEU	4.3
1	C	40	THR	4.3
1	D	44	ARG	4.3
1	D	380	ILE	4.3
1	B	398	HIS	4.3
1	B	407	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	393	GLY	4.2
1	C	321	LEU	4.2
1	D	533	LEU	4.2
1	D	42	SER	4.2
1	A	498	HIS	4.2
1	A	361	SER	4.1
1	D	360	LEU	4.1
1	B	496	GLY	4.1
1	C	44	ARG	4.1
1	B	400	ILE	4.1
1	B	395	LYS	4.1
1	C	371	ILE	4.1
1	A	499	PRO	4.0
1	C	494	ARG	4.0
1	D	281	PHE	4.0
1	A	70	LEU	3.9
1	B	405	MET	3.9
1	B	121	ALA	3.9
1	C	23	ASP	3.9
1	B	406	LYS	3.9
1	B	280	ILE	3.9
1	D	389	ASN	3.9
1	A	211	VAL	3.9
1	A	472	GLY	3.8
1	B	392	LEU	3.8
1	A	390	ASP	3.8
1	A	397	ASP	3.8
1	A	398	HIS	3.8
1	A	391	LYS	3.8
1	A	249	ARG	3.8
1	B	71	ILE	3.7
1	C	280	ILE	3.6
1	C	24	ASN	3.6
1	A	400	ILE	3.6
1	B	210	ASN	3.6
1	B	38	THR	3.6
1	C	395	LYS	3.6
1	D	207	GLU	3.5
1	A	257	VAL	3.5
1	B	495	PRO	3.5
1	C	43	GLY	3.5
1	D	470	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	3.5
1	B	352	LEU	3.4
1	B	214	ARG	3.4
1	D	469	GLU	3.4
1	A	395	LYS	3.4
1	A	71	ILE	3.4
1	D	351	HIS	3.4
1	C	464	VAL	3.4
1	A	193	ALA	3.4
1	C	281	PHE	3.4
1	A	197	GLU	3.4
1	C	408	VAL	3.4
1	A	469	GLU	3.3
1	C	391	LYS	3.3
1	B	279	THR	3.3
1	D	192	ALA	3.3
1	D	185	ILE	3.3
1	A	470	ASP	3.3
1	D	22	LYS	3.3
1	A	254	SER	3.3
1	D	280	ILE	3.2
1	A	210	ASN	3.2
1	B	208	LYS	3.2
1	D	121	ALA	3.2
1	D	71	ILE	3.2
1	A	533	LEU	3.2
1	C	514	LEU	3.2
1	C	22	LYS	3.2
1	B	388	TYR	3.2
1	D	500	VAL	3.1
1	D	498	HIS	3.1
1	A	281	PHE	3.1
1	B	255	PRO	3.1
1	B	473	LYS	3.1
1	B	391	LYS	3.1
1	A	399	CYS	3.1
1	C	373	LYS	3.1
1	B	498	HIS	3.1
1	A	500	VAL	3.1
1	A	404	TYR	3.0
1	B	389	ASN	3.0
1	D	70	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	253	VAL	3.0
1	A	493	THR	3.0
1	B	197	GLU	3.0
1	C	320	ASP	3.0
1	A	467	VAL	3.0
1	C	479	PRO	3.0
1	B	402	ILE	3.0
1	D	243	TRP	2.9
1	D	39	LYS	2.9
1	C	361	SER	2.9
1	A	39	LYS	2.9
1	A	10	THR	2.9
1	B	61	LYS	2.9
1	D	255	PRO	2.9
1	D	481	LEU	2.9
1	B	44	ARG	2.9
1	C	498	HIS	2.9
1	D	344	VAL	2.9
1	A	38	THR	2.8
1	C	392	LEU	2.8
1	B	351	HIS	2.8
1	D	147	TRP	2.8
1	A	501	ASN	2.8
1	B	353	GLY	2.8
1	C	133	LEU	2.8
1	B	500	VAL	2.8
1	B	206	ASP	2.8
1	A	495	PRO	2.8
1	A	473	LYS	2.8
1	D	388	TYR	2.8
1	B	281	PHE	2.8
1	B	397	ASP	2.8
1	A	276	ALA	2.7
1	A	242	LEU	2.7
1	C	367	ARG	2.7
1	A	279	THR	2.7
1	B	242	LEU	2.7
1	D	242	LEU	2.7
1	D	208	LYS	2.7
1	B	344	VAL	2.7
1	C	277	PRO	2.7
1	B	514	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	214	ARG	2.7
1	B	401	VAL	2.7
1	D	51	VAL	2.7
1	A	406	LYS	2.7
1	A	408	VAL	2.6
1	C	260	THR	2.6
1	B	81	LEU	2.6
1	B	123	GLY	2.6
1	C	256	GLY	2.6
1	C	71	ILE	2.6
1	B	403	LYS	2.6
1	B	122	GLU	2.6
1	C	21	TYR	2.6
1	B	39	LYS	2.6
1	D	254	SER	2.6
1	A	514	LEU	2.6
1	A	517	LEU	2.6
1	C	315	PHE	2.6
1	C	349	TYR	2.6
1	C	121	ALA	2.5
1	B	348	SER	2.5
1	B	249	ARG	2.5
1	D	209	GLY	2.5
1	C	477	PHE	2.5
1	D	38	THR	2.5
1	A	277	PRO	2.5
1	A	263	ASN	2.5
1	B	133	LEU	2.5
1	B	350	ASN	2.5
1	D	355	ASN	2.5
1	C	185	ILE	2.5
1	C	375	SER	2.5
1	D	210	ASN	2.4
1	C	197	GLU	2.4
1	C	278	SER	2.4
1	C	364	LYS	2.4
1	B	209	GLY	2.4
1	D	347	ALA	2.4
1	D	513	PHE	2.4
1	B	533	LEU	2.4
1	D	497	PHE	2.4
1	C	500	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	513	PHE	2.4
1	D	212	THR	2.4
1	A	243	TRP	2.3
1	C	478	TYR	2.3
1	C	362	ALA	2.3
1	B	346	ILE	2.3
1	C	499	PRO	2.3
1	C	300	THR	2.3
1	D	252	GLU	2.3
1	A	280	ILE	2.3
1	C	279	THR	2.3
1	D	382	ALA	2.3
1	B	408	VAL	2.3
1	B	300	THR	2.3
1	D	477	PHE	2.3
1	B	70	LEU	2.2
1	B	409	GLY	2.2
1	B	212	THR	2.2
1	D	214	ARG	2.2
1	A	122	GLU	2.2
1	C	194	ASN	2.2
1	A	259	ASP	2.2
1	B	243	TRP	2.2
1	C	61	LYS	2.2
1	C	207	GLU	2.2
1	A	270	ASN	2.2
1	A	359	ASN	2.2
1	A	389	ASN	2.2
1	A	252	GLU	2.2
1	D	10	THR	2.2
1	C	209	GLY	2.2
1	D	311	HIS	2.2
1	B	278	SER	2.2
1	C	394	LYS	2.2
1	A	207	GLU	2.1
1	C	122	GLU	2.1
1	D	359	ASN	2.1
1	C	378	ASP	2.1
1	A	147	TRP	2.1
1	B	205	LEU	2.1
1	D	122	GLU	2.1
1	B	196	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	17	ASP	2.1
1	C	302	VAL	2.1
1	A	394	LYS	2.1
1	C	243	TRP	2.1
1	A	352	LEU	2.1
1	B	356	ASP	2.1
1	A	353	GLY	2.1
1	A	255	PRO	2.1
1	A	253	VAL	2.1
1	A	278	SER	2.1
1	A	262	GLU	2.1
1	B	386	ILE	2.1
1	B	250	TYR	2.1
1	B	195	GLN	2.1
1	C	192	ALA	2.1
1	C	389	ASN	2.1
1	B	254	SER	2.1
1	B	354	ASN	2.0
1	C	282	ALA	2.0
1	B	277	PRO	2.0
1	C	195	GLN	2.0
1	D	495	PRO	2.0
1	D	349	TYR	2.0
1	D	241	VAL	2.0
1	D	257	VAL	2.0
1	B	383	SER	2.0
1	A	206	ASP	2.0
1	C	318	GLY	2.0
1	D	23	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th 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
2	NAD	C	670	44/44	0.97	0.14	-0.14	29,34,65,70	0
2	NAD	A	650	44/44	0.96	0.14	-0.19	32,40,65,68	0
2	NAD	D	680	44/44	0.95	0.13	-0.31	26,35,70,75	0
2	NAD	B	660	44/44	0.97	0.12	-0.51	29,40,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.