



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:21 AM UTC

PDB ID : 1M5N / pdb_00001m5n
Title : Crystal structure of HEAT repeats (1-11) of importin b bound to the non-classical NLS(67-94) of PTHrP
Authors : Cingolani, G.; Bednenko, J.; Gillespie, M.T.; Gerace, L.
Deposited on : 2002-07-09
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

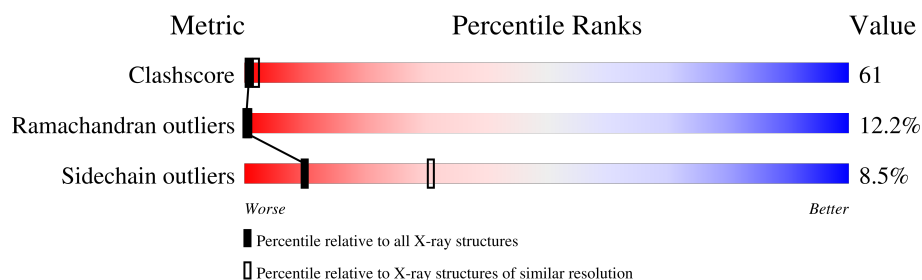
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	485	
2	Q	28	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4020 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 Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	485	Total	C	N	O	S	0	0	0
			3772	2380	627	738	27			

- Molecule 2 is a protein called Parathyroid hormone-related protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	28	Total	C	N	O	0	0	0
			211	136	36	39			

- Molecule 3 is water.

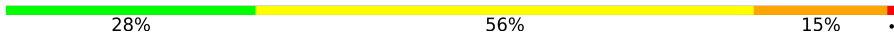
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	37	Total	O	0	0
			37	37		

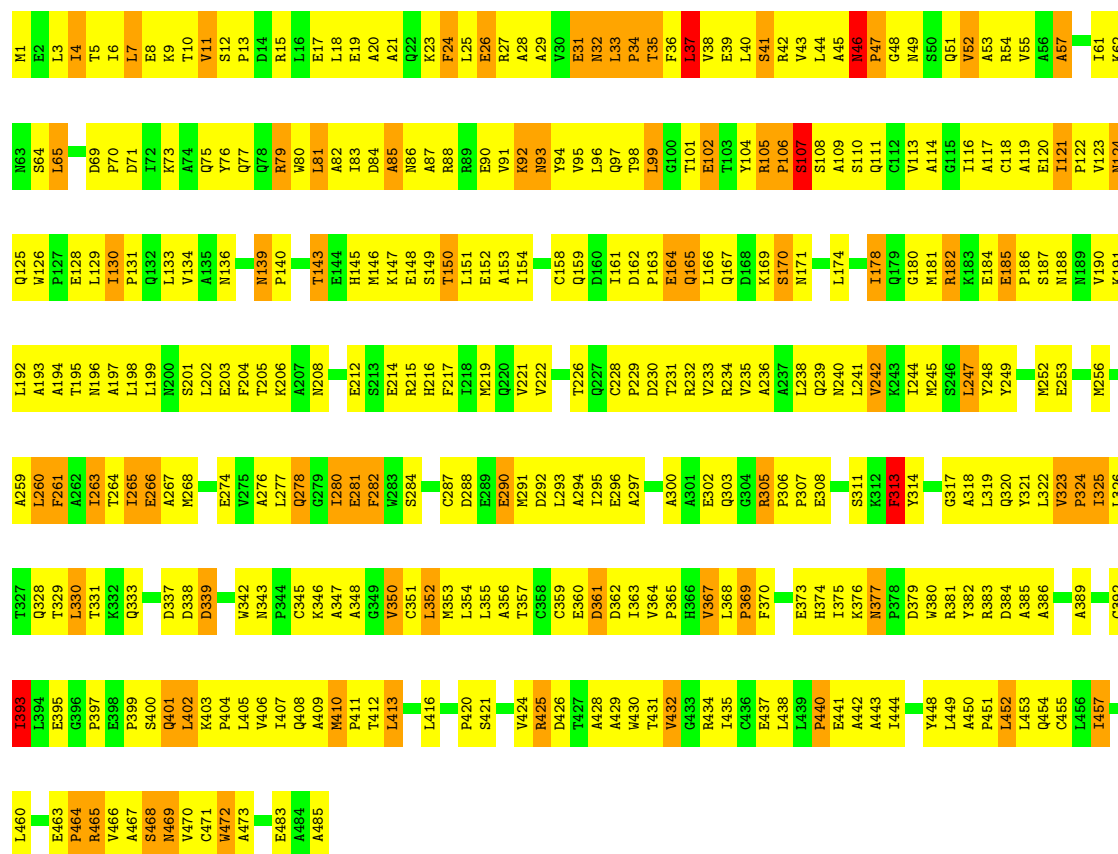
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

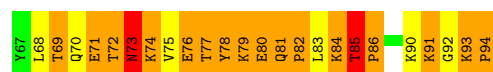
- Molecule 1: Importin beta-1 subunit

Chain S: 



- Molecule 2: Parathyroid hormone-related protein

Chain Q: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	92.79Å 105.45Å 146.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90	Depositor
% Data completeness (in resolution range)	10.0 (50.00-2.90)	Depositor
R_{merge}	0.01	Depositor
R_{sym}	0.01	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.250 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4020	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	S	0.61	0/3842	1.07	23/5232 (0.4%)
2	Q	1.36	2/215 (0.9%)	1.74	5/289 (1.7%)
All	All	0.67	2/4057 (0.0%)	1.12	28/5521 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	92	GLY	N-CA	6.19	1.51	1.45
2	Q	94	PRO	C-O	5.89	1.35	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	263	ILE	N-CA-C	7.71	117.78	110.53
1	S	139	ASN	CA-C-N	7.70	129.46	119.84
1	S	139	ASN	C-N-CA	7.70	129.46	119.84
1	S	185	GLU	CA-C-N	7.01	128.60	119.84
1	S	185	GLU	C-N-CA	7.01	128.60	119.84
1	S	46	ASN	CA-C-N	6.96	128.53	119.84
1	S	46	ASN	C-N-CA	6.96	128.53	119.84
1	S	292	ASP	N-CA-C	-6.89	103.22	111.69
1	S	7	LEU	N-CA-C	-6.70	103.98	111.28
2	Q	78	TYR	O-C-N	6.65	130.82	123.04
1	S	26	GLU	N-CA-C	-6.43	105.06	114.39
1	S	413	LEU	N-CA-C	-6.36	105.18	113.12
1	S	203	GLU	N-CA-C	6.21	119.70	111.75
1	S	457	ILE	N-CA-C	-6.14	104.34	110.30
1	S	313	PHE	N-CA-C	6.08	119.49	111.28
2	Q	73	ASN	O-C-N	5.96	130.52	122.59
2	Q	68	LEU	O-C-N	5.96	128.87	121.84
1	S	284	SER	N-CA-C	-5.65	104.50	111.40
1	S	260	LEU	N-CA-C	5.45	117.03	111.14
1	S	29	ALA	N-CA-C	-5.43	103.25	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	86	PRO	N-CA-C	-5.41	106.14	113.40
1	S	325	ILE	O-C-N	5.29	129.19	122.57
1	S	402	LEU	N-CA-C	-5.16	106.12	112.72
1	S	393	ILE	N-CA-C	5.15	120.05	109.34
2	Q	68	LEU	N-CA-C	-5.12	105.06	113.50
1	S	469	ASN	N-CA-C	-5.11	106.39	113.18
1	S	242	VAL	N-CA-C	-5.07	106.21	111.58
1	S	290	GLU	N-CA-C	5.06	116.61	111.14

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	S	3772	0	3753	438	0
2	Q	211	0	210	50	0
3	S	37	0	0	10	0
All	All	4020	0	3963	482	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 61.

All (482) 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)
2:Q:93:LYS:HB3	2:Q:94:PRO:CD	1.12	1.45
2:Q:93:LYS:CB	2:Q:94:PRO:CD	2.00	1.31
2:Q:81:GLN:CB	2:Q:82:PRO:CD	2.10	1.25
2:Q:84:LYS:O	2:Q:85:THR:HG23	1.45	1.16
2:Q:93:LYS:CB	2:Q:94:PRO:HD3	1.70	1.12
2:Q:81:GLN:CB	2:Q:82:PRO:HD3	1.79	1.11
2:Q:93:LYS:CG	2:Q:94:PRO:HD3	1.79	1.11
2:Q:69:THR:HG23	2:Q:70:GLN:H	1.13	1.10
2:Q:93:LYS:HB3	2:Q:94:PRO:HD3	1.23	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:252:MET:O	1:S:256:MET:HG2	1.53	1.04
2:Q:81:GLN:CB	2:Q:82:PRO:HD2	1.89	1.02
2:Q:93:LYS:CB	2:Q:94:PRO:HD2	1.77	1.02
1:S:130:ILE:O	1:S:134:VAL:HG23	1.60	1.00
1:S:42:ARG:HG2	3:S:505:HOH:O	1.61	0.98
1:S:287:CYS:SG	1:S:355:LEU:HD12	2.02	0.98
1:S:280:ILE:HG21	1:S:347:ALA:HB1	1.44	0.98
1:S:121:ILE:H	1:S:122:PRO:HD2	1.26	0.97
1:S:3:LEU:O	1:S:4:ILE:HG13	1.64	0.97
1:S:99:LEU:H	1:S:99:LEU:HD12	1.31	0.96
1:S:380:TRP:HA	1:S:383:ARG:HE	1.29	0.96
1:S:170:SER:HB2	1:S:208:ASN:HD21	1.30	0.96
1:S:44:LEU:HD13	1:S:57:ALA:HB3	1.48	0.96
1:S:430:TRP:CD1	2:Q:86:PRO:HG2	2.01	0.95
2:Q:84:LYS:O	2:Q:85:THR:CG2	2.14	0.94
2:Q:77:THR:O	2:Q:81:GLN:HA	1.69	0.92
1:S:230:ASP:OD2	1:S:232:ARG:HB2	1.68	0.91
1:S:130:ILE:HG13	1:S:169:LYS:NZ	1.87	0.90
1:S:33:LEU:HB3	1:S:34:PRO:HD3	1.51	0.89
1:S:268:MET:HE3	1:S:280:ILE:HA	1.55	0.88
1:S:130:ILE:HD13	1:S:130:ILE:H	1.38	0.88
2:Q:69:THR:HG23	2:Q:70:GLN:N	1.91	0.85
2:Q:75:VAL:O	2:Q:76:GLU:OE1	1.93	0.84
1:S:238:LEU:O	1:S:242:VAL:HG23	1.76	0.84
2:Q:93:LYS:HB3	2:Q:94:PRO:HD2	0.85	0.84
2:Q:93:LYS:HG2	2:Q:94:PRO:HD3	1.59	0.84
1:S:163:PRO:HB2	1:S:167:GLN:HE21	1.44	0.83
1:S:465:ARG:HG2	1:S:466:VAL:H	1.46	0.81
1:S:322:LEU:C	1:S:324:PRO:HD2	2.06	0.81
1:S:108:SER:O	1:S:111:GLN:HB2	1.81	0.81
1:S:120:GLU:HB3	1:S:126:TRP:HB2	1.62	0.80
2:Q:90:LYS:HG2	2:Q:91:LYS:H	1.46	0.80
1:S:163:PRO:HB2	1:S:167:GLN:NE2	1.96	0.80
1:S:449:LEU:O	1:S:453:LEU:HD12	1.79	0.80
1:S:77:GLN:HB3	3:S:514:HOH:O	1.82	0.79
1:S:40:LEU:HA	1:S:43:VAL:HG22	1.62	0.79
1:S:7:LEU:HA	1:S:10:THR:CG2	2.13	0.78
1:S:62:LYS:HE2	1:S:111:GLN:NE2	2.00	0.77
2:Q:84:LYS:C	2:Q:85:THR:CG2	2.57	0.77
1:S:205:THR:HB	1:S:208:ASN:HD22	1.51	0.76
2:Q:90:LYS:HG2	2:Q:91:LYS:N	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:43:VAL:HA	1:S:46:ASN:HD21	1.50	0.75
1:S:130:ILE:HG12	1:S:131:PRO:HD3	1.67	0.75
1:S:380:TRP:HA	1:S:383:ARG:NE	2.02	0.75
2:Q:85:THR:OG1	2:Q:86:PRO:HD2	1.86	0.74
1:S:76:TYR:HA	1:S:79:ARG:HG3	1.70	0.74
1:S:83:ILE:HG22	1:S:84:ASP:N	2.03	0.73
1:S:430:TRP:CE2	2:Q:86:PRO:HB2	2.23	0.73
1:S:130:ILE:HG13	1:S:169:LYS:HZ2	1.52	0.73
1:S:360:GLU:O	1:S:362:ASP:N	2.22	0.73
1:S:410:MET:HB3	1:S:411:PRO:HD3	1.69	0.73
1:S:121:ILE:H	1:S:122:PRO:CD	2.01	0.72
1:S:130:ILE:HG12	1:S:131:PRO:CD	2.19	0.72
2:Q:79:LYS:HG3	2:Q:91:LYS:HD2	1.70	0.72
1:S:198:LEU:HD23	1:S:240:ASN:OD1	1.90	0.71
1:S:105:ARG:HB3	1:S:106:PRO:CD	2.20	0.71
1:S:33:LEU:CB	1:S:34:PRO:HD3	2.20	0.71
1:S:3:LEU:HD23	1:S:6:ILE:HD12	1.71	0.71
1:S:151:LEU:HA	1:S:154:ILE:HD12	1.71	0.71
1:S:170:SER:CB	1:S:208:ASN:HD21	2.02	0.71
1:S:407:ILE:HG12	1:S:448:TYR:OH	1.89	0.71
1:S:266:GLU:HG3	1:S:267:ALA:N	2.05	0.70
1:S:261:PHE:C	1:S:261:PHE:HD2	2.00	0.70
1:S:130:ILE:HG13	1:S:169:LYS:HZ3	1.55	0.69
1:S:449:LEU:CD1	1:S:453:LEU:HD11	2.22	0.69
1:S:305:ARG:HD3	1:S:306:PRO:HD2	1.74	0.69
1:S:45:ALA:HA	1:S:98:THR:HG23	1.72	0.69
1:S:245:MET:HE1	1:S:256:MET:SD	2.33	0.69
1:S:329:THR:C	1:S:331:THR:H	2.00	0.69
1:S:123:VAL:HB	1:S:125:GLN:HE22	1.58	0.69
2:Q:76:GLU:OE2	2:Q:78:TYR:HE1	1.76	0.69
1:S:399:PRO:HA	1:S:402:LEU:HD12	1.75	0.68
1:S:350:VAL:HA	1:S:353:MET:HE3	1.75	0.68
1:S:457:ILE:HA	1:S:460:LEU:HD12	1.76	0.68
1:S:7:LEU:HA	1:S:10:THR:HG23	1.76	0.68
1:S:166:LEU:HD12	1:S:204:PHE:CE2	2.29	0.68
1:S:333:GLN:HB3	1:S:345:CYS:SG	2.34	0.68
1:S:261:PHE:C	1:S:261:PHE:CD2	2.72	0.67
2:Q:69:THR:CG2	2:Q:70:GLN:H	1.92	0.67
1:S:467:ALA:C	1:S:469:ASN:H	2.03	0.66
1:S:219:MET:HE1	1:S:252:MET:HE1	1.75	0.66
1:S:471:CYS:HB3	3:S:495:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:375:ILE:HG23	1:S:376:LYS:HG2	1.76	0.66
1:S:323:VAL:C	1:S:325:ILE:H	2.04	0.66
1:S:87:ALA:O	1:S:90:GLU:HB3	1.95	0.66
1:S:444:ILE:O	1:S:444:ILE:HG13	1.95	0.65
1:S:114:ALA:O	1:S:117:ALA:HB3	1.96	0.65
1:S:24:PHE:HD2	1:S:24:PHE:C	2.04	0.65
1:S:61:ILE:O	1:S:65:LEU:HG	1.97	0.65
1:S:24:PHE:C	1:S:24:PHE:CD2	2.75	0.65
1:S:405:LEU:O	1:S:408:GLN:HG2	1.97	0.65
1:S:256:MET:SD	1:S:260:LEU:HD12	2.37	0.65
1:S:1:MET:HG3	1:S:24:PHE:HE1	1.62	0.64
1:S:151:LEU:HA	1:S:154:ILE:CD1	2.26	0.64
1:S:261:PHE:HD2	1:S:261:PHE:O	1.80	0.64
1:S:161:ILE:HG22	1:S:162:ASP:N	2.12	0.64
1:S:360:GLU:C	1:S:362:ASP:H	2.05	0.64
1:S:437:GLU:HG2	1:S:438:LEU:HD22	1.79	0.64
1:S:99:LEU:H	1:S:99:LEU:CD1	2.09	0.64
1:S:121:ILE:N	1:S:122:PRO:HD2	2.05	0.64
1:S:219:MET:CE	1:S:252:MET:HE1	2.28	0.64
1:S:319:LEU:HD22	1:S:359:CYS:SG	2.38	0.64
1:S:116:ILE:HG22	1:S:120:GLU:HG2	1.80	0.63
1:S:465:ARG:HG2	1:S:466:VAL:N	2.13	0.63
1:S:151:LEU:HD23	1:S:154:ILE:HD12	1.81	0.63
1:S:300:ALA:HA	1:S:303:GLN:HG2	1.80	0.63
1:S:6:ILE:O	1:S:10:THR:HG23	1.98	0.63
1:S:342:TRP:CZ3	1:S:346:LYS:HB3	2.34	0.63
1:S:377:ASN:O	1:S:383:ARG:HD3	1.98	0.63
1:S:399:PRO:C	1:S:401:GLN:H	2.07	0.62
2:Q:71:GLU:HB3	2:Q:73:ASN:ND2	2.15	0.62
1:S:1:MET:HG3	1:S:24:PHE:CE1	2.34	0.62
1:S:363:ILE:O	1:S:367:VAL:HG22	2.00	0.62
1:S:109:ALA:O	1:S:113:VAL:HG23	1.99	0.62
1:S:119:ALA:C	1:S:122:PRO:HD2	2.24	0.62
1:S:40:LEU:HA	1:S:43:VAL:CG2	2.28	0.62
1:S:11:VAL:O	1:S:11:VAL:HG22	2.00	0.62
1:S:3:LEU:C	1:S:4:ILE:HG13	2.25	0.61
1:S:369:PRO:O	1:S:373:GLU:HB2	1.99	0.61
1:S:226:THR:HG23	1:S:238:LEU:HD21	1.83	0.61
1:S:471:CYS:C	1:S:473:ALA:N	2.55	0.61
1:S:234:ARG:O	1:S:238:LEU:HG	2.00	0.60
1:S:18:LEU:C	1:S:18:LEU:HD23	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:12:SER:HB2	1:S:13:PRO:HD2	1.83	0.60
1:S:453:LEU:O	1:S:457:ILE:HG13	2.02	0.60
2:Q:84:LYS:C	2:Q:85:THR:HG22	2.25	0.60
1:S:364:VAL:HB	1:S:365:PRO:CD	2.31	0.60
1:S:374:HIS:HB3	1:S:382:TYR:O	2.00	0.60
1:S:204:PHE:HD1	1:S:204:PHE:O	1.85	0.60
1:S:32:ASN:OD1	1:S:35:THR:HB	2.02	0.60
1:S:83:ILE:CG2	1:S:84:ASP:N	2.64	0.60
1:S:76:TYR:CA	1:S:79:ARG:HG3	2.32	0.59
1:S:123:VAL:HB	1:S:125:GLN:NE2	2.17	0.59
1:S:28:ALA:HB1	1:S:32:ASN:HB3	1.84	0.59
1:S:95:VAL:HA	1:S:98:THR:OG1	2.03	0.59
1:S:121:ILE:C	1:S:123:VAL:H	2.11	0.59
1:S:322:LEU:O	1:S:324:PRO:HD2	2.03	0.59
1:S:105:ARG:HB3	1:S:106:PRO:HD3	1.85	0.59
1:S:256:MET:HA	1:S:260:LEU:HB2	1.84	0.59
1:S:205:THR:CB	1:S:208:ASN:HD22	2.16	0.59
1:S:431:THR:HG22	1:S:435:ILE:HD11	1.85	0.58
1:S:84:ASP:OD2	1:S:86:ASN:HB2	2.04	0.58
1:S:88:ARG:O	1:S:92:LYS:HG3	2.03	0.58
1:S:256:MET:HG3	1:S:314:TYR:CZ	2.38	0.58
1:S:35:THR:O	1:S:39:GLU:HG2	2.03	0.58
1:S:159:GLN:O	1:S:159:GLN:HG2	2.02	0.58
1:S:302:GLU:HG3	1:S:303:GLN:N	2.19	0.58
1:S:403:LYS:N	1:S:404:PRO:HD2	2.19	0.58
1:S:34:PRO:O	1:S:36:PHE:N	2.37	0.57
1:S:123:VAL:HB	1:S:125:GLN:OE1	2.04	0.57
1:S:151:LEU:HD23	1:S:154:ILE:CD1	2.35	0.57
1:S:313:PHE:CD1	1:S:313:PHE:N	2.72	0.57
1:S:322:LEU:C	1:S:324:PRO:CD	2.76	0.57
1:S:83:ILE:HG22	1:S:84:ASP:H	1.69	0.57
2:Q:79:LYS:HG3	2:Q:91:LYS:CD	2.34	0.57
1:S:41:SER:O	1:S:94:TYR:HB3	2.04	0.57
1:S:46:ASN:N	1:S:46:ASN:HD22	2.01	0.57
1:S:76:TYR:C	1:S:79:ARG:HG3	2.28	0.57
1:S:15:ARG:O	1:S:19:GLU:HB2	2.04	0.57
1:S:226:THR:HG21	1:S:263:ILE:CG2	2.35	0.57
1:S:323:VAL:O	1:S:325:ILE:N	2.37	0.56
1:S:7:LEU:HA	1:S:10:THR:OG1	2.06	0.56
1:S:80:TRP:HA	1:S:83:ILE:HG13	1.86	0.56
1:S:3:LEU:O	1:S:4:ILE:CG1	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:471:CYS:O	1:S:473:ALA:N	2.38	0.56
1:S:83:ILE:CG2	1:S:84:ASP:H	2.17	0.56
1:S:331:THR:HG23	1:S:381:ARG:HB3	1.87	0.56
1:S:471:CYS:C	1:S:473:ALA:H	2.13	0.56
1:S:435:ILE:HG22	1:S:435:ILE:O	2.06	0.56
2:Q:76:GLU:OE2	2:Q:78:TYR:CE1	2.59	0.56
2:Q:85:THR:OG1	2:Q:86:PRO:CD	2.52	0.56
1:S:130:ILE:HG21	1:S:169:LYS:HD3	1.87	0.56
1:S:54:ARG:O	1:S:57:ALA:HB3	2.06	0.55
1:S:64:SER:O	1:S:65:LEU:HD23	2.07	0.55
1:S:120:GLU:O	1:S:126:TRP:N	2.38	0.55
1:S:395:GLU:OE2	2:Q:90:LYS:HA	2.06	0.55
1:S:76:TYR:HA	1:S:79:ARG:CG	2.36	0.55
1:S:17:GLU:O	1:S:20:ALA:HB3	2.06	0.55
1:S:380:TRP:O	1:S:383:ARG:HB2	2.07	0.55
1:S:136:ASN:ND2	1:S:146:MET:SD	2.80	0.55
1:S:99:LEU:HD12	1:S:99:LEU:N	2.13	0.55
1:S:169:LYS:HE2	1:S:169:LYS:HA	1.87	0.55
1:S:295:ILE:O	1:S:296:GLU:C	2.50	0.55
1:S:431:THR:O	1:S:434:ARG:N	2.40	0.55
1:S:215:ARG:O	1:S:216:HIS:C	2.50	0.55
1:S:252:MET:HE3	1:S:260:LEU:HD11	1.88	0.55
1:S:346:LYS:O	1:S:347:ALA:C	2.50	0.55
1:S:6:ILE:O	1:S:10:THR:N	2.40	0.55
1:S:320:GLN:HG3	1:S:321:TYR:CD1	2.42	0.55
1:S:205:THR:HB	1:S:208:ASN:HB2	1.89	0.54
1:S:449:LEU:HD11	1:S:453:LEU:HD11	1.89	0.54
1:S:5:THR:O	1:S:8:GLU:HB2	2.07	0.54
1:S:81:LEU:C	1:S:83:ILE:H	2.15	0.54
1:S:364:VAL:HB	1:S:365:PRO:HD3	1.89	0.54
1:S:470:VAL:O	1:S:473:ALA:HB3	2.07	0.54
1:S:164:GLU:O	1:S:165:GLN:HG3	2.08	0.54
1:S:268:MET:CE	1:S:280:ILE:HG12	2.38	0.54
1:S:24:PHE:HD2	1:S:24:PHE:O	1.90	0.54
1:S:143:THR:HB	1:S:146:MET:H	1.72	0.54
1:S:36:PHE:O	1:S:37:LEU:C	2.50	0.54
1:S:79:ARG:O	1:S:83:ILE:HG12	2.08	0.54
1:S:80:TRP:HA	1:S:83:ILE:CG1	2.38	0.54
1:S:151:LEU:HD13	1:S:194:ALA:HB2	1.89	0.54
1:S:348:ALA:O	1:S:352:LEU:HB2	2.09	0.53
1:S:431:THR:O	1:S:432:VAL:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:105:ARG:CB	1:S:106:PRO:CD	2.87	0.53
1:S:407:ILE:HG23	1:S:448:TYR:HE2	1.73	0.53
2:Q:83:LEU:O	2:Q:84:LYS:CB	2.56	0.53
1:S:43:VAL:HA	1:S:46:ASN:ND2	2.23	0.53
1:S:204:PHE:O	1:S:204:PHE:CD1	2.61	0.53
1:S:389:ALA:O	1:S:393:ILE:HG12	2.09	0.53
1:S:92:LYS:HB3	1:S:126:TRP:CZ2	2.43	0.53
1:S:425:ARG:HH21	1:S:463:GLU:CD	2.17	0.53
1:S:192:LEU:O	1:S:193:ALA:C	2.51	0.53
1:S:84:ASP:C	1:S:86:ASN:H	2.16	0.53
1:S:69:ASP:C	1:S:71:ASP:H	2.17	0.53
1:S:239:GLN:HE21	2:Q:74:LYS:CB	2.22	0.53
1:S:7:LEU:CA	1:S:10:THR:HG23	2.38	0.52
1:S:395:GLU:O	1:S:397:PRO:HD2	2.09	0.52
1:S:5:THR:HG22	1:S:9:LYS:HE3	1.91	0.52
1:S:33:LEU:HD13	1:S:79:ARG:HH21	1.75	0.52
1:S:43:VAL:CA	1:S:46:ASN:HD21	2.22	0.52
1:S:280:ILE:CG2	1:S:347:ALA:HB1	2.30	0.52
1:S:410:MET:CB	1:S:411:PRO:HD3	2.38	0.52
1:S:421:SER:HB3	1:S:424:VAL:HG23	1.91	0.52
1:S:45:ALA:O	1:S:47:PRO:HD3	2.10	0.52
1:S:208:ASN:C	3:S:512:HOH:O	2.53	0.52
2:Q:80:GLU:CB	2:Q:83:LEU:HD12	2.40	0.52
1:S:37:LEU:HD23	1:S:37:LEU:H	1.74	0.51
1:S:116:ILE:HG22	1:S:120:GLU:CG	2.40	0.51
1:S:467:ALA:C	1:S:469:ASN:N	2.68	0.51
1:S:235:VAL:O	1:S:239:GLN:HG3	2.10	0.51
1:S:328:GLN:HE22	1:S:382:TYR:HE2	1.56	0.51
1:S:329:THR:O	1:S:331:THR:N	2.42	0.51
1:S:338:ASP:OD1	1:S:339:ASP:N	2.43	0.51
1:S:145:HIS:O	1:S:146:MET:C	2.53	0.51
1:S:92:LYS:O	1:S:96:LEU:HD13	2.10	0.51
1:S:6:ILE:C	1:S:10:THR:HG23	2.35	0.51
1:S:188:ASN:HD22	1:S:188:ASN:N	2.07	0.51
1:S:206:LYS:HD2	1:S:206:LYS:O	2.10	0.51
2:Q:80:GLU:O	2:Q:81:GLN:O	2.29	0.51
1:S:42:ARG:CG	3:S:505:HOH:O	2.36	0.51
1:S:46:ASN:N	1:S:46:ASN:ND2	2.59	0.50
1:S:276:ALA:O	1:S:277:LEU:C	2.54	0.50
1:S:399:PRO:CA	1:S:402:LEU:HD12	2.40	0.50
1:S:6:ILE:CG2	1:S:25:LEU:HD11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:167:GLN:HG2	1:S:204:PHE:HB2	1.93	0.50
1:S:91:VAL:O	1:S:95:VAL:HG23	2.10	0.50
1:S:430:TRP:CD1	2:Q:86:PRO:CG	2.85	0.50
1:S:448:TYR:HA	1:S:451:PRO:CG	2.42	0.50
1:S:76:TYR:CE2	1:S:79:ARG:NH1	2.79	0.50
1:S:248:TYR:O	1:S:252:MET:HG2	2.12	0.50
1:S:235:VAL:HG11	1:S:274:GLU:HG2	1.94	0.50
1:S:11:VAL:HA	1:S:18:LEU:HD12	1.94	0.50
1:S:15:ARG:HG3	3:S:491:HOH:O	2.12	0.50
1:S:36:PHE:O	1:S:39:GLU:N	2.44	0.50
1:S:199:LEU:HA	1:S:240:ASN:HD21	1.77	0.50
2:Q:93:LYS:CD	2:Q:94:PRO:HD3	2.41	0.49
1:S:380:TRP:H	1:S:380:TRP:CD1	2.29	0.49
1:S:380:TRP:HB3	1:S:383:ARG:HH21	1.77	0.49
1:S:121:ILE:C	1:S:123:VAL:N	2.69	0.49
1:S:40:LEU:O	1:S:43:VAL:HG22	2.12	0.49
1:S:122:PRO:CB	1:S:165:GLN:NE2	2.76	0.49
1:S:154:ILE:O	1:S:158:CYS:SG	2.69	0.49
1:S:170:SER:O	1:S:171:ASN:C	2.55	0.49
1:S:193:ALA:O	1:S:196:ASN:HB2	2.11	0.49
1:S:195:THR:CG2	1:S:236:ALA:HB1	2.43	0.49
1:S:440:PRO:HG2	1:S:441:GLU:H	1.77	0.49
2:Q:81:GLN:O	2:Q:83:LEU:N	2.45	0.49
1:S:407:ILE:O	1:S:411:PRO:HD3	2.12	0.49
1:S:18:LEU:C	1:S:20:ALA:N	2.70	0.49
1:S:166:LEU:CD1	1:S:204:PHE:CZ	2.95	0.49
1:S:214:GLU:O	1:S:215:ARG:C	2.54	0.49
1:S:313:PHE:N	1:S:313:PHE:HD1	2.10	0.49
1:S:40:LEU:CA	1:S:43:VAL:HG22	2.38	0.49
1:S:174:LEU:O	1:S:178:ILE:HG13	2.13	0.49
1:S:214:GLU:O	1:S:217:PHE:HB3	2.13	0.49
1:S:326:LEU:O	1:S:330:LEU:HG	2.12	0.49
1:S:32:ASN:O	1:S:33:LEU:C	2.56	0.49
2:Q:79:LYS:O	2:Q:80:GLU:CB	2.61	0.49
1:S:350:VAL:HG12	1:S:351:CYS:N	2.26	0.48
1:S:428:ALA:O	1:S:432:VAL:HG23	2.12	0.48
1:S:122:PRO:CB	1:S:165:GLN:HE22	2.26	0.48
1:S:395:GLU:O	1:S:397:PRO:CD	2.61	0.48
1:S:105:ARG:C	1:S:107:SER:H	2.21	0.48
1:S:377:ASN:ND2	1:S:379:ASP:N	2.61	0.48
1:S:395:GLU:HG2	1:S:438:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:463:GLU:OE1	1:S:466:VAL:HG21	2.14	0.48
1:S:161:ILE:HG22	1:S:162:ASP:H	1.77	0.48
1:S:182:ARG:HG2	1:S:185:GLU:HB2	1.96	0.48
1:S:329:THR:C	1:S:331:THR:N	2.65	0.48
1:S:434:ARG:O	1:S:438:LEU:HD23	2.13	0.48
1:S:5:THR:HA	1:S:8:GLU:HG3	1.95	0.48
1:S:265:ILE:HD11	1:S:322:LEU:HD23	1.94	0.48
1:S:395:GLU:CG	1:S:438:LEU:HD11	2.44	0.48
1:S:123:VAL:HB	1:S:125:GLN:CD	2.39	0.48
1:S:450:ALA:N	1:S:451:PRO:HD2	2.28	0.48
1:S:449:LEU:HG	1:S:453:LEU:HD11	1.94	0.48
1:S:118:CYS:HB3	3:S:488:HOH:O	2.14	0.48
1:S:356:ALA:HB2	1:S:363:ILE:HD13	1.96	0.48
2:Q:78:TYR:O	2:Q:79:LYS:HB2	2.13	0.48
1:S:449:LEU:O	1:S:452:LEU:HB3	2.14	0.47
2:Q:80:GLU:CB	2:Q:83:LEU:CD1	2.91	0.47
2:Q:71:GLU:HB3	2:Q:73:ASN:CG	2.39	0.47
1:S:76:TYR:HA	1:S:79:ARG:CD	2.44	0.47
1:S:261:PHE:O	1:S:265:ILE:HB	2.14	0.47
1:S:471:CYS:O	1:S:472:TRP:C	2.57	0.47
1:S:11:VAL:HA	1:S:18:LEU:CD1	2.44	0.47
1:S:182:ARG:HG3	1:S:185:GLU:H	1.79	0.47
1:S:18:LEU:O	1:S:20:ALA:N	2.47	0.47
1:S:151:LEU:O	1:S:152:GLU:C	2.58	0.47
1:S:374:HIS:ND1	1:S:382:TYR:HB3	2.30	0.47
2:Q:70:GLN:HG3	2:Q:71:GLU:H	1.80	0.47
1:S:383:ARG:O	1:S:386:ALA:HB3	2.14	0.47
1:S:409:ALA:HB2	3:S:494:HOH:O	2.14	0.47
1:S:411:PRO:C	1:S:413:LEU:H	2.22	0.47
1:S:441:GLU:O	1:S:443:ALA:N	2.47	0.47
1:S:133:LEU:O	1:S:136:ASN:N	2.44	0.47
1:S:162:ASP:O	1:S:163:PRO:C	2.57	0.47
1:S:205:THR:CG2	1:S:208:ASN:HD22	2.28	0.47
1:S:399:PRO:C	1:S:401:GLN:N	2.73	0.47
1:S:416:LEU:HD22	1:S:424:VAL:HG11	1.96	0.47
1:S:264:THR:O	1:S:268:MET:HG3	2.15	0.47
1:S:441:GLU:C	1:S:443:ALA:H	2.22	0.47
1:S:148:GLU:O	1:S:149:SER:C	2.58	0.47
1:S:259:ALA:O	1:S:263:ILE:HG13	2.15	0.47
1:S:322:LEU:O	1:S:323:VAL:C	2.58	0.47
1:S:256:MET:HE2	1:S:314:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:430:TRP:CD2	2:Q:86:PRO:HB2	2.51	0.46
1:S:150:THR:O	1:S:151:LEU:C	2.57	0.46
1:S:426:ASP:OD2	1:S:465:ARG:HG3	2.14	0.46
2:Q:79:LYS:HA	2:Q:79:LYS:HD3	1.72	0.46
1:S:150:THR:O	1:S:153:ALA:N	2.47	0.46
1:S:409:ALA:O	1:S:410:MET:C	2.58	0.46
1:S:54:ARG:HH12	1:S:102:GLU:HA	1.81	0.46
1:S:77:GLN:C	1:S:79:ARG:N	2.72	0.46
1:S:130:ILE:H	1:S:130:ILE:CD1	2.13	0.46
1:S:247:LEU:HD22	3:S:513:HOH:O	2.14	0.46
1:S:440:PRO:HG2	1:S:441:GLU:CD	2.40	0.46
1:S:166:LEU:HD12	1:S:204:PHE:CZ	2.51	0.46
1:S:196:ASN:O	1:S:197:ALA:C	2.59	0.46
1:S:252:MET:HE3	1:S:260:LEU:CD1	2.46	0.46
1:S:300:ALA:HA	1:S:303:GLN:CG	2.45	0.46
1:S:467:ALA:O	1:S:469:ASN:N	2.49	0.46
1:S:107:SER:O	1:S:110:SER:OG	2.33	0.46
1:S:429:ALA:CB	1:S:466:VAL:HG13	2.46	0.46
2:Q:79:LYS:HB3	2:Q:91:LYS:HZ2	1.80	0.46
1:S:106:PRO:O	1:S:107:SER:C	2.60	0.45
1:S:199:LEU:CA	1:S:240:ASN:HD21	2.29	0.45
1:S:230:ASP:O	1:S:231:THR:C	2.57	0.45
1:S:85:ALA:HA	1:S:88:ARG:NE	2.31	0.45
1:S:91:VAL:C	1:S:93:ASN:H	2.24	0.45
1:S:18:LEU:O	1:S:19:GLU:C	2.58	0.45
1:S:88:ARG:HB3	1:S:92:LYS:HE3	1.97	0.45
1:S:121:ILE:O	1:S:123:VAL:N	2.50	0.45
1:S:69:ASP:C	1:S:71:ASP:N	2.73	0.45
1:S:226:THR:HG21	1:S:263:ILE:HG21	1.98	0.45
1:S:368:LEU:N	1:S:369:PRO:HD2	2.31	0.45
1:S:37:LEU:HD23	1:S:37:LEU:N	2.28	0.45
1:S:77:GLN:C	1:S:79:ARG:H	2.24	0.45
1:S:180:GLY:O	1:S:191:LYS:HA	2.15	0.45
1:S:323:VAL:HB	1:S:324:PRO:HD3	1.99	0.45
1:S:464:PRO:O	1:S:465:ARG:C	2.60	0.45
1:S:27:ARG:O	1:S:31:GLU:HB3	2.16	0.45
1:S:33:LEU:CB	1:S:34:PRO:CD	2.92	0.45
1:S:187:SER:HB3	1:S:190:VAL:HG23	1.98	0.45
1:S:287:CYS:O	1:S:288:ASP:C	2.59	0.45
1:S:330:LEU:HD11	1:S:352:LEU:HD12	1.98	0.45
1:S:47:PRO:HG3	1:S:101:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:105:ARG:O	1:S:107:SER:N	2.48	0.45
1:S:483:GLU:C	1:S:485:ALA:H	2.25	0.45
1:S:161:ILE:CG2	1:S:162:ASP:N	2.79	0.45
1:S:413:LEU:O	1:S:416:LEU:HB2	2.17	0.45
1:S:291:MET:O	1:S:294:ALA:HB3	2.17	0.44
1:S:23:LYS:O	1:S:26:GLU:N	2.49	0.44
1:S:412:THR:HG22	1:S:412:THR:O	2.16	0.44
1:S:454:GLN:HA	1:S:457:ILE:HD12	1.98	0.44
1:S:124:ASN:N	1:S:125:GLN:OE1	2.50	0.44
1:S:468:SER:C	1:S:471:CYS:SG	3.00	0.44
1:S:195:THR:HG22	1:S:236:ALA:HB1	2.00	0.44
1:S:228:CYS:SG	1:S:229:PRO:HD2	2.57	0.44
1:S:38:VAL:O	1:S:39:GLU:C	2.60	0.44
1:S:44:LEU:HD13	1:S:57:ALA:CB	2.33	0.44
1:S:102:GLU:HG2	1:S:107:SER:HB2	1.99	0.44
1:S:145:HIS:C	1:S:147:LYS:N	2.73	0.44
1:S:406:VAL:O	1:S:409:ALA:N	2.50	0.44
1:S:212:GLU:OE1	1:S:212:GLU:N	2.37	0.44
1:S:80:TRP:CZ2	1:S:88:ARG:HA	2.53	0.44
1:S:69:ASP:O	1:S:71:ASP:N	2.51	0.44
1:S:182:ARG:HD2	1:S:184:GLU:OE2	2.18	0.44
1:S:222:VAL:HG11	1:S:241:LEU:HG	1.99	0.44
1:S:368:LEU:O	1:S:370:PHE:N	2.50	0.44
1:S:452:LEU:O	1:S:455:CYS:SG	2.74	0.44
1:S:166:LEU:HD13	1:S:204:PHE:CZ	2.53	0.43
1:S:240:ASN:HD22	1:S:240:ASN:HA	1.63	0.43
1:S:253:GLU:HA	1:S:314:TYR:OH	2.18	0.43
1:S:360:GLU:C	1:S:362:ASP:N	2.72	0.43
1:S:129:LEU:C	1:S:131:PRO:HD2	2.43	0.43
1:S:323:VAL:N	1:S:324:PRO:CD	2.81	0.43
1:S:449:LEU:CG	1:S:453:LEU:HD11	2.48	0.43
2:Q:76:GLU:O	2:Q:77:THR:CB	2.66	0.43
1:S:181:MET:O	1:S:182:ARG:C	2.62	0.43
1:S:330:LEU:O	1:S:385:ALA:HB2	2.19	0.43
1:S:281:GLU:OE1	1:S:281:GLU:HA	2.18	0.43
1:S:353:MET:O	1:S:354:LEU:C	2.59	0.43
2:Q:69:THR:CG2	2:Q:70:GLN:N	2.62	0.43
1:S:21:ALA:HA	1:S:24:PHE:HB3	2.01	0.43
1:S:73:LYS:O	1:S:77:GLN:HB2	2.19	0.43
1:S:188:ASN:N	1:S:188:ASN:ND2	2.67	0.43
1:S:233:VAL:O	1:S:233:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:130:ILE:HD13	1:S:130:ILE:N	2.19	0.43
1:S:277:LEU:HD11	1:S:342:TRP:O	2.19	0.43
1:S:465:ARG:HA	1:S:468:SER:OG	2.19	0.43
1:S:457:ILE:HA	1:S:460:LEU:CD1	2.47	0.43
1:S:469:ASN:C	1:S:471:CYS:N	2.75	0.43
1:S:95:VAL:C	1:S:97:GLN:H	2.26	0.43
1:S:105:ARG:HB3	1:S:106:PRO:HD2	2.00	0.43
1:S:154:ILE:H	1:S:154:ILE:HG13	1.51	0.43
1:S:84:ASP:O	1:S:88:ARG:HG3	2.19	0.42
1:S:364:VAL:N	1:S:365:PRO:HD2	2.34	0.42
1:S:178:ILE:HG23	1:S:221:VAL:HG11	2.01	0.42
1:S:6:ILE:HG21	1:S:25:LEU:HD11	2.01	0.42
1:S:51:GLN:O	1:S:55:VAL:HG23	2.19	0.42
1:S:151:LEU:CD1	1:S:194:ALA:HB2	2.49	0.42
1:S:281:GLU:O	1:S:282:PHE:C	2.63	0.42
1:S:91:VAL:C	1:S:93:ASN:N	2.78	0.42
1:S:149:SER:O	1:S:152:GLU:HB2	2.20	0.42
1:S:293:LEU:HD12	1:S:311:SER:HA	2.02	0.42
1:S:360:GLU:OE1	1:S:360:GLU:HA	2.20	0.42
2:Q:72:THR:HG22	2:Q:72:THR:O	2.20	0.42
1:S:139:ASN:HA	1:S:140:PRO:HD2	1.72	0.42
1:S:169:LYS:HA	1:S:169:LYS:CE	2.49	0.42
1:S:201:SER:O	1:S:202:LEU:C	2.62	0.42
1:S:352:LEU:O	1:S:352:LEU:HD23	2.20	0.42
1:S:33:LEU:HB3	1:S:34:PRO:CD	2.37	0.42
1:S:463:GLU:CD	1:S:463:GLU:H	2.27	0.42
1:S:5:THR:O	1:S:9:LYS:HG3	2.20	0.41
1:S:238:LEU:HB2	1:S:278:GLN:CG	2.50	0.41
1:S:46:ASN:ND2	1:S:49:ASN:OD1	2.54	0.41
1:S:18:LEU:HD23	1:S:19:GLU:N	2.34	0.41
1:S:133:LEU:O	1:S:134:VAL:C	2.61	0.41
1:S:249:TYR:OH	1:S:290:GLU:OE2	2.38	0.41
1:S:416:LEU:HD22	1:S:424:VAL:CG1	2.50	0.41
1:S:88:ARG:C	1:S:90:GLU:N	2.78	0.41
1:S:238:LEU:HB2	1:S:278:GLN:HG2	2.03	0.41
1:S:178:ILE:HA	1:S:181:MET:CE	2.50	0.41
1:S:202:LEU:HD13	1:S:244:ILE:HG13	2.03	0.41
1:S:222:VAL:CG1	1:S:241:LEU:HG	2.51	0.41
1:S:353:MET:HG3	1:S:392:CYS:SG	2.61	0.41
1:S:402:LEU:O	1:S:403:LYS:C	2.63	0.41
1:S:300:ALA:HA	1:S:303:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:307:PRO:O	1:S:308:GLU:C	2.63	0.41
1:S:431:THR:HG22	1:S:435:ILE:CD1	2.48	0.41
1:S:32:ASN:O	1:S:34:PRO:N	2.54	0.41
1:S:75:GLN:C	1:S:77:GLN:H	2.29	0.41
1:S:77:GLN:HA	1:S:77:GLN:OE1	2.19	0.41
1:S:323:VAL:C	1:S:325:ILE:N	2.73	0.41
1:S:343:ASN:OD1	1:S:346:LYS:HD3	2.21	0.41
1:S:375:ILE:CG2	1:S:376:LYS:HG2	2.46	0.41
1:S:379:ASP:OD2	1:S:381:ARG:HD2	2.20	0.41
1:S:438:LEU:HD22	1:S:438:LEU:N	2.36	0.41
1:S:441:GLU:H	1:S:441:GLU:CD	2.28	0.41
1:S:40:LEU:O	1:S:42:ARG:N	2.54	0.41
1:S:52:VAL:O	1:S:53:ALA:C	2.64	0.41
1:S:48:GLY:HA2	3:S:501:HOH:O	2.20	0.40
1:S:91:VAL:O	1:S:93:ASN:N	2.54	0.40
1:S:452:LEU:O	1:S:453:LEU:C	2.64	0.40
1:S:199:LEU:HA	1:S:240:ASN:ND2	2.36	0.40
1:S:170:SER:HB2	1:S:208:ASN:ND2	2.15	0.40
1:S:317:GLY:O	1:S:319:LEU:N	2.54	0.40
1:S:11:VAL:O	1:S:11:VAL:CG2	2.69	0.40
1:S:24:PHE:O	1:S:27:ARG:HG2	2.22	0.40
1:S:403:LYS:N	1:S:404:PRO:CD	2.84	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	S	483/485 (100%)	317 (66%)	116 (24%)	50 (10%)	0	1
2	Q	26/28 (93%)	9 (35%)	5 (19%)	12 (46%)	0	0
All	All	509/513 (99%)	326 (64%)	121 (24%)	62 (12%)	0	0

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	4	ILE
1	S	33	LEU
1	S	34	PRO
1	S	35	THR
1	S	107	SER
1	S	165	GLN
1	S	361	ASP
1	S	393	ILE
2	Q	69	THR
2	Q	74	LYS
2	Q	77	THR
2	Q	81	GLN
2	Q	93	LYS
1	S	41	SER
1	S	82	ALA
1	S	104	TYR
1	S	105	ARG
1	S	121	ILE
1	S	124	ASN
1	S	337	ASP
1	S	442	ALA
2	Q	80	GLU
2	Q	84	LYS
1	S	32	ASN
1	S	186	PRO
1	S	318	ALA
1	S	400	SER
1	S	452	LEU
1	S	464	PRO
1	S	468	SER
2	Q	72	THR
2	Q	73	ASN
2	Q	79	LYS
1	S	37	LEU
1	S	65	LEU
1	S	79	ARG
1	S	85	ALA
1	S	92	LYS
1	S	150	THR
1	S	164	GLU
1	S	170	SER
1	S	182	ARG

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Mol	Chain	Res	Type
1	S	282	PHE
1	S	472	TRP
1	S	57	ALA
1	S	324	PRO
1	S	330	LEU
1	S	369	PRO
1	S	106	PRO
1	S	297	ALA
1	S	420	PRO
1	S	425	ARG
1	S	432	VAL
2	Q	85	THR
1	S	11	VAL
1	S	70	PRO
1	S	323	VAL
1	S	440	PRO
2	Q	82	PRO
1	S	52	VAL
1	S	46	ASN
1	S	47	PRO

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	S	414/414 (100%)	381 (92%)	33 (8%)	11	34
2	Q	21/26 (81%)	17 (81%)	4 (19%)	1	5
All	All	435/440 (99%)	398 (92%)	37 (8%)	10	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	24	PHE
1	S	31	GLU
1	S	37	LEU

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Mol	Chain	Res	Type
1	S	46	ASN
1	S	81	LEU
1	S	93	ASN
1	S	99	LEU
1	S	102	GLU
1	S	107	SER
1	S	128	GLU
1	S	130	ILE
1	S	143	THR
1	S	178	ILE
1	S	247	LEU
1	S	261	PHE
1	S	265	ILE
1	S	266	GLU
1	S	278	GLN
1	S	280	ILE
1	S	281	GLU
1	S	305	ARG
1	S	313	PHE
1	S	339	ASP
1	S	350	VAL
1	S	352	LEU
1	S	357	THR
1	S	361	ASP
1	S	367	VAL
1	S	377	ASN
1	S	384	ASP
1	S	401	GLN
1	S	410	MET
1	S	465	ARG
2	Q	71	GLU
2	Q	76	GLU
2	Q	85	THR
2	Q	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	22	GLN
1	S	46	ASN
1	S	86	ASN
1	S	111	GLN

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Mol	Chain	Res	Type
1	S	132	GLN
1	S	165	GLN
1	S	167	GLN
1	S	200	ASN
1	S	208	ASN
1	S	239	GLN
1	S	240	ASN
1	S	250	GLN
1	S	278	GLN
1	S	333	GLN
1	S	377	ASN
1	S	401	GLN
2	Q	70	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.